S. Wagner • A. Bode • H. Satzger • M. Brehm *EDITORS*

High Performance Computing

in Science and Engineering
Garching/Munich 2012

Bayerische
Akademie der Wissenschaften

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The supercomputer HLRB II at the LRZ in Garching was an SGI Altix 4700 system with 9720 processor cores (Intel Itanium2, Montecito), 39 TByte of shared ccNUMA memory, 600 TByte of attached disk space, and a peak performance of 62.3 TFLOP/s. The machine was in operation between 2006 and 2011 and was ranked no. 10 in the TOP500-list at the time of installation. The image shows the white ccNUMA cables on top of the computer racks.

Five years of High Performance Computing with HLRB II

The Leibniz Supercomputing Centre (LRZ) publishes in the present booklet results of numerical simulations on the High Performance Computer in Bavaria (HLRB II), a SGI Altix 4700 system, achieved in particular between 2009 and 2011. The papers were selected from the review reports of projects that have used the HLRB II.

Regarding the usage of the supercomputer, we notice that the trend in the distribution of application areas seen over the last four years is still continuing. The majority of contributed papers belong to the following fields of research: computational fluid dynamics, astrophysics and chemistry. The strongest increase in submissions comes from the geosciences, which submitted three times as many papers as compared to the last progress report in 2009. The number of papers from the fields of astrophysics and life science has increased more than two-fold. The number of submissions from computational fluid dynamics as well as chemistry has increased by more than 50 percent.

Another trend that we observe is the increase in interdisciplinary science. An excellent example is the submission from the Deutsches SOFIA Institut at the University of Stuttgart, which showcases a combination of astrophysical, mechanical engineering, aero dynamical and optical problems. SOFIA (Stratospheric Observatory For Infrared Astronomy) is a telescope housed on board of a Boeing 747. The project used methods from computational fluid dynamics on HLRB II to understand the complex cavity flow phenomena as well as to investigate means to improve the telescope's performance by mitigating the amplitudes and changing the characteristic frequencies of the pressure fluctuations. The project will continue to use similar methods to investigate the aero-optical properties of the cavity shear layer, which potentially limits the image quality of the observatory during flight.

The variety and quality of the submitted papers shows that HLRB II was a huge success for scientists and helped to solve various problems of broad relevance. This will continue and the number and the depth of projects will significantly increase with the operation of SuperMUC. In June 2012, the LRZ as a member of the Gauss Centre for Supercomputing (GCS), will start the operation of its 3 PFLOP/s supercomputer that will also be part of the European Tier-0 infrastructure of the Partnership for Advance Computing in Europe (PRACE). With its innovative warm-water cooling system, SuperMUC will be one of the most energy efficient supercomputers in the world. it will help to further the understanding and knowledge of scientists from Munich, Bavaria, Germany and Europe and will enable scientist to continue the successful work started on HLRB I and II.

Acknowledgments

Garching bei München, Juni 2012
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Astrophysics

Local Supercluster Simulations

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Introduction

As we look into the past, we observe that at recombination (about 13.7 billion years ago) matter in the universe was homogeneously distributed with very low mean density. As the universe evolved, tiny density fluctuations grew into the observed cosmological structures that surround us: tiny dwarf galaxies, spiral galaxies like our own Milky Way, more massive elliptical galaxies, massive clusters and the largest observed structures: super-clusters of galaxies. Due to the nonlinear nature of the collapse and clustering processes, our understanding of the formation of structure in the universe is mainly based on computer experiments which have been performed during the last two decades on the largest existing supercomputers. Within our project we have performed a number of such simulations on the SGI Altix 4700 of the Leibniz-Rechenzentrum Munich.

Our Milky Way is a spiral galaxy which together with another spiral galaxy of approximately the same mass (the Andromeda galaxy) forms the main members of the so-called Local Group of galaxies. The third largest member of this group is a somewhat smaller spiral (known as the Triangulum Galaxy). In total, the Local Group comprises more than 30 galaxies which are distributed in a sphere of about 10 million light-years across and centred between Andromeda and the Milky Way. At a distance of around 50 million light years from the Milky Way, sits a huge cluster of galaxies (the Virgo cluster) which comprises more than 1000 members. This cluster forms the heart of the local super-cluster which is the most massive structure in the Local Universe. The Local Universe itself is just a tiny fraction of the observable universe. Yet, owing to its proximity, the local universe is also the best known part of the cosmos, since we may observe small objects with very low luminosity. The main aim of the CLUES project (Constrained Local UniversE Simulations) is to study our cosmological neighborhood.

Results

Based on observational data of the galaxy distribution in the Local Universe today, we have reconstructed the initial conditions necessary for our cosmological simulations. The results are constrained simulations that show the evolu-

Figure 1: Slice through a simulation box of 587 million light years.

Figure 2: Distribution of the Cold Dark Matter (left) and the gas (right) in the Local Group, see also [6] for the corresponding movie.

tion of structure in the neighbourhood of the Milky Way. In Figure 1 one can clearly see the simulated nearby galaxy clusters and superclusters. Our simulated Milky Way sits in a small filament south of the Virgo cluster which is nearly the exact same environment as the real Milky Way.

In order to study the formation of the Milky Way and the Local Group in more detail we have increased the resolu-

tion in the region where the Local Group is situated. To run the initial conditions for these simulations we needed almost a terabyte of shared memory at the SGI Altix 4700 . Moreover, we have included in our simulations gas dynamics with radiative cooling, star formation and feedback. Figure 2 shows the distribution of dark matter and gas in the Local Group at redshift z = 0. The stellar disks inside the gas disks are not shown here.

Our simulations have shown that a quiet formation history is typical for a galaxy in the environment of the Local Group [2] . Galactic satellites tend to enter the galaxy along the filament pointing toward Virgo [3]. Interestingly, the two main members of the Local Group, the Milky Way and the Andromeda, have even exchanged some of their satellites throughout cosmic history.

Small scale structure can be observed best within our direct cosmic neighborhood. The standard Cold Dark Matter model predicts too many small scale structures – a challenge known also as the missing satellite problem. The predicted number of low mass galaxies in the Local Volume is an order of magnitude higher than observed in the Arecibo Legacy Fast ALFA survey. Also the locally observed number of mini voids cannot be explained within the standard Cold Dark Matter model. We have shown that Warm Dark Matter solves this discrepancy [4,5]. Depending on the temperature of the Warm Dark Matter particle, the initial density perturbations on small scales are erased. This leads to substantially fewer low mass objects. In Fig. 3 we compare the dark matter, gas and stellar distributions of a galaxy as predicted in the Cold and Warm Dark Matter cosmologies.

On-going Research / Outlook

Using new observational data [1] and a new reconstruction method based on the inverse Lagrangian approximation, we are constructing new initial conditions from which to re-run our simulations. The inverse Lagrangian approach allows a better reconstruction of the positions of the initial perturbations which led (after 13.7 billion years of evolution) to the observed local galaxy population today. The new code for the generation of initial conditions no longer requires excessive shared memory but runs using MPI on a large number of processors. It is well suited for the new SuperMUC system at LRZ.

On the upcoming SuperMUC system we will run a series of new gas dynamical constrained simulations in order to study in detail the gas distribution in the Local Group as well as the formation of galaxies in the Local Universe. To this end we will use the modified Gadget code with the improved feedback model of Cecilia Scannapieco as well as the new Voronoi Particle Hydrodynamics code of Steffen Heß. Both codes use a combination of OpenMP and MPI.

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The home page of the CLUES project is http://www.clues-project.org

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3D simulations of large-scale mixing in core-collapse supernova explosions

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HLRB Project ID: H0072

Introduction

Core-collapse supernovae have been studied by computer models for several decades. However, the physical processes occurring during these blasts are very complex, and the range of time and length scales that need to be resolved in ultimately three-dimensional (3D) computer models cover seven orders of magnitude. Thus, until now astrophysicists can simulate only parts of the event and only in one or two spatial dimensions. In our HLRB project, we have performed the first fully three-dimensional (3D) simulations of a core-collapse supernova over a timescale of hours after the initiation of the blast. A core-collapse supernova occurs when a massive star of at least 9 solar masses has burned almost all its nuclear fuel. The fusion engine in the centre of the star begins to stutter, triggering an internal collapse and thus a violent explosion of the entire star. In the case of SN 1987A, a core-collapse supernova that could be seen with the naked eye as it occurred relatively close by in the Large Magellanic Cloud, the star had about 20 solar masses at its birth.

One of the astonishing and unexpected discoveries in SN 1987A and many subsequent core-collapse supernovae was the fact that nickel and iron, heavy elements that are formed near the centre of the explosion, are mixed outward in big clumps into the hydrogen shell of the disrupted star. Nickel bullets were observed to propagate at velocities of thousands of kilometres per second, much faster than the surrounding hydrogen, and much faster than predicted by hydrodynamic calculations assuming spherical symmetry. In fact, it turned out that the brightness evolution of SN 1987A and of similar core-collapse supernovae can only be understood if large amounts of heavy core material (in particular radioactive nickel) are mixed outwards into the stellar envelope, and light elements (hydrogen and helium from the envelope) are carried inwards into the core [1].

Previously performed core-collapse supernova simulations in 2D (i.e., with the assumption of axial symmetry) showed that the spherical shell structure of the progenitor star is destroyed during the supernova blast and large-scale mixing takes place. However, not all observational aspects could be reproduced by 2D models [2].

Numerical model

We simulated our 3D core-collapse supernova models with the explicit multi-dimensional finite-volume hydrodynamics code PROMETHEUS [3], which is based on the piecewise parabolic method (PPM), an exact Riemann solver, and dimensional splitting. We used a code version that was optimized for the HLRB II SGI Altix 4700 system by changing the OpenMP parallelization of the code to exploit its large number of CPUs and ccNUMA bus system. We ran benchmarks using up to 510 CPUs, i.e, one complete node of the Altix 4700 system, to study the parallel performance of our code. According to these tests, we used 256 CPUs for our 3D simulations, which required a total of about 650 000 CPU hours.

We performed our 3D simulations on a computational grid in spherical polar coordinates consisting of about 78 million zones The equidistant angular grid had a resolution of 1° covering the whole sphere except for a cone with a half opening angle of 5.8° around the symmetry axis of the coordinate system to avoid a too restrictive time step condition resulting from the explicit nature of the hydrodynamics code. We have not observed any numerical artifacts resulting from this grid constraint. The radial mesh was logarithmically spaced between a time-dependent inner boundary, initially located at a radius of 200 km, and a fixed outer boundary at 39 million km. It had a maximum resolution of 2 km at the inner boundary, and a resolution of 400 000 km at the outer one corresponding to a roughly constant relative radial resolution of ~1%.

We allowed for free outflow at the outer boundary, and imposed a reflective boundary condition at the inner edge of the radial grid. During the simulation we moved (approximately every 100th time step) the inner radial boundary to larger and larger radii to relax the time step condition. This cutting of the computational grid reduces

the number of radial zones from 1200 at the beginning to about 400 towards the end of the simulation, but involves only the innermost few percent of the initial envelope mass. We convinced ourselves by means of 2D test calculations that this removal of mass has no effect on the dynamics and mixing occurring at larger radii

The initial model used for our simulations is based on the explosion models of Scheck et al. [4], who followed the onset and early development of neutrino-driven explosions in 3D. We used a tabulated EOS that considers contributions of an arbitrarily degenerate and relativistic electron-positron gas, of a photon gas, and of a set of ideal Boltzmann gases consisting of the 8 nuclear species (n, p, He4, C12, O16, Ne20, Mg24, and Ni56) included in our initial model. Nuclear burning is not taken into account in our simulations. Both in the 3D and 2D simulations we neglected the influence of gravity on the motion of the ejecta. While this has no important impact on the dynamics of the expanding ejecta, the amount of fallback is underestimated. However, that way we could avoid the accumulation of mass near the inner (reflecting) radial boundary, which would have implied a considerably more restrictive time step condition.

Figure 1: Surfaces of the outermost locations with constant mass fractions of 3% for carbon (green), and oxygen (red), and of 7% for nickel (blue). The two panels display two views of the hydrodynamic instabilities at about 9000s shortly after the supernova shock has broken out of the stellar surface. The side length of the panels is about 75 million km. [5].

Results

Our 3D results [5] reveal that the asymptotic velocities of metal-rich clumps are much higher in 3D than in the corresponding 2D models, where the Ni and O carrying dense fingers get stuck in the massive, dense He shell that forms below the base of the H-envelope, and stay co-moving with the He matter there at a velocity of ~1500 km/s [2]. In our 3D models we obtain Ni and O bullets propagating at maximum velocities of 4500 km/s and a large fraction (~15%) of the metal core of the star expands with velocities ≥2000 km/s. The most extended and fastest Rayleigh-Taylor structures, some of which have a mass of several 0.001 solar masses, contain most-

ly nickel. These Ni bullets expand more rapidly than the longest fingers with dominant or appreciable O content, which are smaller on average but much more numerous than the large Ni features (Fig.1). Iron-group nuclei, Ne and Mg are thus carried far into the H layer. They move well ahead of O-rich knots, and both Ni and O overtake the material from the carbon layer in the ejecta (Fig.1). The onion-shell stratification of the star is thus partially turned over during the explosion.

Besides strong mixing of heavy-elements into the H envelope, we also observe H being transported deep into the metal core of the star to regions with velocities ≤1000 km/s and an enclosed mass of less than two solar masses.

A small fraction of the metal core receives velocities ≥6000 km/s initially, which is significantly higher than in our 2D runs (but similar to the peak metal velocities of [2]). These clumps penetrate into the H envelope faster than the He wall builds up keeping their speed of ≥4000 km/s until the time of shock breakout and experiencing much less deceleration than in the 2D models of [2].

The different behavior of the 2D and 3D models is a consequence of differences in the drag forces of the surrounding medium, which affect the propagation of the metal-rich clumps and lead to their deceleration as they plow through the He layer. By means of a simple analytic model we could demonstrate that the different geometry of the bullets (torus-like structures in 2D and quasi-spherical bubbles in 3D) can explain the differences observed in the simulations.

On-going Research

While the 2D/3D differences found in our investigation are most likely generic, the extent of the radial mixing, the size and mass distribution of the metal fingers, their velocities and spatial distribution, and the composition of individual clumps probably depends strongly on the structure of the progenitor star, the explosion energy, and the initial asymmetry of the blast. Having advanced the modeling of mixing instabilities in core-collapse supernova explosions to the third dimension, we therefore plan to explore a wider variety of progenitor stars with the goal to establish a link between explosion models and observations.

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Cosmological hydrodynamical simulations in various cosmological scenarios

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Introduction

Clusters of galaxies are ideal cosmological probes. In first approximation, they can be considered as closed systems, thus their content reflects the overall cosmic composition. In particular their number counts, as well as their internal structure, their redshift evolution and their morphology are strongly dependent on the cosmological model and then permit to probe it. The increased size, range and completeness of observational data obtained using the latest generation of astronomical instruments recently opened the so-called period of precision cosmology, meaning that the basic parameters describing our universe can be in principle determined with a precision of ten per cent or better. Future instruments (like the now running PLANCK satellite and the planned e-ROSITA mission) will help to measure cosmology to even higher precision. Additionally, huge observational efforts will be spent to investigate the nature of dark energy, thanks to a large number of future experiments (like the CFH Legacy survey, DES, JDEM, DarkCam, EUCLID). Having its origin in the fundamental nature of gravity or in the super-symmetric extension of the standard model, the aim of such projects is not only to measure the amount of dark energy present today, but also its redshift evolution, which is needed to trace back its fundamental origin. The quality and quantity of the data in such surveys will allow also to test scenarios where the initial density perturbations are (up to some degree) non-Gaussian, which is a natural prediction of several inflationary models. However, such a precision in cosmology can be reached only through a faithful comparison with the results of detailed numerical models: an example is the number density of galaxy clusters, which represents one of the best tools to discriminate between various cosmological scenarios. Therefore cosmological simulations play a key role in our understanding of the universe. However, galaxy clusters turned out to be extremely complex objects, which have to be understood in much better detail if one pretentds to interpret the forthcoming observations. Therefore it is absolutely mandatory to improve cosmological simulations to obtain precise and comprehensive predictions, specially in the field of large scale structure formation. Thanks to the richness and variety of available observational data, galaxy clusters represent an ideal test toi nvestigate the ability of numerical simulations to make precise predictions.

Results

Simulations are performed using P-Gadget3, a massively parallel Tree-PM-SPH code based on MPI. To improve work-load-balance, time consuming parts on every MPI task, it can make uses of several pthreads or alternatively openMP threads. Typical simulations have been performed on 256/512 CPUs in parallel, consuming ca. 70.000 CPU/h each. The largest cosmological boxes done (including hydrodynamics) produce approximately data outputs of 3.5TB each.

Dark Energy Simulations
The first set of cosmological hydrodynamical simulations investigated the effect of different dark energy models on the properties of large scale structures and galaxy clusters in general. We simulated cosmological volumes of $(300 \text{ Mpc/h})^3$ using 2×768^3 gas and dark matter particles, adopting cosmological parameters from the 3-year WMAP values.

We so far performed simulations for the following dark energy models:
- WMAP3 (standard cosmological constant)
- RP (Peebles & Ratra 2002)
- SUGRA ("Super Gravity" models)
- EQ (2x, extended quintessence with 2 different parameters)

Figure 1 shows a slice through the simulation box at the final time (z=0), emerging the structures of the cosmic network, where galaxy clusters form at the junction of the largest filaments. For each model, we performed both control runs considering only dark matter particles and full hydrodynamical runs including gas cooling and star formation. The first results of these simulations have been already published ([1],[3]). The contemporary presence of evolving dark energy and baryon physics allows us to in-

Figure 1: Maps of the final matter distribution in the different dark energy models as used in [1],[2] and [3].

vestigate the interplay between the different background cosmology and the evolution of the luminous matter. Since cluster baryon fraction can be used to constrain other cosmological parameters such as Ω_m, we also analyse how dark energy influences the baryon content of galaxy clusters. We find that in models with dynamical dark energy, the evolving cosmological background leads to different star formation rates and different formation histories of galaxy clusters, but the baryon physics is not affected in a relevant way. We investigate several proxies of the cluster mass function based on X-ray observables like temperature, luminosity, M_{gas} and Y_{gas}. We conclude that the X-ray temperature and M_{gas} functions are better diagnostic to disentangle the growth of structures among different dark energy models.

The results of these simulations are also used in various other projects. Currently we are preparing a further analysis paper where we investigate the connection between dark energy and the inner structure of galaxy clusters by means of the mass-concentration relation ([2]).

Non-Gaussian Simulations

The second set of cosmological hydrodynamical simulations investigated the signatures of non-Gaussian density fluctuations with different strengths. The goal of these simulations is to estimate the effects of such non-Gausianity of the large scale structures and galaxy clusters in general, evaluating their detectability. One of the most interesting effect is on the halo bias, which for non-Gaussian perturbations has a unique scale dependent signature. To investigate this statistical test, a very large cosmological volume is needed. Therefore we considered boxes of (1200 Mpc/h)³ using 2x960³ gas and dark matter particles. The deviation from Gausianity of the initial conditions is usually parametrized by a dimensionless parameter f_{NL} entering in the inital gravitational potential Φ that it is related to a Gaussian random field ϕ as:

$$\Phi = \phi + f_{NL} \cdot (\phi^2 + \langle\phi^2\rangle)$$

We also investigated the effect of higher order, non-Gaussian signatures parametrized by g_{NL}:

$$\Phi = \phi + g_{NL} \cdot (\phi^3 + \langle\phi^3\rangle)$$

So far we investigated the following models performing dark matter only reference simulations:

f_{NL}=0,±100,±200 and g_{NL}=±10⁵ ,±10⁶.

Figure 2 shows the density maps at high redshift as well as at redshift zero for some of the models considered in [4]. The central column displays the density slice, while the left and right ones shows the differences in the matter distribution for the same cosmological volume but

with positive and negative non-Gaussian contribution. The first results based on these simulations have been already published ([4],[5] and [6]). Using these simulations we calibrated the analytic non-Gaussian description of Matarrese, Verde & Jimenez and LoVerde et al., finding an excellent agreement between the simulations and the analytic predictions (see [4] for more details).

Figure 2: Maps of the high redshift and final matter distribution in models with different level of non-Gausianity as used in [4], [5] and [6].

On-going Research / Outlook

The simulations performed have already allowed us to perform a detailed study of the properties of the large scale structures and galaxy clusters, in various alternative cosmological back-ground models ([1],[3],[4],[5],[6]). Such models differ in the nature of dark energy and in the inflationary model leading to different amounts of primordial non-Gaussianity. Many of the starting or upcoming observational campaigns aim to measure such small differences between the predictions of different cosmological models and large cosmological simulations, as the ones performed inside this project, allow to quantify such effects from the theoretical side. Since these simulations include an hydrodynamic treatment of the gas, they can be used as reference for a much larger number of observational campaigns (specially in X-rays and at radio wavelengths for the SZ effect, where the observed signal is coming from the diffuse medium within virialized objects). The simulations performed so far are already revealing interesting details and are used to compare the performances and the findings of different ongoing or planned observational campaigns.

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Forging gold with HLRB II

Introduction

Simulating neutron-star mergers project h0074 has two major scientific goals: the determination of the gravitational-wave signal as dependent on the only incompletely known properties of high-density matter, and the investigation of the formation of heavy elements in the outflows of these events.

The astrophysical origin of the heaviest elements like for instance gold or uranium is still unknown. While the nuclear processes leading to the formation of these nuclei are relatively well understood, the astrophysical production site providing suitable conditions for these reactions has not yet been identified. From the microphysical point of view it is clear that very high neutron densities are required because heavy nuclei can only be built up by successive neutron captures on lighter nuclei. These extreme conditions suggest that this so-called rapid neutron-capture process (r-process) takes place in an explosive environment. Among the most favored sites for this scenario are collisions of two neutron stars, where small amounts of matter become gravitationally unbound (see Fig. 1), mix into the interstellar medium and thus contribute to the observed element abundances.

Results: element formation

Within our project h0074 we explore neutron-star mergers as the astrophysical production site of heavy elements. To this end we simulate the coalescence of two neutron stars focusing on systems with two stars of 1.35 solar masses, which are assumed to be the configuration to collide most often. The calculations are performed with a relativistic Smooth Particle Hydrodynamics code employing a certain approximation to solve the Einstein field equations with a multigrid solver embedded in our code. The implementation allows to track the composition of the matter, in particular, of the material getting unbound from the merger site. These simulations allow to specify the detailed initial conditions (composition and thermodynamical properties) in the outflowing matter and to follow its evolution. By this we are able to provide the first selfconsistent model for the nucleosynthesis in the ejecta of neutron-star mergers. The element abundances are obtained from a postprocessing proce-

dure of the ejecta trajectories with a nuclear network code, which takes into account all relevant reactions for the r-process. The red line of Fig. 2 shows the nucleosynthesis yields averaged over all gravitationally unbound fluid elements. For heavy nuclei with mass numbers A>130 we discover a distribution which is very close to the one that is observed in the solar system. The same is true for the outflow of a merger of a star with 1.2 solar masses and a star with 1.5 solar masses (blue line).

We find ejecta masses of a few thousandths of a solar mass, which is sufficient to explain the observed abundances. Hence, based on the results of our simulations on the HLRB2 we conclude that neutron-star mergers are indeed a viable scenario for explaining the formation of heavy elements with mass numbers above 130 (see [1] for details). Here, the innovation of our work is based on the fact that our computations do not require any tuning of free parameters or additional assumptions e.g. about the composition or the temperature of the outflowing material because this information is taken consistently from the simulations. Moreover, our calculations are the first which consider nucleosynthesis processes of neutron-star mergers in a relativistic framework, which is important especially when compact objects like neutron stars are involved.

Figure 1: Dynamical stages of a neutron-star merger. Material shown in golden colors gets unbound from the merger site and forms heavy elements.

Figure 2: Element abundance pattern produced in the outflow of a neutron-star merger compared to the observed abundances in the solar system.

Our findings are also relevant for a potentially observable optical signal from neutron-star mergers. The freshly synthesized elements in the outflow are radioactive and their decay to stable nuclei releases energy that powers an optical counterpart. Our simulations reveal that these events can be as bright as a faint supernova, but they fade on much shorter time scales of some hours. Considering also their distance these signals are challenging to observe, but for upcoming optical surveys detections are within reach and will allow to get a handle on the amount of ejecta independent from numerical simulations, which is essential for determining the absolute nucleosynthesis yields.

On-going Research

For the future we plan to investigate the outcome of different binary setups. By such a survey one will be able to obtain the element production folded with the binary neutron star population, which will be a crucial step to finally judge on neutron-star mergers as the major source of heavy r-process elements. Our future analysis will also include mergers of neutron stars and black holes, which have been speculated to contribute to the r-process element production. So, it seems that though the intense efforts of alchemists over the centuries only with the aid of modern supercomputers it is possible to find the recipe for forging gold.

Results: gravitational-wave emission

Beside the investigation of the nucleosynthesis outcome of neutron-star mergers, the capabilities of HLRB2 enabled us to investigate another unknown in the context of neutron stars as the second major goal of the h0074 project. The properties of high-density matter as present in the cores of neutron stars are not yet fully explored. In particular the equation of state determining the pressure at a given density is not precisely known. For instance, at two times nuclear density, a typical density inside neutron stars, the pressure differs by a factor 10 between different theoretical descriptions of the equation of state. The importance of the equation of state is due to the fact that it entirely determines the stellar structure and thus the mass-radius relation of neutron stars. This in turn implies the possibility to gain information about the equation of state by the simultaneous measurement of the mass and the radius of a neutron star. This represents a unique approach to study fundamental properties of nuclear and particle physics which govern the equation of state and which are not accessible by laboratory experiments.

While masses of neutron stars have been measured very accurately in binary systems, stellar radii have not yet been deduced from observations with high precision. Within our project we follow a new path to obtain information on neutron-star radii (see [2]). Neutron-star mergers are strong emitters of gravitational waves. These space-time oscillations propagate away from the

Figure 3: Gravitational-wave frequency as the function of the radius of a neutron star of 1.6 solar masses. The radius is characteristic of the equation of state of high-density matter.

source with the speed of light. Gravitational waves are still awaiting their detection, but with an increased sensitivity the upcoming detectors Advanced LIGO and Advanced Virgo are likely to grasp the first signals. Merging neutron stars are among the prime targets of these instruments and the gravitational-wave signal of neutron-star mergers is known to be affected by the equation of state. This is expected because the properties of high-density matter govern the dynamics.

These facts motivate an extensive survey of the equation of state dependence of the gravitational-wave signal to establish the full functional relation between the observable signal and the equation of state. Thus, we simulate the merging of two neutron stars with 1.35 solar masses for a large and representative sample of theoretically proposed equations of state. The typical outcome of such a merger is the formation of a very massive, oscillating, rotating neutron star (see lower panel in Fig. 1). The oscillations of this merger remnant generate a pronounced peak in the kHz range of the gravitational-wave spectrum. The frequency of this peak turns out to be characteristic for the equation of state employed in the simulation. In particular, it is found that the peak frequency scales very well with the radius of a 1.6 solar-mass neutron star (see Fig. 3). The relation shown in Fig. 3 can be used to determine the neutron star radius by a measurement of the gravitational-wave peak frequency. Considering the involved uncertainties the radius can be measured with an accuracy of a few hundred meters. The results of our computer simulations therefore open the fascinating possibility to measure the size of an astrophysical object millions of light years away and to get in this way deeper insight into fundamental physics on the nuclear and particle level.

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The Physics of Galactic Nuclei

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This ongoing project is dedicated to a detailed investigation of the physics of galactic nuclei. In this report, we concentrate on two highlights of our research done with the HLRB supercomputer.

Star Formation near the Galactic Centre Supermassive Black Hole

Introduction

At the centre of the Milky Way lies a massive object of around 4 million times the mass of our Sun. Observations of this object are already good enough so that any alternative explanation besides a supermassive black hole can be ruled out [1]. Around the black hole one can observe two inclined, counter-rotating discs of stars. These discs of stars are hard to explain with the standard model of star-formation in which stars form in an isolated gaseous cloud that is able to collapse under the influence of gravity. Close to the black hole, tidal forces would tear the cloud apart, preventing collapse of the cloud. Recent models for the formation of the discs of stars still assume that they originate from a gaseous cloud, however this happens in a two step process [2]: First the cloud gets captured and torn apart by the black hole. This leads to the formation of a gaseous disc around the black

Figure 1: Density distribution of the gaseous accretion disc around the supermassive black hole.

hole. This disc grows in mass and at some point becomes gravitationally unstable so that stars can form inside the disc. Formation of a second disc would then require a second cloud being captured by the black hole. The stars observed in those discs show a distinguished feature that can be used to test the above model. Normally stars which formed in a gaseous cloud show a typical distribution of masses. There are many stars which have a low mass like our sun and there are only a few stars with very high masses. However the observed discs show only stars at very high masses [3], a fact that can be used to check the validity of a formation model. In our work we use the Supercomputer at the LRZ to simulate the infall and capture of a gaseous cloud and the subsequent star formation around the supermassive black hole.

Results

Our simulations are done using the smoothed Particle Hydrodynamics (SPH) code GADGET3 [4]. In SPH a fluid is modeled by using particles that represent a small volume of the fluid. The code is written in C using the Message Passing Interface (MPI) for parallelisation. The HLRB was first used to conduct a large parameter study to find a set of initial conditions like cloud infall velocity, cloud size and cloud position that leads to the formation of a disc of stars similar to the one observed at the Galactic Centre. The simulations used 64 CPUs and between one to two million SPH particles. The results show that a cloud of a radius of around one parsec and a mass of roughly a hundred thousand times the mass of the sun is needed. Using those initial conditions we conducted a high resolution simulation with 4.5 million SPH particles on 128 CPUs.

Due to the high velocities and high densities reached inside the accretion disc forming around the black hole, the simulations are numerically very demanding. Each iteration needs a very small timestep so that the high-resolution simulation took one month of runtime to finish.

In Figure 1 we show the gas density distribution of the accretion disc that forms around the supermassive black hole. The bright yellow spots throughout the disc represent dense cores which are the progenitors of stars. The

formation of a star itself is below the resolution limit that we can reach with this type of simulation.

On-going Research / Outlook

In an upcoming publication [5] we will study the details of the fragmentation process and the formation of cores in more detail. The direct comparison with observations will allow us to verify if the formation of the discs of stars from an accretion disc provides a reasonable model. Future work on this subject will include the study of other formation scenarios and the comparison of the likelihood of different formation models. The next generation system at the LRZ, the SUPERMUC, will be well suited for those simulations.

Dusty Clouds During Seyfert Activity

Introduction

In one of our previous HLRB projects, we investigated a scenario, where the central supermassive black hole is fed by slow stellar winds, emanating from a massive nuclear star cluster, as often found in nearby Seyfert galaxies. We found that the final gas distribution typically shows a two-component structure: a dense, turbulent inner disk on parsec scale and a geometrically thick inflow of cold clumps and filaments [6,7]. Viscous processes within the disk are expected to drive gas towards the black hole. Finally reaching the centre, the gas will feed the inner hot accretion disk (unresolved in our simulations) and most probably lead to the onset of a Seyfert activity cycle, which means that the central luminosity gets comparable to the luminosity of the whole galaxy. Then, feedback processes due to this radiation – arising mainly in the UV/optical wavelength range – cannot be neglected anymore. To this end, we implemented a one-dimensional dust radiative transfer module into the PLUTO [8] code. In a simplified setup, we study the radiation pressure interaction with idealised spherical clouds, which possess similar characteristics as the ones found on parsec scale in [7], including the effects of gravity and optically thin line cooling.

Figure 2: Density distribution of the infalling cloud.

Results

We find that the evolution of the clouds can be separated into three different phases (Figure 2):
- the lense phase, where the counteracting radiation pressure and gravitational forces transform the cloud into a lenticularly shaped object
- the clumpy sickle phase: this converging flow leads to a sickle shaped object, which breaks up into cloudlets due to ongoing cooling instability
- the filamentary phase: column density instability due to the radiation pressure transform the cloudlets into long radial filaments

As a consequence of these effects, low column density clouds will be pushed outwards, as the radiation pressure force dominates over gravitational attraction. For the case of sufficiently high optical depth, only a small fraction of the gas is pushed outwards (at the lower column density edges of the cloud), whereas the largest part moves inwards and can contribute to the activation of the nucleus. The separation between these possibilities can be understood in terms of a simple analytical model, which mainly depends on the radial column density or optical depth of the clouds. The results presented in this section have been published in [9].

On-going Research / Outlook

Following up on this previous work and also triggered by recent observations [10], we are currently interested in the detailed simulation of a low mass gas cloud on its way towards the centre of the Milky Way. In the most recent observations, the tidal effects are already visible. The idea of our simulations is to investigate in detail possible scenarios for the origin of the cloud and its final fate. We start with idealised hydrodynamics simulations with the PLUTO code [11,12]. Due to its proximity, this is ideally suited to investigate the detailed physics of such accretion processes as well as a sensitive probe of the central hot atmosphere in the milli-parsec environment of a super-massive black hole and will also give us invaluable insight into the physics of (active) galactic nuclei in general.

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Star Formation in the Turbulent Interstellar Medium and its Implications on Galaxy Evolution

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Introduction

The interstellar gas in galaxies is in a highly turbulent state [1]. For example, gravitational fragmentation of the gas and radiative cooling produce dense star-forming clouds. Observations of non-thermal line broadening indicate supersonic random motions in these clouds, which are interpreted as turbulence. However, it is not clear yet how the turbulence is produced. One possible mechanism are blast waves from supernova explosions of massive stars, which feed energy into the surrounding gas. On the other hand, it is likely that a significant amount of turbulence originates from various dynamical instabilities in the interstellar medium (ISM). This means that the non-linear growth of small perturbations due to gravity, shear, or cooling results in turbulent flows.

In our project, we used simple, highly idealized models of these processes to study statistical properties of the resulting turbulence in three-dimensional computer simulations. Gas dynamics is described by a set of partial differential equations, which are known as Euler equations. To solve these equations, finite volume methods were applied, i.e., space is subdivided into a mesh of small cubic cells. The mean density, velocity and energy of the gas can then be calculated as functions of time for each cell and the three-dimensional gas motions are approximately described by the data from all cells (as many as one billion were used in our simulations). The results we obtained have remarkable implications on the origin of turbulence in the ISM and star formation [2,3,4,5].

Often not a single mesh with constant cell size is used, but finer meshes with smaller cells are inserted in the course of a simulation, to get a more detailed representation of the gas density and motion. The finer meshes are not inserted by hand, but they automatically adapt to the structure of the flow according to a prescribed set of rules. This method is called adaptive mesh refinement (AMR). For turbulent flows, however, it is very tricky to find appropriate refinement rules. In our project, we addressed this problem in an entirely new way [2].

A thriving area of contemporary astrophysics is simulations of whole galaxies. Even with the capacities of the next-generation SuperMUC machine at the LRZ, however, it is by far not possible to compute all details. Consequently, turbulence in the ISM and star formation have to be described at least in part by so-called subgrid scale models, which account for anything that cannot be directly computed on the grid (mesh) of the simulation. In this regard, we were also able to achieve important advances [7].

Results

AMR Simulations

In astrophysical simulations, AMR is usually applied to track down regions of high gas density. This makes sense for gravitationally driven systems. For example, stars are produced in the densest regions of star-forming clouds. However, density enhancements are not always generated by gravity alone. Gas can also be compressed by supersonic turbulence in the ISM. Since the flow velocities largely exceed the speed of sound, shocks are formed that compress the gas to high densities. This can result in a gas distribution as shown in Figure 1. In this simulation, which was performed with the fluid dynamics code Enzo, extended shocks were artificially produced by random

Figure 1: Slice of the gas density in an AMR simulation of supersonic turbulence [2]. The gas is compressed in between colliding shock fronts, which are produced by random forcing, and cloud-like structures begin to form at vertices. Refined mesh pieces covering regions of strong compression are shown in green.

Figure 2: Volume rendering of the vorticity (rotation of the velocity) for the same simulation as in Figure 1. High vorticity (intense blue) indicates turbulent eddies and sheet-like shocks.

forcing [2]. This means that a force field, which randomly varies over large length and time scales, sets the gas into motion. One can think of the forcing as a very simple model for bulk motions in the ISM that may result, for example, from shock waves produced by supernovae.

The new AMR technique we developed for this simulation allowed us to follow the production of turbulent eddies in addition to the gas compression by shocks (see [2] for details of the algorithm). The intensity of eddy-like gas motions is quantified by the magnitude of the vorticity, which is shown in Figure 2. By comparing to a non-adaptive simulation with a single high-resolution mesh, we found an excellent agreement of important statistical properties such as the distribution of density fluctuations.

Scaling Properties and Subgrid Scale Models
A difficulty we encountered was that the Enzo code became very inefficient for intense refinement. The newest version of Enzo, however, has greatly improved in this regard and now we apply our AMR technique even in cosmological simulations. Before these improvements became available, further simulations without AMR were performed with the FLASH code in collaboration with Christoph Federrath (now at Monash University Melbourne) and Ralf Klessen at the Institute for Theoretical Astrophysics in Heidelberg.

The analysis of the simulation data showed that the statistical properties of supersonic turbulence depend on the applied random forcing. For example, the distribution of density fluctuations becomes significantly broader if the forcing tends to compress the gas rather than stir the gas into eddy-like large-scale motions [4]. In [5], we showed that this effect also leads to significantly different mass distributions of gravitationally unstable cores, from which stars can form by gravitational collapse. For the observed core mass distributions, however, also magnetic fields can play a role.

Important indicators of turbulence are the scaling exponents of the velocity fluctuation, i.e., differences of the velocity (and powers thereof) between randomly chosen spatial positions separated by a given distance. By calculating the averaged velocity fluctuations for different distances, power laws with characteristic slopes are obtained. It turns out that these slopes also depend on the forcing [3,4]. Moreover, comparisons with observed scaling exponents suggest that the turbulence production mechanism varies for different star-forming clouds [4]. On the other hand, we demonstrated that the scaling of mass-weighted velocities, as suggested in [6], is nearly independent of the forcing [3]. This suggests that the non-linear dynamics of supersonic turbulence, in essence, is the same, regardless of the forcing.

As a further key result of our studies, we succeeded in testing a new subgrid scale model for supersonic turbulence [7]. This model statistically describes the effects of turbulent eddies, which are too small to be captured by AMR. Apart from diffusion, small-scale turbulence also exerts a so-called turbulent pressure on the gas. In contrast to previous subgrid scale models, which were limited by weak turbulent pressure, our model also applies to the regime, in which the turbulent pressure can become large compared to the thermal pressure of the gas. This is an important requirement for astrophysical simulations.

On-going Research / Outlook

The subgrid scale model for supersonic turbulence and the AMR techniques resulting from this project are the basis for on-going simulations of isolated disk galaxy simulations. To that end, the subgrid scale model was combined with a model for star formation and feedback from supernova explosions [8]. This extension of the model introduces two key innovations: Firstly, the star formation rate is computed depending on the local intensity of turbulence. For the parameterisation of the star formation rate, the statistical properties found in [4] play an important role. Secondly, the turbulent pressure, which is determined by the subgrid scale model, allows for a novel feedback mechanism that produces turbulence on small length scales in addition to gas heating.

Currently, this model is implemented into the new fluid dynamics code Nyx, which has been developed in collaboration with the Lawrence Berkeley National Laboratories. This code is scalable to very large numbers of cores and it will allow us to perform galaxy simulations in a follow-up project at the LRZ.

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Dynamics of Binary Black Hole Systems

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HLRB Project ID: H1021

Introduction

Albert Einstein's theory of general relativity has fascinated scientists for almost a century. Even today, general relativity stands unchallenged as our most accurate description of the gravitational interaction in most of astrophysics. However, due to the complexity of the equations, and also due to a lack of computer power, even a seemingly simple problem like the orbiting motion of two stars could not be computed in the full theory until recently. In Newtonian gravity, the Kepler ellipse is well-known as a solution to the two-body problem. In general relativity, space and time become a dynamic entity called spacetime, which allows new, exotic phenomena. For example, general relativity predicts black holes, whose gravity is so extreme that nothing can escape their event horizon. Another prediction are gravitational waves, which are oscillations of spacetime. Even in special relativity, spacetime is still entirely rigid and unchanging. In fact, two black holes that orbit around each other stir up spacetime, generating gravitational waves that carry away energy. Therefore, instead of stable Kepler ellipses we expect an inward spiraling motion leading to a violent collision and merger of the black holes.

The topic of this project was the numerical solution of the general relativistic two-body problem. The goal was to compute the last phase of the inspiral and merger of two black holes, and the gravitational waves generated in the process. Such simulations pose on the one hand a significant theoretical and technical challenge since the time-dependent Einstein equations have to be solved in the regime of highly dynamic and non-linear gravitational fields. On the other hand, theoretical predictions for the gravitational waves generated in a binary black hole merger are eagerly awaited by a new generation of gravitational wave detectors.

The plan was therefore to map out the parameter space of gravitational wave signals from binary black hole inspirals. Numerical simulations of binary black hole systems have only recently reached the point where for the first time orbiting black holes can be computed for at least one orbit. Previous techniques were limited because of the space-time singularity inside the black holes, and because of instabilities of the analytical and numerical methods. After several breakthroughs around 2005, some of which were contributed by our collaboration, today it is possible to compute 10 to 15 orbits and the merger of two black holes. Over the last few years, several research groups, mostly in the USA but also in Germany, have extended the scientific reach of these simulations. In 2006, our project found itself in the exciting situation that just at the time when new methods became available we also gained access to the internationally competitive HLRB.

Results

With HLRB as our main computational resource, we were able to make significant progress on several fundamental issues of the binary black hole problem. In total, the project supported 43 publications, including 5 Physical Review Letters. About 10 Mio. CPU hours were used over the years. Different parameters of a binary are of interest: the mass of the black holes (in particular their mass ratio), whether they are rotating (the size of the black hole spin), and whether the inspiraling orbits are quasi-circular or eccentric.

First of all, the new methods were applied to the standard case of two black holes with equal mass without spin on a quasi-circular orbit. We established the stability and quantified the accuracy of such simulations. Our work led to the longest and most accurate simulation of this type at the time.

In Figure 1 we show a visualisation of the inspiral of two black holes. A

Figure 1: Final orbits, collision and merger of two black holes. Shown is a visualization of the event horizon, where each black hole is represented by a red tube that indicates its motion as time progresses from bottom to top. As predicted by general relativity, the two black holes spiral inwards and merge to a single, larger black hole.

famous precursor of this plot appeared in a book by S. Hawking and G. Ellis 1973, showing the sketch of a "pair of pants" for a straight head-on collision. The "twisted pair of pants" for orbiting black holes is for the first time based on an actual solution to the Einstein equations, and was featured in the DFG Calendar for the Year of Mathematics 2008.

The simulations required the development and implementation of a computational technique called adaptive mesh refinement, parallelized for HLRB, where numerical resolution is adapted to the physical phenomena that have to be resolved. The gravitational waves of such an inspiral serve as a benchmark for more challenging models. We showed for these and other simulations that numerical relativity is able to make contact with the so-called post-Newtonian approximation, which breaks down in the strongly relativistic regime, but which is an important link to classical physics.

Much anticipated was an answer to the question how inequality of the masses affects the merger. For unequal masses, gravitational waves are emitted asymmetrically. This asymmetry can impart momentum to the merged object, which is referred to as gravitational radiation recoil or simply the "kick". We were able to show that the largest possible kick for unequal masses (without spin) occurs for a mass ratio of about 1:3 and amounts to 175 kilometers per second [1]. This is quite a large number considering velocities of stars in a galaxy. However, completely unexpected was the finding that if the black holes have significant spin in the proper direction, then the final black hole can reach velocities of 2600 km/s [2]. This result was one of the rare cases were a theoretical prediction from numerical relativity triggered a series of astrophysical papers, reevaluating the likelihood for such enormous kicks, discussing why they should be suppressed in actual systems since they are not observed, or even searching for and finding one candidate which might be the first supermassive black hole with such a kick velocity. Another line of investigation concerned high-energy collisions of two black holes. In [3] the question is studied what numerical relativity predicts for the (highly speculative) possibility that two tiny black holes are created and collide in a particle accelerator.

These simulations enabled us to participate in various international collaborations concerned with the computation of gravitational waves for the data analysis challenge of the gravitational wave detectors. Given extremely weak signals buried in the noise of the detectors, providing templates for particular sources like black holes is crucial. As an example, in [4] we provided a template for the case of two spinning black holes with the spins aligned with the orbital motion, showing for the first time how to provide simple templates in this case.

On-going Research / Outlook

After the first exploratory physics studies, we are now involved in high-accuracy simulations of black holes that are required for gravitational wave astronomy. In the

Figure 2: Merger of two orbiting neutron stars. Shown are several snapshots of the density in the orbital plane. The neutron stars collide and merge, leading to the redistribution of the nuclear matter in a rotating disk around a spinning, massive neutron star. In this example gravity becomes so extreme that the star at the center promptly collapses to a black hole. Such computations combine the complexity of black holes with general relativistic fluid dynamics.

last two years we extended our simulations to general relativistic systems including matter [5], see Figure 2. We were able to carry out the longest and most accurate simulation for a very simple equal-mass case, but much more remains to be done. Black holes can be modelled very well as vacuum systems, since essentially the matter that collapsed to form the black hole is trapped inside its event horizon. Given our expertise with black holes, we focus on systems of two neutron stars that are already quite relativistic, and which can easily form a black hole when they merge. General relativistic fluid dynamics poses a number of challenges that will require significant advances in our understanding of the physics and in the numerical methods. The challenge of high accuracy for black holes and neutron stars can only be met by a new generation of supercomputers.

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Global MHD simulations of protostellar jets with radiative effects

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HLRB Project ID: H1223

Figure 1: HH212, a stunning example of a bipolar prostellar jet emitting in molecular hydrogen lines [3]

Introduction

The subject of the work I carried out on the HLRB 2 was the investigation of the effect of radiative cooling on the propagation of protostellar jets and the consequent effect on the observable emissions from these objects.

These highly supersonic jets of gas are ejected from accreting protostars in the early stages of their development, the first 30,000 years or so, labelled the Class 0 phase. The jets at this stage typically extend to some tens of thousands of AU (astronomical unit, 1AU is the distance from the earth to the sun).

Such an outflow interacts with the molecular cloud core in which the protostar is forming, and the resulting superheated gas emits light at particular wavelengths according to the chemical composition, allowing astronomers to observe the traces of the outflow with telescopes, see Figure 1.

The protostar itself is hidden within the dark centre of the molecular cloud, making theoretical investigation of the jet ejection process difficult. However, the appearance of the jet on such large scales gives observational clues which, in conjunction with simulations, can provide constraints for theoretical models.

Modelling Jets with Simulations

Our approach is to model the observed protostellar outflow system as a hydrodynamic or magnetohydrodynamic domain, representing the ambient medium of the molecular cloud, into which a collimated pulsating flow of gas is injected, representing the beam of the jet.

The geometry of jets lends itself quite well to simulation in a cylindrically axisymmetric 2-dimensional domain, which enabled us to carry out our simulations without the performance cost of full 3-dimensional computation. The setup is as shown in Figure 2, where initial conditions are set for the gas of both the ambient medium and the jet.

Figure 2: Schematic of the simulation domain setup [2]

Our simulations examined the effect of key parameters on the jet morphology and emission characteristics. Such parameters include the relative densities of the jet and its surrounding medium, the presence/strength of a magnetic field in the surrounding medium, the chemical composition of the molecular cloud and the level of ionisation of the gas in the jet beam.

We used the PLUTO astrophysical simulation code [1], with an additional module we have written to compute the chemistry and corresponding cooling losses at each grid point for every time step. PLUTO, a grid based finite-volume code, solves the HD/MHD equations in parallel via several possible integration methods, while the integration method used for the chemistry module was a simple but effective semi-implicit backwards difference method. The chemical network consisted of the main chemical species and the dominant set of reactions involved in the

production of molecular H_2, a key coolant and emission source in the gas.

In order to be able to carry out simulations of such large scale objects, while still managing to resolve small-scale shock regions, we used the adaptive mesh refinement capability provided in PLUTO via the Chombo AMR libraries.

Performance and Scalability

The resolution chosen for the production simulations was a base grid of 512x64 grid points, with 4 levels of binary mesh refinement, corresponding to an equivalent resolution of 8192x1024 grid points. For the domain of 5000AU this corresponds to a resolution of 0.61AU per grid zone, which is sufficient to resolve the chemical dissociation and cooling zones behind the shock front.

Figure 3: Increasing load corresponding to increasing wall-time as the jet propagates into the domain [2].

Figure 4: Section of the jet showing the entrainment of molecular ambient material and subsequent emission [2].

As the jet propagates through the domain and the area of interaction between the jet and the ambient medium increases, the computational load of the simulation also increases, as shown in Figure 3.

For the production runs we used the HLRB II's SGI Altix 4700 supercomputer. Some thirty runs were carried out in order to probe the effect of different values for the physical and chemical parameters on the propagation and observable emissions. For early parts of the simulation, where the computational load is small, the performance benefit of having a large number of processors is offset by the communication cost between the processors, so we used a varying number of processors at different stages of the runs, typically starting them with 32 or 64 processors and continuing at 128 or 256 processors. The typical CPU consumption per run was between 5 and 10 thousand CPU hours in total.

Results

The data from the simulations provided a wealth of information on some of the factors affecting the jet propagation, giving insight into how the observed jets work. One interesting result was in illustrating the role of the magnetic field in maintaining the stability of the bow-shock. In the simulation run with no magnetic field, the cooling instabilities in the bowshock caused it to break up, allowing ambient molecular material to enter the jet "cocoon".

The molecular material was then heated by internal shocks from the jet and caused to emit in the ro-vibrational lines of H_2, as shown in Figure 4. This supports the "entrainment hypothesis" where the emissions are thought to arise from ambient matter swept up by

Figure 5: Showing the effect of the magnetic field, seen here increasing from 0μG on the left, through 30, 60 and 118 μG on the right. The white box shows matter from the unstable bowshock breaking up and entering the inner part of the jet in the absence of magnetic fields.

the jet, as opposed to (or in addition to) matter in the jet beam itself. In the case where magnetic fields are present, this is not seen to occur (see Figure 5), and the emissions in these cases are seen to occur directly at the shock, a situation known as "prompt entrainment".

Conclusion

The work described here formed part of my PhD work, which I concluded in 2009. Further details are given in my thesis [2].

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Outflows and Jets from

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Young Stellar Objects in Star Clusters

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HLRB Project ID: H1342

Introduction

Our general picture of present day star formation is based on the collapse of over-dense, gravitationally unstable cores within molecular clouds and giant molecular clouds (GMCs). In the current paradigm of modern astrophysics these protostellar cores are built up in shock regions of compressive, supersonic turbu- lence which pervades the clouds. Therefore, the su- personic turbulence is the main catalysts for pre-stellar condensations in star forming regions. One difficulty arises within this picture of star formation: the super- sonic turbulence decays quickly and has to be main- tained. Astonishingly, it is still not known what are the main driving mechanisms and energy support of the supersonic turbulence observed in the interstellar me- dium (ISM).

The possible energy injection into star forming regions can be external (e.g. large scale gas streams, nearby supernova explosions) or come from inside the the molecular cloud via feedback from the young stars (e.g. ionisation shocks, radiation, stellar winds, jets and outflows). The latter possibility, i.e. turbulence maintained from inside the the MC, could – in principle – lead to self regulation of star formation in such re- gion: strong turbulence results in a low star formation rate which in turn lowers the support of turbulence which results in a higher star formation rate increasing again the strength of turbu- lence. Such a scenario was first proposed 30 years ago where the turbulence is driven by jets and outflows from the young stellar ob- ject within the molecular cloud.

Figure 1: Shows the comparison of the collapse of a turbulent cloud core *without* (top) and *with* (bottom) mechanical feed-back (i.e. collimated outflows). The snapshots are taken at an early time into the evolution. Shown is the column density of the cloud and the star formation sites (i.e. sink particles marked as black dots). Surprisingly, the overall structure in both cases is the same, differences are only noticeable at small scales.

Figure 2: Shows the velocity PDFs in the case *without* (red) and with (blue) outflows from protostellar regions at an early time into the collapse (see also Fig. 1). The fraction of outflow powered velocity fluctuations is small compared to the overall turbulent motions.

Results

We studied the influence of protostellar outflows on the dynamical evolution of molecular cloud cores starting with an unstable, turbulent gas sphere. We used our well tested sink particle approach [Federrath+10] to model the feedback of outflows with parameters deduced from observation. Here we present the re- sults from one comparison study where we ran simula- tions with and without feedback. From these studies it seems that mechanical feedback does not dramati- cally alter the dynamics of collapsing cloud cores (see Fig. 1). Only locally the outflows do have an impact on the gas structure. Sometimes gas gets strong enough compressed at the bow shock of the outflows leading to occasional events of *triggered* star formation. Nev- ertheless the global cloud structure as well as the tur- bulent energy content is barely changed in the pres- ence of outflows (see Fig.2).

Based on our studies on jet and outflow driven turbu- lence we conclude that collimated jets from young stel- lar objects are unlikely drivers of large-scale *supersonic* turbulence in molecular clouds (see also [Banerjee+07]).

On-going Research / Outlook

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http://www.hs.uni-hamburg.de/DE/Ins/Per/Banerjee/research.shtml

Ionization Feedback in Massive Star Formation

1

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Introduction

In this project we have studied radiative feedback effects during the formation of massive stars. Understanding the formation of massive stars is one of the most pressing problems in astrophysics. It has been known for decades that radiation feedback is of great importance in massive star formation, but only very recently detailed, fully three-dimensional radiation-gasdynamical collapse simulations have become possible.

Massive stars influence the surrounding universe far out of proportion to their numbers through ionizing radiation, supernova explosions, and heavy element production. Their formation requires the collapse of massive interstellar gas clouds with high accretion rates to reach their final masses before exhausting their nuclear fuel. Massive stars can ionize the gas around them, creating H II regions, and these H II regions form around accreting protostars once they exceed about 10 solar masses. Thus, accretion and ionization must occur together in the formation of massive stars larger than that. In our project, we have studied in detail how the ionization feedback from the growing massive star affects the accretion process and have successfully compared our numerical models with observations.

Results

In the course of the project, we have performed novel radiation-(magneto-)hydrodynamic simulations that consistently follow the gravitational collapse of a massive molecular cloud, the subsequent build-up and fragmentation of the accretion disk surrounding the nascent star, and, for the first time, the interaction between its intense UV radiation field and the infalling material. We have run these extremely demanding calculations on a combination of the most powerful supercomputers in the world, namely JUGENE at the Jülich Supercomputing Centre (JSC), Ranger at the Texas Advanced Computing Center (TACC) and HLRB II at the Leibniz-Rechenzentrum (LRZ) in Garching. The largest of these simulations consumed more than 500,000 CPU hours on HLRB II, using up to 510 CPUs simultaneously. We have used the adaptive-mesh numerical (magneto-)hydrodynamics code FLASH [1] for our simulations. The technically most dif-

ficult part was to develop a proper method for radiation transfer that could be used for the simulations. To this end, we have adapted and extended the MPI-parallelized hybrid characteristics raytracing method [2] for our purposes. Improving the ray traversal along the adaptive-mesh hierarchy, coupling of the radiation transfer to time-dependent stellar sources of arbitrary number, and adding a non-ionizing stellar and accretion radiation component were among our code development tasks.

Once we had all these improvements at hand, we have performed a set of production runs studying the significance of fragmentation, radiation feedback and magnetic fields on the simulation results [3-6]. The simulation data is of great complexity, and in fact evaluating these unique data sets and comparing them to observations is still ongoing work. An illustration of such a simulation is shown in Figure 1. It displays a density volume rendering of a massive, rotationally flattened structure in which several stars form, one being large enough to emit ionizing radiation. The bubble surrounding the dense ring is created by a magnetic field that gets amplified during the collapse, winds up, lifts disk material and accelerates it perpendicular to the disk. This magnetic bubble interacts with a smaller ionization-driven outflow.

The first problem we tackled with our new method was the question whether the ionizing radiation emitted by the growing star could ever be strong enough to terminate the accretion process. To answer that question,

Figure 1: Volume rendering of gas density for a simulation with magnetic fields. Visualization produced with kind help of Herwig Zilken from JSC.

Figure 2: The ionizing radiation from the massive star creates an H II region (red) and drives a bipolar molecular outflow perpendicular to the disk (blue). However, the radiation never becomes strong enough to terminate accretion.

we have run a collapse simulation of a 1000 solar mass molecular cloud in which we artificially suppressed fragmentation to guarantee that a large enough gas reservoir would be available to grow a 100 solar mass star, which is about the upper limit of observed stellar masses. This experiment was successful (see Figure 2), and there was no sign that ionization feedback could ever become strong enough to cut off accretion [3].

Things change drastically when fragmentation is allowed. The massive accretion flow around the growing star is gravitationally unstable, and if it is allowed to fragment, lower-mass companions form in the vicinity of the massive star. These companion stars starve the central high-mass star of material, intercepting matter that would otherwise be accreted by it, and thereby limit its mass growth. The most massive star in this simulation reached less than 30 solar masses. Thus, it is not the radiation feedback that stops accretion onto the high-mass stars, but the fragmentation of their massive accretion flow. We call this new process "fragmentation-induced starvation" [3,5].

The filaments also play an important role for the growth of the H II regions around the high-mass stars. They are so dense that they can shield the ionizing radiation. As a consequence, the H II region cannot expand monotonically away from the growing star as long as it is still embedded in an accretion flow. Instead, it flickers on very small timescales, because each time a filament approaches the star, the gas behind the filament gets shielded and recombines. The time interval between extended and trapped phases can be as short as 10 years, and indeed changes in H II region appearance similar to the ones we find in our simulations have already been observed, but had remained unexplained [3,7].

Our simulations also reproduce the morphological appearances of H II regions around young stars [3,4]. These morphologies had so far been considered a characteristic of a given H II region, but their physical origin was to a large degree not understood. The simulations show that these morphologies not only change continuously during the evolution of the H II region, but that they also dramatically depend on the viewing angle onto that region. The same H II region would be classified differently when looked at from different directions. Thus, H II region morphologies appear to be nothing fundamental, but instead are simply the result of the complex interplay between the infalling gas and the ionizing radiation.

We have also investigated how magnetic fields influence the H II region morphologies [6]. The external magnetic pressure confines their sizes, so that they are smaller than they would be without the magnetic field. However, their morphological appearance itself appears to be unchanged by the magnetic field. Furthermore, our simulations indicate that magnetic fields do not seem to drive powerful molecular outflows in high-mass star formation, but lead to the formation of rather spherical bubbles instead (see Figure 1). This is somewhat in contrast to observations that do find outflows around massive stars. Further studies that try to resolve this discrepancy are underway.

On-going Research / Outlook

Our results have spawned numerous follow-up questions. If fragmentation of the accretion flow limits the mass growth of massive stars, how do the observed 100 solar mass stars form? Does it suffice to start from an even larger initial gas reservoir?

Another question revolves around the impact of turbulence on massive star formation. How does it affect the fragmentation-induced starvation scenario? Does turbulence change the H II region morphologies or their dynamical evolution?

The observational signatures of H II regions are subject to further studies. Preliminary results indicate that an additional mode of H II region flickering is possible that is also related to the accretion process. Stellar evolution models show that in the earliest stages of a star's lifetime, when the star has just started shining, there is a short phase in which the core is burning deuterium. Stars that accrete at a very high rate can then swell up dramatically, which decreases their ionizing luminosity and leads to a shrinking of their H II region. Current work tries to quantify this effect and find means to distinguish it from the geometrical shielding that we have discovered first.

One key element for this and many other studies will be to look at kinematic information from the H II region, as given by the observation of hydrogen recombination lines. Recently, we have developed a method to generate synthetic recombination line observations from our simulation data. These maps can then be compared to real observations, in particular with the upcoming ALMA telescope, that will be able to look at H II regions with an unprecedented angular resolution and sensitivity. Tests like this will help us to further improve our simulations to deliver an even more realistic model of the formation of massive stars.

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Solar Surface Flow Simulations at Ultra-High Resolution

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Introduction

Bright as it appears in the sky, our sun nevertheless still harbours a significant number of unsolved physical problems. Conceivably, some of them refer to the interior which is not directly accessible to observations. Perhaps the largest problem here is the working of the solar dynamo which creates a global magnetic field exhibiting field reversals every 11 years or so. There have even been periods where the dynamo has been stalling for decades. Seemingly, such periods are associated with epochs of cold climate on earth. Even the surface layers which are observed by a large variety of instruments at solar observatories and aboard of balloons and satellites pose a number of basic unsolved problems. At the same time, the sun can serve as a laboratory for the atmospheres of other stars which can impossibly be observed in such a detail as the solar atmosphere can be. It might seem that for the surface layers which are accessible to direct observation there is little room for computational modelling. This is, however, not at all true. Not only is the interpretation of the observations quite difficult in many cases. The rays of light which we observe transverse various inhomogeneous layers, photons being emitted, absorbed or scattered so that ultimately we get a mixture of photons which have been created in various depths. Setting that aside, inferring physical properties from the analysis of the light may be a difficult task.

Solar Granulation – Setting up the Problem

Near the centre of the sun thermonuclear processes release energy. In the inner two thirds of the sun the energy is transported outwards by radiation. Farther out, the energy transport is affected, however, by convection: hot material rises, cools near the surface and sinks down again. In the solar photosphere (the observable layer) we see the outermost manifestation of solar convection which there mainly takes the form of small convective cells, the granules, with typical diameters of somewhat more than 1,000 km. In the centre of granules the hot gas rises, moves sidewards and sinks subsequently down at the granule's boundaries, forming a network of so-

called intergranular lanes. Such granules are easily observable, and their most basic physics have been successfully modelled since quite some time [1]. Observations have, however, revealed both hydrodynamical and magnetic phenomena near the resolution limit. This leaves, of course, room for phenomena below that limit. An understanding of granulation which is as detailed as is feasible is not only worthwhile in itself and for understanding the properties of turbulence in stars. Above the solar photosphere the chromosphere and the corona are situated the proper description of which is a difficult task. After all, the solar corona has a temperature of approximately 1,000,000 K. Its heating mechanism (hydrodynamical or magnetohydrodynamical) has still not been identified with certainty and can scarcely be understood without proper knowledge of the underlying layers. Regions of enhanced turbulence, witnessed both by observations and by numerical simulations, are the granular downflow lanes (cf. e.g. the extensive review [1]). Here, we concentrate on these. Simulations show strong vortices in such regions. Previous investigations which we have

u3 v_r_n_g 0.4 T6000

Figure 1: This figure and the next one show one and the same portion of the solar photosphere (horizontal extent about 1 Mm), albeit at different times and at different resolution. Fig. 1 refers to resolution in the sense of u2, Fig. 2 in the sense of u3 (see text). The yellow surface is the T = 6,000 K isosurface (approximately the depth until which one can peek from outside). The blue tubes are isosurfaces of the magnitude of the vorticity of the flow and mark vortex tubes.

carried out at especially high resolution have shown the occurrence of a very large number of much smaller vortices than previously known; see [4]. These calculations referred to a so-called exploding granule. Vortices have been sought for and found observationally. Large vortices (about 3 Mm) have been described in [2]. Typical recent work shows a majority of vortices with a typical diameter around 250 km, e.g. [3]. The purpose of the present project was to investigate a normal granule and achieve, in addition, even higher resolution, in order to more fully describe this special type of turbulence.

Results – The Calculations

The simulations were carried out using the ANTARES code [4] for solving the equations of compressible hydrodynamics and radiative transfer using realistic opacities and microphysics. The inviscid part of the hydrodynamic equations is discretized using so-called essentially non-oscillatory (ENO) schemes. These high-resolution schemes give much information per grid-point due to the high order of approximation on the one hand and their ability to cope with shocks or strong gradients on the other. Time-evolution is accomplished using special Runge-Kutta methods. The equation of radiative trans-

u3 v_r_n_g 0.4 T6000

Figure 2: The dramatic difference of the amount of vortex tubes as compared to the previous figure shows the effect of increasing resolution to amounts which are more appropriate to describe the turbulent state of the material.

fer is solved by the method of short characteristics. The specific approach (also to parallelization) is described in [4]. The model uses three grid hierarchies (termed u1, u2, u3). The coarsest grid has an extent of 6 Mm in both horizontal directions and contains several granules. The region of special interest (u3) is 1.2 Mm wide in both directions. The horizontal grid-spacing is 22.2 km for u1, 7.4 km for u2 and 3.7 km for u3. Grid-points for u1, u2, and u3, corresponding to one and the same physical location do, in general, not reside on one and the same node. Thus, there is considerable network traffic for linking the various grid-hierarchies together. We have been pleased with the interconnectivity of the HLRB-2 machine which was appropriate for that purpose. On HLRB-2, every core provides 3 GB of memory. For our overall requirement of 1.1 TB we consequently need more than 350 cores. On the other side, the maximum number of MPI processes

is limited by the domain decomposition. In our case, at most 256 MPI processes could meaningfully be used since otherwise the domains would be unduly small leading, among others, to an unfavourable volume to surface ratio (boundary data of each domain have to be transmitted to their neighbours). It is therefore essential to use a hybrid, namely both MPI and OpenMP, parallelization strategy which, in fact, is provided by the ANTARES code. In a very general vein we would like to state that for codes like ANTARES a programming language combining many of the advantages of FORTRAN for numerics (plus omitting some of its disadvantages), with facilities for parallelization (both shared and distributed memory paradigms) and options for creating threads would highly improve working efficiency of code development. To all those requirements the need for reliable compilers has to be added as well. Contrary to most other clusters on which we have worked, parallel output has not been that crucial on HLRB-2 thanks to its file system which allows for very fast data communication. Analysis of the data (in HDMF-format) has been done locally on workstations using the open source visualization software PARAVIEW.

On-going Research / Outlook

The results of the present project have shown a dramatic dependence of the simulated state of turbulence on the resolution of the calculations. They have been presented at various meetings, see e.g. [5]. The question is, of course, which, if any, effects an even further increased resolution will show. In order to investigate this, we are presently working on a similar model which, at the u3 level, has a horizontal grid size of 2.47 km (instead of 3.7 km) and uses improved numerics. There is an abundance of small vortices, with diameters in the 10 – 20 km range. Compare that with the typical diameters of vortices in current observational surveys such as [3] with typical diameters of most vortices of about 250 km as already mentioned previously. Larger vortices (vortex diameter about 100 km) show quite significant evacuation due to Ccoriolis forces, the density or pressure inside the vortex being only half of the values found in the ambient medium. Figure 2 makes it very clear that the vortex tubes are concentrated near the downflux tubes. Consider that the elevated areas of the temperature isosurface (yellow) mark the upflow regions. It is readily seen that in these regions neither in the atmosphere above the isosurface nor further downwards is there any abundance of vortex tubes. In these high-resolution models a large number of small amplitude acoustic pulses is found which are excited in more or less pointwise sources and transverse the computational domain.

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Formation of Molecular Clouds in Colliding Flows

1

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Introduction

Stars in galaxies form in dense, cold molecular gas clouds which condensate out of the diffuse, mostly atomic, interstellar medium (ISM). Those molecular clouds are the birthplaces of stars in galaxies. It is Still an unsolved problem how those clouds form out of the ISM and what are their fate. In the traditional picture, molecular clouds are quasi-static, virialised objects with slow star formation and a long life time. In such objects, star formation was thought to happen only after a significant delay beyond their formation time. Other studies suggested that molecular clouds are very dynamical objects which start to form stars shortly after they are formed. Furthermore, many analyticaland numerical studies could show that MC can form through thermal and dynamical instabilities in the warm neutral medium (NWM) of the interstellar gas. Such thermal instabilities can be triggered by large scale colliding gas streams [Vazquez+07].

Figure 1: Column density of the inner region of the molecular cloud assembled from colliding streams of warm atomic gas. The dots mark the projected positions of star forming regions.

In this study we set out to test those two ideas including the presence of magnetic fields in our calculations. Magnetic fields are important ingredients that permeate the entire galaxy and the interstellar medium. Their dynamical importance can be inferred, for instance, from the beautiful optical jets associated with young stellar objects where the jets are launched and collimated by magnetic fields.

Results

Within this studies [Banerjee+09, Vazquez+11] we find that the ram pressure from the accretion of WNM gas into the clumps contributes a net ram pressure, in ad- dition to the thermal pressure of the WNM, causing the clumps' densities to overshoot past the typical conditions of the CNM, well into the realm of physical conditions typical of large molecular clouds (see Fig.1). Moreover, since the ram pressure from the diffuse medium is turbulent and fluctuating, it induces transonic turbulence within the clumps which, as a consequence of the joint conditions of ram and thermal pressure balance, must have an rms Mach number comparable to that in the diffuse gas. The transonic turbulence in the clumps induces significant density fluctuations, which then provide the seeds for subsequent local gravitational collapse as the clumps approach their Jeans mass (see Fig.2).

Furthermore, the turbulent velocity dispersion within the clumps increases with their mass, respectively size.

Figure 2: Evolution of the total cloud mass and the ratio of this mass to the cloud's Jeans mass. The entire cloud rapidly grows to contain a large number of Jeans masses hence it becomes globally unstable.

As the clumps grow preferentially in lateral directions this scaling is consistent with those inferred from observations.

We also showed that the transition between such clumps and the diffuse medium is generally sharp, with both media being at roughly the same thermal pressure, similarly to the situation in the classical two- phase medium. However, the clumps contain large density fluctuations within them, of up to one order of magnitude above and below the nominal pressure- equilibrium density value, caused by the presence of thermally unstable gas still in transit towards the cold phase on the one hand, and to local gravitational con- traction on the other. Thus, the boundaries of the clumps, which generally consist of thin layers of thermally unstable gas, often become extended and penetrate deep into the clumps. The clumps are nearly isothermal inside, with temperatures in the range 20 - 50 K, as consequence of the density fluctuations within the clumps and the nearly isothermal equation of state governing the high-density gas.

Another key difference between the classical model and the results of our simulations is that the clumps are formed dynamically by the compressions in the surrounding WNM, implying that they are subject to continuous accretion from the WNM driven by its ram pressure. This in turn causes the clumps' mass and size to grow in time. Thus, the clumps' boundaries are ram-pressure-driven phase-transition fronts and clump growth occurs mainly by accretion through their boundaries, rather than by coagulation, as was the case in earlier models of the ISM. In turn, this mass flux drives the clumps to eventually become gravitationally unstable and collapse.

The magnetic field shows a significant level of alignment with the velocity field, but also large fluctuations in magnitude and direction inside the clumps, suggesting that it has been significantly distorted by the turbulent motions in the dense gas. We also find very similar distortions of the magnetic field structure by turbulent

motions in the case with larger a initial field strengths of 3 µG. This suggests that gas streams and field lines are likely to be aligned in the cases of either a weak or a strong magnetic field (see Fig. 3).

The molecular clumps and the cloud as a whole are dynamical and evolve with time, with important consequences for their ability to form stars. After some 20 Myr of evolution, some regions have already undergone local collapse and started to form stars, while other clumps do not yet show signs of star formation, similarly to an earlier suggestion for clouds behind the spiral arms of the Galaxy. The age spread in star formation times is at least 10 Myr over the entire cloud. During the evolution of the cloud, global gravitational focusing enlarges connected molecular regions in the centre of the cloud. In this central region the gas reservoir is sufficient and gas densities are high enough to allow the formation of massive stars.

On-going Research / Outlook

In an ongoing study we are investigating how feedback from star forming regions via outflows and winds as well as supernova explosions will determine the evolution of those clouds. Key question is, whether the generated turbulence by such feedback processes will self-regulate the star formation in molecular clouds and/or whether the clouds will be entirely disrupted.

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Figure 3: Histogram of the angle between the velocity and B- field vectors. The velocity and magnetic field vectors are clearly seen to show a strong tendency to be either parallel or antiparallel..

Molecular clouds and the Color Magnitude Diagrams

1

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Introduction

To understand the processes that govern the formation of stars and galaxies is of paramount importance to improve our comprehension of the observed Universe. Stars commonly form in molecular cloud complexes, whose evolution is ruled by internal and external processes of heating, cooling and instability type.

The goal of this project is to study how these processes evolve and transform with time the molecular cloud complex in a galaxy whose properties we can observe. To achieve these results, we focused our attention on dwarf galaxies because they are the most common type of galaxies in the Universe [1] and often offer a beautiful example of interaction between a major galaxy and its satellites [2]. While orbiting, these satellites are affected by environmental effects that influence their evolution and affect their star formation history [3,4].

In this study we develop a numerical investigation of dissipative phenomena occurring during the orbital evolution of a dwarf satellite galaxy orbiting around a host galaxy. The goal of this project is to reach a simple and qualitative description of the complicated connections existing between gas consumption processes (e.g., ram pressure, Kelvin-Helmholtz and Rayleigh-Taylor instabilities, tidal forces) and star formation processes in the context of the two extended-body interaction and with special attention to the dwarf galaxies dynamical regime involved in our local volume of galaxies, i.e., the Local Group (LG) [5,6]. Moreover, these dynamical phenomena may leave signatures in the star formation activity and in the colour magnitude diagram of their galaxy stellar content. Thus, once established the theoretical framework that links orbital evolution of dwarf galaxies in the LG and star formation processes, we synthetically reproduced observable quantities

Figure 1: orbital evolution of a dwarf galaxy with pericentre r_p on the MW plane (illustrative image in the background) starting its orbiting at r_p = 200 kpc (1kpc=3261 light years) and eccentricity e=0.25

as colour magnitude diagrams. Finally, this procedure allows us to compare the models predictions with the observational data.

Results

Thanks to the computational resources available at the Leibniz Supercomputing Centre, we succeeded in writing a code which is fast in handling these complex star formation processes. In the developing phase (project pr47zo) we realized a parallel integral-differential equations solver based on a parallelized version of the Runge-Kutta techniques with adaptive step-size control. This integrator has been planned and entirely developed on the SGI Altix 4700 at the National Supercomputer (HLR-BII). It is written in Fortran 95, to be easily interfaced with the pre-existing synthetic colour magnitude generator codes [7,8,9], parallelized with distributed memory Message Passing Interfaces (MPI) protocol, debugged with Totalview and profiled with Scalasca. The typical code runs are tuned to best perform on 650 processors. Higher resolution convergence and control tests have been performed scaling the code to higher number of processors: on 1st May 2011 an high resolution simulation ran on 6500 processors on the HLRBII recording peak performances of 23Tflops/sec.

After the development phase, the project has been reviewed as "Grand Challenge Projects" (project pr42fe) and about 330,000 CPU hours have been assigned. This allowed us to tackle the initially posed challenges once we decided to limit our study to the local sample of dwarf galaxies (LG) and with especial attention to the MW dwarf satellites. Because of its proximity, this set of dwarf galaxies represents an excellent laboratory where to investigate these difficult problems thanks to the richness of available observational data and exquisitely precise constraints. We adopted an external force

Figure 2: Pressure profile corresponding to the galaxy orbit shown in Figure 1. Pressure is measured in solar pressure (P$_{sun}$=1.4 10^4 k$_B$ with k$_B$ Boltzmann constant). The color coding from red to blue indicates increasing younger ages.

Figure 3: Star formation profile corresponding to the pressure profile of Figure 2.

field, representative of the gravitational potential of the Milky Way (MW) and a hot plasma coronal gas (T=10^6-10^{8}K) model where to integrate the orbits of the dwarf galaxies (see Figure 1 for an example of the path that a standard-model of a spherical dwarf galaxy that we followed on its orbit for nine billion years)

Once the orbital path of a standard dwarf galaxy in its last 9 Gyr of evolution is computed, a corresponding profile of the pressure acting on the molecular cloud complex of the primordial dwarf galaxy is determined as the one shown in Figure 2.

Once the pressure is determined as a function of the dwarf galaxies' orbital location, the corresponding star formation processes affecting the molecular clouds can be evaluated and the star formation history of the galaxy under exam estimated. For an initially assigned mass spectrum of the molecular clouds, star formation efficiency ε and destruction time τ can be evaluated as a function of the molecular cloud mass and pressure [10] and from them the star formation rate can be estimated as a function of the instantaneous location and mass of the dwarf galaxy in its orbit around the MW [11]. We see in Figure 3 an example of star formation history of the dwarf galaxy corresponding to the path of the Figure 1.

Finally, from the star formation history, and assuming an initial stellar mass function, we are able to produce the corresponding synthetic theoretical colour magnitude diagram. The latter can be convolved with observational errors and shifted in magnitude and colours in order to be directly compared with the observed CMDs. An example of a theoretical colour magnitude diagram (the Hertzsprung–Russell diagram) can be seen in Figure 4 for a dwarf galaxy orbiting in the orbits of Figure 1.

On-going Research / Outlook

The results obtained so far are organized in two papers. The first explains the method developed here, presents some tests on the code performances and scalability, and it has been recently submitted to Astronomy and Astrophysics [12].

In the second paper (representing our on-going project) we plan to extend and complete the family of orbits previously investigated and to study the relative importance of the instability processes implemented.

The improved capabilities of the forthcoming machine SuperMUC can enormously improve the capabilities of our code by providing a higher number of processors and more CPU time. This machine will ultimately allow us to span thoroughly our model parameters' space and to investigate with more precision the physical processes involved.

Figure 4: Hertzsprung–Russell diagram. The colour code represents the age of the stars.

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Magnetic field amplification during gravitational collapse

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HLRB Project ID: pr42ho

Introduction

Magnetic fields are ubiquitous in the Universe and their study forms an important area of research in modern day astrophysics. Magnetic fields are observed in a variety of astrophysical objects starting from planets like our Earth to stars, galaxies and in galaxy clusters. Recently, sophisticated observations have revealed their presence even in objects which were formed when the Universe was relatively young. In technical jargon, we refer to the early stage of the Universe as high-redshift Universe. In some of our earlier works [1, 2, 3], we investigated the issue of magnetic field amplification during the birth of the First stars both analytically and numerically (the simulations in [2, 3] were performed on the HLRB2 at the LRZ under grant no. h1221). These stars were the first objects to form in our Universe that heralded an end to the cosmic Dark ages. Starting from an initial weak seed magnetic field, our study showed that apart from the regular field amplification by gravitational compression, magnetic fields could also be exponentially amplified by a phenomenon called Small-scale dynamo action [1]. The dynamo is a process where energy in turbulent fluid motions is tapped to amplify the magnetic energy. We concluded that dynamo process can lead to additional amplification of magnetic fields during the formation of these objects.

In this project, we explore in detail the effects of environment on the gravitational collapse and magnetic field amplification using high-resolution three dimensional simulations. We choose initial and environmental conditions that are reminiscent of the conditions in primordial mini-halos that lead to the formation of the first stars in the Universe. Our choice of the initial magnetic field strength allows us to explore both the kinematic regime (where the magnetic field is dynamically unimportant) and the saturation phase when the magnetic field becomes dynamically significant. The key questions which we address in this study are as follows: How does the collapse, growth and saturation level of the dynamo depend on the properties of turbulence in the primordial gas? What information concerning dynamo saturation can be obtained from our study? We also seek to explore the influence of uniform rotation of the primordial cloud on the collapse and field amplification. Beyond the formation of the first stars, we expect that the picture emerging from our study will be of general importance to all gravitationally bound objects. The small-scale dynamo may provide strong seed fields for large-scale coherent magnetic fields in galaxies as well as in the large-scale structure of our Universe. This study will improve our understanding of structure formation in the high-redshift Universe.

Results

In this contribution, we focus on the dependence of the growth rate and saturation level of the dynamo generated field on the turbulent properties of the collapsing cloud. In gravitationally collapsing system, the relevant scale is the thermal Jeans length. This scale is set by the competition between gravity and thermal pressure. Using adaptive-mesh refinement technique, we perform simulations where the Jeans length is resolved by a maximum of 128 grid points. We perform these simulations using about $510 - 1024$ cores on the HLRB2 at the

Figure 1: Time evolution of the spectra of the magnetic field.

LRZ. For more details on the computational techniques and the parameter study, we refer the readers to [4]. We first explore the effect of varying initial strength of turbulence choosing a range of initial turbulent velocities having both subsonic and supersonic values. Initially, the small-scale dynamo provides additional field amplification over compression and later attains saturation. Starting from a 1 micro Gauss field, the total magnetic field is amplified by six orders of magnitude to yield final field strengths of about a Gauss in the central collapsing core. The saturation phase is marked by a distinct change of slope of the small-scale dynamo generated field. The magnetic energy grows at the expense of the turbulent kinetic energy and eventually attains saturation at values pertaining to a fraction of the equipartition value. Next, we varied the initial injection scale of turbulence. Here we compared two cases, one in which the injection scale was on the order of the initial Jeans length of the core and the second, where the injection scale was chosen to be at one-fifth the initial Jeans length. In the latter case, we observe that turbulence decays faster as more kinetic energy has to be initialized on smaller scales to obtain the same overall turbulent energy. This leads to early collapse compared to the former where the initial injection scale was on the order of the initial Jeans length. Once again, we observe both the kinematic and saturation phase of the dynamo. Finally, we explore the effect of uniform rotation on the collapse and magnetic field amplification. The dynamical evolution shows two distinct phases: an initial turbulent decay phase followed by a runaway collapse phase where the turbulence is regenerated by the gravitational collapse. For a detailed analysis of dynamo saturation we plot the time evolution of the magnetic energy spectra obtained by Fourier analysis. This is shown in Fig.1. Since the smaller scale eddies amplify the magnetic field faster, saturation should initially occur on smaller scales and gradually on much larger scales. The magnetic field spectra in Fig.1 show that the peak of the spectrum initially occurs on smaller scales and then gradually shifts to larger scales (i.e., smaller k-values) at late times. To get an idea of the saturation level attained at different scales, we show in Fig. 2, the time evolution of the spectra of the ratio of magnetic to kinetic energies. Consistent with earlier theoretical predictions, the magnetic energy at first attains equipartition with the kinetic energy on smaller scales and subsequently on larger scales.

Figure 3 shows a snapshot of the magnetic field obtained from the same simulation. The vectors denote the direction of the local magnetic field. The color bar denotes the magnetic field strength. The magnetic field exhibits filamentary structure. The field is randomly oriented but with equipartition being gradually attained on larger-scales (see Fig. 2), the field is eventually expected to become coherent.

Figure 3: Snapshot of the magnetic field obtained from the same simulation as in Figs. 1 and 2. Vectors denote the local magnetic field direction.

On-going Research / Outlook

With the help of the supercomputing time granted under pr42ho at the LRZ, we have explored the effect of different environmental conditions on the collapse and magnetic field amplification. For the case of primordial magnetized cloud collapse our simulations have shown for the first time that dynamically significant magnetic fields are generated during the collapse. Since the growth rate of the dynamo is crucially dependent on the Reynolds number and thus on the numerical resolution, we expect that with increasing computational power, higher resolutions will be achieved in future which will improve our understanding of dynamo saturation in collapsing objects. The strong random seed magnetic fields could potentially give rise to large-scale coherent magnetic fields. Such coherent magnetic fields could lead to the formation of jets and magnetic outflows thereby permeating the surrounding medium with magnetic fields. Besides, it remains to be explored what effect such fields have on the fragmentation properties of the cloud. This will have a bearing on the final masses of these stars. Exploring these possibilities with additional physics like primordial chemistry and different feedback effects form the subject area of our research in future.

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Figure 2: Time evolution of the spectra of the ratio of magnetic to kinetic energies. The magnetic energy at first attains equipartition on small scales and then gradually at larger scales.

CoJac: Jet Activity in Cosmological Simulations

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Introduction

How did galaxies form and evolve? What were the most important physical processes? And can we explain the observed properties of galaxies with the currently used models of their formation? These questions go far into the realm of cosmology – the very old question how our Universe formed. In the last decades, computational power and the development of new algorithms and codes has finally allowed us to assess these questions more quantitatively and in their complexity.

Current cosmological simulations do a very good job in building up the early structure in the Universe, in particular since the earliest evolution depends mostly on dark matter which, despite its still mysterious nature, can be modeled computationally in a rather simple way. The details of this evolution at small scales, however, within the groups and clusters of galaxies, is mostly dictated by the "normal" baryonic matter, which interacts hydrodynamically and shows a very rich phenomenology. Gas cools over millions of years, looses its pressure support and collapses under its own gravity, forming stars which again heat up the surrounding gas during their evolution and in particular when they explode as supernovae. In the last decade, very massive black holes in the centers of galaxies have become another very important component since they are capable of highly energetic phenomena as quasars or radio jets, summed up as Active Galactic Nuclei (AGN). Since the galaxies feed the black hole with gas, which itself acts back on the galactic gas, the interaction process of active black holes in galaxies is commonly named "AGN feedback".

Although much progress was made in the field of galaxy formation, simulations are still not able to produce the observed galaxies and often rely on phenomenological recipes, which are not understood in their actual physical mechanisms. As an example relevant for this project, high mass galaxies have non-realistic properties in simulations: By the current epoch, 13.7 billion years after the Big Bang, they are still actively forming stars, shining in blue light and grow to masses much larger than observed galaxies, which are not forming stars anymore and hence appear red. It thus have become very important that now, where large-scale simulations are feasible, the "nasty little details" are re-examined, improved in modeling and then plugged into the large-scale runs. This project aims towards including a physical model for AGN jet feedback based on the detailed studies at small scales which the authors have performed in the past. Although the resolved simulation of jet feedback is not feasible for a large number of galaxies on current supercomputers, the restriction to a single galaxy withiin the large computational domain makes this possible and can yield a much better understanding of the impact and importance of this scenario.

Results

The project consisted of three consecutive parts: (1) testing and implementation of the jet feedback model in the simulations of individual galaxies as well as the large-scale simulation code, (2) the MPI-parallel generation of the initial conditions for the large-scale code, (3) production run of the large-scale simulation with subsequent analysis. While the first two parts were carried out successfully before and during the 6 month project period, the third part could not be completed in time. Hence, after the description of the achieved results, some critical remarks and suggestions about the project conditions are given, hoping that future projects may benefit from that.

Positive and negative feedback from jets

Large-scale cosmological simulations so far have only modeled AGN feedback as negative feedback: gas in and around galaxies is heated by the AGN and reduces the star formation rate in the galaxy since stars are formed

t = 10 Myr   5 kpc   t = 22 Myr   5 kpc

Figure 1: Stars in a massive galaxy without (left) and with (right) an active jet.

Figure 2: Filaments of gas falling onto the massive galaxy at their intersection

only in collapsing clouds of cold gas. While the energy release associated with black hole activity can be very large, in extreme cases corresponding to many times the luminosity of all stars in the galaxy, it is not evident that this ultimately leads to the heating of gas, although the observed decline of star formation in massive galaxies makes this scenario very attractive. In fact, Silk (2005) suggested that AGN activity may result in a strong increase in star formation. In a preparatory study for this project, we have modeled the action of jets launched from black holes and their interaction with the clumpy distribution of gas in an isolated model galaxy. We have explicitly included the formation of stars by the observed Kennicutt – Schmidt law and are hence able to analyze the impact of the jet activity in more detail [1,2]. Up to then, this had not been undertaken yet.

We found that in massive gas-rich galaxies of the early Universe, with gas masses of about 100 billion solar masses, the negative feedback is weak and limited to the very center of the galaxy, where the gas is heated and pushed out of the galaxy. The overall effect is dominated by positive feedback, where the star formation rates increase drastically from 150 solar masses per year to more than 500 solar masses per year. This is due to the enormous energy release that heats gas, builds up large pressures and results in a blast wave driven through the galaxy, which itself compresses pre-existing dense gas clouds that radiate strongly at these higher densities, cool down, lose their pressure support and can form additional stars. Since the galaxy in these simulations was isolated and had no interaction with the dynamic environment found in large-scale cosmological simulations, these effects could not be studied with small-scale simulations. Yet it is obvious that the positive feedback can also be expected for cosmological runs and considerably question the often-assumed negative feedback model.

Jets in Large-scale Simulations

Collaboration with experts of large-scale cosmological simulations from the University of Oxford formed a strong basis for this project due to the combined expertise from both jet physics and cosmology. The generation of initial conditions for the large-scale run on HLRB2 worked with only minor technical difficulties. However, preparatory test runs for the large runs crashed unexpectedly at different locations only after several hours of runtime and caused a large delay until the problem in the implementation of the adaptive mesh refinement of the employed code RAMSES could be spotted and fixed. The inclusion of very small-scale phenomena (around 50 pc) within the large-scale run (100 Mpc box size) made a very strong mesh refinement necessary (~20 levels of refinement), relying on quad-precision for some variables responsible for the domain decomposition. However, test runs with such a large refinement could not be tried on smaller machines due to their memory limitations and hence occurred first on HLRB2. After these problems were fixed, only 4 weeks remained for the project, which only allowed few additional test runs and the very early evolution of the production run.

Suggestions for future projects

We have critically re-examined our project planning and schedule to improve this process on our side, but also would like to give some comments here for potential future improvements on the side of the DECI project initiative and its successors. DECI seeks for excellent and highly innovative projects. Yet, leading-edge projects generally struggle with new problems that did not occur for more standard projects. Hence the project duration is of very high importance. Six months are very short for this and do not allow for much delay due to newly occurring problems. Furthermore, the projects were running over the same time period, meaning that the demand for computational resources strongly increases towards the end of the project, resulting in long queuing times. From our point of view, longer project durations and also potentially staggered starting times are appreciable. Another issue that we have encountered, although it did not become critical for our project, is the medium-term storage of the simulation data. Since the data analysis typically reaches beyond the project runtime, considerable storage requirements persist until after the project duration (during the project, these requirements are nicely met). It would be appreciable if the produced data were easily accessible also beyond the project during (e.g. 1 – 2 year).

On-going Research

The simulation setup and data created for and during this project will be used for a successor project. Furthermore here we include a new implementation of quasar feedback – the second aspect of AGN feedback in galaxy evolution.

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Jupiter's Magnetosphere

1

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Introduction

The outer layer of the Sun is so hot (1.5 million degrees) that particles can escape the Sun gravitational field. As a result, every second, approximately 1.4 million tons of plasma (mainly protons and electrons) are ejected in the interplanetary space, reaching speeds of approximately 400 km/s: this stream of particles constitutes the "solar wind".

The interaction between the solar wind and a magnetized planet (such as the Earth or Jupiter) deforms the dipole magnetic field of the planet, which gives the planet's magnetosphere its typical shape (see Fig. 1): compressed magnetic field lines on the day side and elongated magnetic field lines on the night side (the magnetotail). In addition, since the solar wind interacting with the planets is super-sonic, a bow-shock is formed upstream of the magnetopause (closed magnetic field lines of the planet). When the plasma crosses the bow-shock, it is strongly decelerated and heated; it is then deflected around the magnetopause. At Earth, disturbances in the solar wind (specially when the interplanetary magnetic field displays a strong southward component) may trigger geomagnetic storms, during which polar lights are usually strong. At Jupiter, which magnetosphere is very different from the Earth's, the main auroral features are not driven by the solar wind, but mostly by internal processes.

The Earth's and Jupiter's magnetosphere are very different for several reasons: Jupiter has a short rotation period of 9h55min, in addition the surface magnetic field of Jupiter is 14 times larger than the Earth surface field; finally Jupiter's magnetosphere possesses an important internal source of plasma (the volcanic moon Io releases approximately 1000 kg of plasma every second). The Jovian magnetosphere is consequently the largest planetary magnetosphere of the solar system. On the night side, the magnetotail extends up to the orbit of Saturn.

Due to the strong magnetic forces and the fast rotation of the planet, the plasma inside the magnetosphere rotates around Jupiter (see Fig. 2). Close to the planet, where the magnetic forces are the strongest, the plasma rigidly corotates with the planet (meaning that the angular velocities are the same). At approximately 30 Jovian radii (Rj), the magnetic forces cannot sustain the acceleration of the plasma any more and the plasma start to sub-corotate: this is called the corotation break-down. In a strongly ionized plasma (where positively and negatively charged particles move freely), the magnetic field and the fluid's velocity are tightly linked. Consequently, when the corotation breaks down, the field lines are bent in the azimuthal direction and the electric current system sketched on Fig. 3 is formed. This current system triggers the main auroral emission in Jupiter's ionosphere. The aurorae observed at Jupiter are about 100 times brighter than the aurorae observed on Earth.

Figure 1: Results of a simulation: density contours and magnetic field in the noon-midnight meridian (side view). The solar wind comes from the right.

Figure 2: Results of a simulation: density contours and velocity in the equatorial plane (top view). The solar wind comes from the right.

Figure 3: Sketch of the dayside Jovian magnetosphere. Light gray: the ionosphere (where ion-neutral collisions take place). Dark gray: Io torus (plasma created through ionization). Small gray dots: current sheet. The current and magnetic field are represented by solid and dashed lines, respectively.

The position of the corotation break-down is mainly controlled by the mass-loading rate associated with the moon Io (the higher the mass-loading, the closer to Jupiter the corotation breaks down) and by the height integrated conductivity in the ionosphere of Jupiter (the higher the conductivity, the further the corotation breaks down). The goal of our work is to develop a new model in order to perform 3D simulations of the interaction between the solar wind and Jupiter's magnetosphere (including the mass-loading and the ionosphere). And to then perform numerical experiments to understand how internal sources affect the magnetosphere.

The Model

Our simulations are done in the framework of magneto-hydrodynamics (MHD) where source terms are added in order to account for: 1) the mass loading caused by the moon Io (the newly added plasma modifies, for instance, the density and the velocity of the medium) and 2) the collisions between the neutral particles and the plasma in the ionosphere. These collisions affect: the plasma velocity (the plasma is forced to rotate with the planet in the ionosphere), the temperature (e.g. Joule heating) and the magnetic field (closure of the electric current systems in the ionosphere). By controlling the ion-neutral collision frequency in the ionosphere (which is a free pa-

rameter of the model), we control the ionospheric conductivity. The Io mass-loading rate is also a free parameter of the model. The simulations are performed with the mpiamrvac code [1], using a TVDLF (Total-Variation-Diminishing Lax-Friedrichs) numerical scheme with a finite volume setting on a spherical mesh. These are the first global simulations of the Jovian magnetosphere where the ionosphere is directly included in the simulation domain. Even though we had to enhance the size of the ionosphere in order to resolve it on our mesh (which is too coarse due to numerical constrains).

Results

Figures 1 and 2 show the magnetosphere obtained with our simulations. The main features of the Jovian magnetosphere are clearly visible on these figures. A bow shock is formed upstream of the magnetopause where the solar wind is decelerated, and where the density and magnetic field magnitude increase. The plasma is then deviated around the magnetopause. The dipole field of Jupiter is deformed by the solar wind (Fig. 1), with compressed magnetic field lines on the day side and with elongated field lines in the magnetotail. One can also see (Fig. 2) how the plasma created by Io rotates for a long time around Jupiter before finally being ejected in the magnetotail. In order to study the influence of the internal sources, several simulations were performed for different Io mass-loading rates and different ionosphere conductances. For these simulations, the position of the corotation break-down and the azimuthal velocity profiles are in very good agreements with the theoretical model, the in situ measurements and the remote observations. In addition, the position of the corotation break-down, as expected by theory [2], maps to the auroral region in the ionosphere (see Fig. 4). The auroral emissions of Fig. 4 are more symmetric for high Io mass-loading rates or for low ionospheric conductances. We found that this is due to the position of the corotation break-down (which is strongly influenced by these two parameters). When the corotation breaks down very close to the planet, the dipole field is almost not affected by the distant solar wind and the aurorae are almost symmetric. On the contrary, when the corotation break-down occurs far from Jupiter, the solar wind strongly deforms the field lines, which results in asymmetric aurorae.

On-going Research

We are currently running simulations of Jupiter on a new finer mesh in order to obtain even better simulation results. This will improve, for instance, the scales in the current sheet or the shape of the magnetic field lines. To perform such simulations, we need more than 400,000 CPU-hours per run; meaning that, even when 500 CPUs are used, more than five weeks are required to finish a simulation. This kind of simulation would be impossible without super-computers.

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Figure 4: Aurorae in the northern hemisphere of Jupiter's ionosphere for four different simulations. The dayside is located on the right.

$j_{\parallel}/B$ $(A/m^2/T)$

43

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Formation and heating of galaxy clusters in hydrodynamical simulations

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Introduction

The evolution of the large-scale structure in the Universe is driven mainly by the gravitational force. Within the widely accepted ΛCDM cosmological paradigm, the largest virialised structures (the galaxy clusters) are built by gravitational collapse and merging events of smaller subclumps. The baryonic gas falls into the gravitational well of the newly formed clusters, and is shock-heated to the virial temperature.

While this overall picture is based on robust arguments and can be reliably described by simple analytical scaling relations, the details of the gas heating still need to be explored with more sophisticated tools, namely hydrodynamical simulations. In particular, we wish to understand the thermal properties of the cluster population as a statistical ensemble. These properties are of key importance for making predictions of observational signatures of galaxy clusters, both for the X-ray emission and the thermal Sunyaev-Zel'dovich (tSZ) effect in the sub-mm regime.

We devised a theoretical investigation of this problem by the use of the HPC resources at the LRZ, in particular the SGI Altix 4700 HLRB2 and the new machine SuperMig. Our strategy is based on the combination of three main approaches:
- analytical modelling, taking into account the key ingredients of cluster merging history and the different heating mechanisms;
- numerical simulations of idealized setups;
- numerical simulations of cluster formation in their cosmological framework.

In the first phase of the project we focused on turbulent gas flows in the cosmic baryons, and on their role for the thermal history and the non-thermal phenomena in the intra-cluster medium (ICM). We summarise our main results in the following.

Results

In [1] the evolution of the cosmic structure was followed in a box with a size of 100 Mpc h^{-1} on a side. The simulations have been run using a modified version of the grid-based, adaptive mesh refinement (AMR) hybrid (N-body plus hydrodynamical) code Enzo [2], where a subgrid scale (SGS) model for unresolved turbulence has been implemented [3]. The combination of the SGS model with AMR has been called FEARLESS (Fluid mEchanics with Adaptively Refined Large Eddy SimulationS) and is extremely useful in modelling the evolution of turbulence in strongly clumped flows, like those in galaxy clusters. With this tool it is possible to study not only the injection of turbulence in the ICM, but also in the less dense warm-hot intergalactic medium (WHIM), located in the cluster outskirts and in the large-scale filaments.

The time evolution of the average internal and SGS turbulence energies, e_{int} and e_t, for the two baryon phases introduced above, is shown in Fig. 1. The evolution of e_t is different in the two phases: in the ICM, it has a peak at

Figure 1: Time evolution of the specific internal (solid lines) and SGS turbulent (dotted lines) energies, from [1]. The two lines in the upper part of the plot refer to the ICM, and the other two to the WHIM. The lines are scaled according to the factors in the legends, in order to be accommodated in the same plot.

z = 0.000

Figure 2: Volume rendering of the gas density in a cosmological box, centered on a massive galaxy cluster and showing the surrounding filamentary structure of the cosmological large-scale structure.

redshifts between 1.0 and 0.65, while in the WHIM there is a steady increase to the current epoch.

The interpretation of this result, provided in [1], is the following: the peak of e_t in the ICM corresponds to the major merger epoch for the main halos contained in the simulated box, as it is known that merger events deeply stir the cluster gas and inject volume-filling turbulence in it. The features of turbulence in the WHIM, on the other hand, depend on the gas accretion through the external cosmological shocks, and therefore follow the evolution of the kinetic energy flux through them.

Another problem addressed in [1] is about the dynamical pressure support of the cosmic baryons. It has been found that the turbulent support (both on the resolved and SGS scales) is stronger in the WHIM, and less relevant in the ICM. However, only in a small volume fraction (about 10 percent) the turbulent support is dynamically relevant, with respect to the thermal pressure, for counteracting the gravitational contraction. The implication of this result for the physics of turbulent flows in the cluster outskirts will be studied by means of forthcoming high-resolution simulations.

Data analysis and visualisation

The analysis and visualisation of simulation data has been one of the key activities of the first phase of our project. Both stages play a crucial role for the scientific interpretation of the results, and the ever-increasing size and complexity of simulation output make them as important as the data production itself.

As an example, in Figure 2 we present a volume rendering of the baryon density in a box of 12.8 Mpc h^{-1}, showing a galaxy cluster of mass of about 6×10^{14} solar masses. The visualization has been performed using *yt* [4], a multi-code analysis toolkit for astrophysical simulation data based on Python.

This figure is a snapshot of a full movie produced from simulations of structure formation in galaxy clusters. We refer to [3] for the physical details of the simulations, and for the movies we recall here some of the technical ones (see also [5]). In order to create high quality images and movies (12 frames per second), we produced and stored 550 data dumps of the cluster simulation, corresponding to 1.6 million AMR grid files (about 0.5 TB of data). The subsequent analysis has been performed in parallel, on 220 cores of the *HLRB2*.

The results are a good example of the close link between data handling and high-performance computing, which is the key for fully exploiting the resources available on current and future machines. The final movies are publicly available on the Web ([6]).

On-going Research / Outlook

In the remaining time of this project we plan to focus our computational efforts along two main, complementary directions:

- a suite of cosmological cluster simulations similar to that presented in [3], but featuring AMR criteria suitable for refining turbulent flows in the cluster outskirts. These runs will be also used as a starting point for making predictions on observables in different wavelengths;
- a sample of idealised merger simulations including the SGS turbulence modelling. The simplified setup allows to keep the geometrical complexity to a minimum, and to better disentangle the role of different merger parameters.

Finally, we note here that the current version of the Enzo code (2.x) has a much more efficient management of the AMR and of the output, which permits to make an extensive use of grid refinement with a moderate computational price and a better parallel performance. With this version it will be easier to make use of the existing and upcoming computational resources at the LRZ.

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Gravitational Wave Signals from Compact Binary Coalescence

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Introduction

In this project we have investigated two of the most exciting predictions of Einstein's theory of general relativity: black holes and gravitational waves. Binary systems of two black holes – dead stars, or the supermassive black holes found in the centers of galaxies like our own – lose energy due to the emission of gravitational waves and slowly spiral toward each other. When the two black holes are still far away from each other, they can be described accurately by analytical approximations, describing the black holes as point particles. To accurately track their last orbits and merger, we have to solve the full Einstein equations, without approximations. This is what we have done in this project. The main motivation for this work is the international effort to detect gravitational waves. This is the beginning of a new field of astronomy, with the potential to examine the universe from an entirely new perspective, that of gravitational waves, which generated as massive bodies dynamically distort the surrounding spacetime. The observation of gravitational waves from such sources will give new insights into astrophysics and cosmology, the physics of matter at extremely high densities, but also test general relativity, one of our fundamental theories

of nature. The next generations of large interferometers (LIGO[1], Virgo[2], GEO[3]) are foreseen to observe gravitational wave events for the first time. Black holes are also of extreme astrophysical interest. They are now known to be commonplace in the universe, at the centre of our own galaxy and indeed of every galaxy where they have been looked for. Their presence has a profound effect on structure formation and the evolution of galaxies and star clusters. Understanding their dynamics is of paramount concern. One of the most results in theoretical astrophysics in the last year has been the determination of extreme recoil velocities as a result of black hole mergers – a discovery resulting from our work at LRZ.

Solving the Einstein equations to describe black hole mergers requires high-performance computing. They form a set of coupled partial-differential equations in the form of non-linear wave equations for variables describing the spacetime geometry. Unlike in the Newtonian 2-body problem, these must be solved over an entire 3D domain of space. The techniques for doing this have been developed over the last decades, but only since 2005 has the field advanced to the point that stable and reliable evolutions are possible. The primary result of our simulations are gravitational wave signals, decomposed into spherical harmonic modes, as shown in Fig. 1. The frequency and amplitude increase during inspiral toward the merger, finally the amplitude decreases exponentially at constant frequency during the "ringdown".

Figure 1: Dominant spherical harmonic mode of a gravitational wave signal from a coalescing black hole binary.

Results

We write the Einstein equations as an initial-boundary-value problem to yield a coupled system of second differential order elliptic constraints (equations that do not contain time derivatives), and hyperbolic evolution equations (essentially generalized wave equations with very complicated nonlinear source terms) that preserve the constraints. In the free evolution approach the constraints are only solved initially, and the evolution equations are used to construct a solution in time. There is a great deal freedom in writ-

ing the Einstein equations as a system of partial differential equations, and much research has gone into finding optimal choices. We currently focus on a popular choice with well-studied stability properties, the so-called "BSSNOK" system.

A unique aspect of the black hole problem is the presence of a physical curvature singularity at the centre of each body. In practice, these are treated evolving along time-slices of spacetime which slow down so much in a neighbourhood of the singularity, that is never reached. In this approach however, there is an infinite amount of "space" inside the black hole. Using again a clever choice of coordinates, the interior of the black hole event horizon is mapped to a finite coordinate region at the price of a coordinate singularity – the "puncture". This puncture is allowed to advect across the grid, corresponding to the motion of the black hole, this has become known as the ``moving puncture" approach [4,5]. Discretization in space is performed with standard finite difference stencils (4th to 10th order are implemented). Time integration is performed with a 4th-order Runge-Kutta method, which provides sufficient accuracy and a generous Courant stability limit.

The different scales of the problem are resolved using mesh-refinement techniques, essentially following the method of Berger-Oliger. Typically we use 10-12 refinement levels (refining the grid spacing by factors of 2), roughly half of which follow the movement of the black holes. We typically run three different resolutions, to check convergence at the expected order and compute error estimates.

Our results cover wide range of topics, from exploring the binary black hole parameter space, to theoretical progress in understanding the resulting spacetimes, and progress concerning simulation methods. Overall, we have used about 7 million CPU hours on HLRB-2.

One of our key results has been the first construction of an analytical phenomenological model for spinning binaries [6]. This model is a first step, since for simplicity the spins are chosen parallel or anti-parallel to the orbital angular momentum, and therefore it does not include precession. It does however describe the important "hangup" effect: when the spins are parallel to the angular momentum correspond to a repulsive force between the black holes, and increase the time to merger (as well as the orbital speeds of the holes). Anti-parallel spins accelerate the inspiral. What we have

Figure 2: Horizon distance in Mega-parsecs in dependence of the spin of the black holes. Positive signs denote spins parallel to the orbital angular momentum, and negative signs anti-parallel spins.

found, and studied in some detail, is that the hangup effect significantly increases the amount of gravitational waves emitted. Fig. 2 shows the horizon-distance – the distance to which we can observe optimally oriented binary systems – in dependence on the spin χ of the holes. We have also found that to a good approximation, we can assume that both holes have the same spin – or in other words, the total spin can be measured much more accurately than the individual spins.

Our phenomenological model is already used by the LIGO and Vigo collaborations to analyse the data from their detectors. Another important direct contribution to gravitational wave data analysis has been the NINJA-project [7], a community effort to collect and verify gravitational waveforms from groups like ours, and inject them into real and simulated noise from the detectors, to

Figure 3: Orbital tracks of a precessing binary system at mass ratio 1:3. The black line denotes the motion of the heavier hole, the red line is for the smaller hole.

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test and further improve the sensitivity of current codes which are used to search the signal of gravitational wave detectors for events. Our group has committed the largest number of waveforms to the NINJA data repository, and some of us have played a leading role in organizing the project.

An important task is to compare our numerical results with analytical approximations, in particular the post-Newtonian approximation, and the effective-one-body description. For non-spinning binaries we have demonstrated excellent phase agreement with numerical results in full general relativity. When spins are included, the agreement deteriorates, and we have presented an extensive study for non-precessing binaries in [8].

We have also made significant progress toward the modeling of gravitational waves from precessing binaries, gaining new understanding regarding the problem of determining and tracking the orbital plane of a binary as it precesses during inspiral due to spin interactions. In particular, we have been able to show how the spherical harmonic decomposition of the wave signal can be brought into a simple "normal form", which effectively tracks the orbital angular momentum from the wave signal [9]. The complicated orbital tracks of one of our precessing simulations at mass ratio 1:3 are shown in Figure 3.

On-going Research / Outlook

We are still working on refining our analytical model for the three-dimensional non-precessing parameter space (mass ratio and two spin dimensions). The biggest and urgent challenge for the future is however to model the seven-dimensional precessing black hole parameter space (mass ratio and 6 spin components).

To this end we have recently started a project within the European PRACE framework, where we will perform several dozen challenging simulations as a first step toward a systematic exploration of precessing binaries. Advanced gravitational wave detectors will start operating in 2015, and our current and future work will have important consequences in how searches for gravitational wave signals from spinning black hole binaries will be performed. We are also constantly improving our techniques for carrying out our simulations. In order to meet the accuracy requirements of future detectors like the Einstein telescope [10] or eLISA [11] we have to run more accurate simulations starting at larger initial separations – beyond what is feasible in terms of computational cost with our current techniques. Another important topic for the future will be to evolve black holes in alternative theories of gravity. In order to test Einstein's theory with gravitational wave observations, we need some understanding of what black hole mergers look like in alternative theories!

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The Core Mass Function from Simulations of Magnetised

Gravo-Turbulent Fragmentation in Star-Forming Molecular Clouds

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Introduction

Supersonic turbulence in star-forming molecular clouds create the seeds for gravitational collapse into proto-stellar cores and subsequently into stars. Self-gravity must be the physical mechanism for the final transition of dense gas into bound, proto-stellar cores and stars. Magnetic fields, ubiquitously observed in nearby molecular clouds, may also play an important role in this process. To advance on these issues, we use self-consistent, 3-dimensional hydrodynamical and magnetohydrodynamical simulations of solenoidally (divergence-free) and compressively (curl-free) driven supersonic turbulence, including self-gravity and magnetic fields to investigate the formation of dense, bound cores and stars in an environment typical for interstellar gas clouds. A long-standing problem in astrophysics is explaining the observed distribution of core masses (Core Mass Function, CMF) and stellar masses (Stellar Initial Mass Function, IMF). Continuing our studies of purely non-gravitational turbulent fragmentation, we investigate the mechanisms of turbulent gravitational fragmentation, termed gravo-turbulent fragmentation. We will furthermore included magnetic fields in these simulations to check the validity of analytic theories explaining the CMF and IMF. The final goal of our simulations is the correct prediction of the distribution of cores and stellar masses, and evaluating the role of magnetic fields for these distributions.

Results

We summarise the most important results of our HLRB2 project pr32lo. This project focused on the mass distribution of formed cores and stars, the so-called Core Mass Function (CMF) and Stellar Initial Mass Function (IMF). In

Figure 1: Column density snapshots of two high-resolution simulations of star cluster formation run on HLRB2. The turbulence was driven with purely solenoidal (divergence-free) forcing in the left image, while it was driven with purely compressive (curl-free) forcing in the right image. In both simulations, about 230 star particles have formed (shown as white dots), and about 10% of the original gas mass was consumed by the stars. However, the star formation rate is about 25 times higher in the run with compressive forcing of the turbulence, because compressive forcing produces significantly stronger gas compressions [1].

project pr32lo, we wanted to answer the following scientific questions:

- Does compressive forcing yield a different CMF and IMF compared to solenoidal forcing, and which one matches the observed distribution best?
- What are the time scales, star formation rates and efficiencies of solenoidal and compressive forcing?
- Do the typically observed magnetic fields influence the star formation process significantly?

We were able to address these three questions with high-resolution simulations proposed in pr32lo. Figure 1 shows the two proposed high-resolution runs with solenoidal (left) and compressive (right) forcing, but without magnetic fields. Turbulence was driven with the technique described in Federrath et al. (2010) [1] until a Mach number of about 10 was reached in both cases, which is typical for star-forming molecular clouds. Then, self-gravity and sink particles (see next section) were activated. The number of objects formed was roughly the same in both cases at the time when the simulations were stopped, i.e., when the star formation efficiencies are about 10% in both forcing cases. We prefer not to follow the simulation to later times, not only because the simulations become computationally prohibitive, but mainly because radiative and mechanical feedback processes, e.g., jets and outflows from the newly formed stars, would likely alter the subsequent evolution. We plan to include outflow feedback in future work, though (see outlook below).

The most striking result of the systematic comparison shown in figure 1 is that compressive forcing produced the same amount of star formation (i.e., in terms of mass accreted and number of sink particles) about 25 times faster than solenoidal forcing. If the density distribution is indeed the most important ingredient controlling the star formation rate as suggested by the best star formation theories today (Krumholz & McKee 2005; Hennebelle & Chabrier 2008; Padoan & Nordlund 2011), then the forcing dependence of the density distribution must be taken into account in any successful theory of star formation.

Addressing our third scientific question above is particularly important, because some of the star formation theories mentioned above require magnetic fields to explain the observed distribution of stellar masses. However, the observed magnetic field strengths are moderate, and their importance for the star formation process are highly debated since the last 40 years up to the present. In the second part of pr32lo, we thus proposed to explore the effects of magnetic fields in two simulations. Figure 2 shows the effects of adding

magnetic fields. In both simulations, we modelled self-gravitating turbulence, driven with a natural mixture of modes excited by the forcing. The top and bottom images show runs without and with magnetic fields, respectively. The magnetic field reduces fragmentation, an extremely important result for star formation studies, as it shows that indeed, a magnetic field of the typical strengths observed in the interstellar medium can influence the fragmentation and thus the mass distribution of stars, significantly.

Numerical Techniques

Numerical studies of the 3-dimensional gravitational collapse of interstellar clouds have shown that extreme care must be taken in resolving the physical length scale

Figure 2: Star formation without (top) and with magnetic fields (bottom). Fragmentation is significantly reduced when magnetic fields are included, reflected both in the gas distribution, and in the number of sink particles formed (117 without magnetic fields versus 68 with magnetic fields). The visualisations were made on RVS1 at LRZ.

during collapse and star formation (the so-called Jeans length) to avoid artificial fragmentation. Our adaptive-mesh-refinement (AMR) technique in the FLASH code (URL: http://flash.uchicago.edu) has been modified to accurately follow the gravitational collapse by introducing two state-of-the-art implementations: (1) we use a refinement criterion based on the Jeans length [2], guaranteeing that the Jeans length is always sufficiently resolved, and (2) sink particles to represent collapsing objects on the smallest resolvable length scale [3]. Due to the extreme dynamical range in time and length scales, AMR can only be used to follow the gravitational collapse to a certain cutoff length scale. To maintain numerical stability and to avoid extremely small time steps, sink particles are formed with sizes close to the resolution limit. Sink particles are used to follow star formation in the cloud. This innovative module is the key numerical technique to address the Star Formation Rate as a function of the Mach number and turbulent forcing. Prior to sink particle formation, we define a control volume around each AMR cell that exceeds a given density threshold, and check whether the gas in that control volume

- is on the highest level of mesh refinement,
- is converging towards the centre,
- has a gravitational potential minimum in the centre,
- is gravitationally bound,
- is gravitationally unstable (Jeans 1902),
- and is not within the accretion radius of an existing sink particle.

These innovative checks allow us to measure the Star Formation Rate accurately, compared to sink particle implementations based on a sole density threshold for sink creation, because in our implementation, only gas that is bound and collapsing is turned into stars. As soon as a sink particle is created, it can gain further mass by accreting gas from the grid, if the gas inside the sink particle radius is bound to the particle and collapsing towards the centre. We compute all contributions to the gravitational interactions between the gas on the grid and the sink particles: gas-sinks, sinks-gas, and sinks-sinks, by using direct summations over all sink particles and grid cells with gravitational softening inside the sink particle radius. A 2nd-order leapfrog integrator is used to advance the particles on a time step that allows us to accurately resolve close and highly eccentric orbits of particles during close encounters [3]. The sink particles are fully integrated into the MPI parallelisation of the FLASH code. The sink particle module in FLASH allows us to measure the star formation rate of each individual fragment that forms stars. We can thus quantify the amount of gas truly collapsing and participating in the star formation process, as well as the distribution of dense core masses, the Core Mass Function (CMF) and the Stellar Initial Mass Function (IMF), the origin of which remains an unsolved riddle in astrophysics.

On-going Research / Outlook

With the HLRB2 supercomputer, we were able to run the FLASH code with 256 to 510 cores in parallel. The power of the new systems SuperMIG and SuperMUC will enable even better scaling of our parallel applications, because the internode connections are greatly improved. Thus, we are looking forward to running our code on SuperMUC with thousands of cores.

Scientifically, we aim to investigate feedback processes during star formation in the near future. An innovative outflow model was recently developed to launch physically well-calibrated jets and outflows from newly formed sink particles, the mechanical feedback of which may also drive turbulence and influence the star formation process in a self-regulated fashion. We will perform test runs with outflow feedback in our continuation project on SuperMUC. The jets produced during star formation, however, have extremely high velocities, posing strong constraints on the CFL time step, and thus representing a real challenge for modern HPC systems. We will thus continuously rely on the best, next-generation supercomputing, provided by the LRZ.

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Numerical Simulation of Binary Black Hole and Neutron Star Mergers

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Coalescence of Binary Neutron Stars

Neutron stars (NSs) are very compact objects (with a mass between roughly 1.35 and 2 times that of our Sun but with a radius of less than 15 km) formed in the gravitational collapse of massive stars. NSs are at the center of many fascinating phenomena in the Universe, including gamma-ray bursts (GRBs), supernova explosions, pulsars, and gravitational waves. A large fraction of the current astrophysical research topics in the world focuses on one of the above phenomena. We are especially interested in binary neutron star systems (BNSs), which are particularly interesting because of two main reasons: (1) BNSs are very strong sources of gravitational waves. By measuring the gravitational signal from BNSs we can – among many other things – get information about the structure and equation of state of NSs [1]; (2) BNSs are thought to be the engine powering one type of GRBs. GRBs are the most luminous electromagnetic events occurring in the Universe and emanate from seemingly random places in deep space (for general reviews see [2]). GRBs are divided into two classes on the basis of their duration: Short GRBs (SGRBs, lasting between few milliseconds and 2 seconds) and Long GRBs (longer than 2 sec) [2]. While the origin of Long GRBs has been with some confidence identified with supernova explosions [3], that of SGRBs

Figure 1: Snapshots of the merger of two magnetized neutron stars leading to the formation of the black hole and the magnetic jet.

Figure 2: Rest mass density distribution in a counter-rotating model with a recoil velocity V=300 km/s.

remains unresolved. The merger of BNSs is however the most likely candidate for a subclass of SGRBs, those with a harder spectrum [4]. The typical scenario is based on the assumption that a system composed of a rotating black hole (BH) and a surrounding massive torus is formed after the merger of NS-NS or NS-BH binaries. If the disc has a mass greater than 0.1 solar masses, it could supply the large amount of energy involved in GRBs by magnetic-field and neutrino processes. It is not conclusively known whether this scenario is true, but we are doing progress in this direction.

Results and Outlook

With our work we have recently contributed to solving part of the puzzle [5]. We found that a magnetic funnel forms naturally in BNS mergers (without fine tuning of parameters) and such a funnel is apt to contain the jets that may produce SGRBs. This work of ours made the headlines also on the NASA website [6] and on the popular press. More in detail, we performed accurate and long simulations on supercomputers and clearly demonstrated that a binary merger of two NSs inevitably leads to the formation of a relativistic jet-like and ultrastrong magnetic field, which could serve as a central engine for SGRBs. Because the magnetic-field growth is exponential, the picture emerging from our simulations is rather general and applies equally even to mildly magnetized NSs. In brief, by considering a binary of magnetized neutron stars and solving the Einstein equations, we show that their merger results in a rapidly spinning black hole surrounded by a hot and highly magnetized torus. Lasting over 35 ms (much longer than previous simulations), our study reveals that magnetohydrodynamical instabilities amplify an initially turbulent magnetic field of ~10^{12} G to produce an ordered poloidal field of ~10^{15} G along the black-hole spin-axis, within a half-opening angle of about 30 degrees, which may naturally launch a relativistic jet (see Fig. 1).

Even tough we did not treat neutrinos and radiation processes and so we could not see the development of a jet, the broad consistency of our *ab-initio* calculations with short GRB observations shows that the merger of magnetized neutron stars can provide the basic physical conditions for the central-engine of short GRBs. When considering the gravitational waves from this process, we are very close to establishing a successful matching of our numerical waveforms with approximate but analytic ones. The latter are now computed to a sophisticated level including the description of tidal deformations, and allow the extraction of physical parameters from the comparison with their numerical counterpart. In order to improve the match with the analytic predictions, we have performed very high-resolution simulations for several initial models, in which the stars are rather separated. Our results are published in [9]. The duration of the burst, its electromagnetic energy release, and (as said above) the jet opening angle are broadly compatible with the observations. However our simulations lack a proper treatment of the energy losses via photons and neutrinos, which can provide a fundamental contribution to the energy input necessary to launch the fireball and cool the torus. This additional energy input, whose self-consistent inclusion in general relativity remains extremely challenging, may help to launch an ultrarelativistic outflow very early after the black hole forms and to complete the picture of the central engine of an SGRB.

EM counterparts from the coalescence of Binary Black Holes

The merger of supermassive black holes placed at the centre of two interacting galaxies is expected to produce both gravitational wave emission, to be detected by the planned Laser Interferometric Space Antenna (LISA), and the more classical electromagnetic radiation. A lot of attention has been given in the last few years to the

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possibility of this joint detection, with a scientific impact spanning from accretion disc physics to fundamental cosmology [8]. In the post-merger phase, namely after the black holes from the two galaxies have merged into a single one, the typical behavior of the system is characterized by two distinct but related physical effects having to do with the emission of gravitational waves. The first effect is an abrupt mass loss of the resulting black hole, while the second effect is the recoil that it receives due to the anisotropic emission of gravitational waves. Both of them have a strong impact on the dynamics of the circumbinary accretion disc that has accompanied the evolution of the system. An additional physical effect that needs to be taken into account and has been neglected in previous investigations is that produced by counter-rotation, namely when the disc rotates in the opposite sense of the resultant spinning black hole. Such an effect has been considered in this project, by performing two dimensional numerical simulations of counter-rotating kicked disc after a merger event.

Results

We have solved the general relativistic hydrodynamics equations for a perfect fluid by means of the ECHO code, based on the conservative formulation of the equation. We have assumed a Kerr spacetime metric in Boyer Lindquist coordinates, with a computational grid covering the orbital plane of the disc, to which the vector of the recoil velocity belongs. The radial numerical grid is discretised by choosing N_r = 1200 points, non-uniformly distributed from r_{min} = 100M to r_{max} = 6000M. The azimuthal grid extends from 0 to 2π and the number of angular grid points is N_φ=200. The code is parallelized with the MPI standard and the typical number of processors adopted was 64/128. The temperature of the disc is assumed to be constant in space and in time (isothermal evolution). As a result, there is no need to evolve the energy equation, since the energy can be computed directly from the temperature. However, an equation for the time evolution of the internal energy is actually solved, with the only aim of computing an estimate of the emitted luminosity [9]. As initial models we use thick discs configurations subject to both mass loss and recoiling. The combined effects of mass loss from the central black hole and of the recoil velocity generate a spiral shock pattern that transports angular momentum outwards, and become responsible of an enhanced luminosity.

Figure 1 shows the isodensity curves of the rest mass density in a counter-rotating model when the emitted luminosity reaches its maximum. Because the recoil velocity is not large, the disc has not penetrated into the central cavity at this time. Counter-rotating models have larger extension with respect to co-rotating ones and, in addition, have a larger radius of the maximum rest mass density point. These two facts are ultimately responsible for the different behavior of the light curves, namely the fact that the maximum luminosity of counter-rotating discs is a factor (2–12) higher than in the co-rotating case, depending on the parameters of the initial conditions. When the spin of the black hole is increased, the radius

of the maximum rest-mass density moves towards the center for co-rotating models, while it moves towards larger distances for counter-rotating models. Moreover, when the spin of the black hole is increased, the size of the disc increases for co-rotating models, while it decreases for counter-rotating models. Because of this, changing the spin of the black hole has opposite effects on the emitted luminosity for the two classes of models. Indeed, the fluid compression, and therefore the energy released, is larger if it takes place deeper in the potential well, where the effects of the spiral shock are stronger. This explains why increasing the spin of the central black hole produces more luminous co-rotating discs and less luminous counterrotating ones.

On-going Research / Outlook

The calculations presented here and performed on HLRB2 are very relevant for correlating the electromagnetic signal to the gravitational one, in view of the planned Laser Interferometric Space Antenna (LISA) mission. Future work will consider the contribution of a radiation field, treated according to the recent progress achieved in [10].

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The influence of magnetic fields
on massive star formation

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Introduction

In our research we investigate the influence of interstellar magnetic fields on the formation of massive stars, i.e. stars with masses in excess of one solar mass.

The exact formation mechanism of massive stars is currently highly debated with several different scenarios being proposed[1]. In particular the influence of magnetic fields on the formation mechanism has received attention only recently. Magnetic fields are believed to regulate the star formation efficiency, i.e. how much gas is converted from the interstellar medium into stars. This is mainly done by protostellar outflows and jets during the formation process of stars. These outflow/jets are gas streams ejected by the forming stars which extend up to several lightyears into the surroundings. Magnetic fields also affect the accretion properties of protostars, i.e. stars which are in their formation process.

Figure 1: Protostellar disc formed in the centre of the gas sphere. The white dots represent the protostars formed during the evolution, the black vectors the velocity field in the disc.

Results

For the study of the formation of stars from the interstellar medium under the influence of magnetic fields, the magneto-hydrodynamical equations have to be solved. Due to the complexity of these equations, in general this can only be done numerically by means of large-scale, parallelised computer simulations.

In our work we have performed a number of simulations on HLRB. The simulations required a computational time of more than 1 million CPU-hours and the simultaneous use of up to 500 CPUs per simulation. The simulations are performed with the hydrodynamics code FLASH[2] written in Fortran 90. The code solves the 3-dimensional, discretised magnetohydrodynamical equations on a Cartesian grid. Making use of the adaptive-mesh-refinement (AMR) technique, only those regions which are of particular interest for us are resolved with the highest possible spatial resolution whereas other regions of minor interest are resolved more coarsely. This significantly reduces the number of calculations to be performed and hence the computational time required, thus allowing us to perform the simulations over longer physical timescales.

Initial conditions

The exact initial conditions of the birth places of stars are currently not yet known and most likely also vary significantly from region to region. As we do not simulate a particular region observed by astronomers but rather aim to understand the systematic influence of the initial conditions, we have to perform a number of simulations (~ 15) in our work. The initial conditions in our work vary from simulation to simulation covering a large range in parameter space. This allows us to draw conclusions about the effect of the initial conditions on the formation mechanism of massive stars.

As initial conditions we consider a sphere of interstellar, molecular gas. The sphere has a mass of 100 solar masses and a diameter of 0.8 lightyears. As indicated by observations the sphere is rotating around the z-axis and is

threaded by a magnetic field also parallel to the z-axis. To account for the uncertainty in the strength of the magnetic field and the rotation velocity, we vary both over a wide range covering about 2 orders of magnitude which is in agreement with observational results.

Computational results: Discs

The gas cloud considered has a temperature of 15 K only and is therefore highly gravitationally unstable. After starting the simulations the cloud begins to collapse under its own weight. After about 15.000 years a protostar in the centre of the cloud is formed. The protostars are modelled with so-called sink particles. These are particles which only interact with the ambient gas by gravitational forces and can accrete mass from their vicinity. As the cloud is initially rotating around the z-axis, in some of the simulations a protostellar discs builds up around the protostar rotating with high velocities of up to several km/s (see Figure 1 and [3]).

Figure 1 shows the situation in a simulation with a weak, initial magnetic field 4000 years after the first protostars has formed. As can be seen, due to gravitational instabilities the disc has started to fragment and has formed several more protostars. However, one can still easily recognise the rotating disc structure extending out to a few 100 AU (1AU = distance sun to earth)

When, however, a simulation with a stronger magnetic fieldis considered, the overall situation changes dramatically as can be seen in Figure 2. Here, no rotationally supported disc builds up and the gas falls towards the centre almost radially.

This significant difference of the velocity structure in the discs is a direct consequence of the enhanced magnetic field strength. Magnetic fields are shown to be able to remove angular momentum from rotating objects, i.e. slowing down their rotation velocities. In the simulation

shown in Figure 2 this so-called magnetic braking is so strong that almost the complete angular momentum of the gas cloud gets removed. This behaviour is also observed in simulations of low-mass star formation. These computational results are in sharp contrast to observations, which show that rotating protostellar discs are present already in the earliest stages of star formation. Therefore this problem of a too efficient removal of angular momentum is denoted as the magnetic braking catastrophe.

Computational results: Outflows

A prominent feature of ongoing star formation is the existence of protostellar outflows which are observed around more or less every forming protostar. Outflows are ejected from the protostellar discs due to magnetic forces. Also in our simulations large-scale outflows are observed as shown in Figure 3.

The outflows extend up to several 1000 AU and reveal velocities of up to 15 km/s. Such outflows affect the surrounding medium and also reduce the mass accretion onto the protostars in the discs by removing gas.

In the course of our work, we developed a analytical approach to analyse and describe the outflows in detail. Comparing our approach with the simulation data shows that we can describe the underlying ejection mechanism very well. In particular we are able to explain the different outflow morphologies seen in Figure 3. In case of a weak magnetic field and a fast rotating disc a fast and collimated outflow forms whereas in the run with a strong magnetic field and no rotationally supported disc a bubble like, poorly collimated outflow forms. The poor collimation in the latter case is due to the lack of a strong toroidal magnetic field which is responsible for collimating the outflow and redirecting the outflow velocity into the vertical direction.

Computational results: Accretion rates

During their evolution the protostar formed in the different simulations accrete gas from their surroundings due to their gravitational attraction. Despite the fact that the properties of the protostellar discs vary significantly (compare Figure 1 and 2), the accretion rates for the different simulation are all of the order of 10^{-4} M_{sun}/year varying only within a factor of $\sim$ 3. We attribute this fact to two competing effects of magnetic fields. On the one hand, magnetic braking enhances accretion by removing angular momentum from the disc thus lowering the centrifugal support against gravity. On the other hand, the magnetic field counteracts gravity by exerting an outward directed force on the gas in the disc thus reducing the accretion onto the protostars.

On-going Research

One unsolved problem in star formation is the above described magnetic braking catastrophe, i.e. the rapid removal of angular momentum and the lack of rotationally supported discs. In our current research we try to tackle this problem by a series of new simulations. We adopt a

Figure 2: Protostellar disc for a simulation with a strong magnetic field.

Figure 3: Outflows ejected from the protostellar discs 4000 years after the formation of the first protostar for the same simulations as shown in Figure 1 and 2.

similar numerical setup as in the simulations described before but now add a turbulent velocity field to the uniform rotation.

Analysing the outcome of the simulations we now find that rotationally supported discs build up even in the case of strong magnetic fields in contrast to the previous simulations without turbulence. This is shown exemplarily for one simulation in Figure 4 revealing the formation of multiple, rotationally supported discs.

The reason for this is probably the reduced magnetic braking efficiency in the surroundings of the discs where we find a strongly turbulent velocity field with strong shear flows carrying large amounts of angular momentum. Hence, we are confident that turbulence provides a natural and simple mechanism to circumvent the magnetic braking catastrophe as found in simulations neglecting turbulence.

For the future we plan to explore this particular problem in even more detail by means of further simulations. Our aim is to check whether our findings endure in the case of different initial conditions in particular for gas clouds with lower masses. As for this purpose simulations with very high spatial resolution are required, we have to rely on the availibility of new high performance computers like SuperMUC.

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Figure 4: Multiple formation of rotationally supported discs in simulations with turbulent velocity fields.

FiBY: the First Billion Years simulation

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HLRB Project ID: pr95vi

Introduction

The First Billion Years simulation project (FiBY) consists of the simulation of a cosmological volume at the unprecedented resolution of 1250 solar masses per gas particle with the state-of-the-art N-Body/SPH code Gadget [1]. The aim is to follow the formation of a present day galaxy by resolving the sites of giant molecular clouds ($>10^5$ solar masses) that gave birth to the first generation of stars, their enrichment with chemical elements and feedback from stars, and the transition to the second generation of stars.

Early accretion of gas with primordial chemical abundance onto mini-halos of one million solar masses has been shown to lead to population-III star formation (stars forming free of elements heavier than helium). Within these mini-halos chemical enrichment, however, will take place quickly, and population-III star formation will be terminated. At this point it is not clear if continued accretion of cold primordial gas filaments will be able to rejuvenate population-III star formation or if the sites will change from the intersections of the cosmic filaments to the filaments themselves, which will have implications for the distribution of re-ionizing sources in the early Universe and the mass assembly of galaxies. The remnants of massive population-III stars will most likely end their lives as black holes that will continue to grow. We follow their growth and energetic feedback within our simulation.

The first stars and their remnant black holes are the sources of radiation that ionize the Universe. They begin the process of transforming the Universe from a predominantly cold, dark state into the hot, ionized state in which we observe it today. It is thought that this process of re-ionization was completed by the time the Universe was 1 billion years old (roughly 12.5 billion years ago). During the period of re-ionization, the regions surrounding the earliest generation of stars were dramatically influenced, impacting galaxy formation on large scales as well as star formation and black hole evolution at smaller scales. Our simulation, coupled with a radiative transfer post-processing code, is an attempt to answer questions regarding this phase of early structure formation in the Universe.

The first stellar clusters are the building blocks of proto-galaxies which fresh gas is mainly supplied by cold, dense streams. Once the first galaxies have finished their population-III star formation phase, they will enter an episode of growth that is still dominated by large gas accretion rates through cold gaseous filaments and mergers with other galaxies. We are interested in following the path of these galaxies to intermediate redshifts to understand their properties at later times. This helps to establish if signatures of the early formation epoch are still present and detectable. We investigate further how the star formation rate of the galaxies changes as a function of time and closely monitor how this is related to cold accretion flows. The study of the cold accretion mode is of great interest for explaining the observed high star formation rates at intermediate redshifts and we will investigate

Figure 1: Projected mass density on a slice of the simulation volume when the Universe was approximately 500,000 years old. Proto-galaxies are forming at the intersection of dense filaments (bright, yellow blobs).

how the stage for this period in galaxy formation is set up. The size of the simulated box is ideal for a detailed statistical analysis of the early Universe galaxy population which will be soon observed by ground and space-based telescopes such as ALMA, JWST and E-ELT [2,3].

Results

We performed one of the-highest resolution, hydrodynamical, cosmological simulations to date. We employed a modified version of the code Gadget previously used for another simulation campaign. Gadget is a massively parallel code that uses the MPI library. Gravity is solved with a hybrid algorithm that computes long-range forces on a mesh and shot-range forces with an octal tree. The hydrodynamics is evolved with a smoothed particle hydrodynamics (SPH) algorithm.

Table 1: Technical details of the simulation

Co-moving volume size	$(8 \text{ Mpc})^3$
Co-moving spatial resolution	166 pc
Gas particle mass	1250 $M_\odot$
Total number of particles	5,120,216,064
Number of cores	2048
Peak memory usage (approx)	5.12 TB
Number of snapshots	30
Size of one snapshot	515 GB

On top of the existing physics module for gas cooling, star formation, evolution and feedback, we added specific modules for the physical processes we are now able to resolve. In particular, we implemented consistent formation and destruction of the main molecules responsible for gas cooling down to temperatures of few 100 K.

Preliminary results

The scientific investigation of the simulation outputs is still ongoing, and is requiring the effort of a large fraction of our group. We give a detailed description of the current projects in the next section.

We show in Fig. 1 the distribution of the gas within the simulation box at half the simulated physical time. The very high resolution we employed is seen in the richness of details. Most of the bright (mini-)halo are hosting the formation of the first stars and proto-galaxies. A simulation of this size and amount of data output can only be run on massive parallel super-computers.

On-going Research

Our group is conducting several projects based on the data from the simulation. We give here a summary of the ongoing research.

The transition from population-III to population-II star formation

We are investigating when and how population-II star formation becomes dominant. The transition between

Figure 2: Projected temperature map on a slice of the simulation volume when the Universe was approximately 500,000 years old. Outflows generated by supernova thermal energy are visible around most of the proto-galaxies in the selected region (bright, yellow regions, which are also the hottest regions in the simulation).

the two modes of star formation is quick and related to the fast chemical enrichment and supernova-driven galactic outflows from massive population-III stars. Chemical enrichment within galaxies is the main driver, though energetic feedback from supernovae may pollute the gas to large scale. Mini haloes and proto-galaxies forming in these pre-enriched regions will grow in stellar mass only through the population-II star formation channel. The chemical properties of the first galaxies will be strongly affected by the relative importance of the two star-formation modes.

The assembling of the first galaxies

The assembly of the stellar component of haloes (namely, the galaxies) is a walk through a complex path. Part of the stellar mass is created from dense and cold gas clouds in situ. The gas is mainly supplied by accretion through cold filaments and merges with other haloes. The latter can also bring stars formed outside the galaxy. We are looking into the details of the growth of stellar mass of proto-galaxies with the aim of providing predictions for future observations (e.g. the luminosity and abundance functions of the first galaxies).

The re-ionisation history of the Universe

We are conducting intensive post-processing of the simulation outputs with a radiative-transfer code. The code follows the evolution of regions ionized by stellar radiation. The aim is to investigate the speed at which these regions grow to ultimately understand the topology of

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re-ionisation from the first galaxies. One key ingredient of the evolution of ionized regions is the fraction of photons that are able to escape galaxies and their haloes. Using the high resolution of the simulation we are able to give detailed estimates of it that may be used in analytic models.

The dark component of galaxies

Dark matter distribution within galactic haloes is strongly affected by the presence of gas and stars. Moreover, it evolves due to mergers with other haloes. In the early stage of galaxy assembly, star formation is heavily fluctuating due to the strong effect of supernova feedback and merges. We are investigating how star formation and stellar feedback (which characterise both distribution of the stellar component and the gas), together with mergers, shape the dark matter component.

The shape of galactic outflows

Understanding the enrichment history of the Universe is intimately connected to the efficiency of supernova feedback. The thermal energy injected in the galactic gas by this process is able to expand hot and underdense bubbles (thus generating galactic winds) that extend to scales much larger than the galaxy size or even the hosting dark matter halo. We are studying the characteristic properties of these outflows (e.g. the outflow velocity and mass rate, the size of hot bubbles) to give a detailed description of the process of chemical enrichment. This data will be use for providing predictions of the environment in which quasars live and comparisons with their observational data.

We show in Fig. 2 the projected temperature map in the same volume as in Fig. 1. Feedback from supernovae is responsible of the hot galactic outflows. The hot bubbles follow the distribution of galaxies shown in Fig. 1, and merge in regions of high halo density.

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Chemistry

Computational Catalysis for Energy Carriers

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HLRB Project ID: h0351

Introduction

Chemical conversion of raw materials to target compounds in most cases requires an accelerator, i.e., a catalyst, to run in an energy-efficient way, sometimes even to run at all. A striking example are the catalysts to produce synthetic fertilizers, boosting earth's food supply to nurture 5 billion people more than naturally possible. Due to the rather complex nature of their functions, many catalysts are not well understood and thus have to be improved by vague rules at best, but mostly by trial and error. Computational catalysis as interdisciplinary approach is capable of identifying the most likely functions of a catalyst, i.e., its mechanism, suggesting potential improvements to be tested in experiments. Here we present results for understanding catalysts that help to use preferred energy carriers longer and start to generate them on a renewable basis.

Results

To this end, we carried out quantum mechanical calculations on models of catalysts that induce transformations of hydrocarbon molecules. We calculated the electronic structure, i.e., among other properties, the energy of a geometric arrangement of atoms, molecules, and the surface of a solid, using methods based on density functional theory as implemented in the program package VASP (Vienna ab initio simulation package). VASP is parallelized (with MPI message passing) to run efficiently with 30–60 cores for the problems studied. To identify preferred structures iterative minimization procedures have to be invoked. However determining activation barriers for reactions, which are the backbone of catalytic cycles, notably increases the complexity of the task because not only a number of geometry optimizations are needed, but also "chemical intuition" and a variety of algorithms. In the group of Prof. Rösch a toolbox was developed providing standard and new searching algorithms in a modular fashion for any quantum chemistry code. In this toolbox an efficient parallelization scheme is incorporated to run several instances of the quantum chemistry code in parallel, eventually combining the results to identify barriers (transition states). Even with such efficient techniques identifying one transition state may take several days, translating into 15 and more core-years on HLRBII for the work reported.

Ring opening

This project aims at converting feedstocks as aromatics of non-combustion quality to aliphatic chains possibly without branching, hence combustion quality. Methylcyclopentane (MCP) is often used as a model compound to study ring opening catalysis which can yield 2-methylpentane (2MP), 3-methylpentane (3MP), and n-hexane (nHx), depending on the properties of the metal catalyst. For supported Pt catalysts the fraction of these products depends on the size of the Pt particles. For small particles a statistical distribution of C-C bond scission is found whereas large Pt particles, with a notable fraction of surface facets produce mainly the branched products.

Figure 1: Reaction cascades leading to the different products. Indicated are C-H bond cleavage and formation as well as C-C bond scission.

For C-C bond cleavage, it is beneficial to dehydrogenate first the carbon centers forming the bond where the ring is to open (Fig. 1). The first dehydrogenation step proceeds over barriers of ~90 kJ mol^{-1}, subsequent steps on the same carbon atom become easier with barriers as low as 60 kJ mol^{-1}. After dehydrogenation reactions leading to the branched

Figure 2: Overview over experimental and theoretical product distributions from ring opening reactions and their correspondence

and linear hexane species follow different pathways on a flat surface. For the 4-fold dehydrogenated species (Fig. 1) C-C cleavage occurs after one of the C centers has migrated to a 3-fold-hollow site. A rather low activation energy results for C-C bond breaking, 15 kJ mol^{-1}. For the 3-fold dehydrogenated species, on the way to n-hexane, this migration of the carbon group is not possible for steric reasons; without this pre-activation the system has to pass over a higher barrier, 116 kJ mol^{-1}. Inspection of this transition state leads to the conclusion that a stepped surface may allow easier transfer of the methylated carbon to its preferred site. Indeed a stepped surface lowers the C-C scission step of the nHx precursor by 20 kJ mol^{-1}. This varying behavior of dehydrogenated intermediates on flat and stepped surfaces nicely rationalizes experimental findings: on larger particles only 2MP and 3MP are found while on small particles a statistical mixture of all 3 products is found (Fig. 2).

Biomass conversion

Biomass by nature is a rather heterogeneous mixture of compounds with common sets of functional groups. As a first step we examined the conversion of sugar-derived materials that carry hydroxyl groups. To increase their energy content and to render them compatible with modern combustion engines these hydroxyl groups have to be replaced by hydrogen. In "aqueous phase reforming" processes two competing reactions take place which achieve conversion from biomass into fuels if combined in a suitable ratio. The first reaction is the hydrogen consuming dehydration and hydrogenation reaction to produce aliphatic species. The second reaction is the decomposition of bio-

mass into hydrogen and CO_2. On the model compound propanol, we explored how simple alcohols release hydrogen. On Pt first the hydrogen of the hydroxyl group is removed, then the hydrogen at the carbon center, to be followed by a further oxidation step, to yield finally 2.5 H_2 and 1 CO_2 from the initial –H_2COH unit, leaving behind after the C-C bond cleavage a shorter hydrocarbon chain, ready for further reaction.

Our research showed that yet again small catalyst particles with their higher density of defects, such as steps, lower the barrier of this rate-limiting hydrogen production step from ~100 to 75 kJ mol^{-1}. A second major result is that secondary alcohols (–HCOH– units) cannot react to CO_2, but rather desorb from the surface, producing unwanted ketones. Thus with regard to hydrogen production, it is necessary to decompose sugars and sugar-like molecules starting at the chain end, or the reaction will terminate. As a first step toward describing solvation effects, we approximated the aqueous environment by two layers of water molecules on the surface, but restricted to critical reaction steps in view of the notably larger computational efforts. The aqueous environment was found to facilitate desorption of acetone while propanal remains weakly bound at the surface (Fig. 4).

Figure 4: Desorption of aceton into a water shell as example of hydrogen production starting from a secondary alcohol.

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Figure 3: Dehydrogenation pathway for 1-propanol. Activation energies E_a required to cleave the X-H bond marked by the H in red

Quantum Mechanical Modeling of Actinide Adsorption at Surfaces of Clay Minerals

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HLRB Project ID: h0351

Introduction

Actinide environmental chemistry is a topic of current interest with respect to safety issues of deep geological repositories for highly radioactive waste as well as remediation of contaminated sites of nuclear accidents or former nuclear weapon production. Clays are considered as geological formations for such repositories and technical barriers against distribution of radioactive elements. Clay minerals, ubiquitously present in soils and sediments, have the ability to bind (adsorb) strongly metal ions and exchange them. Therefore, adsorption of actinides on clay minerals represents one of the important retardation mechanisms in the environment. Thus, a considerable experimental as well as recently also computational effort is undertaken to unravel this complex chemistry, aiming at a mechanistic understanding of species and processes at the atomic scale.

Clay minerals are layered aluminum-phyllosilicates. The layers of these minerals are composed of sheets of silica tetrahedra SiO_4 and alumina octahedra $Al(O,OH)_6$. One distinguishes two-sheet minerals, where in each layer a tetrahedral silica sheet is bound to an octahedral alumina sheet, and three-sheet minerals where an octahedral sheet is sandwiched between two tetrahedral sheets. These compositions leading to neutral layers are realized in kaolinite and pyrophyllite, respectively (Fig. 1). Families of other clay minerals are based on the same structural motifs and differ from the two prototypical minerals by substitutions of Si^{4+} ions by Al^{3+} in the tetrahedral sheet or of Al^{3+} by Mg^{2+} in the octahedral sheet. Such substitutions lead to a permanent charge of the layers which is balanced by counter ions, positioned between the layers.

The layered structure of the clay minerals is reflected in the platelet shape of their crystals, typically a few micrometers in size. Such platelets preferentially exhibit "basal" surfaces parallel to the layers and to a lower extent "edge" surfaces perpendicular to the sheets. Basal surfaces formed by tetrahedral sheets are less reactive as they expose saturated oxygen atoms of the SiO_4 tetrahedra. Edge surfaces or basal surfaces of two-sheet minerals formed by the octahedral sheet are more reactive because they exhibit OH groups. The charge of the surfaces is determined by the substitutions creating a permanent charge and by the deprotonation of OH groups leading to a pH dependent surface charge contribution. At acidic conditions (low pH) the surfaces bind protons of the adjacent solution and are positively charged while at neutral to basic conditions (high pH) deprotonation leads to a negative surface charge which is favorable for the adsorption of positively charged metal ions as shown in various experiments.

Topics of research regarding the adsorption of actinide ions are the preferred surfaces of clay minerals, the structure of the adsorption sites as well as the structure and chemical composition of surface complexes formed. Spectroscopic techniques like the analysis of the fine structure of X-ray spectra or the measurement of vibrations of the adsorbed species by infrared spectroscopy provided insight, but a detailed picture at the atomic level is still missing. Such information on adsorbed species and their stability is a prerequisite for a mechanistic understanding and a quantitative physico-chemical description of actinide adsorption.

To contribute to this knowledge, we have carried out quantum mechanical computational studies on the adsorption of actinide species on the surfaces of clay minerals. Electronic structure calculations with methods based on density functional theory as implemented in the par-

Figure 1: Structures and surfaces of clay minerals

allel program VASP (Vienna ab initio simulation package) were carried out to determine electronic and geometric structures as well as energies of adsorption. Surfaces of minerals were modeled as stacks of mineral slabs, separated by vacuum layers to create the surfaces. Surface solvation was approximated by a layer of water molecules. In this way models periodic in three dimensions result which allow the application of well-established computational techniques for crystals. Rather large periodically repeated cells (unit cells) have to be chosen to account for the complex structure of surfaces of clay minerals as well as to separate the adsorbed actinide species well enough so that they can be studied essentially as isolated species. Typically these unit cells comprise 100–250 atoms. The parallelized calculation (with MPI message passing) of an optimized structure of a single adsorption complex took 2-3 days when 24-64 cores of HLRBII were used.

Results

We studied the adsorption of uranium and neptunium on various surfaces of the clay minerals kaolinite and pyrophyllite. These actinides form in aqueous solution stable linear actinyl ions uranyl UO_2^{2+} and neptunyl NpO_2^+ which are surrounded by a first shell of about 5 water ligands bound to the actinide. Several types of adsorption complexes were examined. Experimental studies suggest that at acidic pH adsorbed actinyls keep their shell of water ligands. These so-called outer-sphere complexes do not form direct bonds to the surface (Fig. 2). At about neutral or higher pH, inner-sphere surface complexes are formed with direct bonds of the actinide to surface oxygen centers (Fig. 2). X-ray spectroscopic measurements of averaged interatomic distances from the actinides to neighboring atoms suggest that two such bonds are formed (bidentate complex).

For uranyl adsorption on the octahedral basal surface of kaolinite we compared inner-sphere adsorption complexes with one and two bonds to the surface. As they are of comparable stability, both types of species should be present at environmental conditions. Calculated U-Al distances to the surface agree well with measurements for bidentate complexes. For monodentate complexes they are larger, thus not easy to find in X-ray experiments. Measurements of two U-Al distances in a single probe can be interpreted to indicate the presence of at least two different adsorption complexes as our optimizations yielded only complexes with one such contact. Accordingly, the shorter of these distances may be attributed to complexes bound to deprotonated OH groups, while adsorption to protonated sites yields somewhat longer U-Al distances. Outer-sphere complexes have been modeled on tetrahedral and octahedral basal surfaces of kaolinite. Experimentally these complexes have been characterized as adsorbed species which geometrically are not distinguished from solvated actinide ions. In contrast to this picture our computational modeling showed that outer-sphere uranyl complexes at the octahedral basal surface of kaolinite exhibit a rather short bond to one of their aqua ligands which is directed to the surface. This effect is not obtained for neptunyl which interacts less

Figure 2: Various types of adsorption complexes of uranyl on the octahedral basal surface of kaolinite

strongly with the surface due to its lower charge. The unperturbed structures of solvated ions are essentially recovered only when two layers of water molecules are between the surface and the uranyl ion. Thus, uranyl species which differ from the solvated ion may be inner-sphere complexes or special outer-sphere complexes in direct contact with the mineral surface.

In some cases X-ray spectroscopy fine structure experiments resolved two U-O distances besides the uranyl bond for uranyl adsorbed on clay minerals. The shorter one was interpreted as bond to the surface while the longer one was attributed to bonds to aqua ligands. In optimizations of a large number of uranyl adsorption complexes on basal and edge surfaces of kaolinite and pyrophyllite we observed that short bonds are formed to deprotonated surface OH groups while longer ones exist to protonated OH groups. These latter bonds are comparable in length to the bonds to aqua ligands. Especially at edge surfaces we frequently observed deprotonation of aqua ligands of adsorbed uranyl ions with protons moving to the mineral surface. Thus, the hydroxide complex UO_2OH^+ is obtained as adsorbed species instead of uranyl. This complex shows a rather short U-OH bond which is comparable in length to the short bonds of uranium to the surface.

In summary, with computational modeling one is able to refine considerably the atomistic picture of actinyl adsorption on clay minerals surfaces, opening new ways of interpreting available and future spectroscopic experiments.

On-going Research / Outlook

To further support our results, we complement our modelling of actinyl adsorption on neutral clay minerals by dynamical simulations of adsorption complexes which are computationally more demanding. Also clay minerals with permanently charged layers are studied.

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Ab initio Path Integral Simulations of Floppy Molecular Systems

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HLRB Project ID: h1241

Introduction

The primary goals of this long-term project are to understand the quantum dynamics and to explain the highly non-trivial infrared (IR) spectra of protonated methane, CH_5^+, and all its H/D isotopologues at finite temperatures as well as to investigate the effect of microsolvation by adding H_2 molecules to CH_5^+. Our particular interest in protonated methane is due to several reasons. CH_5^+ serves as the prototype for non-classical carbocations and three-centre–two-electron bonding, it is a key intermediate in superacid and hypercarbon chemistry, and is highly relevant in areas as diverse as astrophysics and plasma chemistry. Its challenge to theory can be traced back to its unusually flat potential energy landscape, which enables complex large-amplitude motion to take place. The resulting fluxionality even persists at very low temperatures due to the quantum-mechanical nature of the highly correlated scrambling motion of the five protons. Thus CH_5^+ certainly is a paradigmatic example of the wide class of floppy or fluxional molecules and an ideal guinea-pig for method testing and method developing.

From the simulations' point of view CH_5^+ is an extremely challenging system. Its interactions cannot be parameterized in terms of force fields. Moreover, it has been shown that nuclear quantum effects are crucial and even thermal fluctuations of the nuclei on top of their quantum-mechanical excitations cannot be neglected. Over the last two decades, classical *ab initio* molecular dynamics (aiMD) methods (allowing for all aforementioned features except for the quantum nature of nuclei) have had success in simulating complex molecular systems. In this context aiMD means that the electronic structure is treated on-the-fly by means of density functional theory (DFT) and the term 'classical' refers to nuclei treated as point-particles. One possible route to account for nuclear quantum effects is to employ classical aiMD at higher temperature in order to emulate zero-point fluctuations by temperature ones. Another way is provided by the formalisms based on Feynman's path integral (PI) quantum statistical mechanics, since they allow for quantum delocalization of nuclei in an elegant and, in principle, exact fashion. In the PI framework, *static* properties of the quantum objects can be obtained by the simulation of more complicated, but classical objects. Such a classical object turns out to consist of many replicas (often referred to as beads) of the system, subject to nearest-neighbour harmonic interactions. Nevertheless, computing *dynamic* properties requires extending the method. A careful investigation of known extensions has shown that centroid MD (CMD) can be used to simulate IR spectra of complex many-body systems, despite having an intrinsic systematic error ('curvature problem') which leads to an artificial red-shift of high frequency spectral bands. At the same time CMD opens the door to assigning isotope-dependent time scales for the motion of nuclei inside molecules in the sense of quasi-classical wave-packets.

The global minimum structure of CH_5^+, see inset in Fig. 2, consists of a CH_3 tripod to which an H_2 moiety is attached via a three-centre–two-electron deficiency bond. The transition state for internal rotation can be obtained by rotating the moiety by 30°. The next transition state serves as a barrier for pseudorotation, i.e. the moiety 'opens' till it forms another symmetry plane, consisting of a carbon atom and protons 2, 4 and 5, and then a new moiety is formed by atoms 2 and 3. These two motions together give rise to hydrogen scrambling, that is, all hydrogen atoms become dynamically equivalent. (1)

Results

Based on the allocated HLRB resources, altogether seven papers and a Ph.D. thesis by A. Witt have been published, see our progress reports and [1-3] for most recent publications, and at least two more papers will be written up. It should be stressed, that this project gained a lot by collaborating with the group of Prof. Schlemmer from Cologne, who measured the IR spectra of all six H/D isotopologues of CH_5^+. We started with computing IR spectra by means of aiMD for each isotopologue at room temperature, which had been shown to nicely reproduce the experimental results at T=110K for bare CH_5^+. It turned out that while the CH_5^+ and CD_5^+ cases remarkably matched the experimental results, all mixed isotopologues featured qualitatively wrong relative peak

Fig 2: Probabilities for atoms to participate in the moiety. See inset for numbering.

intensities. This is due to equipartition, which assigns the same thermal fluctuation sizes to protons and deuterons, whereas their zero-point fluctuations are clearly of different magnitude. The effect on spectra can be quantified by computing the occupation numbers for protons and deuterons to reside in the moiety and tripod. Whereas classical aiMD expectedly yields combinatorial (binomial) distributions, the truly quantum occupation numbers yielded by PIMD are *qualitatively* different. It turns out that protons tend to looser deficiency bond of the moiety where deuterons prefer to reside in the stronger covalent bonds of the tripod. This quantum-induced symmetry breaking of the occupation numbers is the key to understanding complex IR spectra of CH_5^+ isotopologues [1]. Further, we developed a technique that enabled spectral decomposition into the contributions of the underlying isotopomers [2]. These isotopomers' spectra were then re-weighted by the afore-mentioned quantum occupation numbers and re-summed resulting in quantum-corrected spectra, which perfectly matched the experimental ones, see Fig. 1.

Then, using another in-house technique, we exhaustively assigned spectral features to molecular motions. Finally we have computed the spectra by means of CMD and again achieved a perfect match with the experiment, see Fig.1. Last but not least, CMD being a genuine quantum method opens access to the sub-ps quantum evolution in terms of isotope-dependent quantum lifetimes, which have been quantified for the first time for such a complex system [3]. The isotope-specific quantum free energy profiles reveal abundant scenarios of hydrogen scrambling dynamics [3]. These results altogether give a coherent picture of the quantum dynamics in CH5+ isotopologues.

The strategy advocated above can be straightforwardly adopted for larger systems, in particular for micro-solvated species, which is a huge benefit of on-the-fly techniques. A particular interest in microsolvating CH_5^+ is due to the conjecture that adding few H2 molecules can stop hydrogen scrambling. We have intensively investigated the dynamics of CH_5^+ under the impact of microsolvating H_2 molecules. In a nutshell, while this solvation slows down the scrambling motion of CH_5^+ at 110K, it freezes out scrambling at 20K, a temperature at which quantum effects dominate over thermal ones. This effect is illustrated in Fig. 2 where the probabilities of atoms to participate in the moiety are shown. While the quantum simulations show that bare CH_5^+ remains fully fluxional, all microsolvated species feature atoms that do not par-

ticipate in forming the moiety at all, hence illustrating the evidence of a – at least partially – frozen structure.

Performance and Scaling

The CPMD package employed in this project is a Kohn-Sham DFT-based MD code which uses a plane wave basis set and pseudopotentials. There exist several levels of parallelization. First of all, any PI problem parallelizes intrinsically with respect to the number of beads of the system, due to the solely harmonic interaction between the beads. For each individual bead, the Kohn-Sham equations of DFT have to be solved iteratively. This computationally demanding part of the calculation is assigned to processor groups (PGr), which require a high band width/ low latency interconnect. Within a PGr parallelization is realized via MPI for inter-node communication and either MPI or OpenMP/Vector processing for intra-node paralle-lization. Thus, this hierarchical parallelization strategy is highly adaptive and can be optimized for the individual platform. In particular, we used 128 beads in order to achieve convergence for the microsolvated species at 20K. Our runs scaled up to 1024 processors, i.e. 128 PGrs and 8 processors within a PGr. CPMD has proven its efficiency for simulations of this type on a wide variety of platforms including HLRB-II and BlueGene.

On-going Research / Outlook

The first goal of this project, namely understanding the IR spectra and thus dynamics of CH_5^+ isotopologues, is essentially achieved. Altogether, the research performed provides a consistent picture of the (quantum) dynamics of this enigmatic molecule [1-3]. Ongoing work on the microsolvated species is in progress and will be published shortly. The PIMD-based methods have proven to be an efficient tool for investigating quantum dynamics on HPC and definitely have perspective for applications for larger systems, especially in the field of bio-chemistry.

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Vibrations of the hydrogen bond network of water

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Introduction

Water, often dubbed the 'matrix of life', owes its role as the most fundamental solvent in biology to the presence of a three-dimensional network of hydrogen bonds (HB's). It does not only prevent the molecules from evaporating, leading to the stability of the liquid phase over a wide range of temperatures. A delicate balance between HB strength and volatility, the ability to break HB's upon thermal fluctuations without destabilizing the network, allows for fast dynamical processes on the timescale of picoseconds (10^{-12} seconds). While the ability of the water HB network to host a multitude of polar solute molecules is crucial for its properties as a solvent, the repulsion of nonpolar, hydrophobic molecules is a dominating factor for the stability of proteins and membrane bilayers.

Biologically relevant solutes range from simple nutrients, such as carbohydrates and amino acids, to large biopolymers, proteins, DNA and poly-saccharides. While particularly enzymes require the aqueous solvent environment to carry out their biological function, water molecules are often even directly involved in their working mechanism.

Vibrational spectroscopy provides an excellent experimental tool to study the microscopic details of water and aqueous solutions. Infrared (IR) spectroscopy studies the internal vibrations of molecules and is highly sensitive to specific chemical groups and the surrounding molecular structure. A notable example is the sensitivity of the vibrational frequency of OH-bonds in water to the local hydrogen bonding pattern. More complex spectroscopic methods are also able to study dynamical processes, such as the breaking of hydrogen bonds and molecular rotation on the picosecond timescale with femtosecond (10^{-15} seconds) resolution.

Recent developments have significantly improved the accessibility of other frequency windows, such as the so-called terahertz (THz) gap. Experiments in this part of the electromagnetic spectrum, between frequencies used in dielectric spectroscopy and the IR, were until recently limited by the availability of powerful radiation sources.

This has changed significantly within the last decade. This development is of particular interest for studies of water, because this spectral region includes the vibrations of water's HB network. In contrast to infrared spectroscopy, where vibrational motion of chemical bonds within the molecules are observed, THz spectroscopy allows to directly probe the vibration of HB's between molecules. Such experimental studies have recently focussed on water in the vicinity of various biomolecules, the so-called hydration water. A longstanding question regarding the properties of hydration water is to which extent the presence of biomolecular solutes is able to influence properties of solvating water molecules, also dubbed 'biological water', and if such a modification may be of biological relevance.

Experimental approaches, probing the structure of hydration water, found a limited effect on water molecules in direct contact with the biomolecular surface. However, recent THz spectroscopy studies observed a significantly more long ranged effect, which is manifested in an increased absorption coefficient of water molecules in several hydration layers around various biomolecular solutes [1,2]. It is estimated that 2-3 layers of water molecules (corresponding to a hydration shell of 6-7 Å thickness) contribute to this signal for smaller biomolecules, such as simple carbohydrates [1]. A significantly more pronounced effect was found for proteins, representing a more complex biomolecular solute, with an increased THz absorption coefficient in a hydration shell that extends to more than 10 Å from the biomolecule surface [2].

As noted before, THz spectroscopy probes the vibrations of the HB network of water. An increased absorption coefficient for water molecules in the hydration shell of biomolecules therefore indicates a fairly long-ranged modification of the vibrations of the HB network. In contrast to measurements of the average molecular structure, vibrations of the HB bond network are expected to be sensitive to water dynamics, particularly considering that THz vibrations (1 period per picosecond) are on the same timescale as various dynamical processes occur-

ring in water, e.g. rearrangements of the hydrogen bond network, rotational relaxation and diffusion.

A thorough interpretation of these observations is hampered by a limited understanding of the vibrational modes underlying the vibrational spectrum of the water HB network. While at IR frequencies, the **intra**molecular vibrational modes are well known, **inter**molecular vibrations are intrinsically more complex. This is especially the case for the vibrations of the HB network of liquid water, where breaking and formation of new HB's occurs on a similar timescale as the actual vibrational motion.

Molecular simulations are of significant value for this kind of problem as they provide us with an atomistic description of the underlying motions. Force field based molecular dynamics (MD) simulations provide these insights at moderate computational costs, especially for processes occurring on the picosecond timescale. However, an accurate description of the THz absorption spectrum of water is not trivial, because the absorption of HB network vibrations in liquid water is dominated by polarization effects, which includes degrees of freedom of the electronic structure within water molecules. In standard force fields, the electronic charge distribution is typically described by fixed point charges assigned to the simulated atoms. Electronic polarizability is therefore not included in the model. While more sophisticated approaches exist that describe the polarizability of water molecules empirically, it has been proven difficult to reproduce the THz absorption of water correctly. To overcome these problems, we focus on *ab initio* MD simulations of water and aqueous solutions in this study. In this approach the electronic degrees of freedom are treated explicitly in the simulation and electronic polarization effects are described in the most natural way. While in force field based simulations the potential energy and forces acting on each atom are evaluated by an inexpensive empirical expression, *ab initio* MD involves a full electronic structure calculation of valence electrons in each step of the simulation, raising the need for state of the art high performance computing resources, such as the HLRB2 and SuperMUC.

Results

In this study we employed the CP2K simulation package with its Quickstep implementation of *ab initio* molecular dynamics within the frame work of density functional theory (DFT). In our simulations we used the functional of Perdew-Burke-Ernzerhoff (PBE) to describe exchange-correlation contributions to the electronic energy. The CP2K code is parallelized with the message passing interface and for simulations of a periodic system with 128 water molecules we found an excellent scaling for up to 64 cores, resulting in a simulation performance of one picosecond per day. Notably, our simulation scheme includes simultaneous simulations of up to 16 independent simulations of each system for statistical sampling, providing an intrinsic degree of parallelization allowing a usage of up to 1024 cores. Proper statistical sampling required a total simulation time of 420 picoseconds for the

bulk water system, corresponding to 500.000 CPU hours, excluding tests of various temperatures, functionals and empirical correction schemes.

We employed a simulation approach, that involves a moderate increase of the simulation temperature to overcome implicit shortcomings of the PBE functional and the lack of the quantum mechanical zero point energy in simulations, which treat the atoms as classical particles. With this approach we were not only able to reproduce structural properties of water in excellent agreement with experimental results, but dynamical processes on the picosecond timescale, such as hydrogen bond rearrangements and diffusion, were also found to agree with the experimental literature. Most importantly, we were able to reproduce the THz absorption spec-

Figure 1: Comparison of the simulations to experimental data: oxygen-oxygen radial distribution functions (top left, experimental data from Ref. [3]), mean squared displacement and diffusion constant D (top right) and absorption spectrum (bottom, experimental data from Ref. [4]).

trum of liquid water, including an absorption band at 6 THz, which is typically absent in force field based simulations of water. These results are summarized in Fig. 1.

The successful description of the THz absorption spectrum of liquid water allowed us to carry out a detailed analysis of the underlying vibrational motions. We have also focussed on contributions of dipolar couplings, correlated fluctuations of molecular dipole moments of distinct water molecules, which contribute significantly to the overall absorption spectrum.

While the focus of our study is on THz vibrations of the HB network of water, our simulations provide us with information about the full range of vibrational frequencies from the THz region to the IR. A detailed comparison of both frequency domains and analysis of the contributions from electronic polarizability effects, revealed pronounced mechanistic differences underlying the absorption spectrum of water at THz frequencies and in the IR. Molecular deformation due to the excitation of in-

Figure 2: Contributions of correlations of molecular dipoles to the absorption spectrum in the THz frequency range (right) and the IR (left). A comparison is shown between the result including electronic structure information (and hence polarizability, top) and the corresponding result with fixed atomic charges (bottom).

tramolecular vibrations in the IR, such as the OH-stretch vibration, involves a significant change of the molecular dipole moment. The resulting change on the electrostatic interactions with neighboring water molecules leads to a correlated polarization of water molecules within a distance of 3 Å. The correlated molecular dipole moment fluctuations of neighboring water molecules contribute significantly to the total IR absorption. The role of polarizability is apparent when the analysis is performed using fixed point charges instead of the electronic structure information. The aforementioned contributions at IR frequencies vanish in this case as shown in Fig. 2.

At THz frequencies, molecular dipoles of neigboring water molecules also show correlations that contribute to the absorption spectrum. In contrast to the IR, these correlations largely persist when polarization effects are neglected. This indicates correlated motion of the atoms of these molecules, while correlations are mostly restricted to the electronic degrees of freedom in the IR.

Extending our analysis to the correlations of nuclear motion, we were able to show that these correlated motions extend beyond direct neighbors. Correlated vibrational motion extends to molecules separated by 5 Å and more with decreasing frequency. This is in agreement to the assignment of acoustic modes in the HB network of water at THz frequencies. Compared to previous studies, our analysis allows a direct observation of the transition from localized motion of single molecules to collective vibrations at THz frequencies in a real-space representation.

A sophisticated analysis of vibrational modes in temporarily stable patterns of hydrogen bonds was successful in identifying vibrational modes, which demonstrate the

collective character of this vibrational motion. In Fig. 3 the onset of correlated motion at decreasing frequencies is displayed in addition to a corresponding mode that involves a correlated defomation of HB's in a hydrogen bonded cluster of eight water molecules.

The presence of such long-ranged correlations of vibrational motions in the HB network of water provides a detailed microscopic picture for the interpretation of long-ranged effects on the THz absorption coefficient of hydration water, which extends to several hydration layers from the biomolecule surface. For more detailed information on the analysis we refer the interested reader to Ref. [5].

Ongoing research focuses on the influence of polarizability on the vibrational motions in water with a potentially significant impact on the interpretation of force field based MD simulations that lack these effects. Additionally we set out to study the vibrational modes of the HB

Figure 3: The onset of correlated vibrational motion below 10 THz with decreasing frequency (left). A corresponding vibrational mode identified in our simulations involving eight hydrogen bonded water molecules is shown on the right.

network of water in ice. There, the absence of fluctuations of the HB patterns should simplify the identification of vibrational modes, which might, however, persist also in the liquid. Ultimately it will be studied to what degree a small solute, urea, can modify these vibrations.

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Theoretical treatment of magnetic molecules

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HLRB Project ID: h1351, pr63fa

Introduction

Molecular Magnetism is a field of condensed matter physics where the properties of magnetic molecules are investigated [1]. Although it has been known for more than 50 years that molecules can possess magnetic moments, the whole field got an enormous impetus when scientists in the late 1980s discovered that a single molecule can show a magnetic hysteresis loop.

Figure 1: Sketch of the magnetic molecule Mn$_{12}$-acetate. The manganese ions are highlighted in color.

The underlying (classical) picture is this: The spins of the magnetic ions contained in molecules such as Mn$_{12}$-acetate (see figure) form a resulting molecular magnetic moment. At low temperatures this moment is rather large (S=10 for Mn$_{12}$-acetate). Its motion is governed by an anisotropy barrier which means that there are two directions (up and down) in which the magnetic moment likes to point and that it would need to overcome an energy barrier in between. This stabilizes the up and down orientations and leads to the magnetic hysteresis. Since this is exactly the behaviour of a magnetic entity storing a single bit, magnetic molecules appeared to be potential ultimately small next-generation storage devices. But since they are so small, quantum effects are important. In essence the latter result in the fact that the magnetic bistability vanishes at temperatures exceeding one or two Kelvins. Therefore, since the discovery of Mn12-acetate chemists try to synthesize molecules with better barriers and physicists together with chemists try to rationalize the magnetic behaviour in order to provide guidance for future synthesis.

Nowadays the range of research questions has broadened. It includes the investigation of magnetocaloric properties of such substances, i.e. the question whether and how efficient one could cool or heat with these materials by just sweeping the field. Efforts of maintaining and manipulating quantum coherent states are being made in order to construct constituents which might be parts of quantum computers. A last but not least focus is on effects that are driven by magnetic frustration, which labels a situation in which interacting magnetic moments are "not happy" since they cannot align parallel or antiparallel due to competing interactions.

In any case it is the task of theory to model such systems with the aim to understand the magnetic behaviour. From the point of view of many-body theory a molecule is already a giant object since it consists of very many nuclei and electrons, therefore complete quantum solutions are not even within reach. But for many observables it is quite sufficient to consider the magnetic moments of the unpaired electrons together with their mutual interactions only. Such models are mathematically represented by spin Hamiltonians of which the Heisenberg Hamiltonian is one of the most famous. It has a rather simple form

$$H = -2 \sum_{k<l} J_{kl} \vec{s}_k \bullet \vec{s}_l$$

The Hamilton operator represents the energy that stems from the interactions of pairs (k,l) of spins, where J_{kl} represents the strength of the interaction. There are only two basic interactions: the ferromagnetic interaction which tends to align the spin vectors in a parallel fashion and the antiferromagnetic interaction which

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tends to align the spin vectors in an antiparallel fashion. Although this classical description sounds very simple the quantum problem is numerically involved since in quantum mechanics the Hamiltonian is represented by a matrix in Hilbert space whose eigenvalues we need to compute. The dimension of this vector space grows exponentially with the number of spins, i.e. $d=(2s+1)^N$ for N equal spins. This means that for e.g. 10 iron spins of s=5/2 the dimension is 60,466,176. Such a matrix, when stored completely, would need about 30 Petabyte of RAM; the determination of its eigenvalues is virtually impossible.

There are two approaches to ease this problem: use of symmetries and Krylow space methods. Both methods have been utilized at the LRZ, the first in h1351, the second in pr63fa.

Results

Using symmetries is one of the major paradigms in theoretical physics (and quantum chemistry). Besides its mathematical beauty it provides additional inside into physical properties as well as massive help for numerical solutions. The procedure is the following: If an operator such as the Heisenberg spin Hamiltonian, Eq. (1), is quantum mechanically represented in Hilbert space it is given by a matrix with as many rows and columns as the dimension of the space. If symmetry can be used then the Hilbert space can be decomposed into mutually orthogonal subspaces and the matrix needs to be evaluated only in each subspace.

Let's consider a mirror symmetry for instance. Then the Hilbert space can be split up into approximate halfs, and in each the matrix has only half of the linear dimension and needs only a quarter of RAM to be stored. The matrices can be treated one after another, which is the numerical gain. It is clear that one aims at the use of as many as possible symmetries [2]. In the course of the Ph.D. project of Roman Schnalle we could devise a scheme to combine the symmetry of spin rotations SU(2) with arbitrary special permutations (point group symmetries). This is a worldwide outstanding result which together with the computational capabilities of the LRZ allowed us to investigate some of the most interesting archetypical molecules in the field [3]. As one example we would like to show the obtained magnetic susceptibility for a molecular wheel of 10 iron spins with spin quantum number s=5/2 (ferric wheel). The related Hilbert space has a dimension of 60,466,176; it can be split up into small enough subspaces by using the symmetries SU(2) and D_2.

As a second example we would like to demonstrate that one can indeed obtain an energy spectrum that is resolved according to the irreducible representations of the underlying point group, in this case I_h for the icosahedron.

Figure 2: Susceptibility of an antiferromagnetically coupled spin ring with N = 10 and s = 5/2. The exchange parameter is J = -9.6 cm^{-1} [3].

Figure 3: Structure and energy spectrum of an antiferromagnetically coupled spin icosahedron with s=1 [3].

A second approach to the eigenvalue problem is given by Krylow space methods [4] which by the way can be combined with the use of symmetries. The original idea of such methods is to obtain only extremal eigenvalues as for instance the lowest eigenvalue of a Hamiltonian, which is the ground state energy, and a few above the lowest which suffice to explain the low-lying excitation spectrum. These methods work by constructing a special vector space (Krylow space) that is only a tiny subspace of the full Hilbert space, but in this special subspace extremal eigenvalues converge rapidly against the true extremal eigenvalues. The Krylow space is generated by applying the Hamiltonian and its powers up to typically about 100 to a (randomly chosen) trial vector. This is a rather cheap operation compared to matrix diagonalisation, and it can be well parallelized [5].

It turns out that Krylow space methods can as well be used in order to accurately approximate quantum statistical observables, i.e. in order to evaluate the partition function with very high accuracy [6]. To this end not only the extremal eigenvalues in the respective Krylow spaces are used but all eigenvalues and eigenvectors which in essence then provide a coarse grained density of states that allows to approximate the thermodynamic functions. This enables us to model magnetic molecules of

unprecedented size, i.e. with Hilbert space dimensions of up to 10^{10} [7].

A very recent example is given by the molecule $\{W_{72}V_{30}\}$ in which the 30 magnetic vanadium ions (s=1/2) have to be modeled in a Hilbert space of dimension 1,073,741,824. Despite this dimension, its magnetic properties as e.g. the susceptibility, see Figure 4, can be evaluated within a few days e.g. on 510 cores of the old SGI Altix at the LRZ in Garching.

The success of Krylow space methods partly rests on the fact that they can be very efficiently parallelized using openMP directives. Many of the necessary operations are simple matrix vector products. The performance can be even further enhanced if matrix elements do not need to be stored but can be evaluated when needed, i.e. "on the fly" [5]. We tested the scaling on various architectures, it seems to be very close to perfect. Beside tests on the SGI Altix and on SuperMUC at LRZ we run tests on ScaleMP vSMP architectures that consists of Infiniband connected commodity x86-based clusters at Bielefeld University and at RWTH Aachen.

On-going Research / Outlook

The success of our first calculations using the Finite Temperature Lanczos Method opens the prospect that re-

cently synthesized magnetic molecules can be modeled with high accuracy in a reasonable time. A few additional results could already be obtained [9,10].

In addition we are going to investigate deposited magnetic molecules by means of Wilson's Numerical Renormalization Group method.

For the constant and very professional support we would like to thank the LRZ very much.

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Figure 5: Runtime of a typical Lanczos run on various architectures. The scaling is very close to perfect. The higher speed of the x86-based clusters reflects its later production date (2010 vs. 2006 for the Itanium II).

Molecular Switches at Surfaces

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HLRB Project ID: h1281

Introduction

The ultimate goal of nanotechnology is control over molecular scale mechanical and electronic components. An oft-proposed route to this goal is the construction of components from controllable single molecules. An important class of such molecules with obvious applications is formed by those that have properties reversibly and bi-stably modifiable by external stimuli – so-called molecular switches. One example is the azobenzene molecule (H_5C_6–N=N–C_6H_5), which can be bi-stably photo-isomerized between its planar, *trans* and torsioned-twisted, *cis* conformers in both solution and gas-phase. The high yield and stability of this reaction have rendered azobenzene an archetype of molecular switch research with proposed technical applications including e.g. light-driven actuators and information storage media.

Figure 1: Schematic illustration of the geometric decoupling strategy and its failure in the context of the adsorbed azobenzene switch: (a) parent (unsubstituted) azobenzene, (b) expected lift-off by bulky spacer groups and (c) real adsorption geometry according to NIXSW and DFT [7].

For many such applications, switching of molecules at solid interfaces – adsorbed at metal surfaces, for example – is of particular interest [1]. Unfortunately however, the switching properties of azobenzene have proven highly sensitive to the adsorbate–substrate interaction: even at nearly chemically inert close-packed noble metal surfaces, switching of surface-adsorbed azobenzene by light has never been achieved, and switching by excitation with a scanning tunneling microscope (STM) tip has been successful only at Au(111). A natural route to restoring the adsorbate switching ability is to further decouple the frontier π, *n* and π* orbitals responsible for the gas- or liquid phase photo-isomerization from the substrate electronic structure. With these frontier orbitals largely located at the central diazo (–N=N–) bridge an intuitive idea to achieve such a decoupling is to functionalize the molecule with bulky spacer groups that prevent a closer encounter of the photochemically active unit with the substrate. This is precisely the notion behind the arguably to date most studied such adsorbate, tetra-tert-butylazobenzene (TBA) [2]. TBA consists of azobenzene functionalized with four tert-butyl groups at the phenyl-ring meta positions as illustrated in Fig. 1. These 'table legs' were indeed found to enhance the switching efficiency of the adsorbed species, as e.g. indicated by the successful TBA switching by light at Au(111). However, attempts at STM-tip induced switching at ostensibly comparable substrates such as Ag(111) and Au(100) have been unsuccessful, indicating that TBA is not significantly more robust to specifics of the substrate interaction than pure azobenzene.

Theory

These circumstances beg the question, how and to what degree the TBA butyl groups really 'decouple' the photochromic moiety from the substrate. For a corresponding atomic-scale understanding the detailed characterization of the adsorbate geometry and binding constitutes a prerequisite and was the main objective of the work in this project. In contemporary surface science, corresponding analyses are increasingly performed by quantitative first-principles electronic structure calculations. Particularly density-functional theory (DFT) with present-day local or semi-local exchange-correlation (xc) functionals has developed into an un-

paralleled workhorse for this task, with often surprising accuracy particularly with respect to structural properties of the surface adsorption system. For TBA at Au(111) corresponding calculations are already challenged by the extension of the functionalized molecule and the simultaneous necessity to describe the metal band structure within a periodic supercell approach. On a more fundamental level, the real limitation comes nevertheless from sizable dispersive van der Waals (vdW) contributions to the surface chemical bond as characteristic for organic molecules containing highly polarizable aromatic ring systems.

For system sizes as those implied by the adsorption of azobenzene or TBA an appealing and computationally tractable possibility to improve on this situation is a semi-empirical account of dispersive interactions within the framework of so-called DFT-D schemes [3]. In this approach the vdW interactions not described by present-day xc functionals are approximately considered by adding a pairwise interatomic $C_6 R^{-6}$ term to the DFT energy. At distances below a cut-off, motivated by the vdW radii of the atom pair, this long-range dispersion contribution is heuristically reduced to zero by multiplication with a short-range damping function. While the applicability of this approach to adsorption at metal surfaces is uncertain, our recent benchmark study performed for azobenzene at Ag(111) revealed that in particular the most recent DFT-D scheme due to Tkatchenko and Scheffler (TS) [4] yields excellent structural properties, albeit at a notable overbinding [5].

Results

In this project we further explored the generality of this finding by analyzing the adsorption geometry, vibrations and energetics of TBA at Au(111). Comparison against near-edge X-ray absorption fine structure (NEXAFS) and high-resolution electron energy loss spectroscopy (HREELS) measurements, as well as a complete analysis of new TPD data confirms the accurate structural and vibrational predictions reached by the DFT-D TS scheme [6]. The again obtained significant overbinding furthermore supports the interpretation [5] that the neglect of metallic screening is the main limitation in the application of this scheme to the adsorption of organic molecules at metal surfaces. Comparing the TBA data to those for pure azobenzene at Au(111) we find a qualitatively different adsorption geometry for the functional backbone in the case of the *cis* isomer as shown in Fig. 2. For the *trans* isomer, on the other hand, we determine an intriguing structural and vibrational insensitivity of the photochemically active central diazo-bridge to the presence of the bulky spacer groups: The real TBA adsorption geometry as determined by our DFT calculations is much better characterized as the 'suspended bridge' between tilted tert-butyl legs that is shown in Fig. 1 [7]. The role of the bulky spacer groups for the switching efficiency is therefore more subtle than the originally anticipated simple geometric decoupling and will be the topic of continuing work in our group.

Figure 2: Perspective view of the cis TBA adsorption geometry at Au(111).

On-going Research / Outlook

The results of this study have shown uncompromisingly that the subtleties of molecular switching at metal surfaces and the role of frequently employed bulky spacer groups cannot be understood by focusing exclusively on geometric properties of the adsorption complex. Building on the detailed characterization of the azobenzene and TBA at Au(111) system achieved in this project, our on-going and future work therefore now directly addresses the actual transient and non-adiabatic switching dynamics. Parts of this work are currently already performed in project "*Ab initio* description of the isomerization dynamics of surface-adsorbed molecular switches" (project-ID pr63ya). Here, a first suite of (numerically highly demanding) calculations comprises geometry optimizations of the molecule constrained to different electronically excited states. At present we already see a sublime performance of our CASTEP-based approach on the new Super-MIG architecture and will report on these findings in detail in the status report of project pr63ya.

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THz spectroscopy of solvated biomolecules studied by *ab initio* molecular dynamics

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Introduction

The solvation dynamics of molecules is of fundamental importance in chemistry and biology processes, like chemical reactions in solutions and protein folding. In our project, we applied *ab initio* molecular dynamics simulations [1] to investigate the structure, dynamics and vibrational spectroscopes of aqueous solutions of the simple amino acids, *e.g.* glycine and valine, at a later stage along this line of research, small peptides in water as well as their theoretical vibrational spectroscopy at low frequencies of about 50-100/cm. The so-called Tera-Hertz (Thz) spectroscopy is a powerful but still emergent experimental probe to access the (sub)picosecond solvation dynamics in the frequency domain which calls for much more theoretical insights into the underlying molecular phenomena. In particular, computational schemes in terms of maximally localized Wannier orbitals and atomic polar tensors will be applied to decompose the individual contributions from the solute and the water solvent to arrive at a molecular level understanding.

Amino acids, being the basic building blocks of proteins, are particularly interesting as they occur in a neutral form in the gas phase, whereas the zwitterionic form is stabilized in polar solvents with a high dielectric constant such as water at ambient conditions. In the zwitterion, the acidic functional group, -COOH, is deprotonated while the basic group, -NH$_2$, is protonated thus yielding anionic and cationic groups, -COO$^-$ carboxylate and -NH$_3^+$ ammonium, respectively, in a solution and a pronounced molecular dipole moment is a consequence. These charged groups, in turn, are expected to strongly interact with the surrounding water molecules thus structuring the solvent in terms of anionic and cationic solvation shells in close spatial vicinity around the very same molecule.

Results

AIMD [1] simulations based on the iterative Born-Oppenheimer propagation approach are performed using the Gaussian and plane waves mixed-basis method as implemented in the QUICKSTEP module within the CP2K AIMD simulation package.[2] A representative snapshot of the aqeous Glycine solution is shown in Fig.1. Based on our simulations, the average number of hydration water molecules around the ammonium group is found to be three, while the two oxygen atoms of the carboxylate group are asymmetrically solvated, with a total of 4.4 water molecules in the first shell. No evidence for a proper intramolecular hydrogen bond connecting the ammonium and carboxylate groups is found. While the carboxylate group strongly prefers to be coplanar to the other heavy atoms, it is subject to significant out-of-plane fluctuations of up to about ±50°. The hydrogen atoms attached to the α-carbon do not establish proper hydrogen-bonding contacts with surrounding water molecules as expected for hydrophobic alkyl groups. The ammonium group in the zwitterionic glycine rotates efficiently in aqueous solution while the rotation of the carboxylate group is strongly hindered.

By analyzing the electronic structure in terms of approximate molecular dipole moments, it is found that the

Figure 1: Representative snapshot of the aquous Glycine system as used in the present AIMD simulations. Water molecules are depicted by a stick representation, glycine by a ball-and-stick model, and the Wannier function centers are shown by small green spheres, the yellow arrows represent the molecular dipoles.

Figure 2: Distribution functions of molecular dipole moments for (a) glycine and (b) water molecules. In (a) neutral Gly in vacuum (blue), isolated zwitterionic Gly vertically transferred from solution into vacuum (dashed red, see text), and zwitterionic Gly solute itself in the solution (black) are shown. In (b) water molecules in the solvation shells of the ammonium group (blue), carboxylate group (red), α-carbon (green), and all remaining "outer" water molecules (magenta) are shown in addition to pure bulk water (black).

solute-solvent coupling leads to a significant increase of the already large dipole of the solvated zwitterion.

As revealed by Fig. 2a, the average dipole moment for the zwitterionic Gly in the solution is around 16.5 D, while for the virtual isolated zwitterionic Gly it amounts to only 12 D. This implies that the molecular dipole moment of the zwitterionic solute increases by about 40 % due to polarization effects in the solution or in other words mainly due to electronic contributions to solute-solvent coupling. Compared to the zwitterionic Gly molecule in the solution, all the Wannier centers in the isolated zwitterionic Gly transferred into the vacuum feature a uniform shift toward the $-NH_3^+$ group because the electrons relax such as to minimize the dipole moment in vacuum. This response of the electronic structure to a low dielectric environment also explains why the dipole moment of zwitterionic Gly decreases from 16.5 to 12 D upon removal of solvating water molecules. The increase of the dipole moment from neutral Gly to the isolated zwitterionic Gly is due to a structural change and thus the generation of separated charged groups, while the dipole moment difference between isolated zwitterionic Gly in vacuum and zwitterionic Gly in the solution results from the coupling with solvation waters, which is an electronic effect due to solvation. Overall, these two contributions together lead to a total increase of the dipole moment of Gly of about 15 D upon solvation in water.

We also analyzed the approximate molecular dipole moments of the water molecules in the solution and find the solute affects the interfacial water molecules only very mildly, even those in the cationic and anionic solvation shells of the ammonium and carboxylate groups, both in terms of their dipole moments and intramolecular structure. The IR spectrum of Gly(aq) is decomposed into individual contributions from the zwitterionic Gly molecule itself in the solution and from the water solvent. They are compared with the IR spectrum of an isolated zwitterionic Gly molecule, obtained by verticaltransfer

out of the solution into vacuum, and with that of a stable neutral Gly molecule in vacuum at the same temperature. Obviously, some modes disappear due to the structural changes from neutral to zwitterionic, whereas other modes are significantly redshifted due to the interactions with the solvation water molecules. Most prominent is a double peak structure at around 1295 and 1350 cm^{-1}; the lower corresponds to the collective movement of C_α and C_c coupling with the symmetric C_c-O_c stretching and C-H wagging, whereas the higher one stems from the stretching mode of the C_α-C_c bond coupled to the symmetric C_c-O_c stretch and the C-H bending. These features, which are located in the rather transparent window between the libration and intramolecular bending resonances of pure water, can be used as the fingerprint of the presence of Gly in its zwitterionic state in aqueous solution. Another most prominent zwitterionic Gly mode at around 1535 cm^{-1} overlaps significantly with the red wing of the intramolecular bending band of water. This results in a redshift and considerable broadening of the combined band.

On-going Research / Outlook

We emphasize that despite the difficulties of getting statistically converged results in characterizing vibrational modes of aqueous solution, the analysis of the glycine solution trajectories produced on HLRB2 yielded a great deal of insights into structures, dynamics, dipole distributions and their impact on IR spectroscopy. The first part of our results has been published. [3] More deep analysis is going on and following publication is in preparation. Similar methods, like spacial resolved spectroscopy and distance decomposition, as we used in our project of bulk water [4] will be applied on the glycine solution.

As it is completely out-of-reach to produce trajectories of the necessary quality and length without the use of a facility such as the HLRB2, we are very thankful for the supply of the computational resources. The new generation high performance computer – SuperMUC, will allow us to generate much better statistics. Furthermore, it will enable us to investigate larger molecules and more complicated systems such as those currently investigated in experiments.

While during the process of the project the ongoing experiments observed much larger concentration dependence of the absorption cross section in valine solution than in aqueous alanine, we decided to extend the simulations to the even larger Valine molecule. It is not only larger but it has also two entaniomers, L-isomer and D-isomer, where L-valine is proteinogenic. Therefore here we will only focus on L-valine which features three conformers which are all dynamically stable. Such a study would not be possible without having accessing to SuperMUC!

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Electrokinetics in Microfluidic Channels Containing Floating Electrodes

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Introduction

Microchip devices for chemical separation and analysis provide significant advantages in performance, resulting in faster and cheaper analytical procedures using small amounts of sample and reagents. However, the use of smaller geometries means as well that the number of molecules to be analyzed is reduced so that their detection can become a challenging task. Apart from the use of highly sensitive detectors, another option is to employ sample preconcentration after (on-line) sample injection. We report that a bipolar electrode (BPE) can be used to alter the local electric field within a microchannel, and that the resulting field gradient can be used to concentrate and separate charged analytes [1,2,4]. The BPE is a conductive material that is not connected to an external power supply, and therefore, it is free to float to an equilibrium potential. If there is a sufficient potential dropped across the solution above a BPE, it can act as an electrode at which cathodic and anodic reactions occur simultaneously at opposite ends. The goal of this project was understanding and characterization complex interplay of the electrokinetic, hydrodynamic and electrochemical phenomena observed in microfluidic systems with embedded floating electrodes.

Results

The hybrid poly(dimethylsiloxane) (PDMS)/glass microfluidic device (a layout is shown in Figure 1a) and bipolar electrode were fabricated using standard lithographic techniques. The microfluidic channel was made by attaching a PDMS mold containing a micro-channel (6 mm long, 100 μm wide, and ~20 μm high) that connects two macroscale cylindrical reservoirs of ~2.5 mm diameter to a microscope glass slide by O2 plasma bonding. Before fabricating the microfluidic device, a floating electrode was prepared by depositing 100 nm of Au onto the glass slide. Then, photolithographic and etching methods were used to pattern a single 500 μm × 1000 μm electrode.

The microchannel and reservoirs were filled with 1.0 μM BODIPY disulfonate (twice negatively charged fluorescent tracer) in 5.0 mM Tris-HCl buffer. If a potential bias is applied between electrodes immersed in the reservoirs, the BODIPY dye concentrates in the anodic compartment of the channel (Figure 1b). In contrast, the dye moves uniformly from anode to cathode in the absence of the BPE due to bulk electroosmotic flow (EOF). This suggests that the EOF in the system with the bipolar electrode, which initially (locally) dominates electrokinetic transport of the dyes, is offset by an increasing magnitude of counter-directional electrophoretic motion.

Numerical simulations were used to model the local electric field and species concentration distributions in the microfluidic device. The basic equations governing the physical phenomena in the system are the Nernst-Planck, Poisson, and generalized Navier-Stokes equations. The Nernst-Planck equation describes local mass and charge transport due to advection, diffusion, and electromigration; the Poisson equation establishes a relationship between the local electrical potential and the species concentration distributions; the generalized Navier-Stokes equation relates the fluid flow velocity field to the pressure and Lorenz force. Spatiotemporal variations in the concentrations of ionic species of the buffer solution and the tracer molecules in the system are governed by balance equations with reaction terms taking into account the fact that the local concentration of the ionic species can change due to the bulk buffer reactions and/or faradaic reactions.

The above formal description of the processes in the system was implemented as an iterative numerical scheme based on discrete spatiotemporal schemes optimized for parallel computations. In particular, for the solution of the Navier_Stokes, Poisson, and Nernst_Planck equations, the lattice-Boltzmann approach and the numerical approaches described by Warren and by Capuani et al.[3] were implemented. In all numerical schemes, a time step of 1×10^{-5} s and a space step of 10^{-6} m were used. A single simulation required ~24 h using 64 processors of an SGI Altix 4700 supercomputer to analyze the temporal be-

havior of the system for 100 s. The developed numerical model was used for detailed simulation to analyze focusing mechanism observed in the microfludic device with the BPE. When a sufficiently high driving voltage is applied across the channel, water electrolysis is induced at the ends of the BPE. A consequence of this process is the neutralization of the buffer cations (TrisH$^+$) by OH$^-$ generated at the cathode end of the BPE. That is, in the vicinity of the BPE, current can be carried by both electrons (through the electrode) and ions (through the solution above the BPE). This results in complex ion transport due to the combined actions of electromigration and EOF, which in turn leads to an electric field gradient in the solution (Figure 2).

The implication of these results is that tracer molecules coming from the anodic reservoir encounter an increasing electrophoretic force in the opposite direction (back toward the anodic reservoir) as they approach the BPE due to the field gradient. At certain axial positions, the two counter-directional components (anodic electrophoresis vs cathodic advective flow) are balanced. When this happens, tracer molecules become quasi-stationary and locally enriched, with enriched zones being separated for tracer molecules with different electrophoretic mobilities [4].

On-going Research / Outlook

The developed numerical model was used to carry out numerical experiments to simulate and analyze electrokinetic transport in more than 200 microchannel devices with the BPEs of the various geometrical configurations, as well as with various buffer systems, analyte molecules, and surface properties of the channel walls, which determine the direction and velocity of the EOF. Currently, the model is employed to study the effect of the characteristics of the electrical double layer formed at the surface of the BPE on the parameters of electrokinetic transport through the channel.

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Figure 1: (a) Layout of the hybrid PDMS/glass microfluidic device with the Au electrode (500mm×1000 mm) embedded at the center of the (6 mm long, 100 mm wide, and ~20 mm high) microchannel connecting the two macroscale cylindrical reservoirs. (b) Optical fluorescence micrograph of the microchannel with the bipolar Au electrode, showing the concentration distribution of BODIPY disulfonate in 5 mM Tris-HCl buffer after applying a potential bias of 30 V for 240 s (top). Schematic illustration of the proposed mechanism of tracer accumulation in the microchannel with a bipolar electrode (bottom).

Figure 2: Measured (top) and simulated (bottom) electric field strength in the hybrid PDMS/glass microfluidic device with the embedded bipolar electrode (BPE).

Electron transfer processes in molecules at surfaces

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HLRB Project ID: pr28lo

Introduction

Dynamical processes involving the transfer or the transport of electrons are of fundamental importance in many areas of physics, chemistry, and biology [1]. Among the great variety of different types of electron transfer (ET) reactions, ET processes in molecular systems at semiconductor or metal surfaces have attracted considerable interest recently. Important applications where such processes play a fundamental role include photonic energy conversion in organic solar cells, where electrons from a photoexcited electronic state of a molecular chromophore are injected into the conduction band of a semiconductor surface, and voltage driven single-molecule conduction in nano-scale molecular electronics. Obtaining a detailed understanding of the basic mechanisms of ET in these systems, which is a prerequisite for the design and optimization of efficient nanoelectronic and optoelectronic devices, requires theoretical modelling and simulation of the processes at a molecular level.

From the theoretical point of view, the simulation of electron transfer and electron transport at molecule-substrate interfaces is particularly challenging. It requires a methodology able to describe simultaneously a finite system with a discrete energy spectrum, the molecular adsorbate, and an extended system such as a metal or semiconductor surface or a metallic electrode. Furthermore, both photoinduced ET reactions and voltage driven electron transport processes typically involve significant non-equilibrium effects and thus require, in addition to the description of the electronic structure, a dynamical treatment.

Here, we report recent results on the simulation of photoinduced ET processes in molecular systems at surfaces obtained using the HLRB II supercomputer. In particular, we analyze orbital-symmetry-dependent ET in short chain alkanethiolate self-assembled monolayers (SAM) adsorbed at the Au(111) surface [2] and photoinduced ET processes in the dye-semiconductor system alizarin-anatase (TiO$_2$) [3]. Results of simulations of electron transport in single-molecule junctions obtained within the project have been discussed in Refs. [4,5].

Results

To study ET processes in the systems mentioned above, we have used a two-step procedure that combines ab initio electronic structure methods with quantum dynamical methods. In a first step, the systems are characterized using first-principles electronic structure calculations, which provide the parameters (electronic states, energies and donor-acceptor couplings) required in the simulation of the dynamics. To account for the extended nature of the system, the electronic structure calculations use periodic density functional theory within the super-cell approach using slab models large enough to describe the systems with the required accuracy. Specifically, we have employed the Vienna Ab initio Simulation Package (VASP) to solve the Kohn-Sham equations using the projector augmented wave method and a plane wave basis. These methods are well suited for parallel computing environments such as the HLRBII supercomputer. After obtaining the equilibrium structure for the extended system, the donor (d) and acceptor (a) states are constructed using a partitioning technique [6] motivated by the projection-operator approach to resonant electron-molecule scattering. This results in a model ET Hamiltonian of the form

$$\hat{H} = \left|\Psi_d\right\rangle E_d \left\langle\Psi_d\right| + \sum_a \left|\Psi_a\right\rangle E_a \left\langle\Psi_a\right|$$
$$+ \sum_a \left(\left|\Psi_d\right\rangle V_{da} \left\langle\Psi_a\right| + \left|\Psi_a\right\rangle V_{ad} \left\langle\Psi_d\right|\right) \quad (1)$$

In the second step, the model Hamiltonian is used to determine the time evolution of the donor state population in the ET process, which characterizes the ET dynamics and can be compared with the experimental data.

Orbital-symmetry-dependent ET in short chain alkanethiolate self-assembled monolayers
The method described above has been applied to study the photoinduced ET process between a photoexcited donor electronic state and a quasi-continuum of acceptor electronic states in the alkanenitrilethiolate/Au(111) SAM system (see Fig.1). In particular, we have considered the electron injection dynamics from the energetically close

lying π1* and π2* donor states (see Fig. 1) corresponding to the two π* resonances of the CN group that can be selectively monitored using core-hole clock spectroscopic techniques [2]. We first characterized the system and found that the most stable adsorption position at the Au(111) surface was the fcc-bridge like position with the CN axis tilted 70.7° against the surface normal. The simulation of the electronic dynamics (see Fig. 1) reveals ET times of 3.8 fs for the π1* donor state and 46.8 fs for the π2* donor state, respectively. This difference can be explained in terms of the spatial extension of the states. While π2* is essentially localized at the CN group with negligible contributions in the rest of the molecule, π1* shows contributions in the backbone of the SAM as well as in the sulphur atom that binds the organic molecule to the Au(111) surface. The spatial extension of this orbital causes stronger donor-acceptor couplings, ultimately leading to a faster electron injection than in the π2* case. These results indicate that charge transport in organic layers can depend on the nature of the initially prepared electronic state even in situations where the donor states energies show a negligible splitting, providing a way for the selective control of the electron injection dynamics, a fact that has been recently demonstrated experimentally [2].

Photoinduced ET processes in the dye-semiconductor system alizarin-anatase (TiO$_2$)

Understanding and controlling the dynamics of electron injection from an excited electronic state of a dye molecule into the conduction band of a semiconductor is a key step to design efficient nanocrystalline solar cells. These processes are usually characterized by their ultrafast (femtosecond) time scale and their non-equilibrium character. Furthermore, intermediate states localized at the chromophore-substrate interface and electron-vibrational (vibronic) coupling may play an important role in the process. Therefore, the model Hamiltonian (1) had to be extended to include the presence of intermediate states. Moreover, the nuclear degrees of freedom where also taken into account in the simulations using a local low-order polynomial expansion of the diabatic potential surfaces at the equilibrium geometries of the ground state [6]. To simulate the quantum dynamics, we used the multilayer formulation of the multiconfiguration time-dependent Hartree method [7]. Figure 2 depicts the decay of the population of the donor state after photoexcitation. The results show that the photoexcitation of alizarin induces an ultrafast injection of the electron into the semiconductor substrate on a timescale of 10 fs, which is in good agreement with experimental results. A detailed analysis of the results has revealed that the electron injection dynamics in this system is accompanied by significant electronic coherence effects, which manifest themselves in the oscillatory character of the population dynamics shown in Fig. 2. As a result, the ET process cannot be characterized by a simple rate constant. Indeed, the process is described by a two-step mechanism, which involves an intermediate state localized at the dye-semiconductor interface.

Figure 1: Population dynamics of the π1* (black) and π2* (blue) donor states reflecting the ET process from the CN group of the molecule to the substrate.

Figure 2: Population dynamics of the donor state reflecting the electron transfer process from the dye molecule to the semiconductor substrate. The simulations depicted include (solid line) and neglect (dashed line) the effect of the vibronic coupling.

On-going Research / Outlook

Our on-going research within the project involves the study of photoinduced ET processes in a variety of molecule-surface systems. In addition, we investigate electron transport and photophysical properties of molecular nanocontacts with graphene as material for electrodes in architectures where two graphene sheets are connected by a single organic molecule. Compared to metal electrodes, graphene offers a number of advantages as a material for electrodes, in particular, high electron mobility, rigidity and mechanical stability and thus more precise control of the molecule-graphene contact geometries. Furthermore, due to its optical properties, graphene electrodes may facilitate the addressability of the nanocontact by laser light for optoelectronic applications. This project will benefit from the methods developed and the experience acquired in the simulation of electron transfer processes of molecules at metal and semiconductor surfaces.

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Towards the total breakup of two-electron atoms:

Spectra, localization properties and driving effects

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Introduction

Despite the seemingly simple problem of three charged particles with known interactions, there is no comprehensive understanding of the regime close to the total-fragmentation threshold of two-electron atoms and their interaction with external fields. The electron-electron interaction term in the Hamiltonian of the helium atom – which otherwise is just the sum of two hydrogen Hamiltonians with amended nuclear charge – renders the two-electron classical dynamics in general irregular or chaotic, with only small regions of regular motion. On the quantum level, the loss of integrability is responsible for the (at least partial) breakdown of good quantum numbers, and leads to an abundance of intriguing quantum effects, such as the autoionization of doubly excited states (DES), fluctuations in the photoionization cross sections (PCS) at high excitation energies (Fig. 1a,b), and highly correlated planetary states of the doubly excited atom associated to classical configurations (Fig. 1c). Hence, even without any external perturbation, DES of helium represent one of the most challenging – and experimentally accessible – test cases for the theory of quantum chaos.

An interaction with an external field enhances dramatically the complexity of the system. Apart from a vast variety of phenomena occurring in ionization and recombination processes of two-electron atoms, the interaction of two-electron atoms with fields might be of fundamental importance in the context of coherent control and quantum information. Strongly correlated states of the DES of unperturbed helium – the frozen planet states – are expected to transform under near-resonant periodic driving into nondispersive wave packets (NWP) – that is, quantum objects which propagate along classical trajectories without dispersion (Fig. 1c). Closely related to the previous aspect is the possibility to explore the correlated motion of multiple electrons with ultrashort pulses. So far, the correlated two-electron dynamics has been observed in Rydberg states [1].

A clear understanding of all the above issues requires an accurate theoretical treatment, which defines a formida-ble theoretical and numerical challenge [2]. Our approach includes a versatile numerical machinery for the accurate description of such systems, with a minimum of approximations, without adjustable parameters. The major approximation consists of confining the atom to a plane. Even after this restriction parallel coding is mandatory due to the large dimensions of the associated eigenvalue problem. Notwithstanding the two-dimensional character of our model, it provides not only a good qualitative description, but also has a quantitative predictive power [3].

In the following we describe our advances in the understanding of the near-breakup-threshold region and in the search for nondispersive two-electron wave packets.

Results

The spectrum of two-electron atoms is composed of series of states converging to the single ionization thresholds (SIT) I_N (Fig. 1d). Already around I_4 the series start to mix, i.e. states of higher series lie below the SIT of lower series. As the energy approaches the double ionization threshold (DIT) the complexity of the spectrum increases. Good quantum numbers valid for low excitations are

Figure 1: Highly doubly excited states

Figure 2: Expectation value of cosθ₁₂ for resonance states below the 25ᵗʰ SIT. Resonances close to the *Zee* and *eZe* configurations are arranged in series which can be labeled by the approximate quantum number *F*. Highlighted are *eZe* configurations only.

Figure 3: The exact PCS of triplet helium (black line) are dominated by the contributions of the *F=1* series (blue) at energies up to the 14ᵗʰ SIT. Above this energy the contributions of the *F=3* and *F=5* series (red and green lines in b) gain importance, while the contributions of all the rest of DES are negligible.

lost and most of the DES cannot be classified. However, there are series of resonances which can be identified with two one-dimensional classical configurations of the atom, the frozen planet or *Zee* configuration (with both electrons on the same side of the nucleus) and the asymmetric stretch or *eZe* configuration (with both electrons on opposite sides of the nucleus). These resonance states are thus characterized by expectation values of the angle θ_{12} between the electron radii which are close to 0° or close to 180°, respectively (Fig. 2).

Series associated to the *eZe* configuration play a fundamental role in the photoionization process. On the one hand, the fluctuation amplitudes of the PCS decay with energy as $|E|^\mu$ for moderate energy values. The exponent μ is related to the stability exponents of the *eZe* configuration [4]. On the other hand, these series dominate the PCS [5,6]. For instance, the PCS from the ground triplet state of helium is essentially reproduced by the *F=1* series at low energies (Fig 3a). However, as the energy gets closer to the DIT, the contributions of the *F=3* and *F=5* series become important. This has relevant consequences in the above mentioned scaling law which apparently fails as the energy approaches the DIT due to the contributions of these "less" collinear states [3,6]. The existence of these dominant resonances has important implications for the discussion about the existence of an *Ericson regime* in helium with strongly overlapping resonances which induce quasi-random fluctuations in the spectrum (Fig. 1b). Though resonances start to overlap around the 9ᵗʰ SIT, Ericson fluctuations are not found in the PCS yet, since dominant series do not exhibit strong overlap even around the 25ᵗʰ SIT [6,7].

In contrast, series associated to the *Zee* configuration can be neglected in the PCS. These states are weakly coupled to the helium ground state, which probably is the main reason they have not been observed yet. The importance of these planetary states is two-fold: first, they are extremely long-lived states localized in regular islands of the phase space of helium. Second, these states are expected to transform under near-resonant coupling in NWP propagating along periodic stable classical trajectories of the *Zee* configuration as illustrated in Fig. 1c: the projection of the dressed state on the phase space of the outer electron

(x and p) is anchored to the resonance island produced by the periodic driving. The dressed state and the resonance island propagate along a periodic orbit of the unperturbed *Zee* configuration [2]. This result obtained within our planar approach gives evidence for the existence of such NWP, yet still awaits its verification within a full three-dimensional approach and its experimental confirmation.

On-going Research / Outlook

A fully three-dimensional approach for the description of two-electron atoms has been already developed. So far, it has been used for the description of low-lying DES [8]. On-going work is the implementation of the atom-field interaction not only for the description of NWP but also for the investigation of ionization processes and the two-electron dynamics in state-of-the-art pump-probe experiments which involve intense ultrashort XUV and X-ray pulses. Due to the coupling of a rather large number of angular momenta, the full description of NWP still requires further understanding of the properties of planetary states with different angular momenta and their coupling to experimentally accessible states through few-photon processes. This might be relevant for the preparation of the initial state in an experimental realization of NWP.

Apart from our interest in two-electron atoms, our approach is also suitable for the numerically exact treatment of two-electron quantum dots. Here we address fundamental, not fully understood phenomena which are characteristic of many-body systems, such as thermalization and decoherence.

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First-principles simulation of the oxidation of ammonia on RuO$_2$(110)

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HLRB Project ID: pr42pe

Introduction

For a rational improvement of industrial catalytic processes the detailed understanding of the elementary steps in the reaction network is crucial. Quantitative simulations aiming at a *first-principles* based microkinetic description has already led to significant advances in the understanding of simple model reactions with one product (like the CO oxidation [1]). However, this approach is severely challenged by the excessive number of elementary processes in more complex reaction networks offering different possible end products (e.g. reactions that exhibit selectivity). An exhaustive determination of the kinetic parameters of all elementary processes from first-principles represents in most cases still a prohibitive computational cost.

To address such chemical reactions an extended approach based on an iterative sensitivity-guided refinement was developed in this project. This refinement shall identify the rate limiting steps in a reaction network so that the focus of detailed analysis of the computationally demanding first-principles evaluation can be restricted to a minimum. Starting with a basis set of elementary reactions, further reactions were added stepwise and the simulations were re-initiated until a consistent description has been reached. The explicit number of elementary processes that have to be examined at the first-principles level using density functional theory (DFT) was therefore *a priori* unknown.

The methodology was exemplified on the oxidation of ammonia to nitrogen monoxide as a showcase: This first step of the Ostwald process has only two initial reactants but exhibits already selectivity (molecular nitrogen is the competing side product):

$$NH_3 + O_2 \longrightarrow NO \text{ and } N_2$$

Since recent experiments [2] determined promising result for the catalyst RuO$_2$ (110) – a sufficiently high selectivity could be reached at a significantly lower temperature than on Pt (as it is used in the industrial process) – the simulations were performed on this surface.

Results

Before picking an initial setup of basis reactions, a precursory analysis of the active sites of the catalyst surface was recorded in order to identify the active sites of the catalyst. Using *ab initio* thermodynamics [3, 4] the phase diagram of the system was evaluated: This gave valuable insights into the surface occupancy and the corresponding stability concerning different pressure and temperature regimes: The focus is therewith only on one type of active site (see figure 1) in the ensuring kinetic modeling (though the RuO$_2$ (110) surface exhibits in principle two dominant adsorption site types).

Figure 1: Phase diagram at T=500K showing the stability range of ammonia and oxygen adsorbed on the two dominant sites of RuO$_2$ (110): The bridge (br) sites are occupied with oxygen within the whole pressure range observed, while the coordinatively unsaturated (cus) sites are participating in the adsorption and desorption processes.

The statistical kinetic Monte Carlo (kMC) simulations were initiated with a basis set of elementary processes that are described at the first-principles level. These initial reactions suggest themselves from chemical intuition: The stepwise dehydrogenation of ammonia and its successors, NH$_2$ an NH, via oxygen and hydroxyl groups, respectively, as well as the spontaneous decomposition of NH$_x$ species. The synthesis of the products appears then eventually by composition of the atomic com-

pounds. Consequently also the corresponding adsorption, diffusion and desorption processes have to be included. For this purpose a total of 39 energy barriers were evaluated with the nudged elastic band (NEB) method.

KMC simulations with this limited basis set of reactions could not show any agreement with the UHV experiment [2] which served as the benchmark for the microkinetic modeling results. However, the distribution and occurrence of the adsorbates on the surface could be studied within these simulations. To start the refinement cycle possible sources for the deviation from experiment were identified and processes that could find a remedy for these deviations were successively added to the reaction network. The effect of every considered process (or class of processes) on the reaction network was evaluated separately by reinitializing several kMC simulations with only one single improvement attempt at the time to attain a systematic evaluation of each of the variations.

Rct. from ... to	PBE [eV]		RPBE [eV]	
	$E_{forward}$	E_{back}	$E_{forward}$	E_{back}
$NH_3 + O$ / $NH_2 + OH$	0.79	0.09	0.84	0.00
$NH_2 + O$ / $NH + OH$	0.72	0.31	0.68	0.27
$NH + O$ / $N + OH$	0.00	0.65	0.00	0.77
$NH_3 + OH$ / $NH2 + H_2O$	not stable	0.00	not stable	0.00
$NH_2 + OH$ / $NH + H_2O$	0.60	0.42	0.31	0.00
$NH + OH$ / $N + H_2O$	0.00	0.84	0.00	0.70
$N + O$ / NO	0.70	2.25	0.79	2.24
$N + N$ / N_2	0.82	3.50	0.85	3.47

Table 1: Energy barriers for the basis reactions.

The initial list of elementary processes was therewith extended by lateral interactions between NO and other adsorbates. Further the effect of the zero point energy (ZPE) correction of the NO binding energy was considered. In addition hydrogen diffusion reactions along NH_x and OH_x adsorbates were attached to the initial process list:

$$NH_x + NH_y \longrightarrow NH_{x-1} + NH_{y+1} \quad x=1\text{-}3, y=0\text{-}2$$

Finally N_2O as a new intermediate and the corresponding processes were introduced to the initial reaction setup:

$$NO + N \longrightarrow N_2O \longrightarrow N_2 + O$$

To account for the error introduced by the approximated XC-functionals provided by DFT, the energetics of the reaction network as described formerly was evaluated using the PBE as well as the RPBE XC-functional. These functionals are known to mark a somewhat upper and lower boundary, respectively, for the bond-strength of an adsorbate. For a list of the energy barriers of the main reactions evaluated with PBE as well as RPBE see table 1.

Notwithstanding none of these first attempts could *significantly* improve the overall agreement with the experiment. However, all attempts could improve the matching with the experiment in at least one aspect. According to the therewith gained insights further kMC simulations comprising diverse *combinations* of the promising innovation were run to investigate the effect of them on each other. The interplay of the various innovations did indeed further improve the simulation results. Figure 2 shows the turnover frequency (TOF) diagram of the two main products as evaluated in the simulations using energy barriers based on the PBE functional: The oxygen pressure dependency of the desorption of NO and N_2 could be reproduced qualitatively. Furthermore, N_2 appeared to be the main product within the low oxygen pressure regime, while NO desorbs more frequently in the high pressure regime – as it was anticipated in the experiment. Albeit it has to be admitted that the absolute values of the TOFs are still certainly lower than in the experiment. Additionally the change of the simulated TOFs of NO and N_2 sprawl over a broader pressure range than observed in the experiment. However, one order of magnitude in pressure corresponds to an energy span of approximately 20 meV which is within the standard error of DFT. This good agreement could clearly show that the individual processes within the observed reaction network act and *re*-act on each other and therewith have (concerted) effects concerning the overall reactivity (and selectivity) of the catalytic process.

Comprising all adsorption, desorption, diffusion and reaction processes for all species and for both XC-function-

Figure 2: Turnover frequency (TOF) diagram resulting from kMC simulations at $p(NH_3)$=const, T=500K based on PBE energetic. The process list comprises the basis reactions as well as lateral interactions, ZPE correction for NO, H-diffusion and the intermediate N_2O and corresponding processes (straight lines: experimental results [2], dashed lines: simulated results).

als, 105 barriers were approached on a first-principles level to reach a sufficient agreement with the experimental results.

On-going Research / Outlook

The reaction network would further benefit from a detailed analysis of N_2O in its role as a desorbant. Experiments performed under ambient pressure [5] could add supportive information concerning this case.

To approach extended reaction networks in general more efficiently the sensitivity-guided refinement could further be extended by a method to estimate the energetic parameters on a low-cost level in terms of its computational cost, rather than be guided only by chemical intuition.

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Hierachical multiscale modelling of short-contact-time H$_2$ production on Rh

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Introduction

Microscale hydrogen production through short-contact-time partial oxidation of natural gas is expected to play a crucial role in light of the potential for a hydrogen-driven economy, where substantial technological barriers have to be overcome in order to introduce hydrogen into the energy system. Despite the favorable thermodynamics and fast reaction rates, CH$_4$ catalytic partial oxidation on transition metals (such as Rh) has to deal with important challenges that are critical for the technology development. In particular, the understanding of the surface chemistry is a crucial and challenging step in the quest to unravel the molecular level mechanisms underlying the macroscopic phenomena. This asks for a systematic and fundamental analysis of the reactivity at the atomic scale.

Using the CPU time awarded at HLRB, we have successfully performed a systematic first principles analysis of the surface reactivity at the nanoscale for the C1 to syngas chemistry on Rh. Following our original proposal, the analysis has been two-fold. On one side, we have revised and improved the UBI-QEP semi-empirical method [1] by performing a first-principles assessment of the UBI-QEP prediction, with special reference to coverage effects in activation energies. By means of this analysis, we have published a modification of the semi-empirical method, able to estimate activation energies for surface reactions within an uncertainty of +/-10% with respect to DFT calculations at negligible computational costs.

On the other side, for the first time in the literature, we have successfully applied a hierarchical multiscale methodology to the analysis of the water-gas-shift (WGS) and r-WGS reactions. In particular, using the HLRB resources, we were able to derive a new picture of the atomic-scale mechanisms in full agreement with all existing experimental data. This resulted in a strong impact on the rational atomic-scale understanding of millisecond contact time reformers for H$_2$ production at the microscale.

Results

The computational time granted at HLRB has been used to perform DFT-PBE electronic structure calculations for surface reactions. Based on our experience with HLRB-II, the superior interconnect of the HLRB-II system has provided an *excellent nearly linear scaling* up to a maximum of 96 MPI tasks per k-point which cannot be achieved on any other platform we are aware of. Such a unique infrastructure together with the available large numbers of CPUs provided by HLRB-II have been a prerequisite to make tractable the computationally expensive Climbing Image Nudged Elastic Band (CI-NEB) simulations for the location of transition state of the elementary steps at the systematic and wide extent herein investigated. Main results are described in the following.

1. First-principles assessment of the UBI-QEP semi-empirical method

Our initial study, published in Angewandte Chemie Int. Ed. [2], proposed a modification of the UBI-QEP semi-empirical method. This method allows for the calculation of the activation energy of a surface reaction as a function of the thermochemical parameters of the involved species (i.e., binding energies). In the common hybrid approach to UBI-QEP all these parameters are determined e.g. by DFT, which is still computationally much less intense than the explicit calculation of the activation energy.

To test the accuracy of the UBI-QEP semi-empirical method, we performed DFT calculations for a range of dissociation reactions in the context of WGS conversion and steam reforming at Rh(111) and Pt(111).

The theory-theory comparison revealed drastic deficiencies of the hybrid UBI-QEP approach as commonly employed in the literature, with predicted UBI-QEP barriers deviating partly by more than 100% from the reference value. By a systematic analysis of the implementation of the UBI-QEP semi-empirical method, we were able to find out the disagreement to be mainly related to two main reasons (detailed reported in Ref. [2]):

a) the semi-empirical method in its original formulation is completely blind with respect to the position of the TS

b) a thermodynamic inconsistency in the energy diagram arises when the semi-empirical method is parameterized with binding energies calculated according to different methods (e.g., DFT, as it is usually the case in the literature)

As for point a) we were able to prove by the DFT calculations performed at HLRB that the information on nature of the TS is established for many classes of reactions and can enter in the semi-empirical scheme by a tuning of the transition state parameter with selected first-principles calculations.

As for point b), we showed that a straightforward remedy is to simply shift the minimum energy path (MEP), such that its minimum coincides with the proper DFT binding energy.

On one hand this recovers the consistency of the derived activation barriers for the forward and backward reaction with all DFT thermochemistry references. Using this modified parameterization procedure we achieved a significant improvement of the UBI-QEP accuracy against the DFT reference. Considering the negligible computational cost involved in determining the UBI-QEP barriers this remaining uncertainty is perfectly acceptable. With no intention to be fully quantitative, such semi-empirical estimates for the barriers can provide most useful insight into complex reaction networks, where an exhaustive first-principles treatment is prohibitive. Here, the computationally undemanding barrier estimates may serve as initial approximate input for the identification of the prevalent reaction pathways, that require refined kinetic parameters from explicit first-principles calculations. This is the task that we have addressed in the second part of the project for the WGS and r-WGS systems on Rh.

2. Hierarchical multiscale analysis of the WGS and r-WGS reacting systems on Rh

In this work, accepted in Chemical Engineering Science [3], for the first time in the literature we have successfully combined semi-empirical methods and first-principles calculations through a hierarchical approach. In particular, we focused our analysis on the WGS and r-WGS experiments in an annular reactor. For the semi-empirical description of the microscale, we use the UBI-QEP microkinetic model of [4] within a 1D heterogeneous model of the annular reactor. Then, at the specific operating conditions of the experiments, we identified the dominant reaction mechanism through reaction path analysis (RPA) based on the actual species consumption rate. These dominant reaction pathways have been then refined with explicit DFT calculations.

The semi-empirical analysis predicted that for the WGS system, H_2O, upon adsorption on the catalyst, dissociates to OH and H. Then, CO adsorbs on the surface and converts to CO_2 through direct oxidation with OH. Water

dissociation turns out to be the rate-determining-step (RDS) of the reaction network, while all the other dominant steps turn out to be at partial equilibrium. This reveals an overall first order dependence with respect to H_2O and a kinetic independence from CO. For the r-WGS system, RPA showed that the same dominant pathways as in the WGS are followed in the reverse way. In particular, CO_2 converts to CO via reaction with H and the RDS is water formation. This leads to a complex kinetic dependence of the overall rate expression on H_2, CO_2 and CO. This is at variance with experiment, which reports a first order dependence with respect to H_2O and CO_2 for WGS and r-WGS, respectively. In particular, this implies that the RDS of the network cannot be water formation for r-WGS.

In order to understand the reasons behind this disagreement, we proceeded by scrutinizing **the identified dominant pathways** through explicit DFT calculations. For the reaction pathways that govern the CO oxidation via OH, this first-principles refinement performed with HLRB resources revealed that, contrary to what was included in the semi-empirical microkinetic model, the direct oxidation of CO by OH was not an elementary step. Thus, it cannot be considered as an alternative route to the carboxyl mechanism. This peculiar insight was only achieved by virtue of the first-principles analysis, as the semi-empirical UBI-QEP method used for the initial screening is blind with respect to the true nature of the transition state and cannot differentiate whether a reaction step is elementary or not. Following the results from the first-principles analysis we remove this non-elementary step from the full microkinetic model. In order to understand the effect of this modification we repeat the RPA for both WGS and r-WGS. As a result of the improved description of the micro-scale, WGS and r-WGS now follow different dominant reaction mechanisms under the investigated experimental conditions. Specifically, in WGS water activation is the RDS and CO converts to CO_2 through a carboxyl pathway. During r-WGS, instead, CO_2 converts to CO via decomposition to CO and O, skipping the carboxyl-pathway. Moreover, CO_2 decomposition turns out to be the RDS. These results lead to a clear first-order kinetic dependence on H_2O and CO_2 for WGS and r-WGS, respectively, and thus reconcile this new picture of the dominant mechanisms at the molecular level with the **all experimentally observed macroscopic reaction orders for WGS and r-WGS.**

On-going Research / Outlook

The methodology that we have developed and validated in these two years *through the granted CPU time* is of primary interest for the atomic scale understanding of complex chemical processes of real technological interest. In particular, for the case in point the obtained results furthermore underscored the danger of common first-principles analyses that focus on a priori selected dominant paths. Not restricted to such bias, our proposed hierarchical approach thus constitutes a very promising avenue to properly transport the *ab initio* predictive-quality to a new level of system complexity. Even though this approach alone represents already a re-

markable step forward with respect to the state-of-the-art microkinetic modeling, several issues still have to be addressed. Among them, very important features are the following:

1. assessment of the semi-empirical method with respect to structure sensitivity
2. assessment of the semi-empirical method with respect to non metallic surfaces (e.g., oxides)
3. extension of the validation of the procedure to more complex systems such as steam, dry reforming and methanation reactions.

Given the high computational costs connected, the aforementioned issues are tractable only on large and efficient computational infrastructures. Scaling properties are of paramount importance. In this respect, the extraordinary (almost linear) scaling properties of CASTEP on HLRB-II that we have experienced in these two years at HLRB-II computational infrastructure is a necessary requirement to achieve such important goals. For this reason, application for an extension of the project is planned.

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Reactivity of Cu/ZnO nanocatalysts for methanol synthesis

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Introduction

Methanol synthesis represents one of the landmarks of heterogeneous catalysis due to the great industrial significance of methanol as a clean liquid fuel and as a raw material for chemical industry. Heterogeneous catalysis, which represents the basis of the chemical industry, is closely linked with nanotechnology. By appropriately controlling, on the molecular scale, the matter at catalytic surfaces, it is possible to enhance the efficiency of catalytic processes in terms of energy consumption and turnover (selectivity). To optimize a catalyst, understanding the molecular processes which take place in the reaction environment is therefore of utmost importance.

Nowadays, the synthesis of methanol is performed industrially over a highly selective copper catalyst supported on zinc oxide (Cu/ZnO) at temperatures of 513-533 K and pressures of 5-10 Mpa. Minimizing the energy consumption requirements to activate this reaction is economically desirable. The interest in understanding methanol synthesis is reflected in the numerous studies involving this catalytic process, which have led to general consensus on the source of carbon being CO_2, and on Cu being the main active component. However, other aspects such as the reaction mechanism, the identity of the key intermediates, the nature of the active site, and the exact role of ZnO, remain under debate. Experiments suggest, on one hand, that ZnO plays a fundamental role in the creation of the active site, and on the other hand, that the redox properties of the gas phase strongly affect the redox state of the active site. These effects may be fundamental to maintaining catalytic activity on Cu/ZnO [Ref. 1 and references therein].

In the present study our initial goal is to understand the enhanced activity of Cu/ZnO catalysts on the atomistic scale. Therefore we employ *ab initio* electronic structure calculations based on density functional theory (DFT) in its efficient plane-wave basis-set and ultra-soft pseudo-potential approach as implemented in the Cpmd software package [2,3]. DFT based *ab initio* electronic structure calculations can predict with high accuracy the physical and chemical properties of surfaces, that in combination with the *ab initio* thermodynamics (AITD) formalism[4] allow for bridging the so-called materials pressure gap, i.e. environment dependent morphology and reactivity changes of the catalyst surface in contact with a reducing or oxidizing gas phase. After having identified all relevant catalyst surface models we focus on the exploration of the reaction network of methanol synthesis over Cu/ZnO by using the *ab initio* metadynamics sampling method in its extended Lagrangian formulation [4,5]. This procedure has been successfully introduced in the heterogeneous catalysis of methanol over bare ZnO[6] and represents a versatile tool for exploring the molecular and free energy landscapes.

Results

Similar to previous insight into strong metal-support interaction effects of Cu atoms, Cu monolayers, and thin films deposited onto ZnO O-terminated surfaces[6] we obtain a strong directional charge redistribution for our Cu/ZnO catalyst models, see Fig. 1 for an example structure

Fig. 1 PES of adsorption of CO_2 over three Cu/ZnO(oooī) slabs: 1/2H and 3/8H represent monolayers of H adsorbed and Zn-ad the ZnCu cluster alloy. Representative local energy minima structures of adsorption complexes employing Γ-point approximation. Atoms follow the colour code H (blue), O (red), C (cyan), Zn (grey) and Cu (green).

(representative of more than 50 structures investigated). Moreover, adjusting the partial pressures of O_2 and H_2 via AITD we find that the composition of the gas phase which is in contact with the catalyst surface gives rise to a heterogeneity of stable surface phases, i.e. differing shape of the nano catalyst and chemical composition (adsorption/desorption of hydrogen or oxygen). Interestingly, at conditions of the catalytic process a hydrogen covered Cu/ZnO surface is preferred while at this hydrogen rich gas phase an increase of the reducing power of the gas phase favours Cu/Zn alloying and oxygen desorption over other stabilization mechanisms. At these conditions we were able to locate three different phases of our model catalysts differing in their composition and the redox state.

We systematically explored their chemical reactivity using CO_2 as probe molecule over the catalyst surface and mapping the potential energy surface (PES) of adsorption, see Fig. 1. This exploration suggests a redox state and site dependent reactivity that can be directly controlled by sim-

Fig. 2 Free energy landscape and molecular species obtained from an explorative multiple walker ab initio metadynamics of the hydrogenation of CO along at the partially hydroxylated ZnO(000-1) surface hosting a F^0/H_2 oxygen vacancy.[6] Relative free energies ΔF (in eV) are provided according to the colour scale.

ply tuning the physical and chemical properties of the gas phase in contact with the Cu/ZnO catalyst. In the lower part of Fig. 1 we give a selection of configurations with CO_2 adsorbed on different sites of the Cu cluster and on the Cu-free catalyst support, with the latter being the preferred for all three models. The adsorption energies range between 30 and 100 kJ/mol, while CO_2 binds stronger on the reduced catalysts 1/2H and 3/8H in an oxygen rich environment than on Zn-ad present in oxygen poor conditions. The most stable of these structures represent an unbiased starting point to study further reactivity of CO_2 on our Cu/ZnO models in the framework of free energy calculations.

Prior the *ab initio* metadynamics sampling, the atomistic structures were equilibrated in the canonical ensemble (T=550 K) using standard Car-Parinello molecular dynamics (MD)[4]. With more than 160 atoms and using a 25 Ry plane wave energy cut-off, these calculations required 7 CPU-minutes per MD step on the HLRB-II (SGI ALTIX4700). A full metadynamics exploration for

one surface model would have had required ~350,000 proc·hours per surface structure and the metadynamics to resolve the minimum free energy paths (MFEP) approximately 250,000 proc hours per surface structure. However these calculations have been moved to the new petascale SuperMUC machine.

In regard to metadynamics simulations, there exist several levels of parallelization. First of all, any multiple walker metadynamics problem parallelizes intrinsically with respect to the number of replicas (walkers) of the total system. Walkers interact in building up the biasing potential and this interaction requires negligible communication effort. Therefore, on the multiple walker metadynamics level the parallelization is almost ideal, i.e. linear even on a Gigabit interconnect. For each individual walker, the Kohn-Sham equations of DFT have to be propagated in an extended Lagrangian scheme [4,5]. This computationally demanding part of the calculation is assigned to processor groups (PGr), which require a high bandwidth/low latency interconnect. Within a PGr, parallelization is realized via MPI for inter-node communication and either MPI or OpenMP/Vector processing for intra-node parallelization. Thus, this hierarchical parallelization strategy is highly adaptive and can be optimized for the individual platform. Cpmd has proven its efficiency for simulations of this type on a wide variety of platforms during the last decade including HLRB-II.

On-going Research / Outlook

Based on the in-depth understanding of the complex interplay of structural and electronic properties of our models acquired throughout our investigations, now we are performing *ab initio* metadynamics simulations. The on-going exploration of the reaction network of methanol synthesis on Cu/ZnO is being carried out on the new petascale SuperMUC machine employing metadynamics sampling and for the three different catalyst models corresponding to the herein obtained environmental conditions of the heterogeneous catalytic process of methanol synthesis.

After having identified the relevant intermediates of the three reaction networks, the exploration will be refined with the MFEP of the reaction channels that finally lead us to a complete picture of the catalytic process.

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Structures and processes at metal-liquid interfaces

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Introduction

The water–metal interface is of significant interest not only from a fundamental but also from an applied point of view, as in the context of corrosion and catalysis. This is particularly true in electrochemistry, which has attracted a lot of attention recently due to its relevance in hydrogen production and energy storage and conversion, as realized for example in fuel cells. At the same time, modern electrochemistry is becoming increasingly concerned with the development of an atomistic understanding of electrochemical processes. In spite of the complexity of electrochemical interfaces, theoretical studies can contribute significantly to the progress in this field in a similar way this has already happened in the related field of surface science. In particular, electronic structure calculations based on density functional theory (DFT) calculations can nowadays describe in considerable detail the structures of complex interfaces.

While it is of course important to determine the energetically most stable structure of water on metal substrates, in most applications, the metal–water interface under ambient conditions is of interest, i.e. at temperatures around room temperature. For a reasonably good treatment of water-metal interaction, it is advantageous to use ab initio molecular dynamics (AIMD) simulations, wherein the forces necessary to integrate the classical equations of motion are determined 'on the fly' through DFT.

In spite of the numerous studies on the subject of metal-liquid interfaces, there is still a number of gaps that needs to be filled. For example, up until now, little attention has been paid to the fact that under electrochemical conditions and low potentials, the platinum electrode is covered by hydrogen. In the following section we discuss how this fact changes our perception of how water behaves near a platinum electrode, as well as some recent results on understanding water structure on metal surfaces with step defects, bringing us closer to real electrochemical environments.

Results

Water structure on hydrogen-covered electrodes
There is still some disagreement between experiment and theory regarding the hydrogen equilibrium coverage: whereas experiments indicate that at 0 V relative to the normal hydrogen electrode the hydrogen coverage should be about 0.66 monolayer (ML), density functional theory calculations yield a hydrogen coverage of 1 ML. Still, there is a qualitative agreement that there is significant hydrogen coverage, and it is very likely that the presence of these adsorbed species has a profound influence on the structure of the electrode-electrolyte interfaces and on the processes occurring at these interfaces.

We have performed ab initio molecular dynamics simulations to study the structure of water layers on clean and hydrogen-covered Pt(111) electrodes at room temperature. In addition to Pt(111) covered with one monolayer of hydrogen, also hydrogen-covered Pt(111) with a hydrogen vacancy and with one additional hydrogen atom per surface unit cell were considered. The typical structure of a water/H/Pt system is shown in Fig. 1. A quick inspection shows clear signs of disorder in the water bilayers. In order to make a more quantitative description of the disorder in these systems, we have calculated distribution functions of some relevant structural parameters of the first water bilayer in order to more clearly see the extent to which the water bilayer is disordered, through the following parameters:

(1) Planar deviation. The distances of oxygen atoms of the ordered water structure are practically the same all throughout the bilayer. Thermal disorder is measured here as the extent to which oxygen atoms deviate from this planar arrangement.
(2) Hexagonal structure deviation. The angle formed by any three adjacent oxygen atoms in the ordered water structure is almost exactly 120°, and so a honeycomb network of perfect hexagons is one of the most obvious characteristics of the ordered water bilayer. Disorder is measured here as the extent to which O-O-O angles deviate from 120°.

Figure 1. Analyzing the structure of water at the metal-water interface. Clockwise, from top-left: planar deviation, hexagonal structure deviation, orientational inhomogeneity. Surface-adsorbed hydrogen is drawn in yellow.

Figure 2. Snapshots showing proton transfer. The weakly-adsorbed hydrogen atom is shown in brilliant yellow in order to distinguish it from the rest of the hydrogen atoms covering the platinum surface. (a)-(b) transfer from the Pt surface to the interface water; (c)-(f) proton transfer within water molecules.

(3) Orientational inhomogeneity. The two criteria mentioned above refer to disorder observable through the relative positions of water molecules in three-dimensional space. Here, disorder is measured by the orientations of water molecules with respect to the surface and with respect to each other.
(4) O-H bonding. It is interesting to examine what effect the hydrogen cover has on the OH bonds on the nearest water layer. In particular, proton transfer events at the metal-water interface and within the water molecule network are examined.

We find that in the presence of a hydrogen layer on Pt(111), the distance of the water molecules from the metal atoms is increased by more than 1 Å compared to clean Pt(111) indicative of a weakened water-electrode interaction [1]. All considered water bilayers on clean and hydrogen-covered Pt(111) are more disordered than ice, although far from the liquid state.

Surprisingly, a stronger order in the water bilayer on hydrogen-covered Pt(111) in terms of maintaining the honeycomb structure and orientational homogeneity has been found. At room temperature, one would expect less strongly-bound water layers on the metal surface to be more liquid-like, i.e., to have greater disorder, because the water molecules are free to move beyond the periodic constraints of the surface.

It is thus surprising to find more order for the case of water on hydrogen-covered Pt(111). One may argue that the stronger order in the water layer is attributable to the coordination of the water bilayer with the hydrogen cover through long-range hydrogen bonds, given the fact that the hydrogen atoms of the full monolayer do not leave the fcc hollow sites. This explanation is however unapt given that the creation of hydrogen bonds does not lead to greater separation between bonding species, not to

mention the fact that the surface-bound hydrogen atoms are not static and do vibrate within the immediate vicinity of the fcc hollow site. The opposite result is attributed to the fact that the presence of the hydrogen layer weakens the interaction of the water with the surface, and the resulting stronger water-water interaction promotes the unexpected order in the water bilayer. This is consistent with the fact that hydrogen bonding is highly orientational.

Proton transfer events were observed only in the molecular dynamics run with a 13/12 ML hydrogen cover in between platinum and water (Fig. 2). In panel (b) we can see that the top-site adsorbed hydrogen atom moves up to the water layer, as the receiving water molecule prepares to transfer one of its hydrogen atoms to a neighboring water molecule. A series of transfers of hydrogen atoms within the water bilayer is observed, jumpstarted by the initial transfer of hydrogen from the platinum surface.

The weakly bound hydrogen adatom is found to be transferred to the water layer during the 11 ps run time of the AIMD simulations, leading to the formation of hydronium complexes. This suggests that the opd hydrogen on Pt(111) is in a dynamical equilibrium with protons in the water. Aside from the close proximity of the top-site adsorbed opd hydrogen to the water layers, it is also less strongly bound to the platinum surface. In contrast to this loosely bound hydrogen, the rest of the hydrogen cover is relatively intact. Within the limited run time of the molecular dynamics performed, no fcc-bound hydrogen atom was observed to hop out of the fcc threefold-hollow sites.

Proton transfer, while shown to occur, is found to be a relatively rare event if one is to look at all O-H bonds in the water layer. Our results also suggest that proton transfer/exchange in the Pt-water interface is not very likely to occur for hydrogen coverages $\theta \leq 1$ ML.

Water structure on stepped surfaces
Stepped surfaces are particularly interesting as these are present in any realistic surface and often exhibit specific electronic and chemical properties. Recently, vibrational

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spectra of water adsorbed on Au(100), Au(511) and Au(11 11) were measured at low temperatures (140K) using electron energy loss spectrometry (EELS) by H. Ibach [2]. This work was motivated by the observed large reduction in the Helmholtz capacitance or inner-layer capacitance on stepped gold and silver surfaces. Three different structural models for a water layer on Au(511) were proposed, but a final assessment of the true water structure solely based on the vibrational spectra could not be made.

Figure 3. Calculated vibrational spectra of the water layer on Au(100) and Au(511). Experimentally observed modes are indicated by dashed lines.

The structural, electronic and vibrational properties of a water layer on Au(100) and Au(511) were studied by first principles total-energy calculations and ab initio molecular dynamics simulations [3]. On Au(100), it was found that a structural model based on a (2×2)surface unit cell is not realistic.

The most stable structures on Au(100) and Au(511) surface were obtained. From the vibrational spectra of the simulation, several fundamental aspects have been observed. On the Au(100) surface, the OH stretching mode can be found at 3500 cm^{-1} and the non-hydrogen-bonded (NHB) hydrogen stretching mode disappeared, which was caused by the weak reaction between water layers and the Au(100) surface. On the Au(511) surface, three peaks can be found around 3500 cm^{-1} (3300 cm^{-1}, 3500 cm^{-1} and 3600 cm^{-1}), in which the division of two hydrogen-bonded (HB) hydrogen stretching modes might be caused by the influence of the step edge. The simulation results, both the positions and the relative intensity of the peaks agree with the experimental data quite well. AIMD results show that at 141 K on Au(100) the rectangular structure is thermodynamically not stable and on Au(511) the structure we obtained is quite stable. And the charge density difference shows a rather localized and strong polarization at the step edge on Au(511). All of the phenomena indicate a strong reaction between the step edge and the water layer, and rather different electronic properties compared with the flat gold surface.

On-going Research / Outlook

The surface of metal electrodes often contain specifically adsorbed ions such as chlorine coming from the electrolyte environment, and these adsorbed species substantially modify the work function of the metal surface. We show that this phenomenon is not just due to charge transfer alone, but also largely due to the polarization on the adsorbed species. More importantly, we are interested in how the presence of these adsorbed ions affects the water structure at the interface, and on its implications on the electrode potential. Along these lines we are also looking at processes at the solid/electrolyte interface under potential control, particularly on describing the electrocatalytic oxidation of methanol.

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Computational Fluid Dynamics

Interactive Thermal Comfort Assessment Simulations

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Introduction

In modern design and planning processes of large buildings, thermal comfort assessment is mandatory. On the one hand, there is the indoor assessment related to the comfort of people staying inside buildings, on the other hand there is the outdoor assessment related to the impact of heat and pollutant emissions of buildings to the environment. Both assessments should be done in very early design stages as economic savings have the highest potential in this phase due to the possibility of changing design steps easily. Necessary simulations have to be carried out on very different scales (from very small, i.e. local, to very large, i.e. global, effects) and, thus, entail an enormous demand for computing performance as provided by the world's largest supercomputers.

Furthermore, there is strong need for interactive computing or computational steering, i.e. carrying out the simulations in real-time and allowing users interactively to visualise the simulation results and manipulate the scenario/setup, in order to optimise the design process and minimise the costs. Unfortunately, interactive computing and high-performance computing are still a contradiction and, thus, demand for special approaches and sophisticated methodologies in order to bridge the gap between computational steering and supercomputing.

Figure 1: BREP geometry of a power plant containing more than 12 million triangles

Results

For performing thermal comfort assessment, we apply computational-fluid dynamics simulations on varying scales using the Lattice-Boltzmann method. Unlike the classical method using the Navier-Stokes equations, the Lattice-Boltzmann method (LBM) is based on concepts of statistical physics. For the LBM code developed by our group, we use a first order finite difference approach in space and time resulting in a quite simple scheme

regarding implementation and parallelisation. For additional numerical stability of the method, a multiple-relaxation-time model based on d'Humières [1] was used and the simulation of convective airflows was achieved by using the hybrid thermal model proposed by Lallemand and Luo [2].

As input data for this LBM code, a voxel-based structure containing information about boundary conditions is necessary. Based on a hierarchical representation, we benefit from the spatial decomposition of an octree structure for the discretisation of the corresponding domain and all included geometric information – ranging from whole buildings down to small details or the interior of single rooms (furniture) – as any desired level-of-detail is easily to be achieved. Due to the necessity that our code requires an equidistant discretisation, all voxels have to be refined until a certain mesh width. An analysis regarding the parallel performance of our code and the influence of different discretisation widths can be found in [3]. Figures 2a, 2b show the results of simulation runs for a highly detailed power plant model (Fig. 1) on different scales.

To evaluate the efficiency of the code, several scalability studies have been performed on the HLRB2. Figure 3 summarises a strong speedup analysis for different discretisation sizes of the above geometry. Small sizes obviously result to a bad CCR and, thus, hinder good scalability values.

Figure 2b: simulation results on a small scale of the power plant model using the same resolution (i.e. amount of degrees of freedom) as on the large scale in order to investigate physical properties in detail

Figure 3: strong speedup analysis for different domain sizes performed on the HLRB2 (see [3])

Figure 2a: simulation results on a large scale of the power plant model in order to investigate pollutant emissions to the surrounding environment

In order to assess the thermal comfort on a local scale, such as in a room e.g., one approach is to apply empirical relations stated in norms. In Fig. 4, local surrounding temperatures resulting from the LBM code are mapped to a dummy's surface (i.e. numerical manikin) and thermal comfort can directly be assessed by applying well established relations. A more complicated but far more accurate approach would be to couple the LBM code to a human thermoregulation model such as Fiala's model [4]. Due to a bidirectional coupling, boundary conditions from the room influence the manikin and the manikin delivers new boundary conditions for the thermal solver.

Here, computational steering can help to identify setups with better comfort behaviour (small scale) or less impact on surroundings (large scale) on-the-fly, i.e. without separate batch computing and visual post-processing. Users can manipulate the scenario (geometry and boundary conditions) during runtime in order to get an immediate feedback by the running simulation; hence there is a di-

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Figure 4: numerical manikin simulation in an enclosed room - the LBM code computes the domain under natural convection boundary conditions with the manikin as heat source; a thermal analysis can now be coupled to this simulation assessing the thermal comfort in the room

rect relation between cause and effect. Nevertheless, this requires the simulation to run in an interactive instead in batch mode, which is not always supported by supercomputer systems. One possibility though to combine interactive computing and HPC is to run 'small' simulations, i.e. with reduced accuracy, on small interactive cluster systems for a quantitative analysis, before any promising setup figured out by the user is then (automatically) launched as batch job with high accuracy for a qualitative analysis on a supercomputing system as proposed in [5].

On-going Research / Outlook

This work is continued in cooperation with projects financed by the Munich Centre of Advanced Computing (MAC@IGSSE), Technische Universität München, and the King Abdullah University of Science and Technology (KAUST), Saudi Arabia.

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Investigation of the drag reduction capabilities of oscillating riblets

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HLRB Project ID: h1061

Introduction

One important contribution to the energy consumption of pipes and transportation systems like ships, trains and aircrafts is the fluid drag. Depending on the application, the drag may originate mostly from friction or mostly from pressure drag. A pipeline for example spends nearly 100% of its pumping energy to overcome the friction drag. The main purpose of this study is to reduce the turbulent friction drag which is an important step to reduce energy consumption in many applications.

Figure 1: Vortex structures (iso-surfaces of the q-criterion) above a riblet surface (left) and a smooth wall (right).

Figure 2: Sketch of the tilting mechanism.
Lamellas are stiff, and synchronized in their movement.

Background

The discovery that shark skin can reduce the friction drag led to the development of "riblets". Such a riblet structure is a grooved surface being aligned with the main flow. So far, the most effective riblet shape achieved up to 10% drag reduction. An example of such a surface is given in figure 1 along with a snapshot of the near wall vortex structures. The main flow is in x-direction that extends graphically from the lower left to the upper right corner. These vortices are responsible for transporting fast fluid to the wall which increases the drag. The riblets (left) constrain and attenuate this kind of vortices compared to the smooth surface (right). The trade-off is an increase of the wetted area which reduces the benefit.

More recently, simulations and subsequent experiments reported a different technique which achieves up to 50% drag reduction by oscillating a smooth wall laterally to the flow. In contrast to riblets, it is an active method which itself consumes energy. As can be shown theoretically, most of the induced oscillation is dissipated right above the wall which reduces the efficiency.

Approach

The present project is about the combination of riblets and the oscillating wall trying to exploit their individual advantages. Therefore, a simple and effective riblet structure is used to impose a lateral oscillation on the flow. The riblets are modelled by lamellas with a specific height and spacing for which a very good performance has been shown. These lamellas are tilted sinusoidally in time up to a maximum deflection angle of 30° as demonstrated in figure 2. They are stiff, and the tilting mechanism is synchronized among all lamellas. It is assumed that at a certain distance from the wall this mechanism needs less energy to achieve a similar fluid oscillation than the oscillating wall because the riblet tips are deeper in the channel and closer to the vortical structures. The present study focuses on the oscillation period T^+ (being the reciprocal of the frequency) as the main parameter. In addi-

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Figure 3: Drag change in percent to a smooth reference wall during the first half of an oscillation period.

Figure 4: Riblet segment with contours of the phase averaged stream-wise velocity: blue – low velocity; yellow – high velocity. Main flow direction is into the plane. Thick black lines represent the wall and the lamellas. Arrows indicate the secondary motion.

tion to the already mentioned optimal riblet shape, three other riblet shapes were investigated but only at a few oscillation periods.

Computations

The investigation is performed using a Direct Numerical Simulation without the need for a turbulence model. Such simulations are extremely precise which is necessary to capture the important flow features of the turbulence above the riblet structure. On the other hand, they are much more exhaustive in terms of computing power and storage demands.

The flow solver is an in-house code that is used successfully across many projects since many years. A steady development and adaption process assures its suitability for actual and future HPC environments. It discretizes the computational domain by Finite Volumes on a collocated grid and solves the incompressible Navier-Stokes-Equations implicitly in time.

The simulations are performed in a channel at a Reynolds number of 180, based on the wall shear velocity and half of the channel height. The Reynolds number based on the mean velocity and channel height is approximately 5700.

The proposed mechanism depends on many parameters where each should be investigated separately, leading to a very high demand of computing power. But the actual limitation of computing time restricted the present investigation to a few parameter sets.

Results

From a total of 26 parameter sets, the best case improved the drag reduction by approximately 1.5 percentage points compared to the static riblet reference. It must be noted that many promising parameters were not included in the investigation due to computing power limita-

tions. It is likely that the result could still be improved if for example the maximum angle was increased. Moreover, the variation of the riblet height and spacing has shown a large influence, but only four shapes were examined.

The phase averaged drag change distributed over the first half of the oscillation period is shown in figure 3 where negative values correspond to better drag reduction. The second half period is not shown here since it is symmetric to the first one. The graph reveals a strong variation of 10 percentage points between a minimum of -15.3 and a maximum of -5.3%. The favourable minimum is located at the time when the lamellas are at their maximum deflection whereas the maximum is found when the lamellas are in upright position. The reason is that the lamellas descent into slower fluid generating less drag. But when they emerge they move into faster fluid that accelerated during the time of the descent. However, the success of a parameter set depends on the average level of the drag oscillation. This level is a result of the whole system of the actuation and the interaction with the turbulent structures above the riblets.

The contours in figure 4 represent the phase averaged stream-wise velocity at maximum deflection. The data is taken from the most effective case being run at $T^+ = 25$. The flow in the riblet groove is very slow as indicated by the blue colour, and rapidly increasing along with the wall distance. The white arrows represent the phase averaged velocity in the wall-normal and the lateral direction. Hence, they visualise the induced oscillation and its propagation into the channel. As already pointed out, the oscillation induced by the oscillating wall decays rapidly with increasing wall-distance. The same behaviour can be observed for the oscillating lamellas but shifted by their height.

The principle of inducing lateral motion and an improved drag reduction of approx. 1.5 percentage points by oscil-

lating riblets could be demonstrated. But the applicability of the concept is limited because in addition to the manufacturing issues, the energy spent for the actuation was not taken into account.

On-going Research

At present, studies on a mechanism of inducing lateral oscillation passively by using a wavy riblet design are in progress [2]. The riblets are displaced in stream-wise direction sinusoidally and thus forcing the flow to follow the oscillation. This method allows a larger fluid displacement than the actively driven lamellas, decouples the oscillation period from the displacement velocity, and allows using riblet geometries that are easy to manufacture.

In this study, the parameter space is even larger and the size of the computational domain is increased by at least six times. Simulations of such a size would not have been possible on the HLRB2.

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Direct Numerical Simulation of Turbulent Flows with Microstructure

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Introduction

In this report, we present the methodology and some selected results of the Direct Numerical Simulation (DNS) of drag reduction by rigid fibers in a turbulent channel flow. The drag reducing property of polymer additives in turbulent flows, i.e. the Toms effect, has been known since 1948. It has been found that fibers and surfactants can have similar effects. Because of its enormous technological importance a lot of efforts have been made to understand the physics behind this effect. These efforts include theoretical, experimental and numerical investigations. The main problem that hinders a full understanding of the effect arises from the complicated interaction between the flow of the solvent and the suspended additives. The additives are in most cases much smaller than the smallest eddies of the flow, i.e. the Kolmogorov length scale. In this respect, the flow can be considered as the *macrostructure* and the additives can be considered as the *microstructure* of the suspension.

The drag reducing effect arises in very dilute suspensions such that the direct effect of the additives can hardly been measured. In experiments it becomes visible as a so-called *stress deficit* which means that there are stresses in the turbulent flow that can not be directly measured. These are the time average of the non-Newtonian stresses from the additives. However, these time averaged stresses do not contribute to drag reduction. Instead, drag reduction is considered to be the result of the interaction of instantaneous non-Newtonian stresses with the strain field of the turbulent flow. These interactions lead to a modification of the turbulence structure, i.e. a damping of some fluctuation components and an amplification of others. Many open questions are unanswered at this time. The simulations described herein aim to clarify some of the hypotheses raised in the context of drag reduction by fibers.

Numerical investigation of this phenomenon has only recently become feasible. One has to bear in mind the complicated interaction between the micro- and the macrostructure. This can be in general formulated by first principles. However, the large number of degrees of freedom hinders a direct solution of the whole problem. Simplifications have been introduced to make numerical simulations feasible. One-way interaction is able to access the dynamics of very dilute suspensions without modifying the turbulent flow field [1]. The use of moment closures allows for directly formulating transport equations for the non-Newtonian stress field. These moment closures have been partly successful in predicting drag reduction [2], however, they neither can render the complete picture of the process nor they can give quantitative prediction of drag reduction in real configurations.

In this work, we present a two-way coupled direct Monte-Carlo simulation strategy which is applicable to weakly Brownian and even non-Brownian fibers for which the drag reduction is maximum. The turbulent flow field is computed using the DNS in an Eulerian framework. The fibers are treated in a Lagrangian framework. The Eulerian-Lagrangian two-way coupled simulation is presented in the following.

Governing equations

The isothermal, incompressible, turbulent flow of a non-Newtonian fluid is governed by the Navier-Stokes equations in which a term is added representing the non-Newtonian stresses by the fibers. The non-Newtonian stress tensor is to be computed using a rheological model. In this work, the theory of Brenner is used involving the second and fourth moments of the orientation distribution function (ODF) of the fibers [4]. As the fibers can generally be very small, they are subject of Brownian rotary motion which tends to smoothen the ODF. The ODF follows a Fokker-Planck equation describing the evolution of the probability to find a fiber at a specific orientation.

Numerical method

The non-Newtonian Navier-Stokes equations are integrated in time using a finite volume method and a third-order Runge-Kutta scheme. To compute the ODF of the fibers, we employ a Monte-Carlo method [1]. This means that we compute an ensemble of individual (sampling)

Newtonian   Non-Newtonian/Fibrous

Figure 1: Fluctuations of the streamwise velocity component in a wall-parallel plane. Newtonian flow (top) and non-Newtonian flow (bottom).

fibers according to the Jeffery equation which describes the orientation of a fiber in reaction to the strain and rotation tensors of the local flow and a stochastic term representing the rotary Brownian motion. By doing this, the moments of the ODF can be obtained by ensemble averaging. The ensembles are transported on Lagrangian paths. An Eulerian grid would not be able to represent the sharp gradients in the stress field that arise from the fact that the fibers have vanishing spatial diffusion.

Simulation

The drag reduction in a suspension of fibres with respect to a Newtonian fluid is investigated by DNS for the case of turbulent flow between two infinitely extended parallel plates, i.e. a turbulent channel flow. The domain size and the grid are given in table 1. After the flow is fully developed, we introduce the fibers. The fiber parameters are given in table 2. After the introduction of fibers, the flow undergoes a transient mode, in which the bulk velocity increases and a drag-reduced state is reached. Once the flow reached the new equilibrium state, we continue the simulation for some time to collect flow statistics.

L_x	L_y	L_z	N_x	N_y	N_z
$3\pi h$	$2\pi h$	$2h$	128	128	128

Table 1: Domain size and number of grid points

Aspect Ratio	Concentration	# of simulated fibers
100	$nL^3=18$	6.55×10^9

Table 2: Fiber parameters

Note the large number of individual fibers which is required to obtain a smooth representation of the non-Newtonian stress field. The fibers are transported along Lagrangian paths. One of the main numerical tasks in these simulations is the interpolation between Eulerian grid, on which the flow is represented, and the Lagrangian points on which the fibres are located. On each Lagrangian path, 100 individual fibers are solved that give a sample in the stress field.

This simulation is conducted on 128 processing elements of the HLRB2 supercomputer (SGI-Altix). Since the suspended particles (fibers) are the bottleneck of the simulation, the parallelization is done over the fibers. It means that each CPU performs a full simulation of the flow field plus a por-

tion of the particles. After each time step, the non-Newtonian stress due to the fibers is averaged over all CPU's which is achieved by a global communication step. We have achieved about 24 CPU-seconds per time step.

Results

Here, we present some of the results from our simulations. The drag reduction is seen as an increase in the bulk velocity under the action of a constant pressure gradient which drives the flow. The modification of the turbulence structure by the fibers is demonstrated by the fluctuations of the streamwise velocity component, plotted in a wall-parallel plane in Figure 2. The Newtonian flow, i.e. the one without fibers, renders a so-called streaky structure at well defined spatial scales. These structures are considered as the main turbulent structures responsible for the generation cycle of wall turbulence. Although the concentration of the fibers is in the ppm-range, the non-Newtonian flow is smoother and the streak spacing is larger. This goes in hand with a higher anisotropy of the turbulent fluctuations that – as a result – are less effective in generating turbulent stresses. The net effect of the drag reduction results from a balance between the reduction of turbulent stresses and the appearance of non-Newtonian stresses (due to the fibers). The correct prediction of which is crucial to the prediction of the amount of drag reduction. Figure 3 shows that none of the moment closures presented to date can reach the accuracy of the microscopic approach presented herein.

Figure 2: Non-Newtonian stresses. N1: first normal stress difference; N2: second normal stress difference. Lines with symbols: moment closure; lines without symbols: Monte-Carlo simulation.

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Interaction between turbulence and radiative heat transfer in a supersonic channel flow

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Introduction

In turbulent gaseous combustion, radiative heat transfer often plays an important role besides heat transfer by conduction and convection. Thermal radiation in a gas is a phenomenon of much longer range than convection and conduction. Hence, an integro-differential equation is required to predict the directionally dependent radiative heat transfer in an emitting/absorbing gas. Also, radiative properties of gases depend strongly on frequency/wavenumber of radiation. Therefore computation of turbulent flows including radiation effects is prohibitively expensive and effects of radiative heat transfer are frequently predicted using simplified models or even neglected in situations where they might be important. Coelho(2007) provides an extensive overview of current understanding of turbulence- radiation interaction (TRI) and its modelling in reactive low Mach number flows. Among the many interesting issues discussed in this overview, two aspects of TRI may be quoted here, namely, the influence of heat radiation on the flow and species concentration fields on the one hand, and the effect of the fluctuating species and temperature fields on radiation on the other. While most work on TRI has been devoted to the influence of turbulence on radiation, little work has concentrated on the question of how radiation affects turbulence variables. It is the aim of this work to focus especially on the behaviour of the turbulence structure under the influence of thermal radiation in inert, compressible, wall-bounded shear layers using Large-eddy simulations (LES).

Computational details

The flow configuration chosen in this study is a minimal channel with dimensions 3.5Hx 2Hx 1.35H in streamwise, wall-normal and spanwise directions, in order to keep the computational costs reasonable (2H is the distance between the channel walls). The compressible Navier-Stokes equations are solved in a pressure-velocity-temperature form using a 6th order compact central finite difference scheme. Explicit filtering based on the approximate deconvolution method is used for LES. Water vapour is chosen as the emitting/absorbing gas. Computations are also done using a fictitious gray gas to increase the optical thickness of the system artificially and the results obtained are compared to those with water vapour as the medium. The bulk Reynolds and Mach numbers of the flow are about 16000 and 1.26 respectively. The radiative heat transfer equation is solved using the Discrete Ordinates Method (DOM) and the spectral radiative properties of water vapour are modelled using the Statistical narrow band correlated-k (SNB-cK) model. The flow and radiation solvers are coupled using MPI routines so that the radiation code receives pressure and temperature from the flow solver and returns the radiative source term to the transport equation for the temperature in the flow solver. The walls of the channel are kept at 1000K and are treated as black surfaces. Fully reflecting boundary conditions are used in the periodic directions for the radiative transfer equation. Subgrid scale emission and absorption are neglected in this study. A coupled simulation with water vapour as the working fluid based on the SNB-cK model used 96 processors on Altix 4700 and the computational time was 276480 cpuh.

Results

We will now present results from the computations with water vapour as the working fluid. As seen in Fig. 1, the

Fig.1: Mean Temperature in Kelvin versus wall-normal coordinate. Solid line: without radiation, dashed line: with radiation.

effect of thermal radiation is to decrease the mean temperature in the channel core compared to its value when radiation is turned off. The near-wall rise in mean temperature from 1000 K at the wall to 1190 K in the core region is due to kinetic energy dissipation. As a result of emission and absorption of radiated heat between the channel centreline and the wall, the temperature in the core is reduced by about 20 K. Consequently, the mean density falls off more gently from its wall value, has higher amplitudes in the core region and varies inversely with the mean temperature, since the variation of mean pressure in the channel is minimal. In Fig. 2 we see that the near-wall peak value of the streamwise Reynolds stress is reduced due to radiation. Thus, radiation counteracts the effects of compressibility in a channel flow since it is known that the peak value of streamwise Reynolds stress increases with Mach number for a given Reynolds number. Subtle effects of radiation on the streamwise Reynolds stress is observed away from the wall, as well. Fig. 3 shows that the near-wall peak in the streamwise pressure-strain correlation is increased because of radiation, an effect which is again opposite to that of compressibility. Using a fictitious gray gas as the working fluid, we have obtained stronger but similar effects of radiation on the mean temperature, density profiles as also on the turbulence structure confirming the trends presented here (see Ref. [2]).

Conclusions and Outlook

The present study shows that the effects of radiation on the turbulence structure are noticeable even in non-reacting flows provided the optical thickness of the system is non-negligible. Effects of radiation seem to counteract those due to compressibility in supersonic channel flows and these insights should be useful for further development of second-order turbulence models.

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Fig. 2: Streamwise Reynolds stress (normalized with wall shear stress) versus semi-local wall-normal coordinate. Solid line: without radiation, dashed line: with radiation.

Fig. 3: Streamwise pressure-strain correlation (scaled with wall shear stress squared divided by mean viscosity) versus semi-local wall-normal coordinate. Solid line: without radiation, dashed line: with radiation.

DNS of Laminar Heat Transfer affected by Free-Stream Turbulence

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Introduction

In a jet engine the hot exhaust gases of the combustor drive the high and low pressure turbines which power the fan and compressor stages. The high turbulence level of the exhaust gases was found to significantly affect the thermal loading of the turbine blades even in regions where the boundary layer flow remained laminar. In experiments it was observed that the heat transfer in regions of accelerating flow where the blade's boundary layer is laminar (laminar heat transfer) increases with increasing turbulence intensity and decreasing turbulence length-scale [1]. To explain the physical mechanisms involved, it was decided to perform direct numerical simulations (DNS) of heat transfer from a heated flat plate in the presence of an accelerating turbulent flow and DNS of heat transfer from the stagnation region of a heated cylinder affected by an impinging turbulent wake.

Results

The numerical simulations of the three-dimensional incompressible Navier-Stokes equations were performed using a slightly adapted version of the LESOCC code developed at the Institute of Hydromechanics of KIT in Karlsruhe. The code is able to solve flow problems defined on curvi-linear meshes. It uses a collocated variable arrangement with momentum interpolation to avoid a decoupling of the velocity and the pressure fields. Second-order central discretisations were used for the spatial derivatives, while a three-stage Runge-Kutta method was used for the time-integration. The Poisson equation for the pressure was solved using the strongly implicit SIP solver of Stone [2]. For the heat transfer a convection-diffusion equation for the temperature was solved using a second-order accurate central discretisation. The Prandtl number was chosen to be Pr=0.71. The code was parallelised using the standard Message Passing Interface (MPI) protocol. The computational domain was divided into a number of blocks of equal size which were assigned their own processing core to achieve a near-optimal load balancing.

Laminar heat transfer from a heated flat plate

In the first set of simulations [3] a flat plate was heated to a fixed temperature of $T=T_0$ while the oncoming turbulent flow had a temperature of $T=0.7T_0$. The main flow was forced to accelerate by the presence of a free-slip converging wall which gradually decreases the downstream cross sectional area by a factor of 4. The flat plate is modelled using a no-slip boundary condition at the bottom of the computational domain and periodic boundary conditions in the spanwise direction. As shown in Fig. 1, at the inflow plane a steady flow field (u_b/U,0,0) was prescribed, where U is the mean free-stream velocity and ub corresponds to the x-velocity of a laminar Blasius boundary layer profile with thickness 0.04L. On this profile free-stream turbulence (u',v',w') was superimposed that originated from a snapshot of a simulation of isotropic turbulence in a box. The Reynolds number, $\mathrm{Re} = \frac{UL}{\nu}$ of the flat plate simulation, based on the mean free-stream inlet velocity U, the length-scale L (see Figure 1) and the kinematic viscosity n is Re=80,000.

In one of the simulations no free-stream turbulence was superposed on the Blasius profile. In this quasi two-dimensional (2D) base-line simulation the spanwise size was reduced to $\Delta z=0.0003L$ and it was resolved using only 4 grid points. In the streamwise (x) and wall-normal (y) directions 902 x 294 grid points were employed. For the 3D simulations a grid refinement study was carried out in the presence of free-stream turbulence with an intensity of Tu=5% and an integral length-scale of Λ=0.0415L. The spanwise size was set to 0.7L and the total number of grid points ranged from 67.9 to 912.3 Million. The number of processing cores needed to perform these simulations ranged from 64 to 504.

Inside the boundary layer of the simulations with free-stream turbulence a strong correlation was observed

Figure 1: Computational domain for the heated flat plate simulation with incoming grid turbulence

Figure 2: Instantaneous temperature in a cross section of the flat plate boundary layer. The vectors correspond to the instantaneous cross-stream velocity field.

Figure 3: Computational domain of the simulation with a heated cylinder and an incoming wake.

between the streamwise velocity fluctuations u′/U and the instantaneous temperature T/T_0: High values of T/T_0 were consistently found to correspond to low-speed streaks where u′/U < 0, while low values corresponded to high-speed streaks where u′/U > 0. This is exactly what was expected to happen as low-speed streaks contain relatively hot fluid from near the heated flat plate that moved upwards owing to impinging free-stream fluctuations, while high-speed streaks contain relatively cold fluid from the top of the boundary layer that moved downwards.

Because of the accelerating flow, the axes of the free-stream vortices tend to align more and more with the direction of flow. The cross-section through the boundary layer shown in Fig. 2 shows the upward convection of hot fluid on one side of each rotating structure and the downward convection of cold fluid from the free-stream on the other side.

Laminar heat transfer in the stagnation region of a heated cylinder

In the second set of direct numerical simulations [4] the augmentation of laminar heat transfer by a turbulent wake impinging on the stagnation region of a circular cylinder was studied. As illustrated in Fig. 3, the cylinder wall was heated to a constant temperature of $T=T_0$ and was cooled by the oncoming flow with a temperature of $T=0.7T_0$. In the circumferential and the spanwise directions periodic boundary conditions were employed while at the cylinder wall a no-slip boundary condition was prescribed. The spanwise size was set to Δz = 2D. At the top and bottom of the computational domain free-slip boundary conditions for the velocity were combined with an adiabatic boundary condition for the temperature. At the outlet a convective outflow boundary condition was used. At the inlet a uniform flow (1,0,0)U was used, where U is the mean inflow velocity. In one of the simulations an incoming turbulent near wake was introduced at the inlet. The wake data were gathered in a separate DNS of flow around a circular cylinder [5]. The Reynolds number of this flow problem, based on the free-stream velocity and the diameter of the cylinder, was Re=13,200. Up to 338 Million grid points and 480 processing cores were used to do the simulations.

To be able to assess the increase in heat transfer caused by the presence of the incoming wake base-line simulations were performed. In one the inflow was assumed to be uniform, while in another one a velocity deficit was

added to the inflow to match the time-averaged situation in the simulation with the incoming wake.

In the simulation with the incoming wake, immediately upstream of the front of the cylinder vortical structures in the turbulent wake were found to be stretched and to become aligned with the direction of the accelerating flow. As the elongated structures approach the stagnation region of the cylinder pairs of counter rotating structures cause hot fluid from near the cylinder wall to be transported upwards to the free stream while – on the other side of the vortex – cool fluid from the free-stream is transported towards the cylinder wall. As a result the stagnation heat transfer rate was observed to increase by up to 37% at the stagnation point as compared to the simulation with the added time-averaged wake-deficit at the inlet.

Figure 4 shows the footprints (large values of T/T_0) of the elongated vertical structures that promote the exchange of hot fluid from the vicinity of the cylinder wall and cold fluid from the free-stream. At the back of the cylinder the pattern in the temperature contours can be seen to become more irregular as the free-stream flow has turned turbulent.

Figure 4: Instantaneous temperature contours in a plane adjacent to the cylinder wall

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Numerical and Theoretical Investigations of Fluid Turbulence

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HLRB Project ID: h0963

Introduction

The statistical description of fully developed turbulence remains one of the most challenging problems of classical physics. In comparison with other fields of science, like e.g. high energy physics, where field theoretic methods allow for calculations of many central quantities with incredible precision, derivations of fundamental statistical properties of turbulent fields directly from the fluid dynamical equations are, with few exceptions, still far ahead of us. The main reason for this is the nonlinear and nonlocal character of the governing equation of motion, the Navier-Stokes equation. These properties are on the one hand responsible for the highly complex spatio-temporal patterns observable in direct numerical simulations (DNS), see figure 1. On the other hand, the same properties are also the origin of the major obstacle on the way to a statistical description from first principles, namely the closure problem; when deriving evolution equations for moments or probability density functions (PDFs) from the Navier-Stokes equation, the statistical equations contain unclosed terms, which necessitate information from higher-order moments or more points in space. When tackling the problem by analytical means only, the validity of the results depends sensitively on the approximations made, and a too crude approximation can lead to unphysical results. This is one reason why turbulence simulations on modern supercomputers have become an indispensable tool to understand the nature of turbulent flows. Hence, one of the goals of the current project is to supplement the analytical treatment of the statistical problem with results from direct numerical simulations.

Numerical Details and Conducted Simulations

For the direct numerical simulations we make use of the vorticity formulation of the incompressible Navier-Stokes equation. The method used is a standard pseudospectral method [1], in which most of the computations (evaluation of derivatives etc.) are performed in Fourier space. The nonlinear term is treated in real space, reducing the computational efforts from $O(N^2)$, due to the otherwise

Figure 1: Volume rendering of the magnitude of vorticity (left) and velocity (right) from a simulation with 512^3 grid points. The vorticity tends to organize into thin filaments forming an entangled global structure. The velocity appears less clearly structured but displays long-range correlations. Volume rendering produced by VAPOR (http://www.vapor.ucar.edu).

arising convolution sums, to $O(N \log N)$ needed for the Fourier transforms. Here, N is the total number of grid points. Adaptive time stepping is implemented employing a third-order Runge-Kutta scheme [2]. We have conducted highly resolved simulations with up to 1024^3 grid points on a periodic domain, integrated for up to tens of thousands of time steps. Our code is MPI parallelized and employs a slab domain decomposition, enabling us to effectively use up to 1024 cores at a resolution of 1024^3 grid points. Parallel IO is incorporated by the use of MPI-IO. The Fourier transforms are performed by the freely available library FFTW [3]. Additionally, we have implemented the possibility to follow trajectories of (so-called Lagrangian) tracer particles, where relevant quantities along the tracer trajectories are interpolated from the turbulent fields with a tricubic interpolation scheme. The HLRB-II at the LRZ Munich has turned out to be an optimal platform for the current parallelization scheme as the individual cores are comparably performant. A typical simulation basically consists of two stages. First, an artificial large-scale initial condition decays for some large-eddy turnover times, during which a turbulent flow develops. Then an external forcing is applied, and the system eventually approaches statistical stationarity. After this preparation

of proper initial conditions, the actual simulation is performed. Here, the flow field is advanced in the statistically stationary state. During this period, fields (velocity, vorticity, velocity gradients etc.) are stored with a sampling rate sufficient to form a statistical ensemble. The statistical analysis is performed during the post-processing stage. Optionally tracer particles are advected with the flow and stored frequently. In total, a typical 1024^3 run on the HLRB-II required several tens of thousands of cpu hours and produced data in the order of terabytes. Within the project, runs with resolutions between 256^3 and 1024^3 grid points with Taylor-based Reynolds numbers ranging from about 75 to 250 have been performed, giving insight into the Reynolds number dependence of the statistical quantities under consideration as well as resolution issues. It has turned out that long simulation durations are important for the constitution of a proper statistical ensemble. Hence, we have performed simulations for more than 100 large-eddy turnover times at a resolution of 512^3 grid points, where special emphasis has been put on an adequate resolution of the small-scale features of turbulence.

Figure 2: Directly estimated and theoretically reconstructed PDFs of the vorticity, normalized by the standard deviation. The theory yields a good description of the strongly non-Gaussian shape of the vorticity PDF.

Scientific Results

Within the project, a number of scientific questions has been addressed. The first question on the agenda has been to investigate the statistics of the single-point velocity and vorticity probability density functions within the framework of the Lundgren-Monin-Novikov hierarchy (see [4] and references therein), a theoretical framework for the statistical description of turbulent flows introduced in the late sixties of the last century. By exploiting statistical symmetries, it has been possible to derive relations that express the single-point statistics in terms of local correlations. For example, it has been shown that the single-point velocity PDF may be expressed in terms of the conditional statistics of the pressure gradient, the external forcing and the rate of energy dissipation. For the case of the vorticity statistics, a relation expressing the PDF in terms of vortex stretching and enstrophy dissipation conditional on the vorticity has been established. DNS results then have been

used to assess this conditional statistics. Thereby a physical discussion of the unclosed terms has been achieved, finally explaining the often discussed slightly sub-Gaussian shape of the velocity PDF as well as the super-Gaussian shape of the vorticity PDF [4,5]. A comparison between the directly estimated vorticity PDF and the result of a consistency check of the theoretical framework is presented in figure 2. Also two-point statistics has been investigated, especially focusing on the interaction of different spatial scales. Furthermore, the simulations have been used to gather acceleration data along Lagrangian tracer particle trajectories. Here, we have analyzed the multi-time PDFs of the acceleration with respect to Markovian properties. As a result, we have found that only for very long time lags the acceleration along the trajectory can be approximated by a Markov process [6]. This especially has implications for the modeling of Lagrangian tracer particle trajectories, which is, for example, relevant in the context of mixing and dispersion.

Outlook

By joint numerical and theoretical efforts, the current project has led to a comprehensive characterization of the single-point statistics of the velocity and vorticity field, and insights into the temporal correlations in terms of the Lagrangian acceleration statistics have been gained. One of the goals for future research is to obtain deeper insights into the multi-point statistics of turbulence. This is related to one of the most challenging questions of theoretical turbulence research, namely which aspects of the fine-scale structure of turbulence are responsible for the energy and enstrophy transfer across scales. Furthermore, we aim for a deeper understanding of the Lagrangian description of fully developed turbulence with respect to the origin of Lagrangian intermittency and implications for stochastic models for particle trajectories. Direct numerical simulations of fully developed turbulence on modern supercomputers undoubtedly will continue to foster new theoretical ideas.

Acknowledgments

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Shock / Turbulent boundary layer interaction

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Introduction

The design process of supersonic and hypersonic aircrafts requires accurate simulation methods for predicting aero-thermodynamic loads. The need to achieve an optimal and safe design poses the requirement of an accurate estimation of critical quantities such as skin friction, heat-transfer rates, mean and fluctuating pressure. The interaction of turbulent boundary layers with shocks and rarefaction waves is one of the most prevalent phenomena occurring in high-speed flight, which can significantly affect significantly the aero-thermodynamic loads. Accurate computations of such interaction are needed to gain a deeper insight into many aspects of this phenomenon, such as the dynamics of the shock unsteadiness, turbulence amplification through the shock, unsteady heat transfer near the separation and reattachment points, turbulence damping by the interaction with a Prandtl-Meyer expansion.

Forward and backward-facing ramp configurations are often used in supersonic-flight engine inlets for turbo jets and scramjets. Given the importance of such flows, compression-expansion and expansion-compression ramp configurations have been thoroughly investigated from an experimental point of view.

A sketch of the main flow phenomena for a compression-expansion ramp configuration is given in Fig. 1. The undisturbed incoming turbulent boundary layer is deflected at the compression corner. This causes the generation of a compression shock, which penetrates the boundary layer. For sufficiently large deflection angles the adverse pressure gradient within the boundary layer results in a region of mean-flow separation near the corner. A detached shear layer travels above the separation region and reattaches in the inclined part of the compression ramp. A λ-shock system is generated near the separation region. The forward foot of the λ-shock originates from the region of flow separation, and the rearward foot from the region of flow reattachment. Further downstream, the reattached boundary layer reaches the decompression corner and passes through the Prandtl-Meyer expansion. Even further downstream, the boundary layer relaxes again towards a developed zero-pressure-gradient turbulent boundary layer.

In the present work we conducted Large Eddy Simulations (LESs) of the supersonic flow over a compression-expansion ramp. For the first time the computational domain covers the whole compression-expansion ramp and results were compared with an available experiment at identical flow conditions. After assessing the prediction quality of the employed numerical technique by matching directly the experimental parameters, the computational results provided a reliable numerical database for the analysis of different issues such as turbulence evolution and interaction with compression and rarefaction waves.

Figure 1. Main phenomena of a compression-expansion ramp flow.

Figure 2. Speed-up obtained by increasing the number of CPUs.

Figure 2(a) Numerical schlieren picture. (b) Experimental schlieren picture. (c) Isosurface of streamwise vorticity. The clockwise rotation is represented by the blue colour. Counter-clockwise rotation is given in the red.

Results

The computation has been carried out with the INCA software, which solves the compressible Navier-Stokes equations. INCA uses a finite volume method for the discretisation of the underlying governing equations on adaptive Cartesian grids with local refinement that accommodate the resolution requirements of wall-bounded turbulent flows over complex geometries.

INCA employs domain decomposition to split the mesh into a number of sub-domains and allocates them to separate processors. The application subsequently can run in parallel on separate sub-domains, where communication between the different sub-regions is achieved through the MPI communication protocol.

A total number of 32.5×10^6 grid points has been employed, distributed among 514 blocks. A total number of 128 cores were employed for the computation. A total amount of 230400 core hours have been used to carry out the simulation, as long integration times were required to cover the low frequency features of the studied system. An evaluation of the scalability properties of the INCA code on the HLRB2 cluster has also been performed. Fig. 2 gives an estimate of the performance increase with increasing number of processors.

An instantaneous snapshot of the computed schlieren-type visualization in Fig. 3(a) shows good agreement with the experimental schlieren picture in Fig. 3(b). The undisturbed boundary layer (1) is affected by the separation shock (2). The interaction results in the appearance of a reverse flow region (3) and of a separated shear layer (4) with travelling shocklets (5) above it. The compression in the reattachment region leads to the generation of the unsteady second stem (6) of the λ-shock configuration. Figure 3(c) shows a side view along the compression ramp. Despite the flow geometry being two-dimensional, the interaction between the boundary-layer and the shock breaks the spanwise homogeneity. After the boundary-layer reattachment location, a pattern that is related to two streamwise evolving structures is clearly visible. Such structures are indicators of the presence of a pair of counter-rotating streamwise vortices, often called Görtler-like vortices. This pattern extends along the entire deflected part of the ramp and disappears after the passage through the decompression corner. Another objective of the present work is to investigate the dynamics of the shock unsteadiness with the aim of extracting the main properties of the mechanism that govern this phenomenon. For this purpose, the results from the LES have been analyzed by means of Dynamic Mode Decomposition (DMD)[3].

Our results show that the interaction cannot be described by a single mode, but that the superposition of four dominant low-frequency modes is sufficient to recover the essential characteristics. These modes are phase locked and represent an asymmetric cycle for the shock motion as well as the periodic pumping of the separation bubble.

On-going Research / Outlook

Further numerical investigations are currently carried out in the field of the shock boundary-layer interaction. A new configuration with an impinging oblique shock on a supersonic turbulent boundary layer developing on a flat plate is currently being computed, which differs in many ways from the already analyzed compression-expansion ramp configuration.

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Numerical investigation of the noise from modified nozzle geometries

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3

Introduction

Prognoses for the future world-wide air traffic consider a constant grow over the next years. The traffic volume is believed by leading aircraft manufacturers to double in the next 15 years. Inhabitants of near airport regions, have therefore to expect an increasing number of take-offs and landings in the future. Among a rise of other environmental impacts, an increased noise load is to be expected. One aim of research projects funded by the German government and the European Union is the reduction of the noise emission by aircrafts. The noise emission of the turbulent jet behind the jet engine is a major contributor the overall noise especially during take-off. The noise reduction of the jet engine has in recent decades been mainly reduced by a decreased exit velocity of the jet stream. This made an increase of the ratio of secondary to primary stream necessary, but due to size restrictions can this process not be followed for-ever. Aircraft manufactures have therefore been search-ing for other means of reducing the noise. One possible means is the modification of the nozzle geometry by adding for instance serrations at the outer nozzle lip as can be seen in figure 1.

Figure 1: Rolls-Royce Trent 1000 engine on a Boing 787 Dreamliner (This photograph is reproduced with the permission of Rolls-Royce plc, copyright © Rolls-Royce plc 2010)

Nozzle lip modifications are studied experimentally since the 1950s. Their positive effects on the noise have been verified, while a negative effect on the nozzle effi-ciency is possible, that thus affects the fuel consumption during take-off and cruise flight.

Due to the availability of computing resources in the recent decades, the design process of nozzle engines, among other things, became more and more supported by numerical predictions. This can lead to reduced design costs, as the costs for building of prototypes and the con-duction of experiments decrease. Still, reliable numeri-cal prediction methods are needed that can handle the complex flow features of the jet stream and reproduce the changes introduces by nozzle modifications. The aim of our work conducted at the HLRB was to examine the capabilities of our existing prediction method, as well as the development of improvements where necessary.

Methodology

The flow regions where most of the noise is created, is the shear layer between the outer slow flight stream and the fast jet stream from the nozzle that exits the nozzle with nearly the speed of sound. The region that affects the nozzle efficiency most, is near wall region inside the nozzle, where the wall friction defines the losses of the nozzle. The flow in both regions is fully turbulent, which means, a prediction method has to handle these complex flow features properly. The rep-resentation of turbulent flows remains a challenging task for numerical prediction methods. Although Direct Numerical Simulation (DNS) allows the complete reso-lution of all turbulent scales, one has to keep in mind that the ratio between the largest and the smallest tur-bulent scales in a flow field grows with increasing ge-ometry size and flow velocity. As this ratio is very large for realistic jet engines and defines the number of grid points that have to be used, a DNS of a jet engine will remain infeasible for the next decades. The introduc-tion of models to represent the fine scale turbulence in a simulation reduces the computational demand considerably, but is accompanied by uncertainties due

to the approximations of this turbulence model. The time averaged flow field can be calculated using a turbulence model by a so called RANS simulation at low computational costs. The prediction of the broadband jet noise from this data however, requires an additional acoustic model to reconstruct the unsteady information not preserved in the RANS. Large-Eddy Simulation (LES) lies conceptually between the RANS and the DNS. Here, only the larger turbulent scales are resolved, while the effects of the smallest scales are accounted for by a sub-grid scale model. Although being much less computational demanding than a DNS, it proves to be to expensive especially for wall-bounded flows where the turbulent scales near the walls are much finer than the geometries involved.

Hybrid RANS-LES methods aim to overcome the limitations of pure LES by relying on a RANS model in the near wall region and using LES elsewhere. The Detached-Eddy Simulation (DES) used in this work is such a method. It was introduced for bluff body flows in [1], where it showed promising results. As the simulation of nozzle modifications requires a methodology that allows efficient handling of wall-boundary layers, the DES should be explored for jet flows.

Results

DES of short-cowl nozzles
During the project *CoJeN* funded by the European Union, the flow around short-cowl nozzles has been simulated with the DES method. In this project both a clean nozzle acting as reference case and an otherwise similar nozzle with serration were studied. Some results and an overview of the mesh used are shown in figure 2, where the developing turbulent structures in the outer shear layer are visualized. Based on the findings using the standard DES approach, some modification to the DES procedure were made that improved the results (compare figures 2a and 2b).

Using the unsteady simulation data, the far-field noise field has been calculated using the acoustic analogy of Ffowcs-Williams & Hawkings (FWH). The calculated

Figure 3: Power-spectral density of predicted far-field noise levels at a low angle to the jet axis (top, 36°) and a sideline angle (bottom, 105°) versus experimental data; — experiment, — coarse grid, — refined grid

spectra show a good agreement with the experiments and predicted the general trend of a noise reduction due the serrations. More information is given in [2].

Comparison of DES and LES of a co-planar nozzle
To examine the LES capabilities of the DES a direct comparison of LES and DES was carried out for a co-planar nozzle [5]. Special care was taken for the LES simulation to use a similar flow profile at the nozzle exit, as was found in the DES, other numerical parameter were kept similar in both simulations. It was found that DES and LES behave very similarly in the jet region, where the DES is running in its LES mode.

DES of long-cowl nozzles
During the same period, the DES method was used in combination with the FWH procedure to examine its predicting capabilities for a

Figure 2: Iso-surfaces of the density showing resolved turbulent flow structures a) standard DES; b) modified DES, unserrated nozzle; c) modified DES, serrated nozzle; d) serrated short-cowl nozzle surface mesh with every second grid line shown

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long-cowl nozzle with and without serrations. Although the flow structures were clearly affected by the serrations and the predicted far-field overall sound pressure levels showed a reduction for the serrated nozzle [3], some features of the flow field indicated that the comparison of the two cases might be somewhat lacking. As with all structure resolving methods, there is a strong dependency of captured flow structures on the grid used. The fact that for the clean nozzle a much coarser grid had been used, raised questions towards the true reasons of the noise reduction predicted numerically.

To further examine the properties of the DES method some additional studies have been carried out. While the effect of a different length-scale definition for the DES was studied in [4], the effect of a refined grid was examined in [6]. The grid refinement had a large effect both on the flow field and on the calculated far-field noise levels. Some acoustic results are shown in figure 3. In general the acoustic results improved with the data from the refined mesh. The increased levels at higher frequencies are clearly an effect of the refined mesh, as it allows smaller resolved structures which are associated with higher frequencies. At the sideline angle, an augmented level is predicted for all mid-range frequencies from the coarse mesh. This does much improve when the data from the refined mesh is used.

On-going Research / Outlook

Using DES as the modeling approach for broadband jet noise calculations proved to be good alternative to LES, and allows to include the nozzle itself in the simulation without special treatment. Work on the method itself and on other nozzle modification was continued in the project Optitheck funded by the German government (BMWi) and Rolls-Royce Germany.

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Distributed Particle Transport Simulation

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Introduction

Microscale particles dispersed in water that floods very small tubes or channels with a saw-tooth-alike radius profile along their longitudinal axis exhibit a behaviour that contradicts human intuition. If the water swaps forth and back, the particles – on the long term – do not remain at the same position even though the stimuli average out to zero. Instead, they start to wander, they drift. Both the speed and the direction of the drift of each particle depend on the particle's size. This observation and related phenomena have been fascinating researchers and engineers since the 1990s, as they are important for biological systems and pharmacy, environmental sciences and contaminant sediment simulation, or the construction of machines sorting particles or macromolecules according to their different size. Hydrodynamic Brownian motor or drift ratchet are names for the underlying system.

computationally too expensive, even for a supercomputer. The underlying equations are well-known, however, the scientific tools for respective computations are still missing, i.e. the computing algorithms and approaches cannot yet cope with such a complicated setting. The computation times are by magnitudes too long.

In this project, we create, study, and apply a new tool concept broadening the horizon of computability: We combine two simulation codes and make them run in parallel. Both are time stepping schemes, i.e. they split up the simulation into to a sequence of problems, compute the solution of one time step, and then proceed to the next one. One code solves the problem very accurately with high computational demands. The other one approximates the particle's movement without inserting the particle into the fluid. The latter is cheap to compute, i.e. the solution is obtained fast. After a while, we compare the results of the two models, i.e. where the particle is located according to the simulation. If they do, more or less, agree, we throw away the very fine computation, store the solver's state, and continue for a while with the cheap code.

The Challenge

Different models do exist to describe the underlying fluid and particle movements. However, solely stochastic models that work for very simple geometries and only due to many assumptions about the solution can describe the particle behaviour as a probability distribution among the geometry. More precise models computing real particles interacting with the fluid fail – they are

Faxen vs. Lattice-Boltzmann fluid-structure interaction
Our 'cheap' model is based upon the Faxen theorems. For them, we compute the movement of the fluid as if there were no particles at all. It is a straightforward finite differences code with an explicit time stepping scheme. We then take this fluid field and insert a virtual particle. The evaluation of a surface integral yields forces acting on this virtual particle and due to these forces we update its location, its velocity, and its rotation.

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Coarse regular grid (Postprocessing computations)

Fine adaptive grid (FSI)

Our 'expensive yet accurate' model is a Lattice-Boltz-mann solver that interacts with a rigid spherical particle with a speed and a rotation. It is basically an elaborated state-of-the-art fluid-structure interaction (FSI) code with some fluctuations added to the fluid field, i.e. this accurate model picks up the Brownian motion.

Validity of the models

Our experiments reveal that the Faxen code gives a good approximation of the particle movement if and only if the particle is not near to the boundaries of the computational domain and if the fluid flow around the particle is not changing fast, i.e. if the particle is not located in the narrow regions of the domain where the fluid is pressed through small passages. If the particle swims in the wider regions of the geometry far away from the walls, we may stay with the cheap Faxen approximation not taking Brownian motion and the impact of the particle on the fluid into account at all. The comparison of the two models simultaneously running identifies exactly such criticial combinations and tells us whether a Faxen simulation is sufficient

Grid computing, checkpointing, and migration

If solely the Faxen code is running, the computational work is so small (compared to the full simulation with a particle) that it sometimes pays off to stop the simulation, store the fluid field to a file (we write a checkpoint),

and continue with the computation on a local desktop computer. This saves supercomputing time and frees the resources for other users.

If the comparison then decides that the simulation has to switch to the Lattice-Boltzmann FSI code again, we upload the fluid field back to a supercomputer and continue the simulation there. This might be a different supercomputer than the one used before.

Results

The primary goal of this work is not to solve the physical problem described in the introduction. The main goal is to create an environment and an infrastructure to solve this kind of problem. We tested and evaluated it for the particle transport; however, its general concept – that is the switching back and forth between two solvers, between different computers, and between different physical descriptions – is transferable to many kinds of other problems.

For our case study, we observed a significant speedup and efficiency of our computations due to three facts:

1. Meeting the original expectation, the switches to the cheap model pay off in terms of computing time. On the one hand, the solution of each time step is faster. On the other hand, we can increase the size of the individual time steps. We thus observe that the simulation creeps as long as the full fluid-inter-action is required. If we switch to the Faxen mode for a while, the simulation speeds up in terms of simulated time to computing time.

2. Scalability is often, and also in our case, bound to the amount of work, i.e. if a problem is not sufficiently big, we cannot fully load a supercomputer. With our approach, we are able to migrate the simulation from a supercomputer back to a local workstation if it becomes too cheap computationally. The computations remaining at the supercomputer however scale.

3. When we move the simulation back to the supercomputer, the choice is up to us which machine to use. One reasonable strategy is to use the supercomputer with the smallest workload currently or the biggest remaining computing budget. This way, we speedup the simulation time – if we computed everything on one machine, we might have to wait longer until our jobs pass the waiting queue and are processed

On-going Research / Outlook

The developed techniques and algorithms to couple multiple simulations and to move computations from one place to another proofed to be of value for this type of problem and can be used in different contexts as well. We thus outsource them and provide them to the community as independent individual modules. Also the two solvers – Lattice-Boltzmann and Faxen – were improved and tuned successfully throughout the project which is of value for successor endeavours and future studies.

And the particles? They keep on moving and we don't know why. However, we already observed up to now unknown particle behaviour such as low frequency drift modes, and we elaborated a set of tools paving the way for future research. Also, we are working on a way to simulate multiple particles and multiple particles interacting.

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Numerical Simulation of Wing and Nacell Stall

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Abstract

This project is part of a research group funded by the German Research Foundation (DFG) which deals with Wing and Nacelle Stall. Stall phenomena occurring in the intake and their interaction with the airplane's engine are the main focus of this project. Flight situations near the border of the flight envelope like take-off and landing with crosswind conditions are likely to cause intake stall. Since the engine operates at take-off thrust settings already at high loading conditions distortions of the intake flow due to intake stall can cause unstable operation of the compressor and loss of thrust if not properly accounted for. In cruising flight conditions strong gusts may have similar effects. However, flight safety is only one reason for this research, distortions of the intake flow result also in a significant loss of engine efficiency. Therefore better and more understanding of the effect of intake distortions on engine efficiency and performance is needed in order to design engines maintaining safe and highly efficient operation even in the presence of distorted inlet flow. The compressor performance due to distortions is crucial for the engines behavior and its efficiency. Hence computations and experiments were carried out within the collaborative research project considering compressors with distorted inflow conditions to study compressor performance with a distorted inflow. As stall and crosswind phenomena can cause a wide spread of different inflow distortions various cases were studied. First, a total pressure and inflow angle distortion was investigated. These inlet distortions are generated in the experiment upstream of the compressor stage by non-rotating steel bars, while in numerical simulations the total pressure and inflow angle distribution measured downstream of the bars are used as inflow boundary conditions. For disturbed inflow conditions, full-annulus calculations have been carried out for two operating points at peak efficiency and near stall, respectively. The objective of the investigations is to validate the flow solver for compressor flow with distorted inflow and to gain a deeper insight into the influence of this kind of distortion on the compressor flow. The results from time-averaged numerical and experimental data have been compared extensively and the interaction of

flow phenomena like the tip clearance vortex and the inlet distortion has been investigated in particular. Further investigations with different kinds of distortion are still running at the LRZ.

Results

Two operating points were simulated with distorted inflow conditions so far, one at peak efficiency conditions and one at near stall conditions. The 85% characteristic was preferred, since for this speedline more experimental data is available. In a first step the numerical results were validated extensively and physical conclusions were drawn subsequently.

In Figure 1 the compressor stage with the simulated total pressure distributions for the inlet plane, a plane between rotor and stator, and the outlet plane is depicted. At midspan, the extent of the total pressure distortion covers almost a 120° circumferential sector of the annulus and the pressure loss is up to 13% for peak efficiency and 10% near stall onset respectively. In order to validate the global flow behavior the measured and simulated pressure rise characteristics of the compressor stage at 85% of design rotor speed with distorted inflow were compared. The comparison of the operating points reveals a good agreement between measurement and simulation and is hence a strong indication that the numerical simulation captures the general flow behavior quite well. A closer look at the

Figure 1: Numerical calculated total pressure distribution

simulation results at conditions near peak efficiency is depicted in figure 2. The measured and calculated circumferential total temperature distributions between rotor and stator at 50% span are shown. The total temperature distribution is qualitatively well captured in most part along the circumference. The particular circumferential deviation is result of the variation of the flow angle at the inlet of the compressor stage featuring a co-spin in the sector between 90° and 160° and a counter-spin in the sector between 160° and 300°. This leads to higher and less aerodynamic blade loading, respectively and hence to less and more energy addition to the flow. In the sector ranging from 280° to 340°, the measured total temperature profile shows a strong drop, which is not reproduced fully by the calculations. As discussed in [1] the authors suppose that the rotor operates in an unstable flow mode in this particular sector. However, the instability is suppressed in the calculation by the unphysical turbulent boundary layer, caused by the lack of a transition model. A detailed discussion of the results can be found in [1] and [2].

Figure 2: Total temperature increase distribution between rotor and stator, 50% span

After validation a closer look into flow physics was performed. The distribution of blade loading leads to the conclusion that the different passages work in different operating points depending on their relative position to the inlet distortion. Therefore in figure 3 the operating points of the different passages are depicted. Two calculated overall operating points are shown, one related to the average of the distorted total pressure (P_{t5}) and one related to the undistorted total pressure (P_{t4}). The experimental data is related to the undistorted total pressure (P_{t4}), however, for comparison with the operating points of the passages the overall operating point has to be related to the distorted total pressure. Furthermore, the stall lines of the undistorted and distorted compressor were included in order to indicate the stable flow regime. The operating points of the passages show a great spread. As already indicated by the aerodynamic blade loading, the main bulk of undistorted passages have almost the same operating point within the stable area of the compressor map. However, in the sector between 150° and 260° the passages exceed both the undistorted and dis-

torted stall line and are operating beyond the stable operating line. This is possible, provided that enough of the passages work on the stable side. In this case 9 of 28 passages exceed the stability limit. In both CFD and experiment the total temperature rise across the distorted sector indicates no critical stall phenomena. That means for the distorted passages, that although operating at unstable flow conditions, the instability has not enough time to develop fully in these passages. Only in the last part of the distorted sector when the rotor re-enters the undistorted part, experimental results suggest a laminar flow separation as a trend of beginning full span stall. In summary, it can be concluded that the numerical results are in good agreement with the experimental data and that CFD contributes strongly to gain a better understanding of the complicated flow phenomena.

Figure 3: Compressor map with passage operating points, colors due to circumferential position

On-going Research / Outlook

After modeling the distortion by suitable boundary conditions at the inlet plane of the computational domain, it was decided by the project partners to design a new test case which allows for simulations including the distortion generator. Detailed measurements of a compressor with distorted inflow were already carried out successfully at TU Darmstadt and will be used again for extensive flow simulations at the LRZ. First unsteady flow simulations are still running, due to their extreme time consuming character and the high workload of both the HLRBII and the Supzero. The German Research Foundation (DFG) will fund this project for another 3 years and in this time it is planned to create an extensive numerical and experimental data base on compressor performance with non-uniform inflow.

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Simulation of the unsteady flow around the Stratospheric Observatory For Infrared Astronomy SOFIA

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HLRB Project ID: h1142, pr42bo

Introduction

The Stratospheric Observatory For Infrared Astronomy SOFIA, a joint project between NASA and DLR, is a 2.5m reflecting telescope housed in an open cavity on board of a Boeing 747SP aircraft. SOFIA operates in the stratosphere at an altitude above 13km to observe objects in the universe in the infrared region of the electromagnetic spectrum.

Figure 1: View of the SOFIA aircraft during a test flight with open door

The flow over the open port during the observation flights presents challenging aerodynamic and aeroacoustic problems. In general, the flow over cavities such as the SOFIA telescope port is characterized by unsteady flow phenomena associated with prominent self-sustained pressure fluctuations caused by amplified acoustic resonances. In the present case, these phenomenon cause unwanted vibrations of the telescope structure and deteriorates the image stability [1].

Numerical approach

To investigate the pressure fluctuations in the cavity CFD simulations using the DES and URANS turbulence approach were performed with the Finite-Volume RANS-solver TAU that was developed by the Institute of Aerodynamics and Flow Technology of DLR [2]. The code solves the unsteady, compressible, three-dimensional Reynolds-averaged Navier-Stokes equations on unstructured or hybrid grids.

Objectives

The primary objective of these simulations is to understand the complex cavity flow phenomena. In a second step the aim of these simulations is to improve the telescope's performance by mitigating the amplitudes and changing the characteristic frequencies of the pressure fluctuations inside the cavity. This could be reached by installing passive flow control devices upstream and downstream the cavity port. The simulations show that the investigated measures have a high potential to increase the telescope's pointing stability [1].

CFD Calculations on HLRB II

The present computations were carried out on the Linux-Cluster SGI Altix 4700 (HLRB II). The typical grid size for a URANS simulation is about 20 million cells (half model). For parallelization, the domain was equally decomposed into 510 sub-domains to utilize 510 processor cores in parallel. A typical CFD computation using the URANS turbulence model consisted of 6000 physical timesteps with 180 inner iterations per step. One physical time step consumed about 56s of wall clock time, yielding an overall time consumption of about 48000CPUh for one run. The physical time step was chosen to 16.4ms, resulting in a simulated time period of 0.1s under wind-tunnel conditions (1.6s under flight conditions). In the DES simulations the time step was decreased to 5.0ms, 13000 physical time steps (40 inner iterations per time step) were performed to simulate 0.065s under wind-tunnel conditions (1.1s under flight conditions). For DES simulations an additional LES grid block was added in the shear layer zone over the cavity to capture the relevant turbulent structures in this zone. The LES grid block is characterized by a very fine discretisation which is blowing up the grid size up to 56 million cells. The computational cost for the DES run was about 65000CPUh (parallelization on 1020 processor cores).

Results

Among several successfully simulated passive flow control devices the results of the combination of a porous

Figure 2: Shear layer characteristic with a porous fence installed upstream the cavity

fence installed upstream the cavity and a 3D semi-lunar shaped aperture ramp attached to the rear wall of the cavity will be presented in the following. Wind-tunnel results showed that the aperture ramp is the essential device for the observatory: it captures the shear layer, stabilizes it and guides the shear layer over the cavity. Figure 2 shows the shear layer characteristic over the open cavity port issued from DES simulations with the locations of the fence and the aperture ramp. In this case the SOFIA aircraft is flying in 41000 feet at a Mach number of 0.85.

Under this flight conditions the shear layer is characterized by large scale "Kelvin Helmholtz" vortices that are passing the cavity. The propagation and the size of these coherent structures have a significant impact on the excitation of pressure fluctuations inside the cavity. As the picture in Figure 2 shows, the transversal structures are ruptured by the fence. This promotes bursting and creating of chaotic three-dimensional vortices already at an earlier stage further upstream in comparison to the case where no fence is installed and only the aperture ramp is present [3]. In Figure 3 it is illustrated that the shear-layer fence yields a significant decrease of the unsteady loads on the telescope assembly. The repartition of the red zones being an indicator of high pressure fluctuations is reduced.

Next to the passive flow control devices that are affecting directly the shear layer, there are as well approaches to counteract the acoustic resonances inside the cav-

Figure 4: PSD plot averaged over all telescope pressure sensors comparing the baseline configuration with and without baffle plate

ity and hence increase the pointing stability of the telescope. This can be achieved for example by installing baffle plates on the cavity floor in such a way that they increase the acoustic damping and shift acoustic resonance frequencies. In Figure 4 are shown the spectral distributions of the pressure fluctuations acting on the SOFIA telescope simulated with and without baffle plates. It can be observed that the acoustic energy concentrated around 46Hz can be reduced significantly by the use of baffle plates in the cavity.

On-going Research / Outlook

Meanwhile flight test data from the SOFIA envelope expansion flights became available allowing a comparison with the CFD simulations. Although there is a good accordance between the flight test data and the CFD results as to unsteady pressure fluctuations originating in the shear layer and the acoustic frequencies, the amplitudes of the acoustic frequencies are overestimated by the numerical simulations and the wind tunnel results.

To understand the reason for this difference, new DES simulations using the latest TAU solver version, finer grids and new blending functions between the RANS and the LES zone (IDDES) are momentarily being carried out. In addition, the existing SOFIA model will be refined by taking into account structural details within the cavity having acoustic damping properties. The impact of so called resonators has already been proven by 2d CFD simulations of the SOFIA cavity. A further field of research is the CFD based prediction of the aero-optical properties of the cavity shear layer being a potential limiter of the image quality of the observatory during flight.

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Figure 3: Pressure fluctuations on the Telescope Assembly with (left picture) and without using a fence (right picture)

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On the High Order Numerical Investigation of a Scramjet Inlet

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HLRB Project ID: h1143

Introduction

Air-breathing propulsion systems are promising approaches to increase the pay load and hence the economic effectiveness of future but also reusable space transportation systems. Particularly in the field of hypersonic aircrafts the scramjet driven systems prove to be a reasonable alternative to the expensive classical and expendable rocket technology at Mach numbers greater than 5. Furthermore, in hypersonic flow regimes scramjets provide a significantly higher specific impulse than classical propulsion systems can achieve. As a major constraint in designing a scramjet is the supply of compressed air required for the efficient combustion of the fuel-air mixture. Whilst conventional aircraft engines provide the compressed air by means of mechanical compressors, hypersonic air-breathing vehicles achieve that compression through a series of shocks (cf. Figure 1). In order to investigate such a propulsion system both experimentally and numerically, the DFG Graduiertenkolleg 1095 has been established aiming at designing and building a scramjet demonstrator in cooperation with its partners at TU München, RWTH Aachen, University of Stuttgart and the German Aerospace Centre (DLR). Within the scope of the Graduiertenkolleg 1095, the research group of Prof. Dr. Claus-Dieter Munz at the Institute of Aerodynamics and Gas Dynamics (IAG) of the University of Stuttgart focuses on the flow phenomena occurring in the scramjet inlet and their numerical investigation.

In the following, we will present the numerical simulation of the 3D scramjet intake which has been developed

Figure 2: 3D scramjet intake geometry proposed by the DFG Graduiertenkolleg 1095 and its partners

during the second period of the Graduiertenkolleg (see Figure 2) at an incident flow with a free-stream Mach number of 8. As the shock system within the inlet is of fundamental importance, we will discuss our obtained results with respect to its proper resolution.

Numerical Code

Since the simulation of the scramjet intake involves strongly time dependent phenomena, a special unstructured discontinuous Galerkin (DG) code called HALO (Highly Adaptive Local Operator) is being used for the numerical discretization. This fully explicit scheme excels not only in arbitrary high order accuracy in both space and time with a minimum of inter-processor communication, but can also handle unstructured hybrid grids with hanging nodes. The HALO code is characterized by its specific time discretization method [1], [2], [3] enabling a high order time consistent local time stepping mechanism. Furthermore, the main feature of this parallelized code is its ability of optimal scaling for a very high number of processsors. An important evaluation tool for the performance of a code is the so-called scale-up efficiency that expresses the ratio of the calculation time on one processor to the total time needed for performing the calculation on N processors. As indicated in Table 1, the DG-based HALO code yields a very high scale-up efficiency for up to 4080 processors processors at constant load per processor which makes it particularly suitable for very large scale computations.

Figure 1: Schematic illustration of a scramjet propulsion system

# processors	1	1000	2197	4080
Efficiency (%)	-	99.1	97.8	98.8

Table 1: Scale-up efficiency of the HALO code

Within the HALO code, several equation systems are implemented, such as Euler and Navier-Stokes as well as viscous Magnetohydrodynamic (MHD) equations. The present calculations, however, base upon Euler equations.

Shock-capturing

Shock waves pose severe challenges to high order computations. In general, the most common shock-capturing methods can be classified into two main groups: Total variation bounded and artificial viscosity based schemes. One of the most popular total variation bounded schemes is the weighted non-oscillatory (WENO) method [4] that adapts to discontinuities and acts as a local limiter function. A main drawback of WENO is that it does not generally preserve energy, can get expensive for high order calculations and is rather suitable for structured meshes. Artificial viscosity based methods, in contrast, are energy-conserving and are also effectively applicable for unstructured grids. They base on the addition of numerical ("artificial") viscosity to the cells near the shock. Through adding viscosity, the discontinuity will be smeared over a length scale so that it can be resolved in the space of interpolating functions. As the artificial viscosity will be added only in the near-shock region, the shock-affected ("troubled") cells have to be located. For this purpose, so-called indicators scan the whole flow field for discontinuities to identify the troubled cells where the viscosity will be added. In order to evaluate the dependency of shock-capturing on high order simulations, we have performed 3D Euler calculations of a scramjet intake at design conditions (M=8.0 at an altitude of 30km) with an artificial viscosity based shock-capturing technique according to Persson and Perraire [5]. This problem was calculated for three different polynomial degrees p (1, 3 and 5) and local time stepping on an unstructured grid (200,000 elements) with 0.8 to 11 million degrees of freedom on 520 up to 2000 processors. To demonstrate the obtained results, Figure 3 comprises the 2D slice planes displaying the distribution of troubled cells for all investigated cases. Here, one can easily see that the shocks and their respective reflections are being reasonably localized by the indicator. While for a lower polynomial degree p, the applied indicator involves rather "shock regions" than discrete shock-affected cells. This region of shock-affected cells, in turn, diminishes into a discrete alignment of troubled cells along the propagating direction of the shock by increasing the spatial resolution, viz. increased polynomial degree p.

After detecting the troubled cells, the next step is to add viscosity in order to resolve the shocks. Thereby, the concept consists of adding viscosity as less as possible since the main drawback of adding artificial viscosity is the reduction of the time step. While this may dramatically reduce the efficiency of a global time stepping scheme, the used local time stepping method restricts this effect only to the troubled cells. The respective amounts

Figure 3: Visualization of troubled cells for a 2D slice plane

of added artificial viscosity for to the corresponding calculations are depicted in Figure 4. As the occurring oscillations resulting from resolving the shock by means of a polynomial interpolation function with a higher degree have to be damped consequentially stronger than treating the same discontinuity with lower spatial resolution. Thus, the calculations with higher polynomial degrees p require enhanced artificial viscosity which, in turn, is concentrated in the vicinity of the shock and does not affect regions away from the shock.

Figure 4: Visualization of the amount of added artificial viscosity

On-going Research / Outlook

In this report we have shown that the used HALO code was able to perform high-order (p=5) scramjet calculations and further to properly resolve the emerging shocks in the intake of a scramjet propulsion system under real operating conditions. After these promising results, subsequent investigations with respect to Navier-Stokes equations would lay a further important milestone towards a 3D scramjet intake LES calculation.

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Direct Numerical Simulation of Gas Transfer through the Air-Water Interface in a Turbulent Flow Environment

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Introduction

This report presents an overview of our numerical work performed on HLRB2 with the objective of improving the understanding of the physical mechanisms of gas transfer across the air-water interface in turbulent flow environment. One important example of such a process is the absorption of oxygen from the atmosphere into rivers or lakes. For oxygen as well as other gases having low solubility, the transfer process is controlled by the hydrodynamic conditions on the iquid side concentrated within an extremely thin boundary layer (typically 10 - 1000µm). Performing measurement within this layer is very difficult and has hindered the progress in gaining fundamental understanding of the problem. Even advanced optical measurement techniques, such as Particle Image Velocimetry (PIV) and Laser Induced Fluorescence ((LIF), face difficulties in resolving the uppermost boundary layer as well as the minute variations of the turbulent mass fluxes (c'w') in the deeper region. With the present numerical simulations, we aim to fill this gap of knowledge.

The three typical sources of turbulence generation in nature are surface-shear (e.g. wind-shear on the ocean), bottom-shear (e.g. river flow), and buoyant-convective (e.g. turbulence caused by surface cooling in lakes) induced turbulences. The simulations performed on HLRB2 focused on the gas transfer problem with the last two mentioned turbulent forcing mechanisms.

Description of computations

The setup of the computational domain was in accordance with the laboratory experiments performed at the Institute for Hydromechanics (IfH), Karlsruhe Institute of Technology, in which the interfacial gas transfer process induced by grid-stirred turbulence (a convenient analogy to bottom-shear turbulence) as well as by buoyant-convective turbulence was studied using PIV and LIF techniques [1]. To save computing time, only a small part of the fluid domain adjacent to the surface was modelled. The geometrical sizes for the bottom-shear cases (BS1 to BS3) and buoyant-convective case (BC) are given in Table 1. The domain had a uniform grid size in the x and y directions and a slightly stretched grid distribution in the vertical direction to achieve a denser grid near the interface.

Two numerical codes had been applied for the simulations. Initially, an adapted version of the "LESOCC" (Large Eddy Simulation On Curvilinear Coordinates) code [2] was employed. This code discretizes the incompressible 3D Navier-Stokes equations using a second-order-accurate central finite-volume approach, with a collocated variable arrangement. To prevent the decoupling of the velocity and pressure fields due to the cell-centred variable arrangement a momentum interpolation procedure is employed. The Poisson equation for the pressure is solved using a Strongly-Implicit Poisson solver (SIP). During the last half year, also the "KCFlo" code that was developed over the last two years was employed on HLRB2. In this code, a fourth-order accurate WENO-scheme [4] and a fourth order central method had been deployed for solving the convection and diffusion equations for the scalar transport, respectively, in order to aim for a high accuracy in areas of high concentration gradients. For the fluid flow, a fourth order accurate kinetic energy conserving discretisation of the convection [3] and diffusion was combined with a second-order Adams-Bashforth method for the time-integration. The Poisson equation for the pressure is solved using a conjugate gradient solver with a simple diagonal preconditioning.

As in LESOCC, for the parallelisation the computational domain was subdivided into a number of blocks (between 200 to 400 blocks), each of which assigned to one processing core. Communication between processes happens through the standard Message Passing Interface (MPI) protocol. The KCFlo code has been further optimized specifically for our cases and thus runs more efficiently compared to LESOCC.

Case	Grid points	Domain (L)	Code
BS1	$518 \times 518 \times 306$	$20 \times 20 \times 6$	LESOCC
BS2	$512 \times 512 \times 300$	$20 \times 20 \times 5$	KCFlo
BS3	$128 \times 128 \times 300$	$5 \times 5 \times 5$	KCFlo
BC	$400 \times 400 \times 256$	$5 \times 5 \times 5$	KCFlo

Table 1: Typical Runs. L is comparable to 1 cm in the physical setup

Results

Bottom-shear case

In the experiments, the turbulence was generated by an oscillating mesh in the lower part of the tank. As mentioned already, only a small part of the fluid domain adjacent to the surface was modelled and periodic boundary conditions were applied to account for the larger horizontal size of the domain in order to save computing time. At the top, the free surface was modelled using a rigid lid approach with a symmetry boundary condition and at the bottom grid turbulence was introduced. In LE-SOCC this was done by introducing a snapshot of a box of isotropic turbulence into the computational domain. In KCFlo the isotropic turbulence was generated in an LES that ran concurrently with the DNS. Snapshots of a plane from this LES were interpolated to the DNS grid and introduced at the bottom of the DNS. The transfer of the diffused substance into the liquid was forced by keeping the concentration C at the surface saturated, while at the bottom $\partial c/\partial z = 0$. The transfer process was simulated for Schmidt numbers ranging from 1 to 32.

Fig. 1a shows a snapshot of the concentration isosurface of 50% saturation together with an x-cross-sectional plane showing the concentration field. Sequences of such images superimposed with their turbulent background flow-fields visualise nicely how eddy structures impinge on the surface from below. Downwelling motions of such eddies initiate the so called peeling process related to surface renewal events, sweeping part of the concentration boundary layer and transporting this oxygen-rich fluid down into the bulk. The upwelling motions, on the other hand, transport oxygen-poor fluid from the bulk up to the surface and at the same time cause a thinning of the boundary layer leading to a higher gas transfer rate.

Buoyant-convective case

Fig.1b shows the results of the three-dimensional DNS run for the buoyant-convective case with Schmidt number = 500. Periodic boundary conditions on the sides and a rigid lid and free slip conditions at the top and bottom were applied. In the laboratory experiments at IfH, the process of buoyant-convection was initiated by introducing cold air above the water surface which in turn generated a cold thermal boundary layer on the water side. Similarly, in the present BC simulations, the temperature at the surface was set to be 3°C colder than that in the water column and random disturbances of 1% were added at t=10 time-units to induce the buoyant-convective instability. The isosurface in Fig. 1b represents a concentration value of 25% saturation. The present BC case show similar flow structures and transport processes as visualized in the PIV-LIF experiments performed at IfH. Shortly after the instability was initiated, the cold upper layer started to sink down in the form of plumes with a typical mushroom shape. These falling plumes transport oxygen-rich fluid from the surface to the oxygen-poor region in the bulk.

As in the experiments, the 3D-DNS results show that the transfer mechanism with buoyant-convective instability is dominated by the continuous movement of sinking

(a) bottom-shear case (BS)

(b) buoyant-convective case (BC)

Figure 1: Isosurface of concentration. a) for the bottom-shear case with Sc=32 and b) for the buoyant-convective case with Sc=500.

and rising plumes, while the continuous motion of eddy structures approaching the interface from below is the main mechanism controlling the gas transfer in shear-free far-field homogenous turbulent environment.

On-going Research / Outlook

Further DNS runs with different turbulent intensities are currently being prepared. In addition, with the present KCFlo code and supported by the increasing computing capacity of the next generation of high performance computers, we would be able to increase the numerical resolution and then be able to perform simulations at higher (realistic) Schmidt numbers (Sc > 32, maybe even up to 500) for the bottom-shear case. Parallel to the above mentioned simulations, a grid refinement study using a dual-mesh approach for the buoyant-convective case is conducted.

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Simulation of broadband noise from high-lift systems

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Introduction

In order to reach the lift force necessary for flight at low speed using wing shapes optimised for cruise conditions, multi-component high-lift configurations can be considered as a standard solution in the civil aviation industry. However, the increase in lift achieved through these measures is paid for by accompanying complex aerodynamic and aero-acoustic phenomena. As a consequence of geometry-induced flow separation, which leads in turn to the shedding, interaction and reattachment of vortical structures, fluctuating surface forces and noise emission can often be observed.

Today, the unsteady flow around high-lift devices and landing gears is known to be a major contributor to the overall noise levels emitted by airplanes during the landing approach, when the engines operate at reduced power. In order to prevent increasing noise exposure caused by the continuous growth in air traffic, the reduction of aircraft noise is an important issue for aircraft manufacturers. A good understanding of the underlying noise generation mechanisms is essential for the development of noise reduction strategies. Insight can be obtained from numerical simulation, which is well suited to provide detailed flow and sound field information.

In this project a three-element high-lift configuration, consisting of slat, main element and flap, is simulated under typical landing approach conditions using a finite-volume based numerical method. Because deployed slats have already been identified as one of the most prominent airframe noise contributors in parametric wind tunnel tests, the main focus of the simulations here is on slat noise generation. To isolate the effect of wing sweep on the sound emission, two infinite-span test cases are studied and compared at approx. equal lift, an unswept wing and a swept wing yawed with a sweep angle of 30°.

Numerical Approach

While small scale turbulence can be modelled in the test cases under consideration, it is important to re-solve the larger vortices in the simulation, because these energetic flow structures are mostly responsible for the sound generation. The large scale vortical motion is captured using the hybrid Delayed Detached Eddy Simulation (DDES) approach, which is based on the solution of ensemble-averaged transport equations in attached boundary layers and the solution of filtered transport equations within separated flow regions. Although the free-stream Mach number is low at landing approach, compressible calculations are conducted, in order to capture mean flow compressibility effects in the slat gap and to incorporate sound radiation in the simulation. An impression of the resolved flow physics using this unsteady and 3-dimensional approach can be obtained from Figure 1.

Figure 1: Snapshot from the slat region of the unswept wing, showing vortical structures and high-frequency sound waves captured in the DDES.

To minimise computational cost for the calculation of acoustic signals at observer positions located far away from the source region, a two-step approach is pursued, whereby the problem is split into a nearfield simulation and a subsequent farfield extrapolation.

Nearfield simulation

A compressible finite-volume code is employed in the nearfield simulation, which is based on the SIMPLE pressure correction algorithm and of 2nd order accuracy in both time and space. An implicit solver with collocated storage arrangement is used to solve the Reynolds-averaged/filtered Navier-Stokes equations on structured multi-block grids, whereby the decoupling of pressure and velocity fields is prevented through a generalised Rhie & Chow interpolation suitable for the simulation of unsteady flows. Non-reflecting boundary conditions allow sound-waves and convective disturbances to leave the computational domain without major reflections. A hybrid, strain-adaptive variant of the Spalart-Allmaras one-equation turbulence model is used for the representation of unresolved scales in the DDES. The code is parallelised via domain decomposition and the data interchange between processors is realised through the standardised MPI-library.

The structured computational mesh enclosing the high-lift configuration consists of ~25 million control volumes, which were arranged in 622 blocks and distributed for 240 CPUs, whereby an even load balancing was achieved.

Farfield extrapolation

In order to obtain the farfield pressure time-series, an integral solution of the equation of Ffowcs-Williams and Hawkings (FWH) is applied, using unsteady flow data acquired on solid and permeable surfaces throughout the nearfield simulation.

Results

The compressible DDES approach proved capable to capture the unsteady flow field surrounding the high-lift configuration [1]. Both noise generation and noise emission were observable in the simulations. A statistical analysis of the acquired unsteady flow field data was performed, and the results give good reason to conjecture, that the interaction of turbulence with the upper slat trailing edge is the principal source of

Figure 3: Variation of cross-correlation coefficient Rpp in time-delay/distance space. The distance is measured from the observer position (black dot) along the black dashed line (see Figure 2). Vertical lines indicate snapshots displayed in Figure 2, the horizontal dash-dotted line marks the upper slat trailing edge position.

sound emission, at least for the investigated high-lift system and settings.

In figure 2 large correlated regions (red/blue), which correspond to low frequency anti-phase wave radiation, can be traced back to the slat upper trailing edge region, following the images in the top row from left to right. Moving further in reverse time (towards the bottom right picture), weakening colours indicate a correlation decay, however the contours can be seen to follow the free shear layer until they almost reach the point of flow separation at the slat cusp.

From figure 3, which shows the correlation coefficient along the dashed line from figure 2 as contours in time-delay/distance space, it can be deduced, that both the size of the correlated regions and the speed at which they move are subject to a sudden change at the upper slat trailing edge. Here, a part of the energy contained within the vortices moving with the flow is scattered into acoustic waves, which are larger in size and propagate at the speed of sound.

The sound generation mechanism thus can be summarised as follows. Instabilities and disturbances in the

Figure 2: Contours of cross-correlation coefficient Rpp (see Figure 3 for colour legend) between pressure signals in the slat vicinity and the pressure signal at a fixed position (black dot) for increasing time-delay between the pressure time-series.

Figure 4: Dipole-like farfield noise directivities obtained from FWH-integration of fluctuating surface pressures on slat. The line pairs enclose the statistical 95% confidence intervals [2] of the sound-pressure-level (SPL).

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free shear layer lead to formation and rollup of vortices downstream of the slat cusp separation point (see figure 1). These turbulent structures are then transported with the mean flow towards a reattachment point on the inner slat surface, before they are either entrained into the recirculation region or ejected through the slat gap. When they pass the edge at high speed in the gap, strong sound waves are emanated.

As shown in Figure 4, the difference in sound emission from the slat between unswept and swept wing configurations is within statistical error bounds. Thus wing sweep appears to have only weak influence on noise generation.

On-going Research / Outlook

The prediction of noise emission from landing gears currently poses a challenge due to their geometric complexity. With further increase in computing power, such simulations will become feasible.

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Numerical Simulation of the Dynamics of Turbulent Swirling Flames

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Introduction

Stringent emission regulations (for NOx, CO, etc.) have been established for gas turbines. In order to comply with these, lean premixed combustion technology has been introduced for stationary engines. However, under this mode of operation, the combustor is prone to blow-out, flashback, and in particular to thermoacoustic instabilities. These instabilities can lead to very high levels of pressure pulsations in a combustor, possibly resulting in structural damage.

To prevent the appearance of these instabilities, a stability analysis of the combustion system is carried out early in the design process. To perform such analysis, it is necessary to know how the flame responds to flow perturbations. This information is provided by the flame transfer function (FTF), which may be obtained experimentally, analytically, or with numerical simulations. The FTF relates the acoustic velocity fluctuations (u') upstream of the flame with the flame heat release fluctuations (q') in the frequency (ω) domain by the following expression:

$$F(\omega) = \frac{q'(\omega)/\overline{q}}{u'(\omega)/\overline{u}} \tag{1}$$

The fluctuations are normalized with their mean values of heat release $\overline{q}$ and velocity $\overline{u}$.

In this study, the flame dynamics of a perfectly premixed axial swirl burner are investigated. To determine the FTF, Large Eddy Simulations (LES) in combination with system identification (SI) methods are applied: First, a LES simulation of the system under consideration is set up. Once a statistically steady solution is obtained, a broadband perturbation is superimposed on the mean flow at the inlet to generate time series of fluctuating velocity and heat release rate. Then the FTF is reconstructed from the data using methods from system identification based on correlation analysis and in the inversion of the Wiener-Hopf equation. The identification process is shown on Figure 1 and described in [1]. The advantage of using LES/SI methods is that it is possible to obtain the flame re-

sponse with quantitative accuracy over a wide range of frequencies from a single LES simulation run, thus reducing the computational effort significantly.

Additionally, investigations on single burner combustor test rigs often play an important role in the early stages of the design process of gas turbines. However, for annular combustors, single burner experiments are in general not representative of machine conditions due to variations in combustor wall temperatures, combustor cross section size, flame-flame interaction between adjacent burners, etc. Such variations, in general, influence both flow field and flame shape.

Figure 1: LES/System identification process.

In this investigation, the validation of the LES/SI method with experimental data is carried out in a first step. Then the potential of the LES/SI approach to detect the impact on the flame dynamics by variations of conditions is investigated and compared with a reference case. This investigation has a special emphasis on variations of the thermal boundary conditions at the combustor wall, combustor confinement ratio and swirler position. The influence of the differences in the flame transfer functions on stability limits is analyzed with a low-order thermoacoustic model.

Setup and Settings

For the present work, the Finite Volume based LES solver AVBP from CERFACS was used. AVBP exhibits a very good parallelization scaling behavior and it is well suited for massively parallel computations. For the simulations

with broadband excitation on HLRB2, 256 CPUs were used. For the reference case, a mesh with 8 million cells was used. For the identification process in this case, 2.8 million iterations were carried out with a computational cost of 7×10^4 CPUh.

In Figure 2, the computational domain of the axial swirl burner for the reference case with nonadiabatic combustor walls (as in the experimental setup) is shown. Reacting flow calculations of a methane-air mixture with an equivalence ratio of 0.77 at atmospheric conditions and 30 kW of power rating are carried out using the Dynamically Thickened Flame Combustion model with one step kinetics and a thickening factor value of 5.

Three additional cases were simulated to study the impact on the flame dynamics by changing the thermal conditions at the combustor walls, increasing combustor cross section area and changing the position of the swirler with respect to the reference case. These variations are detailed in Table 1.

Figure 2: Scheme of the numerical setup of the reference case.

Case	Comb. Wall Temperature [K]	Swirler position* [mm]	Comb. section [mm²]
Reference	600	z=-30	90×90
Adiabatic	Adiabatic walls B.C.	z=-30	90×90
Combustor size	600	z=-30	160×160
Swirler position	600	z=-130	90×90

Table 1: Cases
***z=0 mm at the combustor dump plane (see Figure 1)**

Results and Discussion

Validation

Validation of simulations against experiments for the mean heat release and FTF was carried out only for the reference case [1]. In experiments, the combustor walls are cooled down using convective cooling, resulting in significant heat loss in the combustion products at the outer recirculation zone. Thus the flame is quenched in the outer shear layer and stabilizes predominantly at the

inner shear layer, with the characteristics of a "V-flame". In the simulations, isothermal nonadiabatic walls are used to take into account the effects of heat losses on flame stabilization. Good agreement between experiments and simulations is found in the spatial and axial heat release distribution. In Figure 3, the identified FTF of the reference case using LES/SI is validated against experiments with good agreement. The amplitude gives us an indication of the dynamic response of the flame, and the phase represents a global time lag response.

Figure 3: Identified FTFs at various conditions from LES/SI. Experiments of the reference case are in circles.

Impact of Parameter Variations on the FTF

Comparing the spatial heat release distributions of the various cases in Table 1 with respect to the one of the reference case, the adiabatic case shows a shorter flame with stabilization in both shear layers, while the case with bigger combustor size shows a longer flame with stabilization mainly in the inner shear layer as in the reference case. The case with a varied swirler position shows small differences on the flame shape with respect to the reference case.

In Figure 3, the identified FTFs of all cases are shown. All cases were excited with the same signal. A different flame response between them is observed. With respect to the reference case, the adiabatic case shows a broader response in frequency and a lower steepness of the phase due to the smaller time lags produced by a shorter flame. For the case with bigger combustor cross section, the amplitude shows similar behavior to the reference case, but with the maximum amplitude slightly higher and at a lower frequency. The phase steepness is higher than in the reference case due to the longer flame. For the case with varied swirler position, both flames showed similar flame shape, but they exhibit a quite different flame response, showing two peaks in the amplitude and an increased modulation of the phase for the case with the swirler at a more upstream position. The mechanism of varied flame response with changes on swirler position has been previously investigated by different authors,

and it is related to the different propagation velocity of axial and tangential velocity fluctuations induced by the swirler. The axial velocity fluctuations travel with the speed of sound while the swirl fluctuations with a convective velocity, which is much lower than the speed of sound. This can induce a constructive or destructive mechanism by interactions between flame kinematics, swirl number fluctuations induced by the different propagation speeds, by generation of vortices at the burner outlet, etc. Thus as the swirler is at a different position, the perturbations will take a different time to reach the flame to create a flame response.

The LES/SI results have confirmed that the FTF depends not only on the burner geometry, but also on the boundary conditions, and that there is a strong influence of the swirler position on the flame response. Using an acoustic network model [1], a stability analysis is carried out to assess the impact of such differences in FTFs on combustor stability limits. The analysis indicates that the variations in the predicted FTF may have a significant impact on stability prediction.

Results indicate that the flame transfer function obtained from single burner combustors - be it by experimental or numerical means – should only be used for stability analysis of multi-burner industrial gas turbines provided that operating and boundary conditions, as well as, combustor geometries are equivalent.

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Numerical investigation of complex multiphase flows with Lagrangian particle methods

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Introduction

We have developed a smoothed particle hydrodynamics (SPH) method to simulate complex multiphase flows with arbitrary interfaces and included a model for surface active agents (surfactants) [1]. In SPH the computational domain is discretized with grid-less particles that are evolved in time. This Lagrangian approach is very powerful when complex geometries with strong deformations can occur. As the governing equations for the particles are solved by particle-particle interactions it is straightforward to include complex physical models at phase interfaces where SPH particles of different phases interact with each other.

Surfactants are modelled in our method with a scalar transport equation that includes bulk diffusion, surface diffusion and transport such as adsorption and desorption between an interface and the adjacent bulk phase. As the surfactant concentration at an interface has an effect on the local surface tension the flow evolution and the surfactant concentration field are coupled leading to very complex physics.

Computational details

Since all particle methods rely on particle-particle interactions their computational effort is strongly increased compared to mesh-based simulation tools. Thus, it is even more important to use efficient algorithms and to make use of High Performance Computing. We implemented our method in a FORTRAN-Code as a client application using the PPM-Library developed at the ETH Zürich [2]. This platform offers a fully MPI-parallelized "particle-method-environment" for the user that handles all details of communication and is optimized for the usage of thousands of CPU's.

Results

In the following section we want to present two applications using our SPH method and present selected results of large scale simulations on the HLRBII architecture.

Figure 1: Drop deformation and breakup in simple shear flow at Ca = 0.4, Re = 1 at T=30.

Drop dynamics in simple shear flow

When drops are exposed to extensional flows (e.g. Couette flow) the viscous stresses at the interface deform the drop and are competing with retarding surface tension forces. Depending on the flow conditions and the physical properties of the fluids the drop can either deform to a steady ellipsoid or break-up into two or more droplets. This phenomenon was already studied decades ago and is well understood. When surfactants occur at the drop interface the behaviour can strongly differ from a clean interface. Due to surface concentration gradients the surface tension on the interface can vary locally and induce so-called Marangoni forces that manipulate the break-up process.

Exemplarily we show in Fig. 1 a stretched drop close before breakup where the interface is coloured with the local interface concentration of surfactant. The same experiment for a clean interface results in a similar breakup but much later.

Surfactants do not only change the dynamics of a breakup mode but can also strongly alter the breakup type itself. Fig. 2 shows the so-called tipstreaming phenomenon due to a low diffusive surfactant. Here, the surfactant accumulates mostly at the tips of the stretched drop and the resulting Marangoni-forces suppress the main break-up mode but produce these very thin fluid filaments that leave the drop. This phenomenon was first found in experiments and is of high interest as the thickness of these fluid filaments can be much smaller than any flow focusing device can achieve currently.

Figure 2: Tip streaming of a drop in simple shear flow in the presence of insoluble surfactant at the interface.

We could reproduce this phenomenon with our model and want to study this effect fundamentally in the future [3]. In the presented simulations we used about 2×10^6 particles and ran the calculations on the HLRBII with 256 CPU's for 40 hours.

Multi-species reaction-diffusion in complex geometries
Besides our main interest of simulating surfactant enriched interface dynamics we use our particle method to study transport processes in complex geometries. We have extended our surfactant model for coupled multi-species reaction-diffusion systems and investigate chromium depositioning in fuel cell cathodes [4].

The cold combustion in fuel cells is a promising alternative energy technology that does not produce greenhouse gases. One of the main problems of solid oxide fuel cells (SOFC) that reduces the efficiency dramatically is the chromium poisoning. The current collectors in SOFCs are made of stainless steel that contains chromium. By chemical reaction volatile chromium can migrate into the porous cathode and react with its surface. This effect degrades the efficiency strongly and has to be controlled.

As we are interested especially in the impact of surface diffusion, we do not simulate an entire fuel cell with an air channel, current collector, anode and cathode but study the species dynamics in a section of the cathode to estimate time scales and the influence of reaction rates and surface diffusion on the distribution of a species in the cathode. Then we can use these results to improve continuous coarse-grid models for porous media and study the depositioning of chromium in a real cathode.

For that purpose we take a pixelmap of a section of a real cathode structure (provided by the Pacific Northwest National Laboratory, Washington, USA) and discretize the pores and the air phase with SPH particles, see Fig. 3. The resolution of the block is $32 \times 32 \times 26$, thus a total of 1,048,576 particles is used.

We impose symmetric boundary conditions in x and y direction and prescribe the species concentration at the top layer of the cathode. Besides diffusion in the bulk chromium can react with the surface and diffuse

along the interface into the cathode. Then, due to local non-equilibrium chromium can desorb back to the bulk phase much deeper in the structure than bulk diffusion can transport the species in this time-scale. As an example we show the bulk and interface concentration field of chromium in the cathode in Fig. 4.

Analyzing different parameter combinations we found that finite chromium reaction rates can cause high chromium concentrations deep in the cathode even at very small bulk diffusivity. This complex interplay has to be further investigated aiming for a better understanding of this poisoning process in order to develop more efficient cathodes.

Figure 4: Surface and bulk concentration profile in the cathode for D_s=0.1 and D_∞=1. at T=8.

On-going Research

A key step in the next period of our project is the validation of our results with high resolution simulations. Consequentially we plan to modify our I/O routines to handle large data produced by the simulations and want to explore the functionality of our program for large number of processors ($O(10^3\text{-}10^4)$). Secondly, we want to increase the complexity of the physical models applied in the simulations to detect the dominating effects. In the present study of drop breakup we only consider surface diffusion of insoluble surfactants, but transport phenomena such as adsorption and coupling with bulk diffusion can be included. For the cathode we want to explore a more complex coupled two-species transport model to represent the competitive species dynamics of oxygen and chromium and use more realistic boundary conditions such as prescribed flux conditions and concentration dependent reaction rates.

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Figure 3: Discretization of a section of a real cathode filled with air with SPH particles.

Low-order model and stability analysis of distributed heat release

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Introduction

With the development of lean- premixed combustion technologies thermoacoustic combustion instabilities have become a recurrent problem. In low order modelling of such instabilities [1] the Flame Transfer Matrix (FTM) relating the acoustical properties upstream and downstream of the flame is obtained starting from a Flame Transfer Function (FTF), that relates the acoustic fluctuations of velocity at the burner with the heat release rate of the flame, with the assumption that the flame is an acoustically compact element. This compactness assumption is only valid for Helmholtz numbers $He = k.L_{flame} \ll 1$, where k is the wave number and L_{flame} the flame length. This work a) extends the applicability of low-order models to non-compact conditions, and b) evaluates the damping potential of distributed heat release on the thermoacoustic stability of a combustion system, combining experimental data with computational fluid dynamics (CFD) results. The low order model approach is meant to handle any heat release distribution, and the current numerical study provides realistic and detailed input flame data to a) fully validate the model and b) access the damping potential of distributed heat release under realistic conditions.

The Large Eddy Simulations (LES) are done using the AVBP code (CERFACS/ France), and results are to be compared to experimental data obtained at the University of Cambridge in the framework of the AETHER/ EU project [2].

Results

The low-order model was extended to non-compact conditions: the heat source is now coupled to the fluctuations of the acoustical variables at the base of the flame, allowing direct input of experimental/ numerical Flame Transfer Functions FTF(s), and the approach was validated/ cross-validated with exact solutions and a Finite Volume acoustic solver.

The LES/ System Identification (SI) method used here consisted on a two step procedure. After obtaining a sta-

Figure 1: (top) View of the full 3D combustor with square cross section and 450mm length, showing flame stabilized on the conical bluff body. (middle) Instantaneous and (bottom) average heat release field for the 30 kW shorter flame.

tistical stabilized solution, the system was excited at the inlet and at the outlet with broadband noise superimposed on the mean flow. These broadband perturbations a) propagate to the flame front and create a response in the heat release of the flame and b) reach the boundaries of the computational domain. The velocity and pressure fluctuations at both upstream and downstream of the flame and the heat release fields were exported at every time step and pre-processed to 1D axial resolved data. A final post-processing with a Wiener-Hopf-Inversion correlation technique will allow finding both FTF and FTM for linear regimes and for a chosen frequency range. This will provide both input data for the extended low- order model, i.e. the FTF, and the FTM used to validate the just mentioned low order model.

Two test cases were considered on the CFD computations. One corresponds to a short flame, similar to a standard swirl-stabilized flame and the other to a longer, high power flame. The short flame, shown in Fig. 1, was successfully stabilized and advanced identification signals were applied to both inlet and outlet of the combustor. Figure 2 shows the energy spectra of the downstream (f_{in}) and upstream (g_{out}) running acoustic waves at, respectively, the inlet and outlet of the combustor, and for reference (o) and acoustically excited (Excit) boundary conditions. The use of specific Characteristic Based non- reflecting boundary conditions allow to minimize the inward running reflections from the inlet and outlet (o), providing a high signal (Excit) to noise (o)

ratio for the frequencies of interest (f > 50Hz). This indicates that the System Identification technique will allow extracting both the Flame Transfer Function and Flame Transfer Matrix.

On-going Research / Outlook

The current LES work will provide detailed input data for validation of the distributed flame model (Nnτ) and further insight into the impact of distributed heat release on combustion system instabilities, covering acoustically compact and non- compact conditions. After comparison and cross-validation of the resulting FTM(s), where specific System Identification techniques will allow obtaining the FTM directly from the LES, a stability analysis of the combustion system used in the experiments will be done using the network model tool. On the current work SI techniques [3] will be applied for the first time to a flame in order to extract, besides the standard FTF, the FTM. It will also include a further validation of the distributed flame approach that, having as input the FTF, average temperature and density fields from the LES, should provide 1D acoustical pressure and velocity fields and an FTM comparable to the post-processed LES results.

Besides the broadband excitation runs used for the LES/SI method, additional simulations with a mono-frequency excitation will be done. This allows not only cross-validation of the broadband excitation results, but also provides details on the turbulence/flame interaction and mechanisms that condition the flame response at a given frequency of interest.

In view of the difficulties in stabilizing a realistic long flame on the LES simulations, the planned output data was only achieved up to now for the low power flame. Refinement of the computational mesh and tuning of the combustion model is expected to provide data closer to the experiments for the higher power/ longer flame. A second on-going task is the challenge of actual post-processing of the raw CFD data in order to obtain the FTF. Specific post-processing routines on FORTRAN have been

developed in collaboration with CERFACS to allow extraction of specific thermo-acoustic variables from the raw, 3D, time series data. The LES mesh used on the current project consists of ~11 million cells that, for the above mentioned tracking of the f and g acoustical waves, requires a computational time step of 1.5e-7 s. Furthermore, the overall excited simulation length is 0.3 seconds to identify low frequency oscillations (Nyquist criterion). Then a LES/SI simulation would need at least 2.0e6 iterations, but due to the high level of turbulent noise characteristic of this configuration 3e6 iterations are necessary for a correct identification.

The intrinsic nature of LES (full three-dimensional resolution of the unsteady Navier Stokes equations) makes it very expensive, requiring massive computing resources. The 3D data for each condition tested consists of around 3E6 time steps, with ~150MB of raw data for each time step solution. Even though small scale testing, consisting on extracting time series of velocity at a reference position and of 1D axially integrated heat release, was successfully concluded, the application to the full time series run is yet to be done.

The final task will include a Stability Analysis, where both experimental and CFD data will be used. This task will combine the flame response (FTF) obtained at the experimental campaign with results from current CFD simulations.

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Figure 2: Energy spectra of the downstream (fin) and upstream (gout) running acoustic waves, respectively at the inlet and outlet of the combustor, for reference (0) and acoustically excited (Excit) boundary conditions. These signals will allow identification of the Flame Transfer Function and Flame Transfer Matrix..

Direct numerical simulation of turbulent bubbly flow

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Introduction and methods applied

Bubble-laden turbulent flows are important for numerous industrial processes and many other applications. This report presents results of Direct Numerical Simulations (DNS) of two-phase flows to investigate the interaction between turbulence and bubbles.

The in-house code PRIME solves the Navier-Stokes equation for incompressible fluid on a Finite-Volume staggered grid with a Runge-Kutta pressure-correction scheme in time. The high-level libraries PETSc and hypre are employed for parallelization and the solution of elliptic equations arising from implicit treatment of viscous terms and pressure correction, respectively. The disperse phase is geometrically resolved and represented via an Immersed Boundary method (IBM). For parallel simulations, a master-slave concept was implemented to track the bubbles over the different subdomains. Details of the method are given in [1].

The need for high-performance computing to carry out these investigations is due to the substantial amount of detail being resolved. In DNS, the computational grid has to be fine enough to resolve even the smallest spatial scales of the flow, without any turbulence model. This means that the computational grid has to be very fine, increasing very rapidly the number of cells needed. The simulation at the origin of Fig. 1, for example, was conducted with 1024 x 232 x 512 = 120 Mio grid points. Also the time step has to be small enough to capture the finest scales of motion, and most of all, the simulations have to be conducted long enough to obtain reliable statistical information. In the case of two-phase flow an additional complexity has to be faced, which is to correctly represent the phase boundary. The phase boundary has to be accurately represented with an adequate number of Lagrangian or marker points used by the IBM in order to properly simulate the interaction between the two phases, which is to correctly evaluate the forces introduced by the presence of bubbles.

Results

Simulations of bubble-laden turbulent vertical channel flows have been performed: the flow is periodic in the streamwise (x) and in the spanwise (z) direction and bound by two walls in y-direction (Fig. 1). Bubbles are lighter than the fluid, therefore experiencing a buoyancy force directed upward so that they rise faster than the fluid. The fluid Reynolds number based on the half width of the channel and on the bulk velocity is 2700, which corresponds to a fully turbulent flow, even in the unladen case.

Figure 1: Computational domain, instantaneous fluid velocity in centre plane and snapshot of bubble positions for simulation SmMany in Table 1.

Figure 2: Mean bubble distribution (top), mean fluid velocity (bottom, left) and mean rise velocity (bottom, right).

Three different simulations performed so far, summarized in Table 1. The same numerical grid was used for all the computations on 256 CPUs of the HLRB-Altix 4700. Each simulation took about 90000 CPUh until a statistically steady state was reached and reliable statistics were collected.

Simulation	Number of bubbles	Bubble diameter	Void fraction
SmFew	384	0.052H	0.29%
SmMany	2880	0.052H	2.22%
LaMany	913	0.075H	2.22%

Table 1: Physical parameters of bubble simulations

Small bubbles, effect of void fraction

The bubble Reynolds number based on diameter and relative velocity is 230-260 in the case SmFew and SmMany. The mean fluid velocity profile is barely modified by the bubbles (Fig. 2). The mean bubble velocity is higher in the case of fewer bubbles because of the so-called "hindrance-effect": the higher the volume fraction, the higher the obstruction between bubbles, resulting in higher drag and a lower mean velocity.

The higher mean velocity in the case of few bubbles visible in Fig. 2 could also be the reason for the different wall normal mean bubble distribution: higher (relative) velocity causes a higher mean drag force, which increases the turbulent dispersion yielding a flatter void bubble distribution. Turbulence intensity, quantified by the Reynolds stress tensor, increases with respect to the unladen flow and has a maximum where bubbles tend to concentrate. In the case of many bubbles, concentrating at the walls, the mean wall shear stress is around 15% higher than in the unladen flow, while for few bubbles (which tend to concentrate at a certain distance from the wall) no such augmentation is noticed.

Elongated flow structures in streamwise direction are found in the bubbly flow which are absent in the unladen flow. A similar phenomenon was reported before for the case of settling heavy particle in a similar configuration. Flow visualizations and two-point correlation functions of the streamwise

velocity show a dual influence of the bubbles (Fig. 3): first, with the introduction of few bubbles, some elongated flow structures are created and the flow seems to be more correlated. But with the introduction of more bubbles the velocity fluctuations are larger and the correlation decreases. In both cases the correlation of the flow is lower than the one in the unladen simulation for small streamwise distances, in the order of magnitude of the bubble diameters: bubbles locally generate turbulence which hampers the local correlation of flow structures.

Same void fraction, effect of bubble size

Larger bubbles rise faster than small bubbles because of the higher buoyancy force, with a mean bubble Reynolds number of around 420. Large bubbles tend to concentrate in the middle of the channel (Fig. 2), in contrast with small bubbles. It is a very complex effect, in which the different shape of the wakes may play a leading role. In fact, the bubble Reynolds number is above the threshold at which bubbles begin to experience a zig-zag behaviour when rising [2], also showing an asymmetric wake, that may push, in the presence of a mean fluid velocity gradient, the large bubbles toward the middle of the channel. Simulations of single bubbles in turbulent flows have been performed separately showing a similar behaviour and others are planned to get a deeper understanding of this phenomenon.

The elongated flow structures generated by the large bubbles are more extended in the streamwise direction and show a higher correlation with respect both to the unladen flow and to the flow with small bubbles. The correlation is locally reduced by the presence of the bubbles, presenting a lower value in the middle of the channel where large bubbles tend to concentrate.

Figure 3: Two-point correlation function of velocity in streamwise direction.

Ongoing work and outlook

At the time of writing another simulation is running on SuperMIG. A polydisperse bubble swarm is simulated with the same total void fraction of two of the previous runs, 2.22%. Half of the volume is made of small bubbles and the other half of large bubbles. An instantaneous top-view of the flow in Fig. 4 shows that the different size of the bubbles causes a clear separation between small and large bubbles, as in the monodisperse cases. This feature is also confirmed by preliminary statistical analyses of the mean void fraction which is currently ongoing. The simulations provide important data for the analysis of the complex phenomena responsible for size-dependent segregation which could so far not be explained. Deeper analysis and modelling is currently performed.

Figure 4: Instantaneous bubble distribution, top view (red: small bubbles; green: large bubbles).

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Investigation of Unsteady Flow Structures in the Wake of a Generic Model

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Introduction

The handling characteristics of a car are strongly influenced by unsteady flow structures at its rear end. To quantify their influence and to optimize future vehicles accordingly these phenomena have to be studied thoroughly. As experimental investigations are often complicated through cumbersome measurement techniques, numerical simulations offer a valuable alternative. Especially the use of high-capacity super computers provides the means for a competitive investigation.

In this project transient numerical simulations, including Large Eddy Simulations (LES) and simulations conducted using the Scale-Adaptive Simulation Shear-Stress Transport (SAS SST) turbulence model as implemented in the open source software OpenFOAM®, were performed. In the preliminary stage of the project the efforts were focused on a strongly simplified car model, the modified Ahmed body [1]. This generic car model has the advantage of a manageable case size and a large base of available experimental data.

Thus, the numerical results can be compared to time-accurate surface pressure measurements and force measurements and the accuracy of the results can be ensured. In a later stage of the project a new realistic generic car model – the DrivAer model – is introduced and simulations of this model will be performed on the new Super-MUC computer.

Background

The unsteady effects at the rear end of a vehicle and in its wake that strongly influence its dynamic behaviour are still not understood sufficiently.

As the flow around a car is highly turbulent it is therefore unsteady. Periodic vortex shedding has been observed in the wake of vehicles. These unsteady wake structures lead to time-dependent pressure forces at the vehicle surface and thus induce fluctuating forces and moments. The unsteady forces influence both the cars safety and

its driving comfort. If the unsteady behaviour is not considered in the vehicles design phase, the vehicle cannot be optimized effectively with respect to these aspects.

A lot of the current investigations are still focused on strongly simplified generic bodies, such as the Ahmed body or the SAE body. This is due to the fact that the unsteady investigation of an actual production car is connected to enormous computational effort and can only be realized with the resources of a super computer.

On the other hand, it is quite complicated to find time-accurate reference measurements of realistic production vehicles. Therefore, in a first step, the unsteady effects at the backlight of the Ahmed model were investigated; the findings will then be transferred on to a realistic generic car model and further unsteady simulations will be performed on the new SuperMUC super computer.

The numerical investigations were performed using the Open Source code OpenFOAM®. The CFD Toolbox Open-FOAM® consists of a very flexible set of C++ modules. These can be used to easily build and adapt e.g. solvers, pre- and postprocessing utilities. OpenFOAM® can be run parallelized on multiple processores, although a drop in performance has been reported with growing parallelization.

In a first step, different steady-state OpenFOAM® Reynolds averaged Navier Stokes equation (RANS) solvers were tested for their ability to correctly reproduce the detachment and even more importantly the reattachment of the flow over a backward facing step. The k-ω-SST model shows the most promising results and was therefore chosen for the preliminary RANS simulations. Starting from a converged RANS solution a LES simulation of the Ahmed body was performed. As a subgrid scale wall model, the Smagorinsky model was chosen.

For the discretization of the convective and viscous fluxes a second-order central differencing scheme was selected whereas the time discretization was approximated by a second-order three point backward scheme. As LES of

complex geometries are still very time-consuming and need a lot of computational resources, the capabilities of the SAS SST model were reviewed for the following unsteady investigations. Preliminary investigations were performed on different meshes of the Ahmed body and compared to both the LES simulation and to experimental results. The SAS SST model is based on the introduction of the von Karman length scale L_{vK} into the turbulence equation of the k-ω-SST model.

This allows the SAS models to dynamically adjust to the resolved structures in unsteady RANS simulations. For attached flows the model gives RANS-like solutions while it shows LES-like behaviour in unsteady regions of the flow field. Thus, the SAS SST model acts quite similarly to the DES model, but is not restrained by whose explicit grid dependence in the RANS region.

Computational Resources

The simulation of transient phenomena is typically connected to high computational requirements as already mentioned above. This is primarily due to the necessary resolution of the computational domain to be able to resolve the small scale turbulent structures and the thereby required small time steps to guarantee convergence. Even a relatively coarse grid of the Ahmed body with approximately 15 million cells at an inflow velocity of 40 m/s needs about 25,000 CPU-hours to reach the converged turbulent state and accordingly even more computational time to be able to draw conclusions about transient phenomena. Simulations of this order of magnitude can only be performed on super computers.

Computational Setup

The computational domain chosen for the Ahmed body has a total length of 8L, a total width of 5W, and a total height of 5H with respect to the model length L, the model width W and the model height H. The body is positioned 5L from the outlet, so the outflow boundary conditions do not influence the wake close to the body. The inflow plane is placed at a distance of 2L upstream of the body to create realistic flow conditions in front of the vehicle. This distance corresponds roughly to 7H and was chosen to minimize the blocking effects.

The simulations were conducted at the inlet velocity u = 40 m/s. That corresponds to a Reynolds number of approximately Re=7x10^{5} with respect to the model height H. The RANS simulations were performed using the

k-ω-SST model. To ensure convergence, the RANS simulations comprised 10000 time steps. For the LES simulation the incompressible and unsteady solver pisoFoam was chosen. In order to limit the maximum CFL number to 0.75 and ensure the convergence of the simulation, the time step was chosen as 2 x 10^{-6} s. At the Ahmed body and the floor wall functions were used. The total simulated time spanned 0.435 s, approximately twice the time a fluid particle would take to transverse the length of the virtual wind tunnel. The unsteady SAS SST simulations were started from converged SST simulations and used the unsteady solver pimpleFoam which adapts the time step to fit a previously chosen maximal CFL number. A fully converged solution of the SAS SST was reached after 1.58s.

Results

The LES results presented in this paper are based on a medium spaced grid. The focus of interest lies on the instantaneous flow field around the rear slant of the body. The data was compared to the experimental data by Lienhart et al.[2] and the experimental data gathered in the Windtunnel A of the Institute of Aerodynamics and Fluid Mechanics at the TU München.

Figure 1 shows the visualization of the vortical structures around the Ahmed model using the Q criterion. The flow separates at the sharp edges between the side of the body and the slant and produces two counter rotating cone-like vortices.

Table 1 shows the comparison of the drag coefficient c_D of the various simulations to the experimental value measured in the Wind Tunnel A at Technische Universität München.

	Experiment	SST	SAS	LES[1]
c_D	0.297	0.302	0.275	0.256
Δ	0	2%	-7%	-14%

1 The LES was performed on a different grid.

Table 1: Comparison of the c_D value of the Ahmed body.

The averaged c_D value calculated during the LES simulation performs poorly when compared to the experimental value. While the flow separates at approximately the right position the separation bubble is overestimated and the flow does not reattach over the length of the slant. As the area of separated flow at the slant is responsible for a large amount of the total drag the poor prediction of the c_D value is not surprising.

Figure 1: Vortical structures in the wake of the Ahmed body visualized through the Q criterion.

On-going Research / Outlook

State of the art research on unsteady automotive aero-dynamics often employs strongly simplified car models, such as the Ahmed body. Due to their high degree of abstraction, however, the insights gained cannot be readily transferred to the development of actual production cars. This is especially true where complex body surfaces are involved, such as the A-pillars, the highly curved rear end, and the wheelhouse region. To close this gap a new reference car model for aerodynamic research the DrivAer body is proposed [3]. Its geometry and validation data will be published to encourage independent studies. Numerical simulations of the DrivAer model, both steady state and time-accurate, will be performed on the new SuperMUC super computer.

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Numerical Investigation of the Flow Field about the VFE-2 Delta-Wing

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Introduction

The industrial application of Delta-Wings is manifold and reaches from the classical aerospace engineering, e.g. highly agile aircraft, aerodynamic devices or control surfaces, to unique environmental technologies, such as devices for snow clearance. In all cases the development of leading edge vortices is exploited.

However, steadiness and stability of these leading edge vortices is essential for controllability, particularly for highly agile aircraft. It is well known that vortices can undergo a sudden expansion often related to vortex breakdown [5]. The occurrence of unsteady vortex breakdown is critical for aircraft. It is physically not fully understood, thus further investigation is required. The on-going investigation is funded by the DFG project "Numerische Untersuchung der instationären Strömung um generische schlanke Deltaflügel' "(DFG-B-506/2). The international Vortex Flow Experiment 2 (VFE-2) Delta-Wing is taken as a generic aerodynamic configuration for which small angles of attack already lead to the development of leading edge vortices.

Underlying Theory

A profound understanding of vortex formation and breakdown requires a comprehensive insight into the complete unsteady flow field. This insight can only be obtained from time-accurate simulations accompanied by experiments. The most complete description of flows in continuum mechanics is given by the Navier-Stokes equations, which describe the exchange of momentum in the fluid considering friction.

Solving the Navier Stokes equations requires very high spatial and temporal resolution. A Direct Numerical Simulation

(DNS) is still not feasible for complex turbulent flows in industrial applications due to the required tremendous computational resources. For simulating the turbulent flow about the VFE-2 Delta-Wing several hundred CPU years using 1 Terra flops would be needed, making a simplification of the Navier Stokes equation inevitable.

Commonly used in industry is the RANS (Reynolds-Averaged Navier Stokes) simulation with appropriate statistical turbulence models. This simplified approach often fails to accurately predict separated and reattached flows. Also in the case of the VFE-2 Delta-Wing results do not compare well with the existing experimental results [9].

Better results are expected from Large-Eddy Simulation (LES). In LES only the large flow structures are resolved while small, stochastic structures are modelled with the help of SubGrid Scale (SGS) models. In Implicit Large Eddy Simulation (ILES) the truncation error of the discretization of the convective terms is deliberately tailored to act as a SGS-model which is therefore implicit to the discretization. One implementation of ILES is the Adaptive Local Deconvolution Method (ALDM) [1, 4] which has shown considerable potential for the efficient representation of physically complex flows in generic configurations, such as isotropic turbulence, turbulent channel flow with periodic constrictions, turbulent boundary layer separation and turbulent cylinder flow [7]. In this project the ILES approach will be used for the essential numerical investigations.

Numerical Method

The Adaptive Local Deconvolution Method (ALDM) turbulence model is incorporated in a solver for the incompressible Navier-Stokes equations with constant density. Continuity is ensured by the pres-

Figure 1: Isosurface of streamwise vorticity colored by streamwise velocity for the VFE-2 Delta Wing at an angle of attack of 13° and a Reynolds number of 0.5 million.

u: -0.1 0.1 0.3 0.5 0.7 0.9 1.1

sure-Poisson equation. The equations are discretized on a staggered Cartesian mesh allowing for an easy control of the truncation error and offering superior computational efficiency compared to body-fitted grids [6]. Bounding surfaces of the flow that are not aligned with the grid are accounted for by the Conservative Immersed Interface (CIIM) approach [8].

For time advancement an explicit third-order Runge-Kutta scheme is used. The pressure-Poisson equation and diffusive terms are discretized by second-order centred differences. Further improvement of efficiency is achieved by modelling the turbulent boundary layer using a wall model [2] and by locally adapting the mesh resolution with Local Mesh Refinement, such as used in [7]. In this context new criteria for the Local Mesh Refinement algorithm based on physical criteria are applied. A further considerable reduction of the number of computational cells is achieved, rendering the simulation much more effective.

Results

The results in this reporting period have been obtained for a Reynolds number Re = 0.5 million based on root chord length and an angle of attack of 13°. The objective is to reach a qualitative agreement with the respective experiments of Furman and Breitsamter [3].
For this angle of attack both, experiment [3] and the current simulation, show vortex formation over half chord length, see Fig. 1. Close to the apex the boundary layer flow accelerates over the leading edge and undergoes laminar-turbulent transition. This is also reflected by the high suction levels visible in Fig. 2. Severe pressure gradients in lateral direction provoke boundary layer separation further downstream. The separation region is indicated by the low pressure regions on the upper surface of the wing (see Fig. 2).

Qualitative results for this specific configuration look very promising. A profound understanding is expected after results have been quantitatively validated with the experimental data. The necessary simulations are on-going.

Figure 2: Cp distribution on the upper (top) and front (bottom) surface of the VFE-2 Delta Wing at an angle of attack of 13° and a Reynolds number of 0.5 million..

Computational Details

For this test case again a SGI-ALTIX with ItaniumII processors have been used. CIIM and the wall modelling consume 2% of the overall computational time, the flux calculation with ALDM accounts for 7% and the Poisson solver uses 83%.

Table 1 summarizes further computational details for the present and planned simulations.

AoA [°]	Re[-] in mio	LE	N_{cells} in mio	N_{CPU}	CPUh in mio
13	0.5	MR	20	1024	0.9
13	1	MR	20	1024	0.9
18	1	MR	40	1024	1.2
18	1	S	40	1024	1.2
23	1	MR	40	1024	1.2
23	1	S	40	1024	1.2

Table 1: survey of conducted simulations (black) and planned simulations (grey). (AoA = Angle of Attack, Re= Reynolds number, LE=Leading Edge, number of cells, number of CPUs, number CPU hours)

On-going Research / Outlook

Since the objective is to investigate vortex bursting process, further investigation at the angles of attack of 18° and 23° is with varying leading edge geometries, i.e. MR= Medium Round and S= Sharp, are planned. As a next step an investigation is planned for actively controlling and preventing the vortex burst with leading edge devices, i.e. oscillating control surfaces.

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Direct Numerical Simulations of turbulent Rayleigh-Bénard convection

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HLRB Project ID: pr47he, pr63ro

Introduction

The large structures occurring in the fluid flow on the Sun's surface, in the atmosphere and oceans of planets, including our Earth, are primarily driven by convection. Their actual shape but also the efficiency of the heat transport is however significantly influenced by the Coriolis force due to rotation. Crystal growth and the ventilation of buildings and aircrafts originate within the same physical framework. Understanding these fundamental processes is thus not only utterly important for geo- and astrophysics, but also in industry.

That is, where the idealisation, the so-called Rayleigh-Bénard convection comes into play: The above mentioned highly complex phenomena are simplified to a fluid heated from below and cooled from above, with solely gravity, and hence buoyancy, acting on it. In most of the theoretical and numerical investigations of natural convection the Oberbeck-Boussinesq (OB) approximation is considered. This means that all physical properties of the fluid are assumed to be independent of temperature and pressure, except the density in the buoyancy term which is considered linearly dependent on the temperature. These assumptions are evidently never fulfilled in reality and the deviations of the flow characteristics due to their violation are called non-Oberbeck-Boussinesq (NOB) effects.

Thus the objective of our studies is to investigate the influence of rotation and NOB effects on turbulent thermal convection, also, but not exclusively, at very high Rayleigh numbers. We address these issues by means of Direct Numerical Simulations (DNS).

Numerical method

We performed high-resolved direct numerical simulations of Rayleigh-Bénard convection making use of the well-tested fourth order finite volume code FLOWSI [2]. The code solves the incompressible Navier-Stokes equations and has shown an almost perfect scalability on the HLRB II cluster (figure 1).

For the purpose of investigating NOB effects, the code has been advanced by taking temperature-dependent material properties into account. Furthermore, we incorporated a module to model the effects of rotation.

The mesh size was chosen in a way to fulfil the criterion by Shishkina et al. [5], which guarantees the resolution of the smallest relevant scales, i.e. the Kolmogorov and the Batchelor scale.

So far, our simulations focussed on two fluids, water (Pr = 4.38) and glycerol (Pr = 2547.9). Their material properties were adopted from experimental data by Ahlers et al. [1]. The parameter ranges for our performed NOB simulations are given in figure 2, together with the estimation of the validity range of the OB approximation according to Gray & Giorgini [2]. In sum, we covered the range of Rayleigh numbers $10^5 \lesssim$ Ra $\lesssim 10^9$ and NOB conditions up to a temperature difference Δ between the top and bottom plate of 80 K.

Self-evidently, we performed the corresponding OB simulations for the purpose of comparison as well. Furthermore, we also conducted DNS for different rotation rates under OB and NOB conditions.

Figure 1: Scaling behaviour of the FLOWSI code (pink diamonds) on HLRB II. The perfect scalability of an ideal code is shown as well (black dashed line).

Figure 2: Validity range of the OB approximation according to Gray & Giorgini [2] for water (top) and glycerol (bottom). The pink stars mark the parameters for our NOB simulations.

However, not only the required resolution but also the necessary computation time to obtain reliable statistics, that is at least several months, pushes us to the limits of nowadays supercomputers.

Results

Our NOB simulations revealed that the temperature dependencies of the material properties are able to significantly influence the global flow structures. In general they lead to a breakdown of the top-bottom symmetry typical for OB simulations. The NOB effects that we observe, include, but are not limited to, different thermal and viscous boundary layers, asymmetric plume dynamics and an increase of the bulk temperature T_c (figure 3 & 4). In glycerol for the NOB case $\Delta = 80$ K we obtain a T_c that is 15 K higher than the arithmetic mean temperature between the plates, whereas in contrast, in the case of water the observed increase of T_c is only about 5 K.

Nevertheless, the Nusselt number Nu and the Reynolds number Re and their scaling with Ra show only a slight deviation from the OB case.

In rotating convection another physical phenomenon plays an important role - the formation of columnar vortices, as seen in figure 3. These so-called Ekman vortices are able to extract hot and cold fluid from the bottom and top boundary layers, respectively, and thereby increase the heat transport. They are also responsible for a persisting mean temperature gradient in the bulk. Their size, and related to that their efficiency, is determined by

the heat diffusivity and viscosity, thus they are sensitive to NOB effects. Indeed, while T_c is the same as in the non-rotating case, the absolute value of the temperature gradient is diminished. In line with this, the enhancement of Nu under rotation is stronger under NOB than under OB conditions.

On-going Research / Outlook

A next step on studying NOB effects will be the inclusion of compressible convective flows, i.e. almost all gases, where the Low Mach Number (LMN) approximation will be used, which generally admits the working fluid to be a non-perfect gas. And since in an astronomical and geophysical context Ra is typically rather in the order of 10^{20}, we plan to go to higher Ra, which are of course computational more expensive, because of the mesh size and the required time for sufficient statistics. Additionally, we plan to test existing and as appropriate develop subgrid scale models and perform large-eddy simulations (LES).

Acknowledgments

Figure 3: Instantaneous temperature isosurfaces of water (Pr = 4.38, Ra = 10^8, magenta indicates the warm, cyan the cold fluid), shown are the non-rotating OB (upper left) and NOB case (upper right), as well as a moderately rotating OB (lower left) and NOB case (lower right).

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Figure 4: Instantaneous temperature isosurfaces of glycerol (Pr = 2547.9, Ra = 10⁹) under OB (left) and the NOB conditions (right).

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Coherent flow structures in indoor ventilation

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HLRB Project ID: pr47vi, pr28xa

Introduction

From a physical point of view, the problem of indoor ventilation is a classical example of mixed convection, which is characterized by complex transport mechanisms resulting from the interaction of natural and forced convection. Responsible for the former type of convection is the buoyancy force resulting from temperature induced density differences, while the latter is driven by an imposed pressure gradient. Investigations of room ventilation often aim at comfortable and healthy conditions in buildings, cars or aircraft (for details we refer to a review by Linden [1]). This can be achieved by reaching a proper balance between natural and forced convection.

In the past turbulent mixed convection of air has been investigated mainly in experiments. Schmeling et al. [2] for example, conducted Particle Image Velocimetry measurements of mixed convection in a rectangular convection cell. Fitzgerald and Woods [3] also considered geometrically simple parallelepiped rooms heated from below by uniform heat sources, without any obstacles inside and Gladstone and Woods [4] a simplified geometry of a naturally ventilated room with a heated floor and two openings to the colder ambient air.

Most of the numerical investigations of mixed convection in air have been conducted either for the laminar flow regime, as reported for example by Ehrhard, or if a turbulent flow was considered, by solving the Reynolds-averaged Navier-Stokes (RANS) equation with different types of turbulence models. A comparative study by Blay et al. [5] who tested some available turbulence models revealed large discrepancy of the RANS predictions of mixed convection, for which they made the turbulence models responsible. In particular, Blay et al. [6] found that some of the RANS simulations predicted large-scale circulations rotating in the opposite directions although the physical parameters were the same. Therefore, reliable turbulence models for accurate predictions of mixed convection in complicated domains with external and internal walls are needed.

For the development of such turbulence models, Direct Numerical Simulations (DNS) or well-resolved Large Eddy Simulations (LES) can provide flow details needed to improve these models. In this respect, Kenjeres et al. [7] computed turbulent mixed convection in rectangular enclosures by means of LES using fine meshes.

Their LES results agreed well with those of DNS which they performed for comparison. Additionally, Nielsen et al. [8] conducted DNS, though their simulations turned out to be underresolved.

The objective of the present study is to establish a data base containing instantaneous and one-point correlations of turbulent mixed convection predicted by well-resolved DNS. To extract the contribution of thermal convection, the obtained results are compared to those of DNS of forced convection. The considered parallelepiped enclosure with four parallelepiped obstacles inside and two inlet ducts and two outlet ducts, represents a generic ventilated room or an aircraft cabin.

Fig. 1. Sketch of the domain: the obstacles are heated and the inflows are cooled.

Fig. 2. Scaling of the code on HLRBII Altix (green) compared to the ideal scalability $t_{wct} \propto 1/\#CPUs$ (black).

Computational domain, numerical method and scaling of the computational code

We consider a computational domain reflecting a box with 4 parallelepiped ducts for the inlet and outlet flows, which are connected to the box as shown in Fig. 1. The length, height and width (without ducts) of the domain are denoted as L, H and D, respectively. Through two thin ducts, located close to the top, cold air enters the domain. The length, height and width of the inlet ducts are L, H/150 and W, respectively. Two outlet ducts extending LxH/20xW are located close to the bottom. There are 4 heated parallelepiped obstacles inside the box, which are elevated at a distance H/20 from the bottom and are orientated in a parallel manner. The length, height and width of the obstacles are L, H/5 and D/10, respectively. The distance between the central obstacles is D/5 and the other distances between the obstacles or between the walls and the nearest obstacle equal D/10.

The DNS are carried out with a well-tested, fourth-order, finite-volume code FLOWSI [9] which is advanced for treating domains with interior walls [10] and parallelized. It showed an excellent scaling behaviour on the HLRB II Altix cluster (see fig.2). The incompressible Navier-Stokes equations were solved in Boussinesq approximation being appropriate for a first attack of the higher parametric range, facilitating comparisons with laboratory and other simulation data, and permit to focus on the most essential physics.

To conduct DNS we use very fine meshes, the mean mesh size of which is smaller than the Kolmogorov microscale.(see Fig. 3). Therefore the parallelization of the code is implemented via a spatial domain decomposition in vertical direction to solve the temperature and velocity equations and via distribution of the decoupled pressure source terms in horizontal direction to solve the Poisson equation, both by using the Message Passing Interface (MPI). The scalability of the code on the National Supercomputer HLRB-II SGI Altix 4700 is shown in Fig. 2 exhibiting a perfect, almost linear behaviour for up

to 1024 CPUs. The simulations were performed using a mesh of 384x512x192 nodes and 1000 time steps for 4 to 64 CPUs and 4096x4096x128 nodes for 100 time steps for 64 to 1024 CPUs normalized to the value at 64 cores.

Results

By means of DNS instantaneous and statistical characteristics of turbulent forced and mixed convection in the above described domain were generated. The working fluid is air with Pr=0.714. Ra = 3e8 and Re = 2.37e4.

In Fig. 4 distributions of the instantaneous temperature computed in this DNS are presented. They illustrate complicated turbulent flow structures which are typical for indoor ventilation problems. The results of our DNS reveal that in the cases of forced and mixed convection different large-scale circulations develop inside the domain, although the same geometry and the same Re are considered. In particular, for Re = 2.37e4 a downward flow is obtained in the case of forced convection, while mixed convection leads to an upward flow in the central part of the domain.

Distributions of the mean heat fluxes at the surfaces of the obstacles reflect large variations, and they strongly depend on the positions of the surfaces (vertical or horizontal) as well as on their locations inside the domain.

The heat flux variations are explained by the flow topology close to the obstacles, which is developed in the ventilated room. This in combination with the dominance of the convective nature of the heat transfer leads to the heat flux variations over the obstacles' surfaces. For the same reasons the heat flux in the interior of the domain is irregular as well. Thus the mean vertical heat flux in the central part of the domain between two central obstacles can be up to 5 times larger than the Nusselt number. The largest values of the heat flux magnitude is obtained near the inlet ducts, where the central buoyancy dominated warm up flow meets the inertia dominated cold inlet flow, due to the high temperature gradients there.

The above obtained and formulated results are general and expected to be valid also for more complicated do-

Fig. 3. Mean mesh size visualized in the central vertical cross-section (left) and ratio between the mean mesh size and the Kolmogorov length scale for Gr = 4.22e8, Re = 2.37e4.

Fig. 4. Snapshots of the temperature, as obtained in the DNS for Ra = 3e8, Re = 2.37e4. The scale ranges from blue (low values) to red (high values).

mains in real indoor ventilation problems. The exact locations, where the inertia dominated cold inlet flows meet the large-scale buoyancy dominated warm flow, are of course model-specific, i.e. they depend on the geometry of the domain and on the balance between the temperatures of the inlet flows and the obstacles as well as on the magnitude of the inlet velocity.

For further development of turbulence models for heat transfer in mixed convection as well as for RANS validation, a DNS data base of instantaneous velocity and temperature felds for different geometrical and physical parameters of the mixed convection system is required. The presented simulations are the first contributions to this data base.

On-going Research / Outlook

The complexity of DNS of turbulent thermal convection grows approximately as the Rayleigh number Ra taken with exponent 1.1. Since we intend to investigate mixed convection in the above described domains for the Rayleigh number up to Ra=1.0e11,(which corresponds to the indoor ventilation in reality), the expected complexity of our future DNS is up to 600 times higher than that of our already conducted DNS. Therefore much more computational ressources and further advancement of the computational code are needed for our studies. The up to now obtained results on DNS of indoor ventilation are discussed in detail in our new paper [11].

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Fluid-Structure Interaction between Thin-Walled Structures and Turbulent Flows

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**Figure 1: Outdoor giant tent
(Khan Shatyr in Astana, Kazakhstan, www.khanshatyr.com)**

Introduction

Fluid-Structure Interaction (FSI) is a topic of major interest in many engineering fields. Beside experimental investigations numerical simulations have become an important and valuable tool for solving this kind of problem. Moreover, the significant growth of the computational capabilities during the last years allows solving more complex coupled problems whereby the physical models get closer to reality.

Our lab cooperates with the civil engineering department of TU Munich and our long-term objective is the coupled simulation of big thin membranes exposed to turbulent flows such as outdoor tents or awnings (cf. Figure 1). To study these complex FSI problems, a multiphysics code was developed.

In order to assure reliable numerical simulations of complex configurations, the whole FSI code needs to be validated at first on simpler test cases with reliable reference data. For laminar flows a few benchmarks are available in the literature, but for the turbulent regime the test cases are very rare and often too challenging. Consequently, the short-term goal of this work is to prove the numerical methodology developed for flexible shells and membranous structures exposed to turbulent flows.

Numerical methodology for turbulent FSI benchmarks

In order to reach the final objective to tackle civil engineering FSI applications, it was decided to use highly advanced solvers for both subtasks (fluid and structural mechanics) and to couple both with a third program. So, the resulting coupling scheme is partitioned and divided into three parts:

- The fluid solver FASTEST-3D is a parallelized finite-volume 3D CFD solver. To model turbulent flows, eddy-resolving schemes such as Large-Eddy Simulations (LES) is chosen [1-4]. Direct Numerical Simulations (DNS) is not applicable here due to their enormous CPU-time requirement. The Reynolds-Averaged Navier-Stokes (RANS) method is not used, because of its inability to predict non-equilibrium turbulent flows. The LES technique is obviously the best choice for highly unsteady turbulent flows involved in FSI applications.
- The structure solver Carat++ [5] developed by TU Munich is a finite-element solver specialized in the prediction of shells or membranes, which are appropriate models for thin structures.
- The coupling program CoMA [6] developed by TU Munich is responsible for the exchange of data between the two specialized solvers. Due to different discretization techniques used in the subtasks, different types of grids and different grid resolutions, grid-to-grid data interpolations are necessary. The exchange is carried out via MPI.

One of the big challenges of this work is the CPU-time requirements. Indeed, to get suitable results in FSI a "strong" coupling is highly recommended. For partitioned solution algorithms this means that a subiteration process is required in each time step in order to guarantee dynamic equilibrium between the fluid and the structure. To reduce the CPU-time consumption a special procedure for eddy-resolving schemes requiring small time steps was developed. For this purpose the CFD solver uses an explicit time-marching scheme, i.e. a predictor-corrector scheme. The predictor step advances the momentum equation in time leading to a prediction

a) T_o

(b) $T_o + 1/4\ \Delta T$

(c) $T_o + 1/2\ \Delta T$

(d) $T_o + 3/4\ \Delta T$

Figure 2: Temporal development of the turbulent flow field and the flexible structure, streamwise velocity distribution in a x-y plane.

of intermediate velocities. Then in the corrector step the mass conservation equation is solved and the velocities are corrected. In the present FSI coupling scheme solely the corrector step is incorporated in the subiteration loop. Consequently, a lot of CPU-time is saved [1].

FSI test case in the turbulent regime (FSI-LES)

The whole FSI code had to be validated. In order to do that each program was first checked separately. FASTEST-3D and Carat++ were validated based on many simple and complicated benchmarks [1-4,7]. The coupling program CoMA was also validated with simple data transfers. Then the whole FSI program was verified on the FSI3 laminar benchmark [8] and gave good results [1]. So the next step was to test it in the turbulent regime.

The FSI-LES benchmark was directly derived from FSI3. The geometry is the same: a flexible plate attached at the backside of a fixed cylinder is mounted into a water channel. The Reynolds number was increased to $Re=10^4$ so that the flow is in the sub-critical regime [1]. To solve this multi-physics problem a grid consisting of 17 million control volumes for the flow and 10x10 shell elements for the structure was used. The FSI computation was run on 144 processors of the SGI ALTIX at HLRB Munich and took about 280,000 CPU-h. In the meantime, the entire code was successfully ported to SuperMUC/SuperMIG.

The structure exposed to the flow leads to the formation of an alternating vortex-shedding behind the cylinder. As a consequence oscillating forces are generated on the structure. The flexible plate begins to deform and after a few seconds reaches a quasi-periodic mode of oscillations. In Figure 2 a complete cycle of the structural oscillations is shown based on the distributions of the streamwise velocity in a x-y plane.

Conclusions and Outlook

To respond to the need in civil engineering to be able to predict turbulent flows around thin membranes, a FSI

code was developed. It uses highly specialized solvers (a FV solver based on LES and a FE solver with shell elements) and a special coupling procedure to reduce the CPU time requirements. Each program was validated separately and the whole FSI methodology was verified on a FSI laminar benchmark. With the help of the computational power of HLRB Munich the FSI code was checked on a FSI turbulent test case and delivers very encouraging results. The next step is to compare numerical FSI simulations with complementary experimental data measured in the water channel of the lab. This part of the work is in progress.

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Direct numerical simulation of the formation of subaqueous sediment patterns

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Introduction

The formation of sediment patterns is a common occurrence in river and marine flows as well as in various technical applications involving shear flow over a bed of mobile sediment particles. The process of erosion of particles from the sediment layer and their deposition at certain preferential locations often leads to bed shapes which are commonly described as *ripples* or *dunes*. From an engineering point of view it is highly desirable to be able to predict the occurrence and the nature of this phenomenon, since the bedform significantly influences flow characteristics such as resistance, mixing properties and sediment transport. These modified flow quantities in turn have far-reaching consequences for the operation of diverse facilities in hydraulics, chemical engineering, etc.

Experiments show that at low flow rates small-scale undulations of the sediment bed appear, having no clear-cut shape [1]. When increasing the flow rate in a given experiment, these ripples give way to the much larger dunes, which have an asymmetric shape with a steeper slope on the downstream side of the crests, where flow separation and recirculation occurs, and which propagate downstream. At even higher flow rates the so-called *anti-dunes* appear which tend to propagate upstream.

Most of the previous theoretical work on the formation of ripples, dunes and similar sediment patterns is based upon the notion that a flat bed is unstable with respect to perturbations of sinusoidal shape. Over the years a number of researchers have studied this stability problem for a variety of flow conditions, in the laminar and turbulent regime. Invoking a disparity in time scales between the flow and the bed shape modification, most approaches have considered the bed shape as fixed for the purpose of the analysis. The hydrodynamic stability problem is then complemented by an expression for the particle flux at a given transversal section of the flow. In most of the contributions the particle flux is supposed to be directly related to the local shear stress [2].

Other approaches take into account relaxation effects through a separate differential equation for the particle number density [3].

Compared to experimental observations current stability results can be broadly described as unsatisfactory, sometimes predicting ripple wavelengths which are off by an order of magnitude. The reason for this disagreement can be linked to a poor description of the dynamics of particle motion near the mobile bed.

Objectives

The objective of the present project is to contribute to the elucidation of the physical mechanisms involved in the formation of sediment patterns driven by (turbulent) shear flow. In practice the contribution will consist of several aspects. First, we will provide a complete description of the flow field as well as particle-related quantities (trajectories, velocities) for idealized flow configurations at low Reynolds numbers. Secondly, we will be in a position to test the various existing theories for pattern formation based upon our data. Third, thorough analysis of numerical data as well as interaction with experiments should allow us to establish an improved model of sediment pattern formation.

We are simulating the development of subaqueous bedforms by means of high-fidelity numerical simulations which resolve all the relevant length and time scales of the turbulent flow as well as the individual sediment particles. We are considering a horizontal channel flow with a very large number of freely moving spherical particles representing the mobile bed. The particles will be initially packed to form a horizontal bed at the bottom of the channel. Flow will then evolve and develop over the bed with time. We will investigate the bedform initiation and evolution processes, at a range of parameter values both in the laminar and turbulent regimes. A detailed account of our numerical method can be found in [4].

Figure 1: Snapshot of instantaneous particle positions in a preliminary simulation of the motion of an isolated dune on a smooth surface, driven by channel flow. The particles are colored with respect to their vertical distance from the bottom wall (blue for the lowest and red for the highest). White lines represent Streamlines of the driving flow field.

Results

We have taken the opportunity to perform several preliminary simulations on HLRB2 before it was shut down in October 2011 (please note that we have been granted computing resources for this project on August 2011) to demonstrate the feasibility of performing direct numerical simulation of the phenomenon of sediment pattern formation. The carried out simulations consist of the propagation of an isolated dune on a smooth surface similar to the experimental setup described in [5]. Initially a conical heap, made up of more than 26,000 heavy spherical particles, was submerged in a quiescent fluid. The fluid flow rate was then ramped up to generate a turbulent flow at a bulk Reynolds number of about 3000. The particle heap immediately starts to migrate and deform. Figure 1 shows a snapshot of the particle positions during the course of the simulation. As a result of a complex interplay between the particles and the driving flow field, a croissant-shaped structure with horns pointing downstream is observed to evolve. This shape is characteristic of the so-called "Barchan" dunes. The streamlines shown in figure 1 clearly show the separation and recirculation of the driving flow at the front of the particle structure. Note that the streamwise/wall-normal cross-section of the dune is strongly non-symmetric, with the downstream edge being much steeper.

On-going Research / Outlook

We are looking forward to the new Petaflop system "SuperMUC" where we are planning to carry out our production runs. As mentioned earlier, the production runs consist of the simulation of subaqueous bedforms in a horizontal channel flow at a range of values of the control parameters (e.g. Reynolds number, Galileo number, Shields parameter). We will have small- to large-scale simulations on computational domains containing up to over 2 billion grid points and consisting up to 500,000 spherical particles. We will carry out the runs on 256 up to 1024 cores.

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Aircraft Wake Vortex Evolution in Ground Proximity and at Cruise Altitude

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HLRB Project ID: pr63zi

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Introduction

As an unavoidable consequence of lift aircraft generate a pair of counter-rotating and long-lived wake vortices that pose a potential risk to following aircraft. The prescribed aircraft separations to avoid wake vortex hazards contribute significantly to capacity restrictions of large airports. But also during cruise severe encounters of wake vortices have been reported. Wake vortex behavior is largely controlled by the prevailing meteorological conditions and the interaction with the ground. The most important meteorological parameters are wind, wind shear, turbulence, and temperature stratification.

The Deutsche Zentrum für Luft- und Raumfahrt (DLR) develops wake vortex advisory systems for airports [1,2] and en route which aim at optimizing the air traffic with respect to the measured and predicted wake vortex behavior. As part of such systems simple probabilistic wake vortex prediction models are required that predict wake vortex behavior accurately, robust, and fast [3]. Highly resolving large eddy simulations (LES) conducted on the HLRB II supercomputer provide valuable insights in the physics of wake vortex behavior under various conditions. These LES contribute indispensable guidance for the development of the real-time/fast-time wake vortex models.

Results

Wake vortices in ground proximity
A particular risk prevails during final approach, where the vortices can not descend below the flight path, but tend to rebound due to the interaction with the ground. Moreover, the possibilities of the pilot to counteract the imposed rolling moment are restricted due to the low flight altitude of aircraft above ground. Figure 1(a) shows the interaction of the wake vortices with the turbulent structures generated by crosswinds at the ground surface. At a non-dimensional vortex age of 1.2 the vorticity sheet generated by the lee (rear) vortex detaches from the ground and starts rotating around the primary vortex. Triggered by crosswind streaks the secondary vorticity sheet transforms into so-called omega loops wrapping around the primary vortices and

initiating vortex decay. Under unfavorable crosswind conditions the rebounding upwind vortex may hover over the runway directly in the flight corridor of a landing aircraft.

The introduction of a barrier at the ground surface may substantially accelerate vortex decay in the critical area close to the threshold where most vortex encounters occur as shown in Figure 1(b). Such a setup specifically exploits properties of vortex dynamics to accelerate wake vortex decay in ground proximity with the following characteristics: (i) early detachment of strong omega-shaped secondary vortices, (ii) omega shape causes self-induced fast approach to the primary vortex, (iii) after the secondary vortex has looped around the primary vortex, it separates and travels both ways along the primary vortex, again driven by self induction, (iv) the artificially generated secondary vortex connects to the regular ground effect vortex and thus obtains continued supply of energy, (v) the highly intense interaction of primary and secondary vortices leads to rapid wake vortex decay independent from natural external disturbances.

(a) Without barrier

(b) With barrier

Figure 1: Wall resolving LES of wake vortex evolution in ground proximity with turbulent crosswind (a) without and (b) with a barrier on the ground surface at t* = 1.2. Iso-surface of vorticity magnitude ($|\omega| = 1.5$ s^{-1}) colored by span-wise vorticity component.

Figure 2 shows the evolution of vortex circulation in cross-wind with and without a barrier. Field experiments will be conducted to demonstrate the efficiency of this way to provoke premature vortex decay in the most critical flight phase prior to touch down. Similarly as illustrated by this example for ground effect, most environmental effects like turbulence, stratification, and shear can be understood by analyzing the interaction of vorticity of the primary vortices and secondary (baroclinic) vorticity structures [4]. Also effects like vortex bursting or the formation of vortex funnels can be explained by the interaction of coherent vorticity structures [5].

Figure 2: Evolution of vortex circulation in cross-wind with and without a barrier.

Wake roll-up during cruise

The wake vortex evolution depends not only on environmental conditions such as atmospheric turbulence, temperature stratification and wind shear, but also on the specific aircraft geometry and the configurations for cruise, take-off or landing. A novel wake initialization approach is developed where a realistic aircraft wake is generated in a LES domain by sweeping a high-fidelity RANS flow field through the domain. Using this approach a simulation was performed from the wake roll-up behind the DLR-F6 wing-body model until the vortex decay [6].

Figure 3 shows the wake roll-up and the subsequent evolution of a vortex pair. Here the ambient turbulence is characterized by a normalized eddy dissipation rate of $\varepsilon^* = 0.01$. The flow field is visualized by two levels of iso-vorticity surfaces (red: $|\omega^*| = 250$, blue transparent: $|\omega^*| = 65$). The midpoint in flight direction corresponds to the normalized time labeled in each figure. Wingtip vortices and fuselage wake have large vorticity magnitudes in the beginning. The jet-like fuselage wake decays relatively quickly while the wingtip vortices preserve high vorticity. The decayed fuselage wake and the vorticity from the inboard wing wrap around the wingtip vortices adding disturbances around them. A stable vortex pair appears in Fig. 3(b). At $t^* = 8.8$, the vortex pair is highly disturbed and almost decayed.

On-going Research / Outlook

Numerical simulations and field measurements indicate that approaching aircraft frequently fly close to or even through not fully decayed wake vortices in ground proximity. In order to develop most efficient and safe wake vortex advisory systems for approach and landing the mechanisms which secure the safety of current operations must be understood and considered appropriately. To archive these, the further understanding of wake vortex behavior near the ground and during cruise is required [5].

By using the previous HLRB II system it became possible to investigate wake vortex evolution in various environmental conditions including the ground with reasonable mesh resolution. The next generation supercomputer will enable a major step forward to the understanding of the impact of ground roughness, specific aircraft characteristics, and flight maneuvers on the wake vortex evolution and decay.

(a) $x^*=6.0$ ($t^*=0.04$)

(b) $x^*=305$ ($t^*=2.07$)

(c) $x^*=1300$ ($t^*=8.8$)

Figure 3: Evolution of aircraft wake and the resulting wake vortex pair at cruise conditions, where two different levels of vorticity magnitude are shown by red and blue transparent surfaces.

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Interface-resolved direct numerical simulation of turbulent channel flow with suspended solid particles

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HLRB Project ID: pr95ba

Introduction

Fluid flow with suspended solid particles is encountered in a multitude of natural and industrial systems. Examples include the motion of sediment particles in rivers, fluidized beds and blood flow. Despite the great technological importance of these systems our understanding of the dynamics of fluid-particle interaction is still incomplete at the present date. Recently, however, significant progress has been made based on data provided by new experimental methods as well as numerical simulations. While most past investigations of numerical type have been performed in the context of the point-particle approach, it has now become possible to simulate the motion of a considerable number of finite-size particles including an accurate description of the surrounding flow field on the particle scale. Although the complexity of recent particle-resolved simulations (in terms of Reynolds number, number of particles and computational domain size) is still limited, new insight into the physics of fluid-particle systems is beginning to emerge from such studies.

Previously we have simulated turbulent flow in a vertically-oriented plane channel seeded with heavy spherical particles with a diameter corresponding to approximately 11 viscous (near-wall) turbulent length scales at a solid volume fraction of 0.4% [1]. The pressure-driven upward flow (at constant flow rate) was found to be strongly modified due to the particle presence, with increased wall-shear stress and strongly enhanced turbulence intensity. The average relative flow, corresponding to a Reynolds number (based on particle diameter) of approximately 135, leads to the establishment of wakes behind individual particles.

The objectives of the present study were two-fold. First, we wish to determine the influence of the streamwise length of the computational domain upon the largest flow scales. For this purpose we have performed simulations analogous to the ones presented in [1] but with twice the value of the original streamwise period. The influence of the domain size is elucidated through comparison of statistics between the two data sets. Second, in the present study we intend to provide data for a more complete description of the turbulent fluid-particle interaction in vertical channel flow. To this end we have now generated an enormous data-base which can be analyzed with respect to further aspects of the flow dynamics, previously not available to the community. The numerical method employed in the current simulations is identical to the one detailed in [2].

The current simulation was initialized with an exact periodic extension of a flow field taken at an instant towards the end of the simulation of reference [1]. For this purpose, fluid and particle data in the streamwise interval [0,8h] was copied from the reference field. In order to obtain data in the interval [8h, 16h], data was generated by applying the shift x=x'+8h to the reference field. It should be emphasized that no explicit perturbations whatsoever were added to the initial field. Subsequently, the extended simulation was run while different quantities were monitored in order to determine whether the system has developed sufficiently such as to "forget" the initial state. Data covering the initial 36 bulk time units of the present simulation has therefore been disregarded when computing averages.

A total of 155 bulk time units have been simulated for this flow case, out of which approximately 95 were performed on the system HLRB-II at LRZ. The runs were typically carried out on 512 cores (i.e. the number of grid nodes treated by each core corresponded to 128x128x256). The execution time for each full time step was approximately 60 seconds. Each instantaneous flow field (stored in IEEE double precision) represents a data volume of 65 GB. A number of 120 such fields have been accumulated over the course of this project.

Results

Mean fluid and particle velocity profiles as well as particle concentration profiles and the mean spanwise component of the angular particle velocity were analyzed. It was found that these average quantities

Figure 1: Instantaneous flow field (showing half the channel width) indicating high/low velocity regions as red/green isosurfaces as well as strong vortical regions in grey color. Particles are shown in yellow.

are not significantly affected by an increase of the box size from Lx/h=8 to 16. The observed small differences in these quantities are attributed to statistical uncertainty (limited sampling of the largest flow scales). Concerning correlations between fluctuation velocities for both phases, it turns out that all coefficients which involve the streamwise velocity components are affected by the prolongation of the domain, whereas the remaining correlations (involving only wall-normal or spanwise components) are essentially unchanged. This result is attributed to the "growth" (in size) of the largest flow scales in the prolonged domain, as discussed below.

Figure 1 shows instantaneous data indicating high/low streamwise velocity values as well as regions of intense vortical motion. At the Reynolds number based upon the average relative velocity of the present spheres and their diameter, an isolated particle in ambient surroundings would exhibit a steady, axisymmetric, separated wake. Due to the background turbulence and collective effects, particle wakes are considerably more complex in the present flow. We notably observe unsteady shedding of lambda-shaped vortices, which would otherwise only set in at significantly higher Reynolds number values. Animations of the flow field and the particle motion show that the particle motion in the buffer layer is directly influenced by high- and low-velocity streaks during close encounters.

Concerning the largest flow scales, visual inspection does suggest that these structures are essentially correlated over the full box length. This observation has also been confirmed quantitatively through analysis of spatial correlation functions. These results imply that a considerably larger streamwise period would be needed in order to warrant a complete spatial decorrelation of all scales. However, a quantitative estimate of the required length can unfortunately not be extracted from the present data.

On-going Research / Outlook

Thanks to the smooth operation of the system HLRB-II it was possible to efficiently (in terms of data loss and queueing time) generate high-fidelity flow data. We would like to thank all of the staff at LRZ for their support. The accumulated data-base will now be analyzed w.r.t. a number of additional statistical quantities. Some of the aspects which we intend to elucidate are the following: perform a Voronoi analysis of the spatial structure of the dispersed phase; analyze the statistics of particle acceleration; perform particle-conditioned averaging of the fluid flow field. These tasks are left for future projects.

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Highly-resolved simulations of trailing-edge cutback film cooling

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Introduction

Gas turbines for power generation and aircraft propulsion play an important role for meeting the fast-growing electricity and air transportation needs worldwide. In order to address both the economic and ecological goals of reducing operating costs and greenhouse emissions, respectively, it is of vital importance to further increase the thermal efficiency of future gas turbines. One way to increase the thermal efficiency of the engine is to increase the turbine inlet temperature. This temperature is determined by the combustion process and currently ranges up to 2000 K. Clearly, such temperature ranges lie far beyond the melting point of the most advanced high-temperature materials and can only be achieved by employing additional cooling technologies. These technologies prevent the hot parts of the turbine from catastrophic failure due to excessive thermo-mechanical strains and, thereby, ensure a reliable and efficient operation of the engine. The fundamental cooling practice is to extract cool air from the compressor of the engine and to provide it to the turbine components which are exposed to maximum heat loads. One such component is the trailing-edge section of the blade, which features a cutback on the pressure side as shown in Fig. 1(a). The coolant is first channelled through the interior of the blade and is then ejected onto the exterior surface over which a protective cooling film is formed. Because the cool air must be extracted from the compressor it does not perform work and, therefore, amounts for a thermodynamic loss. Consequently, the design goal is to minimize the amount of coolant while still maintaining an acceptable cooling performance.

Motivation

Previous experimental and numerical studies reported on a counter-intuitive be-haviour of the cooling effectiveness [1]. While one would expect that an increase in the amount of coolant yields an increase in the cooling effectiveness, the opposite was observed: the cooling effectiveness decreased. It was found that the instantaneous mixing between the hot and cool gas flows is characterized by the formation of large coherent structures. These structures were deemed responsible for the above behaviour; however, the detailed transport processes remained unclear. In order to further the understanding of the turbulent momentum and heat transfer mechanisms associated with large coherent structures, numerical experiments using direct and large-eddy simulations (DNS and LES) were conducted on the HLRB II-system at LRZ.

Numerical experiments

The numerical experiment was performed for two engine-relevant configurations as depicted in Fig. 1(b). The geometry and flow conditions are largely in accordance with physical experiments in [1], but included several modifications for optimum computational efficiency. For both configurations, the hot gas in the mainstream has the state of a fully-developed turbulent boundary layer with zero-pressure gradient. In contrast, the state of the cool gas depends on the internal geometry of the

Figure 1: (a) Schematic of high-pressure turbine blade with cutback on pressure-side of trailing-edge; (b) Generic representation in simulation setup.

Figure 2: Streamwise evolution of the adiabatic film cooling effectiveness.

Figure 4: Pinfin case, M = 1.1: Visualization of flow structures (grey) past the pinfin array.

coolant channel. It is either a fully-developed turbulent channel flow, or a fully-developed turbulent flow past an array of staggered cylinders. These so-called pinfins play an important for the internal convective cooling of today's turbine blades. Here, the focus is not on their role for the internal convective cooling, but on their impact on the film cooling performance. The ratio of the cool-gas to hot-gas temperature is 0.75. The blowing ratio M is the cool-gas to hot-gas mass flow. This is the key quantity for the present study, because its variation allows for controlling the turbulence and, thereby, the film cooling performance.

The DNS and LES were performed using the in-house flow solver LESOCC2 [2] and employed between 19 and 190 million control volumes. The computational setup was extensively validated by comparison with experimental and numerical data and it was found that the setup was suitable for the present investigations [3,4,5,6].

Selected results

Figure 3: Reference case, M = 1.1: Visualization of large coherent structures (grey) and spanwise averaged temperature fluctuations (positive: red, negative: blue).

Figure 2 presents selected DNS results of adiabatic cooling effectiveness along the turbine wall. For the reference case, the cooling effectiveness decreases by 44% as the blowing ratio is increased from M = 0.5 to 1.1. This is the counter-intuitive behaviour. The analysis of the statistical data revealed for the first time that the turbulent heat fluxes are dominating the total heat transfer in the trailing-edge cooling situation [4]. It should be emphasized that these fluxes can only be obtained via highly-resolved simulations, because statistical turbulence models employ modelling assumptions and adequate measurement techniques do not exist. The results show that the magnitude of the turbulent heat flux vector in-

creases with increasing blowing ratio. However, not only the strength but also the composition of this vector determines the heat transfer. It is shown that the counter-intuitive behaviour occurs when the turbulent heat flux vector has a strong wall- and upstream-directed component. The analysis of the instantaneous flow field reveals that both clockwise and counter-clockwise rotating flow structures are formed in this case, see Fig. 3. These flow structures transport cool gas away from the turbine wall (negative fluctuations) and entrain hot gas (positive fluctuations) towards the wall and in the upstream direction.

The situation changes drastically in the pinfin case. Figure 2 shows that an increase in blowing ratio from M = 0.5 to 1.1 results in an increase of the cooling effectiveness by +31%. When comparing the cooling effectiveness of the M = 1.1 cases for the two configurations, the gain is even higher (+120 %). The reason for this behaviour is closely related to the turbulent wakes from the pinfin array, see Fig. 4. These wakes prevent the formation of large coherent structures and, therefore, cause a higher cooling effectiveness.

On-going Research / Outlook

The DNS data are presently post-processed. The analysis focuses on both instantaneous and statistical mechanisms of the turbulent heat transfer and the impacts on the cooling performance. Moreover, the DNS data are employed for turbulent heat transfer modelling [5].

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Numerical Simulation of Cavitating Flows

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HLRB Project ID: pr95ma

Introduction

This project focuses on numerical analysis of the dynamics of cavitating flows within injection systems and micro valves of modern automotive engines, as well as of the flow around pump- and turbine blades. Cavitation occurs in a liquid if the pressure locally drops below the vapor pressure. In this case the liquid evaporates and the fluid becomes a liquid/vapor mixture. The collapse of the vapor clouds in regions of higher pressures are often very violent and cavitation-induced erosion of the surrounding material is likely to occur. All simulations of cavitating flows are performed with our in-house CFD codes CATUM [3] and INCA [1], which are 3D finite volume methods for body-fitted grids (CATUM) or immersed boundaries on Cartesian grids (INCA). Both allow for high quality predictions of complex flow phenomena including unsteady shock formation and wave propagation due to collapsing vapor clouds within compressible two-phase flows of low and high Mach numbers.

The project is split into different sub projects, which all focus on different aspects of cavitation phenomena.

Results

Simulation of injection systems and cavitating hydrofoils
During the whole project different setups have been simulated where cavitation plays an important role of the performance of the device. This is especially the case for hydrofoils, which are used in turbines and pumps, and for injection systems. Figure 1 depicts one snapshot in time of the vapor volume iso-surface for a hydrofoil-like shaped structure. Within the blue surfaces the liquid has already evaporated due to the small pressure and the fluid mostly consists of vapor. This simulation used about 300000 CPU hours.

Cavitation erosion
The collapse of vapor clouds results in high pressure peaks, which can damage the surrounding material. Based on physical criteria a novel 'collapse detector' has been developed [2]. This technique allows the identification and quantification of collapse events. With this detector erosion sensitive areas and the stress profile over time can be estimated. Figure 2 illustrates the de-

Figure 1: Cavitating flow above a hydrofoil-like shaped surface. Iso-surfaces of the vapor fraction of 10% at one instant in time. Inside the blue surfaces the fluid mainly consists of vapor. Flow from left to right.

tected collapses. The configuration is a nozzle-target flow, where the exit of the nozzle is directed towards the center of a disc. Cavitation occurs due to the deflection of the liquid and the vapor clouds collapse in the high pressure region at a certain radial distance. The top of figure 2 shows the regions of detected collapses and the bottom shows the time history of the collapses, which can be used for subsequent FEM simulations.

Modeling of turbulence
Turbulence modeling is still a major scientific challenge. Existing validated turbulence models for perfect gas need to be assessed for cavitating flows, where the density of the fluid can vary a few orders of magnitude. An existing and powerful LES-method has been extended to enable simulations of cavitating flows [1]. Figure 3 depicts a simulated cavitating shear layer. This is one of the more fundamental investigations of the interaction of turbulence and cavitation. Also engineering setups are investigated. By simulating devices of fuel injection systems we evaluate numerical models that fully include turbulence phenomena, as well as simpler models, such as physically inviscid approaches.

Dissolved gas
If the liquid includes dissolved gas, the flow field and flow structures can dramatically change. The research in this area is just at the beginning. Different physical models have been investigated. First results indicate that the numerical simulations are able to predict the tendencies as seen in experiments.

Post-processing of highly dynamical flows
Most simulations of cavitating real-world applications produce a lot of data, typical 1TB or above for a single

Figure 2: Typical outputs of the developed collapse detector to predict cavitation erosion. Top: Detected collapses on a disc. The strength of the collapses and their position can be evaluated. Bottom: The time history of the collapses can be used to estimate a stress profile for the material.

simulated setup. The flow field is highly unsteady and special post-processing algorithms help to identify the most important features of the flow. Therefore, statistical analysis using cross-correlations [4] provides the most important flow characteristics while minimizing the amount of data.

HPC

The very small physical time steps (dt≈10^{-11} s - 10^{-9} s) and the required fine resolution in space necessary to observe the small scale structures of the flow require the use of high performance computing systems. The typical number of time steps is of the order of 10^6 and the typical total grid sizes are of the order of 10^7 for 3-D simulations of real-world applications. Up to 480 cores on the HLRBII have been used to simulate and investigate cavitation erosion of complex devices.

For the turbulence research of cavitating flows up to 1000 cores have been used.

On-going Research

The focus on future research in our group is on cavitation erosion, turbulence modeling and flows with dissolved gas. The stress profile of the collapse detector will be coupled with FEM simulations to quantify erosion rates of the material. A highly complex LES simulation of a nozzle is in progress. This reference simulation allows us to investigate the influence of turbulence on cavitation and simpler turbulence models can be assessed against this. The estimated computing time will be around 2 million CPU hours. We investigate novel models to take important effects of gas content within the liquid and the vapor into account. Here, a large series of smaller simulations (≈10000 CPU hours each) are required to perform generic optimization of model parameters to fit experimental observations.

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t = 0.0997 ms

Figure 3: Lambda2-criterion showing vortical structures within a turbulent cavitating shear layer. Vapor regions (not shown here) are generated due to low pressures inside the vortices.

Multiscale modeling of particle in suspension

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Introduction

Particles suspended in a fluid represent a common scenario embracing physical processes that occur at different spatial scales[1]. A granular particle is typically with size between 100µm up to 10mm, in which range the agitation of solvent molecules does not play a role and the motion of the particle can be considered as deterministic. A colloidal particle is characterized by a typical size between 10nm up to 100µm, in which range the particle feels strong effects from solvent molecules and the resulted motion of the particle is Brownian and diffusive. The multiscale modeling of such a particle in suspension is not only important to improve our understanding of the bulk rheological properties of a complex particulate material, but is also becoming an indispensable tool to optimize specific functionalities of novel devices operating under microfluidics conditions. The physics becomes even more complicated when the host medium itself has a non-Newtonian behaviour, such as some complex fluids where macromolecular structures introduce viscoelasticity in the solvent. It is therefore extremely important to develop simultaneously theoretical and numerical models to fill the gap with rapidly evolving industrial applications.

Most of the numerical schemes rely on a deterministic discretization of the hydrodynamic equations and are therefore limited to large Péclet number (defined as

Figure 2: diffusion coefficient of a colloidal particle near a plane rigid wall.

ratio of shear rate and mass diffusion) flow of supra-micron-sized particle suspensions. In several micro-flow conditions the thermal noise, which manifests itself as the diffusional motion of the suspended objects, plays a key role in the dynamics. For example, an accurate description and measurement of the diffusive motion of a colloidal particle may be used as a highly sensitive probe for structure properties, both in distance and orientation, in the presence of complex boundaries[1]. Moreover, in a microrheology experiment, the Brownian motion of a colloidal particle gives a quantitative measurement of properties of the non-Newtonian surrounding medium[2].

Smoothed dissipative particle dynamics (SDPD) is a Lagrangian method, which does not need a mesh to discretize the targeted fluid system, but uses particles to characterize the flow[3,4]. Each SDPD particle can be considered as a coarse-grained meso/macroscopic portion of fluid with defined quantities, such as, mass, density, pressure, velocity, temperature and so on. The GENERIC framework allows us to obtain a discrete version of the Navier-Stokes fluid equations that determines the pressure, viscous and stochastic forces between each pair of SDPD particles in a short range r_c as shown in Fig. 1, in such a way that the fluctuation-dissipation theorem is satisfied [5,6]. A physical particle, such as a colloid can be represented by freezing a group of SDPD particles inside its solid domain, solving its rigid body dynamics through extra equations of motion.

Figure 1: short range interaction of smoothed dissipative particle dynamics.

Results

The first approximation for the dynamics of a micro/mesoscopic spherical particle suspended in a Newtonian medium was given by Albert Einstein in 1905. Since then other people extended his solution to the case of a particle near a wall[7]. Although this extended solution existed for half a century already, it has been extremely difficult for experimentalist to measure the particle's diffusion coefficient due to the difficulty of tracing a sub-micron particle for a sufficiently long time. This is straightforward in numerical simulations, as the whole dynamics history of a colloidal particle can be recorded, from which the diffusion coefficient can be calculated, as shown in Fig. 2. D_0 is the diffusion coefficient for a free particle and $D_\perp$, $D_\parallel$ are normal and parallel components of the diffusion coefficient for a colloidal particle near a plane rigid wall. Closer to the wall, the particle's motion is hindered by the wall due to a hydrodynamic interaction. Moreover, Fig. 2 shows anisotropy in the form of reduced mobility in the normal direction to the wall.

Another interesting physical problem is represented by a suspension of spherical particles in a fluid confined between two parallel walls. In our simulations the solid phase occupies almost 59% of space of the system undergoing constant shear motion. The suspension shows an increased resistance (higher viscosity) with respect to a simple fluid. In Fig. 3 we present the microstructure of such particle suspension by plotting the spatial-temporal averaged radial distribution function (RDF) of all solid particles.

Figure 3: RDF of particles in a suspension under shear flow.

The RDF represents the probability of finding a neighbouring particle around a given one. On Fig. 3, the upper wall is moving to the right and the lower wall is moving left. As a result, more particles tend to align in the compressive axis (from top left to bottom right) and have more closed distance than other orientation. Such a preferred alignment reflects the presence of a string or cluster like colloidal micro-structure, which makes the whole system more dissipative and increases its overall resistance.

Another interesting application of our model is represented by the possibility of simulating microrheology. The microrheology technique allows one to obtain the viscoelastic properties of a complex fluid from the diffusive movement of an embedded colloidal probe particle, through a generalized Stokes-Einstein relation. This way of proceeding is very profitable compared with the traditional rheological techniques because it allows to obtain rheological information of higher frequencies and from smaller quantity of fluids. However, the range of application of the microrheology is still not clear. This is because it is not known how the hydrodynamic interactions between particles or the boundaries can affect the probe. Even the shape of the probe itself might affect the measured rheological properties. Once again, numerical simulations look a very reasonable approach to check the validity of this technique. Using SDPD for a viscoelastic fluid[5], we can check the accuracy of the results in microrheology and obtain, as it can be seen in Fig. 4, the elastic and storage modulus G' and G"), that characterize the viscoelastic properties of the system, for different frequencies[2]. Finally, the results can be compared with the analytical solution for the viscoelastic fluid to check the validity of the assumptions.

On-going Research / Outlook

The numerical scheme, which has been implemented on the Altix 4700 over the last couple of years, is becoming a useful tool and has opened possibilities to study more interesting micro/mesoscopic flow phenomena. Future topics of investigation which includes, for example, three-dimensional simulations of a concentrated spherical particle suspension under shear flow, dynamics of a non-spherical (ellipsoid, dicolloid) particle near a wall or viscoelastic instability/turbulence of a non-Newtonian flow over a periodic array of cylinders[8].

Figure 4: The storage and loss moduli of a viscoelastic fluid obtained from two simulations of microrheology compared with the analytical results.

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As the space is limited in this report, please check our webpage for further publications and animations of this project.
http://www.aer.mw.tum.de.

Computer Science

waLBerla – Hyper-scale fluid simulations with lattice Boltzmann

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4

Introduction

The waLBerla project (widely applicable lattice Boltzmann solver from Erlangen) is the collaborative effort of a number of scientific co-workers from the University of Erlangen-Nürnberg. The idea was to build a software framework for the simulation of fluid flow that would both be applicable to a wide range of problems and flow scenarios, while at the same time designed to be ready to run efficiently on modern super computers (*hyper-scale computing*). By 2005, when waLBerla started, the lattice Boltzmann method for fluid simulations seemed like a promising approach to fit these needs [1, 2], and it has since continued to do so with a rapidly growing community of researchers [3]. The main applications for waLBerla were (and still are) [4]:

- Blood flow in arteries
- Free-surface liquid-gas flows such as bubbly flows or foams
- Particle suspensions like in sedimentation processes, fluidization or colloids
- Potentials and charged particle agglomerates in flows
- Transport phenomena in porous media and complex geometries

The simulation of flows is a computation intensive task, especially if one's aim consists in dealing with real-world scenarios. So, from early on, the development of waLBerla was naturally targeted towards supercomputers such as the HLRB II system of the Leibniz Rechenzentrum.

Results

A considerable part of the program code of the waLBerla project has been developed on and for the HLRB II system [4], and is now continued on its bigger brothers – which will be mentioned in the next section. Here we present the most important and beautiful results from that period. In order to realize particulate flows like suspensions (e.g., paint, blood, juice), where the suspended particles can be assumed to be rigid bodies, the waLBerla simulations can be coupled with a rigid body physics engine. The latter then calculates the motion of the particles from the stresses exerted by the surrounding fluid flow. To correctly simulate full freedom of motion, the particles are treated as voluminous objects with fluid stresses acting on the according surfaces. This way, also rotational movement of suspended bodies may be induced by fluid flow. However, the surface of the moving particle in the flow forms a boundary for the fluid phase and therefore a dynamical boundary treatment is necessary.

For real-life applications one often deals with millions or billions of particles. Therefore, one of the challenges was to realize the fluid structure interaction in a distributed manner that exploits an arbitrary number of CPUs available, by splitting the simulation domain into several patches. In [5], waLBerla was used to simulate more than 9 million fully resolved suspended particles on the HLRB-II machine. The article not only describes the method details but also the various performance results, and the programming techniques used to obtain them. E.g., the use of external C functions with variable length arrays enables the compiler to optimize loops that commonly arise in the lattice Boltzmann calculations, and leads to a significant performance gain. Figure 1 shows the simulation of fluidized particles.

The same code was later used for scaling experiments on up to 294912 processor cores for simulations containing 264 millions of particles in a fluid simulation [7].

Figure 1: Fluidization of particles in a flow by coupling waLBerla with the physics engine p.e.

An efficient method for free surface flows has also been developed within the waLBerla project. The interface between two immiscible fluids, a liquid and a gas (e.g., water and air), is what is called a free surface. waLBerla's free surface method was especially developed to simulate and predict the behaviour of foams, which are arising in industrial applications. Later on, the method has also successfully been used for the simulation of liquid transport in fluid cells.

Figure 2 shows the visualization of a waLBerla simulation of gas bubble development in a liquid. From an algorithmic point of view these simulations extend the lattice Boltzmann scheme by means of a volume of fluid approach that tracks the interface between liquid and gas phase, including a reconstruction of the surface curvature to model surface tension. In [6], the efficient parallelization of the method within waLBerla is demonstrated. Since for distributed calculations the bottleneck is typically the exchange of data between processes, inter-process communication must be kept as local as possible. However due to possible non-local topological changes of the free surface, non-local communication is sometimes unavoidable. However, with the advanced optimization strategy of described in [6], a parallel efficiency of 90% could be achieved on up to 4080 cores of the HLRB-II cluster

On-going Research / Outlook

By the year 2012, waLBerla project is still flourishing. A new generation of scientists keeps developing and extending the project onto new grounds. The software framework has been restructured in favour of better modularization to allow easy adaption of the framework for new application specifications. This way a maximal flexibility and extendibility is maintained to support the

different needs of the increased number of users - without too much overhead and the possibility to reuse functionality added by other users. In addition, the framework now allows programmers to optimize their code for different hardware platforms: Via so-called functionality selectors it is possible to have different processes running on different hardware. This allows the development of applications for heterogeneous hardware (e.g., applications that run efficiently on both CPU and GPU, or a combination of both) [8].

On the application side the waLBerla framework is currently further extended and used for the simulation of food froth (e.g., cream or bread) where the consistency of a foam has to be controlled during the manufacturing process of cereals. Other waLBerla based projects rely on the experience with particulate flows. E.g., the simulation of floating bodies in free surface flow as shown in Figure 4, or simulate electro osmosis with charged particles in flow. The latter exploits the versatility of the framework by adding an additional solver for the electromagnetic fields. All of these applications are extremely resource intensive and target on the new generation of high performance computing systems. With waLBerla we try to build a bridge that allows complex applications to access massively parallel hardware in a well organized, highly efficient way

Figure 3: Floating objects in free surface flow.

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http://www10.informatik.uni-erlangen.de

Figure 2: Simulation of foams with a waLBerla's free surface lattice Boltzmann approach.

Fast Matrix Methods
for Quantum Control Algorithms

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Introduction

Fast and parallelized matrix methods have been developed and exploited for addressing the challenge of calculating quantum dynamics. As an interface to far-reaching applications, quantum control theory is a powerful framework for devising algorithms to steer quantum devices with optimal figures of merit. Controlling quantum systems experimentally is central to many branches of quantum technology including nanotechnology, quantum information processing and spectroscopy. However, to find such steerings is a (classically!) computationally demanding task, as the matrix dimensions and resource requirements grow exponentially with the size of the quantum system.

From a numerical linear algebra point of view, quantum control algorithms make heavy use of both matrix exponential calculations and computation of sequences of matrix products. Hence, the main task within the project was the improvement of these numerical tasks by massive parallelization.

Results

The project has achieved progress allowing to use high-end parallel clusters: this includes tailored preconditioning and parallelization of matrix multiplication, matrix exponentials by Chebyshev series --- all these using matrix symmetries of the quantum system Hamiltonians. Thus a fully parallelised C++ version of the quantum control algorithm GRAPE was used [1], where 128 CPU nodes of the HLRB-II cluster brought a speed-up by more than a factor of 500 as compared to the runtime on a single node.

The main concept to parallelize the GRAPE-code was to distribute the M control matrices uniformly to all available processors, to compute the individual matrix exponentials sequentially on the responsible processors and to find an appropriate parallelization scheme for the forward and backward propagation, i.e. the computation of all M interior matrix-matrix products.

Figure 1: Runtime for the computation of one matrix exponential for different matrix sizes.

Matrix exponentials: In the first stage of the code, the matrix exponentials were calculated via the eigendecomposition of the Hamiltonians. We could improve this task by using Chebyshev-series methods, which allow to exploit the sparsity structure of the control Hamiltonians [1,2]. Figure 1 depicts the benefit of using the polynomial Chebyshev approach.

Prefix problem: Previously, the parallelization for the prefix problem was based on a coarse-grain tree-like approach. Using a 3D fine-grain approach where the individual matrix multiplications are parallelized, could help to obtain another speed-up by factor of 2-3 [2,3] as well as better scalability on the parallel cluster, see Figure 2.

Figure 2: Comparison of runtimes for the matrix-multiplication prefix problem, executed on different numbers of available cores.

Figure 3: Runtime for one iteration of the GRAPE algorithm. Comparison of the old version and the current version for different problem instances in a 10-qubit system.

for one individual contraction have complexity $O(nD^5)$ for periodic boundary conditions (PBC) and complexity $O(nD^3)$ for open boundary conditions (OBC). Table 1 illustrates the computation time for one individual contraction of two 100-qubit MPS tensors of different ranks D (the so-called bond dimension).

	D=20	D=40	D=60	D=80	D=100
OBC	0.072	0.150	0.238	0.310	0.380
PBC	1.4	33.0	233.7	886.5	3142.6

Table 1: Runtime [in seconds] for the computation of one contraction in the simulation of a n=100-qubit system with open boundary conditions (OBC) and periodic boundary conditions (PBC).

The presented enhancements in the computation of both matrix exponentials and matrix-multiplication prefix problem lead to an acceleration of the runtime for one iteration in the entire GRAPE algorithm. Fig. 3 provides a comparison of the runtimes of one GRAPE iteration required by the previous and the current version. Although the number of processers has been chosen to be M/2, which is the optimal choice for the tree-like approach, we obtain an acceleration of factor 2. For any other number of available processors we would expect even better runtime results.

More recently, we have expanded the original quantum control algorithm GRAPE [4] by incorporating more efficient second-order methods (BFGS) as well as by allowing for hybrid combinations between concurrent and sequential update of the control amplitudes [5]. In order to address the typical standard problems of numerical quantum control, the GRAPE algorithm has also been made available as a broadly applicable (fully modular) MATLAB package under the name DYNAMO [5].

However, matrix numerical methods over the entire Hilbert state space of quantum systems soon reach a limit due to the exponential growth of the state space, e.g. for n two-level systems, the state space is 2^n-dimensional. Therefore, in quantum mechanics, a general most challenging problem arises: what is the exact smallest eigenvalue (i.e. ground-state energy) of a matrix (representing the Hamiltonian) which is so large in dimension that it cannot even be stored on a computer but is just given in parameter form?

To this end, physicists developed concepts like Matrix Product States (MPS) for linear one-dimensional topologies or Projected Entangled Pair States for two-dimensional problems. In [6] we have addressed these problems in a unified way to show how computations, such as tensor contractions, can be performed efficiently while being versatile with respect to the coupling topology. The computation of ground states and ground-state energies is usually based on a variational ansatz for the Rayleigh-quotient minimization in the relevant representation format. Hence, the calculation of inner products of two vectors given in some representation format such as MPS is one of the key subroutines in simulation programs. As shown in [6], the costs

On-Going Research / Outlook

Moreover, by exploiting matrix symmetries in typical quantum mechanical Hamiltonians, another factor of two in parameter space can be saved [7] when using our unified versatile tensor contraction modules [6], which shall be parallelized in a follow-up project. We anticipate that these modules will be most useful in two of the major challenges in current numerical quantum physics, (i) the calculation of ground-state energies of Hamiltonians with 2D coupling topologies and (ii) in quantum simulation, where the entire time evolution of many-body systems has to be calculated such that the bond dimension D is kept tractably low by tensor-contraction methods. The latter will be key for extending the calculation of quantum many-body dynamics to optimal control of large-scale systems, where typically thousands of trajectories have to be calculated, see [1,2,4,5].

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Efficient Parallel Algorithms
for Ordinary Differential Equations

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Introduction

Today's most powerful supercomputers utilize tens or hundreds of thousands of processing elements to gain an overwhelming performance. This development generates an urgent demand for software that can exploit this massive potential for parallelism. Our working group searches for new algorithms and data structures that can make efficient use of the resources provided by modern parallel computer systems. One of our major goals is the development of efficient algorithms and software for the parallel solution of *initial value problems* (IVPs) of large systems of *ordinary differential equations* (ODEs).

Systems of ODEs occur as mathematical models for the simulation of time-dependent processes. The initial value represents the state of the process to be simulated at the start of the simulation. The simulation of the process, i.e., the solution of the ODE IVP, then consists of computing a sequence of time steps that move forward the simulation time. At each time step, the ODE system as mathematical model is used to compute how the process to be simulated develops during the small time interval covered by the current time step. The existing numerical solution methods for ODE IVPs differ in the computations performed at each time step. Some of the well known methods are Euler's method, Runga-Kutta (RK) methods, and Adams methods.

The solution of ODE IVPs can be computationally intensive for the following reasons:
- Depending on the process to be simulated and the desired level of detail, the ODE system can consist of a large number, e.g., millions of equations.
- The work associated with each equation that has to be performed at each time step can be computationally intensive.
- A large number of time steps may be necessary to achieve sufficient accuracy within the simulated period of time.

Therefore, many solution methods with potential for parallelism have been proposed. An overview of the fundamental work on parallel ODE methods can be found in [1].

Basically, three types of parallelism that can be available in the solution of ODE IVPs are distinguished:
- *Parallelism across the method (task parallelism):* Independent tasks available in the computational structure of the method, e.g., independent stages in iterated RK methods, are computed on different processor cores.
- *Parallelism across the ODE system (data-parallelism):* The ODE system is partitioned into disjoint subsets of equations such that each processor core is responsible for one of these subsets.
- *Parallelism across the steps:* Time steps are computed in parallel, for example, by overlapping adjacent time steps.

Parallel ODE methods can either use only one or a combination of these types of parallelism. Our focus lies on efficient solvers for computationally intensive large ODE systems which consist of millions of equations or even more. These large ODE systems are solved in parallel by exploiting parallelism across the ODE system, and, additionally, if available, parallelism across the method.

Methodology

We perform systematic scalability analyses of algorithms for the parallel solution of ODE IVPs. The results of these analyses are then used to improve the preexisting algorithms investigated and to develop new algorithms which can be executed efficiently on modern parallel computer systems.

This work involves theoretical approaches, but also largely depends on practical evaluations of algorithms and implementations on physical large-scale computer systems with different architectures where the scalability of the implementations is investigated by analyzing their runtime behavior on different numbers of processor cores. The program codes are implemented in either C or C++ using POSIX Threads, MPI or a mixed programming model.

In particular, the following approach is used to improve scalability:

1. *Improving the locality of memory references:* Improving locality reduces the number of cache misses and usually results in a better parallel execution time and a higher scalability. In particular, if the ODE system is large, e.g., consisting of millions of equations, large amounts of data have to be moved between memory and CPU cores. In this situation, a higher locality can help reducing contention on the interconnection system within and between compute nodes.

2. *Improving inter-processor communication:* Communication costs often exert a dominating influence on the scalability of a parallel program. Thus, minimizing these costs is essential for efficient usage of large parallel computer systems.

3. *Exploiting special properties of the ODE system:* Advanced program transformations to improve locality and reduce communication costs are possible if the solution method exploits special properties of the ODE system.

4. *Reducing processor idle times by dynamic work distribution:* Waiting times resulting from inter-processor synchronization may, in some situations, be reduced by distributing the computations dynamically to the participating processor cores.

5. *Exploiting multilevel parallelism:* Many ODE solution methods show potential for parallelism on multiple levels, e.g., the instruction level, the data level and maybe multiple task levels. Exploiting this potential, for example, by partitioning the processor cores into groups and replacing global communication operations by more efficient group-local communication operations, can enable a reduction of the execution time and an improvement of the scalability.

Results

With the help of HLRB II embedded and iterated RK methods, extrapolation methods and Adams-Bashforth methods have been investigated. Several different transformations on the source code level have been devised, in particular, modifications of the loop structure and modifications of the data structures. As one of the main results, we showed that by exploiting a special coupling structure between the equations (limited access dis-

tance) occurring in many large ODE systems the working space of important loops, i.e., the amount of data repeatedly accessed by these loops can be reduced using a pipeline-like loop structure and, thus, the locality of memory references and scalability can be improved. Further, we could show how a limited access distance can be exploited to reduce storage space and communication costs for many ODE methods, for example, embedded RK methods [2]. Embedded RK methods were also used as example to demonstrate the applicability of dynamic load balancing strategies to ODE methods. The interaction of task and data parallelism was studied for extrapolation methods [3]. Figures 1–3 show selected scalability results.

On-going Research / Outlook

The focus of our current work is the use of adaptive techniques such as adaptive scheduling and automatic selection of parameters and implementation variants. The use of adaptive techniques in numerical software has initially been proposed for linear algebra algorithms (self-adaptive numerical software (SANS) initiative [4]). Currently, we advance this approach to parallel ODE solution methods. We expect that adaptive techniques will be able, on the one hand, to relieve the user from difficult choices of implementation parameters, and, on the other hand, to improve the efficiency of the codes by automatically exploiting special properties of target platform and IVP and by automatically adapting to the current runtime situation.

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Figure 1: Strong scalability (fixed problem size) of general and specialized Adams-Bashforth codes with different loop structures and different data structures implemented with POSIX Threads simulating a vibrating string

Figure 2: Strong scalability (fixed problem size) of general and specialized Adams-Bashforth codes with different loop structures implemented with MPI simulating a vibrating string

Figure 3: Weak scalability (problem size increased with number of processes) of specialized extrapolation codes with a pipeline-like loop structure implemented with MPI simulating a chemical reaction.

Geo Sciences

Computational seismology

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Introduction

Computational wave propagation has become an increasingly important discipline of seismology and will become even more relevant as the observed data volumes increase. After several years of code developments the focus is now on solving scientific problems with the tested and benchmarked research codes. Here we report results based on two flavours of numerical methods: the spectral element method and the discontinuous Galerkin method.

Within the last few decades a number of different numerical methods for modelling and inversion of seismic waveforms has been developed, including basic finite difference schemes, Fourier pseudospectral methods, finite element approaches, and spectral element methods (SEM). The Discontinuous Galerkin (DG) method has been applied only within the last few years but has already become a well-established numerical method. It is suitable for the simulation of seismic wave propagation in general and able to handle complex geometries as well as heterogeneous media using an arbitrary high approximation order in space and time (ADER-DG). Features like local time-stepping and p-adaptivity in each tetrahedral cell lead to a complex load balancing problem.

In the field of seismic tomography we are now moving into a new era: while so far seismic data were reduced to a few travel time observations of some seismic phases (e.g., P and S waves) the aim is now to use the information contained in the complete waveforms of the observations. In the section on seismic tomography we show the first application of this concept to tomography on a continental scale. The tomographic inversion of the subsurface structure under Australia demonstrates that - given the current computational power - inversion based on complete 3-D wave propagation solvers is feasible and leads to much improved tomographic models.

We use a similar concept to investigate whether it is possible to recover earthquake source characteristics by time reversing seismic wavefields. In theory, time reversing the complete seismograms as source injected at the receiver locations constitutes the adjoint field and leads to a first update for the seismic source process. The results shown indicate that the concept works in principle but that a very high station density is necessary to quantitatively recover source characteristics.

Results

Full waveform inversion.

These new simulation capabilities must now be used to further our understanding of the Earth's 3D structure. Detailed knowledge of subsurface heterogeneities is essential for studies of the Earth's dynamics and composition, for reliable tsunami warnings, the monitoring of the Comprehensive Nuclear Test Ban Treaty and the exploration for resources including water and hydro-carbons.

Full waveform tomography is a tomographic technique that takes advantage of numerical solutions of the elastic wave equation. Numerically computed seismograms automatically contain the full seismic wavefield, including all body and surface wave phases as well as scattered waves generated by lateral variations of the model Earth properties. The amount of exploitable information is thus significantly larger than in tomographic methods

Fig. 1: Horizontal slices through the relative lateral variations of the shear wave speed at different depth in the Australasian region

Fig. 2. Focusing of seismic wave fields at the surface after reinjection from a typical surface seismic network using time reversal.

that are based, for example, on measurements of surface wave dispersion or the arrival times of specific seismic phases. The accuracy of the numerical solutions and the exploitation of complete waveform information result in tomographic images that are both more realistic and better resolved.

We developed a novel technique for full 3D waveform tomography for radially anisotropic Earth structure. This is based on the combination of spectral-element simulations of seismic wave propagation and adjoint techniques. The misfit between observed seismograms and spectral-element seismograms is reduced iteratively using a pre-conditioned conjugate-gradient scheme.

The application of our method to the upper mantle in the Australasian region allows us to explain the details of seismic waveforms with periods between 30s and 200s and it provides tomographic images with unprecedented resolution. The final model explains data that were not initially included in the inversion. This is strong evidence for the effectiveness of the inversion scheme and the physical consistency of the tomographic model.

Time reversal
Time Reversal is a promising method to determine earthquake source characteristics without any a-priori information (except the earth model and the data). It consists of injecting flipped-in-time records from seismic stations within the model to create an approximate reverse movie of wave propagation from which the location of the source point and other information might be inferred. The backward propagation is performed numerically using a spectral element code. We investigate the potential of time reversal to recover finite source parameters, test it on a synthetic data set, the SPICE Tottori benchmark model, and on point source moment tensor sources. The results shown in Fig. 2 indicate both the potential and

the problems with this approach depending on the seismic network geometry and density. The time reversal approach is leading an increasingly important role in understanding large earthquake source processes.

Dynamic earthquake rupture
An earthquake is currently understood as a slip developing at a frictional interface between two lithospheric blocks. Dynamic rupture is the process by which the physical behaviour and the initial conditions at faults are predescribed and the solver then calculates the rupture dynamically during the simulation. We implemented the option to have frictional boundaries in the Seissol package based on the discontinuous Galerkin approach (see Fig. 3).

The fact that Seissol uses tetrahedral grids will allow in the future to simulate and understand rupture along faults with complex shapes and initial stress conditions. The physics of the earthquake rupture under such conditions is still poorly understood.

Fig. 3. Snapshots of a dynamic rupture simulation of the M7.4 Landers earthquake that shook California in 1992.

On-going Research / Outlook

All the results presented indicate that the 3-D modelling tools for seismic wave propagation can now be used to model actual observations. The parallelized algorithms based on implementations with Fortran-MPI have been used on O(1000) processors, and show good scaling behaviour. However, for the next generation hardware, more tests and optimization is required to render the algorithms performant on O(100k)-core hardware. We intend to accomplish this through collaborations within the SPPExa initiative and the EU project VERCE (www.verce.eu).

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Modelling the impact of transport (aviation, ships and land traffic) on the climate

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HLRB Project ID: h1112

Introduction

How does human transport affect the Earth system? It is very likely that shipping, aviation, and road traffic, already at a high level today, will increase for the near future; hence the need to determine their impact. In addition to this topic, our modelling work on HLRBII focused on interactions between atmospheric chemistry, aerosols, and climate. The results are highly relevant to society and contribute to the assessments by the Intergovernmental Panel on Climate Change and the World Meteorological Organization. An important part of our effort is devoted to model development and validation in order to maintain our position at the cutting edge of scientific progress.

Our workhorse is the model system EMAC. Its core consists of an atmospheric general circulation model coupled to modules for atmospheric chemistry and aerosol microphysics. All of it is implemented in the Modular Earth Submodel System, MESSy [1]. We are able to set up EMAC appropriately for a wide range of scientific questions. For instance, we can choose among different horizontal and vertical resolutions and can include or exclude schemes of arbitrary complexity for atmospheric chemistry and aerosols. In EMAC, the range of numerical methods comprises spectral transformation, finite differencing, a semi-implicit leap-frog scheme with time filter, and a Rosenbrock sparse-matrix technique. Parallelization follows the distributed-memory concept. EMAC scaled on HLRBII up to 256 cores using a horizontal resolution of 2.8° by 2.8° in latitude and longitude, 90 vertical layers from ground to 80 kilometers above sea level, and comprehensive atmospheric chemistry. A simulation year consumed about 13000 CPU hours, most of it associated with the chemistry scheme.

Results

In addition to gaseous pollutants, ships, aircrafts, and road vehicles emit particles so small that they essentially become part of the air and travel with the winds. Referred to as aerosol, these particles reflect and absorb

Figure 1: Modelled annual-mean soot concentrations in µg/m³ at the Earth's surface.

sunlight and act as nuclei for water droplets and ice crystals. The particles have different characteristics, depending on composition, shape, and size. The dark and rugged soot aerosol (see Figure 1), for instance, is particularly efficient in absorbing sunlight and giving rise to ice crystals.

In order to simulate the impact from shipping on the Earth's climate, we compared two different setups. One simulation accounted for the global shipping emissions, the other not. It turned out that the shipping-aerosol particles brighten near-surface clouds over the oceans which, as a result, reflect more sunlight back into space. The effect owes its importance to those remote ocean regions where shipping constitutes by far the largest source of pollution. Our results indicate that the cooling due to the altered clouds even outweighs the warming from the shipping-related greenhouse gases. However, the impact on the clouds is closely related to the high sulphur content in maritime fuels. Additional simulations with emissions from bio fuels instead of heavy oil revealed a significantly weaker effect.

Pollution-aerosol particles, the very small ones in particular, are known to induce and aggravate cardiovascular as well as respiratory disorders. Our simulations show that the atmospheric transport from far away contributes appreciably to the total shipping-induced burden along the European coastlines. The impact on the continental regions, in contrast, appears to be small.

The effect of aging alters the physical and chemical properties of the aerosols and represents a major scientific issue. For example, ship emissions occur at high concentrations in relation to the atmospheric background. During the subsequent dilution of the exhaust plume, the pollutants are subject to a complex processing which current global models are unable to resolve spatially and temporally. As a remedy, we developed for EMAC a suitable parameterization which has now become operational.

Note that there are other processes which transform the aerosol particles also on a longer time horizon. Through their role as ice crystal nuclei, soot and mineral dust influence the properties of cirrus clouds high up in the atmosphere, and hence the radiation at the Earth's surface. The ability of the aerosol particles to form ice crystals mostly vanishes as they develop a liquid coating through collision with liquid aerosol and condensation of gases. Our simulations indicate an important aviation-related contribution to the total soot burden at heights in the atmosphere where cirrus clouds can occur. However, determining the associated impact on the clouds has to account for the emergence of the liquid coatings on the initially bare particles. Pioneering simulations with a specifically upgraded aerosol scheme showed that the condensation process mentioned above is of primary importance for the coating formation.

Feedback mechanisms associated with atmospheric chemistry can modify the response of the Earth's climate to increased contents of greenhouse gases like carbon dioxide. For a detailed analysis of these feedbacks, we performed several simulations; a reference case against which we compared perturbation simulations with different burdens of carbon dioxide. Our chemistry simulations necessitated the implementation of a mixed-layer ocean scheme into EMAC. The scheme accounts for the uppermost layer in the ocean, subject to mixing from wind-induced waves, but neglects the deeper regions. The reason is that it takes the deep ocean centuries to come into equilibrium with respect to a perturbation in greenhouse gases; too long with respect to the computationally demanding chemistry scheme. With the mixed-layer ocean, however, equilibrium is reached after only twenty simulated years. It turned out that the chemistry slightly dampens the warming of the Earth's surface in response to a higher burden of carbon dioxide, mostly due to negative feedbacks regarding ozone and water vapor.

EMAC accounts for the full interaction between atmospheric motion, radiation and chemistry; an ideal setting for simulating the Antarctic ozone hole. The latter develops nearly every Austral spring due to the presence of man-made ozone-depleting substances and causes strongly enhanced levels of ultraviolet radiation at the Earth's surface. EMAC reproduces the ozone hole in case its winds are forced to match with observations (see Figure 2). Without the forcing, however, it simulates weaker than observed winds high above the Antarctic continent, just like many other atmospheric models. As a result, the ozone hole is absent despite a realistic burden of ozone-depleting substances. Having conducted various test simulations, we were able to track the complicated causal chain down to an excessive activity of weather cyclones around Antarctica. Correspondingly, EMAC does yield an ozone hole in case we impose for the Southern Ocean a smaller than observed north-south-ward temperature contrast.

On the other hand, the presence of interactions between atmospheric chemistry and motion impedes an important quantification procedure. Quantifying the effect of road-traffic pollutants, for instance, on atmospheric composition and climate requires a comparison of two simulations with different emissions. Once emitted, the pollutants are subject to atmospheric transport which differs among the two simulations and disguises the desired emission signal. Even for binary identical initialization, the two simulations will display non-identical transport because the different chemical states impact on atmospheric motion, giving rise to the famous butterfly effect. We managed to suppress any of the interaction path-ways and are now in the position to apply the procedure mentioned above on an operational basis.

On-going Research / Outlook

Building upon our achievements on HLRBII, we continue working with EMAC on SuperMIG. We are now able to determine better the effects upon the Earth system from different transport sectors and types of pollutants, dispose of a mixed-layer ocean scheme, of a mode where atmospheric motion and chemistry are decoupled, and find ourselves in a better position to tackle the ozone-hole problem.

In addition, we are entering other fields: the impact of methane on climate and atmospheric chemical composition, the impact of gravity waves on atmospheric motion, the effect of geo-engineering on atmospheric ozone, issues related to the nesting of fine regional grids into the rougher global mesh, and a more detailed evaluation of EMAC.

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Figure 2: Modelled mass mixing ratio of ozone at 22 kilometers above sea level for 30 September 2003.

Global high-resolution gravity field determination

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HLRB Project ID: pr32qu

Introduction

The Earth's gravity field is of primary interest for many scientific applications and disciplines. It is directly linked to the physical shape of the Earth, the so called geoid (cf. figure 1). The geoid is an irregular surface that coincides approximately with the mean sea surface and which can be regarded over the continents as a continuation of the mean sea surface below the topography. As the gravity potential is constant on the geoid, there is no water flow between points located on it, which is why the geoid is appropriate as general reference and zero level for height systems. In oceanography the geoid serves as important reference surface for modelling sea level change and ocean currents. The deviation of the geoid from the ocean sea surface, the dynamic ocean topography is one of the main drivers of ocean currents and has a fundamental importance for climate change studies. Improved knowledge about the gravity field is the only way to realise the geoid.

Furthermore geophysicists obtain information about mass distributions and density in the Earth's interior by the gravity field. It is also sensitive for mass changes on the surface, such as continental water flows or melting of ice sheets.

Due to its meaning for different scientific disciplines, the gravity field is a very important topic of research and issue of this project

Motivation to use HLRB-II

There exist various kinds of gravity field observations, which can be used in the process of gravity field determination. On the one hand there are terrestrial or airborne

measurements by absolute or relative gravimetry, which provide gravity field observations for certain areas on the Earth as well as observations, derived from satellite altimetry measurements, which cover ocean areas. On the other hand the gravity field is observed by special satellite gravity missions (cf [1]). The main advantage by satellite gravity measurements is that the measurements globally cover the Earth. However the gravity field signal is damped in satellite height, whereas terrestrial or altimetric measurements content the full gravity signal. The combination of all different kind of observations with their different characteristics enables a high accurate global gravity field determination. As to deal with the huge number of observations it is necessary to use a powerful computer system, which was provided by LRZ's HLRBII. For example there exist several terrestrial and airborne data sets with together more than 200 million observations, while the satellite gravity mission GOCE measures more than 500000 observations per day.

The gravity field is represented by spherical harmonics, a generalization of the concept of Fourier series for the sphere. This means, the goal of gravity field processing is to determine spherical harmonic coefficients. The coefficients are obtained by least-square adjustment. The corresponding normal equation systems can be very large. This is the second and even more important reason for the usage of HLRBII. Up to now spherical harmonic coefficients were usually estimated based on full normal equations systems up to spherical harmonic degree and order 360 (corresponding to about 130000 parameters and a 126 GByte normal equation system). The coefficients of higher degrees were calculated by block-diagonal techniques. As only full normal equation systems enable independent stochastic modelling of all data sets and only full normal equation systems provide variance-covariance matrix

Figure 1: The geoid, the physical shape of the Earth

Figure 2: Gravity anomalies (10⁻³m/s²)

information, an approach was implemented at HLRBII which enables to deal with full normal equations systems up to significantly higher degrees (e.g. degree and order 620 corresponding to about 385000 parameters and a 1TByte normal equation system).

Technical procedure

Until now calculations on HLRBII were performed on the base of full normal equations systems to spherical harmonic degree and order 620. All programs are based on FORTRAN90. The first program is used to process the observations and to assemble the normal equation systems per observation group. This program is based on a one-dimensional BLACS process grid, where each process prepares a certain part – theses parts correspond to specific spherical harmonic coefficient groups - of the normal equation matrix. The next programme, again organized in a onedi mensional BLACS process grid, combines the normal equations of the different observations groups together. All IO operations were handled by newly developed routines, because they seem to be more robust for example to MPI-IO routines. After combination a third program performs solution and inversion of the normal equations. This program is organized in a two dimensional BLACS grid, where the normal equations are distributed block-cyclic. For solution and inversion SCALAPACK routines are used. The inversion step is required to obtain error information for the spherical harmonic coefficients. After this step a fourth program estimates variance components, which describe the optimal relative weighting between the observations groups. With this information the stochastic model can be optimized and all steps starting from the combination can be recalculated. Last but least the variance-covariance matrix can be propagated into global distributed errors. See [2] for more information.

Results

The result of the processing chain is a set of spherical harmonic coefficients up to degree and order 620. These coefficients can be expanded in any functional of the gravity field like gravitational potential, geoid heights, gravity anomalies and others, which are used in Earth science studies. Figure 2 shows gravity anomalies, calculated from these spherical harmonic coefficients.

Gravity anomalies are gravity accelerations, reduced by a (approximately) constant factor of 9.8 m/s². It can be seen that gravity anomalies are correlated with topography and bathymetry. Mountains such as the Andes or the Himalaya, ocean trenches as well as tectonic plate boundaries are mapped by gravity.

The gravity field is as indicated in the introduction fundamental for many scientific applications and we can for example use our solution to provide a geoid as reference surface for oceanography. Figure 3 displays the mean dynamic topography, i.e. the difference between the mean ocean surface and the geoid at the Atlantic coast in North America. The Gulf Stream is here clearly visible. This is just one example for many Earth science related products, which can be calculated from global gravity field models and shows its importance to observe the system Earth (cf[1]).

Figure 3: Mean dynamic topography [m]

Outlook

The successor of HLRBII, SuperMUC will open new possibilities, which will permit enhanced gravity field research. In this project further terrestrial data sets shall be included in the calculations, especially in areas where little or bad quality data was used so far. Furthermore the preprocessing of observations shall be refined in order to improve the quality of the gravity field solutions. Also in the field of stochastic modeling further progress shall be achieved. A main goal for the future is to enhance the maximal spherical harmonic degree for calculations based on full normal equation systems. We aim are here for calculations up to degree and order 720, what corresponds to about 520000 parameters and a normal equation system of approximately 2 TByte.

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Direct numerical simulation of sediment erosion

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5

Introduction

The meandering shape of rivers, the erosion of soil in mountains and the transport of soil over large distances into the ocean are examples that illustrate how sediment erosion and sediment transport alter the shape of our landscape. Engineers require formulae for the onset of sediment erosion in order to predict the consequences of sediment erosion and sediment transport or to design protections against sediment erosion. The existing formulae are mostly based on the approach of Shields [1] and provide estimates based on bulk properties of the flow. However, this approach has been found to have low predictive qualities and to lead to unsatisfactory large differences in the estimates. As a result, the focus of related research in the past decades has shifted towards the fundamental aspects involved in sediment erosion and sediment transport.

At the core of the problem is the interaction of a turbulent flow field with a sediment layer - both being of complex nature. The interaction is established on one hand by a hydrodynamic force induced by the turbulent flow on a sediment particle, which then can lead to the onset of sediment erosion. On the other hand the presence of sediment modifies the turbulence structure of the flow by posing a rough wall boundary condition or by interacting with the flow structures when suspended in the flow.

In order to deepen the understanding of the problem it seems reasonable to first reduce the complexity. Simplifications can be done by considering straight channel flow instead of meandering channel flow and by studying a sediment bed of mono-sized spheres in a reproducible structured arrangement instead of a water-worked bed of natural gravel involving a range of sediment shapes and sizes. Also it seems necessary to address some knowledge gabs to related problems before approaching the full complexity of the problem.

While the effect of fixed roughness elements on the turbulent flow has been studied since the beginning of turbulence research [2], few studies considered the effect of the flow (i.e. force and torque) on the fixed roughness elements [3-5], relevant to infer about the onset of sediment erosion. Data provided by simulations in this project helped to address this gap of knowledge [6]. In recent years some researchers employed experimental techniques to study the onset of sediment erosion [7-9]. The focus of the research was on identifying the flow structures related to the onset of sediment erosion. While [9] estimated the onset of sediment erosion based on fixed sphere results, [7] and [8] considered truly mobile particles. The studies identified long streamwise elongated structures of positive streamwise velocity fluctuations in the vicinity of the particle as part of a potential mechanism that lead to the onset of sediment erosion. However, it was not fully clarified if the results of fixed particles can be used to predict the onset of sediment erosion.

In the present study we approach the problem of the onset of sediment erosion by using direct numerical simulation. The potential of this method in providing a full picture of the processes was demonstrated previously by [10]. The numerical method employed is described in [11].

Figure 1:
Instantaneous flow field in small sphere case (left) and large sphere case (right).
Red (blue) surfaces are iso-surfaces of the streamwise velocity fluctuation at values + 3 u_τ (-3 u_τ).

Here, implications of fixed sphere results on sediment erosion are presented and compared with the result of direct numerical simulations of sediment erosion utilizing truly mobile spheres.

Results

The simulations are based on simulations of flow over a layer of fixed spheres in squared arrangement above a rigid wall which is additionally roughened by particle caps staggered to the spheres above. Two particle diameter are con-sidered a small sphere case in which $D+= D\ u_\tau / \nu =11$ and a large sphere case with $D+= 50$. Here, D denotes the particle diameter, u_τ the friction velocity and ν the kinematic viscosity. The bulk Reynolds number is $Re =U\ h / \nu =2900$ in both cases, where U is the bulk velocity based on the open channel height h. An illustration of the setup is provided in figure 1 which shows the instantaneous flow fields in both cases visualized by iso-surfaces of the streamwise velocity distribution. A detailed description can be found in [6] and [12].

The potential for sediment erosion is first studied by defining a critical Shields number based on fixed sphere results. The concept of a critical Shields number is commonly used by engineers based on empirical studies with mobile spheres (cf. range of experiments as identified by [1] in figure 2). When applied to the fixed sphere results of the present simulations this leads to the prediction of a lower critical Shields number for the large spheres [6] which is in disagreement with experimental evidence based on truly mobile spheres.

Therefore, simulations with truly mobile sphere have been carried out and analyzed in detail [12]. The results are provided in figure 2 which shows the Shields number, Sc, of single simulations with mobile spheres in the small and the large sphere case. Two types of erosion events have been considered: multiple particle erosion and single particle erosion events. In case of multiple particle erosion the entire layer of spheres was mobile and could erode in the other cases only few particles in an otherwise fixed bed where mobile and could erode.

As can be seen in figure 1 focus has been given to the multiple erosion events. Here, the simulations follow the trend reported in the literature and shown in form of a shaded area as indicated by [1]. The obtained critical Shields number is in both cases considerably larger as reported in the experiments which can be related to the much shorter duration time of the simulations compared to experiments. Also, it should be stressed that figure 2 show results of single simulations and do not resemble statistical mean values.

In addition to the multiple particle erosion, single particle erosion simulations have been carried out for the small sphere case. Figure 2 shows that in these cases a much higher critical Shields number is obtained. This might be related to a joint effect of the higher particle sheltering in case of single erosion events and the fewer number of mobile particles.

Figure 2: Critical Shields number, S_c, in direct numerical simulations of the onset of sediment erosion with truly mobile particles as a function of the particle diameter in viscous units D^+.

On-going Research / Outlook

In order to account for the particle-particle and particle-wall contact a simple repulsion force has been utilized. Future studies will focus on the implication of the contact model on the study of sediment erosion. Also additional simulations with single mobile particle in the large sphere case would be beneficial to shed light onto the role of collective effects in the onset of sediment erosion. Furthermore additional simulations would be required to provide sound statistical evidence of the studied phenomenon.

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Simulation of 3-D seismic wave propagation in a synthetic Earth

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HLRB Project ID: pr32mu, pr95bu

Introduction

Long-standing questions in the study of Earth's deep interior are about the origin of seismic heterogeneity and the nature of flow in the mantle. Understanding the dynamic behaviour is important as the flow drives plate tectonics and controls the way the Earth looses its heat. Thus, it is a crucial factor in tectonic modelling or in simulations of the geodynamo and the thermal evolution of the Earth. A better understanding of these aspects is of great societal importance. For example, the continuous drift of tectonic plates relative to each other results in a build up of stress at the plate boundaries. This stress can eventually exceed the yield stress of rock, thus leading to (often disastrous) earthquakes.

Most of our knowledge on deep Earth structure and flow comes from the analysis of recordings of seismic waves that travel through the Earth after large earthquakes. Similar to medical tomography, seismic tomography allows us to "see" the present day elastic structure of Earth's mantle in 3-D. During the last two decades, a variety of such 3-D models were built from different datasets. However, seismic tomography can only provide a limited resolution; that is, only a blurred and distorted image of Earth's structure can be obtained. This is a consequence of errors in the data and the non-uniform distribution of earthquakes as well as seismic receiver locations, which mainly cover continental regions. A second problem inherent to any tomographic inversion is that an infinite number of models will fit the data equally well, a problem known as non-uniqueness of the solution.

Geochemical observations also offer important constraints on Earth's structure and evolution, providing compelling evidence for compositional heterogeneity within the mantle. Geophysical techniques, including seismology, can provide detailed information on such heterogeneity. However, despite substantial improvements in seismological methods and a dramatic increase in the amount and quality of available data, interpretations of images from seismic studies remain hampered by trade-offs between thermal and chemical effects. As a consequence, the distribution of chemical heterogeneity within Earth's mantle and, accordingly, its role in governing mantle dynamics, remains poorly understood.

Imaging Earth's interior structure at higher resolution and the convergence towards consistent models serving as a 3-D seismic reference is currently one of the most pressing challenges of modern global seismology today. So far, tomographic studies only used the arrival times of a very limited set of seismic phases from all of the information that is contained in a seismogram. In addition, most studies were based on ray theory, thus completely neglecting the wave character of seismic disturbances.

In order to improve conceptual models of mantle flow, the major challenges in seismology today are to efficiently mine the wealth of information contained in seismic waveforms and to constrain the relative contributions of thermal anomalies and compositional variations to the observed seismic heterogeneity. High expectations to gain new insight currently lie within numerical simulations of wave propagation through complex three-dimensional structures.

Modern computational tools for seismic wave propagation incorporate a large range of physical phenomena and are able to produce synthetic datasets that show a complexity comparable to real observations. Also, computing whole waveform synthetic seismograms at relevant frequencies became feasible on a routine basis in recent years thanks to rapidly growing computational resources. However, it has long been not clear how to introduce geodynamic considerations into seismological forward simulations in an efficient and consistent manner, and how to benefit from expensive large-scale simulations for our understanding of deep Earth structure and dynamics. This was the motivation to develop a novel method, in which we generate synthetic 3-D mantle structures based on dynamic flow calculations that serve as input models in the simulation of seismic wave propagation.

Here, we present the results of our new multi-disciplinary approach that combines forward modelling tech-

Figure 1. Snapshots of the three-dimensional wavefield in one of our geodynamic models. 3-D global wave propagation was simulated for an earthquake in the Fiji Islands region using a spectral element technique. The wavefield is depicted by green and magenta colours together with the shear wave velocity variations in the model, for which vertical cross-sections and iso-surfaces are shown on a blue to brownish colour scale ranging from -2 to 2 per cent. Surface topography is also shown for parts of the globe for geographic reference [1].

niques from geodynamics, mineral physics and seismology. The thermal state of Earth's mantle at present-day geologic time is predicted by 3-D high-resolution mantle circulation models using a finite-element method. The temperature field is then mapped to seismic velocities. For this task, we take advantage of recent progress in describing the state of dynamic Earth models in terms of elastic properties through thermodynamically self-consistent models of mantle mineralogy. The predicted models of seismic heterogeneity are then implemented in a spectral element code for the simulation of 3-D global wave propagation. Using state-of-the-art techniques to solve the wave equation in 3-D heterogeneous media, this approach allows us to capture the correct physics of wave propagation.

Both, the geodynamic as well as the seismic simulations require large-scale high-performance calculations. The computational resources provided through the supercomputing platform HLRB II at the Leibniz Supercomputing Centre (LRZ) allowed for the first time to simulate seismic wave propagation in synthetic Earths; that is, we are now able to compute synthetic seismograms completely independent of seismic observations. This means that we can test geodynamic hypotheses directly against seismic observations, which may serve as a complementary tool to tomographic inversions. More specifically, it is for the first time possible to study frequency-dependent waveform effects, such as wavefront healing and focusing/defocusing in mantle structures with realistic length-scales; that is, in a physically consistent manner.

Results

One specific question that we addressed with our joint forward modelling approach is the origin of two large regions of strongly reduced seismic velocities in the lowermost mantle (the so-called African and Pacific superplumes). Several seismological observations are typically taken as an indication that the superplumes are being caused by compositional variations and that they are "piles" of material with higher density than normal mantle rock. However, a large number of recent geodynamic, mineralogical and also seismological studies argue for a strong thermal gradient across the core-mantle boundary (CMB) that might provide an alternative explanation through the resulting large lateral temperature variations. We tested the hypothesis whether the presence of such a strong thermal gradient in isochemical whole mantle flow is compatible with geophysical observations.

Figure 2. Comparison of the standard deviation (SMAD = scaled median average deviation) of traveltime variations in our geodynamic model to that of the observations. Intermediate and light shaded areas show the range of values inferred from the data [2]. Blue lines: simulated P-wave traveltime variations. Red lines: same for S-waves. Solid and dashed lines show SMAD curves for two different measurement techniques [1].

We have computed synthetic seismograms and a corresponding dataset of traveltime variations for one of our synthetic mantle models assuming a pyrolite composition for the mantle mineralogy. Synthetic seismograms for periods down to 10 seconds were computed for the predicted structure using 486 cores on HLRB II. Altogether, we simulated the seismic wavefield for 17 earthquakes distributed evenly over the globe. The wavefield of each earthquake was "recorded" by a very large number of virtual seismic stations in order to achieve a relatively homogeneous illumination of our model even with a low number of seismic sources. In total, we obtained each ~350,000 cross-correlation traveltime measurements at a dominant period of 15 s for compressional (P) and shear (S) waves.

The traveltimes of observed seismic waves, to which we compared our synthetic dataset, show a peculiar behaviour of their statistics as a function of the turning depth of the waves in the mantle: The standard deviation of P-wave traveltime variations stays almost constant with depth, while that of the S-wave traveltimes increases strongly towards the CMB. This increase in case of S-waves is particularly strong below a depth of around 2000 km (cf. Fig. 2). Such a difference between P- and S-waves is not expected in a chemically homogeneous mantle in the framework of ray-theory, which forms the backbone of seismology.

Using full wavefield simulations, we find, however, that the standard deviations of P- and S-wave traveltime variations in our geodynamic model show the same peculiar behaviour as the observations. This is a remarkable result in light of the isochemical nature of our mantle circulation model and highlights the importance of taking the correct physics of wave propagation into account in the interpretation of long-period seismic data. Most important, our comparison shows that isochemical whole

mantle flow with strong core heating and a pyrolite composition is capable of explaining the statistics of seismic observations. The standard deviations of our synthetic P- and S-wave traveltimes do not only show different trends with depth, but are also matching those of the observations well in terms of their magnitude. While this finding does not necessarily mean that there is no chemical heterogeneity present in the lower mantle, it shows that complex large-scale variations in chemical composition are not required by the dataset studied here.

On-going Research / Outlook

One particular aspect that we currently strive to clarify in the elastic representation of geodynamic heterogeneity is the suspected existence of a mineral phase named post perovskite (the high pressure polymorph of magnesium silicate $MgSiO_3$). The elastic properties of the mantle will be affected by the existence of this phase, which would cause strong shear wave velocity variations across the phase transition while the velocity of compressional waves would change only slightly. To better constrain the relative importance of thermal anomalies and variations in chemical composition for generating seismic heterogeneity, the comparison presented here needs to be repeated with postperovskite included in the mineralogical conversion.

Seismic datasets are rapidly growing not only due to an increasing number of seismic stations, but also due to the fact that traveltime measurements are now starting to be done at multiple frequencies. In this study, we have focused on a single frequency band. In future, it will become important to understand also the multi-frequency datasets from a forward modelling perspective complementary to using them for tomographic inversions. A limitation that we still face is that memory requirements are huge in order to simulate seismic wave propagation up to the highest frequencies used in seismological studies on a global scale (around 1Hz; that is, 1 s shortest period). SuperMUC, the successor system to HLRB II will certainly help to bring us closer to the goal of covering the whole range of frequencies relevant for deep Earth studies.

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High Energy Physics

Simulation of lattice QCD at realistic quark masses

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6

Introduction

Quantum Chromodynamics (QCD) is the underlying quantum field theory describing the strong interactions. Lattice QCD currently provides the only *ab initio* method for performing QCD calculations in the low-energy regime, and for acquiring a quantitative description of the physics of hadrons and nuclei with controlled systematic errors. To reliably connect hadron physics with QCD, extreme computing resources are required.

Since the cost of full QCD computations grows with a large inverse power of the quark mass, initial calculations were restricted to relatively heavy quarks. However, in order for lattice calculations to capture the physics of quarks and gluons in captivity, and reach the needed accuracy requested by the experiments, simulations at physical quark masses, on large volumes and at small lattice spacings are required. That is becoming possible now due to algorithmic developments and major investments in computing power. Due to lack of space I will focus on *recent progress made in developing a quantitative understanding of hadron masses*.

QCD contains six flavors of quarks. In this report we shall only consider the lightest three quarks, up (u), down (d) and strange (s), with $m_l = (m_u + m_d)/2 \approx 4$ MeV and $m_s \approx 100$ MeV. The QCD interaction is flavor blind. Neglecting electromagnetic and weak interactions, the only difference between quark flavors comes from the quark mass matrix. We have our best theoretical understanding when all three quark flavors have the same masses, because we can use the full power of flavor SU(3) symmetry. Nature presents us with just one instance of the theory, with $m_s/m_l \approx 25$. Interpolating between these two cases enables a systematic investigation of flavor symmetry breaking.

Results

The calculations are done on space-time lattices of size up to $48^3 \times 96$ and lattice spacings down to 0.07 fermi.

By working on a discrete grid, the path integral becomes finite dimensional, and can be evaluated by stochastic simulation techniques, such as the Monte Carlo method. One needs to choose an action, which reduces to the continuum value at zero lattice spacing and gives the best physical description of the system, with minimum errors, using the available computing power. The particular clover action used here has a single iterated mild stout smearing for the hopping terms. Together with the tree level Symanzik improved gluon action this constitutes the Stout Link Nonperturbative Clover or SLiNC action. Further details are given in [1].

Starting from the SU(3) symmetric point, $m_u = m_d = m_s$, our strategy is to keep the singlet quark mass $m = (m_u + m_d + m_s)/3$ fixed at its physical value. As we move from the symmetric point to the physical point along the path m = constant, the s quark becomes heavier, while the u and d quarks become lighter. These two effects tend to cancel in any flavor singlet quantity. The cancella-

Figure 1: The masses M_H of the baryon octet H=N, Λ, Σ and Ξ as a function of the pion mass squared. All masses are given in units of their SU(3) symmetric value.

tion is perfect at the symmetric point, and we have found that it remains good down to the lightest points we have simulated so far [2].

In Figure 1 we show, as an example, the masses of the baryon octet (N, Λ, Σ and Ξ) as a function of the pion mass squared $M_\pi^2 \sim m_l$. A fan structure is seen with masses radiating from the common SU(3) symmetric point. Although we have included quadratic terms (in m_l) in the fit, there is really very little curvature in the results. This shows that the Gell-Mann–Okubo relations work all the way from the SU(3) symmetric point to the physical point. This is a remarkable fact.

What does that teach us? The hadron masses receive contributions from two basic sources, the gluonic excitations of the vacuum, as well as the hadron sigma terms. The sigma terms come from the vacuum connected expectation value of the u, d and s quarks in the Hamiltonian

$$\sigma_l^H = m_l \langle H|(uu+dd)|H\rangle \, , \, \sigma_s^H = m_s \langle H|ss|H\rangle \, .$$

While the (flavor singlet) gluonic excitations are approximately independent of the quark masses, the hadron sigma terms σ_l^H and σ_s^H, which are sensitive to chiral symmetry breaking effects, are linearly dependent on m_l and m_s, respectively. The absence of curvature in Figure 1 thus suggest

$$M_H - \sigma_l^H - \sigma_s^H = M_{H'} - \sigma_l^{H'} - \sigma_s^{H'}$$

for any two hadrons H, H'.

Figure 2: The sigma terms σ_l^H and σ_s^H at the physical point for H = N, Λ, Σ and Ξ.

In Figure 2 we show recent [3] results of a direct calculation of the hadron sigma terms of the baryon octet. The light-quark sigma term σ_l is found to be largest for the nucleon N and smallest for the cascade hyperon Ξ, while σ_s is found to be smallest for the nucleon and largest for the cascade hyperon. By comparing the hadron mass splittings in Figure 1 with the respective sigma terms in Figure 2, it can readily be seen that the breaking of flavor symmetry in hadron masses is indeed entirely accounted for by σ_l + σ_s. Other contributions, for example nonanalytic terms

arising from the cloud of virtual pions, as suggested by chiral perturbation theory, appear to be negligible.

In Figure 3 we give our final results for the hadron masses of the vector meson octet, the baryon octet, as well as the baryon decuplet, and compare them with their experimental values. Good agreement with the experimental numbers is found, which is an absolute highlight of lattice QCD.

Figure 3: The octet and decuplet meson and baryon masses (red circles) compared to experiment. We use the pion and kaon (K) masses to determine m_l and m_s. The overall scale is set by the mass of the baryon octet at the SU(3) symmetric point.

On-going Research / Outlook

The calculations reported here have been done at a single lattice spacing. To reliably extrapolate the results to the continuum limit and gain control over discretization effects, the calculations need to be repeated at smaller lattice spacings. That will require much larger lattices and PFlop/s scale computing resources.

Several of the reported hadrons are resonances, which receive contributions from scattering states at small pion masses. So far the contribution of scattering states has been neglected. In an on-going project we are computing the $\pi\pi$ and πK as well as the πN and KN phase shifts to obtain the masses and widths of the low-lying meson and baryon resonances, including the $f_0(600)$ (formerly called σ), $\Delta(1232)$ and N(1535). That requires entirely new techniques.

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Nonlinear gyrokinetic investigation of multiscale plasma microturbulence

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6

Introduction

One of the key physics problems on the way to efficient nuclear fusion based power plants are plasma microinstabilities being excited by the enormous temperature and density gradients in such devices. They cause anomalous heat and particle transport which significantly degrades the plasma confinement quality, thus preventing self-sustaining plasma burning in present-day experiments. Hence, extensive experimental studies are dedicated to understanding and predicting turbulence features. They are accompanied by numerical simulations which are typically based on the gyrokinetic theory - the latter essentially involving a reduced, i.e. 5-dimensional, Vlasov equation per species being coupled by Maxwell's equations.

Along these lines, the research activities on HLRB2 were aiming at exploring the significance of turbulence types on scales whose transport contributions have traditionally been neglected in simulations and experimental diagnostics for various practical reasons, e.g., due to the dramatically increased effort in addressing those scales. HLRB2 thus helped to perform pioneering and stimulating work, particularly pointing at the possible substantial transport generated by hyper-fine-scale turbulence – even in a bath of large-scale turbulence which potentially could have a suppressing effect.

Results

All simulation results presented in the following are based on the nonlinear gyrokinetic GENE code which has now been developed and maintained for more than a decade at IPP, Garching, and more recently by an international team of developers. Here, the discretized nonlinear gyrokinetic equations are solved on a fixed, five-dimensional (three spatial and two velocity space dimensions) grid which is aligned with the magnetic field lines in order to reduce the computational requirements describing highly anisotropic plasma turbulence structures. Furthermore, a so-called δf-splitting technique consistent with the ordering used in the derivation of the gyrokinetic theory is employed so that only the fluctuating parts of each distribution function are propagated in time. The phase space and time operators are treated separately, following the so-called method of lines. While the time stepping is typically done with a fourth-order explicit Runge-Kutta scheme in the initial value solver mode, the numerical schemes in the spatial directions depend on the chosen type of operation. Large fusion devices where the gyroradius is much smaller than the machine size may be simulated in the local approximation. Here, all profiles are evaluated at a single radial position which allows for the application of pseudo-spectral methods in both perpendicular space directions. For smaller devices, GENE has been recently enhanced to consider the full radial profile information which requires changes in the numerical schemes, e.g., by using finite-difference techniques in the radial directions like they are always used in the third spatial direction (parallel to the background magnetic field) and the velocity space directions.

For an efficient use of high-performance architectures, GENE is hybrid-parallelized, i.e. all core parts can be run in parallel using the OpenMP and/or the MPI paradigm. The latter is achieved through domain composition in the species, in the velocity space directions and in two of the three spatial directions (all three in the nonlocal code, respectively). At present, the code has demonstrated a good to excellent scaling behaviour on up to 262k cores, thus being well prepared for upcoming systems like SUPERMUC.

One of the main scientific topics being addressed in the HLRB2 projects is the relevance of hyper-fine scale turbulence on the electron gyroradius scale in the presence of the traditionally considered microturbulence on the much larger ion gyroradius scales being spatio-temporally separated by $(m_i/m_e)^{3/2}$.

Figure 1: Snapshot of turbulent structures of the electrostatic potential on various scales mapped to a torus and in a small cross-section at the outboard midplane.

This simultaneous and self-consistent treatment is naturally extremely challenging but absolutely necessary to reassess previous findings being restricted to the single scales thus artificially excluding any potential cross-scale coupling effect.

Even when using a reduced ion-to-electron mass ratio of $m_i/m_e=400$ the minimum number of direct space grid points evaluates to 768x384x16x32x8 per species in the five phase-space coordinates. To ensure a reasonably well resolved quasi-stationary state of the nonlinear simulations, on the order of 10^5 time steps are required which yields a total computational amount of 100-200 kCPUh per simulation, at least.

Summarizing, we have shown that massively parallized multiscale simulations predict a tendency towards a scale separation between ion and electron heat transport[1,2]. In contrast to its ion counterpart which is only driven by large scales, the electron heat channel may thus exhibit substantial or even dominant high wave number contributions carried by ETG modes and short-wavelength TEMs. Therefore, these investigations might help to understand residual electron heat fluxes in cases where the low-k drive becomes small compared to the ETG drive, as for instance in discharges with dominant electron heating, high β, or transport barriers. However, due to the enormous computational requirements, most of these simulations have been run in idealized geometries – see, for instance, the circular flux surface shape in Fig. 1 - and with reduced physics. Hence, interfaces to several experimental data bases – for instance, of the tokamak experiments DIII-D, Tore-Supra and ASDEX-Upgrade - have been established recently in order to check, at least in the linear regime, whether similar turbulence signatures can be found in real life parameter spaces, see for instance Ref. [3].

Figure 2: Linear growth rate as function of radius and wave number for a specific ASDEX-Upgrade discharge. The color encodes positiv (red) and negative (blue) real frequencies.

A corresponding example can be found in Fig. 2 where the linear growth rate of the dominant microturbulence type at wave number k_y is plotted as a function of the latter and the radial position ρtor for ASDEX-Upgrade based profiles and magnetic equilibria. Clearly, high-k_y (hyper-fine scale) modes are strongly excited and propagate in electron diamagnetic drift direction (negative frequency) while the traditionally considered wave number range $0.05<k_y\rho_s\lesssim1.0$ is here dominated by ion temperature gradient driven modes drifting in the opposite direction (positive frequency). Based on the aforementioned nonlinear simulation

results, a substantial electron heat flux fraction should thus arise from smallest scales and should furthermore gain importance towards the plasma edge where the hyper-fine scale growth rate peak tends to be much larger compared to the peaks at lower k_y. Figure 2 additionally reveals that a second mode with negative frequency may be present a largest scales. Such micro-tearing modes have also often been neglected in the past. Their appearance for realistic parameters, however, has triggered new interest and research as will be discussed in the next section.

On-going Research / Outlook

As a spin-off of the aforementioned HLRB2 results, micro-tearing modes have been investigated in a dedicated research project [4] and have been shown to also potentially contribute significant fractions of the electron heat transport. However, a complete answer on the relevance of these turbulence types would even go far beyond the previous studies and involve triple-scale (super-/sub-/ion-gyroradius-scale) simulations in order to capture possible cross-scale couplings. It is therefore left as a task for future exascale systems.

On the other hand, GENE has recently been extended to consider not only radially localized simulations volumes but also radial domains covering large fractions up to the whole minor radius (compare Fig. 1 and 3) thus allowing to address small fusion devices or transport barriers where the local approximation tends to be less meaningful[5].

Figure 3: Ion gyroradius scale temperature fluctuations for ASDEX-Upgrade as computed with the new global GENE code.

However, such global simulations are naturally much more expensive and hence they have been restricted to either ion- or electron-gyroradius scales only. Especially for the understanding of transport barriers – being a crucial task for the design of advanced tokamak scenarios – multiscale simulations in the global framework are called for to gain new insights and constitute a significant step towards a numerical tokamak.

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http://gene.rzg.mpg.de

Dynamical lattice QCD with Ginsparg-Wilson type fermions

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Introduction

Almost all visible matter is made out of hadrons, in particular neutrons and protons, the building blocks of all nuclei. Hadrons come in two varieties, baryons and mesons. Three quarks form a baryon and a quark-antiquark pair forms a meson. Since quarks and gluons have not been observed as isolated elementary particles one assumes that they are permanently confined. Another important observation is the unexpected lightness of the pion, the lightest meson, which is understandable if the pion is a so-called Goldstone boson of a spontaneously broken symmetry. The broken symmetry is the symmetry between left-handed and right-handed massless quarks and is thus called "chiral symmetry".

The Quantum Field Theory of quarks and gluons is called Quantum Chromodynamics (QCD). It introduces the strong interactions between quarks as mediated by gluons. The basic formalism is simple to write down in terms of an action functional for the bare quark- and gluon fields. Its evaluation is tremendously difficult. Closed analytic solution is impossible and perturbative expansions work only at very high momentum transfer and cannot provide information on binding properties like the mass of the hadrons. On the other hand one expects that QCD is capable to explain all features of strong interaction and all properties of hadrons ab initio. In 1974 Kenneth Wilson suggested to formulate QCD on a space-time grid. This opened the path to a non-perturbative, computer-accessible approach. In 1979 first computer calculations by Mike Creutz showed promising results. Monte-Carlo integration ("simulations") of the high dimensional quantization integrals – one has typically several million variables to deal with – became the method of choice. It was obvious that for a complete calculational approach, which included both, gluons and quarks non-perturbatively and dynamically, extreme compute power would be necessary. On the way towards that goal various simplifications and approximations have been studied. Only in recent years some of them could be relaxed and computations close to the actual parameters of Nature became possible.

Results

In order to really understand the physics of hadrons, one has to perform lattice simulations in which chiral symmetry is not massively destroyed by lattice artefacts, i.e., one has to perform simulations with chiral quarks. Such simulations are, however, extremely costly and so far all large volume simulations done world-wide had to make rather significant approximations. We have studied two different fermion realizations which approximate chiral symmetry better than the usually used Wilson fermion action.

Fixed point fermions
Bern is since decades an established center of chiral perturbation theory (ChPT), i.e., the low-energy limit of QCD. Therefore, it was natural for the Bern-Regensburg group to concentrate on the determination of the low energy constants (LECs) which parameterize ChPT. This can be done on very small volumes which are either hypercubic (ε-regime) or elongated in the time direction (δ-regime) but requires very good chiral symmetry, which we realize with Fixed-Point (FP) fermions.

Chirally improved quarks
The chirally improved (CI) fermions used by the Graz-Regensburg group are based on an approximation, which allows us to reduce the computational costs very substantially. CI fermions are used primarily to investigate excited hadron states.

Our early studies worked in the so-called quenched scenario, i.e., neglecting dynamical vacuum loops of the quarks. In the current project we included the two light quarks u and d in a fully dynamical Monte Carlo simulation.

The Hybrid Monte Carlo algorithm combines a molecular dynamics evolution of the (gluon) gauge field configurations which was implemented for the CI action, in a way

suitable for larger lattices and parallelization on the ALTIX. Several improvements (like Hasenbusch preconditioning, single/double precision implementations of the conjugate gradient inverter, better memory organization, optimized inter-node transfer) led to a significant speed-up (by a factor of more than 2). The currently running program executes and performs nicely on 128 nodes for lattice size $16^3 \times 32$ and on 576 nodes for lattice size $24^3 \times 48$. The CI fermion action used allowed us to work on relatively coarse lattices for linear spatial size 2.4 fm and still being able to study the system at several pion (i.e. quark) masses down to roughly twice the experimental mass values.

Figure 1: Extrapolation of the energy levels obtained for the rho-meson channel towards the physical pion mass [2].

Figure 2: Meson masses for light quark isovector mesons (and excited states) as resulting from the extrapolation to the physical point [2].

Figure 3: Meson masses for isovector mesons (and excited states) with one light and one strange valence quark as resulting from the extrapolation to the physical point [2]; right-hand part: two strange-antistrange mesons.

In the variational method we used and improved one computes cross-correlations of a large set of different hadron interpolators (in our case constructed from gauge-covariantly smeared quark sources of various widths). Diagonalization then leads to eigenmodes corresponding to the ground state and low lying excited hadrons. We also included heavier (strange) valence quarks and determined such masses for mesons and baryons with strangeness.

The quark masses are extrapolated towards the physical point. Fig. 1 shows an example for such an extrapolation for the so-called rho-meson, where we also find signals for an excited state, i.e. another meson.

Figs. 2 and 3 show the meson masses in the light quarks sector and in the light-strange quark sector as obtained from the extrapolation to the physical point. We find generally good agreement with experiment. However, we miss signals from the expected two-particle channels, which should mix in a simulation with dynamical quarks. This needs further study.

The analysis of the baryons for a subset of ensembles was presented in [1] and a complete analysis, also including finite volume effects is in progress.

We have been utilizing the obtained gauge configurations also for other, related studies: i) In a series of papers we investigate the chiral content of the rho and rho' mesons (see, e.g. [3]). We point out that in the infrared a leading contribution to $\rho' = \rho(1450)$ comes from a different chiral representation than the ρ. This allows critical comparisons with the predictions of the quark model. ii) We also find signs for the much-discussed 'tetraquarks'. iii) We also calculated the axial coupling constant of the positive and negative parity states of nucleons. This led to intriguing results concerning a possible effective restoration of chiral symmetry in excited hadrons.

Outlook

We are presently computing the quark propagators for the ensembles of gauge field configurations on the larger lattices and from them the hadron propagators. A study of the baryon spectrum and of the observed finite volume effects is in progress.

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Further information on the discussed and related projects can be found here:
http://www.physik.uni-regensburg.de/forschung/hep/
http://physik.uni-graz.at/lattice/

Twisted Mass QCD: Phenomenological Applications at Light Quark Masses Non-Perturbative Light Quark Physics

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Abstract

We present results of lattice QCD simulations with mass-degenerate up and down and mass-split strange and charm dynamical quarks using Wilson twisted mass fermions at maximal twist at two values of the lattice spacing. We measure with high statistical precision the light pseudoscalar mass m_{PS} and decay constant f_{PS} and determine low energy parameters of chiral perturbation theory. We also calculate the mass of the D-meson which contains a dynamical charm quark accessible only within the setup of this project.

Introduction

The beginning of this century has assisted to radical improvements in theory, algorithms and supercomputer technology, leading to a far increased ability to solve non-perturbative aspects of gauge field theories in a lattice regularized framework. Following this path of improving the lattice setup, in this project we have extended existing simulations of lattice QCD by considering in addition to the u,d light dynamical quark flavours also the effects of the strange and charm sea quarks.

By including – for the first time – a dynamical charm, we are now able to directly study its contribution to physical observables and to quantify the so far uncontrolled systematic effect present in lattice QCD simulations where the charm flavour in the sea is absent. In this report we will discuss simulations with twisted mass dynamical up, down, strange and charm quarks. We realise this by adding a heavy mass-split doublet (c,s) to the light degenerate mass doublet (u,d), referring to this setup as N_f=2+1+1 simulations. This formulation was introduced in [1, 2] and first explored in [3]. The results of this project are published in [4, 5]. The simulation algorithm used is described in detail in ref. [6].

Results

As one of the main outcomes of the project we show in fig. 1 the very precise data for the so-called pseudoscalar

decay constant. In our setup, this quantity has the advantage that it does not need a renormalization which simplifies significantly the computation.

The solid line in the graph is a fit to chiral perturbation theory, which provides an effective low energy description of QCD and which works very well, as the good agreement with the lattice data shows. Such fits allow to determine non-perturbatively the low energy constants of chiral perturbation theory and we give the results of our analysis in table 1.

In fig. 2 we show the mass of the D-meson. The D-meson is the lightest meson containing a charm quark and can only be computed dynamically with the setup of this project. As the figure indicates, the D-meson can be computed reliably. The star symbol in the figure denotes the physical value of the D-meson and the slight mis-match with the lattice results demonstrates that a re-tuning of the bare parameters of the lattice theory is required to reproduce the physical value.

In summary, in this project we have performed a first exploration of lattice QCD simulation including the complete first two quark generations as dynamical degrees of freedom. The outcome of this project has been very successful and we could demonstrate that very accurate results for the light quark flavours can be obtained which can be fitted to chiral perturbation theory. As a result, the

	β=1.95
$\bar{l}_3$	3.70(7)(26)
$\bar{l}_4$	4.67(3)(10)
f_0	121.14(8)(19) MeV
$2B_0\mu_{u,d}/m_\pi^2$	1.032(21)(3)
$\langle r^2 \rangle_s^{NLO}$	0.724(5)(23) fm^2

Table 1: Results of the fits to $_\chi$PT for the ensemble at a ≈ 0.078 fm. Predicted quantities are: the low energy constants $\bar{l}_{3,4}$ the charged pseudoscalar decay constant in the chiral limit f0, the mass ratio $2B_0\mu_l$ / at the physical point and the pion scalar radius. The first quoted error is statistical while the second estimates systematic uncertainties.

Figure 1: The pseudoscalar decay constant f_{PS} as a function of the mass parameter $2B_0\mu_l$ for two values of the lattice spacing a≈0.078 fm (ß=1.95) and a≈0.086 fm (ß=1.90).

Figure 2: The mass of the D-meson, m_D as a function of the pseudo scalar mass m^2_{PS}. This quantity can be computed dynamically only with the setup of this project. The star symbol represents the physical value of the D-meson.

values of the low energy constants in table 1 were obtained. In addition, we could demonstrate that the mass of the D-meson (and also the K-meson) can be computed with good precision.

We consider the present results to be encouraging to proceed with the N_f=2+1+1 flavour research programme of the European Twisted Mass Collaboration (ETMC) in which this project is embedded. In particular, we want to perform the non-perturbative renormalisation with dedicated runs for N_f=4 mass-degenerate flavours, an activity which we have started already. Furthermore, we want to compute the quark mass dependence of many physical quantities towards the physical point where the pion assumes its experimentally measured value.

We are currently performing simulations at a significantly different and lower lattice spacing than the one presented here. Both strategies, smaller quark masses and smaller lattice spacings, will allow us to estimate systematic effects on a quantitative level and to obtain in this way accurate physical results in our N_f= 2+1+1 flavour simulations with statistical and systematical errors fully under control.

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Exploring Lattice QCD with Exact Chiral Symmetry

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6

Introduction

The largest fraction of the mass of ordinary matter surrounding us is generated by the strong interaction taking place inside protons and neutrons. The theory describing the strong interaction - Quantum Chromodynamics (QCD) - is build upon elementary particles, quarks and gluons, interacting through the exchange of colour charges. Asymptotic freedom provides an elegant mechanism to weaken the strength of the interaction at high energies. It is thus possible to perform accurate predictions, relying on the perturbative expansion of QCD, which have been thoroughly tested in high-energy experiments. The understanding of these phenomena is so precise that current experiments at the Large Hadron Collider (LHC) rely on QCD to subtract what is now considered a "background" to possible signals of physics beyond the Standard Model of particle physics.

The situation is however significantly more involved in the low-energy regime of QCD. In this case, the strength of the interaction is large and a complete analytical control of the theory is yet unknown. Solving this problem remains one of the greatest challenges in theoretical physics.

The current theories of particle interactions heavily rely on symmetry principles. In the Standard Model, a central role is for instance played by gauge symmetry. In the limit of massless quarks, the Lagrangian of QCD respects chiral symmetry. This symmetry is however spontaneously broken implying that Nambu-Goldstone bosons will appear in the physical spectrum. In practice, quarks are not massless particles and therefore chiral symmetry is also explicitly broken by mass terms. However, the masses of the two lightest quark flavours -the up and down quarks- are indeed small with respect to the typical scales of hadronic physics. This implies that the effects of chiral symmetry – and its spontaneous breaking – have to be present in the spectrum of QCD and in many low-energy processes.

The properties of hadronic states such as mesons (e.g. pions or kaons) are given by those of a valence quark and anti-quark inside an extremely complex vacuum where gluons and sea quarks are being exchanged.

The pions are the lightest particles in the QCD spectrum spectrum and can assuredly be interpreted as the approximate Nambu-Goldstone bosons of the spontaneous breaking of chiral symmetry. This symmetry also plays a prominent role in the study of hadronic matrix elements of the effective weak Hamiltonian parametrising, for instance, kaon decays and mixing. These processes are being extensively studied both theoretically and in experiments.

Lattice QCD and Chiral Symmetry

Lattice QCD [1] is a rigorous way to address the above mentioned problem of dealing with QCD in the regime of low energies where perturbation theory is not reliable. In a discretised Euclidean space-time, the inverse of the lattice spacing acts as an ultra-violet cutoff to regularise QCD. At a finite value of the lattice spacing, observables will depend on the cutoff. However, physical results can be obtained when removing the cutoff by performing the continuum limit extrapolation. By fixing the physical volume of the system it is furthermore possible to achieve a complete implementation of the dynamics of QCD by numerical methods. An interesting aspect of these studies is that the masses of sea and valence quarks are input parameters and can therefore be varied in order to explore the mass dependence of physical quantities.

A proper discretisation of QCD on the lattice has to guarantee that all the symmetries of this theory are present in the continuum limit. On the other hand, it is desirable that these symmetries are preserved also in the discretised theory since this provides important constraints and a better control of the systematic uncertainties affecting the results of the simulations. Due to a no-go theorem, the implementation of a fermionic action preserving chiral symmetry on the lattice seemed, for a very long time, to be destined to fail. It is one of the major advances on the field to have been able to define a lattice version of chiral symmetry which circumvents the no-go theorem [2].

The overlap operator proposed by Neuberger [3] provides a discretisation of the Dirac operator preserving chiral symmetry on the lattice. Although being a neat way to implement this symmetry, overlap quarks are in practice extremely expensive from the computational point of view.

Figure 1: Dependence of the pion decay constant f_π on the lattice spacing a. The black triangles label the unitary setup. The other symbols refer to the mixed action, each symbol labelling a particular way to match the sea and valence quark masses. All matching conditions lead in the continuum limit to a value consistent with the unitary approach. In addition, the expected quadratic scaling behaviour on the lattice spacing is verified for both unitary and mixed action data.

Indeed, the solution of the Dirac equation can be two orders of magnitude more expensive for overlap quarks than for lattice fermions that break chiral symmetry, e.g. Wilson twisted mass (Wtm) fermions [4]. This becomes quickly prohibitive when considering overlap sea quarks since not only the Dirac equation has to be solved very frequently in this case, but furthermore, state of the art algorithms to simulate dynamical overlap fermions still show a poor scaling on the lattice volume.

Results

The strategy that we have explored in our project at the HLRB system consisted in (i) profiting from the important advances achieved over the last few years in simulating QCD with Wilson-type sea quarks while also (ii) preserving chiral symmetry at the level of the valence quarks where it is known to provide important simplifications. Such an approach is referred as a mixed action, because a different discretisation of the fermionic action is used in the sea (Wtm quarks) and in the valence (overlap quarks) sectors. Furthermore, for both overlap and Wtm formulations it is possible to guarantee that the continuum limit extrapolation of physical observables does not depend linearly on the lattice spacing but only quadratically thus significantly reducing the uncertainties in the final results.

Although very attractive for practical studies of QCD, mixed actions can also introduce potential difficulties. The main goal of our study has been to perform a systematic study of the parameter space in order to identify the regime in which mixed actions are well under control. An additional motivation has been that such a detailed investigation was missing in lattice QCD studies while several groups are currently performing or planning to use a mixed action approach.

The main issue to address in mixed actions studies is related to the the absence of symmetry between sea and valence quarks, something which breaks the unitarity of the lattice theory. Furthermore, it is important to check whether subtle effects could arise from the fact that chiral symmetry is present in the valence but not in the sea. For instance, chiral symmetry allows for the presence of exact zero-modes of the Dirac operator which could induce large effects in infrared physics if they are not properly suppressed by the fermionic determinant involving sea quarks only.

In the following, we refer to the case of observables using sea and valence Wtm quarks as the "unitary" setup and to the case of quantities using overlap valence quarks and Wtm sea quarks as the "mixed action" setup. The first step in controlling the mixed action is to impose that sea and valence quark masses are equal. This can be achieved by matching the unitary and mixed action pion masses m_π. We can then consider another observable, e.g. the pion decay constant or the nucleon mass, and compare its unitary and mixed action values when reducing the lattice spacing towards the continuum limit. Fig. 1 illustrates this behaviour for the pion decay constant f_π. We observe that a common value of the unitary and mixed action determinations of f_π is achieved in the continuum limit. This demonstrates the restoration of the unitarity of the theory. However, in order to obtain such a result in a small physical volume – the lattice size is L~1.3fm – it was necessary to use in the mixed action a modified definition of f_π for which the zero-modes of the Dirac operator were subtracted. An important observation arising from our study [5] is that the constraint $m_\pi \times L > 4$ is needed to completely suppress the effects of the zero-modes. Our study thus provides constraints on the regime of quark masses, volumes and lattice spacings where the results of the mixed action can be considered to be under control.

Outlook

We are currently extending this analysis to other observables to check if the current constraints are valid elsewhere. As already mentioned, we observe that these constraints significantly depend on the zero-mode effects. We are currently performing a direct study of their distributions since an index theorem relates them to the topological structure of QCD. Finally, we plan to profit from the conclusions of this project to devise an ulterior study in which a proper control of the mixed action and of the effects of chiral symmetry could allow to clarify longstanding and remarkably difficult problems such as the ΔI=1/2 rule in Kaon decays. From our current studies, it appears that a petascale system – such as superMUC – is needed to approach such an ambitious project.

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Lattice Studies of Resonances

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HLRB Project ID: pr58na

6

Introduction

Understanding the full spectrum of hadrons from first principles is a key objective of theoretical particle physics. Hadrons are bound states of strongly interacting quarks. The theory which is believed to describe the strong interactions is called Quantum Chromodynamics (QCD). Computing the masses of hadrons based on this theory requires non-perturbative methods. The most successful approach today is based on numerical simulations of a formulation of QCD in discrete rather than continuous space-time called Lattice QCD. Based on this method the masses of a larger range of hadrons could be computed, for instance the masses of the light stable hadrons [1].

An ab-initio computation of such experimentally well-known hadron masses is an important validation of both the theory and the methodology. However, most of the particle states are not stable. To study these so-called resonances using theoretical particle physics methods, like Lattice QCD, continues to be a major challenge. In this project the focus is on a particular class of resonances, the resonances of scalar mesons.

The spectrum of light scalar mesons (i.e. the scalar mesons with masses below 2 GeV) is still a puzzle. For instance the masses of the nonet of the light scalar mesons, which have masses just below 1 GeV, cannot be explained assuming a bound state of two quarks $q\bar{q}$. This description seems, however, to fit to the heavier nonet consisting of mesons with masses which are heavier than 1 GeV. One possible explanation could be that scalar mesons are a mixture of tetraquark states and heavy $q\bar{q}$ states [2]. There are indications that this is not the full picture since there is evidence that some of the scalar mesons are hadronic molecules bound by strong meson-meson interactions [3]. Given this puzzling situation the Particle Data Group made in a review the following statement: "Scalar mesons are especially important to understand because they have the same quantum numbers as the vacuum $J^{PC} = 0^{++}$. Therefore, they can condense into the vacuum and break a symmetry like a global chiral $U(N_f) \times U(N_f)$. The details of how this symmetry breaking is implemented in Nature is one of the most profound problems in particle physics." [4]

Methodology

The computations are performed in a workflow consisting of two stages. First, dynamical gauge configurations are generated using parameters which make these configurations particular suitable for the observables we want to compute. Then, taking these configurations as input, correlation functions are computed and, finally, physical observables extracted.

As QCD can be discretized in various ways we have to decide for one particular formulation, i.e. action. In this project we are using the SLiNC action which comprises Wilson-type fermions [5]. The fermionic part of the action is tuned such that first order discretization errors are eliminated. In this pilot project it is important to keep discretization effects small as we will not be able to afford simulations at different lattice spacings a. (Only this would give us full control over this source of systematic errors).

In our simulations we include two degenerate light quarks and one strange quark. Since for these kind of computations simulating at the physical quark mass is not feasible we have to compromise to a unphysical simulation point. In our current simulations the masses of the light quarks correspond to a pion mass of 250 MeV. We expect this to be sufficiently small to capture the relevant physics. The strange quark mass is tuned such that the sum of the 3 quark masses is (almost) the same as at the physical point, i.e. our strange quark is lighter than in the real world. (This choice is of particular advantage in this project as it allows us to avoid inclusion of $K\bar{K}$ scattering states.) The lattice is relatively fine with $a \approx 0.08$ fm. The size of the lattice, $V = 32^3 \times 96$, has a particular long extension in time direction which is important to suppress contributions from states propagating in opposite time direction. The spatial extension for a given pion mass has to be selected such that we can capture several energy levels using multiple momenta.

To compute the physical observables we are interested in, we have to compute both quark-quark and meson-meson correlators. This used to be numerically prohibitively expensive, but thanks to techniques developed in

recent years this task has become feasible. We employ the so-called distillation method introduced in [6] and, e.g., successfully applied to vector meson decays [7]. Due to the size of the lattice we have to further modify the techniques and use stochastic methods.

Initial Results and Outlook

During the initial phase of the project we have generated a set of configurations. These are currently being used to tune the distillation method. The distilled operators are constructed from the M lowest eigenvectors of the gauge-invariant lattice Laplacian:

$$\Box_{\mathbf{xy}}(\mathbf{t}) = \sum_{\mathbf{m=1}}^{\mathbf{M}} \mathbf{e_x^m}(\mathbf{t}) \, \mathbf{e_y^{m\,\dagger}}(\mathbf{t})$$

where $1 \leq M \leq L^3$. For the simulation parameters used in this project we expect M to be O(100). First results seem to confirm this expectation.

In a next step we will start computation of correlators for a larger set of configurations. This will allow us to extract first estimates of the relevant physical observables.

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Life Sciences

Micromechanical behavior of DNA

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7

Introduction

The topic of the project is relevant to the development of novel single-molecule manipulation techniques in biophysics and bio nanotechnology where complex DNA-liquid interactions occur. The goals of the project are to verify the proposed numerical method by comparing the results for simple flow conditions with available numerical and analytical results, to analyze the dynamics of the DNA macromolecule exposed to an uniform and shear flow, perform simulations corresponding to the more complex experimental flow conditions.

Recently the task attaching one DNA molecule specifically with both ends to different microscopic contact pads on surfaces has been carried out for the first time with respect to the construction of DNA-templated nanowires and networks. These investigations show unambiguously that DNA molecules can be specifically integrated into microfluidic channel systems and be manipulated by hydrodynamic flows.

Because mesoscopic length scales (from nanometres to micrometers) dominate the overall behaviour of DNA, macroscopic approaches such as finite-volume or finite-element based discretizations of the continuum-flow equations, and microscopic approaches, such as molecular dynamics (MD), are not applicable since they cannot resolve the mesoscopic structures, neglect thermal fluctuation effects, or are limited to characteristic length scales near the lower bound of microfluidics. Therefore a number of research groups pursue mesoscopic approaches which can resolve DNA molecular structure, and recover hydrodynamic forces and thermal fluctuation effects as well.

In this project we describe a use model based on smoothed dissipative particle dynamics (SDPD), which is suitable for the numerical simulation of complex flows. The method inherits the favourable properties of Smoothed Particles Hydrodynamics (SPH) [1] for complex flows and the efficient representation of mesoscopic effects. Immersed polymers are taken into account in simulations by a straight-forward modification of the SDPD-particle interactions of particles containing parts of the polymer. The method is validated by the comparison with theoretical results of generic cases [2].

Figure 1: Polymer is modelled as a chain of beads in the "ocean" of solvent particles.

The polymer is embedded into a number of special SDPD particles (denoted as polymer beads) which represent the segments of the polymer molecule. For typical particle sizes a bead would contain mainly solvent and the volume fraction of the polymer segment is small. Therefore, polymer beads interact hydro dynamically, with additional forces due to the chemical bond between the polymer segments contained in neighbouring polymer beads. These additional forces are taken into account by a finite extensible non-linear elastic (FENE) potential

Computational details
In the influential review articles Larsen listed the following forces important for polymer simulations. They all are captured in SDPD model:
- Viscous drag: included in SPH equations
- Entropic elasticity: FENE spring
- Brownian forces: captured by Generic formalism
- Hydrodynamic interaction: included via sol-vent SDPD particles.
- Excluded-volume: in SDPD particle cannot penetrate due to strong potential forces

Figure 2: Polymer bead distribution in Poiseuille flow

- Internal viscosity: polymers beads are also interacting with normal SDPD forces
- Self-entanglement: polymer chain can en-tangle with itself but big number of beads is required.

A typical simulation procedure is illustrated in Figures 1. The polymer chain is immersed in a domain full of SDPD particles.

An implementation of the model with focus on performance was done in FORTRAN 90 using PPM library which hides the complexity of the parallel implementation from the client author:

- PPM: Highly Efficient Parallel Particle-Mesh Library, http://www.mosaic.ethz.ch/Downloads/PPM
- H5Part: An API scheme to store particle data, http://vis.lbl.gov/Research/AcceleratorSAPP
- fgsl: FORTRAN interface to the GSL, http://www.lrz-muenchen.de/services/software/mathematik/gsl/fortran

Figure 3: Ensemble images of the DNA. Shear rate increases from top to the bottom. Black solid line is a wall position. Crosses mark the region with highest bead density.

The parallelization strategy is based on domain de-composition. Communication is performed using ghost-particle layer between neighbouring sub-domains. In case of PPM-client we use only a subset of mapping options provided by the library.

The performance of single processor code achieved on HLRB is around 10^4 particles processed per second per one processor.

Results

A study of polymer confined in the channel and exposed to a Poiseuille flow was also performed. In Fig. 2 the span-wise distribution of polymer mass is shown. We found that the profile is affected by Schmidt number: for lower Schmidt number the depletion region is pronounced at the centre of the channel; for high Schmidt number the polymer concentration tends to be higher in the centre with smaller off-centre peaks [2]. Our simulations results are generally confirmed by the recent experimental study of and more detailed mesoscale simulation.

Another results are related to a DNA molecule tethered on wall surface and exposed to shear flows, it exhibits different mechanical properties due to the different hydrodynamic force and wall-chain interaction. The distributions of DNA beads in the flow-gradient plane for three cases with small, moderate and large shear rates are shown in Fig. 3.

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"In silico" Phosphate Transfer:

From Bulk Water to Enzymes

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7

Why Study Triphosphate Hydrolysis?

Enzymes are protein molecules that function as catalysts to accelerate a myriad of important chemical reactions in nature that would not otherwise occur on a relevant timescale. One such reaction, which plays an integral part in the biochemistry of living organisms, is the hydrolysis of a group of molecules known as nucleoside triphosphates (NTPs). Their most intriguing property is the fact that cleavage of their so-called "energy-rich" phosphoanhydride bonds by specific enzymes leads to a variety of different functions. These encompass such widespread applications as a short-term chemical energy store to drive muscle contraction in the case of ATP, and as second messengers in cell signalling pathways in the case of GTP [1]. Indeed, the malfunction of this reaction is known to be a factor in diseases such as cancer.

When examined more closely, this enzymatic reaction is essentially the addition of a water molecule to the NTP thereby splitting it into two parts, namely the corresponding nucleoside diphosphate (NDP) and an inorganic phosphate molecule, P_i. It is more commonly known as hydrolysis. NTPs are unexpectedly stable in aqueous solution and rapid cleavage of the phosphoanhydride bond only happens when it is catalysed by a suitable enzyme or, alternatively, by a substantial change in the pH of the solution. The exact mechanism of this reaction, not only in solution, but also in various enzymes, has been the subject of intense discussion for a number of years, see [2, 3] for some reviews. Despite these efforts, the reaction pathway is still largely unknown – even in bulk water - although it is assumed to proceed by one of the following mechanisms: dissociative, associative or substrate-assisted catalysis.

Simulation Philosophy: Exploring Free Energy Landscapes

To obtain a picture of any reaction mechanism one needs to examine the system on a molecular level. Recent advances in simulation techniques and computer technology make it possible to study such reactions "in silico" in-stead of in the wet laboratory. As an enzymatic reaction is ultimately a dynamical process, a theoretical method must be able to describe the time-dependant behaviour of the system in question. Classical Molecular Dynamics (MD) is a multifaceted simulation technique that calculates the motion and distribution of the particles in an N-body system by solving Newton's equations of motion iteratively and relates these to experimental observables, e.g. thermodynamic properties, through statistical mechanics [4]. Often, a rearrangement of the electronic structure plays an important role in a reaction so one has to look beyond current empirical force fields and treat the electrons explicitly in the framework of *ab initio* simulation methods [5]. This unfortunately restricts the computable size of a particular system to a few hundred atoms, depending on the method used. The huge size of even a single protein molecule surrounded by its biologically relevant solvation shell (10^5-10^6 atoms) easily renders it computationally intractable for all but the most rudimentary simulation methods and a balance

Figure 1: Free energy surfaces plus molecular configurations sampled along the lowest free energy pathway of the hydrolysis reaction in a) an acidic water solvent (TS=Transition State), b) in a pH neutral water solvent (INT=Intermediate).

between a realistic model and the computational coc1st of simulating the system has to be found. One solution is to employ QM/MM methods, in which only a small part of interest is described using the more exact quantum mechanical (QM) electronic structure methods, the remainder of the protein and its solvent are described using the much more efficient, but less accurate, molecular mechanics (MM) force field methods [5, 6].

Chemical reactions are ultimately governed by the shape of their free energy landscape as the reaction progresses from reactants to products along the pathway of lowest free energy. This often involves overcoming large energy barriers, so-called transition states, meaning it can take up to milliseconds for a reaction to occur, making it unlikely to happen on a QM/MM timescale at finite temperatures (i.e. ~10–100 ps). As the free energy landscape of large, complicated systems is, dimensionally speaking, huge, and, energetically speaking, rugged, an enhanced sampling procedure must be employed that confines the exploration to the relevant regions of this surface only and efficiently visits both deep and shallow minima. In our calculations, this is achieved by the metadynamics method, in which a history-dependant potential is added to the dynamical trajectory of carefully chosen variables which are capable of describing the reaction in question [7]. These can be structural order parameters such as bond lengths, angles or coordination numbers.

The programme employed in this study is CP2K, an open source FORTRAN 95 code which performs *ab initio* MD simulations [8]. It is well parallelized and particularly suited to large scale clusters as its implementation leads to an overall scaling near to $O(N)$ for smaller systems; for larger systems the diagonalisation of the Kohn-Sham matrix can lead to slightly less favourable scaling performance. The calculation of the intermolecular potentials that describe a system of atoms involves such routines as fast Fourier transform (FFT), matrix diagonalisation and eigenvalue problems; the trajectory is ultimately produced by numerical integration using symplectic integrators. Therefore, parallel algorithms tuned to running on large scale machines have recently paved the way to modelling such reactions in protein systems involving hundreds of thousands of atoms. An additional gain in the scalability of such large systems can be achieved using multiple weakly-coupled "walkers" which explore and reconstruct the same FES simultaneously [9]. As the communication load between the walkers is negligible the method is intrinsically parallel and scales linearly with the number of walkers. Thus, on a large-scale parallel machine it is possible to reconstruct the FES of a reaction accurately within a reasonably short simulation time.

A First Glimpse of Hydrolysis and Ongoing Research

To be able to capture the influence an enzyme has on a particular reaction a suitable reference system without the protein environment is required, therefore, the hydrolysis reaction was initially studied in bulk water [10]. Using *ab initio* metadynamics above we obtained the

Figure 2: The hGBP1 dimer complex investigated in the ongoing QM/MM Simulations.

FESs of the hydrolysis of an NTP under both acidic and neutral pH conditions and observed two different reaction mechanisms, see Fig.1a) and b). A possible intermediate was observed in the pH neutral solution. However, a clear-cut picture was not obtained, as the mechanisms exhibited both dissociative and associative characteristics. There was substantial solvent interaction, including many proton transfers within the water solvent, which ultimately led to the concept of an assisting water molecule facilitating the addition of the water molecule to the NTP. Such a complex scenario can only be seen in a bulk solvent environment in which all waters are treated on equal footing with the reactant via *ab initio* simulations.

These results will serve as references for mechanisms and barriers obtained from ongoing simulations of the same hydrolysis reaction in a specific protein, see the GTPase depicted in Fig. 2, enabling us to investigate what effect the protein environment has on the FES and, ultimately, on the enzymatic reaction pathway. For such large systems "all QM" simulations are no longer feasible so that QM/MM approaches must be used. Numerical simulations on large, highly parallel machines are therefore fundamental to exploring the nature of processes happening on a timescale which is often too short to be captured by experimental techniques. Improvements in parallel algorithms together with increasingly powerful hardware such as the SuperMUC are required to keep pace with the ever-increasing size of protein systems as the quest towards modelling a "real life" scenario continues.

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Revising the Seed Plant Tree of Life with Supercomputers under Maximum Likelihood

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7

Introduction

Understanding the genetic and genomic basis of plant diversification has been a major goal of evolutionary biologists since Darwin first pondered his "abominable mystery", the rapid diversification of the angiosperms in the fossil record. In the computer age, the relationship between a set of organisms and their diversification history can be inferred from their molecular sequence data, i.e. DNA or protein sequences, and represented in a phylogenetic tree. Advances in high-throughput sequencing techniques lowered the cost for obtaining molecular data significantly and have boosted both, the interest in molecular phylogenetics as well as its quality. For example, in plant phylogenetics, previous hypotheses from molecular data were often disputed due to the small sample of genes and/or organisms used in the analyses and various conflicting typologies for the five basic seed plant groups have been obtained over time. This has changed since progress has been made in generating genome-scale plant phylogenies. However, plant molecular phylogenetics has long relied on plastid genomes and only a few nuclear markers to infer relationships, but nuclear genome analyses of plants have only recently started to appear in literature. Yet, the incorporation of nuclear phylogenomic information would accomplish two important goals. First, the phylogenetic patterns discovered using nuclear genomic information could be used to corroborate the many well-supported plastid relationships, and to shed light on those relationships that are still at odds. Second, nuclear phylogenomic information can be used to derive new hypotheses for the function of plant genes that are relevant to major divergence events in plant evolution.

Unfortunately, the obvious benefits of phylogenomic analyses come at the price of almost prohibitive computational requirements. Only the availability of large-scale HPC infrastructures and the development of highly efficient and massively parallel tools for phylogenetic inference in recent years rendered such analyses feasible at all.

Results

We aligned protein sequences from 150 plant species that belong to 101 different genera, representing a broad taxonomic range of angiosperms and extant gymnosperms. The resulting multiple sequences alignment contained 10,768,363 columns. From that alignment we derived a smaller sub-alignment that only contained those genes that were present in at least 30% of all species and in which multiple taxa belonging to the same genus were collapsed into a single taxon. This alignment contained 101 taxa and had a length of 1,660,883 amino acid residues.

We performed Maximum Parsimony (MP) tree inferences (including bootstraps) on both alignments with PAUP* and TNT. On the smaller alignment we additionally performed Maximum Likelihood (ML) analyses with RAxML. Due to the rather modest computational requirements of MP-based tree inference, those computations could be carried out with the standard sequential versions of PAUP* and TNT by only exploiting the embarrassing parallelism that is inherent to bootstrap analyses on the 504-node BlueHelix cluster at the Cold Spring Harbor Laboratory. ML analyses, on the other hand, are much more demanding with regards to both, computational as well as memory requirements. Even to accommodate the smaller alignment, we had to employ the MPI-parallel version of RAxML we had previously developed and which is able to distribute the computations as well as its datastructures over multiple nodes [1]. It also implements the CAT-approximation to accommodate rate heterogeneity among sites which reduces the memory and computational requirements to approximately a quarter of the typically used GAMMA model. RAxML additionally features a rapid bootstrap algorithm that reduces the runtime of phylogenetic analyses by another order of magnitude. The majority of ML analyses have been carried out on the HLRB2 supercomputer at the Leibniz Computing Centre, utilizing 2 million CPU hours. Some computations have additionally been carried out on the Woody Cluster at Regionales Rechenzentrum Erlangen and the Infiniband cluster at the Technical University of Munich. In total, we were able to con-

duct 20 full tree searches from different starting points under both CAT and GAMMA and compute 223 rapid bootstrap pseudo-replicates. As the full tree searches under CAT produced better results than the GAMMA model, we performed the bootstraps under CAT as well.

The basic topologies for all three trees inferred under MP and ML are essentially identical (the figure depicts the ML tree with ML and MP bootstrap support values). The bootstrap supports suggest that the inferredd tree topologies are robust overall. All trees corroborate the same monophyletic groups of seed plants, as revealed in all previous morphological analyses and most molecular analyses, namely the seed plants, the cycads, the conifers, the gnetophytes, and the angiosperms. Moreover, all of our analyses support the gymnosperms as a monophyletic group which is congruent with all comparable molecular data sets to date, and in contrast to most morphological analyses, which retrieve gymnosperms as paraphyletic. The differences between molecular-based topologies of the gymnosperms mainly involve the placement of the gnetophytes. The position of the gnetophytes among seed plants, is indeed one of the most interesting unresolved issues in plant systematics. Our inferred genome-wide phylogeny supports the gnetophytes as basal extant gymnosperms. It is noteworthy that in this phylogenomic view of the seed plants, the basic topology of the angiosperm tree used by the Angiosperm Phylogeny Group (APG II, III) is supported with only minor changes.

A controversial topology that is present and well supported in all our of phylogenomic trees is the placement of the monocots between Nuphar and magnoliids. Our phylogenomic tree firmly places the magnoliids as sister to the eudicots, and the monocots as sister to the magnoliids plus the eudicots. The bootstrap support percentages along the backbone of the angiosperms also show that overall, our phylogenomic analysis provides a robust topology for this important group. For a comprehensive discussion of the results, please refer to [2].

On-going Research / Outlook

The continuing rapid accumulation of molecular sequence data will drive the demand for tools and infrastructures that are able to perform large-scale phylogenomic analyses. At the same time, the complexity and degree of parallelism of HPC infrastructures that are able to provide the computational power and memory necessary for such analyses increases steadily. Future research will therefore concentrate on further algorithmic improvements of RAxML and exploitation of additional levels of parallelism.

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http://nypg.bio.nyu.edu/bp
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Chaperone proteins in the crash test

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Introduction

Proteins are complex molecular machines performing their function upon tight regulation. An intriguing example is the chaperone protein Hsp90. Chaperones are helper proteins – they assist other proteins in finding their native most stable structure. As such, they are essential for most cells to survive. This is even more the case for cancer cells, as they are world champions in producing proteins and thus need to cope with highly crowded cell interiors in which the folding of a protein into its native functional state is extra-ordinarily challenging. Chaperones like Hsp90 are thus of primary importance for the survival and proliferation of cancer cells, and thus the growth of cancer. For this reason, these proteins represent a primary group of targets for anti-cancer drugs.

Designing strategies to block Hsp90 function in cancer cells would be greatly aided by deciphering the mode of function of this fascinating molecular machine. Experiments have revealed that Hsp90 undergoes a transition between an open and a closed state, which is an essential feature of its function and regulation. The opening and closure transitions are controlled by the binding of a small nucleotide molecule, namely ATP, which then will be transformed into ADP and finally released again.

But how is the binding of these small molecules in one very restricted protein region coupled to large-scale dynamical transitions of the protein from an open into a closed state and vice versa? How can the protein 'sense' the binding of the molecule and propagate this information into distant regions of the protein scaffold? Could one reveal the distribution of stress in the protein upon perturbing it by a small molecule, analogous to the stress field analyzed during the crash test of a car?

Experiments on Hsp90 to date are not yet able to reveal dynamic information of a pro-

Figure 1: Graphical representation of the simulation system. The protein HtpG (red/white, balls) in the middle of a rhombic dodecahedral water (opaque red, lines) filled box. Sodium (blue, balls) and chlorine (green, balls) represent the physiological salt concentration in cells.

tein at high time resolution. The most advanced experiments can give very detailed information on the spatial resolution (fluorescence resonance energy transfer [1] or hydrogen/deuterium exchange [2]).

Validation by experiment: Hsp90 opening and closing
These complex calculations are based on many parameters and assumptions. To make sure, that the results of these calculations are useful, the basic findings have been compared to experimental results that have not been used to build the simulated model in the first place. To this end, we compared the opening and closing of the protein in our simulation with data from fluorescence resonance energy transfer [1]. The results of the simulations are in a good agreement with the experimental results.

Sophisticated experiments suggested that these motions are happening in timescales of seconds, which however presents an upper limit due to the limited time resolution at hand [2]. Our dynamic trajectories at femtosecond resolution, however, showed that the motion of parts of the protein can be much faster than expected (Figure 2). More specifically, we showed that the large domain movement in Hsp90 required for activation of the protein can happen in the timescale of nanoseconds.

Going beyond experiments: Hsp90 in the crash test
How is this large opening and closing motion involved in activating the protein linked to the binding of the small molecule of ATP? To answer this question, the results of the simulation have been analyzed with a method that had been invented in our group, the force distribution analysis. Just like in a crash test for cars, the internal molecular stresses can be revealed within the protein scaffold. Obviously, we did not calculate the stress distribution in Hsp90 due to high forces upon hitting a wall, but when the small ligand ATP is bound to the protein. We could demonstrate, that the effect of the ligand is

apo

ADP

ATP

Figure 2: left: Line representation of HtpG after a molecular dynamics simulation of 20 ns. right: electron microscopy pictures of the unbound/ apo state (top), the ADP bound state (middle) and the ATP bound state (bottom) as a reference [3]. Results

not just restricted to the vicinity of the binding niche, but force is very selectively channeled through a large helical structure in the protein from the binding area of ATP to a part of the functional part of the protein that is responsible for opening and closing of the protein (Figure 3). Thus, our high resolution technique based on high-performance computing was able to detect the network of forces responsible for signal transmission in a protein on an atomistic scale. On this basis, biochemical mutations for the protein could be proposed to validate our proposed model of the mechanism of the protein.

On-going Research / Outlook

Our results on the intriguing case of molecular chaperones demonstrate that by means of a novel force distribution analysis, the communication pathways in com-

plex molecules like proteins can be deciphered, helping to re-engineer functional mechanisms in protein molecular machines. Applications of this approach to other proteins and protein complexes is promising given that the computational power at hand will increase steadily in the future, a prerequisite for the convergence of molecular stresses investigated here.

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Figure 3: Graphical representation of the result of a force distribution analysis. The two domains of the protein (blue and gray) communicate along a pathway (orange). The comunication interface between both domains is shown in a stick representation.

Coupled Problems in Computational Modeling of the Respiratory System

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Introduction

Mechanical ventilation is a vital supportive therapy for critical care patients suffering from acute lung diseases in view of oxygen supply. However, pre-existing lung injuries predispose patients to a number of complications which are collectively termed ventilator associated lung injuries (VALI). VALI mainly occurs in the walls of the alveoli, i.e. the small lung compartments constituting the blood-gas barrier. Understanding the reason why alveoli still become damaged or inflamed despite recent developments towards more "protective" ventilation protocols is a key question sought by the medical community. Computational models of the respiratory system can provide essential insights into involved phenomena. In particular, computational models offer the possibility to predict data that cannot be measured in vivo such as local alveolar strains and stresses which are relevant for the development and progress of VALI. However, establishing reasonable models is difficult since the lung comprises more than 20 generations of bifurcating airways ending in approximately 500 million alveoli. This complexity inhibits a direct numerical simulation resolving all relevant structures from the onset. Therefore, as a first step, we have developed detailed computational models of distinct parts of the lung, i.e. the tracheo-bronchial and the alveolar region, which will later be combined to one overall "virtual lung" model [1].

Methods

All simulations were performed with our multi-purpose finite element (FE) software platform BACI [2]. BACI has been and is developed within an object-oriented C++ environment. Parallelization is based on domain decomposition methods using MPI. State-of-the-art solution techniques for nonlinear and linear systems of equations as well as for coupling of several physical fields are incorporated in BACI and are continuously developed further in our group. For the implementation of efficient parallel sparse linear algebra operations, BACI makes use of the open-source software framework "Trilinos" (Sandia National Laboratories).

Results

There is an ongoing debate about how turbulence in the upper airways affects flow and pressure in lower airway generations. As opposed to previous simulations, we considered a pulsatile inflow condition, allowing the development of turbulence over a pulse cycle to be investigated, which is obviously more physiologically realistic. Our results (see, e.g., Figure 1) suggest that turbulence effects in the bronchial airways are rather weak and can completely decay as early as the third generation, depending on both geometry and flow distribution.

Figure 1 Contours of phase-averaged velocity in the laryngeal and tracheal region. Contours of velocity are plotted at the locations L1–L4 indicated along the trachea (taken from [3]).

Figure 2 Comparison of pressure contours, for light activity, at maximum inspiration. Left: 3D model with free outflow. Right: 3D model considering peripheral impedances (taken from [4]).

Due to limitations on the number of airways visible on CT scans, only a part of the airway tree can be resolved in 3D. Therefore, realistic boundary conditions need to be applied at the outlets of the 3D domain in order to consider the effect of the unresolved peripheral region appropriately. For this purpose, we have developed a reduced-dimensional model of the non-imageable vessels [4]. Briefly, the 3D airway model is supplemented by simplified 1D trees attached to every 3D outlet. By considering the unresolved peripheral impedances, reasonable outflow boundary conditions are derived for the resolved 3D domain. With these boundary conditions, we found that the maximum pressure in the tracheo-bronchial region is approximately 44% higher than in previous models neglecting peripheral impedances (see also Figure 2).

As a next step, we also studied the influence of the surrounding tissue on both air flow and stresses in the airway walls. To solve the fully coupled non-linear fluid-structure interaction problem, a monolithic approach with algebraic multi-grid preconditioning was utilized (see, e.g., [5] and [6]). We found that essential features of the velocity distribution, such as locations of high velocity jets and recirculation zones, remain the same. However, a fivefold reduction in airway wall stresses was

observed for airway models embedded in lung tissue. In addition, we also found that the distribution of stresses slightly changed (see Figure 3)

Our detailed model of the tracheo-bronchial region enables us to quantify the distribution of pressure and flow into the peripheral regions. Since alveoli are the major site of VALI, we have also developed a comprehensive model of individual alveoli allowing us to determine local stresses and strains in the tissue. In contrast to former studies, our model is based on a realistic 3D geometry obtained from micro-CT imaging. We found that strains in individual alveolar walls are up to 400% higher than averaged global tissue strains (see Figure 4). Consequently, resolving the realistic alveolar morphology is crucial when investigating phenomena of VALI.

Figure 4 Strain distribution in a cube of lung tissue. Red color indicates strain "hot spots" at risk of overdistension (taken from [7]).

Outlook

Ongoing work is concerned with combining our detailed models of the tracheo-bronchial and the alveolar region to one overall "virtual lung" model. For validation purposes, we plan to correlate our simulation results with medical data obtained for patient-specific disease conditions. In the future, we hope to gain further insights into how different ventilation protocols affect local stresses and strains and, thereby, the development and progress of VALI.

Figure 3 Tissue stress normalized by the maximum stress. Left: Airways without surrounding lung tissue. Right: Airways embedded in surrounding tissue.

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Dynamics and interactions of membrane-spanning protein helices

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HLRB Project ID: pr42ri

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Introduction

Individual cells of biological organisms are enclosed and substructured by lipid membranes. These lipid membranes are built from a great variety of different lipid molecules and integral membrane proteins. The task of membrane proteins is to mediate regulated fusion of cells, allow for solute exchange with the cell exterior, regulate release of cellular products, mediate lipid translocation between inner and outer membrane leaflets etc. Proteins are anchored by helical transmembrane domains (TMDs) that frequently guide assembly of proteins to larger functional complexes as a result of specific helix-helix interactions (Langosch and Arkin, 2009). In addition, TMDs are intrinsically dynamic structures in a sense that the hydrogen-bonds that give them their shape experience local and transient open/close reactions (Fig. 1).

It is clear that recognition between TMDs and their transient shape changes, viz. backbone dynamics, must influence each other. Both aspects are connected to their interactions with surrounding lipids which is likely to underly the ability of TMDs to facilitate the fusion between membranes and the translocation of lipids between different membrane leaflets, termed lipid flip-flop. TMD interaction and dynamics also appear to affect their ability to serve as substrates for intramembrane proteases. Specifically, both factors have been suggested to define the specificity by which the TMD of amyloid precursor protein is cleaved to fragments eliciting Alzheimer's disease (Fig. 2).

Results

Our own work focuses on the biophysical basis of the interdependence of helix-helix recognition, helix dynamics, and helix-lipid interaction. At the same time, we try to understand the impacts of these phenomena on a variety of biological issues, such as membrane fusion, lipid translocation, and intramembrane proteolysis. We thus work on a number of paradigmatic TMDs from suitable

Fig. 1 Schematic depiction of a cell (cut open to visualize intracellular structures) with an enlarged patch of plasma membrane (adapted from Nelson and Cox, 2008) and magnifications illustrating interactions and backbone dynamics of transmembrane helices.

Fig. 2 A scheme illustrating how TMD-TMD interaction, TMD dynamics, and TMD-lipid interaction influence each other in ways that are likely to have a strongly regulatory role for various biological processes, like membrane fusion, lipid flip, and intramembrane proteolysis.

model proteins and develop an array of model TMDs to test our hypotheses by design. Computational work on these TMDs complements and interprets our experimental approaches.

So far, we have investigated the dynamics of our de novo designed model TMDs in isotropic solvent matching experimental conditions using the molecular dynamics algorithm NAMD with the CHARMM force field (Phillips, et al., 2005). The results show that the backbone dynamics i) increases at the termini of the helices and ii) depends on the primary structure. The dependence on sequence is particularly important since the helix-destabilizing amino acid types found here have previously been found to be overrepresented in the TMDs of membrane fusogenic proteins and isolated TMDs are known to induce membrane fusion in vitro. Further, this work yielded mechanistic insights into the molecular determinants of backbone dynamics (Quint, et al., 2010). Specifically, we found that the nature of the amino acid side chains imposes certain restrictions on their flexibility within the helix and that they interact less favorably with each other along the helix backbone than the side chains of helix-stabilizing residue types. To our knowledge, this is the first systematic description of TMD helix backbone dynamics. These results obtained by MD simulations are validated by comparing them with experimental results. Indeed, they closely fit experimental work (CD spectroscopy, hydrogen/deuterium-exchange) since the results from >100 ns trajectories could be used to calculate experimental data recorded over several hours with good accuracy!

On-going research/outlook

In one project, we have simulated the dynamics and TMD-lipid interactions of certain model TMDs in lipid bilayer patches with mixed lipid types. The resulting trajectories are currently evaluated in terms of TMD dynamics and lipid structure. Preliminary results indicate that the dynamics of membrane-embedded helices are strongly reduced by the membrane as expected from theoretical considerations. Further, backbone dynamics appears to influence the rigid-body movements of the TMDs in the membrane as well as the interaction with the lipids surrounding them. The beauty of the MD approach is that the multitude of potential protein/lipid interactions can be differentiated and their dependence on backbone dynamics can be analyzed. By a detailed analysis we hope to be able to understand how TMD dynamics influences lipid structure. The biological significance of this project is that this work will shed light on the mechanisms by which TMDs enhance membrane fusion and lipid translocation between membrane leaflets.

In another project, we have investigated the backbone dynamics of the amyloid precursor protein TMD. This TMD is subject to cleavage at various sites by γ-secretase which ultimately leads to the build-up of peptides that lead to Alzheimer's disease. Since the toxicity of these peptides depends on their size and size depends on the site of cleavage, we try to understand how indi-

vidual cleavage events are influenced by the structure and dynamics of this TMD helix. Our results imply that certain mutations that change the cleavage pattern do so by changing local backbone structure/dynamics. Ongoing work in the Alzheimer field addresses the impact of TMD-TMD dimerization on backbone dynamics. Again, this work is complemented by experimental approaches to yield a holistic picture.

A third project adresses another membrane protein, sulph-hydryl oxidase, whose TMD self-interacts in a sequence-specific way. Experimental work identified amino acids that are responsible for mutual recognition of these helices and computational work resulted in a homodimeric structure that matches the computational results. In addition, our preliminary results suggest that interaction is modulated by the lipid environment, thus invoking further experimental work.

Taken together, analysis of these different paradigmatic model systems will shed light on the systematic connection between self-interaction, dynamics, and lipid interaction of TMDs.

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Population based gene-environment interaction analyses for asthma

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Introduction

The exceeding proportion of unexplained heritability in adult height [1] has raised a debate on the importance of single nucleotide polymorphisms (SNPs) for multifactorial diseases and traits. For asthma the situation is less clear, but a similar picture is anticipated [2]. Complementary explanations for heritability may be found in copy number variation, epigenetic modification, gene expression, and genetic epistasis [2]. A further potential mechanism involves interaction of environment and genotype [3]. This can be considered as a modification of environmental effects by the underlying genotype or modification of genetic effects by the environmental exposure.

The aim of the present study was to perform a genome wide scan for gene environment interactions for asthma phenotypes including 582,575 SNPs. The underlying population consisted of a stratified subsample of 1708 children of the GABRIEL advanced studies (http://www.gabriel-fp6.org/index.htm) representing 9,996 children from four study centers. As environmental exposure, childhood exposure to farming was investigated since its inverse relation to asthma has been consistently found in many populations all over the world [4], and various interactions with farming or farm related exposures have been reported for asthma from the ALEX and PARSIFAL studies [5-8].

As statistical method various approaches were explored: First, a full gene environment interaction was analyzed using a logistic regression model including the marginal effects of the genetic and of the environmental effect and additionally an interaction term. The second approach was based on the analysis of gene environment associations separately in the groups of diseased (cases) and healthy individuals (controls). Weighted averaging of the estimates of both groups as suggested by Mukherjee and Chatterjee enhances statistical power by focusing on the informative cases and simultaneously reducing bias from neglecting the controls [9]. Furthermore, we improved the two step method proposed by Murcray et al. [10] by calculating unweighted averages of the estimates of both

groups (step 1A). We furthermore introduced a step 1B, in which we stratified the sample for the environmental exposure and ran GWASes in the exposed and unexposed stratum separately. Again unweighted averages were calculated. The resulting chi-square values of step 1A and step 1B were summed and the corresponding p-value was derived from a chi-square distribution with two degrees of freedom. The resulting p-values were compared to the square root of the significance level 0.05 divided by the number of SNPs according to the Bonferroni method to correct for multiple testing. Only significantly associated SNPs were subsequently tested in a full gene environment interaction analysis (step 2) thereby reducing the number of statistical tests. Again Bonferroni correction was applied but now referring only to the number of SNPs tested in step 2. Since both steps are asymptotically independent statistical power was again enhanced.

The statistical analyses were performed in R. Parallelization was achieved using R's package "multicore". Usually 128 to 510 cores were used in parallel with best performance at 510 cores.

Figure 1: Genome wide interaction analysis for asthma phenotypes. Bonferroni corrected interaction p-values are plotted against the genomic SNP position. The red line represents the effective significance level of 0.05. The blue dots represent the p-values for interactions of farming and related exposures with asthma, the red dots with atopic asthma, and the green dots with non-atopic asthma. The yellow diamonds mark genes represented by at least two SNPs.

Figure 2: Power calculation for the genome wide interaction analysis for asthma with farming as environmental exposure. The power to detect full effect concentrations (blue lines), mild cross-over interactions (red lines), and strong cross-over interactions (green lines) is given for interacting allele frequencies ranging from 0.1 to 0.9 for genome wide significance, (α=0.05 corrected for 500,000 SNPs).

Results

The scientific achievements of the projects were published in the Journal of Allergy and Clinical Immunology [11]. In the genome wide screen, 97 SNPs emerged to interact with farming or related exposures for asthma with Bonferroni-corrected step 2 p-values below 0.05 (Figure 1).

To assess the interaction type we compared the associations of genotype and asthma separately for the exposed and unexposed individuals. The SNPs were coded for the interacting allele, i.e. for a protective effect in the exposed and a risk effect in the unexposed group. In the unexposed group the OR were around unity representing full effect concentrations or greater unity indicating cross-over interactions. Partial effect concentrations with inverse associations in the unexposed were not detected. In the exposed group none of the SNPs had an OR close to unity; hence effect concentrations in the unexposed group were absent. Some of the interacting SNPs had low minor allele frequencies (<0.1); more frequent SNPs with minor allele frequencies > 0.3 were not found to interact.

A simulation study was performed to assess the extent of interaction detectable with the power of the present data set. The power to detect a significant cross-over interaction for asthma with farming at a genome wide level of significance in 500,000 SNPs was above 80% within the range of interacting allele frequencies 30%-80% (Figure 2A). Within the same range there was >50% power for full effect concentrations. The power for partial effect concentrations was rather low (below the blue line in Figure 2). These power estimates take into account the multiple comparisons in a genome wide study. Hence, the study was well powered to detect significant gene-environment interactions for common genetic polymorphisms. Nonetheless we did not discover novel genes with common polymorphisms specifically interacting with the farming environment.

Overall these findings may indicate that the strong protective effect of a farming environment is neither due to the genetic make-up of the farming population per se nor to common genetic polymorphisms interacting with these particular exposures. This implicates that environmental exposures or the lack thereof can determine the new onset of childhood asthma. Conversely, in an unexposed population, genes such as those identified in the GWAS meta-analysis are causal factors for childhood asthma. In this scenario, both genetic and environmental components may independently contribute to distinct mechanisms underlying this condition.

On-going Research / Outlook

Sensitivity analyses have shown that the proposed statistical method has a slight false positive rate. This rate should be quantified and compared to other statistical methods as those described above. In order to quantify this rate at an appropriate resolution on a genome wide level about 1 million SNPs have to be simulated for each of about 100 scenarios. This estimation is based on the estimated number of putative independent loci in the human genome [12].

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Cosolute effects
on protein secondary structures

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HLRB Project ID: pr63ca

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β-sheet

α-helix

extended
strand

Figure 1: Illustration of the three different structures of the model peptides used in the computational study: extended strand, beta-sheet, and alpha-helix. The displayed peptides are polyalanines.

Introduction

Proteins are macromolecules that fulfill a wide range of tasks in biological cells after they have assembled into a certain spatial structure, the native fold. The stability of the correctly folded native structure versus other possible conformations of the chain depends on thermodynamic quantities like temperature and pressure as well as on the presence of other molecules in the surrounding solution. These so-called cosolutes are ubiquitous in cells: they are metabolites, messenger substances, osmoregulators, amongst others. Some of the osmoregulators denature proteins and others stabilize their native fold. Thus, by a permanent, systematic variation of the mixture of cosolutes in a cell it is possible to counteract harmful influences on protein structures and functions

(which can also include cosolute effects themselves). Striking examples are the use of trimethylamine N-oxide (TMAO) against the effect of hydrostatic pressure in deep-sea animals or the accumulation of sugars and glycerophosphorylcholine in the human kidney against the denaturation by urea, a side product of protein metabolism [4].

So far, the impact of cosolutes on proteins is not yet understood on a molecular scale: Why is a substance a denaturant or a stabilizer, and why is a substance inducing helical structures? Do direct specific interactions between the cosolute and the protein decide over the fate of the protein structure or do cosolutes rather exert their influence indirectly by modification of bulk solvent properties? In case of the former: Do cosolutes act via interac-

tion with certain sidechain groups of the proteins or via interactions with the backbone of the molecule?

Answers to all these questions do not only help to elucidate the mechanism of protein stabilization in nature (in general and under extreme conditions). They also provide knowledge, which is needed in order to design artificial additives with tailored effects on protein solutions in biotechnological applications.

Our presented study deals with the cosolute urea, which is a protein denaturant and is commonly used as such in experiments that address questions of protein stability and folding thermodynamics.
We study urea's effect on protein secondary structures by molecular dynamics simulations of model peptides with different structures in aqueous urea solutions of various concentrations. The simulation package Gromacs 4.5 is used [1]. Figure 1 displays the examined peptide conformations: an extended strand, an alpha-helix, and a beta-sheet. All simulated molecules are homopeptides. Since they consist of one type of amino acid, the conformational dependence of cosolute effects can be studied for a single type of residue independently. A simulation of such a model peptide in urea/water solutions of different concentrations yields $\Gamma_{u/w}$, the preferential binding or exclusion of urea and water molecules at the peptide. Together with the urea/water bulk structure, this input is needed for the calculation of the free energy of transfer per residue of the peptides from pure water to urea/water solutions [2]:

$$\frac{d\Delta G_{tr}^{w\to u/w}}{dc_u} = -k_B T \left[\frac{\Gamma_u}{c_u} - \frac{\Gamma_w}{c_w}\right]\left[1 + c_u\left(\frac{\partial \ln y_u}{\partial c_u}\right)_{p,T}\right]$$

High statistical accuracy of these spatial distributions of molecules requires long-timescale molecular dynamics simulations and thus supercomputing facilities.

Results

Figure 2 presents the calculated transfer free energies (TFEs) for the three conformations of polyalanine in Figure 1. All TFEs are negative, which implies that all three

Figure 3: Thermodynamic cycle relating the urea induced change in folding equilibrium between the structures A and B to the TFEs of the structures from water to urea solution.

conformations favor urea/water solutions over water. The solvent transfer of the extended peptide strand, however, is more favorable than the transfer of the helix, which in turn is more favorable than that of the beta-sheet. This qualitative relation is not only observed for alanine residues as shown in Figure 2, but also for the other amino acids we have studied, glycine, leucine and serine (data not shown). A difference in TFE between two conformations means that the folding equilibrium between the two is affected by urea and shifted towards the structure with the more negative TFE. This is illustrated by the thermodynamic cycle in Figure 3, which connects the TFEs to the free energies of conformational change in water and aqueous urea solution. For the examined model peptides it means that urea shifts the equilibrium from the folded structures (helix and sheet) towards the extended strand, which is consistent with the fact that urea is a protein denaturant. Furthermore, our simulations predict, that urea has a stronger effect on the denaturation of beta-sheets than on the denaturation of alpha-helices.

The strength of a denaturant or stabilizer is often quantified by the so-called m-value. It describes the cosolute influence on the equilibrium between two structures A and B as a linear function of the cosolute concentration c_c:

$$\Delta\Delta G = \Delta G_{A\to B}^{c/w} - \Delta G_{A\to B}^{w} = m \cdot c_c$$

According to the thermodynamic cycle in Figure 3 the cosolute induced change $\Delta\Delta G$ is given by the difference of the TFEs of the two considered conformations from water to cosolute solution. The values for $\Delta\Delta G$ for the three possible equilibria between the examined polyalanine secondary structures are presented in Figure 4. At low concentrations they obey indeed in good approximation a linear dependence on the urea concentration,

Figure 2: Calculated TFEs from water to urea solutions of given concentrations for alanine peptides of the three different conformations shown in Figure 1.

Figure 4: Differences in TFE between two different conformations of the same polypeptide chain. They describe urea's influence on the folding transition between the two structures.

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which renders the definition of an m-value for the helix-strand, sheet-helix, and sheet-strand transition possible. The m-value determined from the slope of $\Delta\Delta G$ for the helix-strand unfolding transition is -0.2 kJ per mol alanine residues and mol/l urea. Hence, it is in the same order of magnitude as the experimentally determined value for urea's unfolding of a helix, that consists to two thirds of alanine, which is -0.1 kJ per mol amino acids and mol/l urea [3].

On-going Research / Outlook

The comparison with experimental data and the observed qualitative trends shows that the computational results are in good agreement with experimental findings. Thus, it is feasible to further analyze the performed simulations and to look at parameters that are difficult to measure directly in experiments. Thereby, we can gain insights into the origin of the calculated values for the TFEs. Questions, which are addressed in the ongoing analysis and further computations are: Why is the TFE of the stretched chain more negative than the one of the helix and the sheet? Can the differences in TFEs be traced back to a single parameter describing the conformations like the solvent accessible area? What is the effect of intramolecular hydrogen bonding present in the folded structures but not in the stretched conformation? What is the nature of the molecular interactions between the model peptides and the solution components and what is their effect on the TFE?

In the future we want to include further model peptides with other secondary structures into our investigations. Moreover, we want to turn our focus to other cosolutes, which – in contrast to the denaturant urea – stabilize the native fold of proteins. The direct comparison of analogous simulation results for protein denaturants and stabilizers will help to reveal the molecular origin of the variety of observed cosolute effects on proteins.

Solid State Physics

Numerical simulations of correlated electron systems

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Introduction

In many-particle systems, emergence corresponds to the notion that the whole becomes very different from the sum of its parts. This definition of complexity lies at the heart of modern research from biology to solid state physics and leads to an unlimited wealth of phenomena. In correlated electron systems, emergence is the fundamental concept, which allows us to understand and characterize phases of matter. For instance, a superconducting state consisting of 10^{23} electrons can be characterized by a single complex function of position, a magnetically ordered state by a position dependent vector pointing in the direction of the magnetization. This characterization of states in terms of a function of spatial coordinates (local order parameter) is at the heart of the Landau theory of phase transitions.

Can all states of matter be classified with a local order parameter? The answer is no. One prominent example, which has been discovered experimentally in the group of L. Molenkamp in Würzburg, is the family of so called topological insulators [1]. This state of matter is characterized by a topological quantity. By definition, topological states cannot be described by studying the system locally but rely on global properties. This stands at odds with the Landau concept of local order parameters. Spin-Hall topological insulators are insulating in the bulk but are conducting on the surface. The metallic surface is a so-called helical liquid since the spin orientation is tied to the velocity of the electron. The potential application of such phenomena in the domain of spintronics is still in its infancy.

Another example of states of matter which elude a classification in terms of a local order parameter are spin liquids, states that can be identified with Mott insulators. The latter have become famous for being the parent compounds of high-temperature superconductors. In a Mott insulator, electronic correlations lead to the localization of the charge degree of freedom of the electrons, thereby generating an insulating state. However, as opposed to band insulators and at an energy scale set by the charge gap, the spin degree of freedom remains unquenched. In general, as the temperature drops down to absolute zero, the spins will order to form a magnetically ordered state. In spin liquids, this does not occur since quantum fluctuations are strong enough to hinder order down to the lowest temperature. There are many types of spin liquids, which can be realized in contrived models. Although a liquid, this state of matter has topological order, however of a different type than topological insulators [1]. One big success of recent large-scale numerical simulations is the discovery of spin liquid states in generic models of correlated electron systems, in particular, the Hubbard model on the honeycomb lattice [2]. The understanding of the physics of this model is one of our present interests, which summarizes aspects of our achieved and future research.

Results

One big achievement in the past grant periods is the numerical calculation of the Kane-Mele Hubbard model on the honeycomb lattice. The honeycomb lattice with a zig-zag edge is shown in Figure 1. Here we have considered
a) half-filling (one electron per site)
b) a Hubbard U-term which incorporates a screened Coulomb repulsion, by penalizing double occupancy of a site by two electrons
c) a hopping matrix element t between adjacent sites and
d) a spin-orbit term set by λ.

Figure 1: Honeycomb lattice with zig-zag edges.

It is remarkable that this model is amenable to large-scale quantum Monte Carlo simulations [3,4] and shows a fascinating phase diagram (see Fig. 2). The numerical method we use here is a so-called auxiliary field Quantum Monte Carlo method [5]. It is based on a path integral formulation where the interaction is decomposed with a Hubbard-Stratonovitch field which mediates the electron correlation. The integration over this field is carried out with Monte Carlo methods. For a given tolerance of stochastic errors, the approach scales as $N^3\beta$ where β is the inverse temperature and N the number of sites. This scaling is an exception to the rule that interacting fermionic systems correspond to exponentially hard problems.

In light of the above, one will appreciate the richness of the phase diagram shown in Fig. 2. Let us start in the bottom left corner where electronic correlations and the spin-orbit coupling are switched off. This corresponds to the Dirac fermion semi-metallic (SM) state of graphene which is presently attracting considerable interest. Staying at U=0, and turning on the spin-orbit coupling reveals that the SM state is unstable towards a topological band insulating (TBI) state with helical edges. When correlations become large, magnetism emerges. This state corresponds to an antiferromagnetic Mott insulator (AFMI) where the spin degrees of freedom are frozen. The state breaks time reversal symmetry and hence the topological protection of the TBI. In the parameter range, where metallic and antiferromagnetic phases compete, a quantum spin liquid (QSL) phase emerges.

On-going Research / Outlook

Up to date, we know what the spin liquid phase is not: It is not adiabatically connected to a band insulating state. The further characterization of this state constitutes a computationally tractable challenge. It relies on the optimization of the code so as to reach considerably larger lattice sizes, as well as algorithmic developments which will allow us to detect topological order numerically. The optimization of the code relies on reorganizing the data structure so as to guarantee that virtually all the CPU time goes into the BLAS zgemm matrix multiplication. We then rely on an optimal implementation of this routine on the local architecture. We are presently testing this portable optimization scheme and are confident that it will work.

States of matter are characterized by their excitations. In the case of continuous phase transitions, from ordered to disordered states, one expects the excitations of the disordered phase to condense so as to form the order of the ordered state. Following this idea we can understand the phase transition from the TBI to the AFMI in terms of a Bose condensation of spin excitons in 2+1 dimensions. Our numerical results to date hint that the transition from the QSL to the AFMI is continuous. The understanding of this transition will require considerably more work and will shed light on the nature of the spin-liquid state. In particular, it can potentially answer the question of fractionalization of the spin into spinons in the QSL phase. In this case anomalous exponents are expected.

Figure 2: The zero temperature phase diagram of the Kane-Mele Hubbard model on the honeycomb lattice [3,4]. The calculations on which this phase diagram is based include systems with up to 648 electrons. See text for a description.

As apparent from the phase diagram in Fig. 2, the interplay between spin-orbit coupling and correlations reveal rich phase diagrams. Heavy fermion systems which also play a central role in our project, have both: a strong spin-orbit coupling as well as electronic correlations. Whether these systems can develop correlation driven topological band structures is a question which we can and will address in the following grant periods.

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Tuning the two-dimensional electron gas at the LaAlO$_3$/SrTiO$_3$(001) interface

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HLRB Project ID: h0721

Introduction

Transition metal oxide heterostructures have recently attracted significant attention because of the novel functionality that emerges at their interfaces. A prominent example is a system comprised of the two simple band insulators LaAlO$_3$ (LAO) and SrTiO$_3$ (STO) where a two-dimensional electron gas (2DEG) [1], magnetism [2] and superconductivity [3] emerges. Furthermore, experiments [4] show that the electronic properties can be tuned by the LAO thickness: the system undergoes a transition from insulating to conducting behavior at around four monolayers (ML) LAO. This insulator-to-metal transition (IMT) can be controlled reversibly via an electric field, e.g. by an atomic force microscope (AFM) tip, and several electronic devices based on this feature have been proposed [5]

Understanding and controlling this behaviour is of key importance for the development of electronics and spintronics devices. To this end density functional theory as a material-specific approach can provide valuable insight in the underlying mechanisms. A central aspect in the emergence of these unexpected electronic phases is the violation of charge neutrality at the interface: in the (001) direction LAO consists of charged (LaO)$^+$ and (AlO$_2$)$^-$ planes, while in STO formally neutral (SrO)^0 and (TiO$_2$)^0 planes alternate. Because both cations change across the interface, two distinct interfaces can be realized: an electron doped n-type with a LaO layer next to a TiO$_2$ layer and a hole-doped *p*-type interface with a SrO and AlO$_2$ next to each other.

Results

To gain fundamental understanding in the thickness induced insulator-to-metal transition we have performed DFT calculations on LAO films on STO(001) with varying thickness of LAO. The results demonstrate that an internal electric field emerges in thin polar LAO overlayers on STO(001) [6], expressed in an upward shift of the O 2p bands as they approach the surface [see layer resolved density of states of a 4 ML LAO film on STO(001) with an *n*-type interface (Fig. 1)]. The lattice responds by a strong

polarization visible in the outward relaxation of La-ions and the buckling in the subsurface AlO$_2$ layers (see also Fig. 4a, orange line). The lattice relaxation has a crucial effect on the electronic properties: if the atoms are fixed at their ideal bulk positions, all systems are metallic [6]. The lattice polarization allows several layers of LAO to remain insulating. However, the band gap decreases with each added LAO layer and finally at around 5 monolayers of LAO an *electronic* reconstruction takes place. Remarkably, the closing of the band gap is *indirect* in real space as resulting from an overlap of the valence band maximum defined by the O 2p band in the surface layer and the conduction band minimum marked by Ti 3d states at the interface.

Furthermore we explored the effect of a SrTiO$_3$ capping layer on the electronic properties [7]. The calculations show that adding just a single STO layer induces the IMT already in 2 ML LAO/STO(001) [formerly insulating with a band gap of ~1.2 eV]. The analysis of the band structure (Fig. 2) demonstrates that the origin is of electronic

Fig. 1 Side view of the relaxed structure (left) and layer resolved density of states (LDOS, right) of 4 ML LAO on STO(001). Note the lattice polarization and the internal electric field within LAO.

nature and is associated with a dispersive O 2p surface band, similar to a surface state in STO(001) that extends 0.8 eV above the subsurface O 2p band and marks the top of the valence band at the M point of the Brillouin zone. On the other hand the bottom of the conduction band lies at the Γ point and is determined by Ti 3d states in the interface layer. Thus the closing of the band gap is *indirect* both in real and reciprocal space.

The electron density distribution in 2STO/2LAO/STO(001) integrated between -0.3 and 0.0 eV shows electrons of Ti $3d_{xy}$ character in the interface layer and holes in the O $2p_\pi$ bands at the surface. The presence of two types of carriers with different mobilities is confirmed in Hall and magnetoresistance measurements [7]. This electron-

Fig. 2 Band structure of a) 2LAO/STO(001) with indirect band gap and b) 2STO/2LAO/STO(001) where the band gap closes due to an overlap of an electron band at Γ with a hole band at M.

hole bilayer where the carriers are just 1 nm apart represents a playground to explore excitonic phenomena.

The influence of metallic contacts is a further relevant aspect that needs to be understood in order to incorporate LAO/STO in electronics devices. The DFT calculations reveal that a metallic overlayer alters significantly the electric field within the polar $LaAlO_3$ film (Fig.3 a). For Al or Ti metal contacts the electric field is eliminated, leading to a suppression of the thickness-dependent insulator-to-metal transition observed in uncovered films. Independent of the $LaAlO_3$ thickness, both the surface and the interface are metallic, with an enhanced carrier density at the interface relative to $LaAlO_3/SrTiO_3(001)$

Fig. 3 a) LDOS of 2 ML LAO/STO(001) covered by 1 ML Ti. b) Electron density integrated between E_F-0.65 eV and E_F gives insight into the Ti 3d orbital occupation both in the surface layer and within SrTiO₃.

after the metallization transition. Moreover, the carriers occupy different orbitals (orbital polarization) depending on the distance from the interface (Fig. 3b).

For transition (Fe, Co, Pt) and noble metal contacts (Cu, Ag, Au) a finite and even enhanced (Au) internal electric field develops within $LaAlO_3$. In fact Au is an exception as the Ti 3d conduction band remains unoccupied, lying above the Fermi level (Fig. 4b). Results for a representative series

Fig. 4 a) Variation of lattice polarization (oxygen-metal ion bucking) and (b) occupation of Ti 3d bands within STO(001) for a series of metallic contacts on 2LAO/STO(001).

of metallic overlayers on $LaAlO_3/SrTiO_3(001)$ (Na, Al; Ti, Fe, Co, Pt; Cu, Ag, Au) reveal broad variation of band alignment, size of Schottky barrier, carrier concentration and lattice polarization at the $LaAlO_3/SrTiO_3(001)$ interface (Fig. 4). These correlate with the size of work function of the metal on $LaAlO_3$ which provides guidelines how to control the carrier density at the $LaAlO_3/SrTiO_3$ interface by the choice of the metal contact [8].

On-going Research / Outlook

The achieved results point to a series of parameters that can be used to tune the properties of oxide surfaces and interfaces and realize novel charge, magnetic and orbitally ordered states.

To gain fundamental understanding of the new physics arising at complex oxide interfaces ongoing work within h0721 concentrates on the influence of further parameter such as adsorbates, dopands or the crystallographic orientation. Work funded by DFG, SFB/TR80 and BaCaTeC.

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Simulation of Thin-film Solar Cells

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HLRB Project ID: h0672

Introduction

In this project, we deal with the simulation of thin-film solar cells. The characterizing feature of these types of solar cells is their low thickness of typically 3μm, leading to lower production cost when compared to classical silicon photovoltaic technologies. They consist of absorbing (e.g. silicon) and conductive (e.g. ZnO) layers, and a back reflector made of silver. The optical properties of these layers of different media highly depend on the frequencies of incoming light.

Figure 1: Structure and roughness profile of a tandem solar cell.

For our simulations, the superposition of these frequencies approximates the spectrum of sunlight, which agrees with the solar cell's most common usage scenario. The propagation of light through the solar cell is governed by Maxwell's equations, which are the basis for the discrete model used in our simulations. The absorption model assumes that each photon that gets absorbed in the silicon layer generates one electron worth of output current. The objective of the project is to predict the power output of solar cells and help improve their quantum efficiency, i.e. the rate of conversion of light to electrical power in the cell.

Efficiency

The decisive factor for the efficiency of a solar cell is its ability to convert photons into electrons while they pass through its absorbing layers. This efficiency can in general be improved by diffusive coatings and changes of the surface roughness of the cell's layers. In addition to changing the surface profile, doping certain layers with nano particles or nano rods can also enhance the layer's diffusive properties and thus improve the cell's light trapping behavior. All these measures help prolong the trajectory that light takes through the cell before it exits, thus increasing the probability of absorption. Simulations allow us to study the properties of a wide range of different surface designs and roughness profiles under various angles of incidence of incoming light. As such simulations represent an inexpensive way to predict the effect of design parameters on the quantum efficiency without the need to physically construct solar cells.

Challenges

Due to limitations imposed by available compute power and memory, only a small portion of a real-world solar panel can be simulated. In order to deal with this situation, the model can be adapted to treat this portion as a periodic structure that extends infinitely many times on the horizontal plane. By this trick, the simulation can be chosen to be as large or small as desired. However, large simulations much better agree with real-world solar cells, as the typical surface structures that characterize a solar cell require a certain physical dimension and spatial resolution. Therefore, simulations of a sensible scale with reasonable error tolerances at this time require the use of high performance compute clusters.

Figure 2: Strong and weak scaling behavior with different numbers of processors per compute node.

Consequently the simulation framework needs to scale well onto highly parallel system architectures. This parallelization effort was part of the project with the aim of removing performance bottlenecks from the code and increase computational throughput.

Results

We were able to validate the simulation results against measurements of test coatings provided by Malibu F&E, a subsidiary of Schüco. These measurements include both the roughness profile of the solar cell under investigation and the efficiency of the measured cell as a function of frequency.

Figure 3: Measurement and simulation results for a tandem cell.

The first is used as input to model the interfaces between layers, while the latter provides the frame of reference to evaluate the simulation results against. The differences in quantum efficiency between the real-world cell and its simulation counterpart are explained by a lack of material dependent input data of the PN junction, an additional layer in the cell that cannot be modelled accurately without an appropriate description of its electromagnetic properties. Furthermore, the roughness profile of the lower layers of the tandem cell cannot be obtained by standard measurements. Therefore, the profile of a different amorphous silicon cell had to be used as a substitute. Considering these factors, the simulation results show high agreement between measured and simulated data.

Using simulations, arbitrary interface roughness profiles can be generated and evaluated for their efficiency potential. One particular such kind of surface profile is for example a pyramidal structure for its geometrical simplicity and single scale granularity of roughness.

	Amorphous silicon	Microcrystalline silicon
Simulation	10.35	8.56
Experimental Data	10.82	9.30

Table 1: Short circuit current density measured in mA/cm².

Figure 4: Simulation results of quantum efficiency for different angles of incidence in parts of the spectrum.

Our simulation based studies thus strive to support industry partners in their efforts to produce next generation high efficiency photovoltaics.

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Material-specific investigations of correlated electron systems

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HLRB Project ID: pr28je

Introduction

Electrons in solids move in the electrostatic potential of atomic nuclei and interact with each other via Coulomb forces. In many materials each electron experiences the other electrons only as a static cloud of negative charge. Such materials are called weakly correlated. However, there is an important class of materials where such a simplified picture does not hold, i.e. the electrons dynamically modify their surrounding electron cloud and are themselves influenced by the effects of this modification. These materials typically contain transition metals or rare earths and are called strongly correlated. The complex feed-back phenomena that govern the dynamics of strongly correlated electrons pose a challenge for a theoretical description. Even the simplest models, in which only the interaction among electrons on the same atom is considered, defy an exact solution. One of the few successful approximate approaches is the so-called dynamical mean-field theory (DMFT), which becomes exact in the limit of infinite spatial dimensions. This theory can be applied (Ref. [1]) by using powerful numerical simulation techniques.

Figure 1: Phase diagram showing correlated band insulator and Mott insulator phases as well as the region where two solutions of the DMFT equations exist. Here and in subsequent figures U and T are measured in units of W/4. Inset: Double occupancy as a function of interaction strength for two temperatures (Ref. [2]).

Figure 2: Spectral function for U=5 (correlated band insulator) as a function of temperature (Ref. [2]).

Results

Specifically we have adapted DMFT to study the behavior of covalent insulators (Ref. [2]); materials examples are FeSi, FeSb2, and CoTiSb. In these special insulators, like in metals, the number of electrons fluctuates on all atoms as the electrons move between atoms in the crystalline solid. However, unlike metals, these materials are not conductors, because the electrons are confined to chemical bonds due to an associated binding energy. In the language of correlated electron physics such a material is said to have a charge excitation gap. Introducing an electron-electron repulsion of strength U on each atom the system may choose between two options: i) bond formation, when electrons are shared by neighboring atoms - a scenario favored at small U, ii) each electron is confined to its respective atom, which leads to the formation of local magnetic moments - a scenario favored at large U. We have investigated the intermediate regime between these two limits where the physical properties become strongly temperature dependent.

Figure 3: Uniform (Q=[0,0]) spin (s) and charge (c) susceptibilities and local spin susceptibility for U=4 (correlated band insulator); Ref. [4].

The important control parameters are the overall bandwidth W, which is a measure for the tendency of electrons to move between atoms and thereby to spread out in the crystal, the bare band gap V, which quantifies the energy gained by forming a chemical bond between neighboring atoms, the Coulomb repulsion U, which is the energy needed to place two electrons on the same atomic orbital, and the temperature T. In Fig. 1 we show the overall U versus T phase diagram of our model ansatz for covalent insulators. The limiting cases i) and ii) are identified at weak and strong U, respectively. The transition between the two distinct phases, i.e. the correlated band insulator and the Mott insulator phase, proceeds through a continuous crossover for T>0.07 (in units of W/4), while for lower temperature there is a discontinuous first order transition with a coexistence region.

In a next step we fix the interaction strength U=5 and vary the temperature T in the band-insulator phase. Figure 2 shows the corresponding single-particle spectral functions. This quantity is experimentally accessible in photoemission experiments; it determines the intensity for the removal of an electron at a selected (negative) energy or for the injection of an electron (positive energy). The gap around zero at low temperatures indicates that the material is an insulator. The significant change of the spectral function with increasing temperature is typical for correlated materials. An interesting feature of the present model is the evolution from an insulator at low T to a metal at high T with a continuous gapless spectral function. This is a remarkably unusual temperature evolution, because in most materials the electrical conductivity decreases upon heating. The temperature dependence of the conductivity was explicitly calculated in Ref. [3].

The second unusual behavior is observed in the magnetic (or spin) susceptibility, which determines the magnetization of a material in an external magnetic field. In non-magnetic metals, e.g. Al, the susceptibility is weak and temperature independent. Magnetic metals instead, e.g. Fe, are magnetized spontaneously without an external magnetic field; above a critical temperature their magnetization disappears and the susceptibility decreases

as 1/T with increasing temperature. The present model exhibits a remarkably different magnetic behavior as shown in Fig. 3. At low T the uniform, long-wavelength susceptibility behaves as in a non-magnetic material. However, upon heating the susceptibility rapidly grows and eventually reaches the 1/T behavior typical for magnetic materials.

There is a close connection between the magnetic and the transport properties of the present model for covalent insulators. From analyzing the numerical results we arrive at the following physical picture: At low temperatures the electrons are confined to the chemical bonds formed between the atoms, and thus do not participate in conducting the electrical current. Each bond contains two electrons with opposite magnetic moments, their magnetic response therefore cancels. With increasing temperature the chemical bonding is disrupted and each electron tends to localize to an individual atom. An applied magnetic field can now align their moments with the external field, which is reflected in a substantial increase of the magnetic susceptibility.

On-going Research / Outlook

The effect of electronic correlations in band insulators is still far from being completely understood. More recently our studies were extended to LaCoO3 and related materials, which exhibit similar temperature dependencies of magnetic and transport properties. Although the microscopic mechanisms are distinctly different a useful lesson can be learned from acomparison. In a broader perspective we continue the investigation of correlated multi-band systems, which continue to surprise by unexpected physics.

Figure 4: Charge susceptibility throughout the Brillouin zone . At a high temperature (T=1/5, red) the susceptibility is almost constant. At low temperatures (T=2/15, green, and T=1/15, blue) the uniform susceptibility (q=[0,0]) drops to zero, due to the opening of band gap; unpublished.

Since the challenging part of our computational algorithm is a Quantum Monte Carlo (QMC) random walk, the code is readily parallelized. The computational requirements of the continuous-time QMC are comparatively simple; fast processors in parallel are needed, but not extensive memory. Since the random walks on different CPUs are independently performed, fast network communications are not required either. The new generation of high-performance computers on the Petascale will likely allow us to compute material specific properties of more complex systems. Therefore, we expect that materials' properties tailored towards specific purposes might become predictable. To this end new algorithms will have to be developed to efficiently use the supercomputers' resources.

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First-principles calculations for diluted magnetic semiconductors

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Introduction

The diluted magnetic semiconductors (DMS) are ordinary semiconductors from IV, III-V, II-VI groups of periodic table doped usually with transition metals (TM) from the 3-rd row, such as Mn, Co, Fe, V. They posses conventional properties of semiconductors and exhibit also some unconventional properties like half-metallicity, i.e. the metallic behaviour is in the one spin channel only while the band structure in the other spin channel preserves the energetic gap. The most interesting advantage of these systems for the experimental community is probably the magnetism, and great potential of DMS to be used in spintronics devices [1]. For theoreticians, DMS pose a challenge for various models and ab-initio methods since the long-range classical interactions mix in these crystals with strong electronic correlations at impurities and their close neighbors. Another complication for physicists is disorder and clustering of dopants in groups of atoms showing unpredictable mutual interactions. All above facts make the field of DMS one of the most hot research spots.

To be used in fabrication of spintronics devices, materials must show ferromagnetism at least at room temperature. So far none of such reports established in the community due to different sample preparations and a variety of factors which are difficult to control. Also the theoretical predictions are not conclusive, since the magnetic dopants belong to the class of problems for which the most widely used method, i.e. the density functional theory (DFT) in the local density approximation (LDA) or in the generalized gradient approximation (GGA) flavor, fails to predict correctly the band structure and all derived from it properties. One of the methods, to improve the description of strongly correlated systems, is the pseudopotential self-interaction correction (pSIC) scheme. Therefore, we implemented this method to the very popular "quantum espresso" code, and we improved the equations for forces [2]. We performed also calculations with the LDA+U method and used the obtained magnetic couplings in the Monte Carlo simulations of classical Ising spins to estimate the Curie temperatures for the ferromagnetic phase transition.

The main system of our investigations is silicon doped with rhenium [3]. Silicon is a basic material for electronic devices and together with germanium it is intensively studied as a host material for DMS. Rhenium has not been studied theoretically as a dopant for DMS so far. It deserves special attention due to much stronger hybridization with the host than the 3rd row TMs. The experimental studies for rhenium in amorphous silicon open a challenging prolem why room temperature ferromagnetism in this material disappears when samples stay at ambient conditions for a few months.

Results

The basic information about new DMS under investigation is energetic preference for the formation of impurities at various crystal sites and their charged and magnetic states. We checked five lattice positions for the impurity in silicon: the substitutional site (S), the tetragonal interstitial site (I), the hexagonal interstitial site (H), the exchanged position where the interstitial site is occupied by Si and the close substitutional site is occupied by Re (E), the divacancy configuration where two silicon atoms are removed and the Re atom is placed in the middle of the removed bond (D) [3]. All formation energies (with respect to the substitutional site) and magnetizations are collected in Table I.

	S	I	E	H	D
Ef	0.00	0.23	1.19	1.80	2.24
M	0.99	0.00	0.00	1.83	2.33

Table 1: Formation energies (Ef) for the single sites with respect to the formation energy of the S site [in eV] and magnetic moments (M) in the cell [in Bohr magneton], calculated within the GGA method.

The most stable substitutional configuration has low magnetic moment of 1 Bohr magneton in contrast to the Mn impurity, which has the high spin moment of 3 Bohr magnetons within the GGA method. Presented results were obtained from the calculations of the 64-atom cell doped with one Re atom. The interstitial Re is nonmag-

netic within the GGA method since the impurity d-states fall into the conduction band due to the underestimation of the silicon band gap, which is a common problem in semiconductors described by the DFT method. The same problem remains within the DFT+U method since the silicon gap cannot be improved by the method, which corrects only the position of the d- or f-states. Hence, within the DFT and the DFT+U methods, the interstitial impurities in Si:Re cannot be described properly. To study the magnetic interactions between the impurities, wihin the DFT or DFT+U methods, we need to restrict our investigations to substitutional impurities only. Such calculations showed that these interactions are long-ranged and stronger in the case of the second method. The obtained energy differences between the ferromagnetic and antiferromagnetic states where used in the Monte Carlo simulations of Ising spins [4], and the estimated Curie temperatures at two doping concentrations are collected in Table 2.

x	T_{FM}(GGA)	$T_{FM/SP}$(GGA+U)
3%	84	230-350
5%	190	690-820

Table 2: Critical temperatures [in K] for the ferromagnetic (FM) phase transition within the GGA method and for the ferromagnetic/super-paramagnetic (FM/SP) phase transition within the GGA+U method for two concentrations (x) of impurities.

For the DFT+U method, we show the range of temperatures at which the magnetic clusters start to form, since due to very strong magnetic interactions the uniform magnetization of samples is followed by another magnetic phase at lower temperatures, i.e. superparamagnetism. This is a phenomenon connected to the very large relaxation times for spins in strong magnetic clusters.

In order to include the interstitials into our system, we implemented the pSIC method and checked two energeticaly low lying configurations S and I [5]. The slightly more opened gap of Si allows the d-states of the interstitial Re to fall below the conduction band, and in a result the magnetic moment is equal to that of the substitutional site. The densities of states (DOS) for both impuri-

Figure 1: Density of states (DOS) for single Re impurities in the cell in the substitutional and the interstitial site calculated with the pSIC method.

Figure 1: Density of states (DOS) for single Re impurities in the cell in the substitutional and the interstitial site calculated with the pSIC method.
Figure 2: Formation energies of neutral and charged impurities with respect to the neutral substitutional site.

ties obtained within the pSIC scheme are presented in Figure 1.

The energy of the interstitial site is higher than that of the substitutional site. Therefore, the migration of impurities in the crystal is less plausible. The formation energies of S and I impurities and their charged and magnetic states as functions of the Fermi level position with respect to the valence band maximum is presented in Figure 2.

From the crossing of charged negative substitutional impurity and charged positive interstitial impurity, which is below the energies of both neutral rhenium atoms, we can derive a very interesting conclusion about the charge transfer from the I-case to the S-case. Indeed, the calculations with both impurity types in the one larger cell (96 atoms) confirm this prediction and both rhenium sites are nonmagnetic. This is bad for the DMS but a co-doping of such systems revives the magnetism again, and the n-type is more efficient for the magnetic moment of the whole system than the p-type. The neutral impurity pairs of different types: SS, II and SI are energetically more favorable than single impurities, and the pair which formation energy is the lowest is a mixed pair, a bit higher in the energy is the II pair, and finally the SS pairs lay about 0.5 eV higher than the lowest SI pair. The most favorable pair has the formation energy per impurity lower than the formation of single Re sites of 1.9 eV.

As we can see, the problem with physical description of DMS is complex and needs further simulations with clusters containing more than 2 impurities in the cells, and also further code development which we announce in outlook.

The calculations presented here need strong computing power, because the interactions are long range and the cells achieve the size of about 250 atoms, while we stay at the quantum mechanical accuracy, and we have to optimize the positions of atoms around impurities. Therefore, we performed the calculations parallel in the k-points in the reciprocal space.

We also implemented a new method, the pSIC scheme, to the popular quantum espresso code. Without these

hardware and software tools the subject would be untreatable. Also the classical Monte Carlo simulations of Ising spins for the estimate of critical temperatures need quite strong computer power, since the impurities in the supercells are randomly distributed and the size of classical cells is large. Numbers of impurities for concentrations of a few percent achieve thousands and Monte Carlo measurement numbers are of order of millions.

On-going Research / Outlook

There are four classes of further problems which seek to be calculated in the future for DMS: 1) larger clusters of impurities (more than two) should be calculated, since in the experiment the transition-metal atoms tend to form islands, 2) electron and hole co-doping would need a better method than the simplified pSIC approach, 3) impurity states at the Fermi level should be treated with inclusion of dynamic correlations, 4) non-collinear magnetic order should be considered.

The clusters of impurities need to be embedded in larger supercells, which means that their size will approach 1000 if we add the interactions between clusters (these are important for a good estimate of Tc). All above needs to be optimized geometrically since the energy gain for lattice relaxation is higher than the energy difference between the ferromagnetic and the antiferromagnetic configurations.

The exact positioning of impurity states, especially the unoccupied states, which form the electron traps must be calculated with a method including the quasi-particle excitations, e.g. GW method. We have implemented this method to the quantum espresso code, together with the mixed-basis (we added gaussians) and with extensive use of the crystal symmetry, in order to be able to employ pseudopotentials with more valence electrons (deeper atomic shells are important in the description of these kind of electronic correlations). In the next step we will need more cpu cores to run this code parallel in the k+q point rotations.

The problems with strong correlations at the Fermi level need to be solved with the dynamical mean field theory, which includes also the temperature. This way one can answer the question how the temperature changes the single site magnetism, and within the dynamical cluster approximation one can say about the temperature dependence of interactions between the impurities. This is very important, since at the moment we perform only zero-temperature ab-initio calculations and simulate thermodynamics on the classical level. We are almost ready with the code development to deal with this problem.

Finally, we also pursue the implementation of the pSIC approach together with the non-collinear spin to be able to work with the full Heisenberg hamiltonian instead of the simple Ising model.

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Symmetries and the conductance of graphene nano ribbons

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Introduction

Symmetries play an important role in physics, as they pose tight restrictions on physical laws and phenomena. One of the most important symmetries is *time reversal symmetry*: physical laws remain unchanged if the arrow of time is reversed. For a classical particle, reverting the arrow of time means reverting its velocity. Time reversal symmetry then dictates that the particle's trajectory – regardless of how complicated it is – will be traced back *exactly* if the particles velocity is turned around (see Fig. 1a). This equality of forward and backward moving particles is a very striking example of the restrictions of time reversal symmetry.

Indeed, if time reversal symmetry is broken, a very different picture emerges. For example, time reversal symmetry is broken in an external magnetic field, where forward and backward moving particles are deflected in opposite directions due to the Lorentz force. In this case, reverting the direction of motion of the particle will result in two very different trajectories (see Fig. 1b). Only if the direction of the magnetic field is also reversed, are identical trajectories possible.

In the quantum regime, where particles also have a distinct wave character, the effect of time reversal symmetry is best understood in terms of the quantum mechanical phase. Time reversal symmetry then dictates that the phases of forward and backward moving particles must be equal. If time reversal symmetry is broken by a magnetic field, the original and the reversed path acquire different phases (shown as different colors in Fig. 1c) even if the trajectories themselves are disturbed only marginally by the field.

Indeed, an external magnetic field is typically the only way to break time reversal symmetry. However, Mondragon and Berry [1] proposed a (hypothetical) neutrino billiard, where forward and backward moving particles acquire different phases when reflected by the walls. In this case, time reversal symmetry is rather broken by the walls, not a magnetic field.

Such a neutrino billiard is thus a way to probe our understanding of the fundamental principles of physics. Unfortunately, it is only a *gedanken experiment* and impossible to realize as such in practice. However, the recent discovery of graphene allows to effectively probe the same physics.

Results

Graphene is a two-dimensional sheet of carbon atoms arranged in a honeycomb lattice (Fig. 2a). It possesses various unique properties and is very promising for future electronic applications. Consequently, the Nobel prize was awarded for its discovery in 2010 [2]. One unique aspect of graphene is its electronic band structure which features a linear, Dirac-like dispersion otherwise only known

Fig. 1: Time reversal symmetry in physics. (a) Regardless of how complicated the trajectory of a classical particle, it will be traced back exactly if the particles direction of motion is turned around. (b) This is not true any more if time reversal symmetry is broken by a magnetic field B, and the particle is deflected by the Lorentz force. (c) In the quantum mechanics regime, a magnetic field can have more subtle effects: Even if the trajectories do not differ significantly, forward and backward moving particles can accumulate very different phases (represented as different colors along the paths).

from high-energy physics in fundamental particles as the neutrino. However, unlike the neutrino case there are two Dirac cones at different points of the Brillouin zone (Fig. 2b). These two Dirac cones are time-reversed partners, i.e. reverting the arrow of time not only reverts the velocity of electrons, but also interchanges the Dirac cones. It is thus the presence of the two Dirac cones that prevents per se the kind of time reversal symmetry breaking predicted in a neutrino billiard.

However, under certain conditions graphene may effectively appear absolutely equivalent to neutrinos: If only long-range impurities, such as Coulomb impurities, are present, the two Dirac cones are decoupled. In this case, although strictly speaking present, the real time reversal symmetry that interchanges the Dirac cones becomes ineffective, as electrons in different cones do not interact.

In this limit, only a "wall" is needed to obtain the physics of the neutrino billiard, and this is obtained by cutting structures out of the graphene sheet. Of particular interest are narrow, straight ribbons (graphene nanoribbons). These come in two main variants, namely zigzag (Fig. 2c) and armchair (Fig. 2d) nanoribbons, distinguished but the shapes of their edge. Armchair ribbons are further distinguished into metallic and semiconducting (related to their electronic properties) depending on their width, with one third of all ribbons being metallic, and two thirds being semiconducting. Changing the width by one row of atoms can change the character from metallic to semiconducting and vice versa.

Fig. 2: (a) Carbon atoms in graphene are arranged in a honeycomb lattice. (b) The band structure of graphene features two Dirac-like dispersions at the K and K' points. These two Dirac cones are time-reversed partners, but remain uncoupled if only long-range disorder is present. (c) and (d) Zigzag and armchair graphene nanoribbons, respectively.

For zigzag nanoribbons with only long-range disorder it was in principle known that time reversal symmetry is effectively broken [3]. Through a careful analysis of the Dirac equation we could show that also metallic armchair ribbons feature an effectively broken time reversal symmetry, whereas time reversal symmetry is intrinsically conserved in semiconducting armchair ribbons. The microscopic origin of this effective time reversal symmetry breaking is exactly the same as in the neutrino billiard: forward and backward moving particles acquire different phase shifts due to reflections at the ribbon edges.

Fig.3: Weak localization correction δG as a function of magnetic field B from the simulations. δG is the conductance measured relative to the conductance at zero magnetic field. Data is shown for zigzag and armchair (ac) ribbons.

How can this effective time reversal symmetry breaking be observed in an experiment? It turns out that a simple current measurement through a nanoribbon suffices, as we can make use of a phenomenon called *weak localization* which is intimately related to time reversal symmetry. The conductance (inverse resistance) of a nanostructure is smaller the more electrons are scattered back from the structure. Since paths going in opposite directions (as in Fig. 1a) accumulate the same phase if time reversal symmetry is present, they interfere constructively, enhancing backscattering and leading to a decreased conductance compared to the case with broken time reversal symmetry.

In an experiment one can then measure the conductance as a function of magnetic field. Usually one then observes an increase in the conductance with increasing magnetic field, as for zero magnetic field time reversal symmetry is present and hence conductance decreased, whereas in a magnetic field time reversal symmetry is broken and conductaance enhanced. However, if time reversal symmetry is (effectively) broken already *without a magnetic field*, the conductance should be independent of magnetic field.

To show that our predictions for graphene nanoribbons are testable in experiment, we have performed quantum transport simulations using realistically large systems containing tens of million atoms. The computational cost of these simulations requires supercomputers such as the HLRB2.

In Fig. 3 we show the results of the weak localization behavior as obtained from the simulations. Indeed, we observe a strong magnetic field dependence of the conductance for semiconducting armchair ribbons as expected for preserved time reversal symmetry. In contrast, we see no or only little magnetic field dependence for zizgzag and metallic armchair ribbons, as expected for broken time reversal symmetry at zero field. In addition to this we also see a magnetic field dependence for zigzag ribbons with certain parameters where there is a source of scattering between the cones due to the

interplay of the zigzag edge and the long-range disorder which is beyond the scope of this article.

Apart from the fundamental perspective, ribbons with effectively broken time reversal symmetry are also interesting for applications, as they can conduct a certain amount of current (corresponding to one conductance quantum) without dissipation, i.e. heat production (see the article linked below for more information).

Outlook

An experimental observation of this effective time reversal symmetry breaking requires a good control of the fabrication of graphene nanoribbons. First of all, the ribbons should not have defects on the atomic scale, since these would scatter between the Dirac cones and restore time reversal symmetry. Further, the edges must be controlled up to atomic precision (an additional row of atoms turns a metallic armchair ribbon into a semiconducting one). The recent, fast experimental progress on fabricating and controlling graphene edges however gives hope that our predictions can be tested in the near future.

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In this booklet, the Leibniz Super-computing Centre (LRZ) reports on the results of numerical simulations performed in particular between 2009 and 2011 on the High Performance Computer in Bavaria (HLRB II). The papers were selected from the review reports of projects that have used the supercomputer.

HLRB II was in operation between 2006 and 2011. Its architecture was an SGI Altix 4700 system, based on Intel Itanium2 processors (Montecito). The machine had 9720 processor cores, 39 TByte of shared ccNUMA memory, 600 TByte attached disks and a peak performance of 62.3 TFLOP/s. It was ranked no. 10 in the Top500-list at the time of installation.

The articles provide an overview of the broad range of applications that require high performance computing to solve challenging problems. For each project, the scientific background is described, along with the results achieved and the methodology used.

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