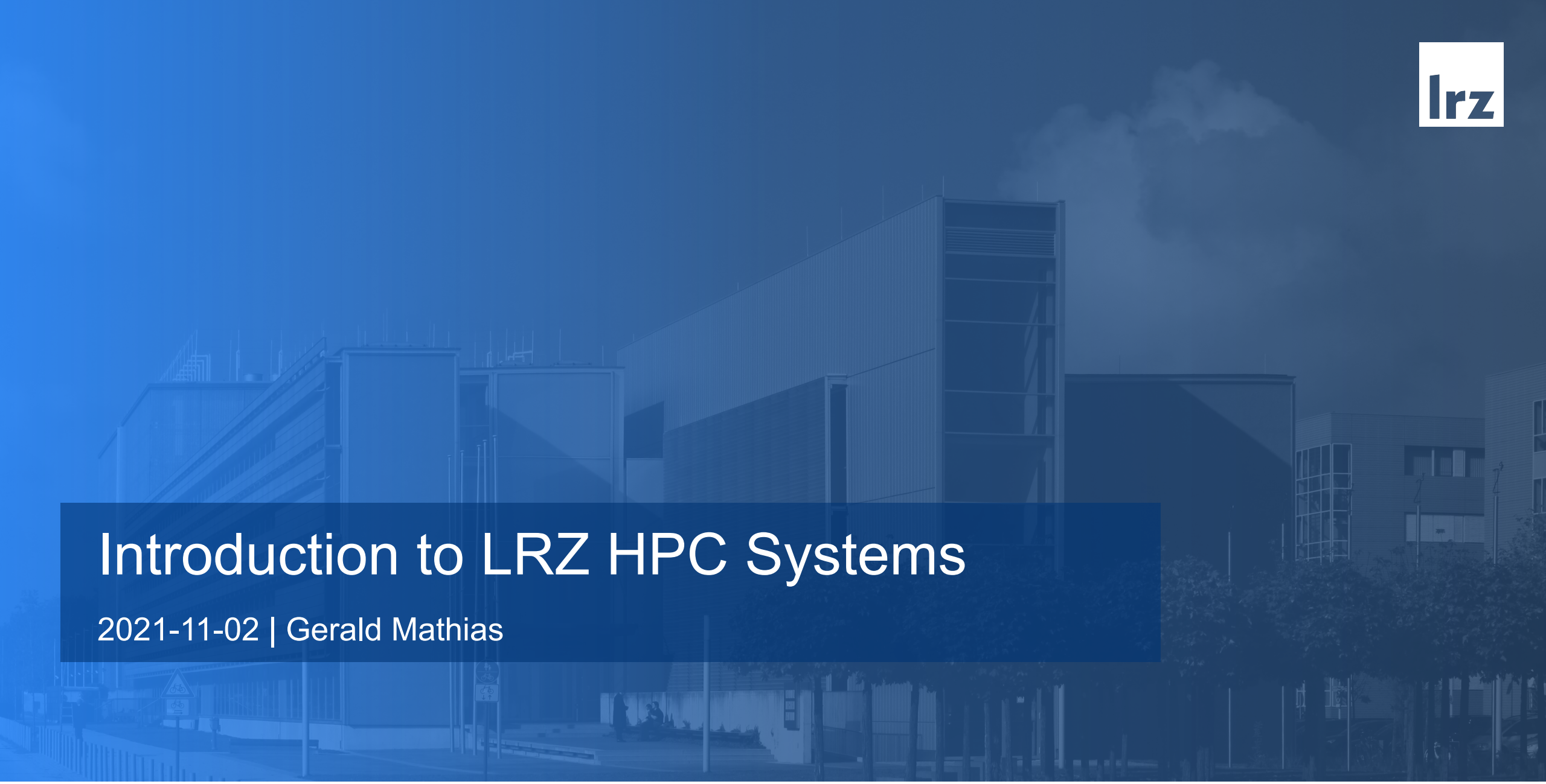


# Introduction to LRZ HPC Systems

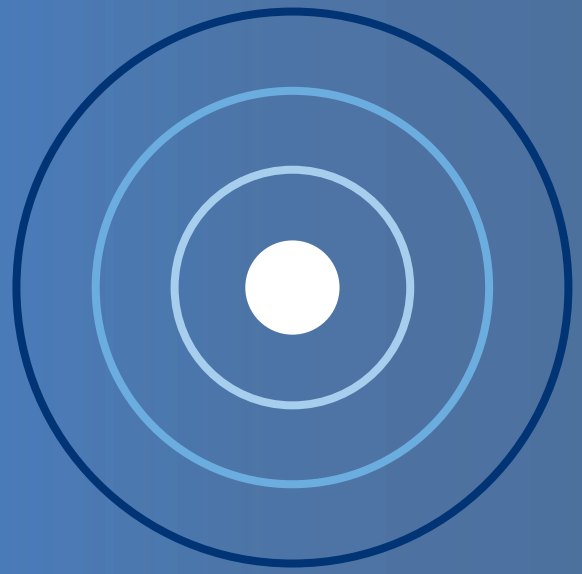
2021-11-02 | Gerald Mathias

# Leibniz-Rechenzentrum (LRZ)/ Leibniz Supercomputing Centre

of the Bayerischen Akademie der Wissenschaften/ Bavarian Academy of Sciences and Humanities

**250**
employees
approx.

**56**
years of
IT support



Computer Centre
for all Munich Universities

Regional Computer Centre
for all Bavarian Universities

National Supercomputing Centre
(GCS)

European Supercomputing Centre
(PRACE)

# For European Research

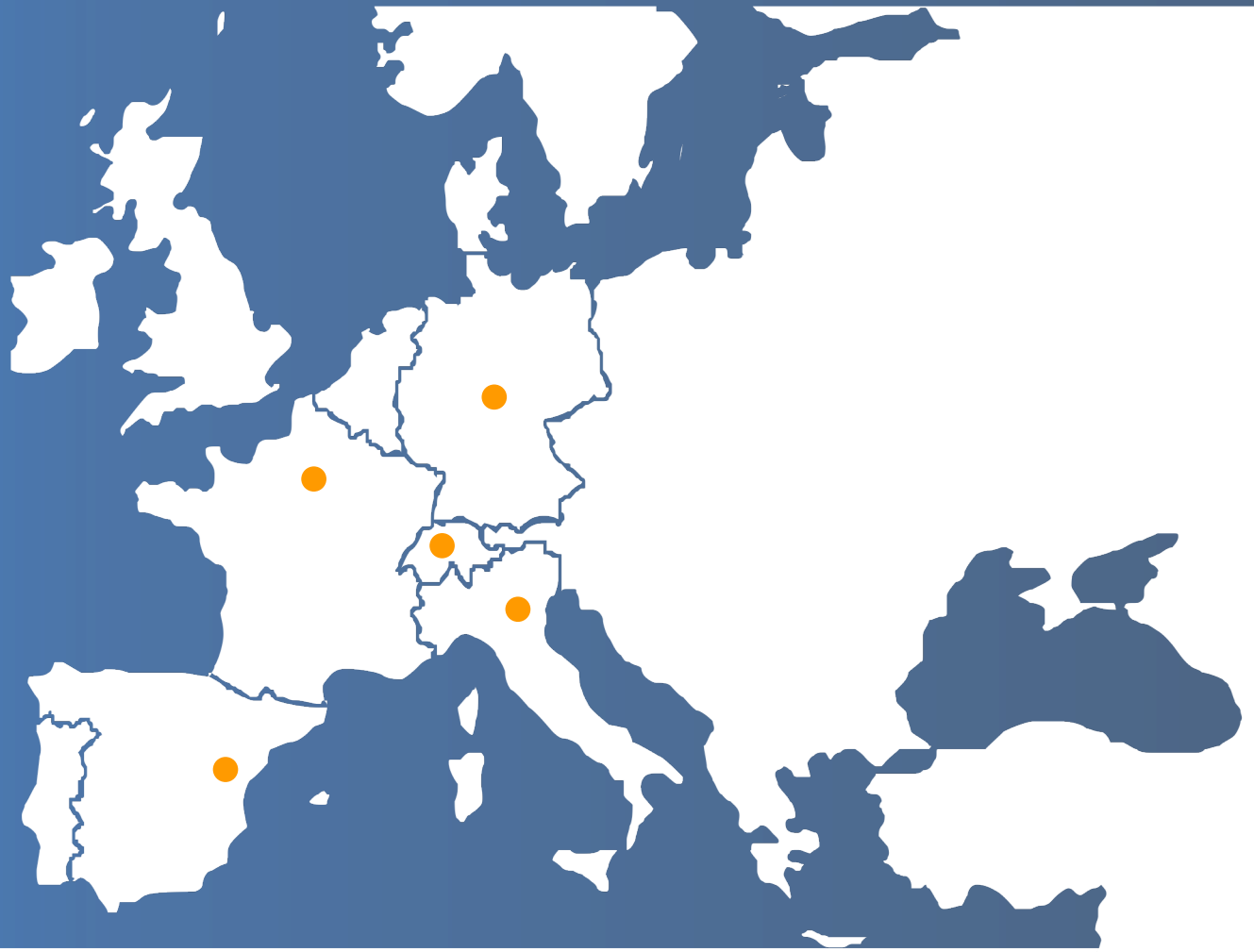
**Partnership for Advanced Computing in Europe (PRACE) |** 25 Countries

Federated, pan-European Tier-0 supercomputing infrastructure

Hosting Members:

- GCS  (Germany: LRZ, HLRS, JSC)
- BSC (Spain)
- CSCS (Switzerland)
- CINECA (Italy)
- GENCI (France)

PRACE 2: 2017 – 2020




Lenovo
Lenovo
SuperMUC-NG

# SuperMUC-NG: Intel / Lenovo

| | thin | fat |
|---|---|---|
| Processor type (205/240 W TDP) Xeon Platinum 8174, 24 cores | Intel Skylake | Intel Skylake |
| Number of cores per node | 48 (2x24) | 48 (2x24) |
| Memory per node | 96 GB | 768 GB |
| Nominal frequency | 2.7 GHz | 2.7 GHz |
| AVX-512 frequency (all cores active), current default frequency | 2.3 GHz | 2.3 GHz |
| Floating point operations per clock (Fused MulAdd = 2) | 32 | 32 |
| Total number of nodes of this type | 6336 | 144 |
| Number of islands with this node type (792 nodes / 144 Nodes) | 8 | 1 |
| Fat Tree with island, pruning 1:3.8 between islands | | |
| | | |
| Total Cores | 311,040 | |
| Total Nodes | 6480 | |
| Total Memory | 719 TByte | |
| „Peak Performance“ | 26.9 PF | |
| Linpack (Nov 18: rank 8, **Jun 19 and Nov 19**: rank 9) | 19.5 PF | |
| *Cf. Vector Triad RINF  vd=va*vb+vc  (Average/Large+OpenMP)* | *1.0 / 0.2 PF* | |

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# SuperMUC-NG

## IBM Spectrum Scale (GPFS) Parallel File System

- SCRATCH/WORK
  - 50 PByte capacity
  - 500 GByte/s I/O bandwidth
- LRZ DSS: Data Science Storage for Long Term Data Storage
  - 20 PByte capacity and
  - 70 GByte/s I/O bandwidth
- HOME
  - 256 TB + 256 TB Replika
  - 28 Gbytes/s SSD Tier, 7 Gbyte/s HDD Tier, 40000 IOPS


## OpenStack Compute Cloud (100 GigE)

- 32 nodes with 2x Intel Xeon 6148 processors, 192 Gbyte
- 32 nodes with 2x Intel Xeon 6148 processors,
  2x Nvidia Volta 100 GPUs, 768 GByte memory
- 1 huge memory node with 8x Intel Xeon 8160 processors,
  6144 GByte memory

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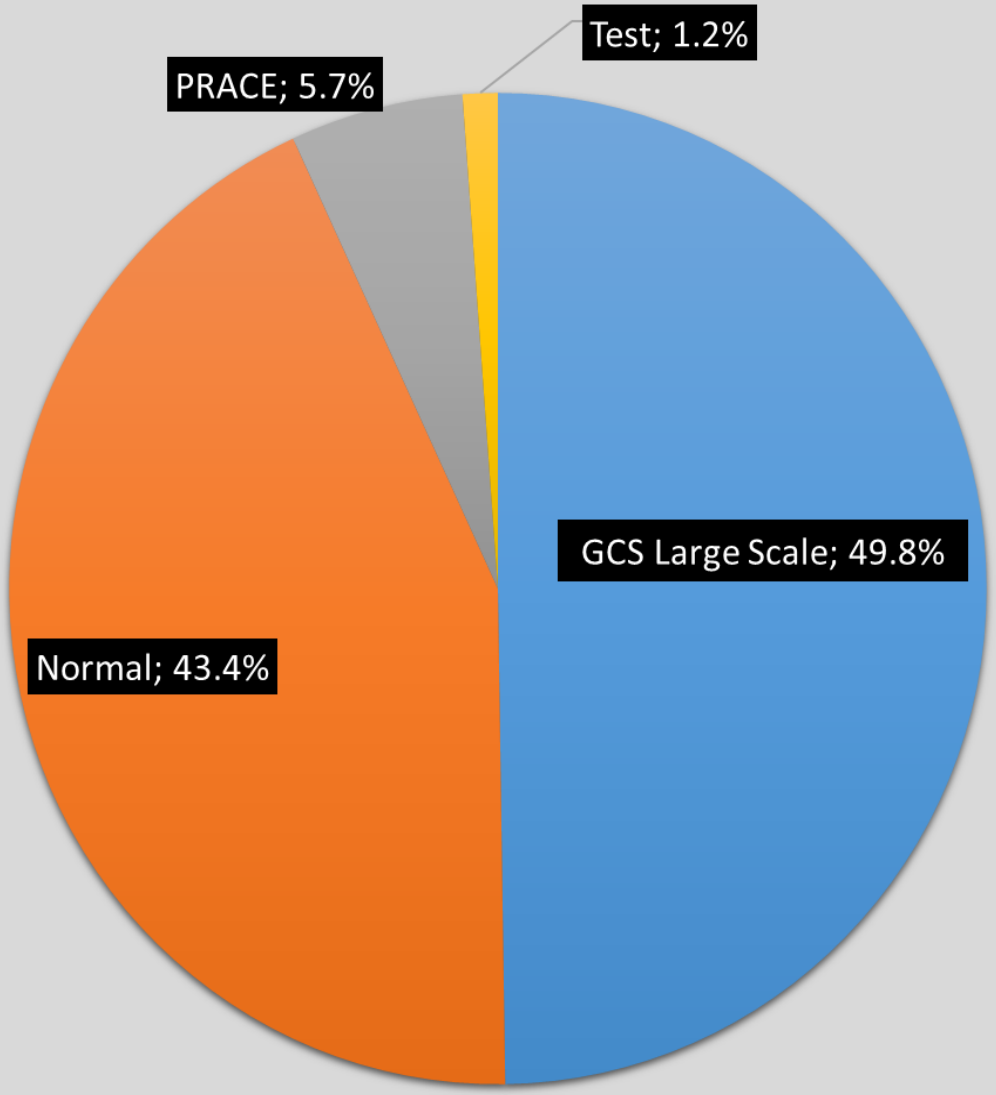
# Coming 2023:
# SuperMUC-NG Phase 2

- ~250 Compute nodes
  - 2 Intel SapphireRapids CPUs
  - 4 Intel PonteVecchio accelerators

- *Distributed Asynchronous Object Storage* (DAOS) for AI and ML workloads
- Programming: Intel OneAPI software stack
- Course series planned for 2022

# Usage 2019/2020




up to 2.6 G core-h / year

*main scientific areas*

- 28% CFD / engeneering
- 20% elementary particle physics
- 18% astrophysics
- 8% condensed matter

# System Access
# Test Accounts and Compute Projects

Scientists in Europe are eligible, proposals for computing time are reviewed.

- Scientists with affiliation in Germany
  https://doku.lrz.de/display/PUBLIC/Access+and+Login+to+SuperMUC-NG
- European scientists apply via
  https://prace-ri.eu/hpc-access/preparatory-access/
  https://prace-ri.eu/hpc-access/project-access/

# System used today: CoolMUC2

- Nodes were part of the SuperMUC Phase2 system installed in 2015
- Dual Intel Haswell nodes (2x14 cores)
- TIER-2 system.

Login onto the system via secure shell from
a terminal window (Linux/macOS)

On Windows systems, install putty https://www.putty.org/

```
:~> ssh -Y lxlogin[1-4].lrz.de -l xxyyyzz
```

Please use login nodes for compiling but not for compute!

# SLURM Batch System

**Submit a job:**

```
sbatch --reservation=hcow1w21 job.sh
```

**List own jobs:**

```
squeue –M cm2_tiny
```

**Cancel jobs:**

```
scancel -M cm2_tiny jobid
```

**Interactive Access:**

```
module load salloc_conf/cm2_tiny
salloc --partition=cm2_tiny --time=00:30:00 --reservation=hcow1w21export
OMP_NUM_THREADS=28
srun --reservation=hcow1w21 ./myprog.exe
exit
```

or: `srun --reservation=hcow1w21 --pty bash`

Reservation is only valid during the workshop, for general usage on our Linux Cluster remove the "--reservation=hcow1w21"

Details: https://doku.lrz.de/display/PUBLIC/Running+parallel+jobs+on+the+Linux-Cluster
Examples: https://doku.lrz.de/display/PUBLIC/Example+parallel+job+scripts+on+the+Linux-Cluster
Resource limits: https://doku.lrz.de/display/PUBLIC/Resource+limits+for+parallel+jobs+on+Linux+Cluster

# Example OpenMP Batch File

```
#!/bin/bash
#SBATCH -o /dss/dsshome1/0B/a2c06ae/test.%j.%N.out
#SBATCH -D /dss/dsshome1/0B/a2c06ae
#SBATCH -J test
#SBATCH --clusters=cm2_tiny
#SBATCH --partition=cm2_tiny
#SBATCH --nodes=1-1
#SBATCH --cpus-per-task=28
#SBATCH --get-user-env
#SBATCH --reservation=hcow1w21
#SBATCH --time=02:00:00
module load slurm_setup
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK
./myprog.exe
```

# Environment Modules

- Used by most centres
- provide standard software environment by the computing centre
- modular installation of software
- provide multiple versions of a package/compiler/library
- central software installation

Which modules are loaded?

```
:~> module list
Currently Loaded Modulefiles:
 1) admin/1.0                  5) intel/19.0.5
 2) tempdir/1.0                6) intel-mkl/2019.5.281
 3) lrz/1.0                    7) intel-mpi/2019.7.217
 4) spack/staging/20.1.1
```

*Good practise*

Use `module list` in batch scripts and compile scripts to document run/compile conditions.

➡️ helps debugging problems

# Environment Modules

## Which modules are provided?

```
# complete list
:~> module available
/lrz/sys/spack/.../linux-sles15-skylake -
abinit/8.10.3-intel19-impi
adios/1.13.1-gcc8-impi
adios2/2.5.0-intel19-impi
bigmpi/0.1-intel19-impi
blitz/1.0.1-gcc8
...

# selected package
:~> module av likwid
-/lrz/sys/spack/.../linux-sles15-skylake -
likwid/4.3.3-gcc8-msr     likwid/5.0.1-gcc8-msr
likwid/4.3.3-intel19-msr  likwid/5.0.1-intel19-msr

------ /lrz/sys/.../files_sles15/tools -------
likwid/4.2  likwid/4.3  likwid/4.3-perf
```

## Find module by keyword

```
:~>  module search compiler
- /lrz/sys/spack/.../linux-sles15-x86_64 -
          gcc/8.4.0: Compilers:GNU compiler collection:GCC
          gcc/9.3.0: Compilers:GNU compiler collection:GCC
       gcc/9.3.0-nv: Compilers:GNU compiler collection:GCC
       intel/19.0.5: Compilers:HPC languages:Intel Fortran/C/C++
       intel/19.1.1: Compilers:HPC languages:Intel Fortran/C/C++
         llvm/8.0.0: compiler:clang:llvm
         llvm/9.0.0: compiler:clang:llvm
matlab-mcr/R2019a-generic: applications:scientific programming
           framework:MATLAB compiler runtime
matlab-mcr/R2019b-generic: applications:scientific programming
           framework:MATLAB compiler runtime>
        perl/5.30.0: Compilers:tools:perl interpreter:scripting
```

# Environment Modules

## What does a module do?

```
:~> module show elpa
-------------------------------------------------------------------
/lrz/sys/spack/release/21.1.1/modules/haswell/linux-sles15-haswell/elpa/2020.05.001-intel19-impi-openmp:

setenv          ELPA_SPEC /.../21.1.1/opt/haswell/elpa/2020.05.001-intel-4pvo3pf/.spack/spec.yaml
conflict        elpa
prepend-path    LD_LIBRARY_PATH /.../21.1.1/opt/haswell/elpa/2020.05.001-intel-4pvo3pf/lib
prepend-path    LIBRARY_PATH /.../21.1.1/opt/haswell/elpa/2020.05.001-intel-4pvo3pf/lib
prepend-path    C_INCLUDE_PATH /.../21.1.1/opt/haswell/elpa/2020.05.001-intel-4pvo3pf/include
prepend-path    INCLUDE /.../21.1.1/opt/haswell/elpa/2020.05.001-intel-4pvo3pf/include
prepend-path    PKG_CONFIG_PATH /.../21.1.1/opt/haswell/elpa/2020.05.001-intel-4pvo3pf/lib/pkgconfig
setenv          ELPA_LIB /.../21.1.1/opt/haswell/elpa/2020.05.001-intel-4pvo3pf/lib/libelpa_openmp.a
setenv          ELPA_SHLIB {-L/.../21.1.1/opt/haswell/elpa/2020.05.001-intel-4pvo3pf/lib -lelpa_openmp}
```

`prepend-path:` extend path variable

`setenv:` provide environment variable

**Hint**: Use module-provided variables in makefiles, the command line and in shell scripts!

# Environment Modules

## Loading and unloading

```
:~> module av gcc
--- /apps/modules/data/development -----
gcc/4.9.4 gcc/5.4.0 gcc/6.2.0 gcc/7.3.0 gcc/8.1.0

# load new module
:~> module load gcc
:~> module list
Currently Loaded Modulefiles:
 1) gcc/8.1.0
# change current module (unload & load)
:~> module switch gcc gcc/7.3.0
:~> module list
Currently Loaded Modulefiles:
 1) gcc/7.3.0
# unload the module
:~> module unload gcc
:~> module list
No Modulefiles Currently Loaded.
```

## Aliases and defaults

```
:~> module alias
--- Aliases ------------------------
intel-mkl/2019 -> intel-mkl/2019.5.281
intel-mkl/2019-gcc8 -> intel-mkl/2019.5.281
intel-mkl/2019-seq -> intel-mkl/2019.5.281
intel-mpi/2019-gcc -> intel-mpi/2019.7.217
intel-mpi/2019-intel -> intel-mpi/2019.7.217
intel/19.1 -> intel/19.1.1

---------- Versions ----------------
admin/default -> admin/1.0
allinea-reports/default -> allinea-reports/18.3
amber/default -> amber/18
amira/default -> amira/2019.3
```

depends on the local module-file setup

# How was the module build: ${PACKAGE}_SPEC

```
:~> module load elpa
:~> less $ELPA_SPEC
spec:
- elpa:
    version: 2020.05.001
    arch:
      platform: linux
      platform_os: sles15
      target:
        name: haswell
        vendor: GenuineIntel
compiler:
      name: intel
      version: 19.0.5.281
    namespace: fixes015x
    parameters:
      openmp: true
      optflags: true
      cflags: []
      cppflags: []
      ...
```

```
 dependencies:
 intel-mkl:
        hash:
       3zuek252xqyrotkmqbbzq7e3q6tyjv4h
        type:
        - build
        - link
      intel-mpi:
        hash:
       xi6c5vue36rwmzhw4zqexs2yfymaho3z
        type:
        - build
        - link
    hash:
       4pvo3pf7eqkymzf7agava74m7wm5ptij
- intel-mkl:
    version: 2020.1.217
    arch:
      platform: linux
      platform_os: sles15
      target:
        name: haswell
```

the .spec file contains all relevant information for the dependency tree.

# Environment Modules: Intel OneAPI Software Stack

## Loading intel-oneapi

```
:~> module av intel-oneapi
---/lrz/.../environment ---
intel-oneapi/2021.1  intel-oneapi/2021.2
intel-oneapi/2021.4
:~> module load intel-oneapi
intel-oneapi-mpi: using intel wrappers for mpicc, mpif77, etc

Loading intel-oneapi/2021.4
  Unloading conflict: intel-mpi/2019-intel intel/19.0.5 intel-mkl/2019
  Loading requirement: intel-oneapi-compilers/2021.4.0 intel-oneapi-mkl/2021 intel-
oneapi-mpi/2021-intel intel-oneapi-itac/2021.4.0
```

unloads intel default modules and loads
intel-oneapi versions

# Environment Modules: Intel OneAPI Software Stack

## Loaded and available

```
:~> module list
Currently Loaded Modulefiles:
 ... 4) spack/21.1.1   5) intel-oneapi-compilers/2021.4.0  6) intel-oneapi-mkl/2021
7) intel-oneapi-mpi/2021-intel 8) intel-oneapi-itac/2021.4.0  9) intel-oneapi/2021.4
:~> module av intel-oneapi
---- /lrz/sys/spack/.../linux-sles15-x86_64 ----
intel-oneapi-advisor/2021.4.0    intel-oneapi-ipp/2021.4.0    intel-oneapi-mkl/2021.3.0
intel-oneapi-ccl/2021.4.0        intel-oneapi-ippcp/2021.4.0  intel-oneapi-mkl/2021.4.0
intel-oneapi-clck/2021.4.0       intel-oneapi-itac/2021.4.0   intel-oneapi-mpi/2021-gcc
intel-oneapi-compilers/2021.4.0  intel-oneapi-mkl/2021         intel-oneapi-mpi/2021-intel
intel-oneapi-dal/2021.4.0        intel-oneapi-mkl/2021-gcc8   intel-oneapi-tbb/2021.4.0
intel-oneapi-dnn/2021.4.0        intel-oneapi-mkl/2021-seq    intel-oneapi-vpl/2021.6.0
intel-oneapi-dpcpp-ct/2021.4.0   intel-oneapi-mkl/2021.1.1    intel-oneapi-vtune/2021.7.1
intel-oneapi-inspector/2021.4.0  intel-oneapi-mkl/2021.2.0
```

more tools for code analysis, machine learning libraries, MKL versions etc.
(more to come soon)

# Tasks for the hands-on

Modules

1. Log on to the `lxlogin[1-4].lrz.de`
2. Which modules are automatically loaded?
3. Identify available compilers.
4. Why are module files for intel compilers in different directories?
5. Find the module of the latest Intel MKL version.
6. Load the `intel-oneapi` stack.

SLURM:

7. Write a bash ”Hello World” script
8. Write a batch script to run it with SLURM.
9. Run in in interactive mode on a node.