



Leibniz Supercomputing Centre
of the Bavarian Academy of Sciences and Humanities

The background of the slide is a photograph of a modern, multi-story building with a glass and metal facade, likely the Leibniz Supercomputing Centre. The image is overlaid with a semi-transparent blue filter. The building has several windows and a prominent vertical structure on the right side.

Leibniz Supercomputing Centre

Using oneAPI on SuperMUC-NG | 08.11.2022 | Nisarg Patel

Motivation



Map of Intel Toolkits



Intel oneAPI Base Toolkit

- Intel oneAPI Collective Communications Library
- Intel oneAPI Data Analytics Library
- Intel oneAPI Deep Neural Networks Library
- Intel oneAPI DPC++/C++ Compiler
- Intel oneAPI DPC++ Library
- Intel oneAPI Math Kernel Library
- Intel oneAPI Threading Building Blocks
- Intel oneAPI Video Processing Library
- Intel Advisor
- Intel Distribution for GDB*
- Intel Distribution for Python*
- Intel DPC++ Compatibility Tool
- Intel FPGA Add-on for oneAPI Base Toolkit
- Intel Integrated Performance Primitives
- Intel VTune Profiler

Intel oneAPI HPC Toolkit

- Intel oneAPI DPC++/C++ Compiler
- Intel C++ Compiler Classic
- Intel Cluster Checker
- Intel Fortran Compiler
- Intel Fortran Compiler Classic
- Intel Inspector
- Intel MPI Library
- Intel Trace Analyzer and Collector

Intel AI Analytics Toolkit

Intel oneAPI IoT Toolkit

Intel oneAPI Rendering Toolkit

Intel-oneAPI components on SuperMUC-NG



- Intel-oneAPI components are provided via Environmental Modules.

Core Intel-oneAPI components for LRZ HPC

(provided as a standalone modules)

- Intel-oneAPI-Compilers
- Intel-oneAPI-MPI
- Intel-oneAPI-MKL

Other Intel-oneAPI components for LRZ HPC

(provided as a toolkit module)

- Intel-oneAPI-Toolkit
 - Collective Communications Library
 - Data Analytics Library
 - Deep Neural Networks Library
 - Threading Building Blocks
 - Video Processing Library
 - Advisor
 - DPC++ Compatibility Tool
 - Integrated Performance Primitives
 - VTune Profiler
 - Inspector
 - Trace Analyzer and Collector

What is an Environmental Module?



- Modules provide a flexible way to configure and access various applications, compilers, tools and libraries dynamically by managing the shell environment
- In other words modules allow for the dynamic modification of environment variables such as;
 - library paths
 - binary paths
 - license server settings
 - application specific configurations

```
>module show intel-oneapi-compilers
-----
/lrz/sys/spack/release/22.2.1/modules/x86_64/linux-sles15-x86_64/intel-oneapi-compilers/2022.2.0:
conflict      intel-parallel-studio
conflict      intel
setenv        INTEL_ONEAPI_COMPILERS_WWW https://doku.lrz.de/display/PUBLIC/Intel+Compilers
setenv        IFORTCFG dummy.cfg
setenv        ICCCFG dummy.cfg
setenv        ICPCCFG dummy.cfg
setenv        CC icx
setenv        CXX icpx
setenv        CPP {icx -E}
setenv        FC ifx
setenv        FORT_BUFFERED true
setenv        FORT_BLOCKSIZE 16777216
module-whatIs compilers:fortran/c/c++/dpc++:icx:icpx:ifx:ifort:icc:icpp:INTEL-ONEAPI-COMPILERS
-----
```


Intel-oneAPI components are provided via Environmental Modules



```
>module avail intel-oneapi-compilers intel-oneapi-mpi intel-oneapi-mkl intel-oneapi-toolkit
----- /lrz/sys/spack/release/22.2.1/modules/x86_64/linux-sles15-x86_64 -----
intel-oneapi-compilers/2021.4.0  intel-oneapi-compilers/2022.1.0
intel-oneapi-compilers/2022.0.1  intel-oneapi-compilers/2022.2.0

----- /lrz/sys/spack/release/22.2.1/modules/x86_64/linux-sles15-x86_64 -----
intel-oneapi-mpi/2021-gcc          intel-oneapi-mpi/2021.5.1-gcc    intel-oneapi-mpi/2021.7.0-gcc
intel-oneapi-mpi/2021-intel        intel-oneapi-mpi/2021.5.1-intel  intel-oneapi-mpi/2021.7.0-intel
intel-oneapi-mpi/2021.4.0-gcc      intel-oneapi-mpi/2021.6.0-gcc
intel-oneapi-mpi/2021.4.0-intel    intel-oneapi-mpi/2021.6.0-intel

----- /lrz/sys/spack/release/22.2.1/modules/x86_64/linux-sles15-x86_64 -----
intel-oneapi-mkl/2021              intel-oneapi-mkl/2022            intel-oneapi-mkl/2022.1.0
intel-oneapi-mkl/2021-gcc11        intel-oneapi-mkl/2022-gcc11     intel-oneapi-mkl/2022.2.0
intel-oneapi-mkl/2021-seq          intel-oneapi-mkl/2022-seq
intel-oneapi-mkl/2021.4.0          intel-oneapi-mkl/2022.0.2

----- /lrz/sys/spack/release/22.2.1/modules/x86_64/linux-sles15-x86_64 -----
intel-oneapi-toolkit/2021.4.0      intel-oneapi-toolkit/2022.2.0    intel-oneapi-toolkit/2022.3.0
```

Intel-oneAPI toolkit module



```
>
>module load intel-oneapi-toolkit/2022.3.0

>
>module list
Currently Loaded Modulefiles:
  1) admin/1.0          4) spack/22.2.1          7) intel-oneapi-mkl/2022.2.0
  2) tempdir/1.0       5) intel-oneapi-compilers/2022.2.0  8) intel-oneapi-toolkit/2022.3.0
  3) lrz/1.0           6) intel-oneapi-mpi/2021.7.0

>
>module avail
- /dss/lrzsyst/sys/spack/release/22.2.1/modules/x86_64/linux-sles15-x86_64/.intel-oneapi-toolkit/2022.3.0 -
intel-oneapi-advisor/2022.3.0  intel-oneapi-dpcpp-ct/2022.2.0  intel-oneapi-tbb/2021.7.0
intel-oneapi-ccl/2021.7.0      intel-oneapi-inspector/2022.3.0  intel-oneapi-vpl/2022.2.0
intel-oneapi-clck/2021.7.0     intel-oneapi-ipp/2021.6.1        intel-oneapi-vtune/2022.4.0
intel-oneapi-dal/2021.7.0      intel-oneapi-ippcp/2021.6.1
intel-oneapi-dnn/2022.2.0      intel-oneapi-itac/2021.7.0
```


Questions?