



Onboarding amplitUDE

HPC Services in UDE

VI-HPS Tuning Workshop TW 47

02.06.2025 – Dr. D. Brands / J. Mir

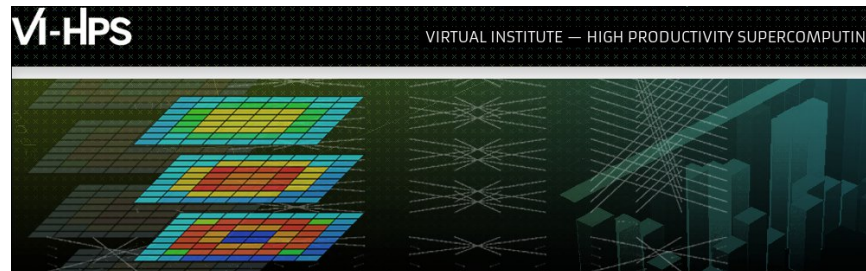


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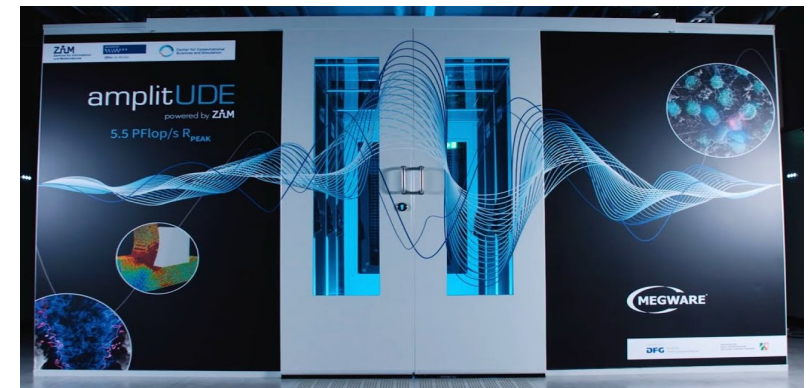
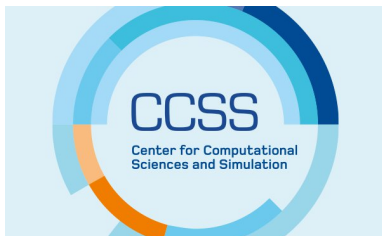


Agenda

- **HPC Resources at UDE**
- **Software Stack and Tools**
- **Access and VPN**
- **Research Support, Trainings, and Workshops**

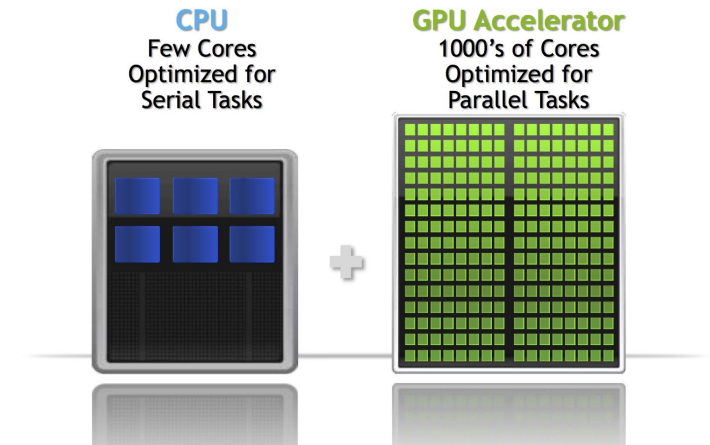
Introducing amplitUDE

- Officially inaugurated on December 2, 2024
- Represents a €7.5 million investment co-funded by the German Research Foundation (DFG) and the State of NRW
- Funded by DFG State Major Instrumentations (“Großgeräte”) organised by Center for Computational Sciences and Simulation (CCSS) and ZIM
- Hosted and managed by ZIM



amplitUDE: Technical Specifications

- **Supplier:** MEGWARE GmbH, Germany
- **Compute Nodes:**
 - 252 CPU Nodes (2x Intel® Xeon® Platinum 8480+):
 - 184 Standard Nodes (512 GB RAM)
 - 55 High-Memory Nodes (1 TB RAM)
 - 13 Super High-Memory Nodes (2 TB RAM)
 - 19 GPU Nodes (2x Intel® Xeon® Platinum 8480+):
 - 18 Nodes with 4x NVIDIA H100 GPUs with 80 GB
 - 1 Nodes with 2x NVIDIA H100 GPUs with 80 GB
 - *Coming Soon (4 Nodes with 8 NVIDIA H200 GPUs with 141 GB)*
- **Networking:** Mellanox InfiniBand NDR200 with Blocking Ratio 1:1.66
- **Storage:** Lustre File System with ~2.1 PB usable capacity
- **Energy Efficiency:**
 - Ranked #8 globally on the “Green500” list for energy-efficient supercomputers
 - Direct liquid cooling with heat recovery



Quelle: <https://blogs.nvidia.com/blog/whats-the-difference-between-a-cpu-and-a-gpu/>

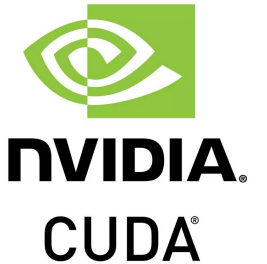
Software Stack & Tools

■ Slurm Workload Manager

- amplitUDE and magnitUDE use Slurm for resource management

■ Modules System

- Pre-installed software packages via environment modules e.g., Anaconda, CUDA
- Machine learning libraries (TensorFlow, PyTorch)
- Commercial Software like MATLAB, Intel One API, ANSYS, etc.



■ Customizable Environment

- Users can load specific modules or create isolated environments tailored to their workloads using conda, pip, etc.

Software Stack & Tools

■ Module System

- Softwares are installed on the amplitUDE and maintained by the HPC-Team.

Frequently used commands:	
list modules/software available	<code>module avail</code>
list modules/software loaded in the current session	<code>module list</code>
load a specific module/software	<code>module load <moduleName></code>
show information about a module	<code>module show <moduleName></code>
help on the <code>module</code> tool	<code>module help</code>

Software Stack & Tools

```
[cbm107c@login2 ~]$ module avail
```

/cluster/modulefiles/apps

```
alphafold/2.3.2_troubleshooting      lammps/stable-29Aug2024-openmpi-nvcc-cuda  q-e/7.4-openmpi-5.0.3-gcc  starccm/18.06.007-R8
ansys/R2024R1                        mathematica/14.0                          q-e/7.4-openmpi-nvcc-cuda  starccm/19.06.009-R8
cp2k/2024.1-psmp                     ovito/3.6.0-gcc-11.4.1                    r/4.4.0-gcc-13.3.0
lammps/stable-29Aug2024-openmpi-5.0.3-gcc  plasticity/1.4.0-openmpi-5.0.3-gcc        starccm/17.06.008-R8
```

/cluster/modulefiles/compiler

```
cmake/3.29.6  gcc/13.3.0
```

/cluster/modulefiles/mpi

```
openmpi/5.0.3-gcc      openmpi/5.0.5-gcc-11.4.1-wv3zim  openmpi/hpc-x-4.1.7-intel
openmpi/5.0.3-intel24  openmpi/5.0.7-gcc-11.5.0         openmpi/hpc-x-4.1.8-gcc
```

/cluster/modulefiles/intel-oneAPI

```
advisor/2024.0      compiler32/2024.0.0  dpct/2024.0.0  intel_ipp_ia32/2021.10  mkl/2024.0  tbb32/2021.11
advisor/latest      compiler32/latest    dpct/latest     intel_ipp_ia32/latest   mkl/latest   tbb32/latest
ccl/2021.11.0       dal/2024.0.0         dpl/2022.3      intel_ipp_intel64/2021.10  mkl32/2024.0  vtune/2024.0
ccl/latest          dal/latest           dpl/latest      intel_ipp_intel64/latest  mkl32/latest   vtune/latest
compiler-rt/2024.0.0  debugger/2024.0.0    ifort/2024.0.0  intel_ippcp_ia32/2021.9   mpi/2021.11
compiler-rt/latest   debugger/latest       ifort/latest    intel_ippcp_ia32/latest   mpi/latest
compiler-rt32/2024.0.0  dev-utilities/2024.0.0  ifort32/2024.0.0  intel_ippcp_intel64/2021.9  oclfpga/2024.0.0
compiler-rt32/latest  dev-utilities/latest   ifort32/latest   intel_ippcp_intel64/latest  oclfpga/latest
compiler/2024.0.0     dnnl/3.3.0            inspector/2024.0  itac/2022.0              tbb/2021.11
compiler/latest       dnnl/latest           inspector/latest  itac/latest              tbb/latest
```

/cluster/modulefiles/nvidia

```
cuda/12.3.2  nvhpc/23.9
```

/cluster/modulefiles/tools

```
anaconda3/2023      hh-suite/3.3.0-openmpi_5.0.3-gcc  scalasca/2.6.1-gcc-11.4.1
cube/4.8.2-gcc-11.4.1  hmmer/3.4                          scalasca/2.6.2-gcc-11.5.0
```

SLURM Partitions & Data Storage

■ CPU and GPU Partitions

```
[username@login1 ~]$ sinfo
```

PARTITION	AVAIL	TIMELIMIT		
STD-l-12h	up	12:00:00		
STD-m-48h	up	2-00:00:00		
STD-s-96h*	up	4-00:00:00		
HIM-l-12h	up	12:00:00		
HIM-m-48h	up	2-00:00:00		
HIM-s-96h	up	4-00:00:00		
SHM-l-24h	up	1-00:00:00		
SHM-s-96h	up	4-00:00:00		
GPU-big	up	2-00:00:00		
GPU-small	up	2-00:00:00		
STS	up	1:00:00	8	ndstd[001-008]
FST	up	8:00:00	8	ndstd[001-008]

■ Storage

- homes
 - Classical Unix-Home
 - UDE central fileserver
 - Quota 50 GB
- HPC-Home
 - \$HPC_HOME
 - Lustre parallel file storage
 - Quota 500 GB
- Scratch
 - \$SCRATCH
 - Lustre parallel file storage
 - Managed via HPC workspaces
 - Quota 10 TB

SLURM Partitions & Data Storage

■ Workspace

- To create a workspace
 - `ws_allocate <ws_name> <lifetime>`
- To check list of workspaces
 - `ws_list`
 - `cd /lustre/scratch/<your-workspace>/`

■ Data Transfer

- `scp -r /path/to/local/file <username>@gateway.amplitude.uni-due.de:/lustre/scratch/<your-workspace>/`
- Enter password + 2FA

Reservation for VI-HPS Tuning Workshop

■ Slurm Reservation

- `scontrol show res`
- `sbatch --reservation=VI-HPS_Tuning_Workshop_Duisburg-Essen job.slurm`

```
[root@mgmt1 ~]# sinfo -T
```

RESV_NAME	STATE	START_TIME	END_TIME	DURATION	NODELIST
VI-HPS_Tuning_Workshop_Duisburg-Essen	INACTIVE	2025-06-02T00:00:00	2025-06-05T23:59:59	3-23:59:59	ndgpu[002,010],ndhim[051-055],ndstd[001-008,082-083]

```
[root@mgmt1 ~]#
```

Access and VPN

■ Access / eduVPN

- Direct connection to the HPC-systems is only possible from the network (intranet) of the UDE.
- Otherwise a VPN-connection must be established
- The login process using **ssh** is done with a 2FA-authentication (password + OTP-token).
=> Activation of 2FA-authentication in selfcare-portal (<https://selfcare.uni-due.de>)
- The jump host can be accessed via ssh
 - `ssh USERNAME@login.hpc.uni-due.de` use alternatively IP: 134.91.131.245
 - Afterwards, `ssh amplitude`
- Alternatively, in your `$HOME/.ssh/config`

```
Host login-ampl
  HostName login.hpc.uni-due.de
  User [USERNAME]
  RequestTTY force
  RemoteCommand ssh amplitude
```

Internet Access on amplitUDE

■ Proxy

- Internet access from within the cluster is restricted and must pass through a proxy with a white listing
- Environment variable are already set by default:
`HTTPS_PROXY, https_proxy, HTTP_PROXY, http_proxy` pointing to proxy on `134.91.129.97:3128`
- If it fails nevertheless ...
 - `bash-5.1$ curl -I downloads.linaroforge.com`
 - `curl: (7) Failed to connect to downloads.linaroforge.com port 80: Connection refused`
- ... HPC support must add the URL to the white list.  Try again

```
bash-5.1$ curl -I downloads.linaroforge.com
HTTP/1.1 301
Moved Permanently
[...]
Location: https://downloads.linaroforge.com/
[...]
bash-5.1$ curl -I https://downloads.linaroforge.com
HTTP/1.1 200 Connection established
[...]
bash-5.1$
```

Empowering Researchers with amplitUDE

■ Access & Onboarding

- Managed by ZIM in collaboration with the Center for Computational Sciences and Simulation (CCSS)
- Streamlined application process to encourage early adoption by researchers



■ Comprehensive Documentation

- Guides for account setup, job submission, data storage management, and software usage



Landing page for HPC at UDE



Vielen
Dank

Join mailing list for
more training updates



escience-training-join@lists.uni-due.de

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