



# RWTH Compute Cluster Software Environment

HPC Intro 2022

Daniel Schürhoff

# Agenda

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## ■ Philosophy

- Single Cluster Image
- Single Cluster File System

## ■ Access to the Cluster

## ■ Software Environment

- (RHELcomp) CentOS Linux release 7.9, as less mods as possible
- Linux distribution RPMs (yum) – unmodified
- module system
  - <https://hpc-wiki.info/hpc/Modules>

## ■ Batch system SLURM => presentation of Mr. Wagner

## ■ Account

- RWTH & FZJ members : SelfService
  - (FZJ members need TIM/IdM)
- External users:
  - compute time application
  - With this you can get an account

- **Firewall: use VPN if outside of RWTH and other trusted networks**
  - Cisco Any Connect
- **Login via SSH**
  - Remote Desktop Sessions (FastX)
  - SSH with Multiplexer (screen, tmux)
- **CLAIX18: login18-1.hpc.itc.rwth-aachen.de (also 18-2 ...18-4)**
  - Batch System: SLURM,
  - default modules: intel/19.0, intelmpi/2018

## ■ Common Software easy to use

→ `module list`

Lists all loaded modules

→ `module avail`

Which modules are available?

→ `module load/unload 'modulename'`

Self-explanatory

Modules are grouped -> load Group to see available modules

→ `module switch 'modulename1' 'modulename2'`

# Available Modules

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## ■ **DEVELOP:**

clang, cmake, cuda, cudnn, ddt, forge, gcc, gmake, intel, intelaxe, intelitac, intelixe, intelmpi, intelvtune, likwid, nagfor, nccl, ninja-build, nvhpc, openmpi, pgi, python, python, reports, studio, totalview

## ■ **MATH:**

gurobi, gurobipy, maple, mathematica, r-project

## ■ **CHEMISTRY:**

abinit, cantera, cosmoconf, cp2k, dalton, gamess, gaussian, gaussview, gromacs, lammps, liggghts, openbabel, openmx, qe, siesta, turbomole, vasp, xtb

## ■ **CONTAINERS:**

datascience-notebook, horovod, pytorch, tensorflow

## ■ **And many more**



# Modules Best Practise

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- **Do not load/unload modules in the .zshrc**

- **If in doubt, start over with:**

  - `module purge`

- **(Re-)Compile your application correctly**

  - Binaries from other systems/clusters should be recompiled

  - Use current modules

    - default compiler (intel/19.0), if in doubt: older releases

    - default Intel MPI (2018), if in doubt: older releases (2019 'experimental')

  - `$FLAGS_FAST (-xSSE4.2 -axCORE-AVX2,AVX)`

  - don't forget to enable debugging and optimization (in that order)

    - `-g -O3`

# Summary

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- **Please use modules!**
- **(Re-)Compile your application correctly**
- **use envvars we set for you! \$FC \$CC \$CXX \$MPIFC \$....**

```
$ $MPICC -g $FLAGS_FAST mpihelloworld.c  
$ $MPIEXEC $FLAGS_MPI_BATCH a.out
```

- **consult documentation**

→ <https://hpc-wiki.info>

← general concepts

→ <https://help.itc.rwth-aachen.de/service/rhr4fjjuttff>

← RWTH specifics



# All the links – Step-by-Step

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## ■ Create Account (and/or a compute time project):

→ [www.rwth-aachen.de/selfservice](http://www.rwth-aachen.de/selfservice)

→ [www.itc.rwth-aachen.de/hpc-projects](http://www.itc.rwth-aachen.de/hpc-projects)

## ■ Download and use VPN (or be in University Network):

→ <https://help.itc.rwth-aachen.de/service/vbf6fx0gom76/article/51b128e3749740d3ab0bffa27acb6906/>

## ■ Connect via SSH or FastX:

→ SSH: <https://help.itc.rwth-aachen.de/service/rhr4fjjutttf/article/10c8f0d9b0064013aa439f0b504cc806/>

→ Gitbash (4 Windows): <https://git-scm.com/download/win>

→ FastX: <https://help.itc.rwth-aachen.de/service/rhr4fjjutttf/article/25f576374f984c888bb2a01487fef193/>

→ Nodes: <https://help.itc.rwth-aachen.de/service/rhr4fjjutttf/article/0a23d513f31b4cf1849986aaed475789/>

## ■ For Software please use the provided Modules (see above)

## ■ Consult Documentation:

→ <https://hpc-wiki.info>

← general concepts

→ <https://help.itc.rwth-aachen.de/service/rhr4fjjutttf>

← RWTH specifics

→ For questions we have the Service Desk: [servicedesk@itc.rwth-aachen.de](mailto:servicedesk@itc.rwth-aachen.de)



**Thank for your attention.**

Daniel Schürhoff