RWTH Compute Cluster Software Environment

HPC Intro 2022

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Agenda

- **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**

Access

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

Access

- **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

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Module System

- **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

- **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

- **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

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Summary

- **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/rhr4fjjutttf   ← RWTH specifics

All the links – Step-by-Step

- **Create Account (and/or a compute time project):**
  - → www.rwth-aachen.de/selfservice
  - → 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

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Thank for your attention.

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