RWTH Compute Cluster Software Environment

HPC Intro 2021

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Agenda

- **Philosophy**
  - → Single Cluster Image
    - → Exceptions confirm the rule.
    - → Now: "May you live in interesting times“ (purported to be a Chinese curse)
- **Software Environment (Sw)**
  - → (RHELcomp) CentOS Linux release 7.x, as less mods as possible
  - → Linux distribution RPMs (yum) – unmodified
  - → (binary-distributed) ISV software
  - → (source code) ISV software

  } module system https://hpc-wiki.info/hpc/Modules
- **Batch system**
  - → ~~IBM(Platform) LSF~~
  - → SLURM => presentation of Mr. Wagner

Access

- **Account**
  - → RWTH & FZJ members : SelfService[1]
    - → (FZJ members need TIM/IdM)
  - → External users:
    - → compute time application[2]
    - → With this you can get an account

- **[1] www.rwth-aachen.de/selfservice**
- **[2] www.itc.rwth-aachen.de/hpc-projects**

Access

- **Front Ends**
  - → firewall: use VPN if outside of RWTH and other trusted networks
  - → login via SSH
    - → recommended: Remote Desktop Sessions (FastX) [4]

- ~~**(old) Bull era: cluster, cluster-linux, cluster-x, …**~~
  - ~~→ Batch System: LSF,~~
  - ~~→ default modules: intel/16.0, openmpi/1.10.4~~
- **(new) CLAIX18 era: login18-1, login18-x-2, …**
  - → Batch System: SLURM,
  - → default modules: intel/19.0, intelmpi/2018
- **[4] https://help.itc.rwth-aachen.de/service/rhr4fjjutttf/article/0a23d513f31b4cf1849986aaed475789/**

New module defaults

- **same Linux, same RPMs…**
  - → batch system: LSF → SLURM ← your old batch scripts won‘t work!
  - → intel/16.0 → intel/19.0
  - → openmpi/1.10.4 → intelmpi/2018 ← your [Open MPI] binaries won‘t run!

- **„Where is my lovely version XYZ (that one from my student time)?“**
  - → likely in DEPRECATED. Don‘t try to ride that dead horse forever.

New module defaults

- **openmpi/1.10.4 → intelmpi/2018 ← [Opem MPI] binaries won‘t run!**
- **!!! RECOMPILE YOUR APPLICATION !!!**
  - → well, old binaries *could* still be able to run…
    - → after some ‚module switch‘ commands
  - → - serial and Open MP applications –*quite sure*
  - → - Intel MPI binaries – *highly likely*
  - → - Open MPI binaries – *likely* for 3.x, *maybe* for other versions
  - → … you don‘t ride your grandpa‘s VW Beetle, don‘t you?
- **old binaries optimized for old CPUs (e.g. -xHost, -fast) won’t use new CPUs at full grade (no AVX2…)**

CLAIX18 – Software

- **old binaries *could* run, but would be inefficient, highly likely**
- **recompiling/linking all of your software – use:**
  - → default compiler (intel/19.0), if in doubt: older releases;
  - → default Intel MPI (2018), if in doubt: older releases (2019 ‘experimental’)
  - → -xHost on [login18*] front end for optimize for CLAIX18 CPUs
    - → won’t run on old CPU’s (incl. CLAIX16 CPU’s!)
  - → $FLAGS_FAST (-xSSE4.2 -axCORE-AVX2,AVX)
    - → will run fine everywhere (also on old hardware)
  - → don‘t forget to enable debugging and optimization (in that order)
    - → -g -O3

CLAIX18 – Software

- **use modules! e.g. for Open MPI (3.1.3) :**

```
$ module switch intelmpi openmpi
```

- **use envvars we set for you! $FC $CC $CXX $MPIFC $....**

```
$ $MPIFC -g $FLAGS_FAST  mpihelloworld.f90
$ $MPIEXEC $FLAGS_MPI_BATCH  a.out
```

- **consult documentation**
  - → https://hpc-wiki.info ← general concepts
  - → https://help.itc.rwth-aachen.de/service/rhr4fjjutttf ← RWTH specifics

Summary

- **Alles bleibt beim Neuen…**
  - → Same new, same new…
- **Critical changes:**
  - → LSF → SLURM,
  - → new (versions of) software and default modules (incl. pre-loaded MPI)
- **!!! RECOMPILE YOUR APPLICATION !!!**
- **`$FLAGS_FAST`**

CLAIX18 – Documentation & Support

- **Documentation:**
  - → https://hpc-wiki.info ← general concepts
  - → https://help.itc.rwth-aachen.de/service/rhr4fjjutttf ← RWTH specifics
  - → https://hpc-wiki.info/hpc/Modules ← Module System
  - → https://hpc-wiki.info/hpc/Nodes → RWTH Hardware ← Nodes

- **Support:**
- **Service Desk: servicedesk@itc.rwth-aachen.de**

- **"Please don't shoot at the pianist, he is doing his best."**

Thank for your attention.

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