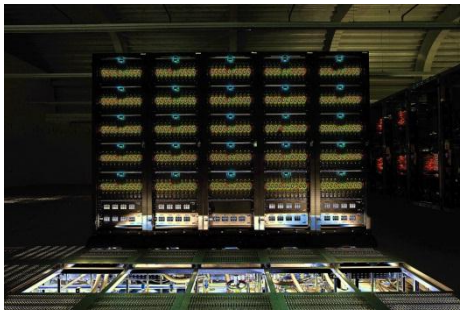
The RWTH Compute Cluster Environment

Introduction



Source: D. Both, Bull GmbH

Tim Cramer

19.03.2012

How to login

Frontends

cluster.rz.RWTH-Aachen.DE	cluster2.rz.RWTH-Aachen.DE
cluster-x.rz.RWTH-Aachen.DE	cluster-x2.rz.RWTH-Aachen.DE
cluster-linux.rz.RWTH-Aachen.DE	cluster-linux-opteron.rz.RWTH-Aachen.DE
cluster-linux-xeon.rz.RWTH-Aachen.DE	cluster-linux-nehalem.rz.RWTH-Aachen.DE

- Use frontends to develop program, compile applications, prepare job scripts or debug programs
- limited CPU time of 20 minutes
- login / SCP File transfer:
  - `$ ssh [-Y] user@cluster.rz.rwth-aachen.de`

    `$ scp [[user@]host1:]file1 [...] [[user@]host2:]file2`

Why to use the batch system?

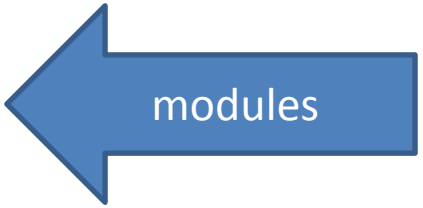
- **Use of backend nodes via our batch system for large calculations**
  - Contra:
    - Jobs sometimes need to wait before they can start
  - Pro:
    - Nodes are not overloaded with too many jobs
    - Jobs with long runtime can be executed
    - Systems are also used at night and on the
    - Fair share of the resources for all users
    - The only possibilty to handle such a big amount of compute nodes
- **LSF documentation / example scripts**
  - **https://wiki2.rz.rwth-aachen.de/**
  - **http://www.rz.rwth-aachen.de/hpc/primer**

Module System (1/2)

- **Many compilers, MPIs and ISV software**
- **The module system helps to manage all the packages**
  - List loaded modules
    - `$ module list`
  - List available modules
    - `$ module avail`
  - Load / unload a software
    - `$ module load <modulename>`
    - `$ module unload <modulename>`
  - Exchange a module (Some modules depend on each other)
    - `$ module switch <oldmodule> <newmodule>`
  - Reload all modules (May fix your environment, especially with a NX session)
    - `$ module reload`
  - Find out in which category a module is:
    - `$ module apropos <modulename>`

Module System (2/2)

```
$ module avail
------------ /usr/local_rwth/modules/modulefiles/linux/x86-64/DEVELOP ------------
acumem/1.0.6                    java/1.5(default)
acumem/2009.2(default)          java/1.6
gcc/3.4                         openmpi/1.3.3(default)
gcc/4.2                         parawise/3.1(default)
gcc/4.3                         pgi/10.0
gcc/4.4                         pgi/10.1
gcc/system-default(default)     pgi/10.2
intel/11.0                      pgi/10.3(default)
intel/11.1(default)             pgi/7.1
intel/11.1.056                  pgi/8.0
intel/11.1.059                  python/2.4.2
...                                     ...
------------ /usr/local_rwth/modules/modulefiles/GLOBAL ------------
BETA      DEPRECATED GRAPHICS   MATH      TECHNICS   VIHPS
CHEMISTRY  DEVELOP    LIBRARIES  MISC      UNITE
```



Environment Variable

RWTH AACHEN UNIVERSITY

- **For convenience we provide several environment variables**
  - Set by the module system

Variable	Function
$FC, $CC, $CXX	Compiler
$FLAGS_DEBUG	Compiler option to enable debug information.
$FLAGS_FAST	Enables several compiler optimization flags.
$FLAGS_OPENMP	Enables OpenMP support.
$MPIFC, $MPICC, $MPI	MPI compiler wrapper.
$MPIEXEC	The MPI command used to start MPI applications.
$FLAGS_MPI_BATCH	MPI options necessary for executing in batch mode.
$FLAGS_OPENMP	Compiler option to enable OpenMP support.
$OMP_NUM_THREADS	Sets the number of threads for OpenMP applications.
$FLAGS_MATH_INCLUDE	Include flags for mathematical libraries (e.g. Intel MKL)
$FLAGS_MATH_LINKER	Linker flags for mathematical libraries (e.g. Intel MKL)

RWTH AACHEN UNIVERSITY

We provide laptops and some exercises

- Login with your PC Pool Account (it‘s not the same as for the cluster)
- If you don’t have an account:
  Use the local user “hpclab”
- Use PUTTY or the NX Client to login to the cluster (now with HPC Account)
- Feel free to **ask questions** or prepare your own job scripts

Source: D. Both, Bull GmbH