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Betriebseinheit für
technisch-wissenschaftliche
Infrastruktur

Introduction to High-Performance Computing

Session 03
HPC Environment, Modules, Compiler, and Toolchains

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HPC User Environment

the user environment on a HPC cluster consists of:

- the operating system (OS)
  - e.g. RHEL Linux (all HPC systems in top500 have Linux-like OS)
  - basic functionality (login, create and edit files, …)
- data storage
  - one or more file systems
  - temporary, short and long term storage
- software
  - scientific applications
  - libraries
  - compiler
- job scheduler

File Systems

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HPC File Systems

- typically on a HPC system different file systems are available

  http://www.fz-juelich.de/ias/jsc/EN/Expertise/Datamanagement/JUDAC/Filesystems/filesystems_node.html

Name	Description	Features
`$TMPDIR` or `/scratch`	temporary storage provided on a per job basis, deleted after job often local disk or similar	very fast I/O, up to a few TB, no backup
`$WORK`	temporary storage for job data, maybe kept after job, typically parallel file system attached to interconnect	fast, parallel I/O, up to PB, no backup
`$DATA`	mid-term storage for job output, parallel filesystem or NFS	up to PB, maybe with backup
`$HOME`	NFS storage, long term and secure, for program codes, initial conditions	few 100GB, full backup, snapshots
`$ARCH`	permanent archive, storage for finished projects, tape library	few PB, possible slow read

File Systems

http://wiki.hpcuser.uni-oldenburg.de/index.php?title=File_system_and_Data_Management

- central Enterprise Spectrum Scale storage (ESS)
  - used for home, data, group and offsite directories
  - NFS mounted over 2x 10Gb Ethernet
  - full backup and snapshot functionality
  - can be mounted on local workstation using SMB
- shared parallel storage (GPFS)
  - used work directory only
  - data transfer over FDR Infiniband
  - no backup
  - can also be mounted on local workstation using SMB
- local disks or SSDs for scratch
  - CARL compute nodes have local storage (1-2TB per node)
  - EDDY compute nodes have 1GB RAM disk (for compatibility)
  - usable during job run time

Directory Structure

- on every filesystem (**`$HOME`**, **`$DATA`**, **`$WORK`**) users will have their own subdirectory
  - e.g. for **`$HOME`**

```
drwx------    abcd1234   agsomegroup   /user/abcd1234
```

  - default permissions prevent other users from seeing the contents of their directory
  - user can give permissions to others to access files or subdirectory as needed (user‘s responsibility)
  - file and directory access can be based on primary (the working group) and secondary (e.g. the institute) Unix groups
  - recommendation: keep access restricted on **`$HOME`** and if needed share files/dirs. on **`$DATA`** or **`$WORK`**

https://wiki.hpcuser.uni-oldenburg.de/index.php?title=File_system_and_Data_Management#Managing_access_rights_of_your_folders

File Systems

File System	Env. Variable	Path	Used for
Home	`$HOME`	`/user/abcd1234`	critical data that cannot easily be reproduced (program codes, initial conditions, results from data analysis)
Data	`$DATA`	`/nfs/data/abcd1234`	important data from simulations for on-going analysis and mid term (project duration) storage
Work	`$WORK`	`/gss/work/abcd1234`	data storage for simulation runtime, pre- and post-processing, short term (weeks) storage
Scratch	`$TMPDIR`	`/scratch/<job-dir>`	temporary data storage during job runtime
Offsite	`$OFFSITE`	`/nfs/offsite/user/abcd1234`	long term storage for inactive data, only available on login nodes

- `$HOME`, `$DATA` and `$OFFSITE` have backup for disaster recovery and daily snapshots for file recovery
- quotas are use on all file systems to limit the amount of data that can be stored by a user

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Quotas

https://wiki.hpcuser.uni-oldenburg.de/index.php?title=File_system_and_Data_Management#Quotas

- on every file system default quotas are in place
  - `$HOME`, `$DATA` and `$OFFSITE` have 1TB, 20TB and 12.5TB, respectively
  - the number of files is also limited (`$HOME`: 500k, `$DATA`: 1M, `$OFFSITE`: 250k)
  - `$WORK` has 25TB and no limit on number of files
  - maybe increased upon request (if resources are available)
- soft and hard quotas
  - in addition to the soft limit above, there is also a higher hard limit
  - if usage is over soft quota a grace period of 30 days is triggered
  - after grace period no data can be written to the affected directory by user

➔ check your usage with **`lastquota`** and clean up your data on work regularly

Group Directories

- group directories are available upon request
  - storage on the ESS
  - can be mounted via SMB (only version 2 or better)
  - path: **`$GROUP`** or **`/nfs/group/agyourgroup`**
  - should be used for data shared among members of the same group, in particular to avoid multiple copies of the same file
  - group leader is owner of directory
  - default rights are set so that anyone in group can read and write to group directory

File System Shares

https://wiki.hpcuser.uni-oldenburg.de/index.php?title=Local_Mounting_of_File_Systems

- you can mount your **`$HOME`**, **`$DATA`** and **`$WORK`** as well as **`$OFFSITE`** and **`$GROUP`** directories on your local workstation
- server address for mounting are

$HOME	**//smb.uni-oldenburg.de/hpc_home**
$DATA	**//smb.uni-oldenburg.de/hpc_data**
$WORK	**//smb.hpc.uni-oldenburg.de/hpc_work**
$OFFSITE	**//smb.uni-oldenburg.de/hpc_offsite**
$GROUP	**//smb.uni-oldenburg.de/<groupname>**

  – for Windows connect a network drive (and replace “/” with “\”)
  – for Linux add information in **`/etc/fstab`**

File System Use

- applications with high I/O demands can put a lot of stress on the used file system
- I/O-performance depends on the I/O profile
  - I/O with few but large files is better than many small files
  - sequential I/O is better than random access
- pick the right file system for your I/O profile
  - local disks or SSDs are best for I/O with small block sizes
  - parallel files system (`$WORK`) is best for large files and parallel I/O
  - `$HOME` and `$DATA` (and all NFS mounted directories) should be avoided for I/O at runtime

simple I/O performance tests can be done with **`dd`**

https://www.thomas-krenn.com/de/wiki/Linux_I/O_Performance_Tests_mit_dd

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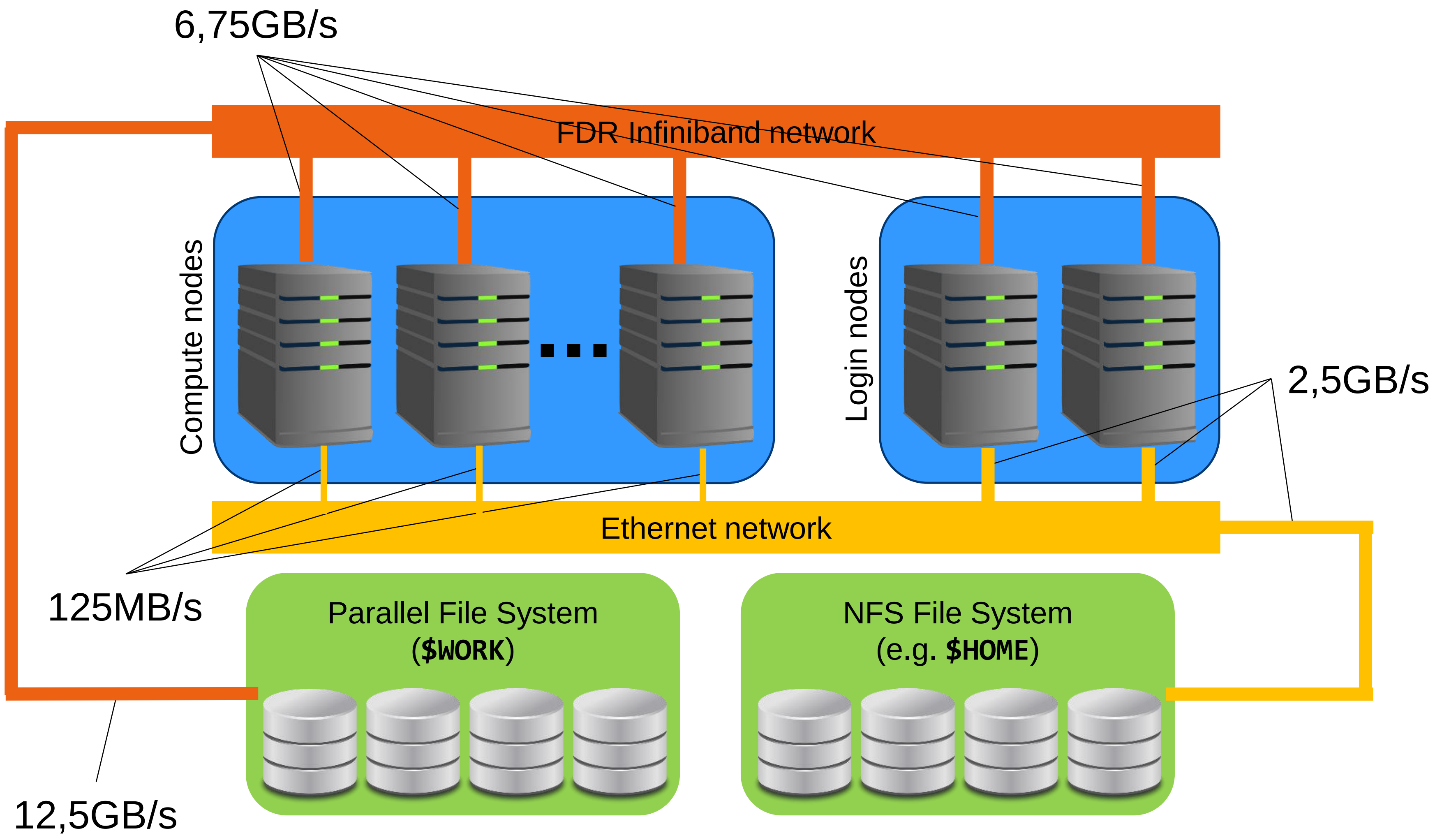
File System Bandwidth Limits



Note, that the maximum bandwidth is shared for the whole node/cluster

Best Practices for File System Use

- if your job is doing heavy I/O use **`$WORK`** or **`$TMPDIR`**
  - I/O bandwidth to **`$WORK`** is more than 10GB/s (shared for the whole cluster), compared to 125MB/s at most to **`$HOME`** and **`$DATA`**
  - try to use parallel I/O and avoid using many small files
  - **`$TMPDIR`** is best for small files and random access (in particular in the partitions **`mpcb.p`** and **`mpcp.p`**)
- keep your data on **`$WORK`** while it is being processed
  - data that is currently not needed can be moved to **`$DATA`**
  - consider creating compressed archives and organise your data
  - only keep important data and delete as much as possible when a project is finished
  - use **`$GROUP`** if you frequently need to share data within your group to avoid unneccessary copies of data

Best Practices for File System Use

- user-specific directories will be deleted when the account expires
  - files are only kept for 180 days
  - make sure you copy files you want to keep elsewhere (e.g. a group directory)
- reducing your file system footprint
  - the size but also the number of files count (especially if there is a backup)
  - clean up your directories whenever you finish a project or no longer need some files
  - files you want to keep can be packed in an archive file

```
$ tar cf project.tar project/      # create tar-file
                                   # to reduce number of files
$ zstd --rm project.tar            # compress files for smaller size
```

Final Remarks File Systems

- setting file permissions
  - add execute (**`x`**) permission to directories to allow **`cd`**
  - add read (**`r`**) permission to directories to allow **`ls`**
  - avoid adding write (**`w`**) permission for group or others on directories (you cannot change ownership of files)
- checking quotas
  - use the **`lastquota`** command to find out how much diskspace your are using
  - also weekly e-mails to all users

What will (not) change with the next cluster?

- every user will get a new **`$HOME`** and **`$WORK`**
  - old directories will be available for migration period
- both **`$HOME`** and **`$WORK`** will be on a new parallel file system
  - faster file I/O over Infiniband
  - snapshots and backup for **`$HOME`** but not for **`$WORK`**
- **`$DATA`** and **`$OFFISTE`** will be available as before
  - also group directories **`$GROUP`**
- no local HDDs or SSDs anymore
  - a **`$TMPDIR`** will be provided on a fast NVME-server
- I/O performance will increase for all directories
  - probably a factor of two

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Software and Modules

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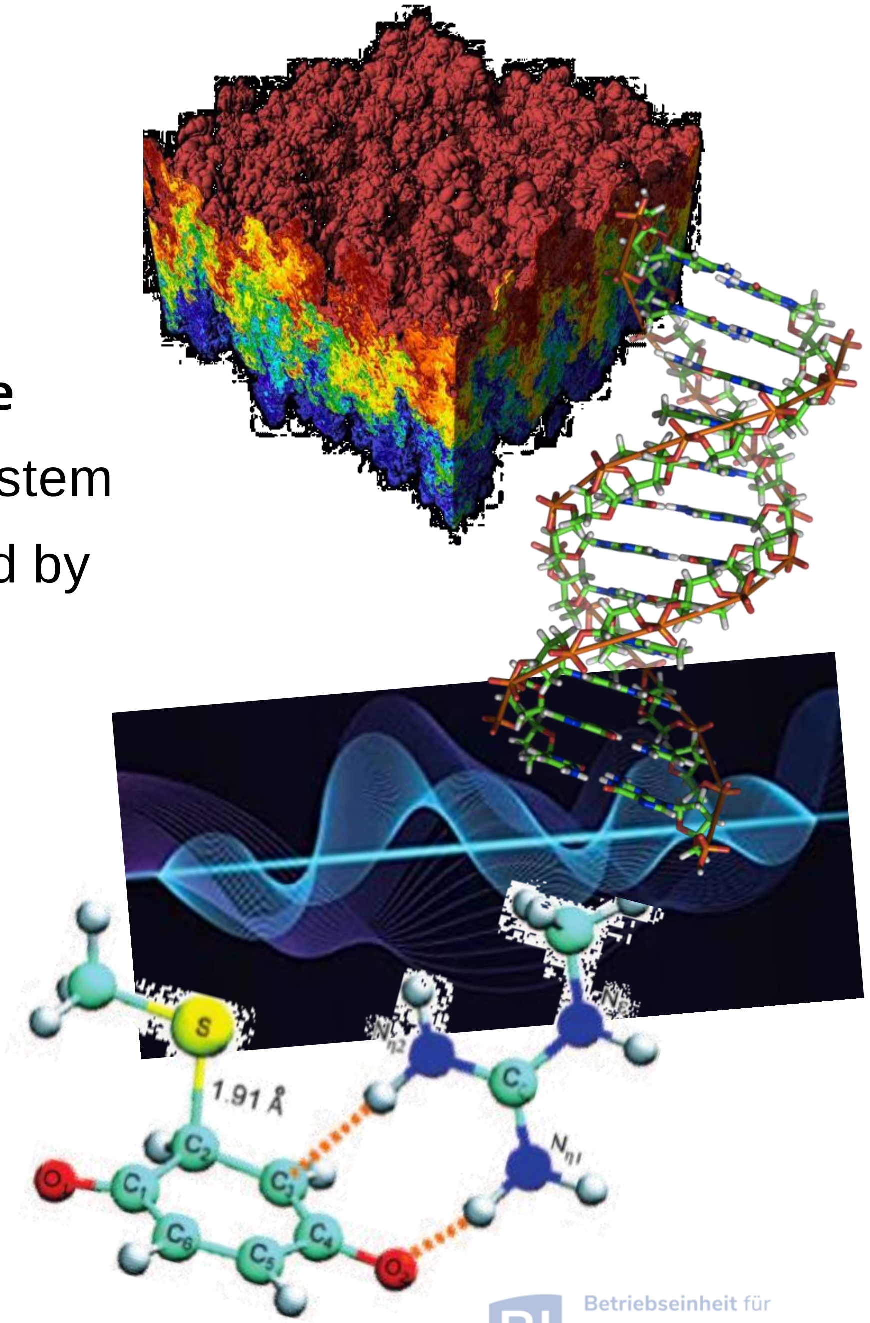
Using Installed Software

- software is installed centrally on the cluster
  - main path: **`/cm/shared/uniol/software`**
  - installed applications are optimized for system
  - can be used by all users (unless restricted by license terms)
  - own software can be installed, too, e.g. in **`$HOME`**
- installed software includes
  - compilers
  - libraries (MPI, numerical libraries,…)
  - scientific application
  - overview and help in the HPC wiki



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Environment Modules

- Linux settings are defined by environment variables

```
$ echo $HOME                    # home directory
/user/abcd1234
$ echo $PATH                    # where to look for applications
/cm/shared/apps/slurm/current/sbin:/cm/shared/apps/slurm/current/bin:/us
r/local/bin:/usr/bin:/usr/local/sbin:/usr/sbin:/opt/ibutils/bin
$ env                           # full list
HOSTNAME=hpcl002
TERM=xterm
. . .
```

  – applications require correct settings of environment variables (e.g. the **`PATH`**-variable)
  – environment modules are used to make predefined changes to the environment using the **`module`**-command

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The **`module`**-command

- the environment settings for installed applications are managed using modules
  - example: loading a module for **`SAMtools`**

```
$ module load SAMtools/1.9-GCC-8.3.0
$ samtools --version
samtools 1.9
Using htslib 1.9
Copyright (C) 2018 Genome Research Ltd.
$ which samtools
/cm/shared/uniol/software/8.3/SAMtools/1.9-GCC-8.3.0/bin/samtools
[abcd1234@carl]$ echo $PATH
/cm/shared/uniol/software/8.3/SAMtools/1.9-GCC-8.3.0/bin:/cm/shared/...
```

  - after the module is loaded, the application can be used
  - the variable **`$PATH`** has been modified (among other things)

The **`module`**-command

- available modules can be displayed and searched for
  - displaying all modules (also work with **`spider`**)

```
$ module available
----------------- /cm/shared/uniol/modules/8.3/bio --------------------
  . . .
  SAMtools/0.1.19-foss-2019b      SAMtools/1.9-GCC-8.3.0  (L,D)
  . . .
```

  - very long list of available modules
  - modules can be highlighted with **`(L)`** for loaded and/or with **`(D)`** for default
  - add application name to get shorter list
- show currently loaded modules

```
$ module list
Currently Loaded Modules:
  1) slurm/current  2) hpc-env/8.3  3) GCCcore/8.3.0  ...
```

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The **module**-command

https://wiki.hpcuser.uni-oldenburg.de/index.php?title=User_environment_-_The_usage_of_module_2016

- find modules

```
$ module available [module-name]
$ module spider [module-name]
```

  - list all modules [with given module name]
  - both commands are case-insensitive and understand regular expressions when using option **-r**

- load/unload

```
$ module load <module-name>
$ module remove <module-name>
```

  - to return to a default state

```
$ module restore
```

- information about modules

```
$ module list
$ module help <module-name>
$ module spider <module-name>
```

The **module**-command

- you can define, save, and restore your own module collections

```
$ module load SAMtools Python      # to load some modules
$ module save mycollection         # to save currently loaded modules
Saved current collection of modules to: "mycollection"
$ module purge                     # unload all modules
$ module restore mycollection      # restore previously saved collection
Restoring modules from user's mycollection
$ module list
Currently Loaded Modules:
  1) slurm/current                 7) ncurses/6.1-GCCcore-8.3.0      13) Tcl/8.6.9-GCCcore-8.3.0
  2) hpc-env/8.3                   8) bzip2/1.0.8-GCCcore-8.3.0      14) SQLite/3.29.0-GCCcore-8.3.0
  3) GCCcore/8.3.0                 9) XZ/5.2.4-GCCcore-8.3.0         15) GMP/6.1.2-GCCcore-8.3.0
  4) zlib/1.2.11-GCCcore-8.3.0    10) cURL/7.66.0-GCCcore-8.3.0      16) libffi/3.2.1-GCCcore-8.3.0
  5) binutils/2.32-GCCcore-8.3.0  11) SAMtools/1.9-GCC-8.3.0         17) OpenSSL/1.1.1d-GCCcore-8.3.0
  6) GCC/8.3.0                    12) libreadline/8.0-GCCcore-8.3.0  18) Python/3.7.4-GCCcore-8.3.0
```

  – if no name is given for **`save`** or **`restore`**, the collection **`default`** is used

The **ml**-command

- the **module**-command (as well as some subcommands) can be abreviated
  - any command **module subcmd** can be replaced with **ml subcmd**
  - the **ml**-command also may have different meanings depending on the context

```
$ ml                                        # same as module list
Currently Loaded Modules:
  1) slurm/current   2) hpc-env/8.3
$ ml av                                     # same as module available
. . .
------------------- /cm/shared/uniol/modules/core ---------------------
   slurm/current (L)      hpc-env/8.3     (L)
. . .
$ ml SAMtools                               # same as module load SAMtools
```

hpc-env Modules

- in the module core-section you can find a number of **hpc-env** modules

```
$ module available
------------ /cm/shared/uniol/modules/core ---------------
  hpc-env/6.4   (D)    hpc-env/8.3       (L)
  hpc-env/8.1          hpc-uniol-env
  hpc-env/8.2          hpc-uniol-new-env
```

  - these modules provide some basic settings (e.g. **$DATA**, loading the Slurm module) and make a specific module stack available
  - the version corresponds to a specific **GCC** version and all modules in the stack are based on this **GCC** version
  - the non-version modules are older and not based on a specific **GCC**
  - most software is installed in **hpc-uniol-env**, **hpc-env/6.4** and **hpc-env/8.3**
  - if you login you will find **hpc-uniol-env** loaded, this can be changed (e.g. with **module save**)
  - only one **hpc-env** module can be loaded at any time

Modules

- why use modules
  - modules allows multiple versions of the same application to be installed
  - modules change all the environment settings as needed
  - modules know about dependencies and conflicts

- modules and jobs
  - modules have to be loaded within a job script (as needed)
  - modules loaded when the job is submitted are remembered by SLURM (but you may submit a job later again with different modules loaded)

Compiler, Libraries and Toolchains

Compiler

- different compilers available (from vendors and also open-source)

```
---------- /cm/shared/uniol/modules/compiler -----------
   CUDA-Toolkit/8.0.44              NAG_Fortran/5.2
   GCC/4.9.4-2.25                   PGI/12.10
   GCC/5.4.0-2.26                   PGI/15.10
   GCC/6.2.0-2.27          (D)      PGI/16.10       (D)
   LLVM/3.8.1-goolf-5.2.01          icc/2016.3.210
   LLVM/3.8.1-intel-2016b           ifort/2016.3.210
   LLVM/3.9.0-intel-2016b  (D)
```

   – Intel compiler usally gives very good performance (icc and ifort)
   – using different compilers may help to better understand your code
   – some compiler support special hardware (e.g. GPUs by PGI)
   – always load one compiler (don‘t use OS GCC)

Example: **`RandomWalk.cpp`**

- download the code **`RandomWalk.cpp`** (and the other RandomWalk files) from Stud.IP
  - the code simulates a 2d random walk, each step of lenght one in random direction, prints out distance from start after N steps
  - expected distance is SQRT(N)
  - compile with GCC or ICS

```
$ gcc RandomWalk.cpp –o RandomWalk
$ ipcp RandomWalk.cpp –o RandomWalk
```

  - run with one argument for seed, e.g.

```
$ ./RandomWalk 12345
```

  - timing with

```
$ time ./RandomWalk 12345
```

Libraries

- libraries are available as modules
  - numerical libraries provide optimized solutions of general problems

```
------------ /cm/shared/uniol/modules/numlib -------------
   ATLAS/3.10.2                 Octave/4.0.3
   Armadillo/7.500.1            OpenBLAS/0.2.19
   CLHEP/2.2.0.4-intel-2016b    Qhull/2015.2
   Eigen/3.2.9                  ScaLAPACK/2.0.2
   FFTW/3.3.5-gompi-5.2.01      SuiteSparse/4.5.3
   FIAT/1.6.0-intel-2016b       cuDNN/5.1-CUDA-8.0.44
   GMP/6.1.1   (D)              cvx/2.1
   GSL/2.1                      imkl/11.3.3.210
   Hypre/2.11.1                 leda/6.3
   LinBox/1.4.0                 maple/18
   MATLAB/2016b                 maple/2016            (D)
   MPFR/3.1.4                   stata/13
   NTL/9.8.1
```

Example: Matrix-Matrix Multiplication

- basic linear algebra is available in many different numerical libraries
  - OpenBLAS, Lapack, MKL, …
  - Basic Linear Algebra Subprograms (BLAS) contain e.g. a General Matrix Multiplication (gemm) of the form:
$$C = \alpha A \cdot B + \beta C$$
  - original version written in Fortran
  - used in the **`mm.cpp`** example (**`cblas_dgemm`** is the C-interface for double precision **`gemm`**)

```
// A, B, and C are objects of class SqMatrix but A[0] etc. are
// pointers to first element in matrix which is what dgemm expects
cblas_dgemm(CblasRowMajor, CblasNoTrans, CblasNoTrans,
            n, n, n, alpha, A[0], n, B[0], n, beta, C[0], n);
```

Toolchains

http://easybuild.readthedocs.io/en/latest/eb_list_toolchains.html

- some modules are called toolchains
  - provide a collection of compiler, MPI, and/or numerical libraries

```
------------- /cm/shared/uniol/modules/toolchain ------------------
 foss/2016b       gompi/5.2.01         iimpi/2013b    intel/2016b (D)
 gimpi/6.2016     gompi/6.2.01 (D)     iimpi/2016b (D)
 gompi/4.1.10     goolf/5.2.01         intel/2013b
```

- examples:
  - foss: free and open-source software, currently GCC, OpenMPI, OpenBLAS, ScaLAPACK, FFTW
  - fosscuda: same as foss with CUDA support
  - gompi: GCC, OpenMPI
  - intel: Intel compilers, MPI, MKL

Example: Matrix-Matrix Multiplication

- the code **`mm.cpp`** uses **`OpenBLAS`** which is included in the **`foss`**-toolchain

```
$ ml restore
Resetting modules to system default
$ make clean
rm mm mm.o
$ make
g++ -O2  -c mm.cpp
mm.cpp:7:19: fatal error: cblas.h: No such file or directory
 #include "cblas.h"
                   ^
compilation terminated.
make: *** [mm.o] Error 1
$ ml foss
$ make
g++ -O2  -c mm.cpp
g++ -O2  -o mm mm.o -lopenblas
```

Example: Matrix-Matrix Multiplication

- alternatively, the code can be compiled with Intel MKL
  - requires some code change (different header file)
  - requires changes to Makefile (different libraries to link)
  - result: code runs faster by 25%

```
$ sacct -j 2591679 -o JobID,JobName,Partition,Elapsed,MaxRSS,State,ExitCode
       JobID    JobName  Partition    Elapsed     MaxRSS      State ExitCode
------------ ---------- ---------- ---------- ---------- ---------- --------
2591679      run_mm.job     carl.p   00:06:21             COMPLETED      0:0
2591679.bat+      batch              00:06:21      7336K  COMPLETED      0:0
2591679.0            mm              00:00:33     37600K  COMPLETED      0:0
2591679.1            mm              00:00:32    113412K  COMPLETED      0:0
2591679.2            mm              00:00:33    412420K  COMPLETED      0:0
2591679.3            mm              00:00:32   1592064K  COMPLETED      0:0
2591679.4            mm              00:04:09   6310656K  COMPLETED      0:0
```

What will (not) change with the new cluster?

- module commands and module usage will not change
  - new versions of **`hpc-env`** modules
- **`foss`**-toolchain will be available in a recent version
  - additional toolchain with AMD compiler (?)
  - is the **`intel`**-toolchain still useful (?)
  - no extra **`*cuda`**-toolchain, instead **`CUDA`** can be loaded additionally

Advanced Job Management

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Running Many Jobs

- you may need to run a program on the HPC cluster many times with different parameters
- example: run program **`isPrime`** several (M) times
  - different input parameter (value to test) every time
  - all input parameters are in file **`parameter.dat`**
- strategies:

– simple approach:	make M copies of job script, modify the input parameter in every file, could be automatized, not recommended
– loop approach:	use a single job script with a loop
– job array approach:	use Slurm's job array functionality

Running Many Jobs: Job Arrays

- job or task arrays are defined by Slurm option

```
$ cat array_job.sh
. . .
### settings for job array
#SBATCH --array 1-10:1%4    # define task array
                            # format range:step%tasklimit
. . .
```

  - range of tasks can be defined as **`from-to:increment`**
  - multiple ranges with comma-separated list
  - limiting the number of parallel tasks is possible with **`%tasklimit`** (when tasks have high resource requirements)

Job Arrays

- the same job script is executed for each task in the array
- additional variable **`SLURM_ARRAY_TASK_ID`** is provided

```
$ cat prime_job.sh
. . .
# get parameter from file for each task
parameter=$(awk "NR==$SLURM_ARRAY_TASK_ID {print \$1}" parameter.dat)
echo -n "Task $SLURM_ARRAY_TASK_ID tested if $parameter is prime? "
./isPrime $parameter
. . .
```

the task-ID can be used

– e.g. to number input or output file

– read specific line from input file (as in the example above)

– computations in bash (limited)

Job Arrays

- job array are a powerful tool for task parallel jobs
  - to be preferred over submitting many individual jobs
  - each tasks in a job array should be sufficiently long (e.g. > 1h), due to the overhead for a single task
- requires some strategy for post-processing
  - often Linux tools can do the trick, more complex tasks may require post-processing script in e.g. Python
- additional environment variables for first and last task
  - however, tasks may not complete in the correct order
  - alternatively job dependencies can be used

awk

http://www.gnu.org/software/gawk/manual/gawk.html

- powerful Linux tool that searches the lines of a file for patterns and performs an action on that line
  - similar tools are **`grep`** (pattern matching) and **`sed`** (streaming edit)
  - works well with data files (tables)
  - uses a **`C`**-like syntax

- example: **`prime.awk`**
  - reads all output files from the job array (using **`cat`** to combine them)
  - counts yes and no answers
  - prints final result

Job Arrays: Do‘s and Don‘ts

- do use job arrays whenever you run many almost identical jobs (e.g. parameter studies)
  - don‘t automatically submit 100s or 1000s of jobs simultaneously
- do limit the number of parallel running tasks if individual jobs require a lot of resources
  - there is a setting `MaxJobsPerAccount=250` limiting the maximum number of running jobs for your group
- don’t parallelize very short jobs in a job array
  - individual tasks should run for minutes at the very least, better for hours
  - group tasks for longer job run time and parallelize for groups
- do test
- don’t run tasks if you do not need to

Running Many Jobs

- you may need to run a program on the HPC cluster many times with different parameters
- example: run program **`isPrime`** several (M) times
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- strategies:

– simple approach:	make M copies of job script, modify the input parameter in every file, could be automatized, not recommended
– loop approach:	use a single job script with a loop
– job array approach:	use Slurm’s job array functionality
– parallel approach:	use the Linux command **`parallel`**

The **`parallel`** Command

https://www.gnu.org/software/parallel/

- the **`parallel`** command is a shell tool for executing command in parallel
  - available on the cluster as module

```
$ module load parallel
```

  - example: run **`RandomWalk_task.sh`** ten times in parallel

```
$ parallel -N 1 -j 4 --joblog parallel.log  ./RandomWalk_task.sh {1} ::: {1..10}
Running RandomWalk with seed 2000 on hpcl001
Seed = 2000
Running RandomWalk with seed 4683 on hpcl001
Seed = 4683
```

The **`parallel`** Command

https://www.gnu.org/software/parallel/

- the parallel command can be used in many different ways
  - in the example

```
$ parallel -N 1 -j 4 --joblog parallel.log ./RandomWalk_task.sh {1} ::: {1..10}
```

  - a range is given with **`::: {1..10}`**, alternatively use **`::: $(seq 10)`**
  - with **`{}`** or **`{n}`** the value of the argument is passed to the task
  - the option **`-N`** defines how many arguments are passed to the task
  - the option **`-j`** defines how many tasks can run in parallel
  - an additional logfile is created with the option **`--joblog <logfile>`**

The use of the parallel command should be cited.

Running Many Jobs

- several approaches can be used to run many tasks on the cluster

loop approach:	single job, post-processing could be included, only serial processing, best used if tasks are short (minutes) and total runtime not too long
job arrays:	single **`sbatch`**, one job per task, parallel processing on available resources, tasks should run >1h, limit maximum number of tasks running, overhead for starting tasks
parallel approach:	single job, distributed resources can be used, better control over used resources, little overhead for starting tasks, scripts can be adapted easily

also see https://wiki.hpcuser.uni-oldenburg.de/index.php?title=How_to_Manage_Many_Jobs

Handling Many Output Files

- jobs or job arrays with many tasks in general also generate many output files
  - may degrade performance, use **`$WORK`** or **`$TMPDIR`**
  - you may hit your file number quota
- if possible try to generate single output file
  - might be difficult at job runtime but can be done afterwards

```
$ tar zcf RandomWalk.data.tar.gz RandomWalk*.data  # create a compressed tar-file
$ rm RandomWalk_*.data                             # delete small files
$ tar -zxOf RandomWalk.data.tar.gz | awk -f RandomWalk.awk | sort -g
#steps  expected        mean            std
10      3.162278        2.089732        1.232151
100     10.000000       9.985299        6.881550
. . .
```

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Job Dependencies

https://wiki.hpcuser.uni-oldenburg.de/index.php?title=How_to_Use_Job_Dependencies

- jobs can have a dependency on another job
  - option: **`--dependency`** or short **`-d`**
  - format: **`--dependency <type>:<jobID>[,<jobID>…]`**
    where **`<type>`** can be one of: **`afterany`**, **`afterok`**, **`afternotok`**
- a job with a dependency will not start until the predecessors have completed with the demanded status
  - careful: make sure exit status is correct for your needs
  - additional type **`after:`** jobs starts once predecessors have started
- a special dependency type is **`singleton`**
  - all jobs with the same job name and from the same user have to complete first, can be used to collect results

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Exercises

Exercises

1. Try to compile and run the **`mm`**-code
   - Try to use different toolchains
2. Try to run a job script for an application
   - See next slide for specific example Orca
3. Try to run and compile the **`RandomWalk`**-code
   - Try different compilers
   - Run multiple times as job array
   - Run multiple time using the Linux **`parallel`** command

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Example: ORCA Job

- examples for using installed software on the cluster can be found in the HPC wiki
  - e.g. ORCA (chemistry) http://wiki.hpcuser.uni-oldenburg.de/index.php?title=ORCA_2016
  - download the files for serial runs and submit job
  - use ORCA 3.0.3

  - the job script is rather complex
    - module is loaded
    - files are copied to $TMPDIR
    - application is started from $TMPDIR
    - output is copied to $SLURM_SUBMIT_DIR

Example: Many Random Walks

- task: run RandomWalk several (M=10) times to get the average distance after N steps from multiple runs
  - different seed every time, provided in a file
  - write job script run as one or more SLURM jobs

  - think how to analyse data from M completed runs
    - how to combine the output of M tasks
    - maybe with awk script?