Practical Example: High Performance Computing

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RWTH Compute Cluster

- High-Performance-Computing infrastructure

- Linux-based

- Highly paralellizable

- All RWTH affiliates are granted access, but with limited resource allocation

- More information on the following link.

RWTH Selfservice

- Use Selfservice (https://idm.rwth-aachen.de/selfservice/) to manage university accounts and create HPC-account to use the cluster

- Account and Passwords
  - Account Overview (to check current accounts)

Service/Account	Username	Status	Action
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- Create Account (to set up a new one)

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SSH and Cluster Login

- Use established *Secure Shell Protocol (**ssh**)* connection to log in to the front-end cluster nodes with your username and password

- $ ssh <username>@<server-address>

SSH and Cluster Login (subject to change*)

Server-name	OS	Purpose
login18-N.hpc.itc.rwth-aachen.de	Rocky Linux 8	Front-End Dialogue System CLAIX2018 N={1,2,3}
login18-4.hpc.itc.rwth-aachen.de	CentOS 7	Front-End Dialogue System CLAIX2018
login.hpc.itc.rwth-aachen.de	CentOS 7	Front-End Dialogue System CLAIX2016
login18-x-N.hpc.itc.rwth-aachen.de	Rocky Linux 8	Remote Desktop sessions N = {1,2}
login18-g-N.hpc.itc.rwth-aachen.de	Rocky Linux 8	GPU-System N = {1,2}
login-g.hpc.itc.rwth-aachen.de	CentOS 7	GPU-System (2016)
login18-t.hpc.itc-rwth-aachen.de	Rocky Linux 8	Tuning processes
login-knl.hpc.itc.rwth-aachen.de	CentOS 7	KNL (highly parallelizable)
lect.hpc.itc.rwth-aachen.de	Rocky Linux 8	Dedicated to lectures

SSH and Cluster Login

- Use established *Secure Shell Protocol (**ssh**)* connection to log in to the front-end cluster nodes with your username and password

- $ ssh <username>@<server-address>

- In the case of the RWTH cluster:

- $ ssh <TIM>@login18-N.hpc.itc.rwth-aachen.de

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SSH and Cluster Login

- Special nodes for intensive I/O operations

copy18-1.hpc.itc.rwth-aachen.de	2 x 40 Gbit/s
copy18-2.hpc.itc.rwth-aachen.de	2 x 40 Gbit/s
copy.hpc.itc.rwth-aachen.de	2 x 10 Gbit/s

- Use these nodes if you need to transfer large files

Cluster Available File Systems

Name	Path	Backup	Quota (file)	Quota (#files)
$HOME	/home/<TIM-Kennung>	yes	150 GB	-
$WORK	/work/<TIM-Kennung>	no	250 GB	-
$HPCWORK	/hpcwork/<TIM-Kennung>	no	1000 GB	50000
$TMP	*Local Ext4/XFS storage*	no	-	-
$BEEOND	*BeeGFS On Demand*	no	-	-

Source code
Configuration files

Output files
Working data

IO intensive job,
large files

Cluster - mount drive

- Use *sshfs* to mount remote directory to local machine:

  - $ sshfs <TIM>@copy18-1.hpc.itc.rwth-aachen.de:<Path> <local Path>

- Unmount with:

  - $ sudo umount -l <local Path>

- Access to cluster only from eduroam or through RWTH VPN

  - https://help.itc.rwth-aachen.de/en/service/vbf6fx0gom76/article/6a2cfd0933604cd28eaaa69194ff8d16/

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Cluster - Batch Jobs

- Job handling system - SLURM

- SBATCH [option] command [arguments]

- Slots

Parameter	Function
-c, --cpus-per-task <numcpus>	Number of threads/processes for an OpenMP/Hybrid script
-n, --ntasks <numtasks> --ntasks-per-node <numtasks>	Number of threads/processes for an MPI job
-N, --nodes <numnodes>	Number of nodes/hosts for the job

- List of slurm commands:

  - https://help.itc.rwth-aachen.de/en/service/rhr4fjjutttf/article/3d20a87835db4569ad9094d91874e2b4/

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Cluster - Batch Jobs

- Further job parameters

Parameter	Function
-J --job-name=<jobname>	A name for the current job
--mem-per-cpu=<size>	Required RAM per allocated CPU
-o, --output=<filename>	Name for a report file, containing the standard output of the job
-t, --time=d-hh:mm:ss	Time for job execution, after this time the job is killed
-A, --account=<project>	Submit a job for a specific project
--gres=gpu:<type>:2	Requesting two GPUs per node

- Batch documentation - https://slurm.schedmd.com/sbatch.html

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Cluster - Batch Jobs

- **sbatch** job.sh - sends job, declared in job.sh, to the scheduler

- After defining the slurm parameters, don't forget to write the script you want to execute

- You job might need to load some modules, update environmental variables or activate condo environments.
  - **module** load Python/3.9.6
  - **module** avail # Lists all available modules
  - **export PATH**=~/.local/bin:$PATH
  - **conda activate myenv**

Cluster - Example Scripts

```bash
#!/bin/bash

### Job name
#SBATCH --job-name=MYJOB

### File for the output
#SBATCH --output=MYJOB_OUTPUT

### Time your job needs to execute, e. g. 15 min 30 sec
#SBATCH --time=00:15:30

### Memory your job needs per node, e. g. 1 GB
#SBATCH --mem=1G

### The last part consists of regular shell commands:
### Change to working directory
cd /home/usr/workingdirectory

### Execute your application
myapp.exe
```

Cluster - Monitor Jobs and Resources

- Use **squeue** to monitor current jobs in progress:
    - squeue -u <TIM> # to only view your jobs

- Use **scancel** to stop current jobs from executing
    - scancel -u <TIM> # cancels all your jobs
    - scancel -n <JOBID> # cancels job with ID=JOBID

- Use **quota** to see how much space you're occupying

- Use **r_wlm_usage -q** to view your accounting information

- More info:
    - https://help.itc.rwth-aachen.de/service/rhr4fjjutttf/article/13ace46cfbb84e92a64c1361e0e4c104/

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Cluster - GPU Nodes

- Login to a GPU node by:
  - **ssh** <TIM>@login18-g-1.hpc.itc.rwth-aachen.de

- See GPU usage with **nvidia-smi**

```
Tue May  7 17:24:20 2019
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 418.43       Driver Version: 418.43       CUDA Version: 10.1     |
|-------------------------------+----------------------+----------------------+
| GPU  Name        Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf  Pwr:Usage/Cap|         Memory-Usage | GPU-Util  Compute M. |
|===============================+======================+======================|
|   0  Tesla V100-SXM2...  Off  | 00000000:62:00.0 Off |                    0 |
| N/A   42C    P0    54W / 300W |      0MiB / 16130MiB |      0%   E. Process |
+-------------------------------+----------------------+----------------------+
|   1  Tesla V100-SXM2...  Off  | 00000000:89:00.0 Off |                    0 |
| N/A   42C    P0    54W / 300W |      0MiB / 16130MiB |      0%   E. Process |
+-------------------------------+----------------------+----------------------+

+-----------------------------------------------------------------------------+
| Processes:                                                       GPU Memory |
|  GPU       PID   Type   Process name                             Usage      |
|=============================================================================|
|  No running processes found                                                 |
+-----------------------------------------------------------------------------+
```

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+-------------------------------+----------------------+----------------------+

+-----------------------------------------------------------------------------+
| Processes:                                                       GPU Memory |
|  GPU       PID   Type   Process name                             Usage      |
|=============================================================================|
|  No running processes found                                                 |
+-----------------------------------------------------------------------------+
```

GPU-id
and type

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+-------------------------------+----------------------+----------------------+
|   1  Tesla V100-SXM2...  Off  | 00000000:89:00.0 Off |                    0 |
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+-------------------------------+----------------------+----------------------+

+-----------------------------------------------------------------------------+
| Processes:                                                       GPU Memory |
|  GPU       PID   Type   Process name                             Usage      |
|=============================================================================|
|  No running processes found                                                 |
+-----------------------------------------------------------------------------+
```

GPU-id
and type

GPU memory

Cluster - GPU Nodes

- Login to a GPU node by:
  - **ssh** <TIM>@login18-g-1.hpc.itc.rwth-aachen.de

- See GPU usage with **nvidia-smi**

Compute model: 1 person

```
Tue May  7 17:24:20 2019
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 418.43       Driver Version: 418.43       CUDA Version: 10.1      |
|-------------------------------+----------------------+----------------------+
| GPU  Name        Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf  Pwr:Usage/Cap|         Memory-Usage | GPU-Util  Compute M. |
|===============================+======================+======================|
|   0  Tesla V100-SXM2...  Off  | 00000000:62:00.0 Off |                    0 |
| N/A   42C    P0    54W / 300W |      0MiB / 16130MiB |      0%   E. Process  |
+-------------------------------+----------------------+----------------------+
|   1  Tesla V100-SXM2...  Off  | 00000000:89:00.0 Off |                    0 |
| N/A   42C    P0    54W / 300W |      0MiB / 16130MiB |      0%   E. Process  |
+-------------------------------+----------------------+----------------------+

+-----------------------------------------------------------------------------+
| Processes:                                                       GPU Memory |
|  GPU       PID   Type   Process name                             Usage      |
|=============================================================================|
|  No running processes found                                                 |
+-----------------------------------------------------------------------------+
```

GPU-id
and type

GPU memory

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Cluster - Exercise - GPU with python

- Sing in to the cluster
    - $ **ssh** <TIM>@login18-g-2.hpc.itc.rwth-aachen.de

- Check if you're successfully in the group
    - $ groups #should see lect0094 among others

- Load modules and install some libraries locally
    - $ **module** load Python/3.9.6
    - $ **module** load cuDNN/8.6.0
    - $ **module** load CUDA/11.8
    - $ **export PATH=~/.local/bin:$PATH**
    - $ **pip3** install --user tensorflow pandas scikit-learn
    - $ **pip3 install** --user matplotlib tensorrt numba

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Cluster - Exercise - GPU with python

- Create a new directory and copy the files needed:

    - $ **cd** ~/

    - $ **mkdir** BioInfo

    - $ **rsync** -rp /home/lect0094/sample BioInfo

    - $ **cd** BioInfo/sample

- Edit (**vim**) your email address and submit job (**sbatch** run.sh)

- Check status regularly ($ **squeue** -u <TIM>)

Practical Example: Linux Basics

The Operating System UNIX

- UNIX Development
  - 60s: MULTICS: MULTiplexed Informaion and Computing Service
  - Developed by MIT, Bell Labs and General Electrics
  - Written in Programming Language 1 (PL1) and Assembly

  - Thompson and Ritchie later create UNIX, written in C

Linux – Basic Commands (Revisit)

- command parameter1 parameter2 *…*

- *man* – **man**ual. Displays manuals for linux packages *(try man man). Displays useful information about how to use the package.*

- *pwd* – **p**rint **w**orking **d**irectory. Displays the current working directory

Linux – Basic Commands (Revisit)

- *ls* – **lis**t. Displays the content of a directory
  - ls -l ~/Pictures

-rw-r--r--	1	martin	martin	101685	Apr 29	13:23	Selection_001.png
-rw-r--r--	1	martin	martin	39835	Apr 29	14:37	Selection_002.png
-rw-r--r--	1	martin	martin	76985	Apr 29	14:48	Selection_003.png
-rw-r--r--	1	martin	martin	27096	May 2	14:04	Selection_004.png
-rw-r--r--	1	martin	martin	62783	May 3	11:58	Selection_005.png
-rw-r--r--	1	martin	martin	65201	May 6	16:11	Selection_006.png
drwxrwxr-x	2	martin	martin	4096	Apr 24	11:41	Temp

- Access rights   Links   Owners/ Groups   Size   Last Modified   Filename

Linux – Basic Commands (Revisit)

- *ls* – **lis**t. Displays the content of a directory

  -rw-r--r--   1   martin   martin   101685   Apr 29   13:23   Selection_001.png

  - Access rights:
    - Type: (**d**)irectory, (**l**)ink, (**-**) a file
    - Rights: (**r**)ead, (**w**)rite, e(**x**)ecute
    - Sequence: *user group anybody*

  - Owner/Group:
    - Owner – first column: *martin*
    - Group – second column: *martin*

- Either can be changed with *chmod* and *chown/chgrp* respectively
- Run executable with full path or from directory with "*./file*"

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Linux – Basic Commands (Revisit)

- *cd* – **c**hange **d**irectory. Switches to a new directory, supplied as a parameter

- *mkdir* – **m**a**k**e **dir**ectory. Creates a new directory

- *rm* – **r**e**m**ove. Removes a specified file or directory ("-r")

- *cp* – **c**o**p**y. Copy a file or directory ("-r")
- *scp* – **s**ecure **c**o**p**y. Copy a file to or from a remote source
- *rsync* – **r**emote **sync**. A fast copying tool. Also works for remote copy

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Linux – Basic Commands (Revisit)

- *ln* – **lin**k. Link a file into a new directory

- *echo* – Prints a string to standard output

- *cat* – con**cat**enate. The content of a file is printed to standard output

- *wc* – **w**ord **c**ount. Counts the number of words, rows ("-l") pr characters ("-c") in a file.

Linux – Basic Commands (Revisit)

- pipe ("|") - connect commands

- output (">") and input ("<") for a specific program. Output can also concatinate to existing content, without deleting (">>")

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Linux – Environment Variables

Variable	Description
PATH	Colon separated list of directories, which will be searched through when entering a name of executable
HOME	The pathname of the home directory.
SHELL	The currently used shell program
USER	The current username

```
$ echo $PATH
/usr/local/sbin

$ export PATH=~/.local/bin:$PATH
$ echo $PATH
/home/martin/.local/bin:/usr/local/sbin
```

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Linux – Vim

- A further development of Vi

- Open-Source editor for use inside the Terminal

- Open file with "$ vim filename"
  - Type "i" for insert (edit)
  - ESC to go back to entry menu
    - :q – exit without saving
    - :wq – save and exit
    - :q! - force exit without saving

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Further Readings

- Linux tutorials:
  - https://www.tutorialspoint.com/unix/
  - https://ryanstutorials.net/linuxtutorial/

- SLURM – batch system
  - https://slurm.schedmd.com/documentation.html
  - https://doc.itc.rwth-aachen.de/display/CC/Using+the+SLURM+Batch+System
  - https://hpc-wiki.info/hpc/SLURM#Jobscript_Examples