Introduction to the MaRC3a Cluster

Hessisches Kompetenzzentrum für Hochleistungsrechnen (HKHLR)

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What is an "HPC Cluster"?

- Historically (1960s-1970s): No "personal computers"
  - University computing center is running "The Computer"
- If you had to calculate something:
  - Apply for compute time, drop off the punch cards with your program
  - Wait a few days
  - Come back to collect your results (as a printout)
- ***The same general concept* - with lots of added automation and convenience features - *is still used on HPC clusters even today!*...**
- ...but the needs of both software and users have changed.

Figure: IBM punchcard sorting machine (MZG A4, own picture)

What is an "HPC Cluster"?

- Today: (Almost) everyone has a personal computer...
- **...but the needs of scientific computing have been growing faster than the abilities of personal hardware!**
  - Simulations in physics, chemistry, or meteorology would take days, weeks or even *years* to complete on a current personal computer
  - Data sets are getting too large to store on local diskspace (several Terabytes or even Petabytes)
  - Memory needs are outscaling personal hardware (up to Terabytes, even more for large calculations)
  - Research might need 1000's or 10,000's of calculations (search over parameter space, trainig DNNs, iterating over large data sets)
    - ⋆ These might be individually small, but *only a few can be run concurrently* on a personal computer

What is an "HPC Cluster"?

- Can't research groups just buy and run hardware by themselves? Possible! But:
  - Quite expensive
    - ★ Single 64-core server with 256 GB RAM: ~5,000-15,000 EUR
    - ★ Single 64-core server with 256 GB RAM + 4 server-grade GPUs: ~30,000-40,000 EUR
  - Needs maintenance
    - ★ Additional personnel for administration, updating, support, repair
  - Idle times still cost money
    - ★ Electrical power, cooling
  - Needs appropriate housing
    - ★ Probably can't be run from "under the desk" (fire regulations, noise, power draw)
- **Conclusion: Not every research group - or even department - can afford to buy, house, run, and maintain their own hardware infrastructure for scientific computations!**

What is an "HPC Cluster"?

- Result: University computing centers have moved from having "The Computer" to having "The Large Bunch Of Interconnected Computers"
  - i.e. a **Cluster**
- Using the cluster (mostly) follows the same paradigm as outlined above...
  - Submit your calculation: Define resource needs and what program(s) to run
  - Wait until your calculation completes
  - Collect the results
- ...but you can submit calculations from anywhere (as long as you can login to the cluster)
- ...and lots of your and other's calculations can run concurrently
- ...and complex hierarchies can be in place to automatically (and -ideally- fairly) decide priority of calculations (i.e. who goes first)

What is "MaRC3a"?

- Further problem: HPC clusters do not count as 'basic infrastructure'
  - Difficult to get funding (except for NHR centers or special national projects)
  - Common solution: Project-related funding by one or several departments / research groups / interdisciplinary projects, with the computing center offering consultation, housing, and support
- In case of MaRC3a: Primary stated purpose is "calculations in the field of bioinformatics, pharmaceutical chemistry and theoretical physics"
- Primary project initiator: SYNMIKRO, with additional contributions from several other departments and research groups
  - Hardware contributors get special "owner" privileges (higher priority, longer max. job runtimes) on their own hardware
  - Agreement: Unused compute power is made available to all members of the university

Figure: MaRC3a hardware overview (diagram by Marcus Lechner)

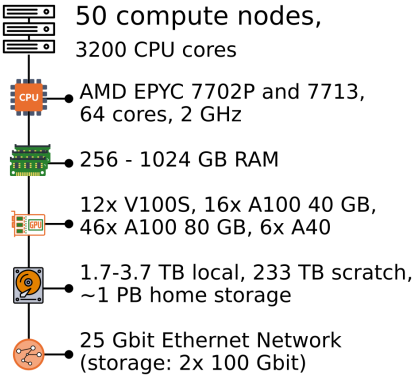
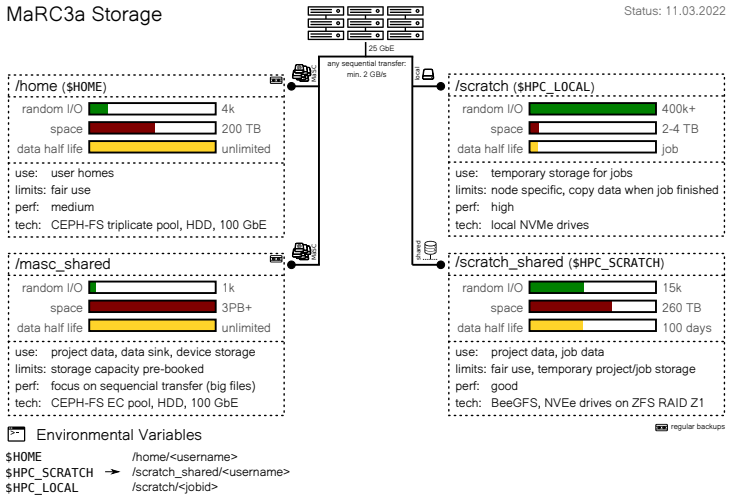


Figure: MaRC3a storage overview (diagram by Marcus Lechner)



Personal requirements

- Must have a university (mail) account (i.e. <user>@staff.uni-marburg.de)
- Leader of research group needs to sign cluster usage agreement
  - Via web form:
    `https://admin.staff.uni-marburg.de/hpc-agreement_en.html`
  - Also names one or more "HPC Managers"
- HPC Managers can then register members of the group for cluster access
  - Also via web form:
    `https://admin.staff.uni-marburg.de/hpc-user_en.html`
  - Need to *register themself as a user* if they want to work on the cluster
- Users need to have their Login Shell set to a value *other than 'rssh'*
  - Web form: `https://admin.staff.uni-marburg.de/aendshell.html`
  - Up to personal preference; default recommendation is 'bash'

Technical requirements

- Software to be used must be able to run on Unix/Linux systems
- Most software (with special exceptions) must be able to run *unattended* and from the commandline, i.e. *no UI*
- Ideally: Software is able to use computational resources *efficiently*
  - Some software packages are already parallelized
    - ⋆ Task: Find out how to explicitly control parallelization
    - ⋆ Task: Find out most efficient parallel settings
  - Some code can be parallelized with additional libraries, e.g. Python or R code
    - ⋆ Task: Find a feasible parallelization solution
  - Some projects just need to perform lots of calculations
    - ⋆ Task: Find a solution to manage job submission and organization of results
    - ⋆ Using builtin functions like job arrays, or scripting, or other additional tools

- Once access has been granted, connecting to the cluster is done via an *SSH client*
- All Linux distributions and current Windows versions (Win 10, Win 11) have a builtin terminal command (`ssh`)
- Alternatively, there are some UI clients:
  - puTTY (lightweight, already installed on many university computers)
    - ⋆ Download available at `https://www.putty.org/`
  - MobaXTerm (all-in-one solution including file browser and XServer for running UI programs on remote machines)
    - ⋆ Download available at `https://mobaxterm.mobatek.net/`

Other than for software on HRZ-installed computers (OPSI), we cannot give support nor warranty for privately installed software. It is *your* responsibility to keep this software up to date and to make sure that it does not pose a security risk!

- **The MaRC3a cluster can only be accessed from the university network!**
  - Computer is at the university and either connected via cable or through eduroam/UMRnet WLAN: No further action required
  - Connecting from home: Only through university VPN! See: `https://www.uni-marburg.de/en/hrz/services/vpn`

Connecting via commandline

- `ssh -X -C -p 223 <username>@marc3.hrz.uni-marburg.de`
- Enter your staff password when prompted

Connecting via UI client

- Hostname: "marc3.hrz.uni-marburg.de", port: 223
- User credentials: Staff username and password

Commandline options

- `scp -P 223 <source> <target>`, remote sources or targets have the format `<user>@<server>:<path>`
- E.g. (with my username "sittr") copying *to* the cluster:
  `scp -P 223 test/some_file.txt sittr@marc3.hrz.uni-marburg.de:/home/sittr/test`
- Copying *from* the cluster:
  `scp -P 223 sittr@marc3.hrz.uni-marburg.de:/home/sittr/test/some_file.txt ./test`
- Copying whole folders: Add '-r' (for "recursive"), i.e.
  `scp -P 223 -r <source> <target>`
- Alternative to SCP: `rsync` (more capabilities, but also more complicated)

GUI options

- SSH clients with builtin file browser (e.g. MobaXTerm)
- Linux file browsers (Nautilus, Nemo, ...) have a "connect to server" function - same settings (hostname, port, user credentials) apply as for connecting via ssh

MaSC storage

- MaRC3 has a direct connection to the MaSC storage cluster
- If you have files in the SMB share on MaSC, these are directly available on MaRC3 under `/masc_shared/<your_group>`
- **Avoid heavy IO directly between MaRC3 jobs and masc_shared!**

Recommended: Enabling passwordless login on MaRC3a

- On your local machine, generate a key pair:

  ```
  ssh-keygen -t ecdsa -b 521
  ```

  Setting a passphrase for the private key is optional but recommended
- Copy the public key to the cluster:

  ```
  scp -P 223 id_ecdsa.pub <user>@marc3.hrz.uni-marburg.de:/home/<user>/.ssh
  ```
- Connect to the cluster (via password) and add the public key to the authorized_keys file:

  ```
  ssh -p 223 <user>@marc3.hrz.uni-marburg.de
  ```

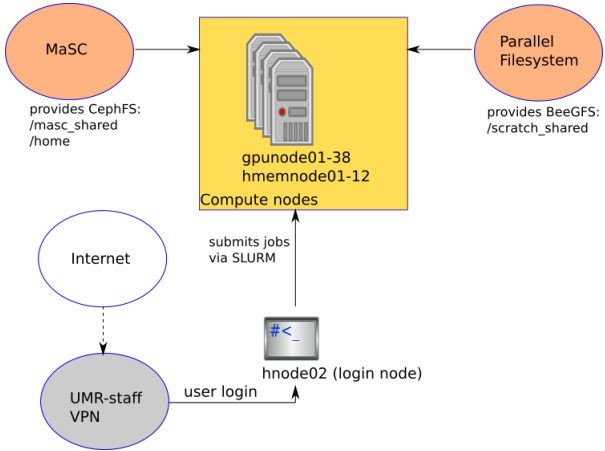
  ```
  cat .ssh/id_ecdsa.pub >> .ssh/authorized_keys
  ```
- Subsequent logins will automatically use the public key instead of the password

- After login, you arrive at the *command prompt*
- The default interface is Linux *bash* (*B*ourne-*A*gain *Sh*ell)
- Everything is done via typing in commands
- We can only give a very limited overview here

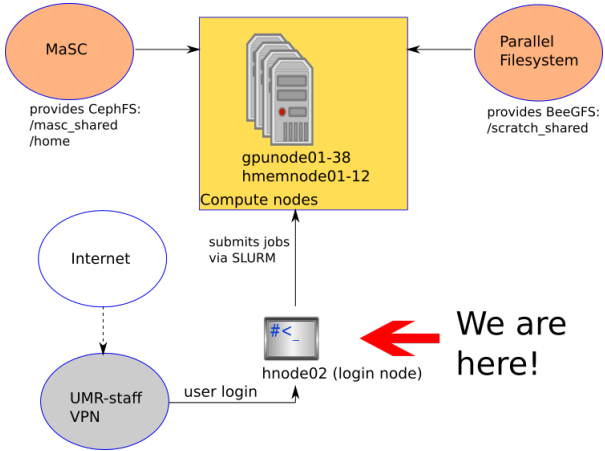
listings/marc3_prompt.sh

```
1 ##########################################################################
2 # Welcome to the MaRC3a system.                                          #
3 ##########################################################################
4 * [...some public messages and general info...]                         *
5 ##########################################################################
6
7 Last login: <date> from <address>
8 [<username>@hnode02 ~]$
```

Cluster Structure

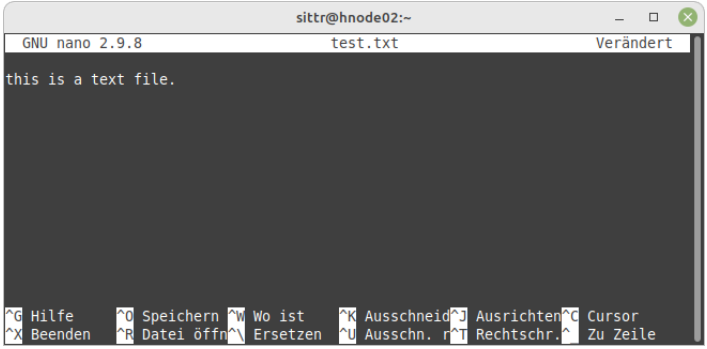


Cluster Structure



- `ls <path>` - list contents of *path*
- `cd <path>` - "change directory" / jump to *path*
- `cp <source> <destination>` - copy file from *source* to *destination*
- `cp -r <source> <destination>` - copy folder including its contents from *source* to *destination*
- `rm <path>` - "remove" / delete file at *path*
- `rm -r <path>` - delete folder at *path* including its contents (**be careful with this!**)
- `man <command>` - open the manual / help page for *command*
- `<command> --help` - print help text for *command*

- `nano` is a (comparatively) beginner-friendly commandline text editor
- Usage: `nano <filename>`
- Commands are displayed at the bottom (`"^"` stands for CTRL/STRG key!)
- Save with STRG+O, exit with STRG+X



- Lots of different software on the cluster means lots of different *dependencies*
- Might want to have several versions of a software or library installed side-by-side
- How to reliably establish a *runtime environment* with the correct versions?

→ **Environment Modules**

- Allows to mix and match software versions to build the correct runtime environment
- Can enforce dependencies and avoid mixing of mutually exclusive software
- Reproducible environment for every job run

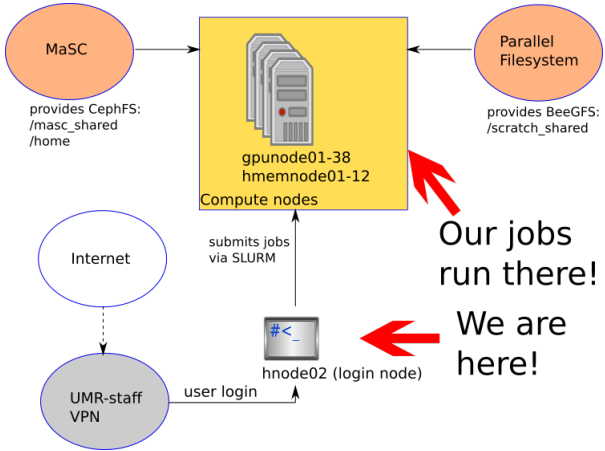
Module Commands

- `module load <modulename>` - load module *modulename*
- `module unload <modulename>` - remove module *modulename*
- `module list` - list loaded modules
- `module avail` - list available modules
- `module spider <modulename>` - list all available versions of *modulename*
- `module purge` - remove *all* currently loaded modules

- Many more commands available - see `module --help`
- Tip: In jobscripts (see below), always lead with a `module purge` to ensure a clean working evironment

So, how do I start my calculation?

- We need a system that distributes available computation resources:
  - According to preset priorities - reflect group membership, access to exclusive / special resources
  - Fairly - everyone gets a turn *eventually*
  - Efficiently - maximize calculation throughput and balance loads
  - Automatically - minimize the need for manual adjustment
- Solution: **Job Scheduling System**
  - Several implementations available, largely same feature set: Oracle Grid Engine (former Sun Grid Engine; used on MaRC2), SLURM, LSF, ...
  - On MaRC3a, we use the "Slurm Workload Manager" (formerly known as Simple Linux Utility for Resource Management)
  - To do its job, the scheduler needs informations about the calculation you want to run


MaSC
provides CephFS:
/masc_shared
/home
Parallel
Filesystem
provides BeeGFS:
/scratch_shared
gpunode01-38
hmemnode01-12
Compute nodes
Our jobs
run there!
Internet
submits jobs
via SLURM
We are
here!
hnode02 (login node)
UMR-staff
VPN
user login

You need to provide:

- *What* the calculation needs (# of processes, amount of memory, ...)
- *Which* environment it needs to run (→ Modules)
- *How* to run it (execution command and program parameters)

The Scheduler decides:

- *Where* to run it (whichever node can provide the stated amount of resources)
  - Less resources required → more opportunities to "fit in"
- *When* to run it (priority of waiting jobs depends on current cluster load, needed resources, user or group membership, ...)
  - Every job will run **eventually**

So, how do I tell the scheduler what it needs to know?

- Via *job script*

SLURM Job Scripts

- Format: Shell script
- Three sections:
  - SLURM parameters (lines start with `#SBATCH`)
  - Environment setup (lines (usually) start with `module`)
  - Calculation command(s) (can take the form of any shell command, most likely something like `<program> <parameters>`)

Job Script Example

listings/marc3_job_example.slurm

```
#!/bin/bash

#SBATCH --time=00:20:00
#SBATCH --ntasks=2
#SBATCH --output=example.out
#SBATCH --mem-per-cpu=100M

module purge
module load gnu9
module load openmpi4

mpicc --version
```

listings/marc3_job_example_comments.sh

```
-> "Shebang" (tells the system the type of script)

-> Set max. job runtime
-> Set amount of processes
-> Set where console output goes
-> Set the needed amount of memory per core

-> Remove all modules to start with a clean environment
-> Load the gcc 9.x module
-> Load the openmpi 4.x module

-> Print the version of "mpicc" and exit
```

Do we actually *need* the resources that are requested here?

Most important parameters (i.e. `#SBATCH` lines):

- `--time=<DD-HH:MM:SS>` → maximum job runtime; default: 3 days
- `--partition=<name>` → which node subset to run on; can be automatically chosen depending on `--time`, `--gpus`, and `--ntasks` requirements; default: "normal"
- `--ntasks=<num_tasks>` → amount of processes; default: 1 **or**
- `--ntasks-per-node=<num_tasks>` **and** `--nodes=<num_nodes>` → explicitly set process distribution
- `--cpus-per-task=<num_threads>` → how many threads to start for each process; default: 1
- `--gpus=[type:]<num>` → amount of GPUs (types: v100s, a100, a40; no type given: can run on any GPU); default: 0
- `--mem=<mem_in_mb>` → amount of *total* memory per node, **or**
- `--mem-per-cpu=<mem_in_mb>` → amount of memory *per cpu*; default: 1000

Some more important parameters:

- `--mail-user=<address>` **and** `--mail-type=<type>` → send a mail for certain events (commonly useful: END; also available: BEGIN, FAIL, ALL, ...)
  - *Only works with university addresses!* (i.e. `<user>@staff.uni-marburg.de`)
  - In case of END, also displays resource utilization (important to gauge reservation parameters for future jobs!)
- `--output=<filename>` → place console output (STDOUT, STDERR) into the set file name; default: `slurm-<job_ID>`
- `--error=<filename>` → place STDERR output into the set file separately; default: goes into the same file as STDOUT
- `--account=<account_name>` → use specified account for this job; only relevant if you are part of multiple groups with different cluster access rights

How do I choose the correct parameters for my job?

- If a job steps over its requirements (memory, time limit), it will be killed
- Goal: Set requirements so a job "fits into them"
- Initially: Approximate by order of magnitude
  - Will it take one hour, one day, ten days to finish? → `--partition=short|normal|long`
  - Will it need 1 GB, 10 GB, 100 GB of memory?
- Use `--mail-type=END` output to check resource utilization and adjust accordingly
- Advantage of setting memory and time limit restrictions: Scheduler can find idle resources where job "fits in" → Reduced waiting times until job start

Consider reserving a bit *less* memory than the node maximum (e.g. `--mem=250G` instead of 256G) - system kernel and OS also need memory, and the scheduler will take "free memory" into account, **not** "theoretically available memory"!

Okay, I have a job script with parameters now. How to submit it?

- `sbatch <job_script>` submits the job script to the scheduler
  - Pay attention to error messages!
  - SLURM will refuse jobs that cannot run in their current configuration
- `sbatch` can also take any SLURM parameters directly (i.e. `sbatch --ntasks=4 <job_script>`; these will *override* the parameters present in the script
- `scancel <job_ID>` cancels / kills a waiting or running job
- `squeue` displays currently running and waiting jobs
- `sinfo` displays cluster partitions and their current state
- `scontrol show job <job_ID>` displays a running job's details
- `sacct` displays finished jobs (default: only from current day)
- `seff <job_ID>` display resource usage statistics for a finished job

My calculation needs interactive commands, can I start interactive jobs?

- Generally yes, **but:**
- Interactive jobs have, by nature, low efficiency from an HPC perspective (i.e. idle times waiting for input)
- Thus, they are quite restricted in order to not lock down large amounts of compute resources:
  - One running job per user
  - Max. 12 hours of running time
  - Max. 16 CPU cores
  - Max. 1 GPU
- If this is not enough, we can offer support to try and find a solution that works for you
- Starting an interactive job works like this:

```
srun <needed resources and parameters, i.e. --ntasks etc.> --pty bash -i
```

- Local support in Marburg is handled through the "Request Tracker" ticket system
  - **marc3@hrz.uni-marburg.de**
- Central mail address that notifies all employees who are involved with the topic
- Can reach support staff even if individual people are on vacation / on sick leave / busy with other things
- MaRC3a staff:
  - René Sitt (HKHLR member, first- and second-level support, software maintenance, administration)
  - Marcus Lechner (MaRC3a + further hardware addons project coordination, administration, additional support)
  - Clemens Thölken (Additional SYNMIKRO position; administration support for MaRC3a and MaSC)
  - Thomas Gebhardt (Head of Central Systems Department, administration, additional support)
  - Manuel Haim (User management)

- Documentation is provided on the University's "share" pages
- Needs login with staff account
- Will be extended over time
- Address:
  `https://share.uni-marburg.de/de/hrz/it-mitarbeiter/hpc/hpc-user/marc3a-masc`
- Specialized subtopics have their own articles:
  `https://share.uni-marburg.de/de/hrz/it-mitarbeiter/hpc/hpc-user/marc3`