Getting started

This page gives you an overview of the most important aspects of the PALMA-II cluster, how to connect to it and what a typical workflow could look like. Specifics can be found in the subsections for each topic separately.

PALMA-II consist of several hundred compute nodes running CentOS 7 as operating system. Every node consists of 2 Intel Xeon Gold 6140 CPUs containing 18 CPU cores each. Users will first have to connect to so-called login nodes to gain access to the compute nodes themselves. Applications or compute **jobs** can then be started via an interactive session or via job/batch scripts using the slurm workload manager.

Access

To access the PALMA-II cluster you have to connect to one of the **login nodes** via an SSH connection using a terminal emulator. If you are on Linux or Mac OS, you can use the terminal applications that come pre-installed with your OS. If you are on windows you can use PuTTY.

- SSH address: username@**palma.uni-muenster.de**

You will need an ssh-key to access PALMA. Please find further instructions here.

If you need a short introduction on how to use a shell (terminal), please refer to this site.

Filesystem

When you log in to the cluster for the first time, a directory **/home/[a-z]/<your-username>** is created for you. Please use this folder *only* to store your applications. Do *not* store your numerical results in here. Storage in **/home** is limited. For (numerical) results of your computations use the folder **/scratch/tmp/<your-username>**. The environment variable **$WORK** automatically points to the scratch folder.

Directory	Purpose
/home/[a-z]/<username>	Personal applications, binaries, libraries etc.
/scratch/tmp/<username>	Working directory, storage for numerical output (start your applications from here!)
/mnt/beeond	Temporary working filesystem, provided on a per-job basis

There is **NO BACKUP** of the home and working directory on PALMAII as these are not intended as an archive. We kindly ask you to remove your data there as soon as it is no longer needed.

Further information can be found at: Data & Storage

Datatransfer

To transfer data from and to the cluster, you can either use the scp command from a terminal (Linux & Mac OS) or use something like WinSCP (Windows) or FileZilla (all platforms).

An example using *scp* is given below:

Task	Command
Copy a local file to your *home* folder on PALMA-II	`scp -i $HOME/.ssh/id_rsa_palma MyLocalFile username@palma.uni-muenster.de:/home/[a-z]/username/`
Copy a local folder to your working directory on PALMA-II	`scp -i $HOME/.ssh/id_rsa_palma -r MyLocalDir username@palma.uni-muenster.de:/scratch/tmp/username/`

Copy a file on PALMA-II to your local computer	`scp -i $HOME/.ssh/id_rsa_palma username@palma.uni-muenster.de:/scratch/tmp/username/MyData/MyResult.dat /PATH/ON/YOUR/LOCAL/COMPUTER/`

Loading available software

Common applications are provided through a **module** system and have to be loaded into you environment before usage. You can load and unload them depending on your needs and preferences. The most important commands are:

Command	Description
`module avail`	List currently available modules (software)
`module spider <NAME>`	Search for a module with a specific *NAME*
`module load <NAME>`	Load a module into your environment
`module unload <NAME>`	Un-load a module from your environment
`module list`	List all currently loaded modules
`module purge`	Unload **all** module in your environment

Details and specifics can be found in the module system section.

Starting Jobs

Jobs can be started in three different ways using the the slurm workload manager:

1. Interactive (giving you direct access to the compute nodes)
2. Non-interactive (using slurm to directly queue a job)
3. Batch system (submitting a job script)

Type	Command
Interactive	srun <config options> --pty bash
Non-interactive	srun <config options> <my-applications-to-run>
Batch	sbatch my_job_script.sh

Both methods will reserve a certain amount of CPU cores or nodes for a given amount of time depending on your settings. Further information about the submission of jobs, configuration options, example job scripts can be found in the Job scheduling / submission section.

Workflow

An example of a typical workflow on PALMA-II is given below:

Step	Command
1. Connect to the login node of palma	`ssh username@palma.uni-muenster.de`
2. Navigate to your working directory	`cd /scratch/tmp/username/MySimulation/`

3. Load the needed software into your environment	`module load intel/2019a`
	
	`module load GROMACS/2019.1`

4. Start your simulation / computation	`srun -N 4 -n 36 --partition normal --time 12:00:00 gmx mdrun -v -- deffnm NPT`

Monitoring

Please find the Ganglia Monitoring at https://palma.uni-muenster.de/ganglia for the usage of the nodes and OpenXDMod userstats at https://palma2b.uni-muenster.de/