Introduction to Supercomputing at JSC: Hands-On (November 2024)

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Introduction

The largest computers used for computational science have exhibited an exponential increase in the rate of basic operations they can perform since at least the 1990s. For more than a decade, this growth has been enabled not by increasing clock speeds of individual processing units, but by assembling systems that consist of ever greater numbers of processing units. Scientific applications intended to run on these systems are expected to orchestrate many of these computational units to collaborate on solving a given computational problem. Building these kinds of applications is called parallel programming. Parallel programming will only be touched on briefly in this course, but Jülich Supercomputing Centre (JSC) offers several courses that teach various techniques related to the topic.

Scientists who want to run applications on these systems, be they custom made or third-party, are expected to know how to use these systems. Working through this guide will teach you how to:

- access the systems available at JSC,
- navigate the file system,
- find pre-installed software,
- build your own software
- and finally, to run software.

Access

This chapter will teach you how to log in to the systems at JSC.

Getting a JSC account

A basic prerequisite to get access to the HPC systems and other services at JSC is a JSC account. If you do not already have an account (they have the form `<family name><number>`, e.g. `steinbusch1`), one can be created through JSC's user portal JuDoor (click the *Register* button).

Joining a compute time project

To be allowed to log in to an HPC system, your JSC account needs to be a member of a computing time project that has an active budget on the system. This is the case if

- you have successfully applied for test computing time for a test project and are now the principal investigator (PI) of your own project, or
- you have successfully applied for computing time during one of our calls for project proposals and are now the principal investigator (PI) of your own project, or
- you have gained access to a project either by being invited by the PI or project administrator (PA) or by being granted access upon requesting to join a project through JuDoor.

We have created a computing time project for this course with a project ID of `training2436`. To join the project, log in to JuDoor and click *Join a project* under the *Projects* heading. Enter the project ID and, if you want to, a message to remind the PI/PA (one of the instructors) why you should be allowed to join the project. Afterwards the PI/PA will be automatically informed about your join request and can add you to the different systems available in the project. As soon as you are unlocked for the system, the system entry will be shown on your JuDoor main page. You have to accept our Usage Agreement for the system you want to use before you can continue with the next step.

Login procedure

Logging in to our systems is usually done through the Secure Shell (SSH) mechanism, although there are alternatives such as UNICORE and JupyterLab. Our SSH configuration uses an authentication mechanism

based on public and private keys rather than passwords. A pair of public and private keys has to be generated on your personal computer. The private key has to be protected by a passphrase. The public key is then registered for access to the system through JuDoor.

CAUTION

NEVER SHARE YOUR *PRIVATE* KEY!!!

Several software packages can be used for logging in through SSH. The procedure is documented below for some popular choices:

- OpenSSH - a popular choice on GNU/Linux, macOS, and other Unix-like operating systems
- PuTTY - a popular choice on Windows

MULTI-FACTOR AUTHENTICATION

JuDoor offers users the option to enable Multi-Factor Authentication (MFA), which adds an extra layer of security to your account. With MFA enabled, you'll be required to provide a secondary factor of authentication in addition to your password. For example, when logging in to JSC services, you'll be prompted to enter a time-based one-time password (TOTP) as the second factor. In addition, JuDoor allows users to enable MFA for SSH login. Once enabled, when accessing the ssh service on the login hosts of the JSC system, users will be prompted to enter a 6-digit token after successfully authenticating using the ssh public key.

To enable MFA in JuDoor please navigate to the "Account Security" page by clicking the fingerprint icon in the navigation bar or using the account dropdown menu. There you see a list of your accounts. You can start the setup process using the "Start MFA Setup" button. On this page you can find our recommendations for TOTP Apps to use, but any other TOTP App should probably work just as well. You will need to install a compatible App, scan the QR-Code with the App to add the account, and then insert into the form both your current password and the code the App generates. After pressing "Continue" you will be presented with 10 reset codes. These can be used to disable MFA again in case you lose access to your second factor. You should save these at a secure location or print them.MFA will be enabled for your account only after you have confirmed that you have saved these reset codes. MFA is now enabled. The Fingerprint Icon in the Navigation bar now shows your MFA authentication state. Because you have just entered a valid code, you are MFA authenticated and can continue to use JuDoor as normal. The MFA authentication expires after 24 hours or if you open JuDoor from a different browser/device or clear your cookies.

The following actions are secured by MFA in JuDoor and therefore a valid token is needed:

- Joining a project
- Adding an SSH Key
- Removing an SSH Key
- Changing someone's access in a project if you are a PI or PA Actions that require TOTP are marked with a fingerprint icon.

Currently, MFA is an opt-in feature (can be activated on demand). However, at some point in the future, it will become an opt-out feature (activated by default but can be deactivated if desired).

Generating a key pair with OpenSSH

OpenSSH is a set of command line tools, so open up a terminal. We suggest you start by creating a fresh pair of public and private keys (a key pair). To generate a key pair enter the command shown in the code snippet below. The program asks for a passphrase. This passphrase is not used for authenticating to the remote system, but rather acts as an encryption key for the private part of the key pair stored on the local file system. In case the private key file is stolen by an attacker, they will not be able to use the key without knowing the passphrase, so make sure to use one that is hard to guess.

```
$ ssh-keygen -a 100 -t ed25519 -f ~/.ssh/id_ed25519
Generating public/private ed25519 key pair.
Enter passphrase (empty for no passphrase):
Enter same passphrase again:
Your identification has been saved in /Users/bsteinb/.ssh/id_ed25519.
Your public key has been saved in /Users/bsteinb/.ssh/id_ed25519.pub.
The key fingerprint is:
SHA256:tHin8v4j4cyVVe2BEWAinq/vlhFExupY+37s94216uA bsteinb@zam478
The key's randomart image is:
+--[ED25519 256]--+
|       .o+ o.o+. |
|      . +oo  ....|
|       o+    . ..|
|       =.o  .   .|
|      = S.oo     |
|     . +o+o      |
|      .=oo+.    .|
|       o*+oo.. oo|
|       .**+Eoo+o.|
+----[SHA256]-----+
```

If the designated output file (`~/.ssh/id_ed25519`) already exists, the program asks to overwrite it. This is probably *not* what you want, since you might be using the key contained therein. Change the output name by using the arguments `-f ~/.ssh/id_ed25519_jsc` instead of `-f ~/.ssh/id_ed25519`. If you do so, keep in mind that your keys are in a non-default location for the remainder of the course.

Print the contents of the public key to the terminal by entering:

```
$ cat ~/.ssh/id_ed25519.pub
ssh-ed25519 AAAAC3NzaC1lZDI1N [...] 6BRJMTyE4voyqJGm36P+ bsteinb@zam478
```

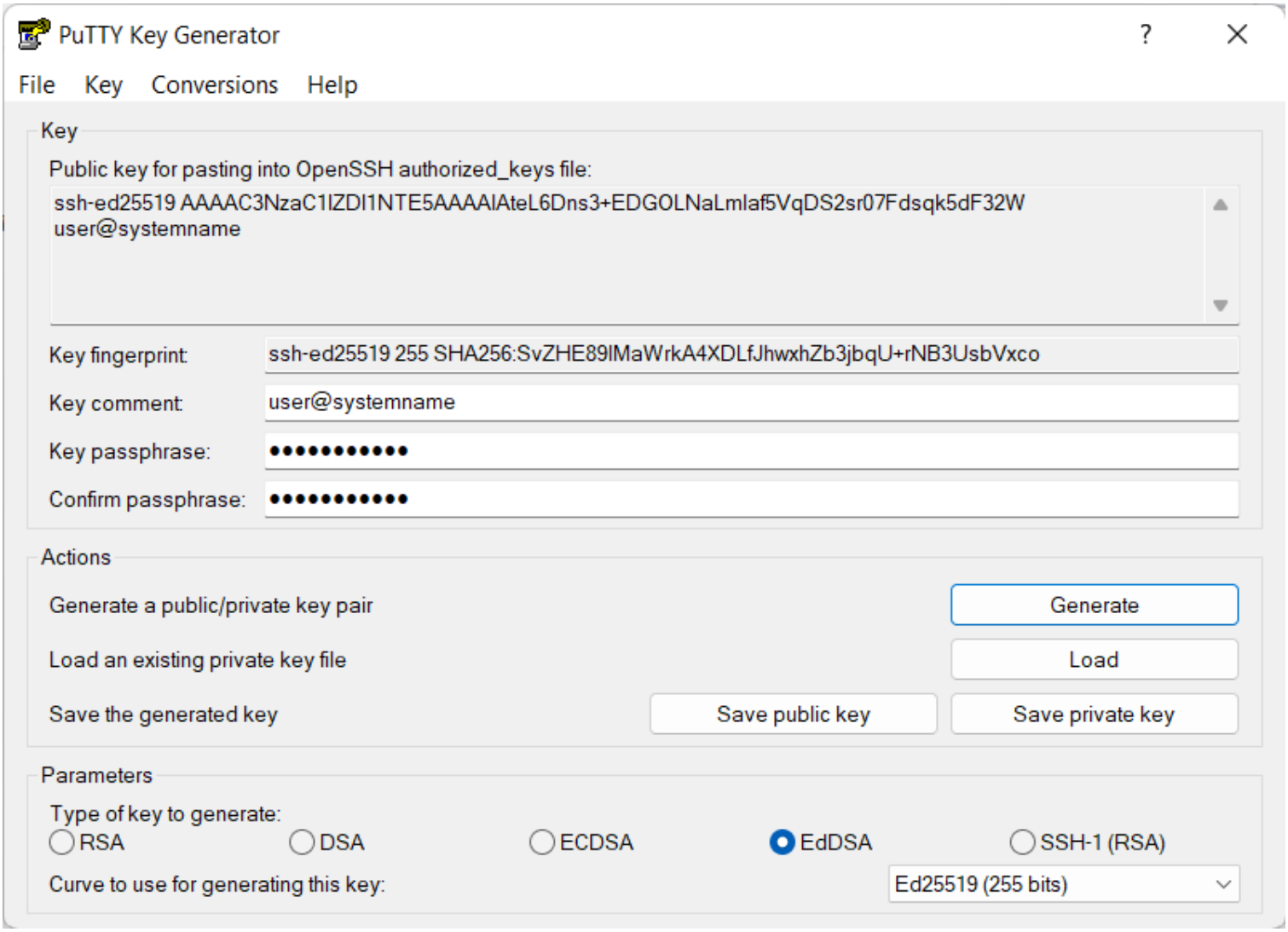
and copy it to the clipboard (do *not* copy the key above! This is only an example, The one you have generated will be different). Continue by uploading the public key to JuDoor.

Generating a key pair with PuTTY

Open `puttygen.exe` to generate a key pair. Select *Ed25519* as the key type then click *Generate* and follow the instructions of the program. Once the key has been generated, enter a strong passphrase that cannot be guessed easily. This passphrase is used to encrypt the key while it is stored on disk so that it cannot be used if it is stolen.

Click *Save private key* to save the private key to a `.ppk` file.

Now copy the contents of the field *Public key for pasting into OpenSSH authorized_keys file* to the clipboard.



INFO

There is a known issue currently with the Windows implementation of OpenSSH. If you see the error message

```
Corrupted MAC on input.
ssh_dispatch_run_fatal: Connection to x.x.x.x port 22: message
authentication code incorrect
```

while trying to log in, please follow the guidance here.

Uploading the public key

Navigate to JuDoor and click on *Manage SSH-keys* next to the entry for the system you want to use under the *Systems* heading. Paste the public key into the form in the field labeled *Your public key and options*

string, but do not submit yet. As a further security measure, you have to specify the systems that your log in attempts will come from. This is done via an additional `from`-clause on your public key, that can contain single IP-addresses and address ranges as well as host names and even wildcard patterns based on either of these.

Specifying a `from`-clause is relatively easy if you have access to a system with a fixed IP-address or an IP-address that changes dynamically, but comes from a range of addresses that can be specified concisely. This is typically the case for systems which are connected to university or research centre networks (even via VPN when working from home). For example, systems connected to the network of Forschungszentrum Jülich will be assigned an IP-address from the range `134.94.0.0/16`, so a valid `from`-clause would be `from="134.94.0.0/16"`. Other institutions will use different address ranges, you should be able to find these out from your institutions network operations centre.

Sometimes, patterns based on host names will work better than those based on IP addresses. For example, Forschungszentrum Jülich assigns host names that end in either `fz-juelich.de` or `kfa-juelich.de`, so a valid `from`-clause could also be `from="*.fz-juelich.de,*.kfa-juelich.de"` (notice how multiple patterns can be combined with a comma in between). Once again, the host names assigned by other institutions will be different. To some extent, this scheme also works for home internet access. Internet providers typically assign IP addresses dynamically drawing from fragmented pools that are hard to specify completely in terms of address ranges, but they often assign host names which follow a pattern that can be found out. The command `nslookup <your IP>` will tell you the host name assigned to your system by the provider (find out your IP either from the JuDoor key upload form or by asking a search engine "what is my ip"). This host name might look something like `2909a2-ip.nrw.provider.net`. Chop name components off the beginning and replace them with `*` to come up with a pattern, e.g. `*.nrw.provider.net`.

Add your `from`-clause in front of the public key you already pasted into the form. The result should be something like:

```
from="134.94.0.0/16" ssh-ed25519 AAAA [...]
```

Then click *Start upload of SSH keys*. It will take a little time for the key you uploaded to JuDoor to be synched to the actual system. Eventually though, you will be able to log in. Once again, we have instructions for

- OpenSSH
- PuTTY

IPv6 connectivity update for JURECA login nodes

For users connecting from machines with a globally routed IPv6 address assigned to them, their SSH clients will favour IPv6. This can lead to issues for users who have uploaded SSH public keys with `from=` clauses based solely on IPv4 addresses or using patterns based on host names which do not match the host names their internet provider assigns to IPv6 addresses.

The long term solution for these issues is to update your `from=` clauses to include patterns based on IPv6 addresses (or host names matching the IPv6 addresses).

A short term solution can be to revert to IPv4 connectivity. This can be done by connecting to a new DNS name which will keep resolving to IPv4 addresses only: `jureca-ipv4.fz-juelich.de`. Another option is to disallow IPv6 in your SSH client. For OpenSSH this can be done with the command line option `-4` or the configuration setting `AddressFamily inet`. In PuTTY the protocol can be overridden with the setting 'Internet protocol version' in the 'Connection' pane.

Logging in with OpenSSH

To log in with OpenSSH, enter the following command:

```
$ ssh -i ~/.ssh/id_ed25519 <account name>@<system name>.fz-juelich.de
```

(Remember to change the location of the key `~/.ssh/id_ed25519` if you saved it to a non-default location.) For example, if I wanted to log in to JUWELS Cluster it would be:

```
$ ssh steinbusch1@juwels-cluster.fz-juelich.de
```

The following table lists the host names of login nodes for the different systems. Pick the one you want to use.

System	Login node host name
JURECA-DC	`jureca.fz-juelich.de`
JUWELS Cluster	`juwels-cluster.fz-juelich.de`

System	Login node host name
JUWELS Booster	`juwels-booster.fz-juelich.de`
JUSUF	`jusuf.fz-juelich.de`

When connecting for the first time, OpenSSH will prompt you to confirm the server key fingerprint:

```
The authenticity of host 'jusuf.fz-juelich.de (134.94.0.184)' can't be
established.
ECDSA key fingerprint is SHA256:tuswM7JtVcWNS5wRCVIfv1h4uRHReHIN77C4zTYaPjs.
Are you sure you want to continue connecting (yes/no/[fingerprint])?
```

JSC publishes SSH fingerprints for its systems through JuDoor. You can find them on the page you used to upload your public key. Either compare the keys or, in newer versions of OpenSSH, you can paste the fingerprint from JuDoor into the prompt to confirm it.

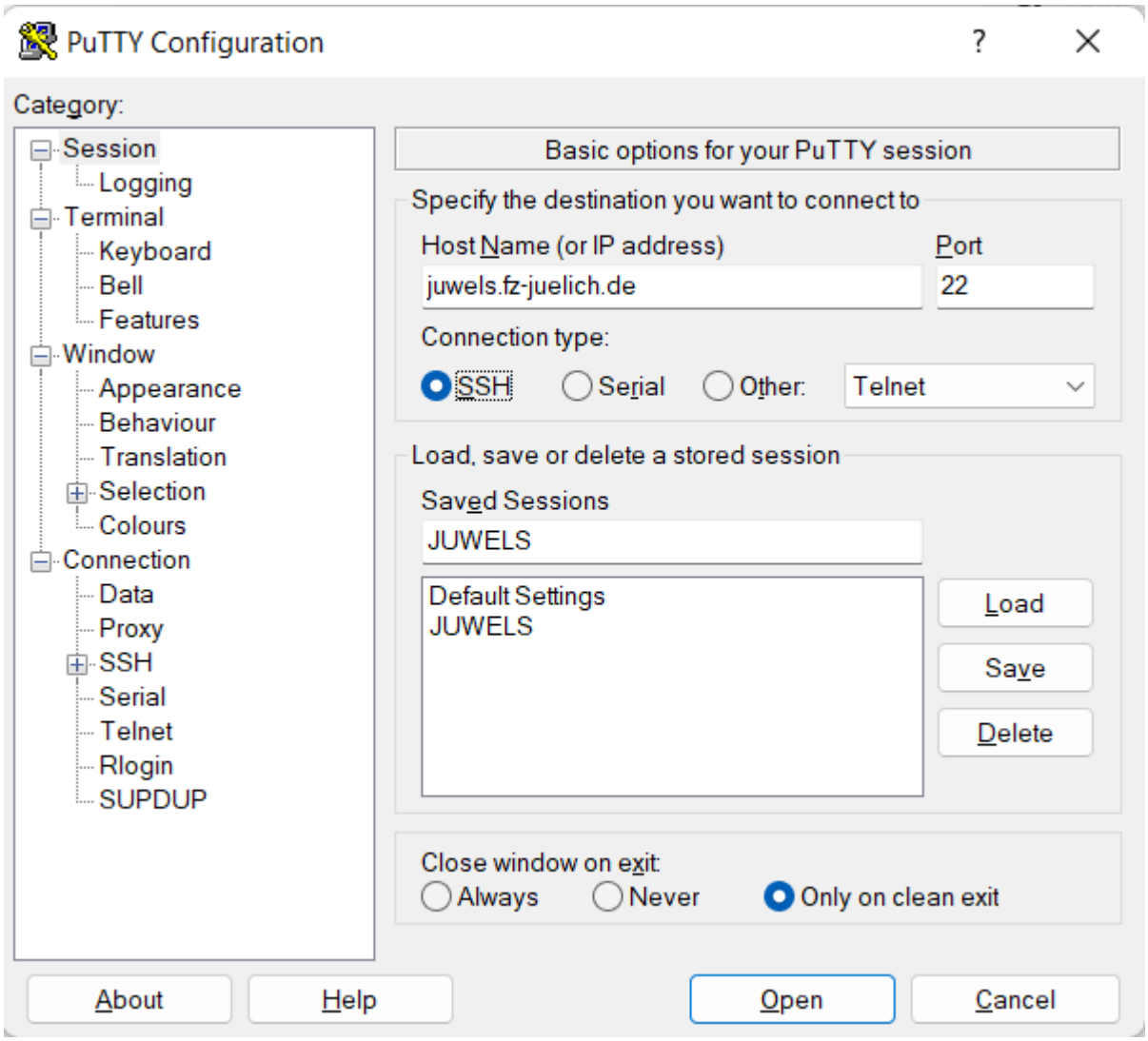
Then you should see an informational message (the *message of the day*, MOTD) followed by a shell prompt similar to the following:

```
**************************************************************************************
*  Welcome to                                                                        *
*       _ _   ___        _______ _     ____                                        *
*      | | | | \ \      / / ____| |   / ___|     Juelich Wizard                    *
*   _  | | | | |\ \ /\ / /|  _| | |   \___ \        for                           *
*  | |_| | |_| | \ V  V / | |___| |___ ___) |      European Leadership            *
*   \___/ \___/   \_/\_/  |_____|_____|____/         Science                       *
*                                                                                  *
**************************************************************************************
                                                              2020-11-19T14:00+0200
 ### Status information JUWELS ###

Known issues:     https://apps.fz-juelich.de/jsc/hps/juwels/known-issues.html

**************************************************************************************
steinbusch1@jwlogin01:~ $
```

Once you have logged in successfully, you can continue with Unix shell basics.

Logging in with PuTTY

Launch `putty.exe` to log in. Set the *Host name* for the system you want to connect to, e.g. `juwels-cluster.fz-juelich.de`.

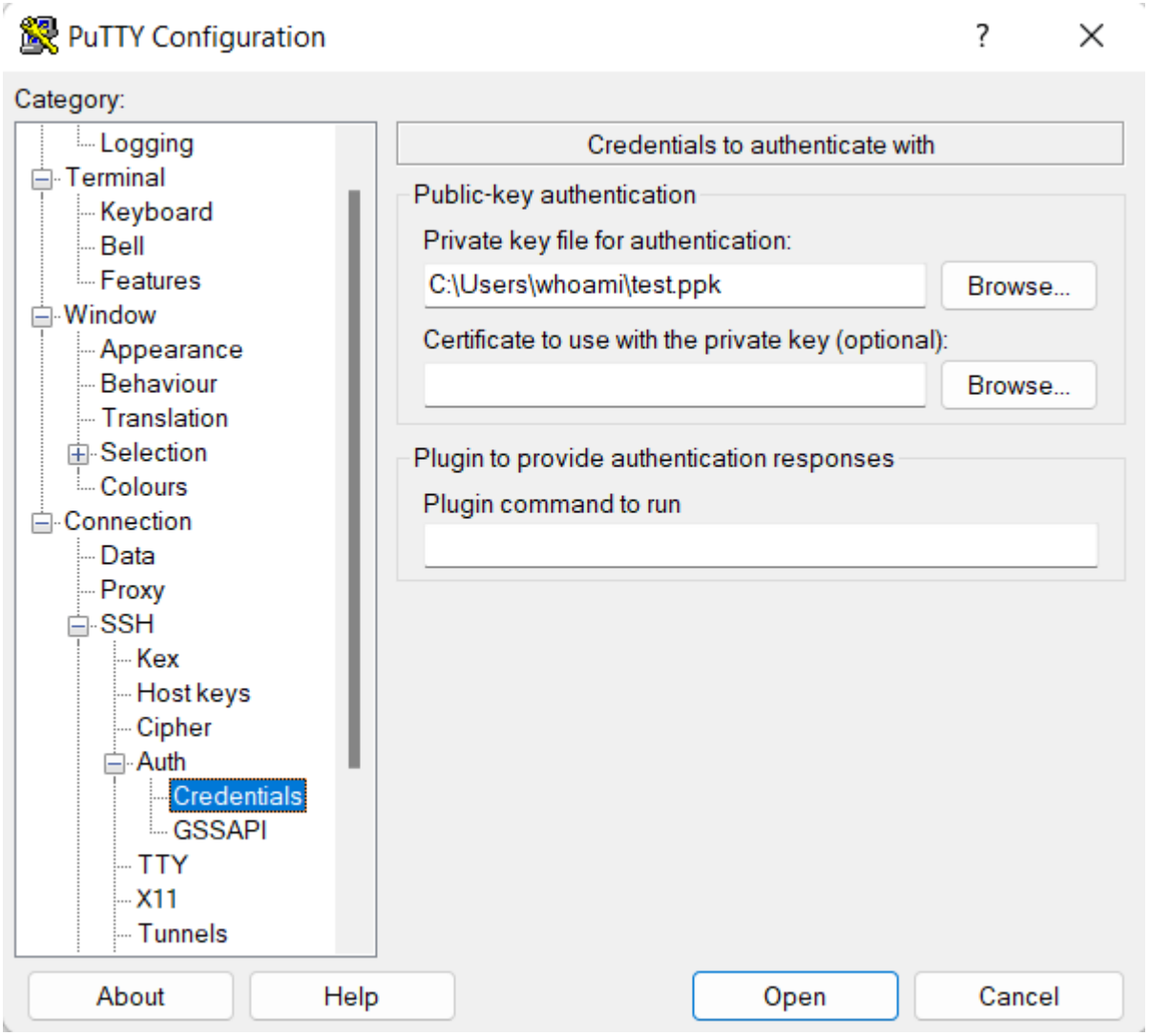


The following table lists the host names of login nodes for the different systems. Pick the one you want to use.

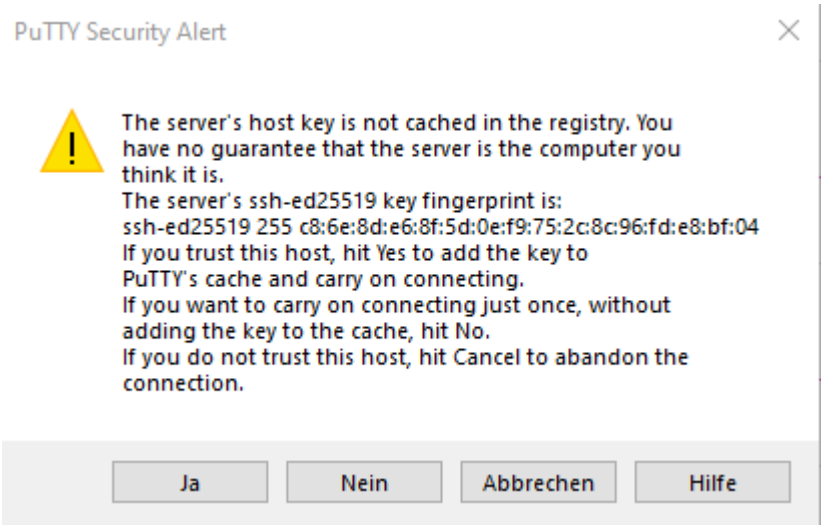
System	Login node host name
JURECA-DC	`jureca.fz-juelich.de`
JUWELS Cluster	`juwels-cluster.fz-juelich.de`
JUWELS Booster	`juwels-booster.fz-juelich.de`

System	Login node host name
JUSUF	`jusuf.fz-juelich.de`

Navigate to *Connection* > *SSH* > *Auth* > *Credentials* and under *Private key file for authentication:* select the key you just generated.



If you want to save this configuration, you can navigate back to the *Session* screen to give the session a name and save it. Now click *Open* to connect. When you connect for the first time, PuTTY will display a dialog like the following:



This is not an error, but a security feature. The server key fingerprint displayed in the dialog has to be verified by comparing it to the known good fingerprint. JSC publishes SSH fingerprints for its systems through JuDoor. You can find them on the page you used to upload your public key.

Once you have logged in successfully, you can continue with Unix shell basics.

JupyterLab

Alternatively, you can use JupyterLab to log in. The authentication credentials are the same as for JuDoor. Once you have logged in, you need to create a JupyterLab instance by clicking *Add New JupyterLab*. On the next screen you must select which system you want to log in to, what project to use for accounting and what part of the system you want to log in to (more about this later), login nodes are the right choice for the moment. Startup of JupyterLab may take a while, but once it is done, you can launch a terminal running a shell on the system of your choice inside the browser. To do so, click *File* > *New* > *Terminal* and you should see a shell prompt similar to this:

```
[steinbusch1@jrl06 ~]$
```

Checking System/Service Status

The root cause of many problems ("I cannot log in", "the system is slow") can be found by checking the JSC status webpage. Here you will find up-to-date status information on the services JSC provides, including upcoming planned maintenances. A traffic-light colour system is used to indicate the state of a system or service, with green systems functioning as expected for most or all users. Yellow systems are degraded, with issues that will impact many users. Red systems are strongly degraded which will impact most or all

users. Finally, dark-red systems are unavailable. Do not fret that you see more systems than what you have access to, as this is a general landing page for all of our systems.

Below our cluster systems you can find information on our storage systems/tiers. If you cannot find files, a certain mount is unavailable or the system becomes unresponsive to filesystem commands like `ls` this is the place to check. Even further down is the status of the services JSC provides, like JuDoor or Jupyter-JSC. Finally there is the status of JSC-support. Check here if you cannot reach JSC support or they do not respond in a timely fashion, if there is no reported issue try contacting them again using a different mode of communication, *i.e.* telephone or email. At the bottom of the page is a description of the traffic-light icons.

You can get further information on the degraded status of the systems and services by clicking on any of the system names, filesystem names or services. Give it a try! There you can also see older issues to help you diagnose problems that may have occured in the recent past.

Further reading

Our online documentation has more information on accessing the systems. It provides further examples of `from`-clauses, discusses configuration of SSH clients to set up short-cuts and gives hints for troubleshooting. If you want more details, you can find the documentation for our various systems here:

- JUWELS documentation: Access
- JURECA documentation: Access
- JUSUF documentation: Access

Unix shell basics

Whether you log in via OpenSSH, PuTTY, or opening a Terminal in JupyterLab, you will be interacting with the system through a Unix shell. Unix shells are text based interfaces that prompt the user to input commands and display the result of executing those commands back to the user. The underlying concepts (the file system, executing programs, etc.) are probably familiar to you, but the text based interface can seem daunting at first. This section will teach you how to accomplish essential tasks on a Unix shell. If you are already familiar with this kind of interface, you may want to skip ahead to the section describing the environment.

Like many operating systems, Unix provides an abstraction for storage media called a file system. Data of various types (text, images, executable code, etc.) is stored in files which can be organized in a tree-like hierarchy of directories that starts at a single root (the "root directory"). Objects in the file system (files or directories) are addressed using strings of characters called "paths" that list the directories one has to traverse to get to an object plus the objects name. The slash `/` serves as the separator between elements of a path and cannot itself appear in file or directory names. Some examples for paths are:

```
/etc
/usr/bin/env
/home/bsteinb/Documents
```

These paths are all "absolute paths", meaning, they describe the location of an objects in relation to the root directory (which is represented by a single slash `/`):

- `etc` is a directory that is found inside of the root directory
- `env` is a file found in the directory `bin` which itself is found in the directory `usr` inside the root directory
- `Documents` is a directory in `bsteinb` which is a directory in `home` which is a directory in the root directory

Since absolute paths can become unwieldy in deep directory hierarchies, Unix also allows relative paths. To this end, every program (including the shell you are using) is executed in a "working directory" (which can be changed during the execution of the program). Relative path specifications are then interpreted in relation to this working directory. They are written without the initial slash `/`. Some examples for relative paths are:

```
Documents
bin/env
../etc/crontab
```

With a working directory of `/usr`, `bin/env` refers to `/usr/bin/env`, just like the absolute path above. The path component `..` above has a special function. It refers to the parent (the containing directory) of a file system object and can appear in both relative and absolute paths. So `../etc/crontab` refers to a file `crontab` in a directory `etc` that can be found in the parent directory of the current working directory. `/home/bsteinb/../janedoe/.bashrc` can be simplified to `/home/janedoe/.bashrc`.

To find out the current working directory of the shell you are using, type:

```
$ pwd
```

The output should be something like:

```
/p/home/jusers/steinbusch1/juwels
```

which is the "home directory" associated with your account on the system. To list the contents of the working directory, execute the `ls` command:

```
$ ls
```

If you are working with a fresh user account, the output of this command might be empty, because there are no files (or only hidden files) in your home directory. To make `ls` display the hidden files as well, add the optional argument `-a`:

```
$ ls -a
```

The output should now be non-empty and contain files and directories with names that start with the period `.`. In Unix, whether a file system item is hidden or not is determined by the first character in its name being the period `.`.

`ls -a` is our first example of a more complex command invocation. It starts with the name of a command (so far, we have seen `pwd` and `ls`) followed by a list of arguments (here `-a`), all separated by spaces. `ls` can be used to list the contents of any directory, by specifying the path of the directory in the last position. To list the items in the `/etc` directory, type:

```
$ ls /etc
```

Most commands and the list of arguments they accept are documented in the Unix manual pages. They can be accessed through a command – `man` – that takes as its only argument the name of the manual page you want to read. For most commands there is a manual page with the same name as the command. To read the manual page for `ls`, type:

```
$ man ls
```

You can scroll through the manual page using the arrow keys. When you are done reading, close the manual by pressing `q` on the keyboard. To find manual pages for a specific topic, you can use the `apropos` command which searches the library of manual pages for a given keyword.

To change the working directory of your shell and all commands you invoke subsequently, use the `cd` command:

```
$ cd /
```

This will take you to the root directory. If you now execute `ls` without specifying a path, it should show you all items in the root directory, e.g.:

```
$ ls
arch   bin   dev  gpfs  lib    media  opt  proc  run   selinux  sys  usr
arch2  boot  etc  home  lib64  mnt    p    root  sbin  srv      tmp  var
```

Invoking `cd` without an argument takes you back to your home directory:

```
$ cd
$ pwd
/p/home/jusers/steinbusch1/juwels
```

Alternatively, the path to your home directory is also availably as the value of an "environment variable". Environment variables map names (strings) to values (also strings) and can be seen as implicit input to commands while arguments on the command line are explicit inputs. The name of the environment variable that contains the path to your home directory is `HOME`. Its value can be inspected using the `printenv` command:

```
$ printenv HOME
/p/home/jusers/steinbusch1/juwels
```

The `printenv` command asks the environment for the value of the variable `HOME` (using the `getenv` function) and prints it to the terminal. In some situations it makes sense, to use the value of environment variables as explicit arguments to a command (e.g. if you want to `cd` to the value of `HOME`). This is supported by a shell mechanism called "variable expansion": mention the name of a variable, prefixed by the dollar sign `$` in a command line and the shell will substitute the value of the variable and pass that as an argument to the command:

```
$ cd $HOME
$ pwd
/p/home/jusers/steinbusch1/juwels
```

The `env` command can be used to inspect the environment. When invoked without any arguments it prints a list of all variables currently defined and their values.

```
$ env
[...]
HOME=/p/home/jusers/steinbusch1/juwels
[...]
```

`pwd`, `cd` and `ls` let you navigate the file system. The following commands can be used to make modifications to the file system. First is `mkdir` which allows you to make a directory:

```
mkdir <directory_path>
```

To create an empty file at a given location, use:

```
```

```
touch <file_path>
```

In your home directory, create two directories and a file:

```
$ mkdir dir1 dir2
$ touch dir1/file1
```

You can use `ls` to confirm that you have created two directories next to each other, one of which contains an empty file.

```
$ ls
dir1 dir2
$ ls dir1
file1
$ ls dir2
```

Files and directories can be moved, copied and deleted with the commands:

```
$ mv <source_path> <destination_path>
$ cp -r <source_path> <destination_path>
$ rm -r <path>
```

Make a copy of `dir1` and check that it also contains `file1`.

```
$ cp -r dir1 dir3
$ ls dir3
file1
```

Move the copy of the file into `dir2`.

```
$ mv dir3/file1 dir2
$ ls dir2
file1
$ ls dir3
```

Finally, remove all three directories.

```
$ rm -r dir1 dir2 dir3
$ ls
```

Lastly, we will mention one way of editing text files: the `nano` editor. To open a file in `nano`, type:

```
$ module load nano
$ nano <file_path>
```

(The `module` command will be explained in detail later on.)

To insert something into the file, just start typing. Save your changes by pressing *CTRL-O*. Exit the editor by pressing *CTRL-X*. The bottom part of the terminal will display more functions which can be reached using certain key bindings. Interaction with the editor, such as specifying a file name when saving, will also happen here.

Change permissions with chmod

To change access permissions for files and directories one can use the `chmod` command. Through the `ls -l` command one can display the current access rights to a file or directory, which will look as follows:

```
-rwxr-xr-x 1 zjupa1 jusers 26080 May 10 16:58 <file>
drwxr-xr-x 5 zjupa1 jusers  4096 May 11 15:52 <dir>
```

The entries from left to right are: access rights, number of files, owner (user), group, size, date of last interaction, file or directory name. The first character in the access rights entry is either a hyphon `-` for files (first line above) or `d` for directories (second line above), followed by three blocks of three characters each: `r`, `w`, and `x` which specify the read, write, and execute access, respectively. A hyphon `-` then means that access is not granted. The first block of three characters specifies the access for the *user* (owner, here: `zjupa1`), the second for the *group* (that owns that file or directory, here: `jusers`), the third for all *others*. For above examples the *user* has all rights, while the *group* and *others* can read and execute but not write.

Access permissions can be changed in either symbolic or numeric mode.

Symbolic mode

In the symbolic mode `chmod` has following syntax:

```
$ chmod [references][operator][modes] <file>/<dir>
```

where references can be `u` for the *user*, `g` for the *group*, `o` for *others*, or `a` for *all*. The operator is either `+` to give a right, `-` to remove a right, or `=` to set rights exactly as specified. Modes are the three access rights `r`, `w`, `x`. Applied to above example

```
$ chmod g+w <file>
```

gives the *group* write rights and result to

```
-rwxrwxr-x 1 zjupa1 jusers 26080 May 10 16:59 <file>
```

while doing

```
$ chmod ug=rx <file>
```

results in

```
-r-xr-x--- 1 zjupa1 jusers 26080 May 10 16:59 <file>
```

Numeric mode

The modes of access rights can also be given in a numeric notation following the syntax

```
$ chmod [numeric notation] <file>/<dir>
```

For a list of numeric values and their translation to `r`, `w`, and `x` access rights for the *user*, *group*, and *others*, as well as for further reference you can consult here.

Environment

Now that you know about the basic Unix commands, this section will teach you about some of the peculiarities of the environment on the systems at JSC.

Active project

The first point to talk about is the *active project*. You already know about accounts and computing time projects and by this point you should be a member of at least one project to have access to one of our systems. However, in general, a single user account can be a member of multiple computing time ("C") projects (and also data projects ("D")) at the same time. You can see the projects that you are currently a member of in your user profile on JuDoor, or, if you are logged in to one of the HPC systems, you can use the `jutil` command:

```
$ jutil user projects
     project    unixgroup      PI-uid project-type budget-accounts
------------ ------------ ----------- ------------ ---------------
       hello        hello    hellopi1            D               -
      chello       chello    hellopi1            C           hello
  training00   training00      coach2            C      training00
```

Certain system resources, like file system space and compute time, are associated with the projects that you are a member of. Performing actions that consume these resources, storing files or running a computation, have to be counted against the resource pool available to the project. This is done by storing files in certain locations or specifying a compute time budget when running computations. It is possible to explicitly specify a project, each time one of these actions is performed. For brevity's sake, one can also make one of the projects the "active project" and then all actions performed in the remainder of the session will implicitly be performed in the context of that project. This can also be done through the `jutil` command:

```
$ jutil env activate -p training2436 -A training2436
```

Now `training2436` is the active project. Any computational jobs will be accounted against its budget and the special file system locations associated with it can be reached through certain environment variables. More about that in the next section.

> **HINT**
>
> In case you are working on different compute budgets we recommend to set the budget explicitly as it is described later in the document to avoid using the "wrong" budget for a specific simulation job.

File system points of interest

Every user account on the systems has a home directory (reachable through the `HOME` environment variable) where the user can store his personal files. However, there is a limit on the volume of data and also the number of files that can be stored in this directory (see more details here). Files stored here are also accessible only to you, which can cause issues if collaborators need them and you do not have access. Furthermore, the file system performance in `HOME` is reduced. It is recommended to use `HOME` only for configuration files. More storage space is granted to computing time projects. At least two directories are created for each project:

- a `PROJECT` directory, that can store medium amounts of data, and offers modest performance and is backed up regularly, and
- a `SCRATCH` directory, that offers high I/O bandwidth and should therefore be used for input and output of computations. However, no back up of these directories is performed and files that have not been touched in 90 days are automatically deleted.

Data projects have access to other storage locations, e.g. the tape based `ARCHIVE` for long term storage of results.

The path of these directories is available as the value of environment variables of the form `<directory>_<project>`, e.g. `PROJECT_training2436` or `SCRATCH_training2436`. If you have activated a project in the previous section, you will also have environment variables that are just `PROJECT` and `SCRATCH` that point to the respective directories of the active project.

Print the contents of `PROJECT_training2436` and `PROJECT`:

```
$ printenv PROJECT_training2436
/p/project1/training2436
$ printenv PROJECT
/p/project1/training2436
```

Change into that directory and see what is already there:

```
$ cd $PROJECT_training2436
$ ls
```

Inside the `PROJECT` directory, make a directory to contain the files that you work on. In order to avoid collisions, use your account name as the name of the directory (the `USER` environment variable contains your user name):

```
$ mkdir $USER
```

There is more information on file system points of interest in the documentation.

Further reading

Our online documentation has more information on the system environment. It describes further file systems covering more specialised use cases and discusses transferring files to and from the systems via SSH and Git. If you want more details, you can find the documentation for our various systems here:

- JUWELS documentation: Environment
- JURECA documentation: Environment
- JUSUF documentation: Environment

Software Modules

HPC centres will usually make some effort to provide software that is commonly used for scientific purposes. This includes compilers, parallel programming libraries like MPI, numerical libraries, and even complete simulation programs. These software packages form a hierarchy of dependencies (simulation programs use numerical and parallel programming libraries, and everything must be compiled with a specific compiler). Towards the bottom of this hierarchy, packages tend to be interchangeable (several compilers for C or Fortran, several libraries implement the MPI standard) and some of the higher up packages perform better when compiled with a certain compiler. It therfore makes sense to offer a range of software packages that implement low level functions and then build a software landscape upon each combination of those low level packages. The two lowest levels in this hierarchy, compiler and MPI library together form a "toolchain". To help keep the complexity of accessing these different collections of software in check, JSC uses a combination of EasyBuild and Lmod to build software and make it available as software modules. During a log in session, modules can be loaded and unloaded using the `module` command to use the software that is provided by them. When you log in, a set of default modules is loaded for you, e.g. on JUWELS:

```
$ module list

Currently Loaded Modules:
  1) GCCcore/.9.3.0 (H)   3) binutils/.2.34 (H)
  2) zlib/.1.2.11   (H)   4) StdEnv/2020

  Where:
   H:  Hidden Module
```

To see what other modules can currently be loaded, type:

```
$ module avail

------------------------ Core packages --------------------------
   Advisor/2020_update3
   Autotools/20200321
   Autotools/20200321                                (D)

   [...]
```

```
   unzip/6.0
   xpra/4.0.4-Python-3.8.5
   zsh/5.8

--------------------------- Compilers ----------------------------
   GCC/9.3.0                          NVHPC/20.9-GCC-9.3.0  (g)
   Intel/2020.2.254-GCC-9.3.0         NVHPC/20.11-GCC-9.3.0 (g,D)
   NVHPC/20.7-GCC-9.3.0       (g)     NVHPC/21.1-GCC-9.3.0  (g)

----------------- User-based install configuration -----------------
   UserInstallations/easybuild

  Where:
   S:        Module is Sticky, requires --force to unload or purge
   g:        built for GPU
   L:        Module is loaded
   Aliases:  Aliases exist: foo/1.2.3 (1.2) means that "module load foo/1.2"
will load foo/1.2.3
   D:        Default Module

Use "module spider" to find all possible modules and extensions.
Use "module keyword key1 key2 ..." to search for all possible modules matching
any of the "keys".
```

The available modules are grouped into categories:

- Core packages, which are independent of the choice of toolchain
- Compilers, which are the first ingredient of a toolchain
- Archictectures, which can be used to load software for different processor architectures. This category does not exist on all systems.

Go ahead and load a compiler:

```
$ module load GCC
```

If you now run `module avail` again, you will notice two additional software categories:

```
$ module avail

------------- MPI runtimes available for GNU compilers -------------
```

```
[...]

--------------- Packages compiled with GNU compilers ---------------
[...]
```

These contain modules that depend on (or were built with) the GCC module that you just loaded. Loading one of the available MPI modules will complete your choice of a toolchain and make more software available:

```
$ module load OpenMPI
$ module avail

------------------------ OpenMPI settings ------------------------
   mpi-settings/CUDA-low-latency    mpi-settings/CUDA (L,D)

--------- Packages compiled with OpenMPI and GCC compilers ---------
[...]
```

If you are looking for a particular piece of software that you know the name of, rather than rummaging through all the toolchains, you can use the `module spider` subcommand, as the output of `module avail` suggests:

```
$ module spider LAMMPS

----------------------------------------------------------------------------
-----------
  LAMMPS: LAMMPS/7Jan2022
----------------------------------------------------------------------------
-----------
    Description:
      LAMMPS is a classical molecular dynamics code, and an acronym for Large-
scale
      Atomic/Molecular Massively Parallel Simulator. LAMMPS has potentials for
      solid-state materials (metals, semiconductors) and soft matter
(biomolecules,
      polymers) and coarse-grained or mesoscopic systems. It can be used to
model atoms
      or, more generically, as a parallel particle simulator at the atomic,
meso, or
      continuum scale. LAMMPS runs on single processors or in parallel using
      message-passing techniques and a spatial-decomposition of the simulation
domain.
```

```
      The code is designed to be easy to modify or extend with new
functionality.

    Properties:
      Built with GPU support

    You will need to load all module(s) on any one of the lines below before
the "LAMMPS/7Jan2022" module is available to load.

      Stages/2022  GCC/11.2.0  ParaStationMPI/5.5.0-1

    Help:
      Description
      ===========
      LAMMPS is a classical molecular dynamics code, and an acronym
      for Large-scale Atomic/Molecular Massively Parallel Simulator. LAMMPS
has
      potentials for solid-state materials (metals, semiconductors) and soft
matter
      (biomolecules, polymers) and coarse-grained or mesoscopic systems. It
can be
      used to model atoms or, more generically, as a parallel particle
simulator at
      the atomic, meso, or continuum scale. LAMMPS runs on single processors
or in
      parallel using message-passing techniques and a spatial-decomposition of
the
      simulation domain. The code is designed to be easy to modify or extend
with new
      functionality.


      More information
      ================
       - Homepage: https://lammps.sandia.gov/
       - Site contact: Support <sc@fz-juelich.de>
```

Loading the LAMMPS module with OpenMPI loaded fails:

```
$ module load LAMMPS
Lmod has detected the following error:  These module(s) or
```

```
extension(s) exist but cannot be loaded as requested: "LAMMPS"
  Try: "module spider LAMMPS" to see how to load the module(s).
```

`module spider` with a specific module version provides details on how the module can be loaded:

```
$ module spider LAMMPS/7Jan2022

----------------------------------------------------------------------------
----------
  LAMMPS: LAMMPS/7Jan2022
----------------------------------------------------------------------------
----------
    Description:
      LAMMPS is a classical molecular dynamics code, and an acronym for Large-
scale
      Atomic/Molecular Massively Parallel Simulator. LAMMPS has potentials for
      solid-state materials (metals, semiconductors) and soft matter
(biomolecules,
      polymers) and coarse-grained or mesoscopic systems. It can be used to
model atoms
      or, more generically, as a parallel particle simulator at the atomic,
meso, or
      continuum scale. LAMMPS runs on single processors or in parallel using
      message-passing techniques and a spatial-decomposition of the simulation
domain.
      The code is designed to be easy to modify or extend with new
functionality.

    Properties:
      Built with GPU support

    You will need to load all module(s) on any one of the lines below before
the "LAMMPS/7Jan2022" module is available to load.

      Stages/2022  GCC/11.2.0  ParaStationMPI/5.5.0-1

    Help:
      Description
      ===========
      LAMMPS is a classical molecular dynamics code, and an acronym
      for Large-scale Atomic/Molecular Massively Parallel Simulator. LAMMPS
has
      potentials for solid-state materials (metals, semiconductors) and soft
```

```
matter
      (biomolecules, polymers) and coarse-grained or mesoscopic systems. It
can be
      used to model atoms or, more generically, as a parallel particle
simulator at
      the atomic, meso, or continuum scale. LAMMPS runs on single processors
or in
      parallel using message-passing techniques and a spatial-decomposition of
the
      simulation domain. The code is designed to be easy to modify or extend
with new
      functionality.


      More information
      ================
       - Homepage: https://lammps.sandia.gov/
       - Site contact: Support <sc@fz-juelich.de>
```

The problem is that LAMMPS is only available in particular toolchain which includes Stages/2022, GCC/11.2.0, ParaStationMPI/5.5.0-1. We could simply reload the MPI module rather than having to reload the entire toolchain, but this can sometimes come with unintended consequences, where what is loaded in a `module load` command is not necessarily unloaded while swapping modules.
For this reason, we also do not recommend using the `module unload` command, although it is available. We would recommend to unload (almost) all modules and start with a fresh environment, using `module purge`:

```
$ module purge
$ module load Stages/2022
$ module load GCC/11.2.0
$ module load ParaStationMPI/5.5.0-1
$ module load LAMMPS
```

The `module` command is part of the Lmod software package. It comes with its own help document which you can access by running `module help` and a user guide is available online.

The JUWELS system is special in terms that it consist of multiple system modules (as opposed to software modules) based on different compute technologies. The software we provide on JUWELS is also split into different hierarchies, one per system module. As JUWELS uses different login nodes for the different system

modules (Cluster and Booster), the correct software collection is loaded automatically based on which login node you use, so we would always strongly recommend using the login nodes of the JUWELS module you intend to compute on.

Further reading

Our online documentation has more information on software modules. It lists the basic tool chains (compiler + communication library + math library) available on our systems and discusses using older software stages. If you want more details, you can find the documentation for our various systems here:

- JUWELS documentation: Software Modules
- JURECA documentation: Software Modules
- JUSUF documentation: Software Modules

Custom software

For some, the software that is made available via the module system is enough to do their daily work. Others will want to bring their own software to the systems. This chapter will teach you how to run software distributed as source code for both compiled programming languages and scripting languages.

Compiled languages

For the three most common compiled languages in scientific computing, C, C++, and Fortran, the basic workflow is very similar. Open the file `hellompi.c` in the `nano` editor (or a different editor of your choice). (`nano` is available as a module, if you want to use it, type `module load nano`.)

```
$ nano hellompi.c
```

Paste the following listing into the file, save and close the editor.

```
#include <stdio.h>
#include <mpi.h>

int main(int argc, char* argv[]) {
  MPI_Init(&argc, &argv);

  int r, s;
  MPI_Comm_rank(MPI_COMM_WORLD, &r);
  MPI_Comm_size(MPI_COMM_WORLD, &s);
  printf("hello from process %d of %d\n", r, s);

  MPI_Finalize();
}
```

Once you have a compiler and an MPI library loaded (e.g. `module load GCC OpenMPI`), the file can be compiled as follows:

```
$ mpicc -std=c11 -o hellompi hellompi.c
```

We will explain how to run the program in a later chapter.

A lot of software is not compiled and installed by invoking the compiler directly, but by using a build system. GNU `make` is installed from the operating system package sources and GNU `autotools` as well as `CMake` are available as modules. More exotic build systems are also available, as are compilers for other languages like Go or Rust.

Scripting languages

Scripting languages have become more popular in scientific computing recently. Modules are available for Python and Julia.

Python

The Python interpreter can be loaded as a module as well as the `mpi4py` package that allows you to use MPI from your Python programs.

```
$ module load Python mpi4py
```

Edit a file `hellompi.py`:

```
($ module load nano)
$ nano hellompi.py
```

And paste the following content into it, then save and exit the editor.

```
from mpi4py import MPI

r = MPI.COMM_WORLD.rank
s = MPI.COMM_WORLD.size

print(f"hello from process {r} of {s}")
```

We will explain how to run the program in a later chapter.

More Python packages are available as modules. For scientific computing, the `SciPy-Stack` collection is especially interesting.

See also Supercomputing Environment Template using Python Virtual Environments venv to create project-based virtual environments that leverage the already installed Python modules on our systems, which are often significantly more performant than defaults from package managers.

Transferring and archiving data

With increasing supercomputing performance the data produced through simulation increases. Data management needs to be considered for every compute time project. In some workflows it could be necessary to get access to storage technology with improved I/O bandwidth. At JSC there are several storage technologies serving different needs. Access is granted for some of the storage technologies through application for a data project which can be submitted at any time. For large data transfers to or from the supercomputer infrastructure at JSC the system JUDAC with the address `judac.fz-juelich.de` delivers maximal bandwidth performance.

Download files from the web (supported only on login nodes!)

> **WARNING**
>
> **This option supported only on the login nodes!**

Only login nodes have a connection to the internet, and allow for file downloads and interactions with git or other version control repositories hosted outside the JSC GPFS. This is not supported on compute nodes.

`wget` is a simple file downloader that allows downloading files using HTTP, HTTPS, and FTP protocols. `wget` supports a number of options allowing to download multiple files, resume downloads, limit the bandwidth, recursive downloads, download in the background, etc.

Here is the typical syntax

```
$ wget <url link to the file>
```

Transferring files and folders from/to cluster

scp

`scp` allows to copy files over a secure, encrypted network connection. As `scp` command uses SSH to transfer data, it requires a password for authentication.

Copy file to the cluster

```
[from your laptop] $ scp [options] /path/to/file/filename <account
name>@<system name>.fz-juelich.de:/path/where/to/copy
```

Download file from the cluster

```
[from your laptop] $ scp [options] <account name>@<system name>.fz-
juelich.de:/path/to/the/file /path/where/to/save
```

To recursively copy a directory, use the `-r` (recursive) option.

rsync

If you already experienced with `scp`, you can test `rsync`. The `rsync` utility provides many advanced features for file transfer.

The syntax is similar to `scp`. Here is an example of file transfer to the cluster with commonly used options

```
[from your laptop] $ rsync -avzP /path/to/file/filename <account name>@<system
name>.fz-juelich.de:/path/where/to/copy
```

Download file from the cluster

```
[from your laptop] $ rsync -avzP <account name>@<system name>.fz-
juelich.de:/path/to/the/file /path/where/to/save
```

Where

- `-a` (archive) preserves the date and times, and permissions of the files;
- `-v` (verbose) option gives verbose output to help monitor the transfer;
- `-z` (compression) option compresses the file during transit to reduce size and transfer time;
- `-P` (partial/progress) option preserves partially transferred files in case of an interruption and also displays the progress of the transfer.

SSHFS

SSHFS allows you to mount a remote filesystem using SFTP.

To mount a remote filesytem you can do the following

- Make sure that SSHFS is installed on your local machine, e.g.

```
[from your laptop] $ which sshfs
```

Output will show where SSHFS is installed. If the result is empty, you need to install it (or tell the shell which directories to search for executable files).

- Create a directory which will be your mounting point

```
[from your laptop] $ mkdir <mountpoint>
```

- To mount remote directory

```
[from your laptop] $ sshfs <account name>@<system name>.fz-
juelich.de:/path/to/directory /path/to/mounting/point
```

- To unmount the filesystem

```
[from your laptop] $ fusermount -u <mountpoint>
```

On BSD and macOS, to unmount the filesystem

```
[from your laptop] $ umount <mountpoint>
```

Alternatives

- On Windows you can use various clients, e.g. WinSCP, FileZilla, PuTTY, etc.
- UFTP (UNICORE FTP) is a file transfer tool similar to Unix' FTP. Its main features include high-performance file transfers from client to server (and vice versa), list directories, make/remove files or

directories, sync files and data sharing. In addition, users can easily share their data even with users who do not have Unix-level access to the data.

- GridFTP is an extension of FTP used within large science projects. It includes features like parallelized FTP streams, fault tolerancy, download of portions of data and authentication and encryption for file transfers.

Archiving files

One of the biggest problems we often encounter when transferring data between remote HPC systems is the transfer of large numbers of files. There is an overhead involved in transferring each individual file, and when transferring a large number of files, this overhead in combination slows down the data transfer dramatically.

This issue can be solved by archiving multiple files into a smaller number of larger files before transferring the data. It is also possible to combine archiving with compression to reduce the amount of data we need to transfer, thereby speeding up the transfer. This can be done for example with `tar` utility.

Here is an example of archiving all data from a specific directory

```
$  tar -cvf <archive name>.tar /path/to/data/to/be/archived
```

Extract data from the archive

```
$  tar -xvf <archive name>.tar
```

Where

- `-c` (create) create new archive;
- `-v` (verbose) option gives verbose output to help monitor the archiving process;
- `-f` (file) filename of the archive;
- `-x` (extract) extract files from an archive.

To create a compressed archive using `tar` we add the `-z` option and add the `.gz` extension to the file to indicate it is compressed

```
$  tar -czvf <archive name>.tar.gz /path/to/data/to/be/archived
```

> **INFO**
>
> Please note that data compression and decompressing can take longer than transferring the un-compressed data.

The extract compressed files from the archive you can use the same way as for uncompressed data as `tar` recognizes it is compressed and decompresses and extracts at the same time.

```
$  tar -xvf <archive name>.tar.gz
```

If you have access to `$ARCHIVE`, data is migrated to tape for long term storage. Tape drives are relatively slow, and retrieval of a file requires retrieval of the specific tape it is stored on. It is heavily recommended that you archive your files by tarring them before placing them in $ARCHIVE. This will allow much more efficient retrieval if you need these files later.

Budgeting

There are a large amount of users involved in using supercomputing resources. In the application phase it is made sure that they are in need of this amount of computing resource. If every user could use unlimited resources, compute time and/or data storage capabilities would be quickly monopolised by a few users. We prevent this through budgeting. There are budgets on compute time, the amount of data and the number of files stored. This ensures that every user can use a portion of the supercomputing facilities at JSC.

Job Accounting

Each computing time project has been granted a certain amount of compute time (core-hours) on an HPC system. This budget is split monthly over the runtime of a project so that a regular project that runs for 12 months has 1/12 of the total amount of the granted core-h available each month. To allow further flexibility we have established a "3-month-window": Core hours that have not been used in the previous month can be used in the current month and will be lost in the next month if they are not used in the current month. Whereby in the current month you can also use the quota of the next month but with a decreased priority of the submitted jobs. The priority will be further decreased if you have used up the quota of the next month as well.

> **CAUTION**
>
> Users are charged for complete nodes they occupy, regardless of the number of CPUs used since the requested compute nodes for your application are not shared among users. The comute time used for one job will be accounted by the following formula: `#nodes * #AvailableCoresPerNode * walltime`.

Jobs that run on nodes equipped with GPUs are charged in the same way. Independent of the usage of the GPUs the available cores on the host CPU node are taken into account.

Detailed information of each job can be found in KontView which is accessible via the button 'show extended statistics' for each project in JuDoor.

Alternatively, you can execute the following command on the login nodes to query your CPU quota usage: `jutil user cpuquota`. Further information can be found in the "Accounting" chapter of the corresponding System Documentation.

Data Quotas

There are limitations on the amount of data and the number of files (inodes) on each file system. The usage of the data within a project is visualized in JuDoor. If you follow the links within JuDoor to KontView, more detailed statistic on data usage are visualized.

WHAT IS AN `inode`?

An inode (index node) is a data structure used in Unix file systems to store metadata about files and directories.
It serves as a unique identifier for each file/directory on the file system. Key points about inodes include:

- Each file has an associated inode that stores its metadata, such as file type, permissions, ownership, timestamps, and pointers to the file's data blocks on disk. Each directory also has at least one associated inode that contains similar information.
- inodes are identified by a unique number within a file system. This inode number is used by the operating system to access the file's metadata and data blocks.
- Each file system has a fixed number of inodes determined during its creation, limiting the maximum number of files it can hold. Running out of inodes can cause issues even if disk space is available. This is one of several reasons large numbers of small files or complex directory trees are not ideal.
- More inodes in a system can mean a longer time to look up files.
- In general, large numbers of small files leads to lower performance or performance issues.

HANDY COMMANDS

View global data usage across all file systems

```
df -h
```

inode usage on all file systems

```
df -i
```

Breakdown of data usage in a directory `dir` (in ascending order)

```
du -h --max-depth=1 <dir> | sort -h
```

List the inode usage in a directory `dir` (in ascending order)

```
du --inodes --max-depth=1 <dir> | sort -h
```

Identify the inode of a file

```
ls -il <file>
```

Identify the inode of a directory

```
ls -idl <dir>
```

Display the metadata of a file or directory

```
stat <file|directory>
```

Applications for a data project, giving access to other data storage facilities than PROJECT or SCRATCH of the compute time projects, can be submitted according to the information here. Applications for data projects are processed in a rolling manner. Therefore, you can apply for a data project at any point in the life of your compute time project, if you should see the need.

Running jobs

Up to now, you have been working on the log in nodes of the system. These nodes are set aside for working interactively on tasks that are needed to prepare your computations, such as compiling your applications, moving input data into place, and writing configuration files for your programs. Since the number of log in nodes for each system is small and they are shared between all users, we ask you to keep the resource consumption on these systems as low as possible. Building software should be restricted to using only a few processes in parallel, simulations and post-processing jobs should be run on the compute nodes. Use the `who` command to see who else is logged in to the log in node you are currently using:

```
$ who
steinbusch1 pts/71       2021-03-11 09:51 (pool-148-54.vpn.kfa-juelich.de)
[...]
$ who | wc -l
59
```

Unlike the log in nodes, users are not given free access to the compute nodes at any time. Instead they form a pool of resources managed by the resource manager software. Due to our collaboration with the company Partec we use "psslurm", which is based on Slurm and optimized for our systems to manage these resources. To run a computation on the compute nodes, you have to specify to the resource manager what amount of resources you need and for which duration. Once the resources have become available, you will be allowed to execute programs on them. Two modes of operation are possible:

- interactive mode where programs can be run on the allocated resources from a shell, possibly repeatedly, and
- batch mode where a shell script describing the commands to run as part of a computation is handed off to the resource manager for asynchronous execution.

Interactive mode

One-shot

The `srun` command is used to execute commands on a set of allocated resources. If no resources are currently allocated, `srun` can infer from its command line arguments what resources are needed, request them from the resource manager and defer the execution of the associated commands until the resources

are available. After the associated commands have been run, the resources are relinquished and running further commands will have to ask for resources again. This one-shot mode can be useful when you want to interactively run a few quick jobs with varying sets of resources allocated for them. Run the `hostname` command to see how `srun` will run commands on different nodes than the log in nodes. The `hostname` command lets you see or change the name of your computer (e.g. name of the login or compute node), which is useful for recognising it on a network or setting it up for different tasks. On JURECA and JUSUF, use this command):

> **WARNING**
>
> Do not forget to replace `YYYYMMDD`, where `YYYY` and `MM` and `DD` are the current year and month and day in the Gregorian calendar, e.g. `20240522`.

```
$ hostname
jrlogin09.jureca
$ srun -A training2436 --reservation hands-on-YYYYMMDD hostname
srun: job 3472578 queued and waiting for resources
srun: job 3472578 has been allocated resources
jrc0454
```

For the JUWELS Cluster and JUWELS Booster, there are a few differences: The name of the reservation on JUWELS Cluster is hands-on-cluster-YYYYMMDD and hands-on-booster-YYYYMMDD on JUWELS Booster. To submit to JUWELS Cluster, you want to be logged in to the Cluster login nodes:

```
$ hostname
jwlogin02.juwels
$ srun -A training2436 --reservation hands-on-cluster-YYYYMMDD hostname
srun: job 9792359 queued and waiting for resources
srun: job 9792359 has been allocated resources
jwc06n213.juwels
```

To submit to JUWELS Booster, you want to be logged in to the Booster login nodes and you have to specify the number of GPUs you want to use

```
$ hostname
jwlogin24.juwels
$ srun -A training2436 --reservation hands-on-booster-YYYYMMDD --gres gpu:4
hostname
```

```
srun: job 4575092 queued and waiting for resources
srun: job 4575092 has been allocated resources
jwb0053.juwels
```

Please keep these differences in mind if you are using JUWELS Booster, they will not be repeated in further examples.

Invocations of the `srun` command have the following syntax:

```
$ srun <srun options...> <program> <program options...>
```

Above we have seen four `srun` options:

- `-A` (short for `--account`) to charge the resources consumed by the computation to the budget allotted to this course (if you have used `jutil env activate -A training2436` earlier on, you do not need this).

> **INFO**
>
> The training account budget can be used till the end of the month. After one would need to specify another budget from an active compute time project.

- `--reservation` to use nodes which have been set aside for this course. For this course we have active reservations for the following systems: JURECA, JUWELS Cluster, JUWELS Booster and JUSUF.

> **INFO**
>
> For JURECA and JUSUF use the following reservation: `hands-on-YYYYMMDD`. To work on JUWELS Cluster or Booster modules, you have to use `hands-on-cluster-YYYYMMDD` or `hands-on-booster-YYYYMMDD` respectively. Do not forget to replace `YYYYMMDD`, where `YYYY` and `MM` and `DD` are the current year and month and day in the Gregorian calendar, e.g. `20240522`.

> **WARNING**
>
> The reservation is active only during the hands-on sessions 9:00-12:00. Outside those time slots everything can be equally done simply removing the `--reservation` option altogether.

- `--partition` specifies which set of compute nodes to request resources from. We typically group nodes of the same hardware type into a partition.
- `--gres` specifies additional resources, other than compute nodes, in this case the presence of four GPUs in the compute nodes.

For the `<program>` we used `hostname` with no arguments of its own.

To run more parallel instances of a program, increase the number of Slurm *tasks* using the `-n` option to `srun`:

```
$ srun --label -A training2436 --reservation hands-on-cluster-YYYYMMDD -n 10
hostname
srun: job 3472812 queued and waiting for resources
srun: job 3472812 has been allocated resources
8: jwc00n002.juwels
9: jwc00n002.juwels
0: jwc00n002.juwels
1: jwc00n002.juwels
6: jwc00n002.juwels
3: jwc00n002.juwels
5: jwc00n002.juwels
2: jwc00n002.juwels
7: jwc00n002.juwels
4: jwc00n002.juwels
```

If you do not tell Slurm that your commands are multi-threaded (`hostname` is not), it will assume each task only needs a single CPU core and pack as many as possible into a node.

> **INFO**
>
> Note also the `--label` option to `srun` which prefixes every line of output by a number that identifies the task that generated the output.

Running more tasks than will fit on a single node will allocate two nodes and split the tasks between nodes:

```
$ srun --label -A training2436 --reservation hands-on-cluster-YYYYMMDD -n 100
hostname
srun: job 3473040 queued and waiting for resources
srun: job 3473040 has been allocated resources
 0: jwc00n007.juwels
```

```
[...]
50: jwc00n008.juwels
[...]
```

Allocations always contain entire nodes exclusively. So your jobs should request a number of tasks that is divisible by the number of tasks which can fit on a node to avoid losing parts of your budget. Running over multiple nodes without intending to is also likely to degrade performance.

You can now also use `srun` to run the `hellompi` program introduced in the previous section on deploying custom software:

```
$ srun -A training2436 --reservation hands-on-cluster-YYYYMMDD -n 5 ./hellompi
srun: job 3471349 queued and waiting for resources
srun: job 3471349 has been allocated resources
hello from process 4 of 5
hello from process 0 of 5
hello from process 3 of 5
hello from process 1 of 5
hello from process 2 of 5
```

Interlude: Partitions

The systems at JSC typically provide more than one pool of resources, called *partitions*. The resources in the different partitions might have different hardware characteristics or cater to different use cases.

The previous examples were run on the default partition of the system you are using, `batch` on JUWELS Cluster and JUSUF Cluster, `booster` on JUWELS Booster and `dc-cpu` on JURECA. You can find out what partitions the different systems have in the documentation for JURECA, JUWELS, and JUSUF.

Of particular interest are the development partitions on each system (look for `devel` in their name). These consist of a small number of nodes which are set aside to prioritise small and short jobs which are typically run as part of development work on your application rather than production use of the system.

Try running the previous two examples using `hostname` on the development partition of your system by specifying it through `srun`'s `-p` option.

> **WARNING**

> Remove the `--reservation` option, because the reservation does not include nodes from the development partition.

We will have a look at other partitions later.

Interactive allocation

If, instead of requesting resources anew everytime you want to run a command on the compute nodes, you want to hold on to a specific set of resources and quickly dispatch a series of commands to run on them, you can use the `salloc` command in combination with `srun`. To do so, you specify the amount of resources you will need for your computations when calling `salloc`. `salloc` will request these resources from the resource manager and block until they are available. Then it will launch a new shell for you from which you can call `srun`, possibly multiple times, to dispatch commands onto the allocated resources.

In the previous section you took a task-centric approach to requesting resources by using the `-n` command line argument to `srun` to specify a number of tasks you want to run. This approach also works with `salloc` -- in fact the way you specify resources is mostly the same between all different modes Slurm supports. However, since the number of CPU cores is always rounded up to the next multiple of the number of CPU cores in a single node, it might make sense to take a hardware centric approach to requesting resources. Using the `-N` command line argument, you can request a number of nodes from the resource manager (remember to specify `--gres gpu:4` for JUWELS Booster):

```
$ salloc -A training2436 --reservation hands-on-cluster-YYYYMMDD -N 1
salloc: Pending job allocation 3475519
salloc: job 3475519 queued and waiting for resources
salloc: job 3475519 has been allocated resources
salloc: Granted job allocation 3475519
salloc: Waiting for resource configuration
salloc: Nodes jwc00n014 are ready for job
$
```

At the new shell prompt, you can use `srun` to run commands without having to specify resources again:

```
$ srun hostname
jwc00n014.juwels
```

By default, Slurm assumes that your program is single-threaded, but still only launches one task per allocated node. This can be changed by specifying the CPUs per task with the `-c` argument.

```
$ srun -c 1 hostname
jwc00n014.juwels
[...]
jwc00n014.juwels
```

If you want to run several commands on a node without having to go through `srun` each time, you can use `srun` to launch a shell on the node:

```
$ srun --pty --cpu-bind=none /bin/bash
$ hostname
jwc00n014.juwels
$ exit
```

> **WARNING**
>
> When using `srun` in one-shot mode, your account is charged for the time it takes to run the associated command. With `salloc` your account is charged for the duration of time you spend in the shell launched by `salloc` (and commands launched by that shell). Once you are done with the allocated resources, do not forget to exit from the shell:

```
$ exit
salloc: Relinquishing job allocation 3475519
salloc: Job allocation 3475519 has been revoked.
$ printenv SLURM_JOB_ID
$
```

If the `printenv SLURM_JOB_ID` prints a number, then you are still inside the allocation.

Batch mode

If the system is relatively quiet and you are asking for a small amount of resources (or working on the `devel` partitions), `salloc` or one-shot `srun` should allow you to work with the system more or less interactively. Large production jobs on the other hand might have to wait an uncomfortably long time for resources and so

running them interactively is not really convenient. Imagine you `salloc` a large number of nodes and while you wait you decide to go have lunch. If the allocation comes through while you are away you will still be charged for the resources even if they idle.

Also, if the systems were only used interactively, resource utilization would drop off in the late hours of the evening and ramp up in the mornings.

To enable better resource utilization and allow users to schedule jobs asynchronously, Slurm offers a batch mode through the `sbatch` command. It too requests resources from the resource manager, but unlike `salloc` which presents you with an interactive shell prompt from which you can call `srun`, `sbatch` runs commands from a shell script (the "job script") without needing user intervention. The resources can be specified as command line arguments to `sbatch`, same as with `salloc` and `srun`, but can also be described in the job script. Open a new shell script in the editor:

```
($ module load nano)
$ nano testjob.sh
```

And enter the following script:

```
#!/bin/bash
#SBATCH --account=training2436
#SBATCH --reservation=hands-on-cluster-YYYYMMDD
#SBATCH --nodes=2
#SBATCH --cpus-per-task=1
#SBATCH --output=mpi-out.%j
#SBATCH --error=mpi-err.%j
#SBATCH --time=00:05:00

module load GCC ParaStationMPI

srun ./hellompi
```

> **WARNING**
>
> Always use the same software stack (e.g. compiler, MPI) that was used to build the software to ensure compatibility and optimal performance. Different versions can cause errors or degrade performance.

Remember to specify `gpu:4` `gres` for JUWELS Booster.

Then save the script and submit it for execution with:

```
$ sbatch testjob.sh
Submitted batch job 3476793
```

After the first line (the shebang line) the script contains specially formatted comments that act like arguments to `sbatch`. These arguments are written in their long form. Previously, you used the short form (e.g. `-N` is the same as `--nodes`). After the block of comments come regular shell commands. Inside the job script, we use the `module` command to make the software modules needed by the job programs available (here the compiler with its runtime libraries and an MPI library). The tasks are once again created using the `srun` command which works the same as before.

The job created by `sbatch` has to wait in a queue until the necessary resources become available. Use the `squeue` command to inspect the queue:

```
$ squeue -u $USER
             JOBID PARTITION     NAME     USER ST       TIME  NODES
NODELIST(REASON)
           3476793     batch testjob. steinbus PD       0:00      2 (Priority)
```

> **TIP**
>
> You can use the `watch squeue` command, which continuously updates and displays information about the status of jobs. It refreshes the output at regular intervals, allowing you to monitor changes in real time.
>
> To exit `watch squeue` you can press `Ctrl + C`. This command interrupts the execution of `watch` and you return to the regular command prompt.

You might have to wait for a while, but eventually your job will be run. While your job is pending in the queue or already running you can execute another command to retrieve further information about your job:

```
$ scontrol show job <JOBID>
```

Once it is running, you will find two files next to the job script, `mpi-err.XXXXXXX` and `mpi-out.XXXXXXX` where `X` are decimal digits. These contain what was written to the standard error and output streams by

your job. Should you need access to the hardware during job execution check out the `sgoto --help` command to log into a compute node during job execution.

Affinity and multi-threading

Computers today are typically equipped with multi-core CPUs which can work on multiple streams of instructions at the same time. The operating system is in charge of deciding which program gets to use which CPU core at a given point in time. Usually, it will let those programs which need access to resources run wherever resources are available, meaning one and the same program can end up using different CPU cores at different points in time. On a desktop machine this is not a problem. In fact it is a good thing, since we typically run far more programs than we have CPU cores available.

In an HPC setting things are different in that the workloads are adapted to use a number of processes or threads which matches the number of CPU cores (normally, you will have `n_processes x n_threads = n_nodes x n_CPU_cores_per_node`). If there is exactly one process or thread per CPU core, it would be wasteful to shuffle them around between different CPU cores. In order to avoid this shuffling, the resource manager assigns to the processes that it spawns an *affinity mask*. An affinity mask is a set of numbers identifying the CPU cores a process is allowed to use. By default, Slurm assumes that the processes you create are single threaded and gives each process access to a single CPU core. Allocate a node for playing around with this mechanism:

```
$ salloc -A training2436 --reservation hands-on-cluster-YYYYMMDD -N 1
salloc: Pending job allocation 3499694
salloc: job 3499694 queued and waiting for resources
salloc: job 3499694 has been allocated resources
salloc: Granted job allocation 3499694
salloc: Waiting for resource configuration
salloc: Nodes jwc00n001 are ready for job
```

Use the `numactl` command to inspect the affinity masks created by Slurm:

```
$ srun --label numactl --show
0: policy: default
0: preferred node: current
0: physcpubind: 0
0: cpubind: 0
0: nodebind: 0
0: membind: 0 1
```

The identifiers of accessible CPU cores are listed in `physcpubind`. Here, the single process that is created has access to a single CPU core, `0`. Now, confirm that different processes will get access to different CPU cores:

```
$ srun --label -n 3 numactl --show
2: policy: default
2: preferred node: current
2: physcpubind: 1
2: cpubind: 0
2: nodebind: 0
2: membind: 0 1
1: policy: default
1: preferred node: current
1: physcpubind: 24
1: cpubind: 1
1: nodebind: 1
1: membind: 0 1
0: policy: default
0: preferred node: current
0: physcpubind: 0
0: cpubind: 0
0: nodebind: 0
0: membind: 0 1
```

The three processes get access to CPU cores `0`, `1`, and `24` respectively. If your processes are not single-threaded, you will have to give them access to more CPU cores (otherwise all threads will run on the same CPU core). This can be done using Slurm's `--cpus-per-task` parameter, or `-c`:

```
$ srun --label -c 24 numactl --show
1: policy: default
1: preferred node: current
1: physcpubind: 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44
45 46 47
1: cpubind: 1
1: nodebind: 1
1: membind: 0 1
0: policy: default
0: preferred node: current
0: physcpubind: 0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
0: cpubind: 0
0: nodebind: 0
```

```
0: membind: 0 1
2: policy: default
2: preferred node: current
2: physcpubind: 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68
69 70 71
2: cpubind: 0
2: nodebind: 0
2: membind: 0 1
3: policy: default
3: preferred node: current
3: physcpubind: 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92
93 94 95
3: cpubind: 1
3: nodebind: 1
3: membind: 0 1
```

INFO

Note how once you specify the number of CPU cores per task, Slurm switches its behavior from creating one process per node to filling the node with as many processes as possible. Each process gets access to 24 different CPU cores.

Copy the following small program into a file `hellohybrid.c`:

```c
#include <stdio.h>
#include <mpi.h>
#include <omp.h>

int main(int argc, char* argv[]) {
  MPI_Init(&argc, &argv);

  int r, s;
  MPI_Comm_rank(MPI_COMM_WORLD, &r);
  MPI_Comm_size(MPI_COMM_WORLD, &s);
  #pragma omp parallel
  if (!omp_get_thread_num())
    printf(
      "hello from process %d of %d, using %d threads\n",
      r, s, omp_get_num_threads()
    );
```

```
  MPI_Finalize();
}
```

And compile it with:

```
$ mpicc -fopenmp -o hellohybrid hellohybrid.c
```

Now run the program:

```
$ srun ./hellohybrid
hello from process 0 of 1, using 1 threads
```

Again, using default settings, Slurm creates a single process and restricts it to a single CPU core. The OpenMP run time library supports shared-memory multiprocessing and allows to query the number of CPU cores accessible to the process. It creates just as many threads (here only one). If you specify a number of CPU cores per process this changes:

```
$ srun -c 24 ./hellohybrid
hello from process 2 of 4, using 24 threads
hello from process 0 of 4, using 24 threads
hello from process 3 of 4, using 24 threads
hello from process 1 of 4, using 24 threads
```

Once more, Slurm fills the node with four processes having appropriate affinity masks. The OpenMP run time figures out that each process is allowed to use 24 CPU cores and creates a team of threads to fill those CPU cores.

> **WARNING**
>
> Do not forget to exit your salloc session at this point.

JSC Affinity Tools

Since we are using psslurm we have implemented a few options different than the default in Slurm. For this reason we are offering two tools that can help you to understand the process affinity on our systems:

1. The command line executable: `psslurmgetbind`

2. An online pinning tool

> **WARNING**
>
> After the update to Slurm version 22.05, the pinning scheme has changed. The pinning tool is still available but it does not give accurate results at the moment.

Further information can be found in the "Processor Affinity" chapter of the corresponding System Documentation.

Further reading

Our online documentation has more information on working with the resource manager. It has detailed lists with the hardware available in various partitions as well as job limits. Also, it discusses advanced topics like multiple job steps, dependency chains and heterogeneous jobs. If you want more details, you can find the documentation for our various systems here:

- JUWELS documentation: Batch system
- JURECA documentation: Batch system
- JUSUF documentation: Batch system

You can also have a look at the official Slurm documentation.

LLview - Detailed Job Reporting

LLview is an excellent tool that provides an overview of currently running and finished jobs, including detailed job reports plus obscure error messages that are hard to find for users. Your jobs crash and you do not know why? This is the first place to check. There is a website for each of our large systems. You can find the link for every system at the lower left corner of the documentation webpage of LLview. To begin check out your system of interest, ideally one you have run jobs on.

Currently Active Jobs

When opening LLview by default it will first show you the list of your currently active jobs, either pending or running. If you are the Principal Investigator (PI) or Project Administrator (PA) for a project and you are in the project view you will see all active jobs from your project. Project mentors also have access to this view.

You filter the list based on the filters below any of the column headings. Clicking on any column heading will cause the jobs to be sorted in ascending or descending order, an arrow will appear next to the column title indicating either ascending (upwards-pointing arrow) or decending (downwards-pointing arrow). In the case a of sort conflict the submission time of a job is used to resolve the conflict, with jobs that were submitted more recently appearing above jobs that started earlier, if sorted ascending. By default jobs are sorted according to ascending job start submit time with your most recently submitted jobs at the top.

Values in red in the list indicate that something may be wrong. For example the average load on a node may be high. Note that this is reported in fractions of the utilization of a single core. A 1.0 therefore means that a single core was fully utilized. This value should ideally be as close as possible to the number of cores a node has.

Important to note is also the state of the job, which you can find on the right. The job can either be pending, if it has been submitted, but is not yet running, or running. Sometimes it can also be completed (CMPL) or error if the job has finished successfully or errored out respectively. These jobs will then be shortly removed from this list.

Clicking on any of the jobs will cause the graphs to be populated at the bottom of the page if the job ran for more than a couple of minutes, depends on how often LLview is able to query the system state. The "Load on Node" gives you an idea of the evolution of the load placed on a node over time. The other two graphs show the evolution of I/O bandwidth and number of I/O operations per second for various storage tiers, you can change the storage tier by clicking on one of them in the bottom right (HOME, PROJECT, SCRATCH, FASTDATA).

The two right-most columns can contain small pictograms, one of a chart and the other is the Adobe PDF icon. If they are available it means that job reports are available for the jobs. The chart pictogram takes you to a webpage-based interactive report. The PDF icon downloads a non-interactive PDF report. These contain detailed information on the job as well as error codes. They with a textual header listing important information regarding the job. Then, if the job ran long enough graphs of various metrics, like CPU and GPU usage, are presented. Finally a list of nodes and error messages is included at the end. The error messages are especially important as these can be Slurm diagnostic error messages that might be difficult for users to find. For more information see the detailed-report documentation.

Jobs Ended Today

This is the same view as the currently active jobs view but for jobs that have finished in the last 24 hours.

Jobs < 3 weeks

This is the same view as the currently active jobs view but for jobs that have finished in the last three weeks.

Live

Here you can see a live view of the system and how jobs are distributed across the supercomputer on a rack level on the left. At the bottom on the left is a scheduling prediction which shows when which jobs are expected to be scheduled. Large jobs also have their names displayed.

On the right you can see the color-coded queue of all jobs, including currently running and finalizing jobs. Clicking on a column title sorts the list either ascending (upwards-pointing arrow) or descending (downwards-pointing arrow).

If this tab has a drop down then you can see different queues, for example for the JUWELS cluster you will be able to see the `batch` and `GPU` queues.

> **INFO**
>
> Note that only the main queues are shown. Queues like the `devel` queue for development are not shown. To see these queues you will have to login to the systems and use `squeue`.

Queue Tab

In the queue tab you can see the queue for all partitions you can submit to. Unlike (Live) the results are not filtered according to the partition and the queue is displayed in the typical LLview fashion.

Further reading

Here you can find the documentation for LLview.

Using GPUs

All systems at JSC have nodes which are accelerated by General Purpose Graphics Processing Units (GPGPUs or just GPUs). In this section, we will discuss basic aspects of using them, inspecting them during execution, assigning them to particular MPI tasks and talking a little about network architecture, which can be important for efficient usage.

Since the GPUs are all made by NVIDIA, using them is accomplished through their CUDA SDK. CUDA is available as a module:

```
$ module load CUDA
```

This example is executed on the JUWELS booster module. To demonstrate how to compile and run a program that uses GPUs, we will use one of the examples included in CUDA. To do this, we must additionally load the compiler `NVHPC` and the MPI version `ParaStationMPI`.
Additionally, we load a settings module that ensures our MPI implentation is properly set up to use CUDA.
The samples directory of the CUDA installation has a number of example codes you can play and learn with.

Here we compile the example using a combination of C++, MPI and CUDA code. We load the necessary modules, navigate into our individual user directories for this project, download sample codes from Nvidia using git, and finally navigate into the download folder and build this software:

```
$ module load NVHPC ParaStationMPI MPI-settings/CUDA
$ cd $PROJECT_training2436/$USER
$ git clone https://github.com/NVIDIA/cuda-samples.git
$ cd $PROJECT_training2436/$USER/cuda-samples/Samples/0_Introduction/simpleMPI
$ make
/p/software/jurecadc/stages/2024/software/psmpi/5.9.2-1-NVHPC-23.7-CUDA-
12/bin/mpicxx -I../../../Common    -o simpleMPI_mpi.o -c simpleMPI.cpp
/p/software/jurecadc/stages/2024/software/CUDA/12/bin/nvcc -ccbin g++ -
I../../../Common  -m64    --threads 0 --std=c++11 -Xcompiler -fPIE -gencode
arch=compute_50,code=sm_50 -gencode arch=compute_52,code=sm_52 -gencode
arch=compute_60,code=sm_60 -gencode arch=compute_61,code=sm_61 -gencode
arch=compute_70,code=sm_70 -gencode arch=compute_75,code=sm_75 -gencode
arch=compute_80,code=sm_80 -gencode arch=compute_86,code=sm_86 -gencode
arch=compute_89,code=sm_89 -gencode arch=compute_90,code=sm_90 -gencode
arch=compute_90,code=compute_90 -o simpleMPI.o -c simpleMPI.cu
```

```
/p/software/jurecadc/stages/2024/software/psmpi/5.9.2-1-NVHPC-23.7-CUDA-
12/bin/mpicxx    -o simpleMPI simpleMPI_mpi.o simpleMPI.o  -
L/p/software/jurecadc/stages/2024/software/CUDA/12/lib -
L/p/software/jurecadc/stages/2024/software/CUDA/12/lib64 -lcudart
mkdir -p ../../../bin/x86_64/linux/release
cp simpleMPI ../../../bin/x86_64/linux/release
```

There should now be an executable called `simpleMPI` inside the `simpleMPI` directory. To run the program, use `srun` like before:

```
$ srun -A training2436 -p <gpu partition> --gres gpu:4 -N 1 -n 4 ./simpleMPI
[...]
Running on 4 nodes
Average of square roots is: 0.667305
PASSED
```

In this command `-A` indicates the account that the compute time is taken from.
`-p` indicates the partition (a specific queue in the cluster, either a "normal" one like `batch`, for particular uses like development or for particular resources, like more RAM, or GPUs).
A partition that contains nodes equipped with GPUs must be specified - `-p develgpus` for JUWELS and JUSUF, `-p dc-gpu-devel` for JURECA, or `-p develbooster` for JUWELS Booster.
You must specify the number of GPUs you want the command being run within `srun` to have access to. `--gres gpu:4` makes 4 GPUs available to the command being run.
It can be useful to set this differently sometimes, for example if you want to run multiple independent tasks on each separate GPU on a node, using `--gres gpu:1`, or on JUSUF, which only has a single GPU per node on its GPU partition.
`-N` indicates the number of nodes, and `-n` the number of tasks, as before.
`./simpleMPI` runs the program we compiled, from the directory we are currently in.

> **INFO**
>
> **Note:** In this output *nodes* means *MPI tasks*. The developers of this code have assumed implicitly that only one GPU with one MPI task is located on one node when creating this software.

GPU Inspection During Execution

LLview is a feature-rich tool we recommend you familiarise yourself with, to monitor your jobs and extract most of the data relevant for many monitoring use cases with low effort from the user side. Nevertheless, logging into the compute nodes during job execution is easy and comfortable and, in some cases, necessary.

In the following bash session on the JUWELS booster a job is initiated through `srun` in the background of this login node session (`&` at the end of the command).
Just hit enter after this line to retrieve the normal command line. The job is simply waiting 600 seconds or 10 minutes - we won't do any useful work, this is just to demonstrate accessing a node of a running job.
We then use `sgoto` to access a specific node during execution.
We then show the usage of the GPUs on that node with `nvidia-smi`.
This command is just to act as an example, and can be exchanged with anything you would like to do on the compute node during job execution.
Afterwards we log out from the compute node with `exit`, put the executed `srun` command from the background to the foreground with `fg` and cancel this execution by hitting `CTRL-C` a couple of times until the normal command line is available.

If you want to try this example yourself, remember top change the sgoto command to the appropriate JobID, followed by a 0 (indicating the first, and in this case only, node in the job).

```
$ srun -N 1 -n 1 -t 00:10:00 -A training2436 -p develbooster --gres=gpu:4 sleep
600 &
[1] 25114
srun: job 5535332 queued and waiting for resources
srun: job 5535332 has been allocated resources
$ sgoto 5535332 0
$ nvidia-smi
Thu May 12 08:49:34 2022
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 510.47.03    Driver Version: 510.47.03    CUDA Version: 11.6     |
|-------------------------------+----------------------+----------------------+
| GPU  Name        Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf  Pwr:Usage/Cap|         Memory-Usage | GPU-Util  Compute M. |
|                               |                      |               MIG M. |
|===============================+======================+======================|
|   0  NVIDIA A100-SXM...  On   | 00000000:03:00.0 Off |                    0 |
| N/A   44C    P0    55W / 400W |      0MiB / 40960MiB |      0%      Default |
|                               |                      |             Disabled |
+-------------------------------+----------------------+----------------------+
|   1  NVIDIA A100-SXM...  On   | 00000000:44:00.0 Off |                    0 |
| N/A   44C    P0    54W / 400W |      0MiB / 40960MiB |      0%      Default |
```

```
|                               |                      |             Disabled |
+-------------------------------+----------------------+----------------------+
|   2  NVIDIA A100-SXM...  On   | 00000000:84:00.0 Off |                    0 |
| N/A   45C    P0    58W / 400W |      0MiB / 40960MiB |      0%      Default |
|                               |                      |             Disabled |
+-------------------------------+----------------------+----------------------+
|   3  NVIDIA A100-SXM...  On   | 00000000:C4:00.0 Off |                    0 |
| N/A   44C    P0    58W / 400W |      0MiB / 40960MiB |      0%      Default |
|                               |                      |             Disabled |
+-------------------------------+----------------------+----------------------+

+-----------------------------------------------------------------------------+
| Processes:                                                                  |
|  GPU   GI   CI        PID   Type   Process name                  GPU Memory |
|        ID   ID                                                   Usage      |
|=============================================================================|
|  No running processes found                                                 |
+-----------------------------------------------------------------------------+
$ exit
logout
$ fg
srun -N 1 -n 1 -t 00:10:00 -A training2436 -p develbooster --gres=gpu:4 sleep
500
^Csrun: sending Ctrl-C to StepId=5535332.0
srun: forcing job termination
srun: Job step aborted: Waiting up to 6 seconds for job step to finish.
```

`sgoto` takes the job id as the first argument and the node number within the job as the second argument where the counting starts with 0.
`nvidia-smi` prints some useful information about available GPUs on a node, like temperature, memory usage, currently running processes and power consumption.

> **NOTE**
>
> In the example above, `nvidia-smi` shows 0% utilisation because the GPUs are not being used. If GPUs were being used, the utilisation metrics displayed by `nvidia-smi` would be non-zero, reflecting the active use of GPU resources.

GPU Affinity

On systems with more than one GPU per node, a choice presents itself - which GPU should be visible to which application task(s)?
This is controlled through the environment variable `CUDA_VISIBLE_DEVICES`, which can be set to a comma separated list of integers identifying devices to be visible to a task.
You can manually define this variable before running your tasks with `srun` if the pinning is going to be the same for every task.

Let us investigate further on this with a practical example.
First, we prepare a device query example, (remembering to reload the modules from the first example if you are completing this in a different session).

```
$ cd $PROJECT_training2436/$USER/cuda-
samples/Samples/1_Utilities/deviceQueryDrv/
make
/p/software/jurecadc/stages/2024/software/CUDA/12/bin/nvcc -ccbin g++ -
I../../../Common  -m64    --threads 0 --std=c++11 -gencode
arch=compute_50,code=compute_50 -o deviceQueryDrv.o -c deviceQueryDrv.cpp
/p/software/jurecadc/stages/2024/software/CUDA/12/bin/nvcc -ccbin g++   -m64
-gencode arch=compute_50,code=compute_50 -o deviceQueryDrv deviceQueryDrv.o  -
L/p/software/jurecadc/stages/2024/software/CUDA/12/lib64/stubs -lcuda
mkdir -p ../../../bin/x86_64/linux/release
cp deviceQueryDrv ../../../bin/x86_64/linux/release
```

This will create the executable `deviceQueryDrv`. During the execution of `deviceQueryDrv` all visible CUDA devices are queried.
The following sbatch script `gpuAffinityTest.sbatch`, written for the JUWELS Booster, executes the assisting bash script `gpuAffinityHelper.bash` which, in turn executes `deviceQueryDrv`.
We perform this in this manner, as we wish to get information from multiple commands inside each task, run in parallel.

```
#!/bin/bash
#SBATCH --ntasks=1
#SBATCH --nodes=1
#SBATCH --time=00:01:00
#SBATCH --partition=develbooster
#SBATCH --gres=gpu:4
#SBATCH -A training2436

module load CUDA NVHPC ParaStationMPI MPI-settings/CUDA
```

```
srun bash gpuAffinityHelper.bash
```

The helper script `gpuAffinityHelper.bash` will be needed to print the environment variable `CUDA_VISIBLE_DEVICES` for every MPI task initiated.

```
#!/bin/bash

#export CUDA_VISIBLE_DEVICES=<comma-separated list of visible gpus>
echo "MPI task" $SLURM_PROCID "with CUDA_VISIBLE_DEVICES ="
$CUDA_VISIBLE_DEVICES

./deviceQueryDrv
```

The automatically set environment variable `SLURM_PROCID` contains the current MPI task ID.
The definition of the environment variable `CUDA_VISIBLE_DEVICES` will be performed by you.
By uncommenting the commented line within `gpuAffinityTest.bash`, `CUDA_VISIBLE_DEVICES` can be defined manually for every task. This allows to you to specify which GPUs are visible for which MPI tasks.
For the moment, leave it commented out.

Execute this example for `ntasks=1` in `gpuAffinityTest.sbatch` and study the output file.

```
MPI task 0 with CUDA_VISIBLE_DEVICES = 0,1,2,3
./deviceQueryDrv Starting...

 CUDA Device Query (Driver API) statically linked version
 Detected 4 CUDA Capable device(s)

 Device 0: "NVIDIA A100-SXM4-40GB"
 [...]
 Device PCI Domain ID / Bus ID / location ID:   0 / 3 / 0
 [...]
 Device 1: "NVIDIA A100-SXM4-40GB"
 [...]
 Device PCI Domain ID / Bus ID / location ID:   0 / 68 / 0
 [...]
 Device 2: "NVIDIA A100-SXM4-40GB"
 [...]
 Device PCI Domain ID / Bus ID / location ID:   0 / 132 / 0
 [...]
```

```
 Device 3: "NVIDIA A100-SXM4-40GB"
 [...]
 Device PCI Domain ID / Bus ID / location ID:   0 / 196 / 0
 [...]
> Peer-to-Peer (P2P) access from NVIDIA A100-SXM4-40GB (GPU0) -> NVIDIA A100-
SXM4-40GB (GPU1) : Yes
> Peer-to-Peer (P2P) access from NVIDIA A100-SXM4-40GB (GPU0) -> NVIDIA A100-
SXM4-40GB (GPU2) : Yes
[...]
Result = PASS
```

Note the value for `CUDA_VISIBLE_DEVICES` at the beginning. For this single MPI task all 4 GPUs are visible.
Additionally, we can see the Bus IDs for all of the GPUs on this node, which can be useful information but is not important for this tutorial.
At the end of the file you can also see the successful interconnectivity tests of the GPUs.

If you do not manually define the environment variable `CUDA_VISIBLE_DEVICES` yourself, `srun` will provide a default:

- for jobs with a single task (`-n 1`) all devices will be visible `CUDA_VISIBLE_DEVICES=0,1,2,3` to that task.
- for all other jobs, only a single device will be visible per task, with the same device being visible to multiple tasks if there are more tasks than GPUs.

Tasks will only have access to the GPUs in the environment variable `CUDA_VISIBLE_DEVICES` for that specific task.

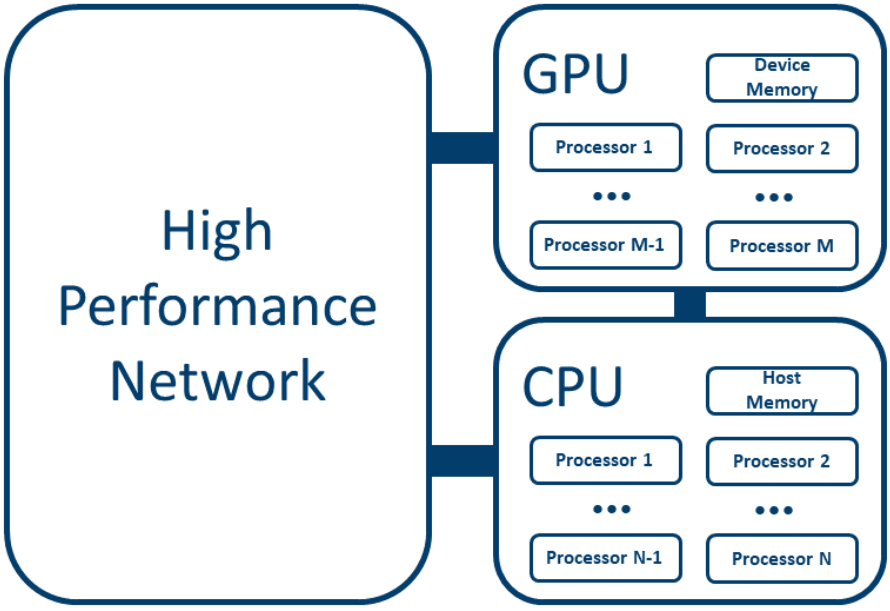
By playing a little with the number of tasks within the scripts stated above you can study the behaviour of the GPU pinning and confirm the default. If this default is not suited to your needs you can uncomment the line

```
export CUDA_VISIBLE_DEVICES=<comma-separated list of visible gpus>
```

and define `CUDA_VISIBLE_DEVICES` as you wish.

Network Architecture Study

The JUWELS Booster delivers a network infrastructure allowing direct data exchange between the GPUs, which can accelerate a workload. These GPUs have internal hardware to store data and are directly connected to the high-performance network (other nodes, storage, etc.).



With this in mind, it becomes clear that the traditional data exchange between two GPUs, with an intermediate hop of data on host memory, will lead to less-than-ideal performance. CUDA-awareness of an MPI implementation is a vital part to increase data exchange performance between GPUs. On JSC supercomputing resources there are preinstalled implementations for CUDA-aware MPI, like `ParaStationMPI` and `OpenMPI`. To enable CUDA-awareness, you need to load the module MPI-settings/CUDA. CUDA-awareness enables passing a pointer to data on the GPU directly to an MPI-directive.

The following example `mpiBroadcasting.cpp` performs three different measurements for speed of data exchange by use of the MPI directive `MPI_Bcast`. `MPI_Bcast` broadcasts data from one MPI process to other MPI processes. In the source code below, at first, data between host memories is exchanged. Secondly, data between GPUs is exchanged by hopping intermediately onto the host memory. At last, data between GPUs is exchanged by use of the direct network connection between the GPUs.

```
#include <stdio.h>
#include <string.h>
#include <mpi.h>
#include <time.h>
```

```
#include "cuda_runtime.h"

int main(int argc, char *argv[])
{
  clock_t start, end; // Time stamps
  double cpu_time_used;
  int myrank;
  int N=100000000; //# elements to broadcast per repetition
  //# broadcasting several repetitions since maximal size of
  // elements to send is restricted through MPI
  int Nbcast=20;

  double *x = new double[N]; // Allocate space on host memory
  double *d_x; // Array on device
  cudaMalloc(&d_x, N*sizeof(double)); // Allocate space on device

  for (int i=0;i<N;i++) x[i] = 1.0f; // prefilling data into allocated memory
  // send data into device
  cudaMemcpy(d_x, x, N*sizeof(double), cudaMemcpyHostToDevice);

  MPI_Init(&argc, &argv);
  MPI_Comm_rank(MPI_COMM_WORLD, &myrank);

  // Initial unmeasured broadcasting due to
  // setup offsets in initializing connections
  for(int i=0;i<Nbcast;i++) {
    MPI_Bcast(x, N, MPI_DOUBLE, 0, MPI_COMM_WORLD);
    MPI_Barrier(MPI_COMM_WORLD);
    MPI_Bcast(d_x, N, MPI_DOUBLE, 0, MPI_COMM_WORLD);
    MPI_Barrier(MPI_COMM_WORLD);
  }

  // host to host memory measurement
  start = clock(); // set the start time
  for(int i=0;i<Nbcast;i++) {
    MPI_Bcast(x, N, MPI_DOUBLE, 0, MPI_COMM_WORLD);
    MPI_Barrier(MPI_COMM_WORLD);
  }
  end = clock(); // set the end time
  // compute cpu time elapsed during the broadcasting
  cpu_time_used = ((double) (end - start)) / CLOCKS_PER_SEC;
  if (myrank == 0) printf("Broadcasting to all host memories \
    took %f seconds. \n", cpu_time_used);

  // device to device with intermediate copy to/from host
```

```
  start = clock();
  for(int i=0;i<Nbcast;i++) {
    cudaMemcpy(x, d_x, N*sizeof(double), cudaMemcpyDeviceToHost);
    MPI_Bcast(x, N, MPI_DOUBLE, 0, MPI_COMM_WORLD);
    cudaMemcpy(d_x, x, N*sizeof(double), cudaMemcpyHostToDevice);
    MPI_Barrier(MPI_COMM_WORLD);
  }
  end = clock();
  cpu_time_used = ((double) (end - start)) / CLOCKS_PER_SEC;
  if (myrank == 0) printf("Broadcasting to all GPUs took %f seconds \
    with intermediate copy to host memory. \n", cpu_time_used);

  // device to device through direct network connection of the GPUs
  start = clock();
  for(int i=0;i<Nbcast;i++) {
    MPI_Bcast(d_x, N, MPI_DOUBLE, 0, MPI_COMM_WORLD);
    MPI_Barrier(MPI_COMM_WORLD);
  }
  end = clock();
  cpu_time_used = ((double) (end - start)) / CLOCKS_PER_SEC;
  if (myrank == 0) printf("Broadcasting to all GPUs took %f \
    seconds. \n", cpu_time_used);

  // Release allocated memory space on host and device
  cudaFree(d_x);
  delete x;

  MPI_Finalize();
  return 0;
}
```

The initial broadcasts are needed to let the network establish connections between the MPI tasks, so it does not make sense to measure these. Some implementations of MPI are setting up network connections between MPI tasks only at first data exchange, to avoid setting up connections that are never required. This is an offset which is not planned to be measured here. `MPI_Barrier` directs all MPI tasks to wait until all data was broadcasted.
As a result there are three times measured and printed - host to host, GPU to GPU through the host, and direct GPU to GPU. This example is executed on 2 nodes with 4 tasks on every node, where each task occupies one GPU.

> ⚠ **WARNING**

> Note that we switch compiler at this stage, compared to previous instructions of this chapter.
>
> Use the same modules for compilation which you are planning to use for execution.

```
$ module load NVHPC CUDA OpenMPI
$ mpicxx -O0 -I$CUDA_HOME/include -L$CUDA_HOME/lib64 -lcudart -lcuda
mpiBroadcasting.cpp
$ srun -N 2 -n 8 -t 01:00:00 -A training2436 -p booster --gres=gpu:4 ./a.out
Broadcasting to all host memories took 4.526835 seconds.
Broadcasting to all GPUs took 7.481972 seconds with intermediate copy to host
memory.
Broadcasting to all GPUs took 2.625439 seconds.
```

The parameter `-O0` deactives any optimizations performed by the compiler, which is needed since a powerful compiler could know at compile time that the same data is initialized for all tasks and then sent around. This could lead to a deletion of the MPI directives at compile time leading to extremely small but erroneous time measurements. Other parts of this command are related to supplying the libraries on which `mpiBroadcasting.cpp` depends.

The data exchange directly from one GPU to another GPU is the fastest. Furthermore, the CPUs on the JUWELS Booster nodes have a relatively small compute performance, to avoid too much overhead and unnecessary power consumption. These nodes are designed intentionally such that as much workload and data exchange as possible should be performed by the GPUs.
You can study the source code and play around with this setup. This will give you valuable insights on how to develop your own software for execution on the JUWELS Booster.

Further reading

Our online documentation has more information on software modules. It lists the basic tool chains (compiler + communication library + math library) available on our systems and discusses using older software stages. If you want more details, you can find the documentation for our various systems here:

- JUWELS documentation: GPU Computing
- JURECA documentation: GPU Computing
- JUSUF documentation: GPU Computing

The CUDA SDK documentation gives you detailed information about how to develop CUDA code. There are also excellent articles in the web for learning CUDA like An Even Easier Introduction to CUDA or An

Introduction to CUDA-Aware MPI.

The JSC regularly offers CUDA courses for HPC, which are an ideal starting point to get into the topic.

Useful Links

In this chapter, you can find a useful collection of links to get more information about several topics. The slides of workshops held at JSC (also from this introductory workshop) you can find here. For the future, the regularly updated master of this working document you can find here. Keep in mind that some template words are left within the document on purpose. You will need to adjust them for your testcase.

System Documentation

JSC offers documentation for the production systems:

- JUWELS
- JURECA
- JUSUF

JSC Services

- JSC Service Status
- JuDoor
- Jupyter Lab
- HDF Cloud

Job Reporting

The Job Reporting service gives you access to PDF reports which contain certain performance metrics that the system automatically collects about your jobs. It also includes an overview over the system utilization and queue. You can access the Job Reporting service for the different systems here:

- JUWELS
- JURECA
- JUSUF

Apply for Computing Time

- The JSC web site describes how to apply for computing time.
- The JSC web site describes how to apply for test projects.

Apply for a Data Project

The JSC web site describes how to apply for a data project.

JSC Course Programme

JSC offers many courses throughout the year covering topics such as parallel programming, machine learning, and visualization. Please have a look at the course programme on the JSC web site.

Supercomputing Support

Our high-level support team supports the users in case of problems on our systems, e.g. porting of the application, parallelisation and performance issues as well as usage of the HPC system. So if you are having a question, you cannot sort out by yourself, by working through this document or by having a look into the documentation, just drop a mail to sc@fz-juelich.de.

AI

An AI-related collection of guides and recipes can be found here.

Manual software installation

- This example shows how to install software on JURECA using EasyBuild, but it
- This tutorial shows how to install additional python libraries via `pip`
- This tutorial shows how to configure a conda environment at a JSC supercomputer.