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Leibniz
Universität
Hannover

# Cluster System Handbook

Leibniz Universität IT Services
Scientific Computing Group

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# Contents

## Preface

This handbook is meant to facilitate your work with the cluster system of Leibniz Universität Hannover. Please take some time to read through this document and do not hesitate to contact the cluster team, cluster-help@luis.uni-hannover.de, if you have any questions. If you think you have no time at all, please make sure you are at least subscribed to the Cluster-News mailing list, in order to receive announcements concerning the cluster system.

Yours sincerely,
Cluster-Team

# I am a new user - Quick Start

Please note: If you have absolutely no time at all, at least read this one page. Please make sure, the following points are met.

- Did you receive an email, confirming your addition to the Cluster-News mailing list? Important announcements, for example maintenance periods, are announced on this list.
- Did you change your password? You can change your password using the command `passwd`.
- Consider the cluster system as a tool to facilitate your research. Mastering any tool takes time. Consider attending an introductory talk and reading this Cluster Handbook.

# About the cluster system

In order to meet the University's demand for computing resources with a lot of CPUs and memory, LUIS is operating a cluster system as part of the service Scientific Computing. All scientists of Leibniz University can use the cluster system for their research free of charge.

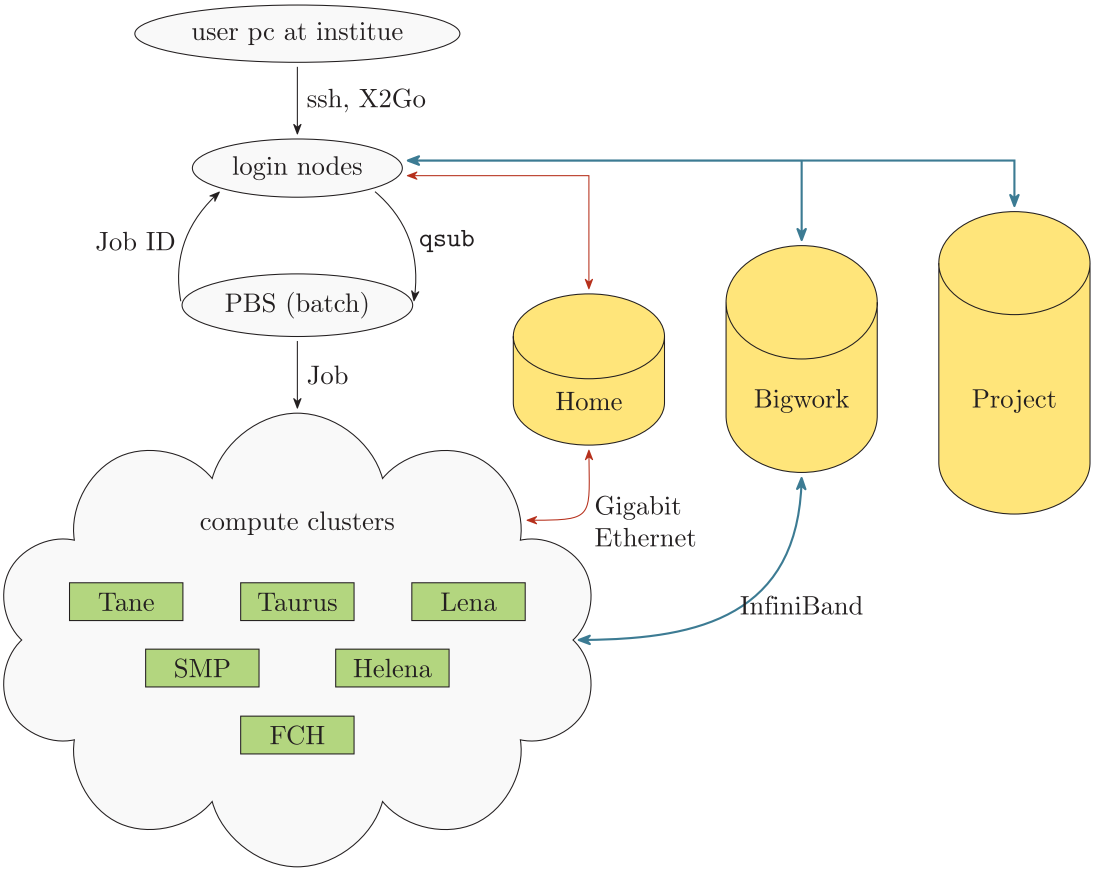


Figure 2.1: Sketch of the cluster system with it's individual components

Resources of the cluster system are largely a DFG major instrumentation. Therefore rules[1] for DFG major instrumentation apply when using the cluster system. Project leaders of your EDV-Project bear responsibility to comply with the DFG rules.

## 2.1 Getting Access

An EDV-Project is the framework under which you will conduct your work on the cluster system. Probably there is already an EDV-Project leader at your institute. In this case this person can create a cluster user account for you using BIAS. In case you need to apply for an EDV-Project yourself, please use form ORG.BEN 4[2].

Please note: Create only one user account per person.

[1] www.dfg.de

[2] User accounting on BIAS is not part of the service Scientific Computing and thus not part of the cluster system

## 2.2 What the cluster system may be used for

Parts of the cluster system are DFG major instrumentation, thus rules for DFG major instrumentation apply when using the cluster system. Furthermore software licenses are valid for research and teaching only. Accordingly the cluster system must only be used for research and teaching activities.

## 2.3 Current computing power

Currently the cluster system consists of the following compute resources:

- 3 Clusters for MPI jobs needing lots of CPUs
  - Lena: 80 nodes; 16 cores each @ 2.4 GHz; 64 GB RAM
  - Tane: 96 nodes; 12 cores each @ 2.9 GHz; 48 GB RAM
  - Taurus: 54 nodes; 12 cores each @ 2.66 GHz; 48 GB RAM
- 22 SMP machines for jobs needing lots of RAM
  - SMP: 4 nodes; 32 cores each @ 2.5 GHz; 256 GB RAM
  - SMP: 9 nodes; 32 cores each @ 2.0 GHz; 256 GB RAM
  - SMP: 9 nodes; 24 cores each @ 2.0 GHz; 256 GB RAM
- 3 Machines with 1 TB of memory
  - Helena: 3 nodes; 32 cores each @ 2.13 GHz; 1028 GB RAM
- Forschungscluster-Housing
  - FCH: 35 machines in various configurations

Please note: The length of support contracts for individual clusters varies. Should you need an identical hardware platform over the next years, please choose Lena.

## 2.4 Forschungscluster-Housing

Additionally institutes can integrate their own hardware for use within the cluster system in the service called Forschungscluster-Housing (FCH). This hardware is accessible only to the respective institute during the day, i.e. between eight o'clock in the morning and eight o'clock in the evening. During night-time all cluster users have access to the Forschungscluster-Housing resources.

If you get directed to a machine that does not fit the name scheme of our main clusters during that time period, it is most likely a FCH participant. For information about having your own hardware in the Forschungscluster-Housing, please get in touch.

## 2.5 Contact & Help

For all cluster related questions, please contact cluster-help@luis.uni-hannover.de.

# Connecting to the cluster system & file transfer

The following addresses should be used to connect to the cluster system:

login.cluster.uni-hannover.de in order to submit jobs.

transfer.cluster.uni-hannover.de whenever you need to transfer data.

Please note: Execution time is limited to 30 minutes on all login nodes.

Thus transfers will be aborted on all login nodes if the execution time limit is reached. On the transfer node execution time is unlimited, but on the other hand it is not possible to submit jobs on the transfer node.

## 3.1 Connecting from Linux or Mac OS

In order to connect to the cluster system from Linux or Mac OS an ssh client is required, which comes with most distributions by default. The following command will establish a connection to the cluster system. Replace username with your cluster user name.

```
ssh username@login.cluster.uni-hannover.de
```

If you need to use graphical programmes on the cluster system, the option `-X`, which enables X11 forwarding, is required.

```
ssh -X username@login.cluster.uni-hannover.de
```

## 3.2 File transfer using Linux or Mac OS

There is a special node dedicated to data transfer with the cluster system. Whenever you transfer data with the cluster system use the special transfer node:

`transfer.cluster.uni-hannover.de`

Files can be transferred to and from the cluster system in a number of ways. For single files `scp` can be used. It is recommended to use `rsync` for file transfers. Additionally you can use FileZilla if you would like to use a graphical tool. Information on how to configure FileZilla for use with the cluster system can be found in section 3.4.

Please note: Use dedicated transfer node for file transfers, because processes are aborted after 30 minutes on the login machines.

## 3.3 Connecting from Windows

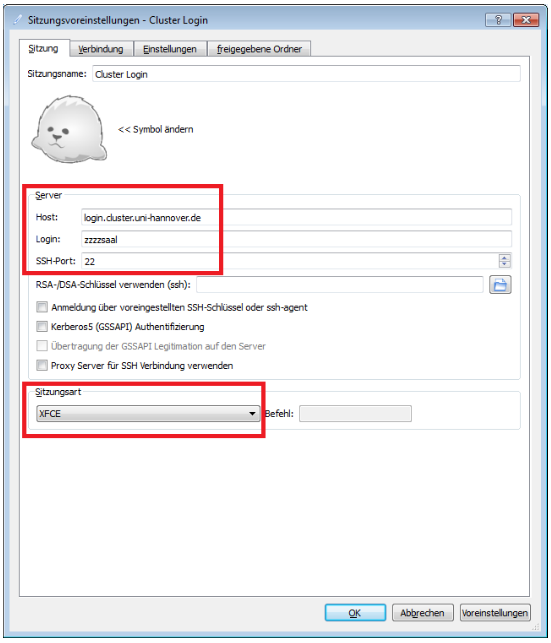
In order to connect to the cluster system from Windows additional software is needed. Using graphical programs on login nodes or compute nodes is possible with the help of an x-window client. Following are instructions on how to install and configure the `X2Go` client under Windows 7 for use with the cluster system. This guide is based on the X2Go-client version `4.0.2.1+hotfix1`, which can be obtained from the following URL. After downloading you may install the program to a folder of your choice.

### 3.3.1 X2Go client configuration

After starting the X2Go client, either using a desktop short-cut or using the start menu, a configuration dialogue is displayed. In this dialogue you should specify a session name and make the following four entries.

1. Host: login.cluster.uni-hannover.de
2. Login: Your user name
3. SSH-Port: 22
4. Session type: XFCE

The completed configuration dialogue is depicted in figure 3.1. Entries in the red boxes have to be set accordingly. Afterwards leave the configuration assistant by clicking the OK button.



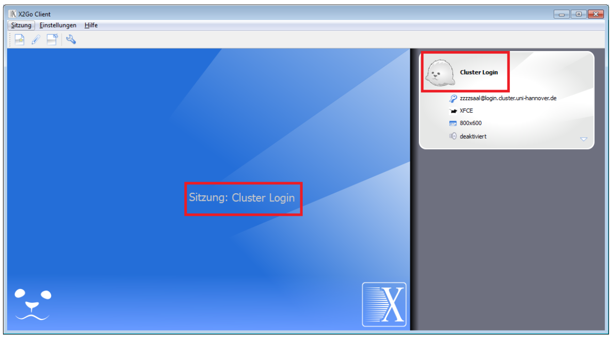
Sitzungsname: Cluster Login

Server
Host: login.cluster.uni-hannover.de
Login: zzzzsaal
SSH-Port: 22
RSA-/DSA-Schlüssel verwenden (ssh):
□ Anmeldung über voreingestellten SSH-Schlüssel oder ssh-agent
□ Kerberos5 (GSSAPI) Authentifizierung
□ Übertragung der GSSAPI Legitimation auf den Server
□ Proxy Server für SSH Verbindung verwenden

Sitzungsart
XFCE
Befehl:

Figure 3.1: X2Go configuration dialogue, entries in red boxes have to be set.

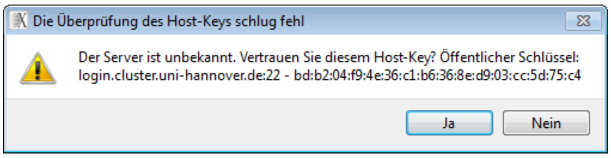
On the right side of the main window the newly created session name is displayed, see figure 3.2. You can start this session by clicking on the session name (in the upper right corner in figure 3.2) or by entering the session name in the dialogue box named session.



Cluster Login
zzzzsaal@login.cluster.uni-hannover.de
XFCE
800x600
deaktiviert

Sitzung: Cluster Login

Figure 3.2: Start a new session by clicking or entering the session name.



Die Überprüfung des Host-Keys schlug fehl

Der Server ist unbekannt. Vertrauen Sie diesem Host-Key? Öffentlicher Schlüssel:
login.cluster.uni-hannover.de:22 - bd:b2:04:f9:4e:36:c1:b6:36:8e:d9:03:cc:5d:75:c4

Figure 3.3: Host key verification dialogue

The first time a connection is established, the login nodes' host-key is unknown. A notification will pop up and you need to accept the host-key (see figure 3.3) by pressing yes.

After a connection was successfully established an XFCE Desktop is displayed as depicted in figure 3.4.

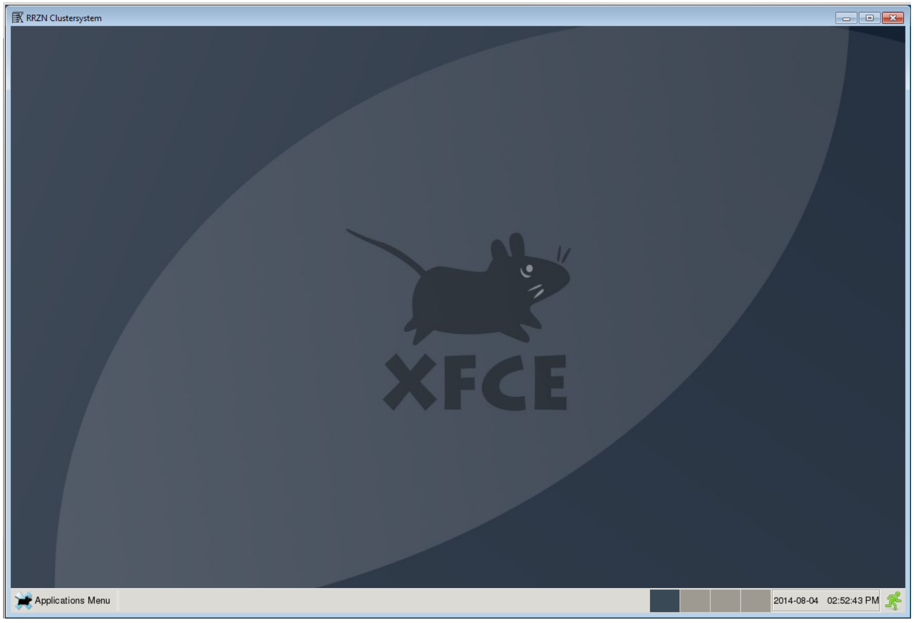


Figure 3.4: XFCE desktop with applications menu in the lower left corner

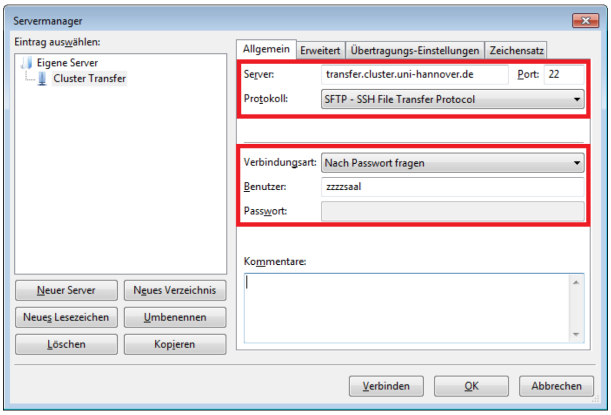
The Applications Menu in the bottom left corner can be used to start a console window and then load modules or submit jobs into the queue. You can open editors e.g. to write or edit batch scripts. Particularly interactive jobs which open graphical program windows can be run. To end your session either go to the Applications Menu or press the little green icon in the bottom right corner of your desktop.

## 3.4 File transfer under Windows using FileZilla

In order to exchange files with the cluster system under Windows, FileZilla client can be used. Following are instructions on how to install and configure FileZilla client version `3.14.1_win64` under Windows 7 which can be obtained from the following URL. After downloading you can install FileZilla client to a directory of your choice.

After installing, open the Site Manager and create a new server which you can then connect to. The following options have to be set, see the red boxes in figure 3.5.

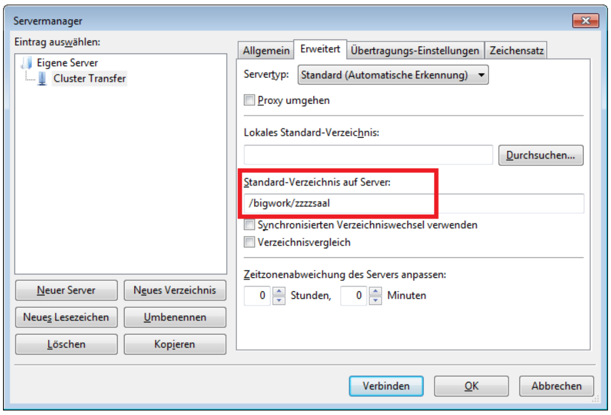
- Host: transfer.cluster.uni-hannover.de
- Protocol: SFTP - SSH File Transfer Protocol
- Logon Type: Ask for password
- User: Your user name



Server: transfer.cluster.uni-hannover.de Port: 22
Protokoll: SFTP - SSH File Transfer Protocol
Verbindungsart: Nach Passwort fragen
Benutzer: zzzzsaal
Passwort:

Figure 3.5: Site Manager: General

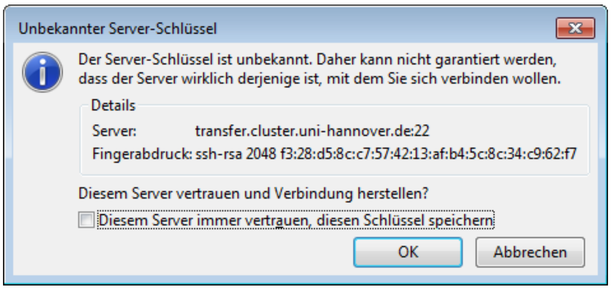
Furthermore it is possible to open the remote connection directly to $BIGWORK. If you do not choose this option the remote directory will be set to $HOME. In order to configure this option, go to the Advanced tab and set Default remote directory accordingly, see figure 3.6.



Servertyp: Standard (Automatische Erkennung)
□ Proxy umgehen
Lokales Standard-Verzeichnis:
Standard-Verzeichnis auf Server:
/bigwork/zzzzsaal
□ Synchronisierten Verzeichniswechsel verwenden
□ Verzeichnisvergleich
Zeitzonenabweichung des Servers anpassen:
0 Stunden, 0 Minuten

Figure 3.6: Site Manager: Advanced

The first time a connection is established the transfer node's host-key is unknown. A notification will pop up and you need to accept the host-key, see figure 3.7.



Unbekannter Server-Schlüssel

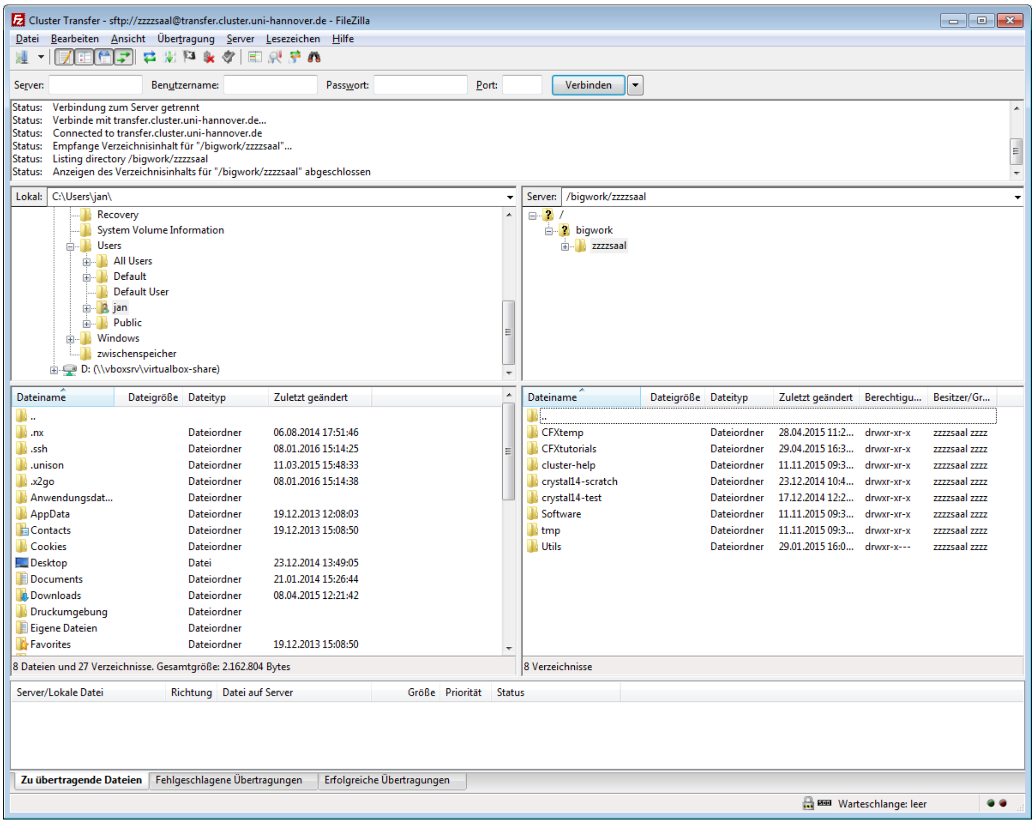
Der Server-Schlüssel ist unbekannt. Daher kann nicht garantiert werden, dass der Server wirklich derjenige ist, mit dem Sie sich verbinden wollen.

Details
Server: transfer.cluster.uni-hannover.de:22
Fingerabdruck: ssh-rsa 2048 f3:28:d5:8c:c7:57:42:13:af:b4:5c:8c:34:c9:62:f7

Diesem Server vertrauen und Verbindung herstellen?
□ Diesem Server immer vertrauen, diesen Schlüssel speichern

Figure 3.7: Host-key verification on first connection attempt

After a connection is successfully established, see figure 3.8, you can exchange data with the cluster system.



Cluster Transfer - sftp://zzzzsaal@transfer.cluster.uni-hannover.de - FileZilla

Server: Benutzername: Passwort: Port:

```
Status:	Verbindung zum Server getrennt
Status:	Verbinde mit transfer.cluster.uni-hannover.de...
Status:	Connected to transfer.cluster.uni-hannover.de
Status:	Empfange Verzeichnisinhalt für "/bigwork/zzzzsaal"...
Status:	Listing directory /bigwork/zzzzsaal
Status:	Anzeigen des Verzeichnisinhalts für "/bigwork/zzzzsaal" abgeschlossen
```

Lokal: C:\Users\jan\

```
    Recovery
    System Volume Information
    Users
      All Users
      Default
      Default User
      jan
      Public
    Windows
    zwischenspeicher
  D: (\\vboxsrv\virtualbox-share)
```

Server: /bigwork/zzzzsaal

```
/
  bigwork
    zzzzsaal
```

| Dateiname | Dateigröße | Dateityp | Zuletzt geändert |
|---|---|---|---|
| .. | | | |
| .nx | | Dateiordner | 06.08.2014 17:51:46 |
| .ssh | | Dateiordner | 08.01.2016 15:14:25 |
| .unison | | Dateiordner | 11.03.2015 15:48:33 |
| .x2go | | Dateiordner | 08.01.2016 15:14:38 |
| Anwendungsdat... | | Dateiordner | |
| AppData | | Dateiordner | 19.12.2013 12:08:03 |
| Contacts | | Dateiordner | 19.12.2013 15:08:50 |
| Cookies | | Dateiordner | |
| Desktop | | Datei | 23.12.2014 13:49:05 |
| Documents | | Dateiordner | 21.01.2014 15:26:44 |
| Downloads | | Dateiordner | 08.04.2015 12:21:42 |
| Druckumgebung | | Dateiordner | |
| Eigene Dateien | | Dateiordner | |
| Favorites | | Dateiordner | 19.12.2013 15:08:50 |

8 Dateien und 27 Verzeichnisse. Gesamtgröße: 2.162.804 Bytes

| Dateiname | Dateigröße | Dateityp | Zuletzt geändert | Berechtigu... | Besitzer/Gr... |
|---|---|---|---|---|---|
| .. | | | | | |
| CFXtemp | | Dateiordner | 28.04.2015 11:2... | drwxr-xr-x | zzzzsaal zzzz |
| CFXtutorials | | Dateiordner | 29.04.2015 16:3... | drwxr-xr-x | zzzzsaal zzzz |
| cluster-help | | Dateiordner | 11.11.2015 09:3... | drwxr-xr-x | zzzzsaal zzzz |
| crystal14-scratch | | Dateiordner | 23.12.2014 10:4... | drwxr-xr-x | zzzzsaal zzzz |
| crystal14-test | | Dateiordner | 17.12.2014 12:2... | drwxr-xr-x | zzzzsaal zzzz |
| Software | | Dateiordner | 11.11.2015 09:3... | drwxr-xr-x | zzzzsaal zzzz |
| tmp | | Dateiordner | 11.11.2015 09:3... | drwxr-xr-x | zzzzsaal zzzz |
| Utils | | Dateiordner | 29.01.2015 16:0... | drwxr-x--- | zzzzsaal zzzz |

8 Verzeichnisse

| Server/Lokale Datei | Richtung | Datei auf Server | Größe | Priorität | Status |
|---|---|---|---|---|---|

Warteschlange: leer

Figure 3.8: Connection to transfer-node established with FileZilla

## 3.5 Connecting from outside the university's network

The cluster system in not reachable from outside the university's network. In order to connect from outside you have to establish a connection with the university's network first, e.g. by using a VPN. The colleagues from the network team provide a VPN service.

LUIS VPN Service

After establishing a connection to the university's network you can connect to the cluster system as usual.

Please note: Connection speed from outside networks will mostly be slower than from your office. This can cause applications which provide a graphical user interface to respond slowly and make working with them hard. If gui windows respond slowly, it is due to the technical nature and not a technical problem with the cluster system.

# File systems

There are two storage systems which make two file systems globally available, i.e. available on every node. These are depicted in figure 4.1.

$HOME Your home directory. Comparatively few space available but with a daily backup. Thus only the most important files should be saved here. $HOME is connected through gigabit ethernet and thus rather slow compared to $BIGWORK.

$BIGWORK Your bigwork directory. Comparatively much space available but without backup. It is meant as a work directory. All computations should write to this directory. $BIGWORK is connected through InfiniBand technology and thus much faster than $HOME. It is referred to as work or scratch file system and should be regarded as such. After finishing work on an idea clear the board, i.e. delete unneeded files.

$PROJECT Your project directory. Each project(from the BIAS point of view) is provided by reasonable large amount of $BIGWORK independent high performance(lustre, InfiniBand) project storage for long time retaining of your data. All members of a project have read&write access to the project storage area which is available at `/project/<your-cluster-groupname>` (or you can use the variable $PROJECT to access your group's project storage). If you wish to save your personal files on project storage, it is recommended that you create the directory $PROJECT/$USER with proper access rights, `mkdir -m 0700` $PROJECT/$USER, and store your files there. Each group's initial quota for project storage will be 10 TB. The project storage is visible on login and transfer machines only, but not from cluster work nodes. This means that the project storage can not be used as an input&output for your jobs running on the cluster work nodes(instead use $BIGWORK). You can use either the cluster login nodes or the transfer(recommended) machine to move your files from $BIGWORK to $PROJECT or vice versa. In general, $PROJECT storage is not intended to be used for heavy computation, instead for long time retaining of your cluster data, which might need to have a fast access to $BIGWORK storage. Therefore, in terms of IOPS it is relatively slower than $BIGWORK storage. Project storage is not backed up.

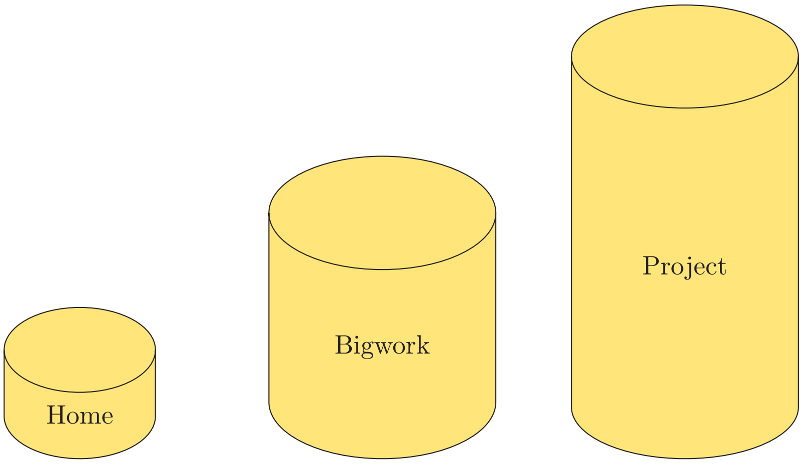
Store your most important data on $HOME, which you can not risk losing and could otherwise not recreate. Simulation's intermediate results should be written to $BIGWORK because these can be recreated by running the simulation again. Here you have much more storage space available which is also connected faster using InfiniBand. When using $HOME to save files during computations you will very likely slow down your computation. Thus make sure all default directories are set to $BIGWORK. These include temporary directories and those automatically set by applications.

Under no circumstances should a link to $BIGWORK be created in your home directory. In this scenario data written to $BIGWORK would be passed through $HOME and from there to $BIGWORK and vice versa for reading data. The environment variable $BIGWORK should be used instead.

Please note: Backing up your data regularly from $BIGWORK to $PROJECT storage or to your institute's server is essential, since $BIGWORK is designed as scratch file system.

## 4.1 Quota and grace time

On both storage systems only a fraction of the whole disk space is available to you, which is your quota. There is a soft quota and a hard quota. A hard quota is an upper bound which can not be exceeded. The soft quota on the other hand can be exceeded. Exceeding your soft quota starts the grace time. During this grace time you are allowed to exceed your soft quota up to your hard quota. After this period you



| $HOME | $BIGWORK | $PROJECT |
|---|---|---|
| ○ /home/username | ○ /bigwork/username | ○ /bigwork/groupname |
| ○ 10 GB soft quota | ○ 100 GB soft quota | ○ 10 TB soft quota |
| ○ 12 GB hard quota | ○ 1 TB hard quota | ○ 12 TB hard quota |
| ○ All cluster nodes | ○ All cluster nodes | ○ login & transfer nodes |
| ○ backup | ○ no backup | ○ no backup |
| ○ Gigabit Ethernet | ○ InfiniBand | ○ InfiniBand |

Figure 4.1: Cluster file systems with specifications

will not be abale to store any more data, unless you reduce disk space usage below the soft quota. If your disk space consumption falls below the soft quota, your grace time counter is reset.

By using the quota mechanism we are trying to limit individual disk space consumption and keep the system performance as high as possible. Please delete files which are no longer needed. Low disk space consumption is especially helpful on $BIGWORK in order to optimise system performance. You can query your disk space usage and quota with the following commands, see also exercise in chapter 4.4.

fquota Display $HOME disk usage and quota.

lquota Display $BIGWORK and $PROJECT disk usage and quota.

Please note: If no free space is left on $HOME you will not be able to login graphically any more. Connecting using ssh (without -X) will still be possible.

## 4.2 Bigwork's file system Lustre and stripe count

Please note: All statements made in this section also apply to $PROJECT storage

On the technical level $BIGWORK is comprised of multiple components which make up the storage system depicted in figure 4.2. Generally it is possible to use $BIGWORK with default values. However, it can be useful to alter parameters, especially stripe count. Setting stripe count manually can result in higher individual transfer rates and increase overall system performance. This not only benefits you but all users of the cluster system.

Data on $BIGWORK are saved on OSTs, object storage targets. Each OST consists of a number of hard disks. By default data are saved to only one OST when writing to $BIGWORK, regardless of data size. This corresponds to a stripe count of one since stripe count indicates how many OSTs will be used to store data. Striping data over multiple OSTs can increase data access time. Transfer speeds of multiple OSTs, i.e. multiple hard disk clusters, are combined.

Please note: When working with files larger than 100 MB, please set stripe count manually according to section  4.5.

Stripe count is set as an integer value representing the number of OSTs to use, with -1 indicating all available OSTs. It is advised to create a directory below $BIGWORK and set a stripe count of -1 for it. This directory can then be used to store all files larger than 100 MB. For files smaller than 100 MB a stripe count of one, which is set by default, is sufficient.

Please note: In order to alter the stripe count of existing files, these need to be copied, see section 4.6. Simply moving files with `mv` is not sufficient in this case.

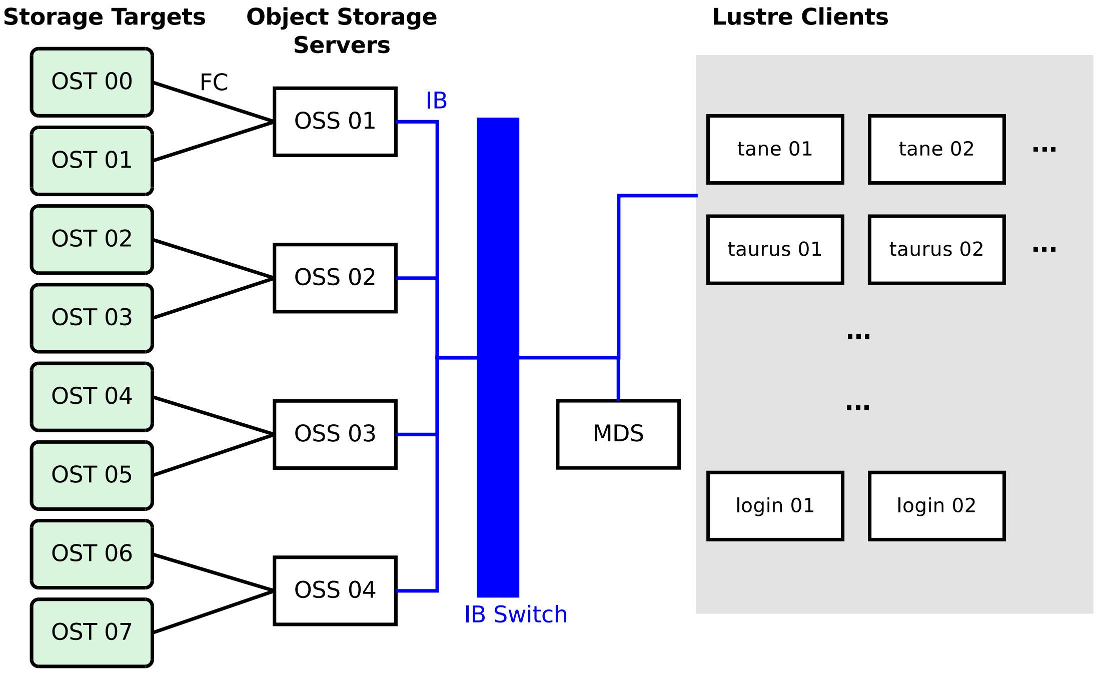


Figure 4.2: $BIGWORK's technical components with object storage targets (OST), object storage servers (OSS), metadata server (MDS) and InifiniBand (IB) switch.

## 4.3 $TMPDIR

Within jobs $TMPDIR points to local storage available directly on each node. Whenever local storage is needed, $TMPDIR should be used.

Please note: As soon as a job finishes, all data stored under $TMPDIR will be deleted automatically.

Do not simly assume $TMPDIR to be faster than $BIGWORK, but test it. $TMPDIR could be used in case of applications that need a temporary directory.

## 4.4 Excercise: Using file systems

```
# where are you? lost? print working directory!
pwd
# change directory to your bigwork directory
cd $BIGWORK
# what is the absolute path of your bigwork directory?
pwd
# change directory to your project directory
cd $PROJECT
# what is the absolute path of your project directory?
pwd
# change directory to your home directory
cd $HOME
# display the absolute path of your home directory
pwd
# display your home quota
fquota
# display your bigwork & project quota
lquota
# make your personal directory in your group's project storage
mkdir -m 0700 $PROJECT/$USER
# copy the directory mydir from bigwork to project
cp -r $BIGWORK/mydir $PROJECT/$USER
```

When displaying your quota, used space is given in kilobytes.
Note: tera, giga, mega, kilo . . .

Used space: 000 123 456 789

## 4.5 Excercise: setting stripe count

```
# get overall bigwork usage, note different fill levels
lfs df -h
# get current stripe settings for your bigwork
lfs getstripe $BIGWORK
# change directory to your bigwork
cd $BIGWORK
# create a directory for large files (anything over 100 MB)
mkdir LargeFiles
# get current stripe settings for that directory
lfs getstripe LargeFiles
# set stripe count to -1 (all available OSTs)
lfs setstripe --count -1 LargeFiles
# check current stripe settings for LargeFiles directory
lfs getstripe LargeFiles
# create a directory for small files
mkdir SmallFiles
# check stripe information for SmallFiles directory
lfs getstripe SmallFiles
```

Use newly created LargeFiles directory to store large files

## 4.6 Excercise: altering stripe count

Sometimes you might not know beforehand, how large files created by your simulations will turn out. In this case you can set stripe size after a file has been created in two ways. Let us create a 100 MB file first.

```
# enter the directory for small files
cd SmallFiles
# create a 100 MB file
dd if=/dev/zero of=100mb.file bs=10M count=10
# check filesize by listing directory contents
ls -lh
# check stripe information on 100mb.file
lfs getstripe 100mb.file
# move the file into the large files directory
mv 100mb.file ../LargeFiles/
# check if stripe information of 100mb.file changed
lfs getstripe ../LargeFiles/100mb.file
# remove the file
rm ../LargeFiles/100mb.file
```

In order to change stripe, the file has to be copied (`cp`). Simply moving (`mv`) the file will not affect stripe count.

First method:

```
# from within the small files directory
cd $BIGWORK/SmallFiles
# create a 100 MB file
dd if=/dev/zero of=100mb.file bs=10M count=10
# copy file into the LargeFiles directory
cp 100mb.file ../LargeFiles/
# check stripe in the new location
lfs getstripe ../LargeFiles/100mb.file
```

Second method:

```
# create empty file with appropriate stripe count
lfs setstripe --count -1 empty.file
# check stripe information of empty file
lfs getstripe empty.file
# copy file "in place"
cp 100mb.file empty.file
# check that empty.file now has a size of 100 MB
ls -lh
# remove the original 100mb.file and work with empty.file
rm 100mb.file
```

# Modules & application software

Please note: Lmod is now set as default software module system. It is automatically activated at login time. Usage of the old software module system is documented in the Appendix. Note that we will no longer neither update existing nor install new software applications there.

The number of packages, i.e. software, which is installed with the operating system of cluster nodes is kept light on purpose. Additional packages and applications are provided by a modules system which enables you to easily customise your working environment on the cluster system. Furthermore we can provide different versions of software which you can use on demand. Loading a module, software specific settings are applied, e.g. changing environment variables `PATH`, `LD_LIBRARY_PATH` and `MANPATH`.

An environment module system which has recently been deployed on the cluster is called `Lmod` (see appendix for an old, TCL based module system, which is still available as a default module system. `Lmod` allows for better performance and implements more functionalities, yet the usual module based commands will work almost the same as before. In addition to some new features, we have adopted a more systematic software naming and versioning convention provided by the `EasyBuild` software installation system. For more information, please visit the Lmod Homepage.

`Lmod` installation on the cluster utilizes a hierarchical software module naming scheme. This means that the command `module avail` does not display all installed software modules instead the modules that are immediately available to load. Upon loading some modules, more modules may become available. Specifically, loading a compiler module or MPI implementation module will make available all the software built with/against those applications.

At the top level of module hierarchy there are modules for compilers, toolchains and software applications that come as a binary and thus do not depend on compilers. Toolchain modules organize compilers, MPI implementations and numerical libraries. Currently the following toolchain modules are available:

- Compiler only toolchains
  - GCC: GCC + updated binutils
  - iccifort: Intel compilers + GCC
- Compiler + MPI toolchains
  - gompi: GCC + OpenMPI
  - iimpi: Intel compilers + Intel MPI
  - iompi: Intel compilers + OpenMPI
- Compiler + MPI + numerical libraries toolchains
  - foss: gompi + OpenBLAS + FFTW + ScaLAPACK
  - intel: iimpi + Intel MKL
  - iomkl: iompi + Intel MKL

See table 5.1 for a list of GNU based toolchains and tables 5.2 and 5.3 for Intel based toolchains installed.

Table 5.1: GNU based toolchains

| Name | GCC | OpenMPI | FFTW | OpenBLAS | ScaLAPACK | LAPACK | Sub-Toolchain |
|---|---|---|---|---|---|---|---|
| foss/2014b | 4.8.3 | 1.8.1 | 3.3.4 | 0.2.9 | 2.0.2 | 3.5.0 | gompi/2014b |
| foss/2015b | 4.9.3 | 1.8.8 | 3.3.4 | 0.2.14 | 2.0.2 | 3.5.0 | gompi/2015b |
| foss/2016a | 4.9.3 | 1.10.2 | 3.3.4 | 0.2.15 | 2.0.2 | 3.6.0 | gompi/2016a |
| foss/2016.04 | 5.3.0 | 1.10.2 | 3.3.4 | 0.2.18 | 2.0.2 | 3.6.0 | gompi/2016.04 |
| foss/2016b | 5.4.0 | 1.10.3 | 3.3.4 | 0.2.18 | 2.0.2 | 3.6.1 | gompi/2016b |

Table 5.2: Intel based toolchains with Intel MPI

| Name | ICC | IFort | IMKL | IMPI | Note |
|---|---|---|---|---|---|
| intel/2016a | 2016.1.150 | 2016.1.150 | 11.3.1.150 | 5.1.2.150 | compiled by GCC-4.9.3-2.25 |
| intel/2016b | 2016.3.210 | 2016.3.210 | 11.3.3.210 | 5.1.3.181 | compiled by GCC-5.4.0-2.26 |

Table 5.3: Intel based toolchains with Open MPI

| Name | ICC | IFort | IMKL | OpenMPI | Note |
|---|---|---|---|---|---|
| iomkl/2016b | 2016.3.210 | 2016.3.210 | 11.3.3.210 | 1.10.3 | compiled by GCC-5.4.0-2.26 |

## 5.1 Working with modules

This section explains how to use software modules.

List the entire list of possible modules

```
module spider
```

The same but more compact output

```
module -t spider
```

Search for specific modules that have "string" in their name

```
module spider string
```

Detailed information about particular version of the module (including instructions on how to load the module)

```
module spider name/version
```

List modules immediately available to load

```
module avail
```

Some software modules are hidden from the `avail` and `spider` commands. These are mostly the modules for system library packages which other directly used user applications depend on. To list hidden modules you should provide the `--show_hidden` option to the `avail` and `spider` commands:

```
module --show_hidden avail
module --show_hidden spider
```

A hidden module has a dot (`.`) in font of its version (eg. `zlib/.1.2.8`).

List currently loaded modules

```
module list
```

Load a specific version of a module

```
module load name/version
```

If only name is specified, the command will load the default version marked with a (D) in the `module avail` listing (usually the latest version). Loading a module may automatically load other modules it depends on.

It not possible to load two versions of the same module at the same time.

To switch between different modules

```
 module swap old new
```

To unload the specified module from the current environment

```
 module unload name
```

To clean your environment of all loaded modules

```
 module purge
```

Show what environment variables the module will set

```
 module show name/version
```

Save the current list of modules to "name" collection for later use

```
 module save name
```

Restore modules from collection "name"

```
 module restore name
```

List of saved collections

```
 module savelist
```

To get the complete list of options provided by Lmod through the command `module` type the following

```
 module help
```

## 5.2 Exercise: Working with modules

As an example of working with the Lmod modules, here we show how to load the `gnuplot` module.

List loaded modules

```
 module list

No modules loaded
```

Find available gnuplot versions

```
 module -t spider gnuplot

gnuplot/4.6.0
gnuplot/5.0.3
```

Determine how to load the selected `gnuplot/5.0.3` module

```
 module spider gnuplot/5.0.3

--------------------------------------------------------------------------------
  gnuplot: gnuplot/5.0.3
--------------------------------------------------------------------------------
    Description:
      Portable interactive, function plotting utility - Homepage: http://gnuplot
          .sourceforge.net/
    This module can only be loaded through the following modules:

      GCC/4.9.3-2.25  OpenMPI/1.10.2

    Help:
      Portable interactive, function plotting utility - Homepage: http://gnuplot
          .sourceforge.net/
```

Load required modules

```
 module load GCC/4.9.3-2.25  OpenMPI/1.10.2

Module for GCCcore, version .4.9.3 loaded
Module for binutils, version .2.25 loaded
Module for GCC, version 4.9.3-2.25 loaded
Module for numactl, version .2.0.11 loaded
Module for hwloc, version .1.11.2 loaded
Module for OpenMPI, version 1.10.2 loaded
```

And finally load the selected `gnuplot` module

```
 module load gnuplot/5.0.3

Module for OpenBLAS, version 0.2.15-LAPACK-3.6.0 loaded
Module for FFTW, version 3.3.4 loaded
Module for ScaLAPACK, version 2.0.2-OpenBLAS-0.2.15-LAPACK-3.6.0 loaded
Module for bzip2, version .1.0.6 loaded
Module for zlib, version .1.2.8 loaded
.............
.............
```

In order to simplify a procedure of the gnuplot module loading, the current list of loaded modules can be saved in "mygnuplot" collection (the name string "mygnuplot" is of course arbitrary) and then loaded again when needed as follows

Save loaded modules to "mygnuplot"

```
 module save mygnuplot

Saved current collection of modules to: mygnuplot
```

If "mygnuplot" not is specified, the name "default" will be used.

Remove all loaded modules (or open a new shell)

```
 module purge

Module for gnuplot, version 5.0.3 unloaded
Module for Qt, version 4.8.7 unloaded
Module for libXt, version .1.1.5 unloaded
............
............
```

List currently loaded modules. This selection is empty now.

```
 module list

No modules loaded
```

List saved collections

```
 module savelist

Named collection list:
  1) mygnuplot
```

Load `gnuplot` module again

```
 module restore mygnuplot

Restoring modules to user’s mygnuplot
Module for GCCcore, version .4.9.3 loaded
Module for binutils, version .2.25 loaded
Module for GCC, version 4.9.3-2.25 loaded
Module for numactl, version .2.0.11 loaded
.............
.............
```

## 5.3 Application software

A wide variety of application software is available in the cluster system. These applications are located on a storage system and are available through an NFS export. If you need a different version of an already installed application, or one that is currently not installed, please get in touch. The main prerequisite for use within the cluster system is availability for Linux. Furthermore, if the application needs a license, we need to have a look at additional questions.

# Working with the cluster system

The reason you decided to use the cluster system is probably it’s computing resources. However, computing nodes are not accessible directly to users. With around 250 people using the cluster system for their research every year, there has to be an instance organising and allocating resources among users. This instance is called the batch system, also called PBS (portable batch system). The cluster system uses TORQUE as resource manager and Maui as scheduler, which upon request allocate resources to users.

Most work with the cluster system is done as jobs. Jobs are the framework with which the computing resources of the cluster system can be used and they are started by the qsub command. Generally qsub has the following form.

```
qsub <Optionen> <Name des Jobscripts>
```

The manual page for `qsub` can be accessed like this.

```
man qsub
```

You can quit reading the manual page by pressing the ’q’ key.

## 6.1 Login nodes

After logging in to the cluster system you are located on a login node. These machines are not meant to be used for large computations, i.e. simulation runs. In order to keep these nodes accessible their load has to be minimised. Therefore processes will be killed automatically after 30 minutes of elapsed cpu-time. Please use interactive jobs for tasks like pre- or post-processing and even some larger compilations in order to avoid the frustrating experience of sudden shut down of your application.

## 6.2 Interactive jobs

The simplest way of using the cluster system’s compute power is by starting an interactive job. This can be done by issuing the qsub command with -I option on any login node.

```
zzzzsaal@login02:~$ qsub -I
ACHTUNG / WARNING:
’mem’ parameter not present; the default value will be used (1800mb)
’walltime’ parameter not present; the default value will be used (24:00:00)
’nodes’ parameter not present; the default value will be used (nodes=1:ppn=1)
qsub: waiting for job 1001152.batch.css.lan to start
qsub: job 1001152.batch.css.lan ready

zzzzsaal@lena-n080:~$
```

In this example a user by the name of zzzzsaal issues the qsub command from the node login02. Following this the batch-system warns about missing parameters and starts a job with ID 1001152.batch.css.lan. Using the short JobID 1001152 is more common. Afterwards user zzzzsaal is located on machine lena-n080 which can be seen by looking at the command prompt, which now shows @lena-n080 to indicate this. This is node number 80 of the Lena cluster. From now on this node’s computing power can be utilised.

This simplest form of an interactive job uses default values for all resource specifications. In practice resource specifications should always be adapted to fit one’s needs. This can be done by supplying the qsub command with options. A listing of possible options can be found in section 6.4. The following example illustrates how user zzzzsaal requests specific resources starting from login node login02 inside an interactive job. For this interactive job the user requests one cpu-core on one machine and 2 GB of memory for an hour. Additionally the `-X` option is used, which switches on X window forwarding, so applications with graphical user interfaces can be used.

```
zzzzsaal@login02:~$ qsub -I -X -l nodes=1:ppn=1 -l walltime=01:00:00 -l mem=2GB
qsub: waiting for job 1001154.batch.css.lan to start
qsub: job 1001154.batch.css.lan ready

zzzzsaal@lena-n079:~$
```

After the job with JobID 1001154 has started, the machine named lena-n079 is ready to be used. An extended example of how to utilise interactive jobs is given in section 6.9.

## 6.3 Batch jobs

In preparation for batch jobs interactive jobs should be used. Within interactive jobs all commands can be entered which are later going to make up a batch script, thus testing functionality. Only if everything works should the commands be put into a batch script line by line. This line to line transcript of an interactive session can be used as batch script. In case you were given a batch script by other people, take some time to enter all the commands in an interactive job. This way you familiarise yourself with what the individual commands do.

In order to request the same resources as with the interactive job from section 6.2 within a batch job, the following can be written to a file.

```
#!/bin/bash -login

# resource specification
#PBS -l nodes=1:ppn=1
#PBS -l walltime=01:00:00
#PBS -l mem=2GB

# commands to execute
date
```

Generally jobscripts can be divided into two parts, resource specification and commands to be executed. Lines beginning with # are comments with two exceptions. The first line here specifies the shell which is used to interpret the script. In this case the shell is bash. Also lines beginning with #PBS are recognised by PBS, portable batch system, as resource specifications. In this case the resources requested are one cpu-core on one machine and 2 GB of memory for an hour. The section with commands to executed only contains a signle command. The date command returns the current date and time.

This file is saved as batch-job-example.sh and can afterwards be submitted to the batch system by issuing the qsub command.

```
zzzzsaal@login02:~$ qsub batch-job-example.sh
1001187.batch.css.lan
```

After submitting the jobscript a JobID is returned by the batch system, in this case 1001187. After the job has finished two files can be found in the directory which the jobscript was submitted from.

```
zzzzsaal@login02:~$ ls -lh
total 12K
-rw-r--r-- 1 zzzzsaal zzzz 137 19. Apr 12:54 batch-job-example.sh
-rw------- 1 zzzzsaal zzzz   0 19. Apr 12:59 batch-job-example.sh.e1001187
-rw------- 1 zzzzsaal zzzz  30 19. Apr 12:59 batch-job-example.sh.o1001187
```

The first file has the extension .e1001187, which holds all error messages which occurred during job execution. In this case this file is empty. The second file has the extension .o1001187 and contains all messages which would have been displayed on the terminal and have been redirected here. By displaying this file's contents this can be verified.

```
zzzzsaal@login02:~$ cat batch-job-example.sh.o1001187
Tue Apr 19 12:59:18 CEST 2016
```

The file contains the output of the `date` command.

Please note: Jobscripts written under windows need converting, see section 6.3.1.

### 6.3.1 Converting jobscripts written under windows

Creating a jobscript under windows and copying it onto the cluster system may create the following error message when submitting that jobscript with `qsub`.

```
zzzzsaal@login02:~$ qsub WindowsDatei.txt
qsub:  script is written in DOS/Windows text format
```

Check this file with the `file` command.

```
zzzzsaal@login02:~$ file WindowsDatei.txt
WindowsDatei.txt: ASCII text, with CRLF line terminators
```

Convert the file to Unix format.

```
zzzzsaal@login02:~$ dos2unix WindowsDatei.txt
dos2unix: converting file WindowsDatei.txt to UNIX format ...
```

Check the file again with the `file` command to see if conversion was successful.

```
zzzzsaal@login02:~$ file WindowsDatei.txt
WindowsDatei.txt: ASCII text
```

## 6.4 PBS options

Following is a list of selected PBS options, which allow job control. These options are valid for interactive as well as batch jobs.

`-N` *name*
: declares a name for the job

`-j oe`
: join standard output and error streams

`-l nodes=`*n*`:ppn=`*p*
: request n nodes and p cpu cores per node

`-l walltime=`*time*
: requested wall clock time in format hh:mm:ss

`-l mem=`*value*
: requests RAM according to value, possible suffix of kb, mb or gb

`-M` *email address*
: list of users to whom mail is sent about the job

`-m abe`
: send mail on (one or multiple selections): a - job abort, b - job beginning, e - job end

`-V`
: all environment variables are exported to the job

`-q` *queue*
: destination queue of the job, see section 6.7

`-W x=PARTITION:`*`name`*
partition to be used, see 6.7

`-I`
job is to be run interactively

More options can be found on the man page, which can be opened with the following command.

```
man qsub
```

## 6.5 PBS environment variables

“When a batch job is started, a number of variables are introduced into the job’s environment that can be used by the batch script in making decisions, creating output files, and so forth. These variables are listed in the following table”[1]:

`PBS_O_WORKDIR`
Job’s submission directory

`PBS_NODEFILE`
File containing line delimited list on nodes allocated to the job

`PBS_QUEUE`
Job queue

`PBS_JOBNAME`
User specified jobname

`PBS_JOBID`
Unique JobID

## 6.6 PBS commands

`qsub script`
Submit PBS job

`showq`
Show status of PBS jobs

`qdel` *`jobid`*
Delete Job jobid

All of the above commands have detailed manual pages, which can be viewed with the following command:

```
man <command>
```

In order to exit the manual page, press `q`.

### 6.6.1 pbsnodes

On the login-nodes the `pbsnodes` command can be used to obtain information about resources. For example, the amount of RAM of one of the “Terabyte-Machines” in the helena queue can be queried.

```
pbsnodes smp-n031
```

[1] Source: http://docs.adaptivecomputing.com/torque/4-2-10

At first the output will seem a little bit confusing. It shows, among others, the following parameter.

```
physmem=1058644176kb
```

This output can be converted into gb. 1024kb equals 1mb, 1024mb equals 1gb etc. ... This way you know the maximum number of RAM you can request on one machine in queue helena is 1009 gb.

## 6.7 Queues & partitions

| Cluster | Nodes | Processors | Cores /Node | Memory /Node (GB) | Partition | Queue |
|---|---|---|---|---|---|---|
| Lena | 80 | 2x Intel Haswell Xeon E5-2630 v3<br>8-cores, 2.40GHz, 20MB Cache | 16 | 64 | lena | all |
| Tane | 96 | 2x Intel Westmere-EP Xeon X5670<br>6-cores, 2.93GHz, 12MB Cache | 12 | 48 | tane | all |
| Taurus | 54 | 2x Intel Westmere-EP Xeon X5650<br>6-cores, 2.67GHz, 12MB Cache | 12 | 48 | taurus | all |
| SMP | 9 | 4x Intel Westmere-EX Xeon E7-4830<br>8-cores, 2.13GHz, 24MB Cache | 32 | 256 | smp | all |
| | 9 | 4x Intel Backton Xeon E7540<br>6-cores, 2.00GHz, 18MB Cache | 24 | 256 | puresmp | all |
| | 3 | 4x Intel Westmere-EX Xeon E7-4830<br>8-cores, 2.13GHz, 24MB Cache | 32 | 1024 | — | helena |
| FCH | 33 | | | | .[2] | all |

There are three queues available:

`all`
: This is the default queue and does not have to be requested explicitly. PBS will route a job to matching nodes.

`helena`
: A queue for jobs with large RAM requirements up to 1 Terabyte.

`test`
: A queue for testing. There is one node with 12 processors and 48 GB of RAM available. Maximum walltime is 6 hours.

In addition to queues there a multiple partitions. Using these partitions you can direct your job to specific machines, for example in the queue all, see table for partition names. Forschungscluster-Housing machines are divided into one partition per institute.

## 6.8 Maximum resource requests

Some maximum values exists, which can not be exceeded. Maximum walltime per job is limited, as well as maximum number of simultaneously running jobs. Furthermore the number of cpus is limited. All these limits apply per user name.

[2] each institute has it's own partition

Walltime Maximum walltime is 200 hours per job

Jobs The maximum number of running jobs per user is 64

CPUs The overall maximum number of CPUs (ppn) all running jobs can use is 768 per user

## 6.9 Excercise: interactive job

```
# start an interactive job, what happens?
qsub -I
# exit this interactive job
exit
# specify all resource parameters, so no defaults get used
qsub -I -X -l nodes=1:ppn=1 -l walltime=01:00:00 -l mem=2GB
# load module for octave
module load octave/3.8.1
# start octave
octave
# inside octave the following commands create a plot
octave:1> x = 0:10;
octave:2> y = x.^2;
octave:3> h = figure(1);
octave:4> plot(x,y);
octave:5> print(’-f1’,’-dpng’,’myplot’)
octave:6> exit
# display newly created image
display myplot.png
```

Interactive jobs are useful for debugging, always use interactive first

## 6.10 Excercise: batch job

Create a file named MyBatchPlot.m

```
x = 0:10;
y = x.^2;
h = figure(1);
plot(x,y);
print(’-f1’,’-dpng’,’MyBatchPlot’);
```

Create a file named MyFirstBatchJob.sh

```
#!/bin/bash -login
#PBS -l nodes=1:ppn=1
#PBS -l walltime=01:00:00
#PBS -l mem=2GB
# load octave module
module load octave/3.8.1
# start octave
octave MyBatchPlot.m
```

Submit the job script

```
qsub MyFirstBatchJob.sh
```

Check files MyFirstBatchJob.sh.o* and MyFirstBatchJob.sh.e*

# Transferring files into the archive

Please note: The archive is operated as part of the service Archivierung and thus not part of the cluster system.

The archive can be used to store results and simulation data permanently. Each account has to be registered for archive use, before using it. This can be done on the BIAS-website after logging in with your user name and password. After clicking on the link entitled Ihren Benutzernamen für die Nutzung des Archivsystems zulassen it takes roughly an hour, before the archive can be used.

## 7.1 Quota

Archival storage in the archive system of Leibniz Universität Hannover is controlled by a quota mechanism. There is a quota on the amount of files as well as storage space. Please see the website of the archive service for further details at `http://www.luis.uni-hannover.de/archivierung.html`.

## 7.2 Transferring data into the archive

In order to transfer data into the archive of Leibniz Universität Hannover, it is recommended to use the cluster's dedicated transfer node, see 3.2 and 3.4.

## 7.3 Login with lftp

The archive can be reached at `archiv.luis.uni-hannover.de` using the `lftp` command.

```
username@clustertransfer:~$ lftp <username>@archiv.luis.uni-hannover.de
```

After entering your cluster user name's password the `lftp` prompt appears.

```
lftp <username>@archiv.luis.uni-hannover.de:~>
```

Now you can use the `ls` command to list your directory contents at the archive. At the same time this is to test an established connection to the archive.

```
 lftp <username>@archiv.luis.uni-hannover.de:~> ls
```

At your first login to the archive system with your account the directory is empty. The `ls` command will not return any listing. You can terminate the connection with `exit`.

```
lftp <username>@archiv.luis.uni-hannover.de:~> exit
<username>@clustertransfer:~$
```

Aliases for `exit` are `quit` and `bye`.

## 7.4 Copying files into the archive

On the cluster system's transfer node change to the directory where the data to be copied are located.

```
clustertransfer:~$ cd $BIGWORK/my_data_dir
clustertransfer:/bigwork/username/my_data_dir$
```

After logging in using lftp the put command is used.

```
clustertransfer:/bigwork/username/my_data_dir$ lftp
<username>@archiv.luis.uni-hannover.de:~>
lftp <username>@archiv.luis.uni-hannover.de:~> put myfile.tar.gz
```

The file `myfile.tar.gz` is located inside the directory we previously changed to in this example. After using `put` to transfer the file it is also available on the archive. The `TAB` key works for completing file and directory names in lftp as well.

Saving multiple small files in the archive is not desired, because at least one copy of the data are kept on magnetic tape. Therefore a constant stream of data is desirable which can be achieved by some large files. It is recommended to use `tar` or `zip` to combine small files into one bigger file. This can also optimize your quota.

In order to transfer multiple (large) files at once, the `mput` command can be used. This is short for multiple put. The `mput` command understands the wildcard `*` as it is used in bash.

```
lftp <username>@archiv.luis.uni-hannover.de:~> mput mydata*.tar.gz
```

## 7.5 Fetching files from the archive

In order to get fetch files from the archive, the `get` command can be used.

```
lftp <username>@archiv.luis.uni-hannover.de:~> get myfile.tar.gz
```

This command puts the file at the location the `lftp` command was issued from which transferred the file into the archive. For fetching more than one file the `mget` command can be used (multiple get). Fetching the file may take some time until transfer starts. This time is needed by the storage robot to find the respective magnetic tape and wind the tape to the position the file is located at.

## 7.6 Some useful commands

Listing the current directories' contents can be achieved by the command `!ls`. An exclamation mark executes the command on the machine lftp was started on. On the contrary listing the current local directory can be done with `lpwd` at the lftp prompt.

It is possible to create directories in the archive using the `mkdir` command.

```
lftp <username>@archiv.luis.uni-hannover.de:~> mkdir myDir
```

Changing directories works in the usual way using `cd`.

```
lftp <username>@archiv.luis.uni-hannover.de:~> cd myDir
```

And back up one directory.

```
lftp <username>@archiv.luis.uni-hannover.de:~> cd ..
```

A local directory can be changed using the `lcd` command, short for local cd.

```
lftp <username>@archiv.luis.uni-hannover.de:~> lcd /bigwork/<username>/datadir
```

## 7.7 Further reading

- man page `lftp`

  ```
  clustertransfer:~$ man lftp
  ```

navigate using the arrow keys and exit with 'q'

- Service Archivierung:
  http://www.luis.uni-hannover.de/archivierung.html

# Citing the cluster system

We welcome citing the cluster system in your publications. If you would like some help phrasing your acknowledgement, feel free to use the examples below. We appreciate it.

Example 1

> Die Ergebnisse/Teile der Ergebnisse, die in dieser Arbeit vorgestellt sind, wurden mithilfe des Clustersystems an der Leibniz Universität Hannover berechnet.
>
> The results presented here were (partially) carried out on the cluster system at the Leibniz University of Hannover, Germany.

Example 2

> Diese Arbeit wurde vom Team des Clustersystems der Leibniz Universität Hannover unterstützt.
>
> We acknowledge the support of the cluster system team at the Leibniz University of Hannover, Germany in the production of this work.

Example 3

> Diese Arbeit wurde unterstützt vom Compute-Cluster, welches von der Leibniz Universität Hannover, vom Niedersächsischen Ministerium für Wissenschaft und Kultur (MWK) und der Deutschen Forschungsgemeinschaft (DFG) getragen wird.
>
> This work was supported by the compute cluster, which is funded by the Leibniz Universität Hannover, the Lower Saxony Ministry of Science and Culture (MWK) and the German Research Association (DFG).

# When your work is done

When you are done working with the cluster system, it would be nice, if you did a few things before leaving.

1. Clean up your directories
   - Clean up $HOME
   - Clean up $BIGWORK
2. Contact us in order to write a contribution to the next Clusterjahresbericht
3. Have your project leader delete your user account

## 9.1 Leaving the Cluster-News mailing list

You can leave the Cluster-News mailing list any time, as it was stated in the welcome email, but we urge you to stay on the list, until your work is done. In case you do not have the welcome email at hand, this is how: send "SIGNOFF CLUSTER-NEWS-RRZN" to listserv@listserv.uni-hannover.de from the email address that you would like to unsubscribe. If it does not work, we can take you off the list manually. It is advantageous to us, if you unsubscribe yourself. This way your request is on file.

# Appendix

## A.1 Working with old software modules

This section is about using software modules which are based on the old "Environment Modules" system.

Please note: As the old module system has several issues that can lead to inconsistencies in the software environment, it has been replaced by the new Lmod based module system. The old modules are still available, but we will not provide neither updates of existing nor installing of a new software.

Run the following command to make available all the old software modules

```
source /sw/modules.sh
```

If you use the csh-family shells:

```
 source /sw/modules.sh
```

The above command has to be run before loading any modules.

To make the old module system your default, add the above line to your `~/.bashrc` or `~/.cshrc` file.

You can work with the old module environment using the following commands:

`module avail` Show all available modules

`module load <modulename> <...>` Load one or more modules

`module unload <modulename>` Unload a module

`module list` Show currently loaded modules

`module show <modulename>` Show which environment variables will be set by a module

Additionally there is a man-page with extensive documentation.

```
man module
```

## A.2 Exercise: Working with modules

```
# find available octave modules
module spider octave

# determine how to load the selected Octave/4.0.0 module
module spider Octave/4.0.0

# load required modules
module load GCC/4.9.3-2.25 OpenMPI/1.10.2

# load module for octave
module load octave/4.0.0

# start application octave
octave
```

## A.3 List of all modules available May 9th 2016

```
abaqus/2016(default)
abaqus/6103
abaqus/6113
abaqus/6121
abaqus/6133
abaqus/6142
abaqus/693
amber/14-gnu
amber/14-impi-intel
amber/14-openmpi-gnu(default)
ansys/13.0
ansys/14.0
ansys/14.5
ansys/15.0
ansys/16.0
ansys/16.1
ansys/16.2
ansys/17.0(default)
ansysem/15.0
ansysem/16.0
ansysem/16.1
ansysem/16.2
ansysem/17.0(default)
aria/2.3(default)
atlas/3.10.0-gnu-4.1.2
atlas/3.10.2-gnu-4.9.1
blas/20090223
blast/2.2.31(default)
blat/3.4
blat/3.5
boost/1.47.0
boost/1.49.0(default)
boost/1.58.0
bwa/0.7.10
bwa/0.7.8
ccpnmr/2.4.0(default)
cfx/12.1
cfx/13.0
cfx/14.0
cfx/14.5
cfx/15.0
cfx/16.0
cfx/16.1
cfx/16.2
cfx/17.0(default)
cgal/4.4
charmm/c35b2-gnu(default)
charmm/c35b2-mpi-gnu
cmake/2.8.7
cmake/3.0.1
cns/1.21-aria2.3-gnu
cns/1.21-aria2.3-intel
cns/1.3-gnu
cns/1.3-haddock2.2-gnu
cns/1.3-haddock2.2-intel
cns/1.3-intel
comsol/3.5
comsol/3.5a
```

```
comsol/3.5a2
comsol/4.0
comsol/4.2
comsol/4.2a
comsol/4.3
comsol/4.3a
comsol/4.3b
comsol/4.3-ckl
comsol/4.4
comsol/4.4-ckl
comsol/5.0
comsol/5.0-ckl
comsol/5.1(default)
cpmd/3.15.1_gnu_openmpi
crystal/09
crystal/14
cst/2012
cst/2013(default)
cst/2014
cython/0.24(default)
elmer/04012016
emacs/23.4
fds/6.1.1_smv-6.1.11
fds/6.4_smv-6.3.6(default)
feko/6.2
feko/6.3
feko/7.0
feko/7.0.2(default)
feko/7.0_hw
fesafe/6.5(default)
fftw/3.2.2-gcc-4.3.3(default)
fftw/3.3.4-gcc-4.9.1
fftw/3.3.4-gcc-4.9.2
fftw/3.3.4-impi-intel-14.0.1.106
fftw/3.3.4-intel-13.0.1.028
fftw/3.3.4-intel-14.0.1.106
fftw/3.3.4-openmpi-gcc-4.9.2
fftw/3.3.4-openmpi-intel-14.0.1.106
fftw/3.3-intel-2011.4.191
fluent/12.0
fluent/12.1
fluent/13.0
fluent/14.0
fluent/14.5
fluent/16.0
fluent/16.1
fluent/16.2(default)
fluent/17.0
fluent.beta/12.0(default)
g++/4.2.4
g++/4.5.1
g++/4.6.3
gambit/2.4.6(default)
gams/23.6.3
gams/23.7.3
gams/23.8.2
gams/24.2.2
gams/24.3.3
```

```
gams/24.4.6
gams/24.5.4(default)
gams_nhus/23.9.5
gams_nhus/24.5.3
gams_nhus/24.5.6
gaussian/g03.E01
gaussian/g09.A02
gaussian/g09.C01(default)
gaussian/g09.D01
gcc/4.2.4
gcc/4.3.3
gcc/4.4.3
gcc/4.5.1
gcc/4.6.2
gcc/4.6.3
gcc/4.9.1
gcc/4.9.2(default)
gdal/1.11.0
gdal/1.8.0(default)
gdb/6.8
gfortran/4.2.4
gfortran/4.5.1
gfortran/4.6.3
gmp/4.24
gmp/4.3.2
gmp/5.0.1
gmsh/2.8.5
gnuplot/4.2.5
graphviz/2.38.0
gromacs/4.0.4_mvapich2_mklseq_d(default
   )
gromacs/5.1.1-openmpi-gcc-4.9.2
gromacs/5.1.2-plumed-2.1.5-openmpi-gcc
   -4.9.2
groops/1.1-mpi-gnu
gsl/1.12
gurobi/6.5.0(default)
haddock/2.2-gnu
haddock/2.2-intel
hdf5/1.8.1(default)
hdf5/1.8.13
hdf5/1.8.9
icc/10.1.015(default)
icc/11.0.074
icc/11.1.046
idb/10.1.015(default)
ifort/10.1.015(default)
ifort/11.1.046
imkl/10.0.3.020(default)
imkl/10.2.1.017
impi/3.2.1.009
impi/4.0.0.025(default)
impi/4.0.2.003
impi/4.1.3.048
intel.compiler/11.1.046(default)
intel.compiler/11.1.069
intel.composer/2011.4.191(default)
intel.composer/2011_sp1.10.319
intel.composer/2013.5.192
intel.license
intel.studio/13.0.1.028
intel.studio/14.0.1.106(default)
```

```
ipython/3.2.0
isight/5.9(default)
itac/8.0.3.007(default)
itac/8.1.4.045
lammps/7Dec15
lapack/3.2
latex/20130723
ls-dyna/8.1.105897(default)
magma/2.20-10(default)
maple/15
maple/16(default)
maple/17
mathematica/10.0
mathematica/10.1.0
mathematica/10.3.0
mathematica/10.4.0(default)
mathematica/8.0
mathematica/8.0.4
mathematica/9.0
matlab/2011a
matlab/2012a
matlab/2012b
matlab/2013a
matlab/2013b
matlab/2014a
matlab/2014b
matlab/2015a
matlab/2015b
matlab/2016a(default)
matplotlib/1.4.2(default)
matplotlib/1.4.3
mkl/10.0.3.020(default)
mkl/10.2.1.017
modeller/9.15(default)
molden/5.0
mpc/0.8.2
mpe2-impi/1.0.6p1
mpfr/2.4.0
mpfr/2.4.2
mpfr/3.0.0
mpich2
msindo/3.4.01
mvapich2/1.4.1-intel(default)
mvapich2/1.8-intel
mvapich2/1.9rc1-intel
mvapich2/2.0b-intel
mvapich2/2.0-pgi-cuda
mvapich2/2.1a-pgi-cuda
nag/nagcl
nag/nagf95
nag/nagfl90
namd/2.10-impi-intel
namd/2.10-openmpi-gcc
netcdf/4.0
netcdf/4.3.2
networkx/1.10
nfft/3.2.4-gnu-4.9.1
numpy/1.1.0
numpy/1.3.0
numpy/1.6.0
numpy/1.6.2
numpy/1.9.0
```

```
numpy/1.9.2
nvidia/5.5
nvidia/6.0
nvidia/6.5
nvidia/7.5.18(default)
octave/3.2.4
octave/3.6.3
octave/3.8.1(default)
octopus/4.1.2-gnu
octopus/4.1.2-intel
octopus/4.1.2-mpi-gnu(default)
octopus/4.1.2-mpi-intel
openblas/0.2.15(default)
opencv/2.4.9(default)
openfoam/1.6-binary
openfoam/1.6-ext
openfoam/2.1.0
openfoam/2.1.1
openfoam/2.2.0
openfoam/2.3.0-SystemMPI-pvbatch
openfoam/2.3.0-SystemMPI-pvbatch-
    offscreen
openfoam/v3.0+(default)
openmpi/1.3.2-intel10
openmpi/1.4.3-gnu
openmpi/1.4.5-gnu
openmpi/1.6.3_gnu_4.5.1
openmpi/1.6.3-gnu_4.9.1
openmpi/1.8.1-intel13
openmpi/1.8.2-gnu(default)
openmpi/1.8.2-gnu-4.9.2
openmpi/1.8.2-intel
openmpi/1.8.3-pgi-cuda
paraview/3.10.1(default)
paraview/3.4.0
paraview/3.8.1
patran/2010(default)
pbs-drmaa/1.0.13
pbs-drmaa/1.0.15(default)
pfft/1.0.8-gnu-4.9.1
pfft/1.0.8-intel-14.0.1.106
pgi/14.1
pgi/14.10
pgi/14.6(default)
pgi/7.2
pgi-mpich/7.2
pgi-mvapich/14.6
phenix/1.10-2155(default)
plumed/2.1.5-openmpi-gcc-4.9.2
```

```
povray/3.6
proj/4.5.0(default)
proj/4.8.0
pydot/1.0.28
python/2.4.6
python/2.6.4
python/2.7.3(default)
python/2.7.9
python/3.4.2
qt/4.7.3
qt/4.8.6
qt/5.3.1
qtiplot/0.9.8.10(default)
qutip/1.1.3
qutip/2.2.0
qutip/3.1.0
R/2.10.1(default)
R/3.0.2
R/3.1.1
rosetta/3.5-impi-intel
rosetta/3.5-openmpi-gnu
samtools/0.1.16
samtools/0.1.19
sas/9.2
schroedinger/2015-3(default)
scipy/0.11.0
scipy/0.14.0
scipy/0.16.0
seqmonk/0.29.0(default)
starccm/10.02
starccm/10.04(default)
starccm/5.04
starccm/7.06-r8
starccm/8.04
starccm/8.06
sun-java/1.6.0_12
sun-java/1.6.0_16
sun-java/1.7.0_55
tcl/8.4.13-gcc-4.9.1(default)
tgicl/2.1
tosca-fluid/2.4(default)
tosca-struc/8.1(default)
totalview/8.11.0
totalview/8.5.0(default)
vtk/5.0.4(default)
vtk/5.4.2
vtk/5.6.1
xerces-c/2.7.0(default)
```