



Leibniz-Rechenzentrum
der Bayerischen Akademie der Wissenschaften



COMSOL at LRZ – a Howto

„LRZ Linux Cluster Systems and COMSOL Workflows”

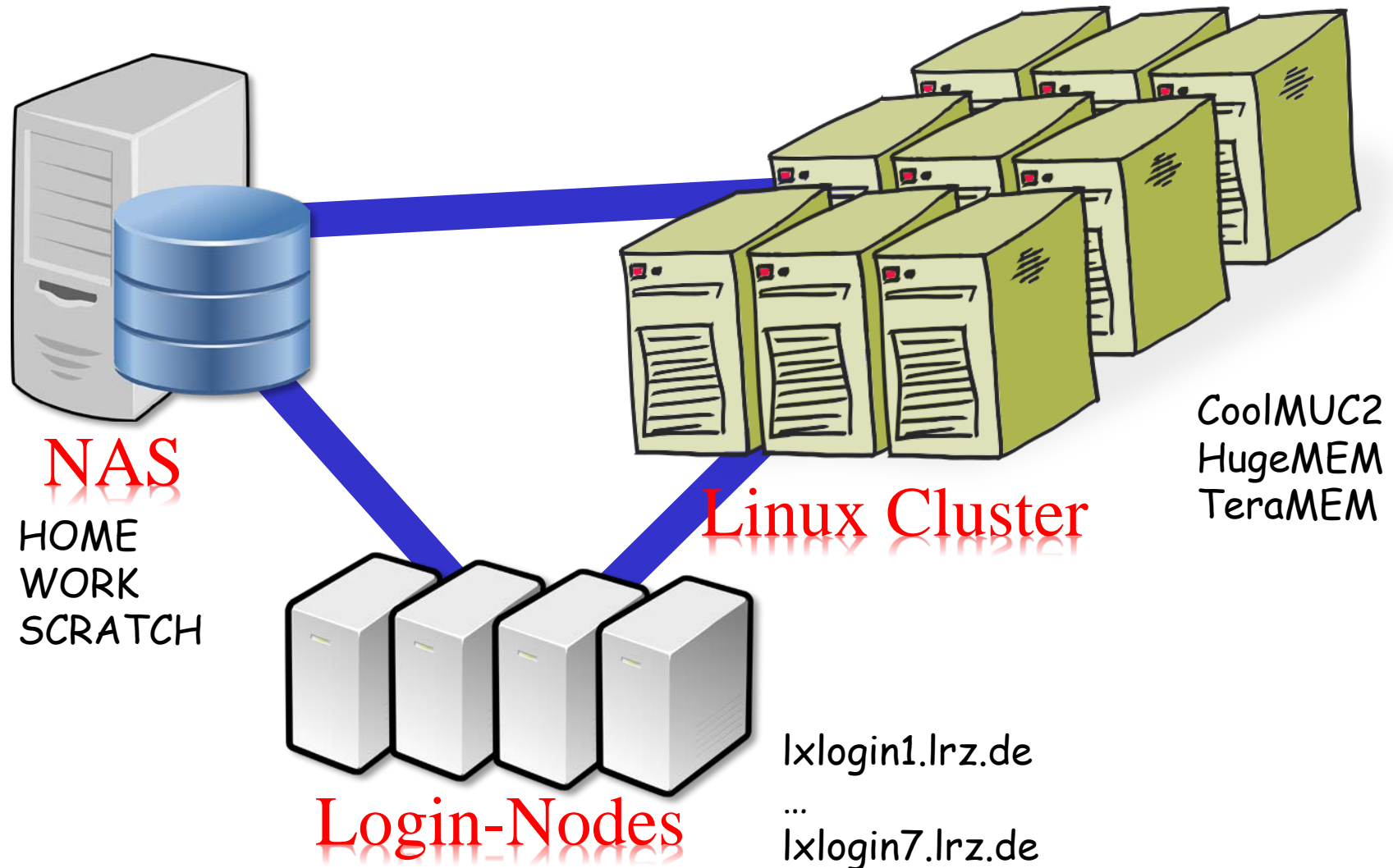
[Martin Ohlerich](#)

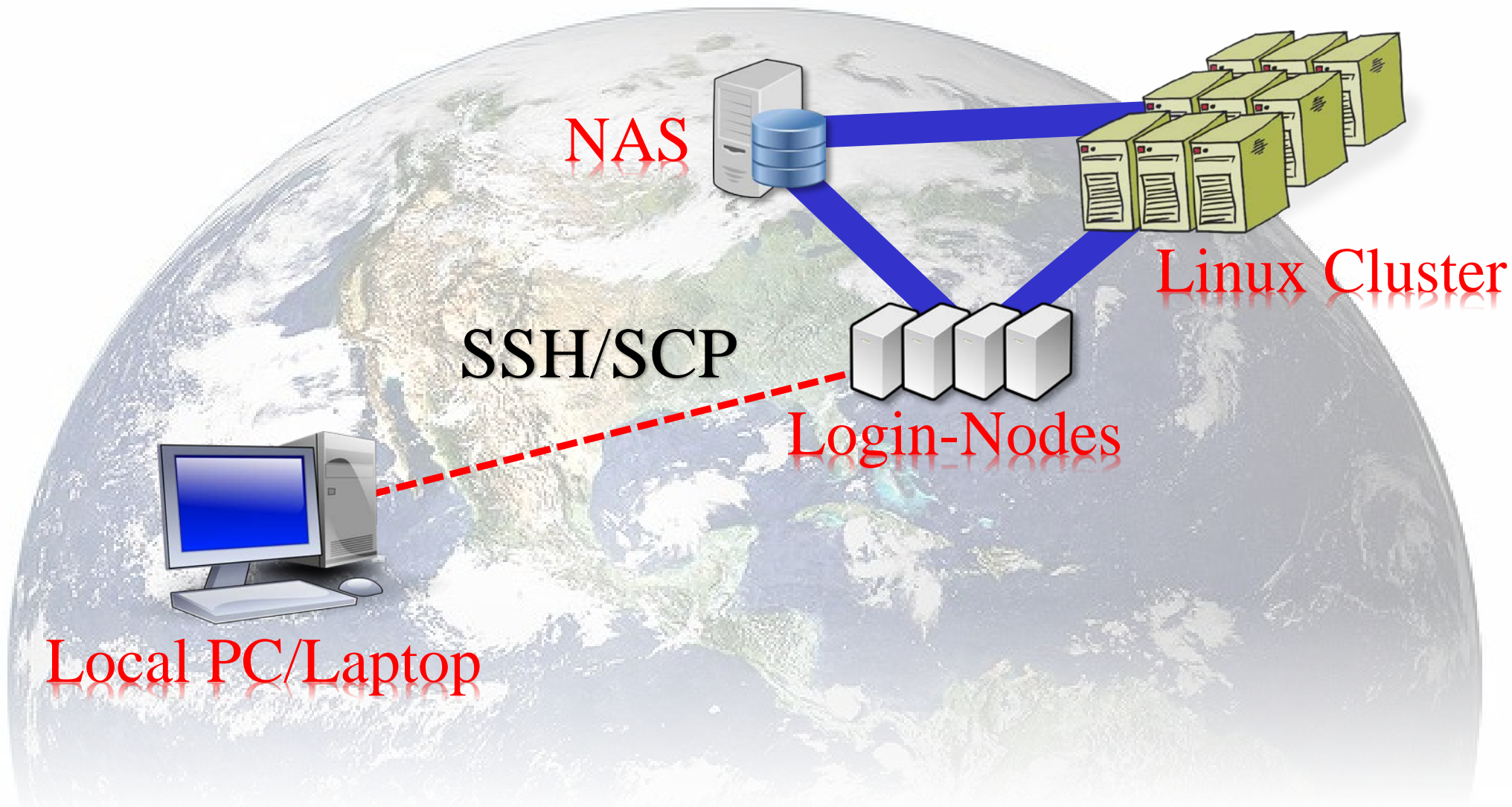
- **LRZ Linux Cluster Systems**
 - *General Overview*
 - *Access/Login*
 - *Basic Usage*

- **COMSOL Workflow Configurations**
 - *A normal Batch Job*
 - *From GUI on a Login-Node*
 - *From GUI on a local PC via a Login-Node*

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LRZ Linux Cluster Overview







Access/Login – SSH/SCP under Linux/MAC

In terminal on your Laptop/PC login on *lxlogin6.lrz.de*

```
$ ssh bla34zak@lxlogin6.lrz.de
```

or, if X-forwarding (graphical applications such as COMSOL GUI)

```
$ ssh -Y bla34zak@lxlogin6.lrz.de
```

Copying files to/from *lxlogin6.lrz.de*

```
$ scp bla34zak@lxlogin6.lrz.de:path/to/file .
```

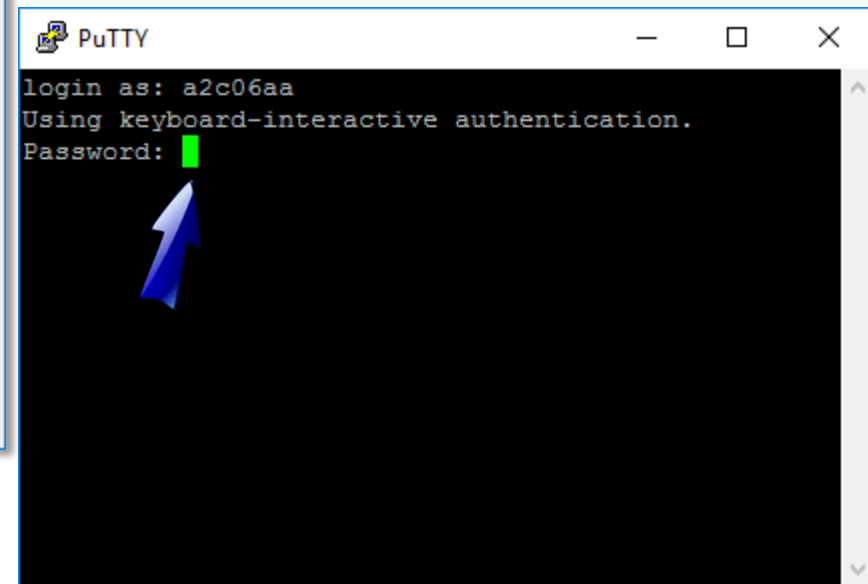
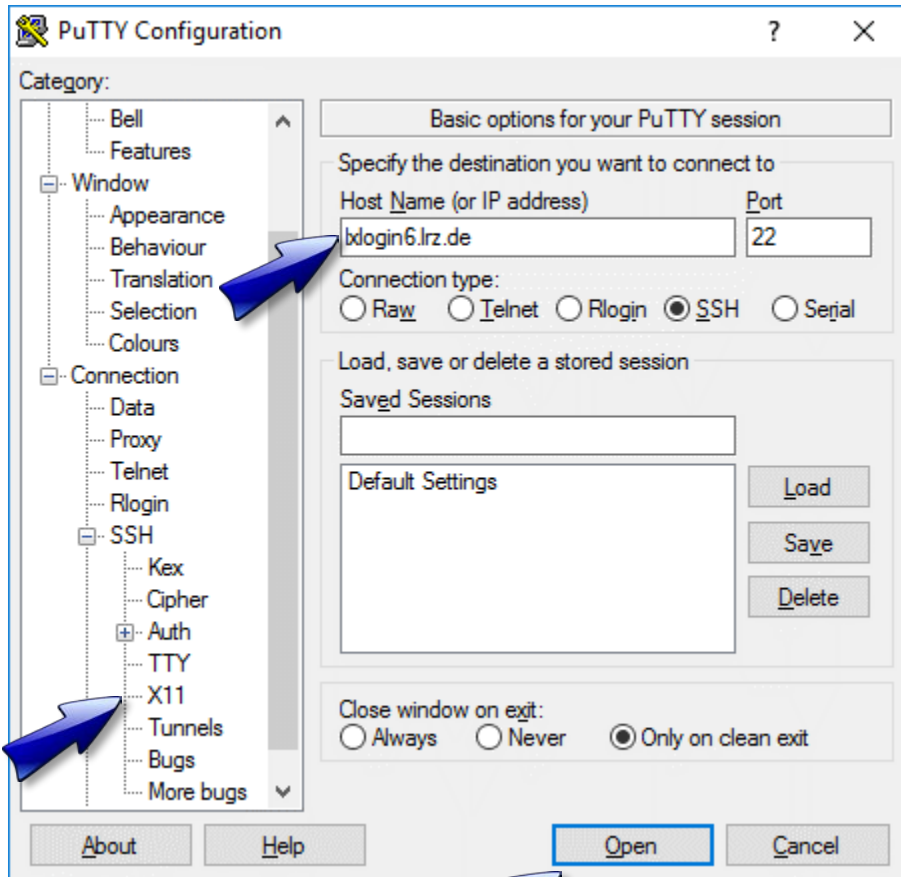
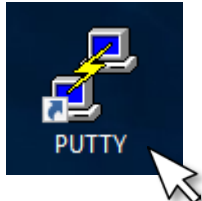
or back

```
$ scp file bla34zak@lxlogin6.lrz.de:path/to/
```

Works also for folders:

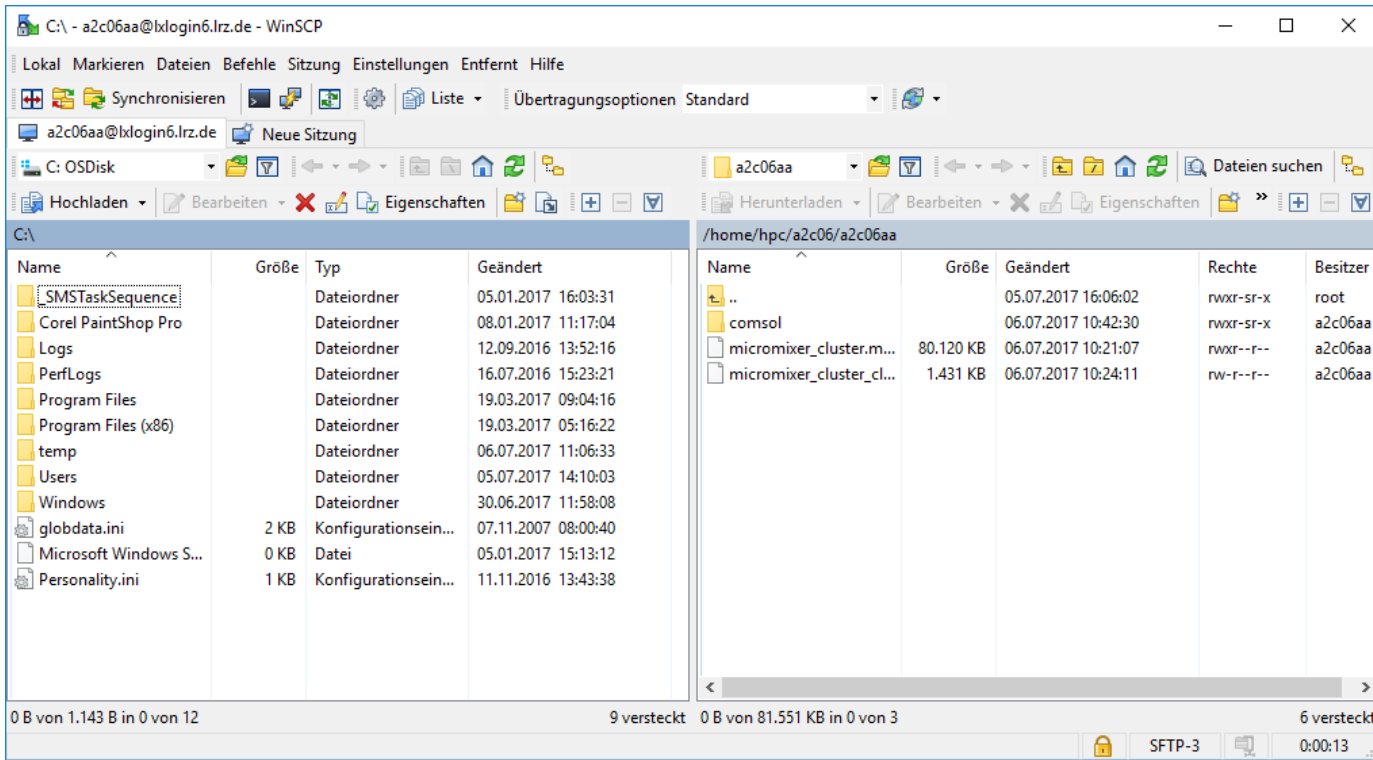
```
$ scp -r folder bla34zak@lxlogin6.lrz.de:path/to/
```

Access/Login – PuTTY under Windows





SCP/File Transfer under Windows/Linux/MAC



WinSCP



FileZilla



Konqueror



Login – Things that make life easier (Linux/MAC)

Local PC/Laptop:

```

$ ssh-keygen -t rsa # generate private-public key pair
Generating public/private rsa key pair. Enter file in
which to save the key (XXXXXXXXXXXXXXXXXXXXX/.ssh/id_rsa):
Enter passphrase (empty for no passphrase):
Enter same passphrase again:
...
$ cat ~/.ssh/id_rsa.pub
ssh-rsa AAAB3NzaC1yc2EAAAADAQA . . .

```



Enter a non-empty, secure passphrase

(different from your login password!)

Copy this public key into ~/.ssh/authorized_keys in the Home directory on lxlogin6.lrz.de !

[\(more information\)](#)



Login – Things that make life easier (Linux/MAC)

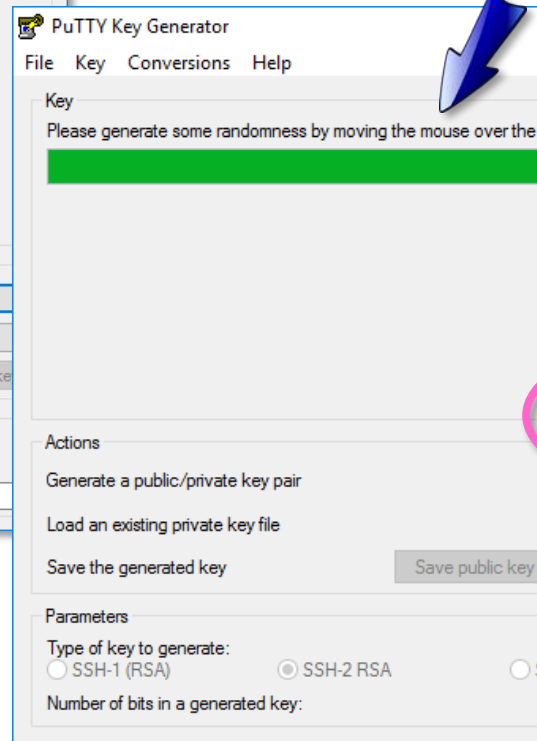
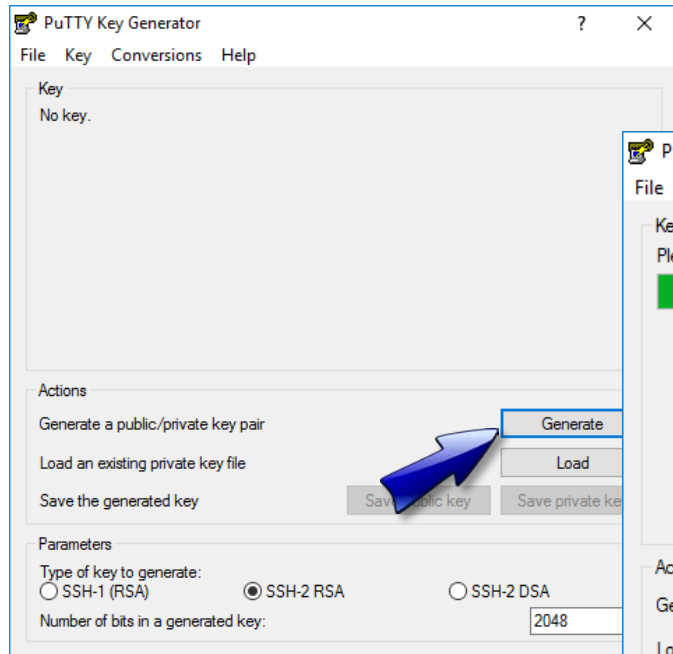
Local PC/Laptop:

Enter the passphrase

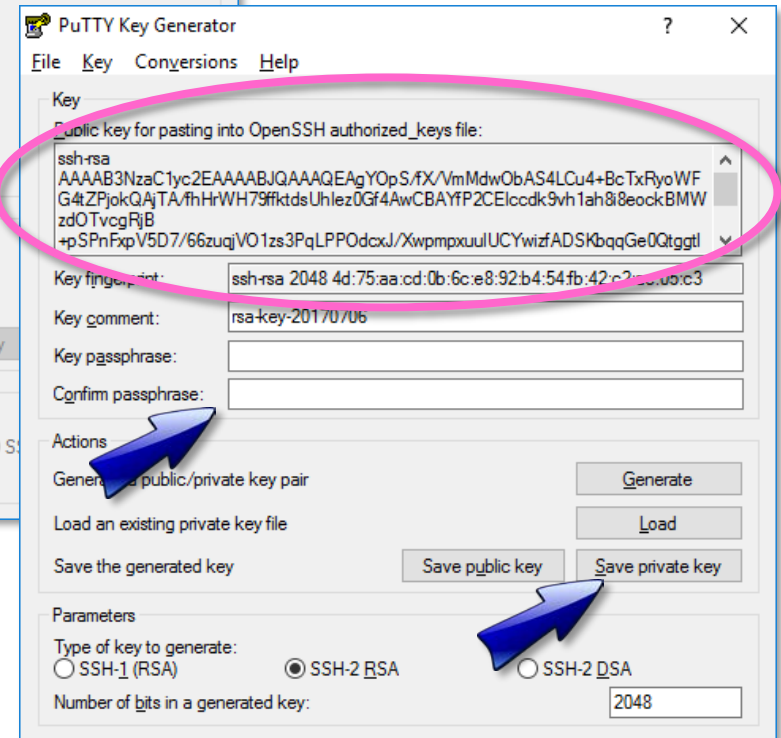
```
$ ssh-add # add ssh key
Enter passphrase for XXXXXXXXXXXX/.ssh/id_rsa:
Identity added: XXXXXXXXXXXX /.ssh/id_rsa XXXXXXXXXXXX /.ssh/id_rsa)
$ ssh bla34zak@lxlogin6.lrz.de
```

No passphrase needed

Login – Things that make life easier (Windows)



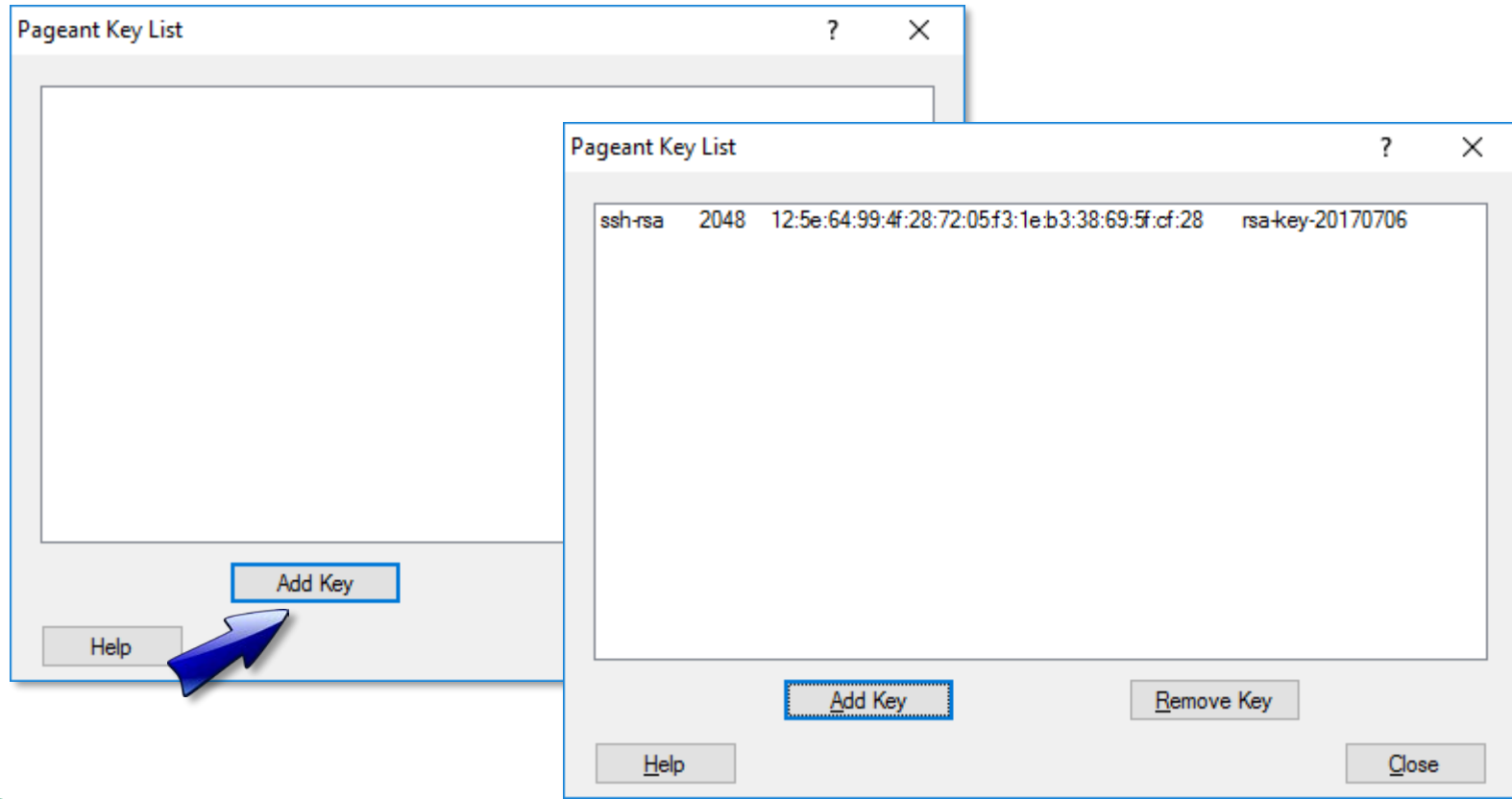
Copy this public key into
~/.ssh/authorized_keys in
the Home directory on
lxlogin6.lrz.de !



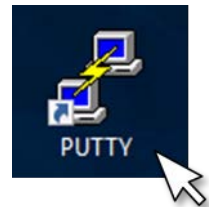
Enter a non-empty, secure passphrase
(different from your login password!)



Login – Things that make life easier (Windows)



Pageant





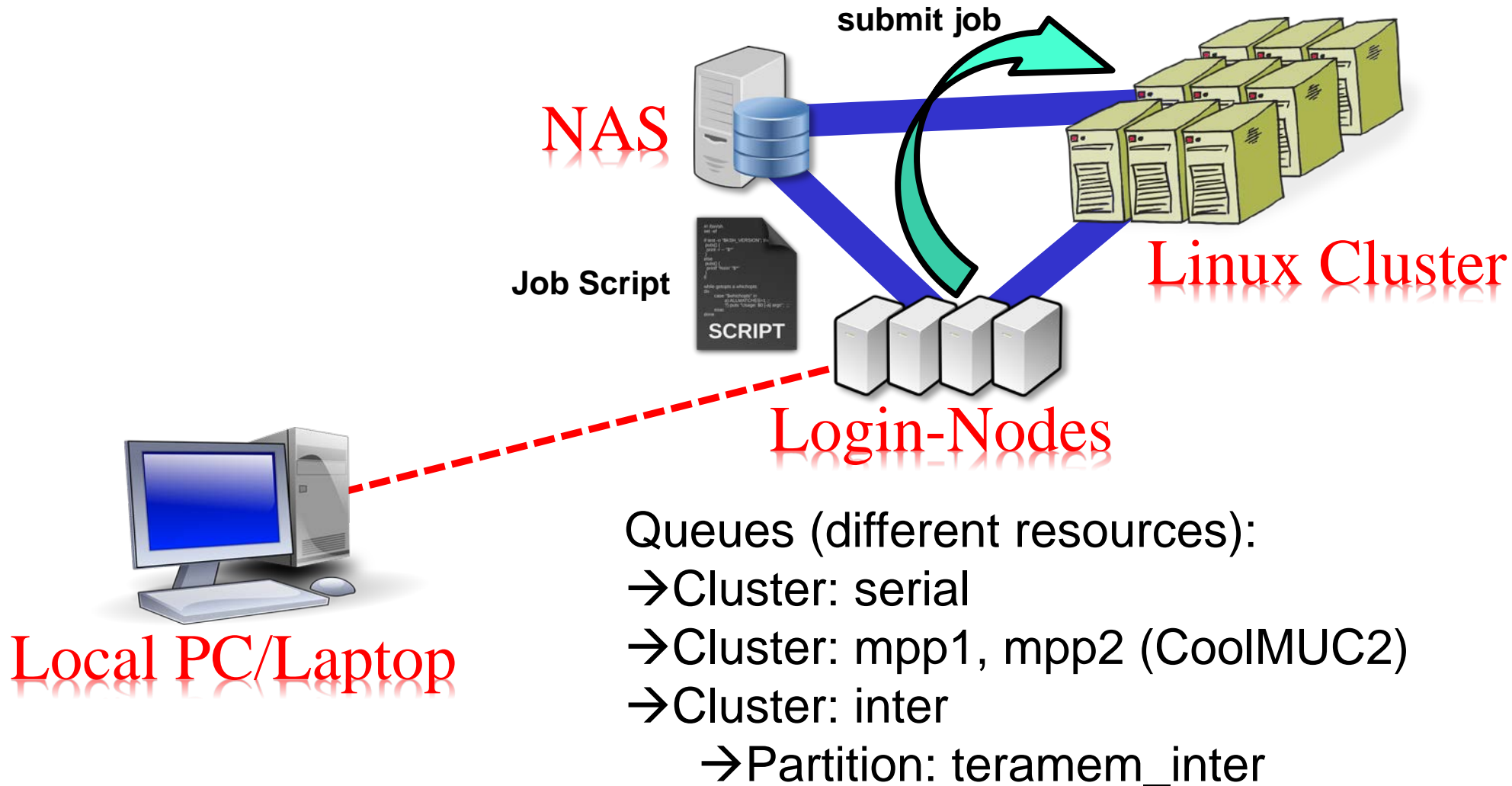
The Environmental Module System

On lxlogin6 (LRZ cluster):

```
$ module help          # get help
$ module list         # list loaded modules
Currently Loaded Modulefiles:
  1) admin/1.0        3) intel/16.0       5) mpi.intel/5.1
  2) tempdir/1.0     4) mkl/11.3         6) lrz/default
$ module avail comsol # search for available mods
----- /lrz/sys/share/modules/files/applications -----
comsol/4.1  comsol/4.2  comsol/5.2a  comsol/5.3(default)
$ module load comsol # load module
$ module unload comsol # remove module
```

Sets *environment variables* (`PATH/LD_LIBRARY_PATH/...`)
and *aliases*

[\(more information\)](#)



On lxlogin6 (LRZ cluster):

```
$ sinfo -M mpp2 # get info about clusters (all)
CLUSTER: mpp2
PARTITION    AVAIL    TIMELIMIT  NODES  STATE  NODELIST
mpp2_batch*  up       2-00:00:00  2  drain* mpp2r04c04s[03-04]
mpp2_batch*  up       2-00:00:00  2  alloc  mpp2r04c04s[01-12]
...
$ sbatch job.sh # submit job.sh to cluster
Submitted batch job 345705 on cluster mpp2
$ squeue -M mpp2 -u $USER # check job status
CLUSTER: mpp2
JOBID PARTITION    NAME        USER        STATE        TIME  TIME_LIMI
NODES NODELIST(REASON)
345705 mpp2_batch  ans_test    bla34zak    PENDING        0:00  20:00
4      (Resources)
$ scancel -M mpp2 345705 # cancel job
```



SLURM – Basic Job Control

On lxlogin6 (LRZ cluster):

```
# get info about pending/running/completed jobs
$ scontrol show jobid -dd 345418 -M mpp2
JobId=345418 JobName=comsol
  UserId=bla34zak (39481) GroupId=a2c06(2351)
  ...
Command=/lrz/sys/applications/comsol/5.3/bin/comsol batch ...
  ...
```

**Very useful when debugging the job submission string
From COMSOL GUI**



SLURM Job Script

```
#!/bin/bash
#SBATCH -o ./job_%j.out      # output of screen
#SBATCH -D .                 # work directory
#SBATCH -J comsol_mpp2      # job name
#SBATCH --get-user-env       # environment
#SBATCH --clusters=mpp2    # which queue
#SBATCH --nodes=4           # CPU resources
#SBATCH --ntasks-per-node=28 # multiples of 28 for mpp2
#SBATCH --mail-type=none    # notification @ state change
#SBATCH --mail-user=<bla34zak@lrz.de>
#SBATCH --time=00:30:00    # estimated run time

. /etc/profile.d/modules.sh # activate environment modules

module load comsol/5.3
mpiexec hostname | sort > mpi_hostfile
comsol batch -inputfile micromixer_cluster.mph \
             -outputfile micromixer_cluster_output.mph \
             -f mpi_hostfile
```



Outline

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On lxlogin6 (LRZ cluster): MPH file prepared

```
...
#SBATCH --clusters=mpp2           # which queue
#SBATCH --nodes=4                 # CPU resources
#SBATCH --ntasks-per-node=28     # multiples of 28 for mpp2
...
mpiexec hostname | sort > mpi_hostfile
consol batch -inputfile micromixer_cluster.mph \
             -outputfile micromixer_cluster_output.mph \
             -f mpi_hostfile
```

On MPP2, you get only complete nodes!

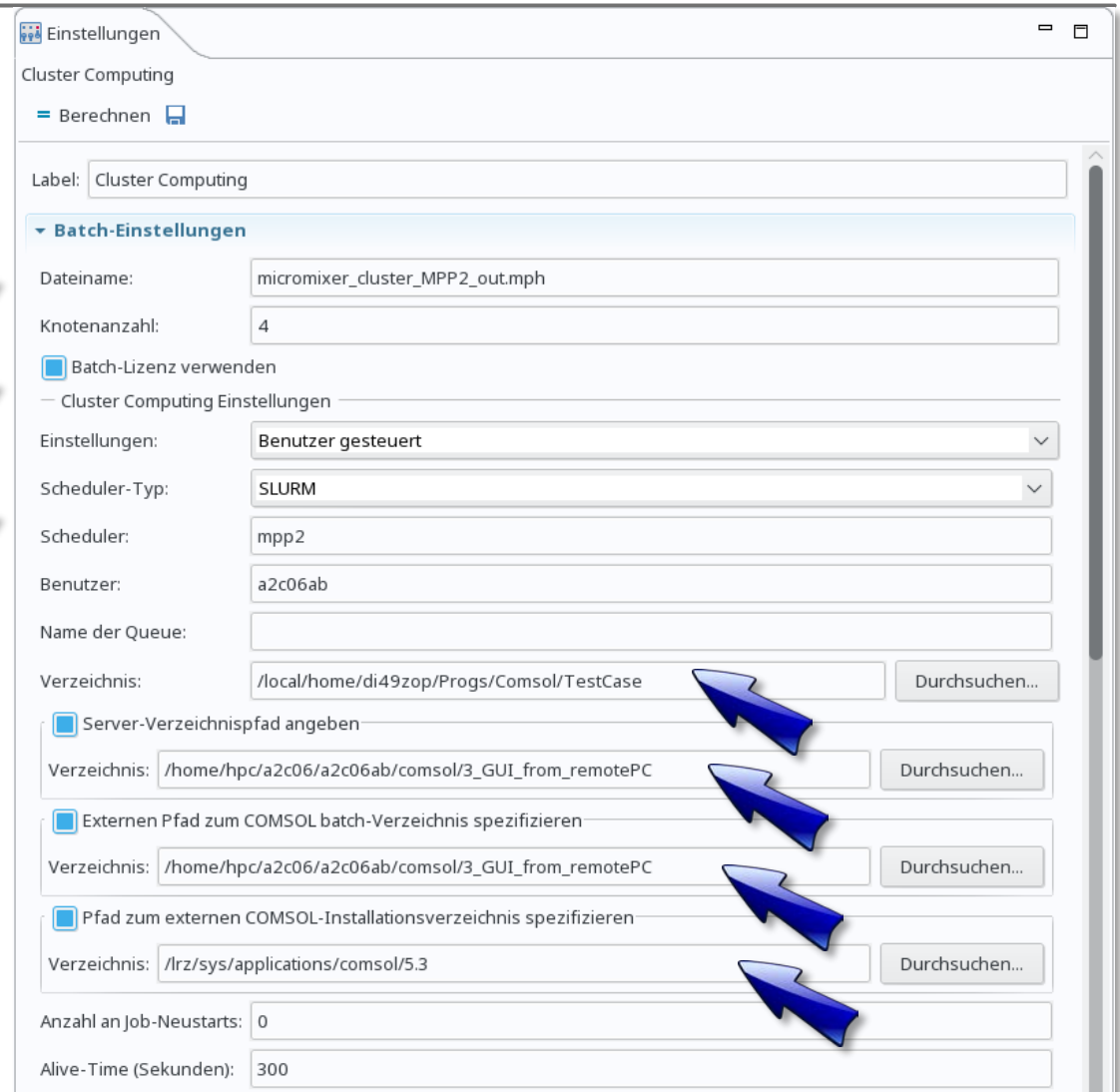
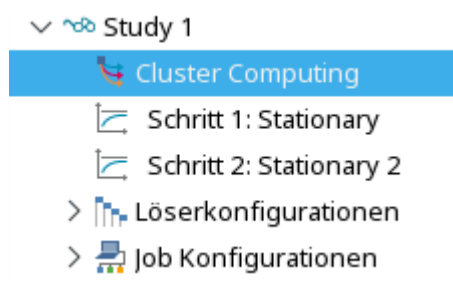


A normal Batch Job

On lxlogin6 (LRZ cluster): ... as before; now hybrid

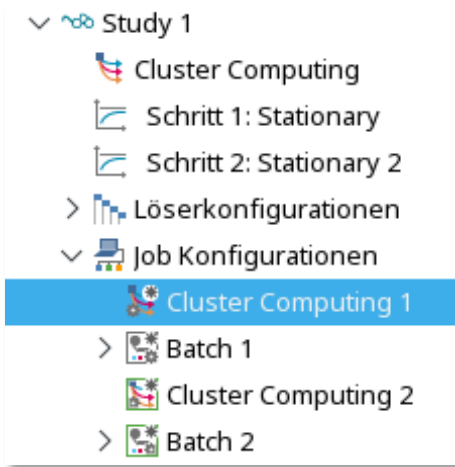
```
...
#SBATCH --clusters=mpp2
#SBATCH --nodes=4
#SBATCH --ntasks-per-node=2
...
mpiexec hostname | sort > mpi_hostfile
export OMP_NUM_THREADS=14
comsol batch -inputfile micromixer_cluster.mph \
             -outputfile micromixer_cluster_output.mph \
             -f mpi_hostfile
```

On Ixlogin6 (LRZ cluster): open COMSOL



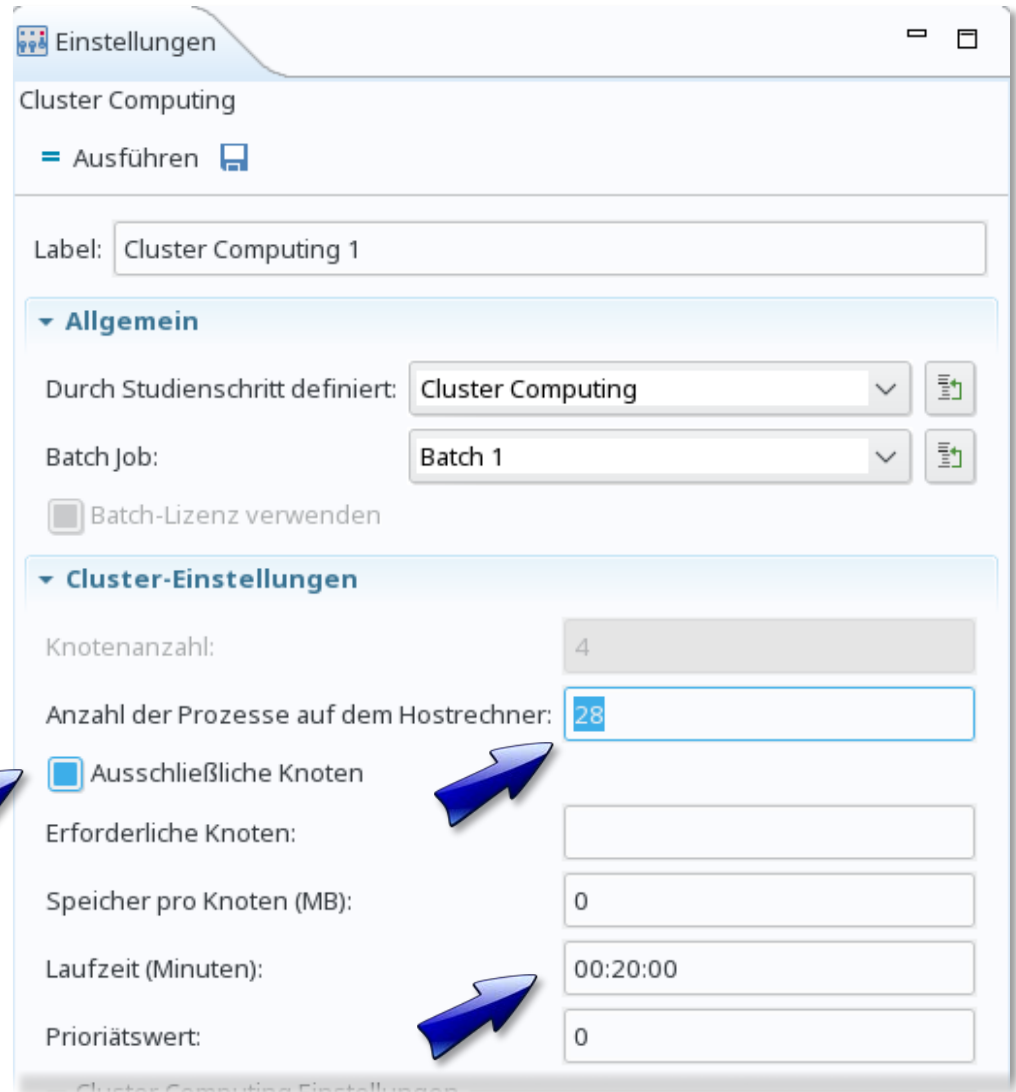


From GUI on Login-Node



Click on *Study 1*
→ = *Compute*

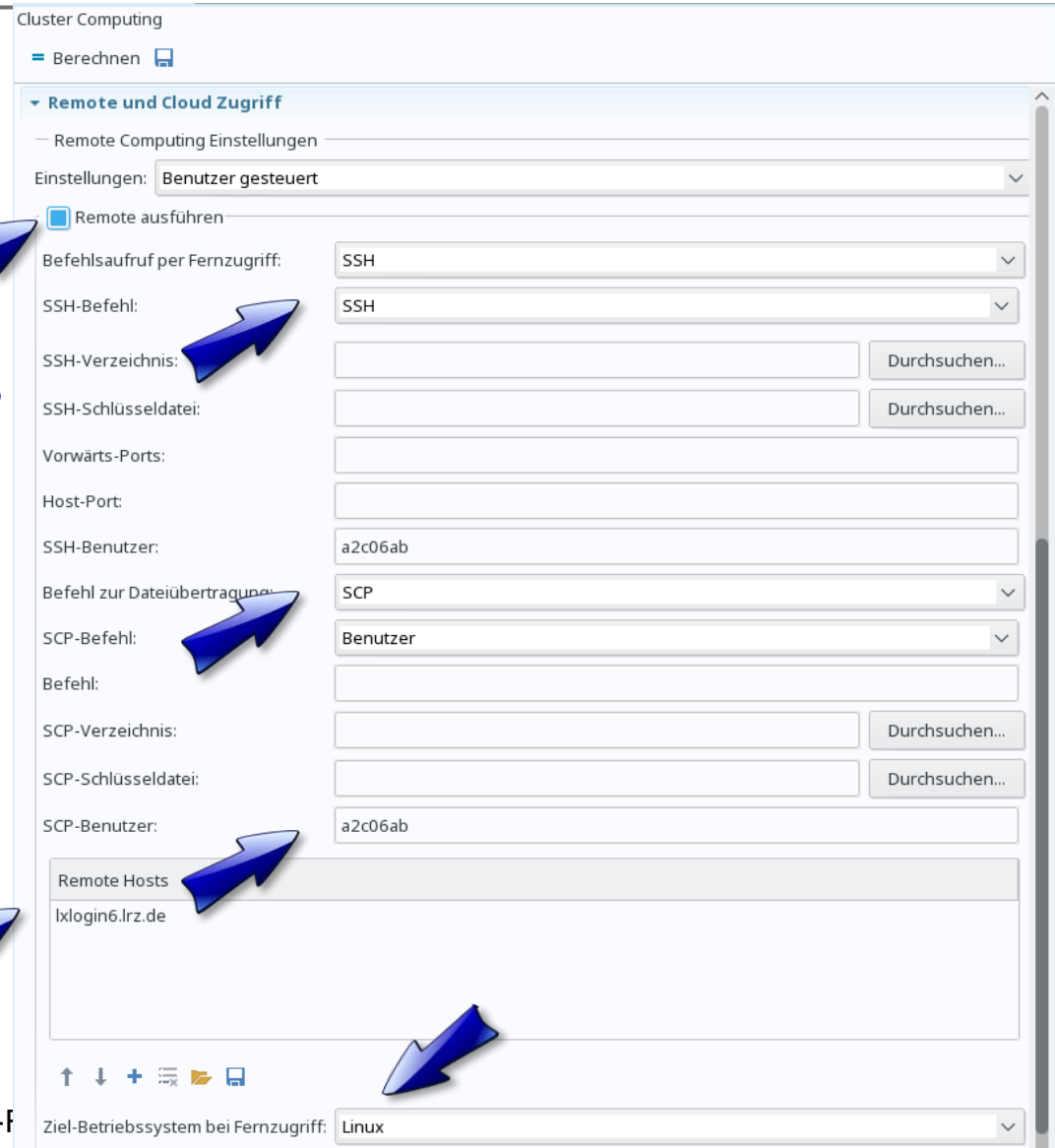
Discussion:
Why two cluster computing nodes?
What means green color?
Differences to Windows GUI?
Batch node? (number of cores)



**On local PC-Laptop:
open COMSOL**

**Cluster Computing settings
as before + *Remote and
Cloud Access***

on Windows:
PUTTY, PSCP



Cluster Computing

= Berechnen

Remote und Cloud Zugriff

Remote Computing Einstellungen

Einstellungen: Benutzer gesteuert

Remote ausführen

Befehlsaufruf per Fernzugriff: SSH

SSH-Befehl: SSH

SSH-Verzeichnis:

SSH-Schlüsseldatei:

Vorwärts-Ports:

Host-Port:

SSH-Benutzer: a2c06ab

Befehl zur Dateiübertragung: SCP

SCP-Befehl: Benutzer

Befehl:

SCP-Verzeichnis:

SCP-Schlüsseldatei:

SCP-Benutzer: a2c06ab

Remote Hosts

lxlogin6.lrz.de

↑ ↓ +

Ziel-Betriebssystem bei Fernzugriff: Linux



General Preferences

Options → Preferences

<ul style="list-style-type: none"> Allgemein Anwendungsbibliotheken Bauteilbibliotheken Client-Server Dateien E-Mail Ergebnisse Geometrie Grafik- und Plotfenster Hilfe Methoden Model Builder Multicore und Cluster Computing Parametrischer Sweep Physics Builder Remote Computing Sicherheit Updates 	<p>Multicore</p> <p>Anzahl der Kerne: <input checked="" type="checkbox"/> 14</p> <p>Anzahl von Sockets: <input checked="" type="checkbox"/> 2</p> <hr/> <p>Cluster Computing</p> <p>Scheduler-Typ: <input type="text" value="SLURM"/></p> <p>Zusätzliche Planer-Argumente: <input type="text"/></p> <p>Zusätzliche MPI Argumente: <input type="text"/></p> <p>MPI Verzeichnis: <input type="text"/></p> <p>Scheduler: <input type="text" value="mpp2"/></p> <p>Benutzer: <input type="text" value="a2c06ab"/></p> <p>Name der Queue: <input type="text"/></p> <p>Batch-Verzeichnis: <input type="text" value="/local/home/di49zop/Progs/Comsol/Test"/> <input type="button" value="Durchsuchen..."/></p> <p><input checked="" type="checkbox"/> Server-Verzeichnispfad angeben</p> <p>Verzeichnis: <input type="text" value="/home/hpc/a2c06/a2c06ab/comsol/3_GUI_from_remoteP"/> <input type="button" value="Durchsuchen..."/></p> <p><input checked="" type="checkbox"/> Externen Pfad zum COMSOL batch-Verzeichnis spezifizieren</p> <p>Verzeichnis: <input type="text" value="/home/hpc/a2c06/a2c06ab/comsol/3_GUI_from_remoteP"/> <input type="button" value="Durchsuchen..."/></p> <p><input checked="" type="checkbox"/> Pfad zum externen COMSOL-Installationsverzeichnis spezifizieren</p> <p>Verzeichnis: <input type="text" value="/lrz/sys/applications/comsol/5.3"/> <input type="button" value="Durchsuchen..."/></p> <p>Befehl Voranstellen: <input type="text"/></p> <p>Befehl Hintenanstellen: <input type="text"/></p> <p>Anzahl an Job-Neustarts: <input type="text" value="0"/></p> <p>Alive-Time (Sekunden): <input type="text" value="300"/></p>
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Visualization (from browser)

rvglrun comsol



Thank you for your
attention!