



bw | HPC – C5

Remote Visualization on bwUniCluster



UNIVERSITÄT
HEIDELBERG
ZUKUNFT
SEIT 1386

Hochschule
für Technik
Stuttgart

Hochschule Esslingen
University of Applied Sciences

Universität
Konstanz



UNIVERSITÄT
MANNHEIM



Universität Stuttgart

EBERHARD KARLS
UNIVERSITÄT
TÜBINGEN



KIT
Karlsruher Institut für Technologie



ulm university universität
uulm



Baden-Württemberg
MINISTERIUM FÜR WISSENSCHAFT, FORSCHUNG UND KUNST

Funding:

www.bwhpc-c5.de

Results visualization – how to do it?

■ Locally

- Download the data on the local PC (scp from JUSTUS to LOCAL station)
 - Visualization programs must be installed
 - Performance?
 - Workflow break

■ X-Forwarding

- Easy to use
- Responsiveness can be bad for interactive graphics
- Only recommended for non-interactive use

■ VNC (Virtual Network Computing)

- Needs a server started on the cluster
- Better performance than X-Forwarding

X-Forwarding

- Login with ssh option -X

- Without X-Forwarding: `ssh <UserID>@justus.uni-ulm.de`

- With X-Forwarding: `ssh -X <UserID>@justus.uni-ulm.de`

Now you can start graphical applications

X-Forwarding

- Login with ssh option -X

- Without X-Forwarding: `ssh <UserID>@justus.uni-ulm.de`

```
module load chem/molden  
molden
```

- With X-Forwarding: `ssh -X <UserID>@justus.uni-ulm.de`

```
module load chem/molden  
module load chem/molpro/2015.1.5  
molden $TURBOMOLE_HOME/bwhpc-examples/methane.xyz  
module load chem/molden
```



bw | HPC – C5

Remote Visualization with VNC

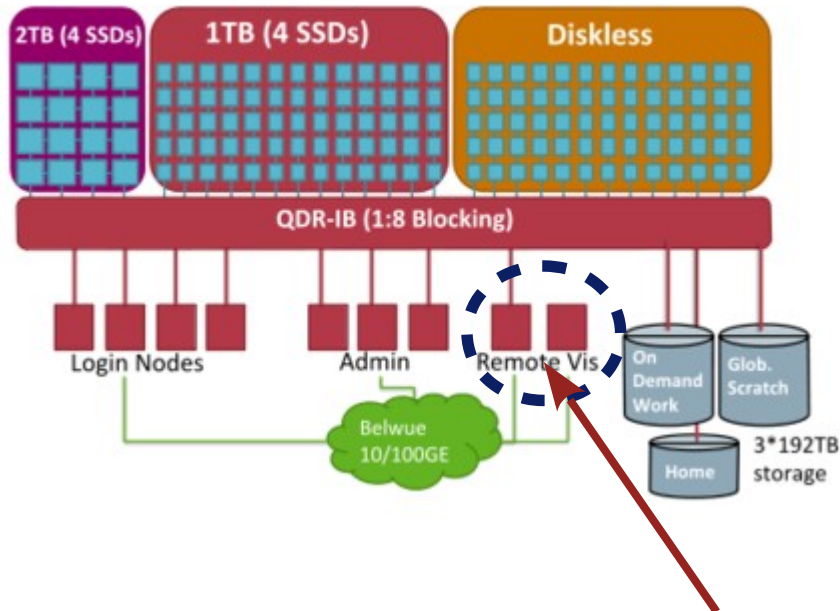




bwHPC – C5

Remote Visualization with VNC

JUSTUS



2 nodes for the remote visualization

NVIDIA K6000

512 GB of RAM

4 TB of the local disk space.

ssh <UserID>@justus-vis.uni-ulm.de

Remote Visualization with VNC

HOW TO DO IT ON JUSTUS?

- login on vis node: `ssh <UserID>@justus-vis.uni-ulm.de`
- start vnc server: `module load vis/tigervnc`
`run_vncserver`
- connect to vnc session via an ssh tunnel:
follow the instructions given by run_vncserver
- Run vis applications within the VNC session
`vmd ...`