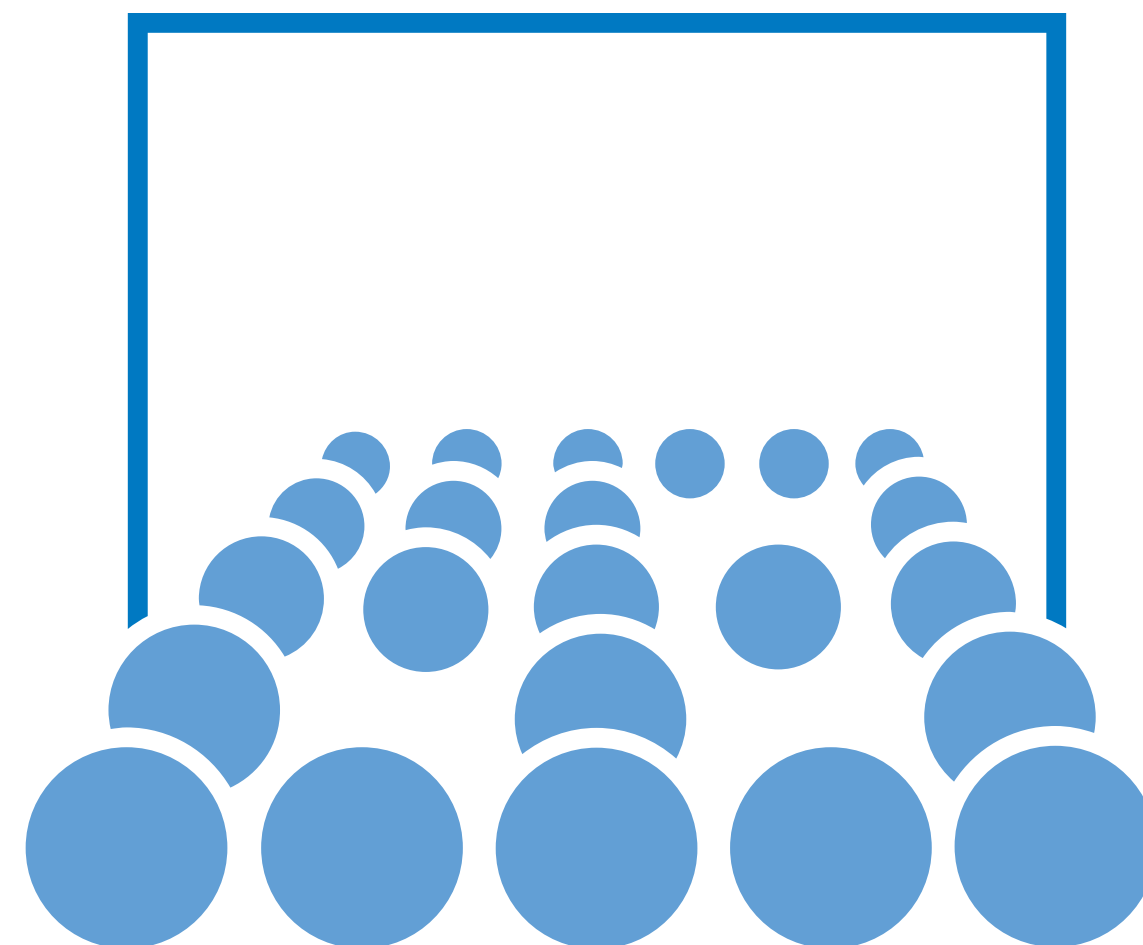


PSE Molecular Dynamics

Session 4: Code Optimization
Alex Breuer, Benjamin Uekermann



MAC-Cluster: Overview

	Intel Sandy Bridge (snb)	AMD Bulldozer (bdz)
Product Name (base frequency)	Xeon E5-2670 (2.6 GHz)	AMD Opteron 6274 (2.2 GHz)
#nodes	28	18
#cores	448	1216 (608 FPUs)
Peak (TFLOPS)	9.3	10.7
Memory (TB)	3.5	4.9

Guidelines

- logins: one login per participant
- change password through: <https://idportal.lrz.de/r/entry.pl>: Passwort ändern on left side, type old one, repeat your new one two times and hit Passwort ändern afterwards.
- ssh xyz@mac-login-amd.tum-mac.cos.lrz.de or xyz@mac-login-intel.tum-mac.cos.lrz.de, within the MWN (VPN client or computing hall)
- I/O goes to \$SCRATCH, nowhere else!
- read the motd carefully
- Documentation & policies
 - http://www.mac.tum.de/wiki/index.php/MAC_Cluster
 - <http://www.lrz.de/services/compute/linux-cluster/intro>

```

breuera — ssh — 80x24
#####
Welcome to the MAC Research Cluster      ##  ##  ##  ##  ##
operated by                             ##  ##  ##  ##  ##
Leibniz Supercomputing Centre           ##  ##  ##  ##  ##
#####

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This cluster offers several different platforms organized as partitions:

PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
nvd        up        infinite   4      idle mac-nvd[01-04]
ati        up        infinite   4      idle mac-ati[01-04]
wsm        up        infinite   2      idle mac-wsm[01-02]
snb        up        infinite  28      idle mac-snb[01-28]
bdz        up        infinite  19      idle mac-bdz[01-19]

NodeName=mac-nvd[01-04] Procs=32 Sockets=2 CoresPerSocket=8 ThreadsPerCore=2
NodeName=mac-ati[01-04] Procs=32 Sockets=2 CoresPerSocket=8 ThreadsPerCore=2
NodeName=mac-wsm[01-02] Procs=64 Sockets=4 CoresPerSocket=8 ThreadsPerCore=2
NodeName=mac-snb[01-28] Procs=32 Sockets=2 CoresPerSocket=8 ThreadsPerCore=2
NodeName=mac-bdz[01-19] Procs=64 Sockets=4 CoresPerSocket=16 ThreadsPerCore=1

partition "nvd" features:
- 4 nodes: dual socket Intel SandyBridge-EP Xeon E5-2670, 128 GB RAM,

```

Some Basics

- X-forward:
`ssh -Y user@mac-login-amd.tum-mac.cos.lrz.de`
- module system:
`module load, list, unload, info`
- Use the Linux Cluster to show your VTune-results:
`ssh -Y user@lxlogin1.lrz.de`
- Compute Interactive:
`salloc --partition=snb -ntasks=1 -cpus-per-task=32 --time=01:00:00`
`srun ./MoISim ARGS...`
- Compute: batch (see example-script at login)
`queue | sbatch | sinfo | sview`
- You are able to login to allocated compute nodes directly:
`ssh mac-snbXX | ssh mac-bdzXX`