Efficient MD simulations at HPC2N

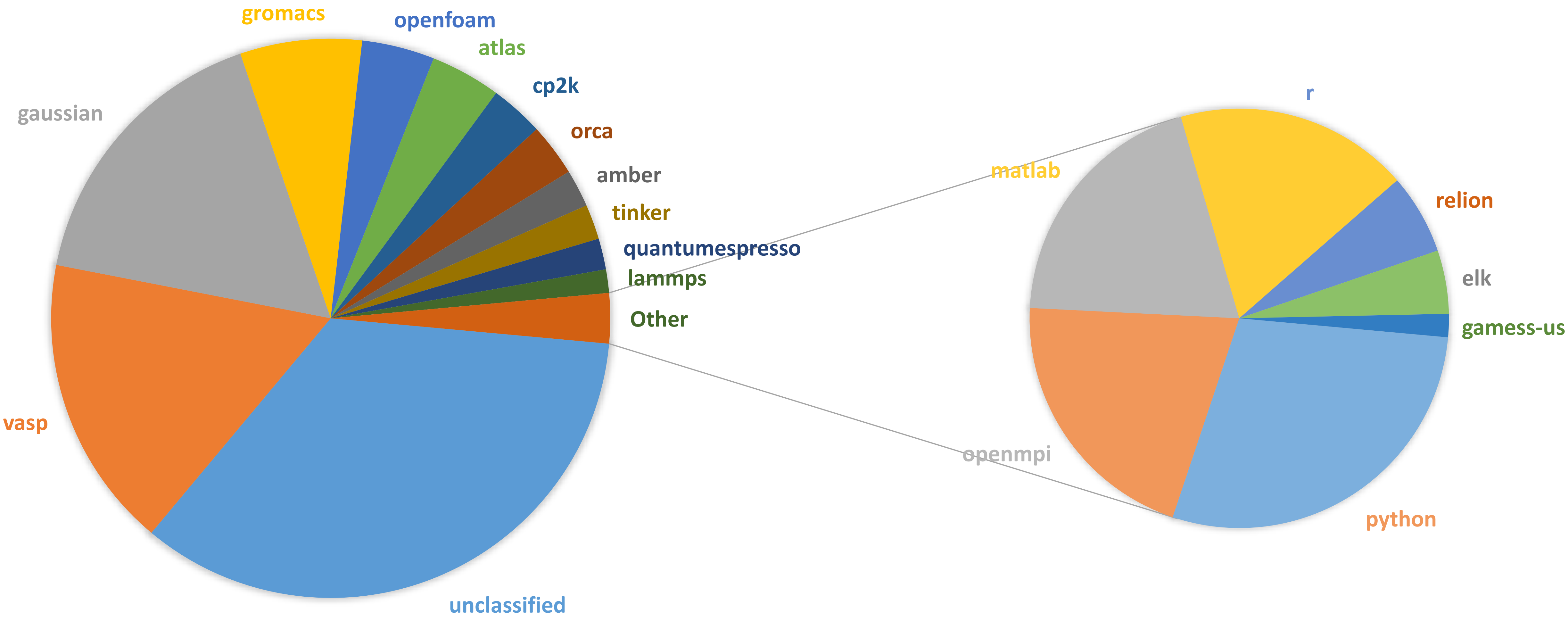
P. Ojeda

Application Expert

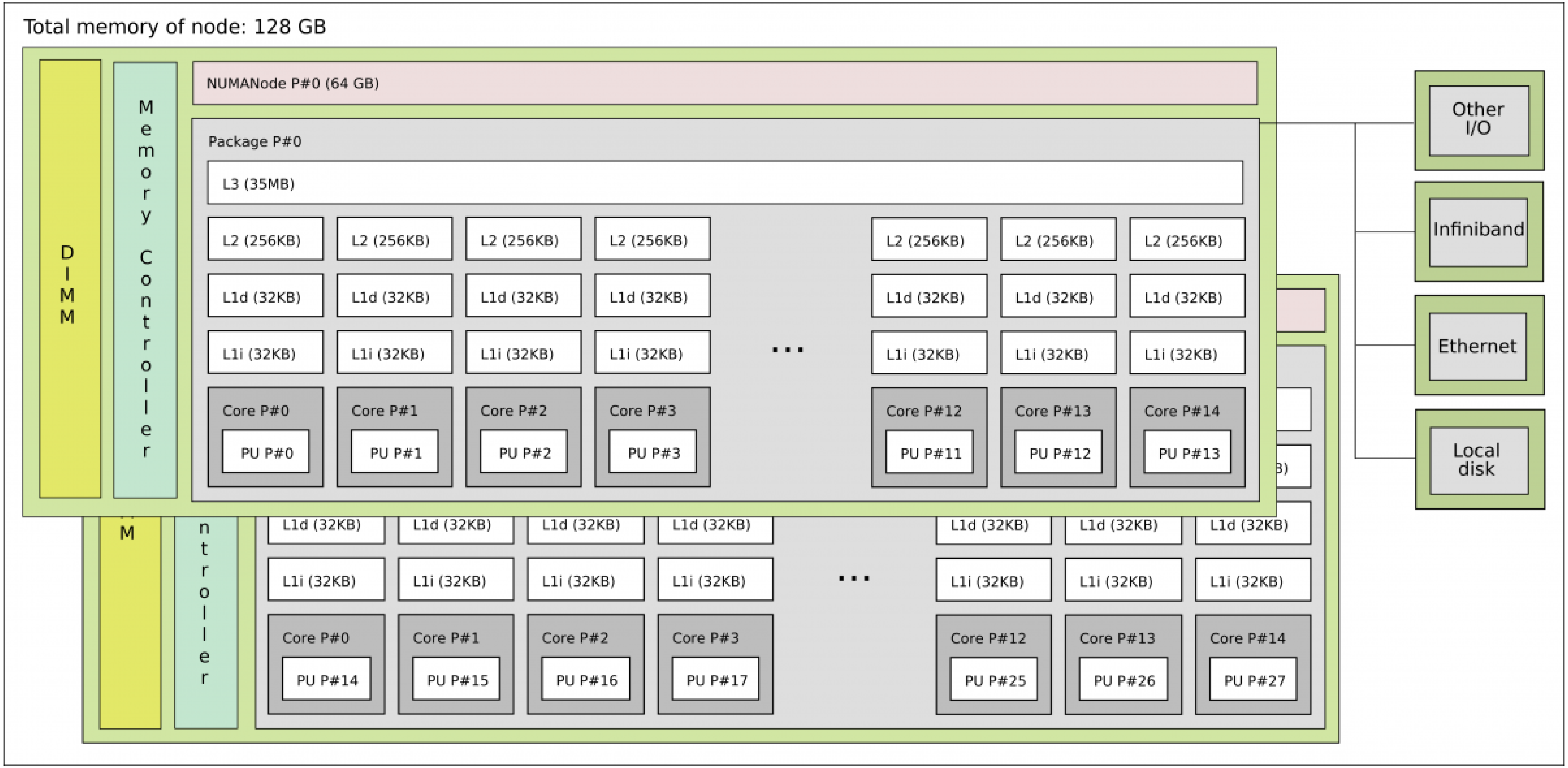
Application Experts at HPC2N:

- Jerry Eriksson
- Åke Sandgren
- Pedro Ojeda (MD, Ab-initio software)

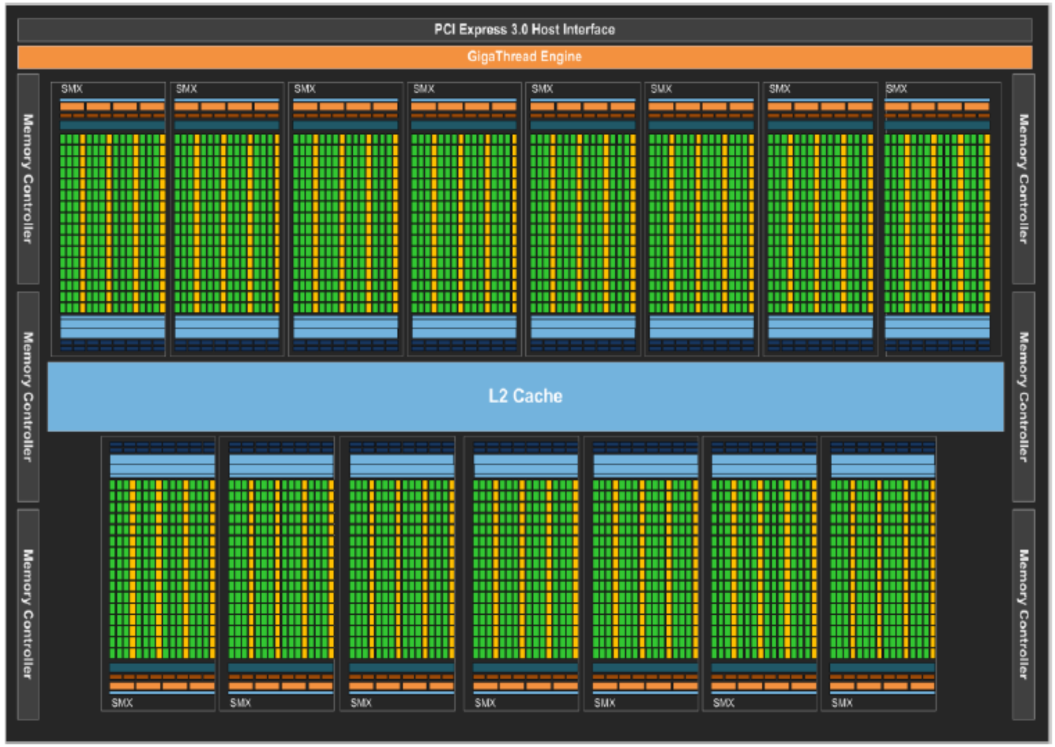
CORE HOURS USED BY DIFFERENT APPLICATIONS (-2021)



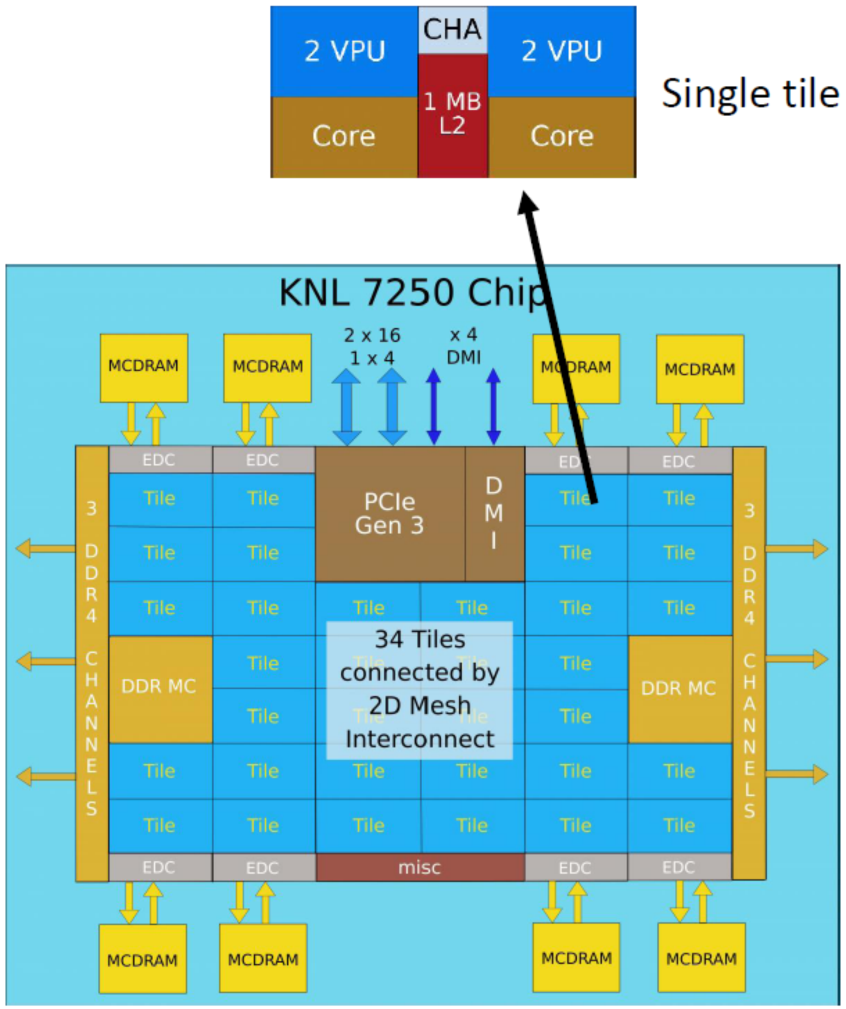
Broadwell node on Kebnekaise



Accelerators



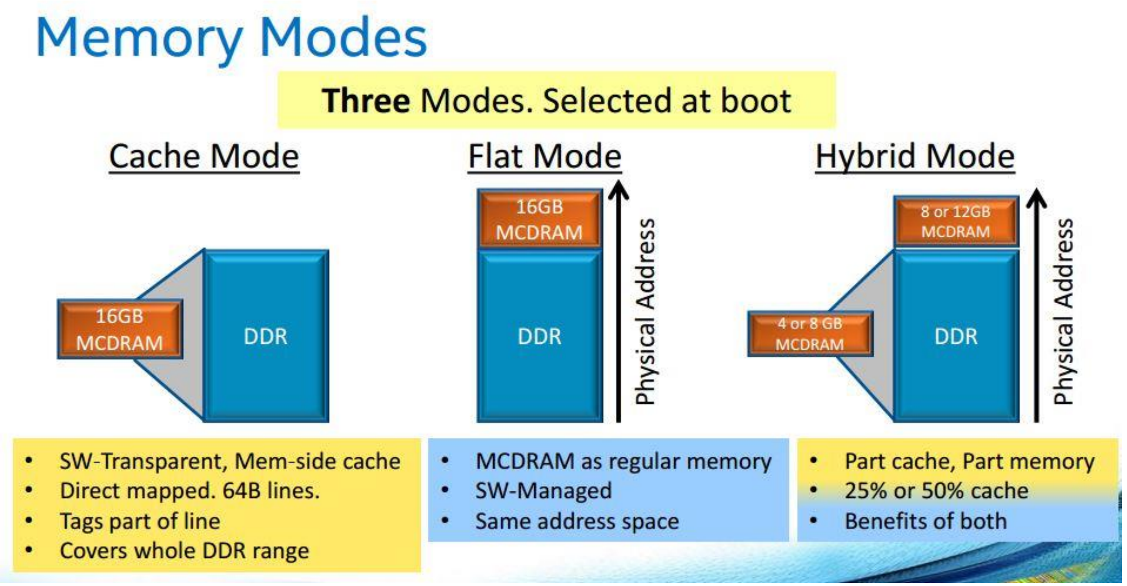
GPU showing the independent units Streaming Multiprocessors (SM).



KNL, composed of several Tiles

$Z(i) = A*X(i) + Y(i)$ (Vector Op. SIMD)

KNL



Memory Modes

Three Modes. Selected at boot

Cache Mode

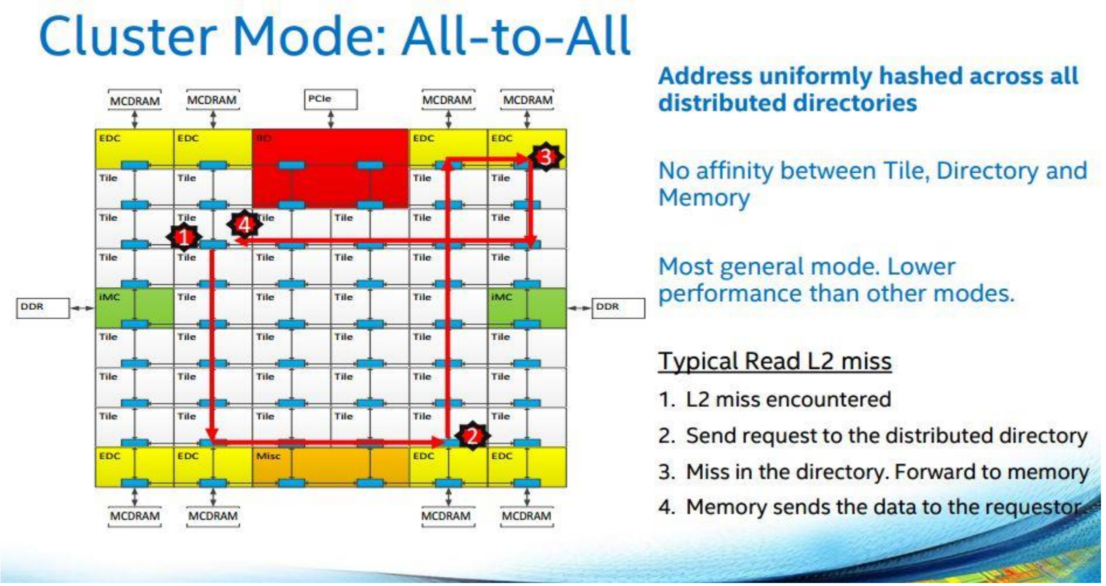
- SW-Transparent, Mem-side cache
- Direct mapped. 64B lines.
- Tags part of line
- Covers whole DDR range

Flat Mode

- MCDRAM as regular memory
- SW-Managed
- Same address space

Hybrid Mode

- Part cache, Part memory
- 25% or 50% cache
- Benefits of both



Cluster Mode: All-to-All

Address uniformly hashed across all distributed directories

No affinity between Tile, Directory and Memory

Most general mode. Lower performance than other modes.

Typical Read L2 miss

1. L2 miss encountered
2. Send request to the distributed directory
3. Miss in the directory. Forward to memory
4. Memory sends the data to the requestor

#SBATCH --constraint=a2a,cache

#SBATCH --gres=hbm:4G

Credits: PRACE Best practice KNL (2017)

KNL

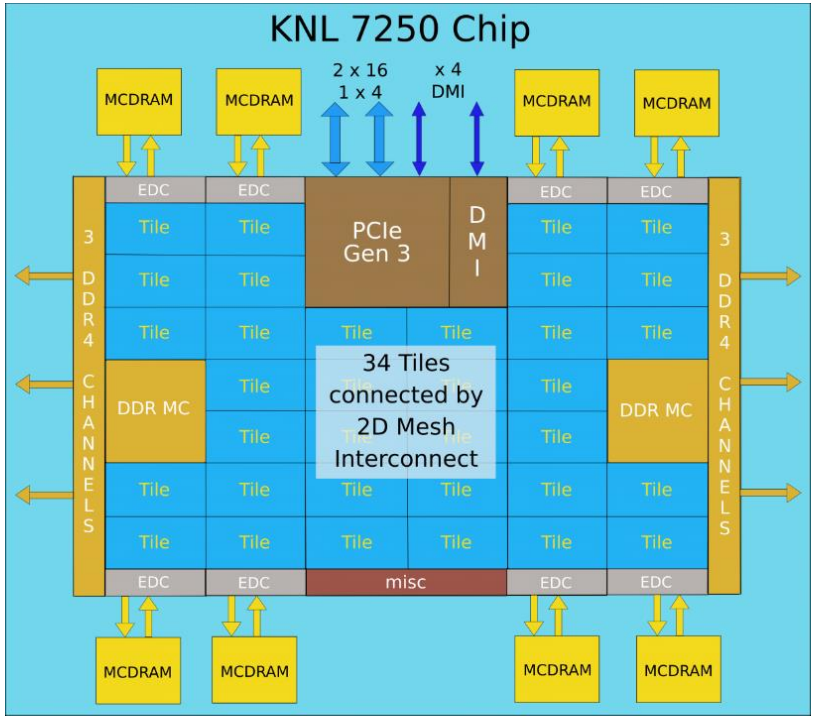
```
#SBATCH --constraint=quad,flat
```

```
numactl -H
node 0 size: 193306 MB
node 0 free: 186258 MB
node 1 cpus:
node 1 size: 16125 MB
node 1 free: 15990 MB
node distances:
node   0   1
  0:  10  31
  1:  31  10
```

More information:
https://www.hpc2n.umu.se/resources/hardware/kebnekaise/knl

KNL Thread affinity

There are physical 68 cores with 4 hyperthreads on each.



Credits: Intel

Bind the threads by using OpenMP env. var.

```
export OMP_NUM_THREADS=4
export OMP_PROC_BIND=spread
export OMP_PLACES=cores
```

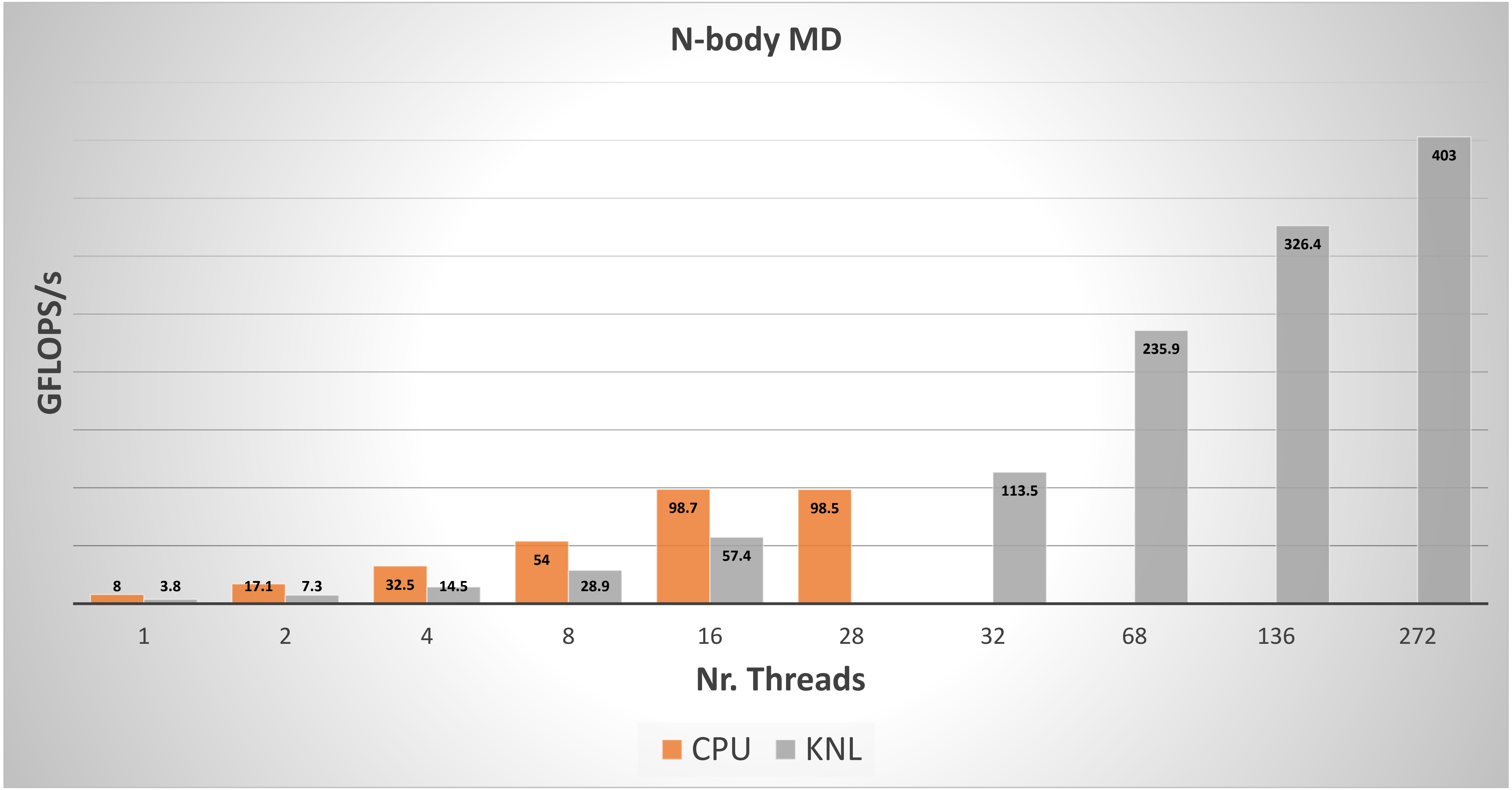
```
srun -n 68 -c 4 --cpu_bind=cores a_knl.out
```

Alternatively, use Intel var.

KNL Thread affinity

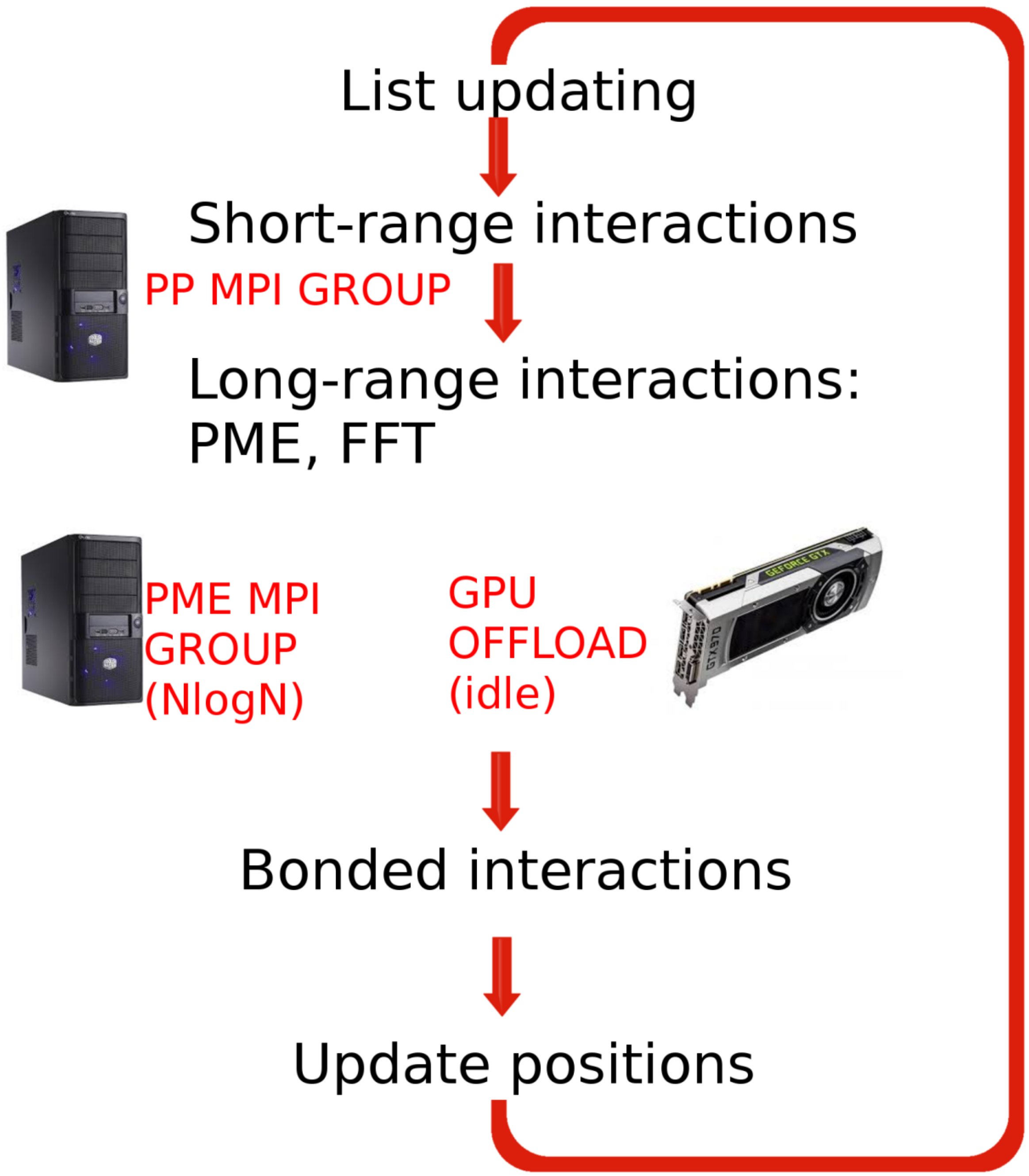
```
#export OMP_PROC_BIND=spread, close, etc.
#export OMP_PLACES=threads, cores, etc.
export OMP_NUM_THREADS=4
srun -n 16 -c 4 --cpu_bind=cores ./xthi
```

```
Hello from rank 0, thread 0, on b-cn1209.hpc2n.umu.se. (core affinity = 0)
Hello from rank 0, thread 1, on b-cn1209.hpc2n.umu.se. (core affinity = 68)
Hello from rank 0, thread 2, on b-cn1209.hpc2n.umu.se. (core affinity = 136)
Hello from rank 0, thread 3, on b-cn1209.hpc2n.umu.se. (core affinity = 204)
Hello from rank 1, thread 0, on b-cn1209.hpc2n.umu.se. (core affinity = 1)
Hello from rank 1, thread 1, on b-cn1209.hpc2n.umu.se. (core affinity = 69)
Hello from rank 1, thread 2, on b-cn1209.hpc2n.umu.se. (core affinity = 137)
Hello from rank 1, thread 3, on b-cn1209.hpc2n.umu.se. (core affinity = 205)
```



KNL are specially performant if one is developer of the MD application

MD workload



List updating

Short-range interactions

PP MPI GROUP

Long-range interactions:
PME, FFT

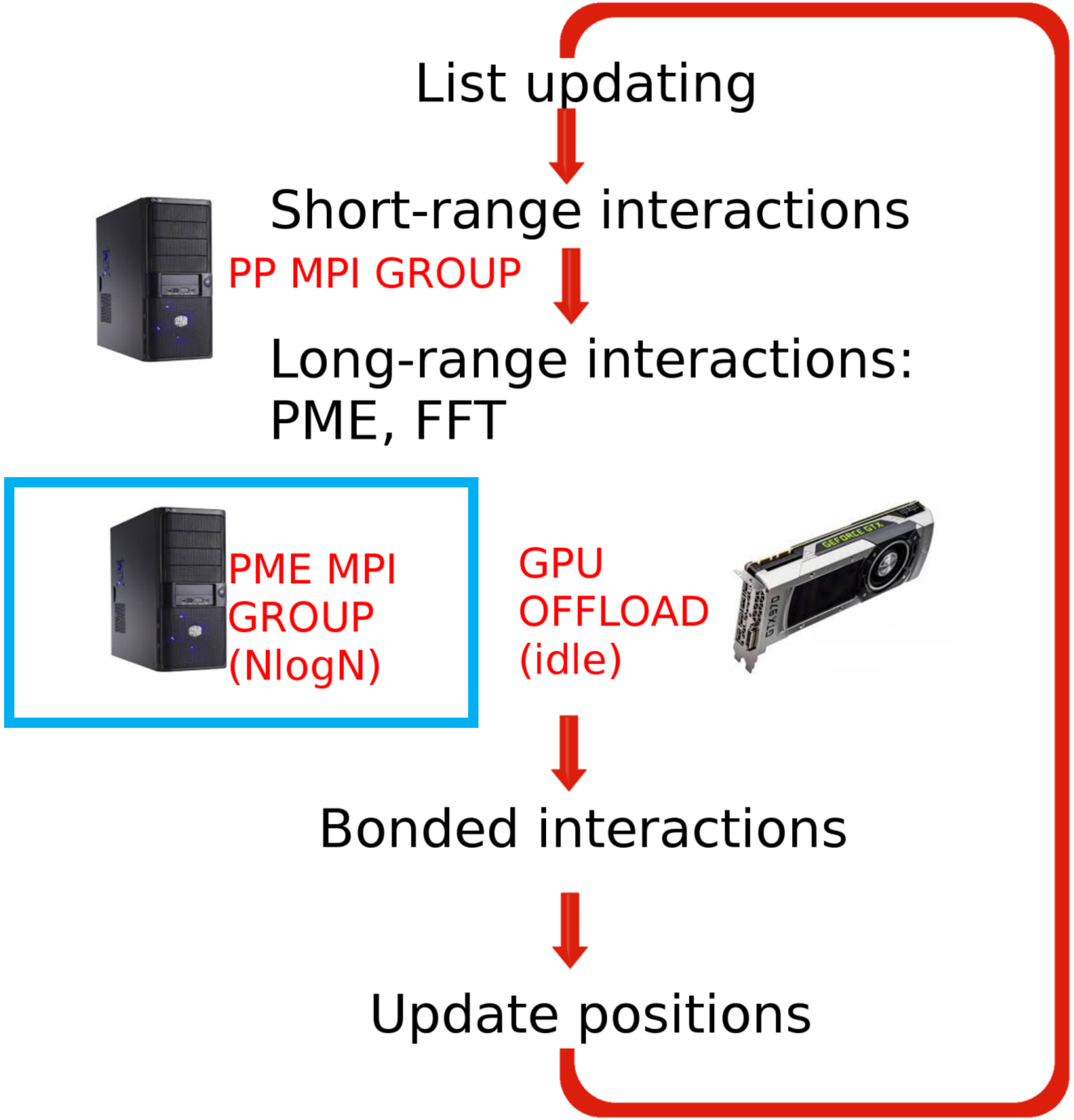
PME MPI
GROUP
(NlogN)

GPU
OFFLOAD
(idle)

Bonded interactions

Update positions

MD workload



List updating

Short-range interactions

PP MPI GROUP

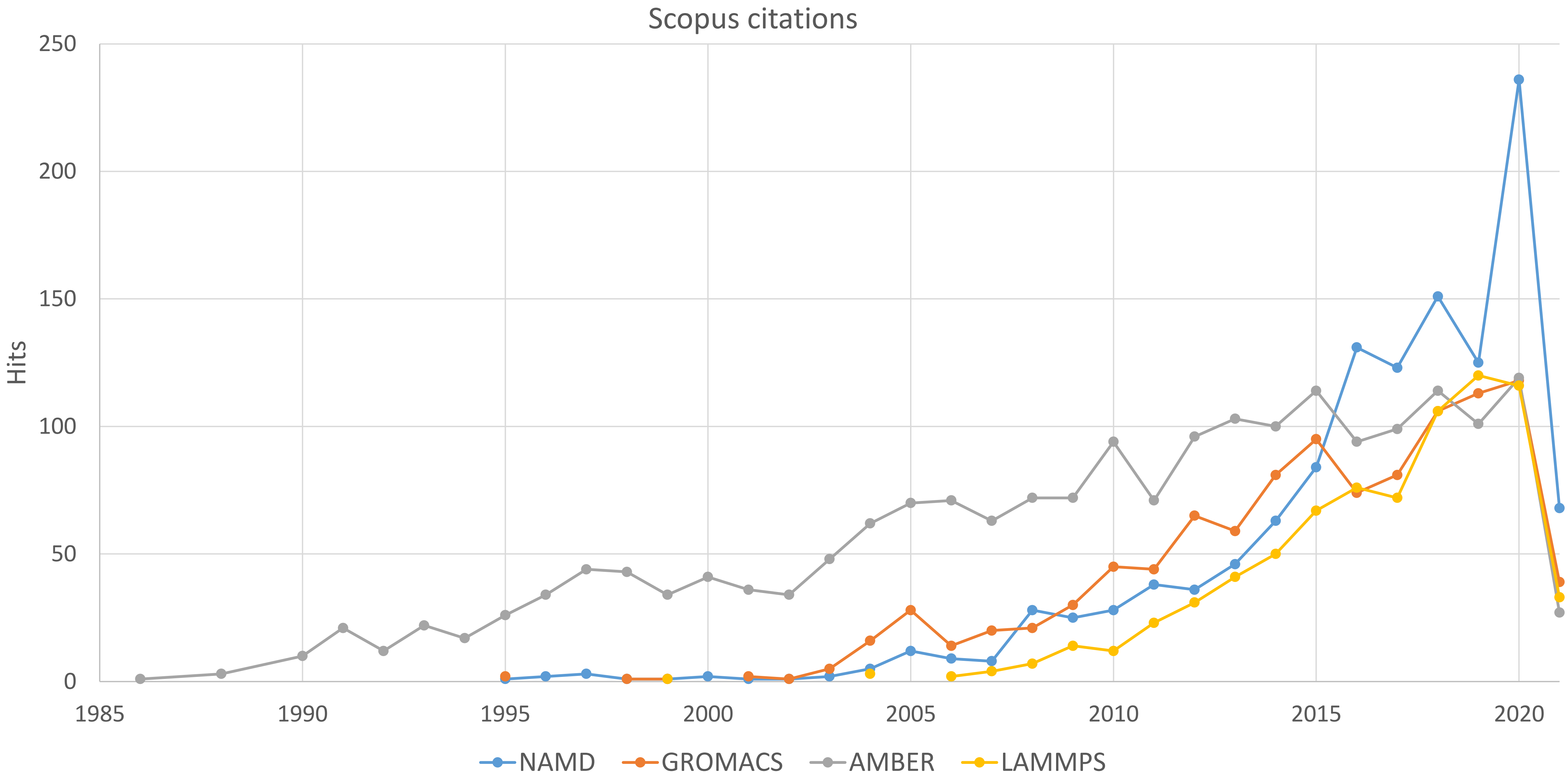
Long-range interactions:
PME, FFT

PME MPI
GROUP
(NlogN)

GPU
OFFLOAD
(idle)

Bonded interactions

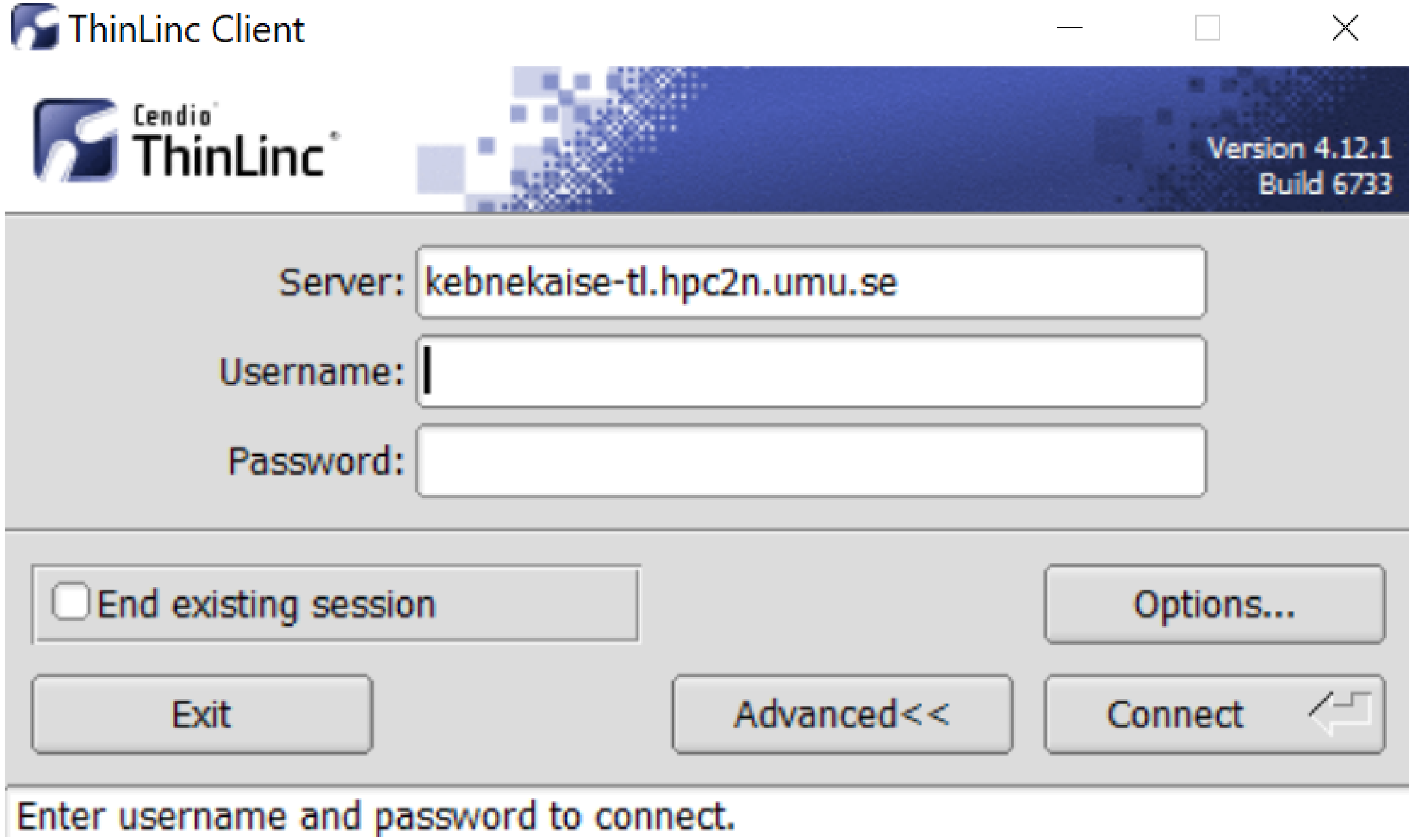
Update positions



Data from www.scopus.com server by searching for the name of the software. In the case of AMBER the keyword dynamics was added.

ThinLinc client

Download and installation site:
https://www.cendio.com/thinlinc/download



Server: kebnekaise-tl.hpc2n.umu.se

Username:

Password:

Enter username and password to connect.

Username and Password are the ones you received for HPC2N

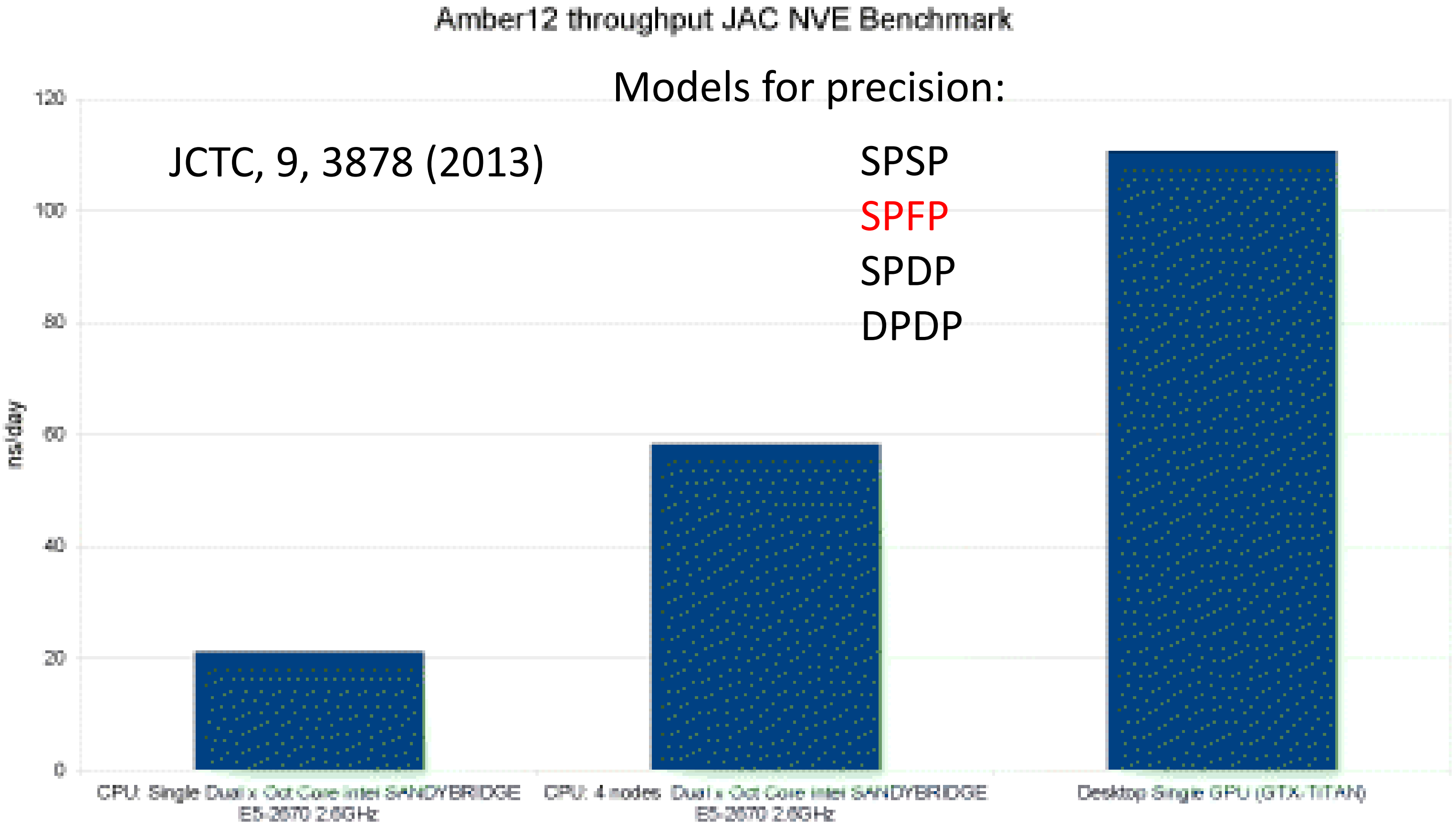
Just the first time you use ThinLinc, got to Options -> Screen and uncheck the box “Full screen mode”

Benchmark

- Solvated protein (1AKI)
- 158945 atoms
- 1.2 nm cutoff radius
- 1 fs time step
- PME for electrostatics
- Input scripts generated in http://www.charmm-gui.org/

AMBER

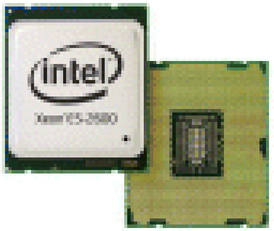
- Collection of independent routines
- It uses Sander/PMEMD for solving the Newton’s equations
- It offers a robust set of analysis tools



JCTC, 9, 3878 (2013)

Models for precision:

SPSP
SPFP
SPDP
DPDP



```
ml GCC/9.3.0  OpenMPI/4.0.3
ml  Amber/18.17-AmberTools-19.12-Python-2.7.18
srun pmemd.MPI -O -i  input.mdin
srun pmemd.cuda.MPI -O –I input.mdin
```

AMBER Tools

- For setting up a simulation (initial structure, solvation, ions, …):

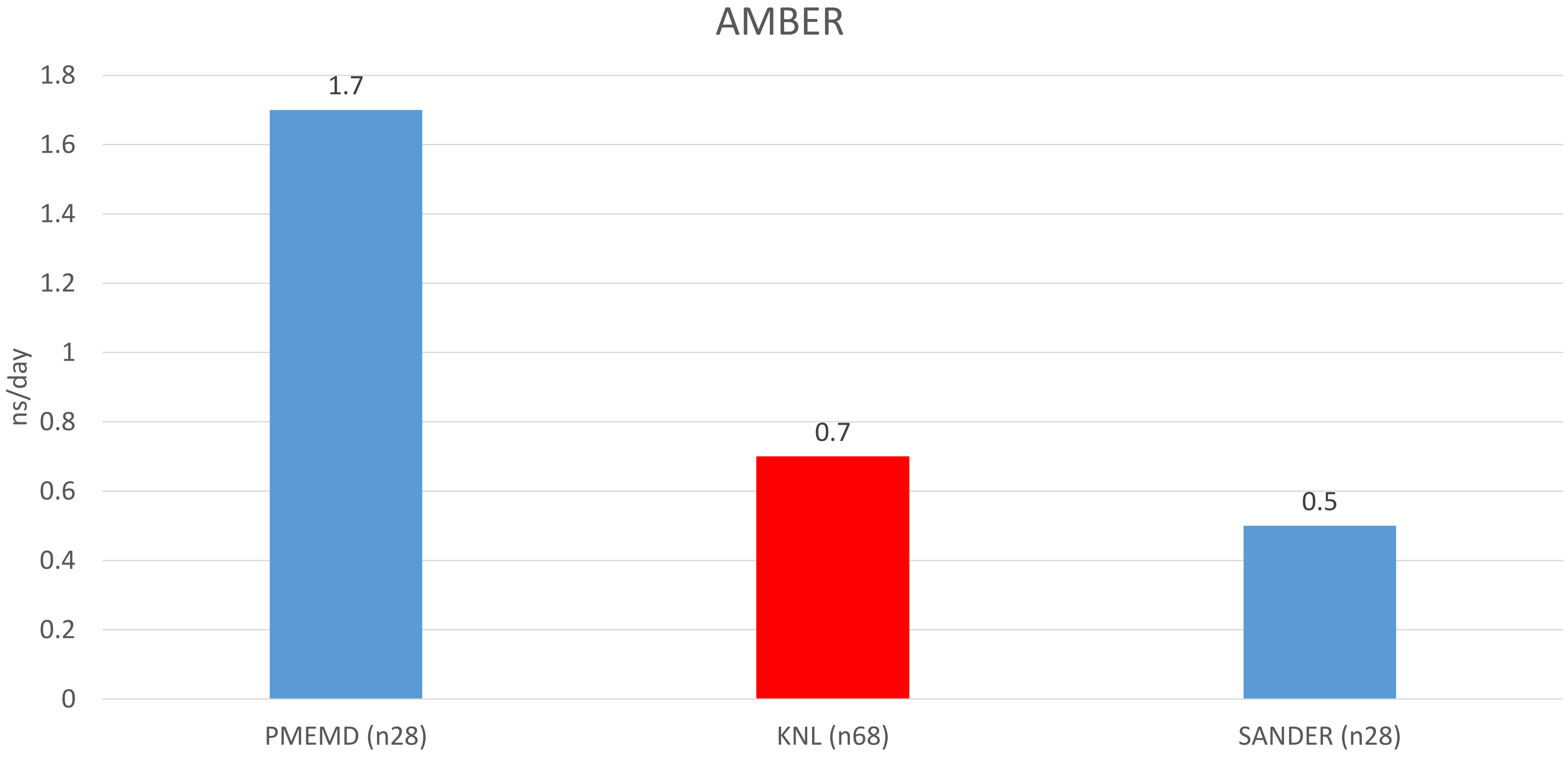
Load the modules:

```
$ml GCC/9.3.0  OpenMPI/4.0.3
$ml Amber/18.17-AmberTools-19.12-Python-2.7.18
```

On the command line:

```
> tleap, antechamber, cpptraj, …
```

AMBER


AMBER
ns/day
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
1.7
0.7
0.5
PMEMD (n28)
KNL (n68)
SANDER (n28)

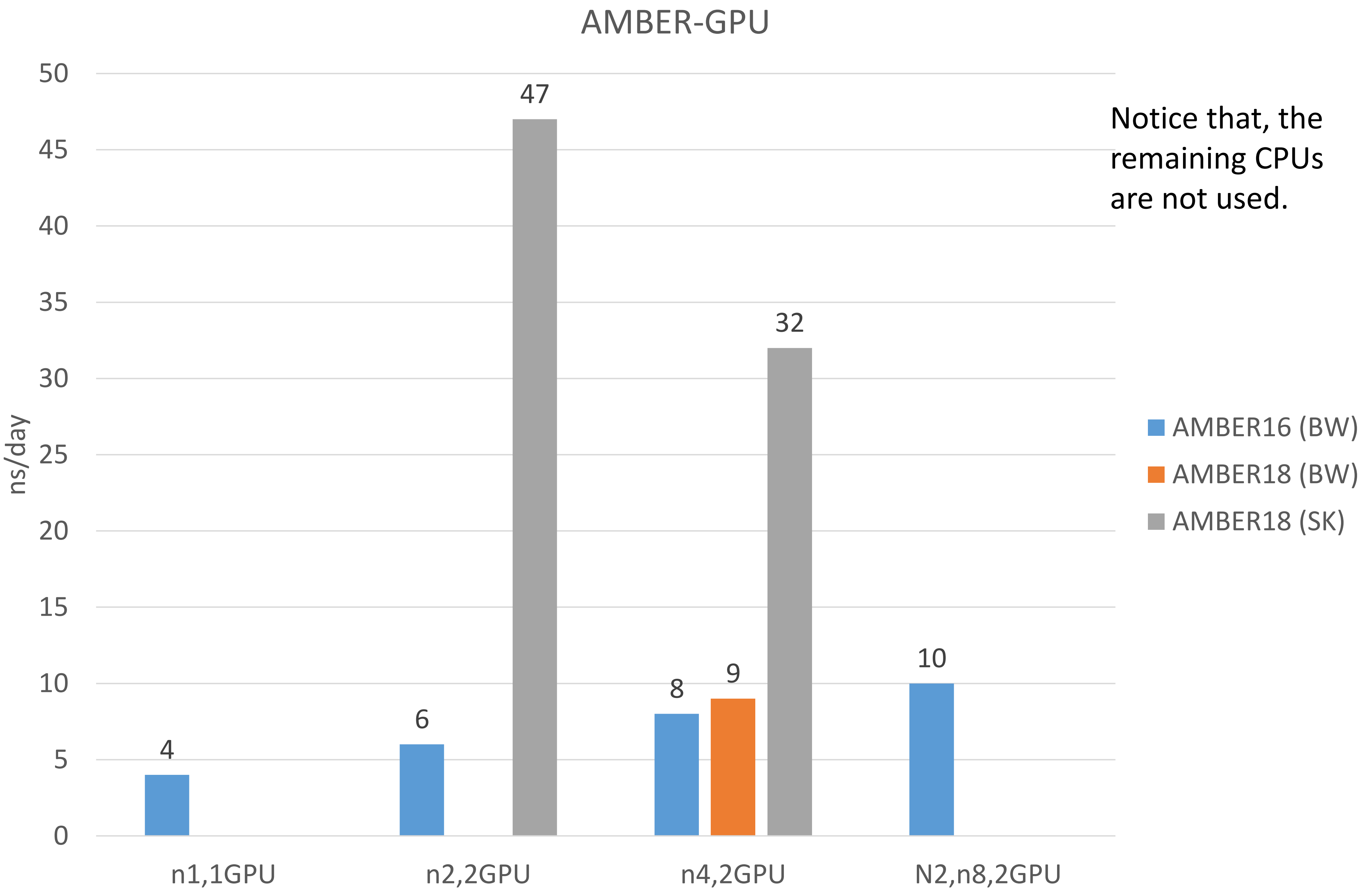
AMBER-GPU

```
#!/bin/bash
#SBATCH -A staff
#SBATCH -t 00:50:00
#SBATCH -N 1
#SBATCH -n 4
#SBATCH --gres=gpu:k80:2
#SBATCH -p batch
#SBATCH --exclusive
#SBATCH --output=job_str.out
#SBATCH --error=job_str.err
#SBATCH --mail-type=END

ml purge > /dev/null 2>&1
ml GCC/9.3.0  OpenMPI/4.0.3
ml  Amber/18.17-AmberTools-19.12-Python-2.7.18

srun pmemd.cuda.MPI -O -i input.mdin -p input.parm7 -c input.rst7 -o input.mdout
```

AMBER

On Kebnekaise, best performance is achieved with 4 MPIs/Node and using 2 GPU cards

Nr. Ranks (-n)	Nr. GPUs	ns/day
2	1	6
2	2	6
4	2	8
8 (single-node)	2	6
8 (multi-node)	2	10



Notice that, the remaining CPUs are not used.

AMBER

- If you observe any issue with a GPU run, go back to the pure CPU version (AMBER 2018 user guide)
- In case you want to perform independent simulations use the variable CUDA_VISIBLE_DEVICES to specify the GPU you will use or better request a single GPU card (--gres=gpu:k80:1)
- GPU enhanced sampling: Gaussian Accelerated MD (JCTC, 11, 3584-3595, 2015)

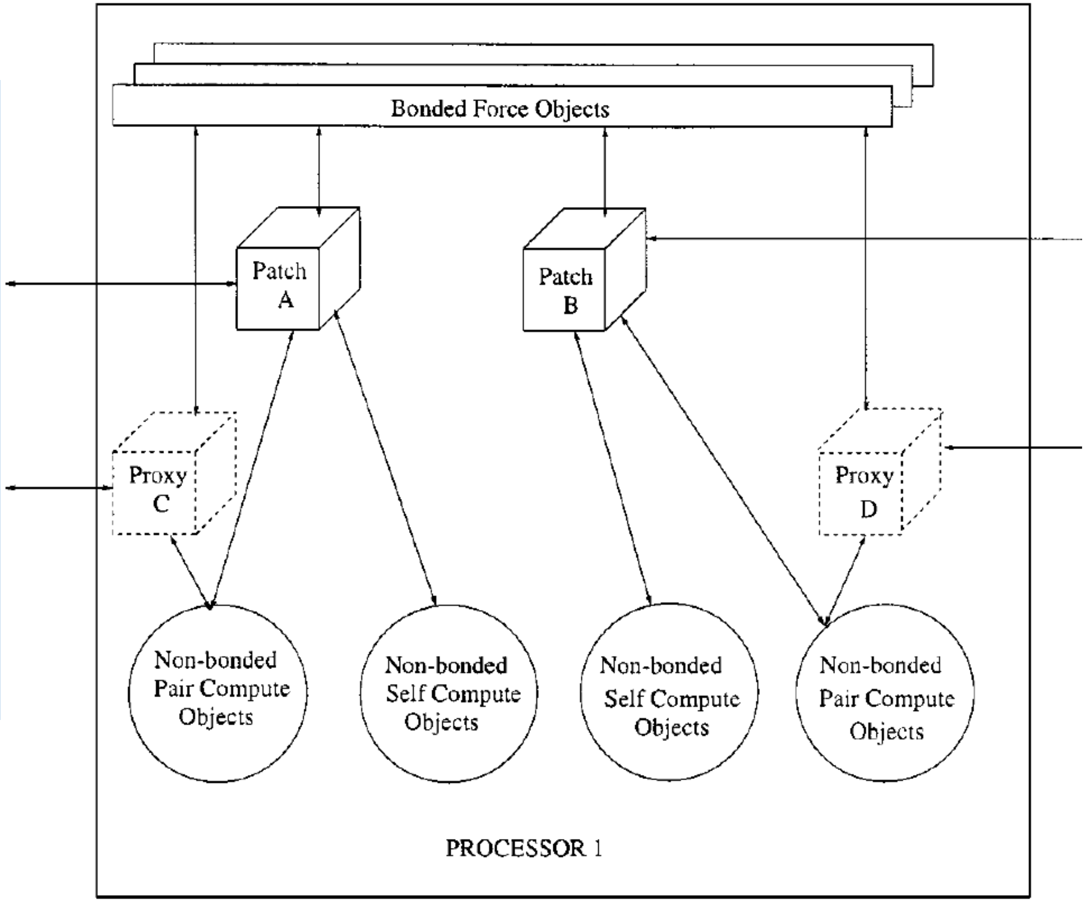
AMBER

Resources

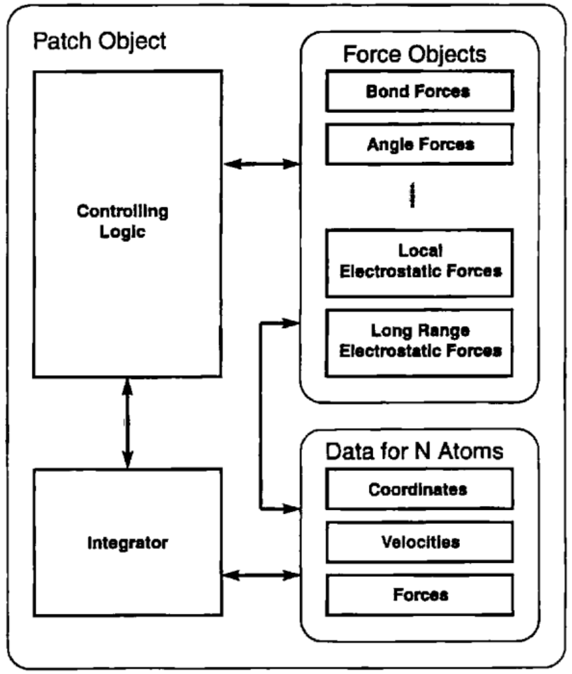
AMBER tutorials
http://ambermd.org/tutorials/

NAMD

- Based on charm++ communication protocol
- It is object-oriented
- Versions: single node, multi-node, GPU, and KNL
- Highly scalable
- Message driven comm.


Bonded Force Objects
Patch A
Patch B
Proxy C
Proxy D
Non-bonded Pair Compute Objects
Non-bonded Self Compute Objects
Non-bonded Self Compute Objects
Non-bonded Pair Compute Objects
PROCESSOR 1

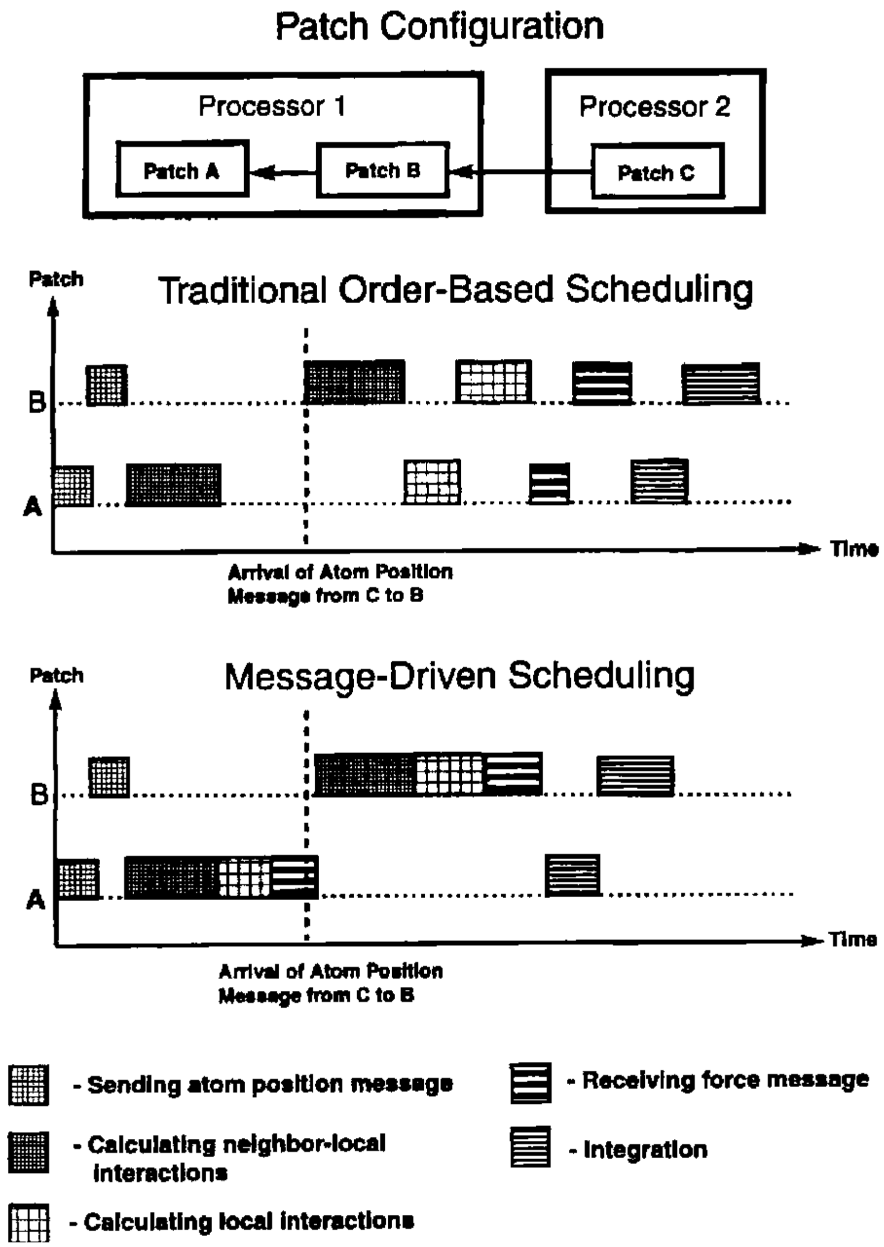
Credits: JCC, 151, 283 (1999)



Credits: The Int. J. Supercomp. Appl. And High Performance Comp., 10, 251-268 (1996)

NAMD

- Based on charm++ communication protocol
- It is object-oriented
- Versions: single node, multi-node, GPU, and KNL
- Highly scalable
- Message driven comm.



Patch Configuration
Processor 1
Patch A
Patch B
Processor 2
Patch C
Traditional Order-Based Scheduling
Patch
B
A
Time
Arrival of Atom Position Message from C to B
Message-Driven Scheduling
Patch
B
A
Time
Arrival of Atom Position Message from C to B
- Sending atom position message
- Calculating neighbor-local interactions
- Calculating local interactions
- Receiving force message
- Integration

Credits: The Int. J. Supercomp. Appl. And High Performance Comp., 10, 251-268 (1996)

NAMD (multiple nodes)

```
#!/bin/bash
#SBATCH -A SNICyyyy-xx-zz
#Asking for 10 min.
#SBATCH -t 00:10:00
#Number of nodes
#SBATCH -N 2
#Ask for 56 processes (2x28 cores on the nodes)
#SBATCH -n 56
#SBATCH --exclusive
#Load modules necessary for running NAMD
ml GCC/9.3.0  OpenMPI/4.0.3
ml NAMD/2.14-mpi
srun namd2 config_file > output_file
```

NAMD (GPU) (single node)

```
#!/bin/bash
#SBATCH -A SNICyyyy-xx-zz
#SBATCH -t 00:50:00
#SBATCH -N 1
#SBATCH -n 28
#SBATCH --exclusive
#Ask for 2 GPU cards
#SBATCH --gres=gpu:k80:2
#Load modules necessary for running NAMD
ml GCC/9.3.0  CUDA/11.0.2  OpenMPI/4.0.3
ml NAMD/2.14-nompi
#Execute NAMD
namd2 +p 28 +setcpuaffinity +idlepoll +devices $CUDA_VISIBLE_DEVICES config > output.dat
```

NAMD

- NAMD will scale if the number of patches >> number of processes

```
Info: Startup phase 5 took 0.00011301 s, 1131.09 MB of memory in use
Info: PATCH GRID IS 7 (PERIODIC) BY 7 (PERIODIC) BY 7 (PERIODIC)
```

- One can dedicate some processors to solve PME long-range part (config file)

```
PMEProcessors 8
Ldb unload PME yes
```

- For the CUDA version, one can offload PME to GPUs:

```
usePMECUDA on
PMEoffload on
```

In the output file you will see:

```
Info: PME RECIPROCAL SUM OFFLOADED TO GPU
```

- Colvars module for free energy calculations can be run on GPUs.

More information:
https://www.ks.uiuc.edu/Research/namd/2.13/ug/node106.html
https://www.ks.uiuc.edu/Research/namd/wiki/?NamdPerformanceTuning

NAMD

- Colvars module for free energy calculations can be run on GPUs

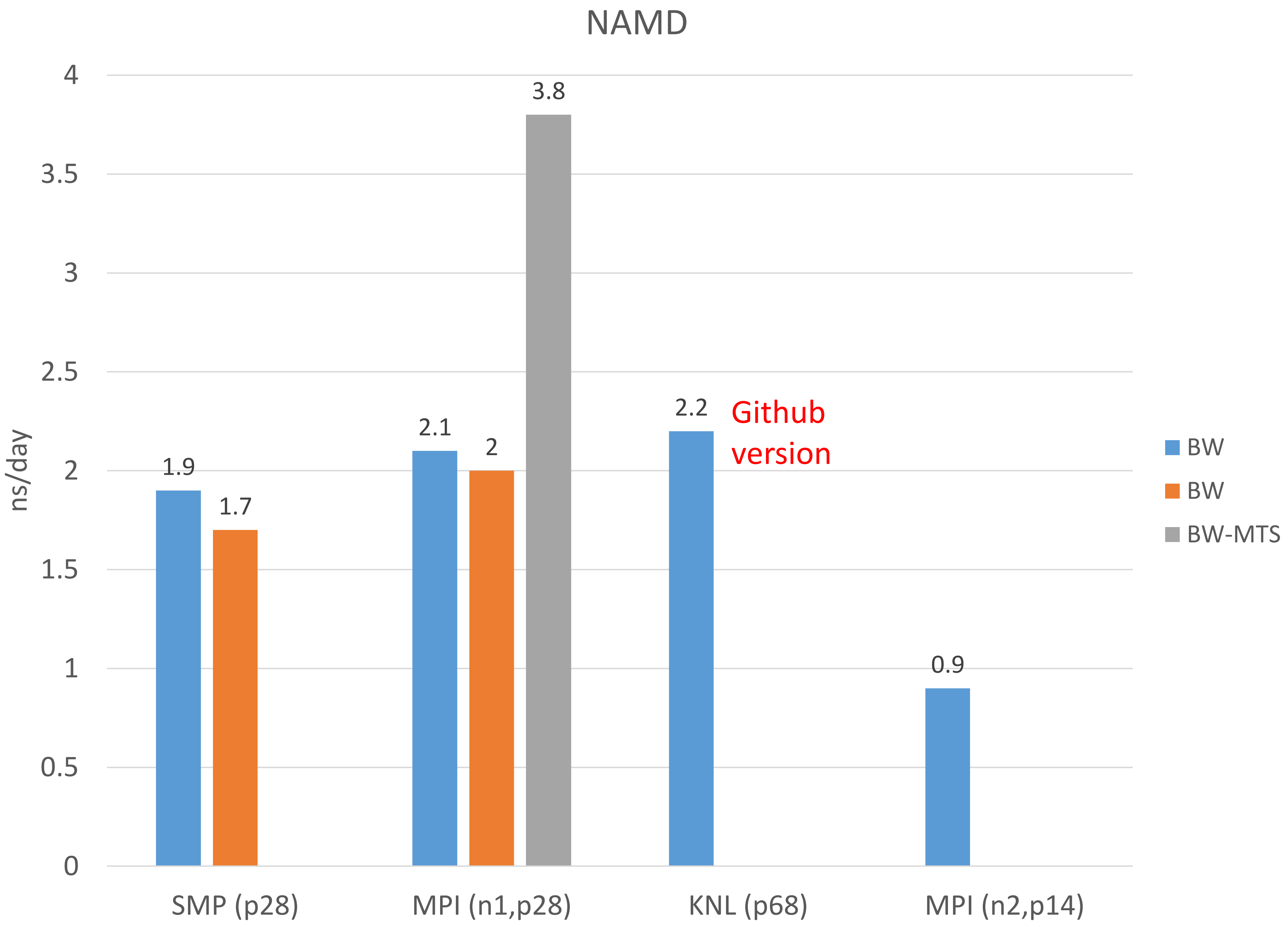
```
colvar {
        name restrain01
        width 0.5
        lowerboundary 0.0
        upperboundary 8.0
        lowerwallconstant 100.0
        upperwallconstant 100.0

        distanceXY {
            main {  atomnumbers {list of atoms} }
            ref { atomnumbers {list of atoms} }
            axis (0.0, 0.0, 1.0)
        }
}
```

Restraint where a channel is asymmetric

http://www.ks.uiuc.edu/Training/Tutorials/science/channel/channel-tut.pdf

NAMD

Use the +setcpuaffinity flag for a 10% speedup for the CUDA version



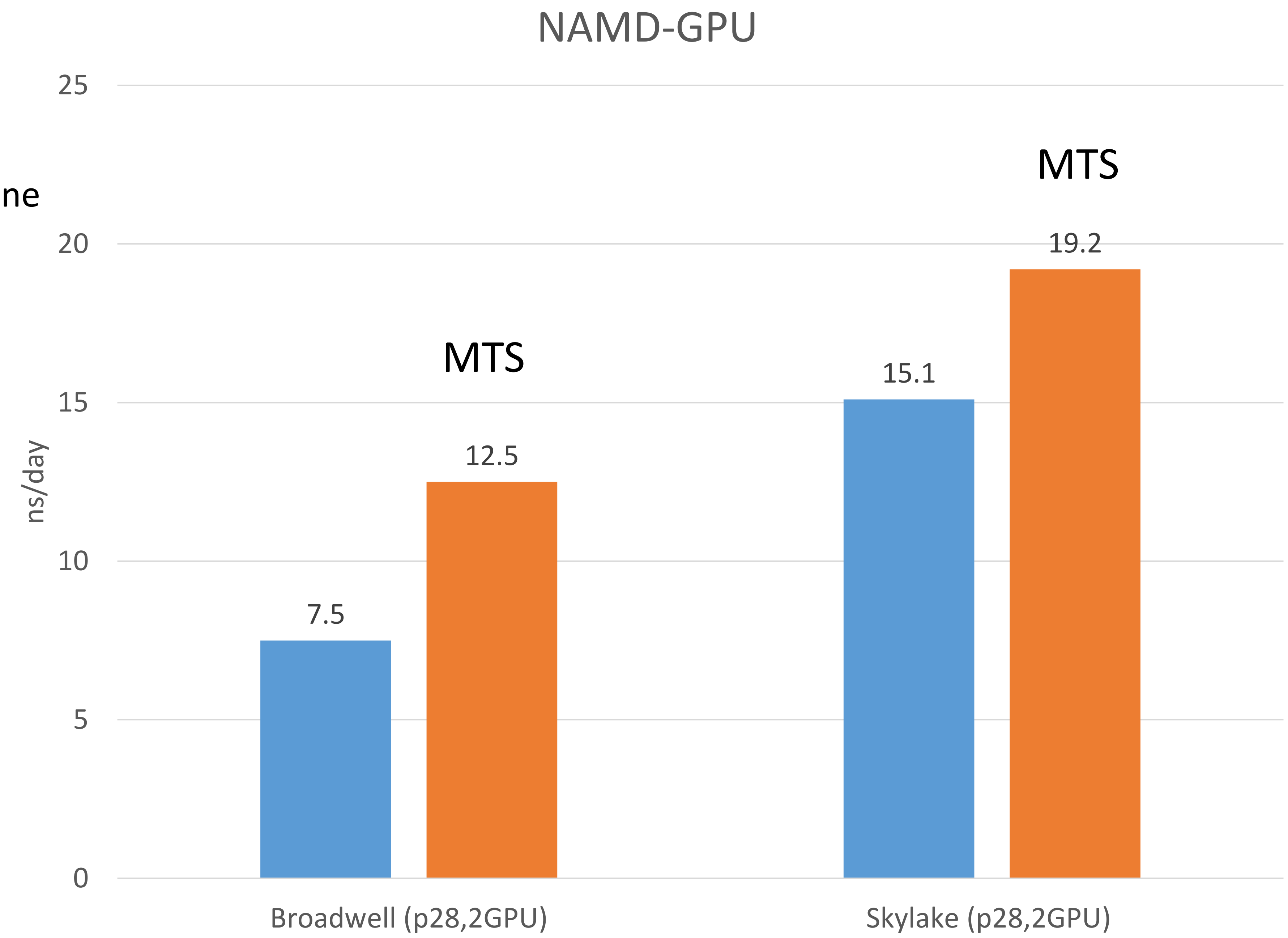
NAMD

With the new Volta GPU cards one can speed up the simulation by 1.6x

#SBATCH --gres=gpu:v100:2

SMP (Skylake)	
Setup	Timing (ns/day)
+p28 (2GPU)	15.1
+p14 (1GPU)	9.8

MTS=Multiple Time Step



NAMD

Resources

NAMD tutorials:
http://www.ks.uiuc.edu/Training/Tutorials/#namd

GROMACS

```
#!/bin/bash
#SBATCH -A SNICyyyy-xx-zz
#SBATCH -t 00:10:00
#SBATCH -n 4
#SBATCH -c 7
# Asking for 2 GPUs
#SBATCH --gres=gpu:k80:2

ml GCC/5.4.0-2.26  OpenMPI/2.0.1 CUDA/8.0.44
ml GROMACS/2016-hybrid

if [ -n "$SLURM_CPUS_PER_TASK" ]; then
    mdargs="-ntomp $SLURM_CPUS_PER_TASK"
else
    mdargs="-ntomp 1"
fi

srun gmx_mpi mdrun $mdargs -npme 0 -dlb yes  -v -deffnm step4.1_equilibration
```

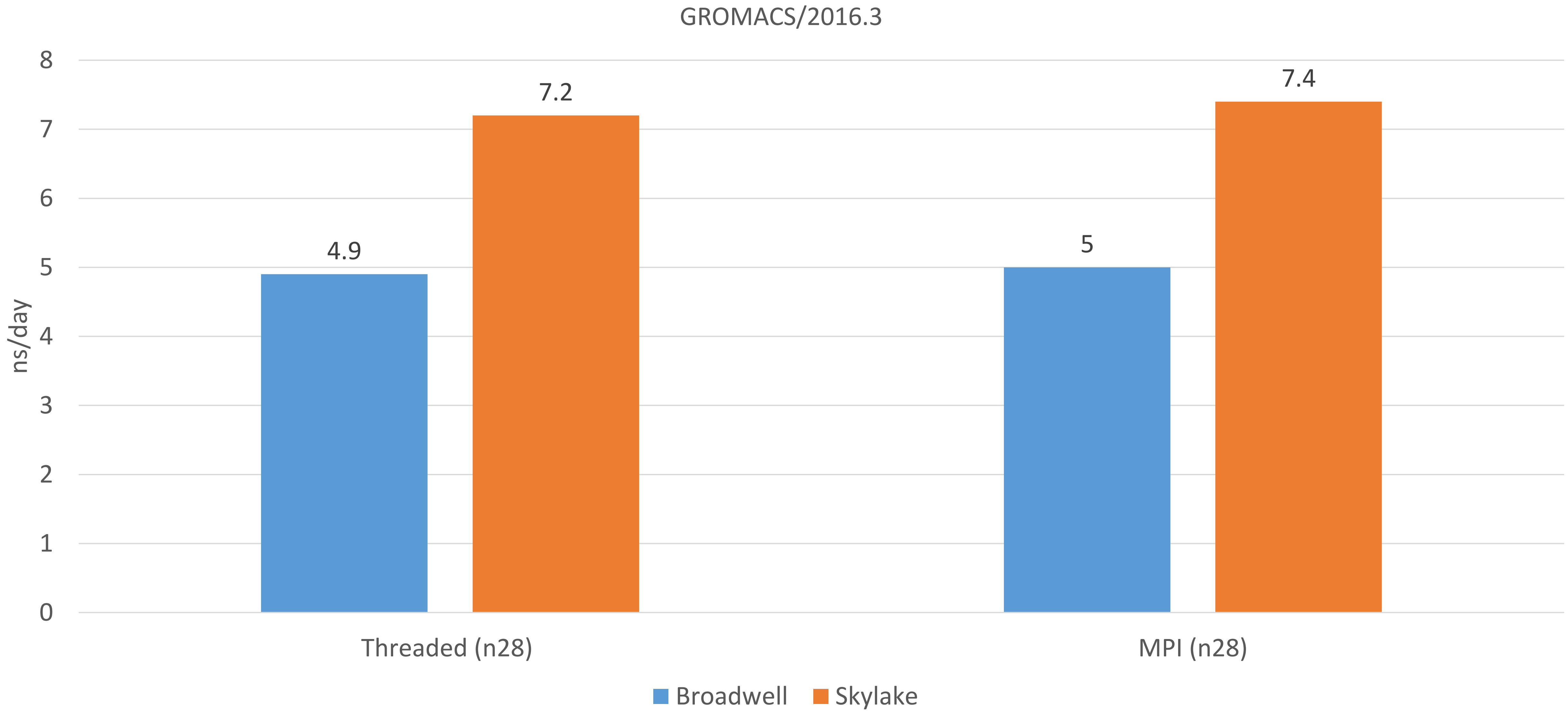
GROMACS recognizes the number of available GPU cards

gmx tune_pme

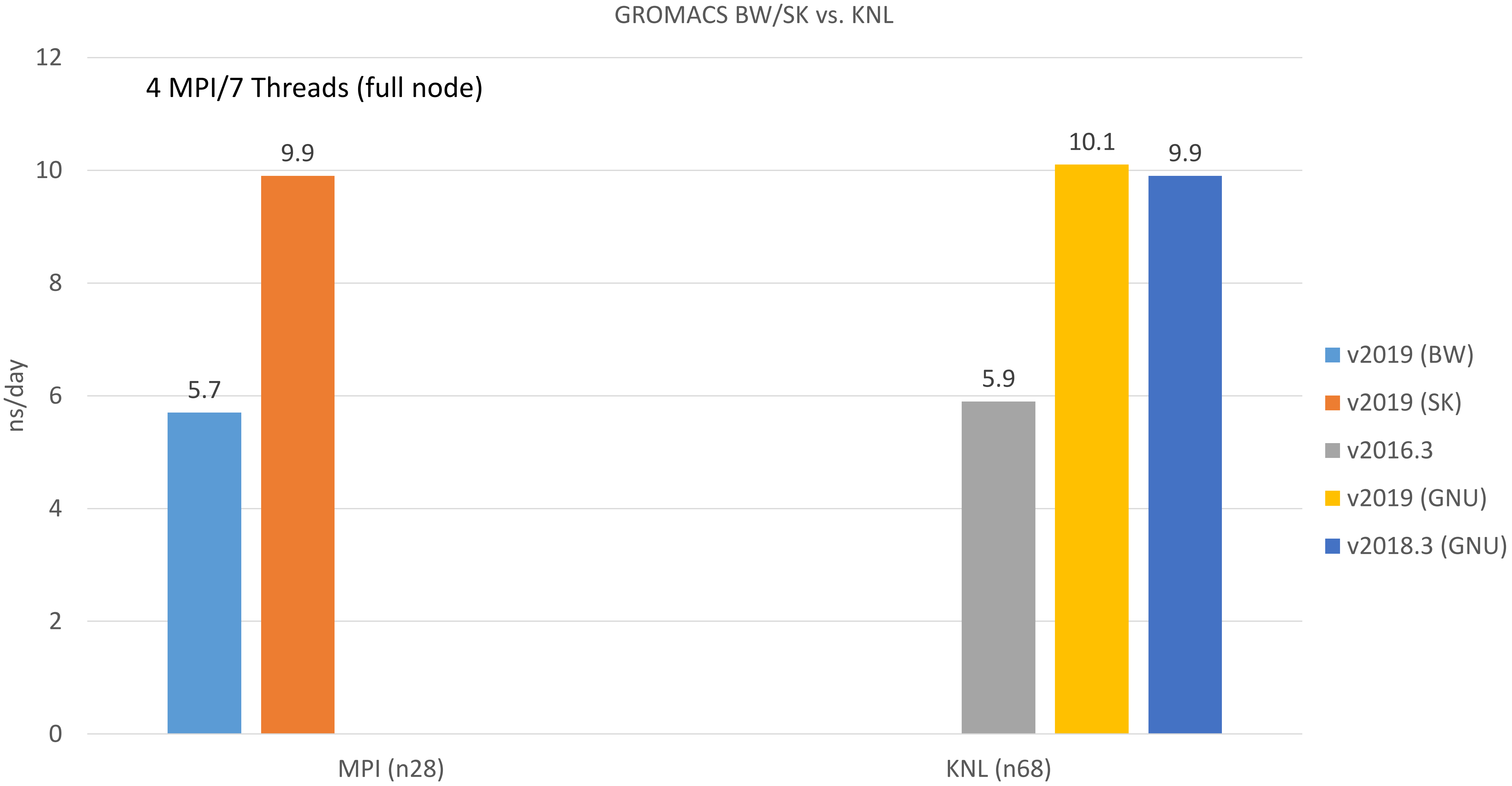
```
Individual timings for input file 0 (npt_bench00.tpr):
PME ranks      Gcycles       ns/day        PME/f    Remark
   0          4355.019      57.776         -      OK.
   0          4547.105      55.335         -      OK.
   0          4289.420      58.659         -      OK.
  -1(  0)    4455.791      56.469         -      OK.
  -1(  0)    4440.157      56.668         -      OK.
  -1(  0)    4275.551      58.850         -      OK.

Tuning took     7.7 minutes.
-----------------------------------------------------------
Summary of successful runs:
Line tpr PME ranks  Gcycles Av.     Std.dev.       ns/day        PME/f    DD grid
   0   0    0         4397.181      133.917       57.257         -      4   1   1
   1   0   -1(  0)    4390.500       99.855       57.329         -      4   1   1


-----------------------------------------------------------
Best performance was achieved with the automatic number of PME ranks (see line 1)
Please use this command line to launch the simulation:

mpirun -np 4 gmx_mpi mdrun -npme -1 -s npt.tpr -ntomp 7 -dlb yes
```

GROMACS

4 MPI/7 Threads (full node)



GROMACS



GROMACS BW/SK vs. KNL
4 MPI/7 Threads (full node)
ns/day
0
2
4
6
8
10
12
5.7
9.9
5.9
10.1
9.9
MPI (n28)
KNL (n68)
v2019 (BW)
v2019 (SK)
v2016.3
v2019 (GNU)
v2018.3 (GNU)

GROMACS KNL

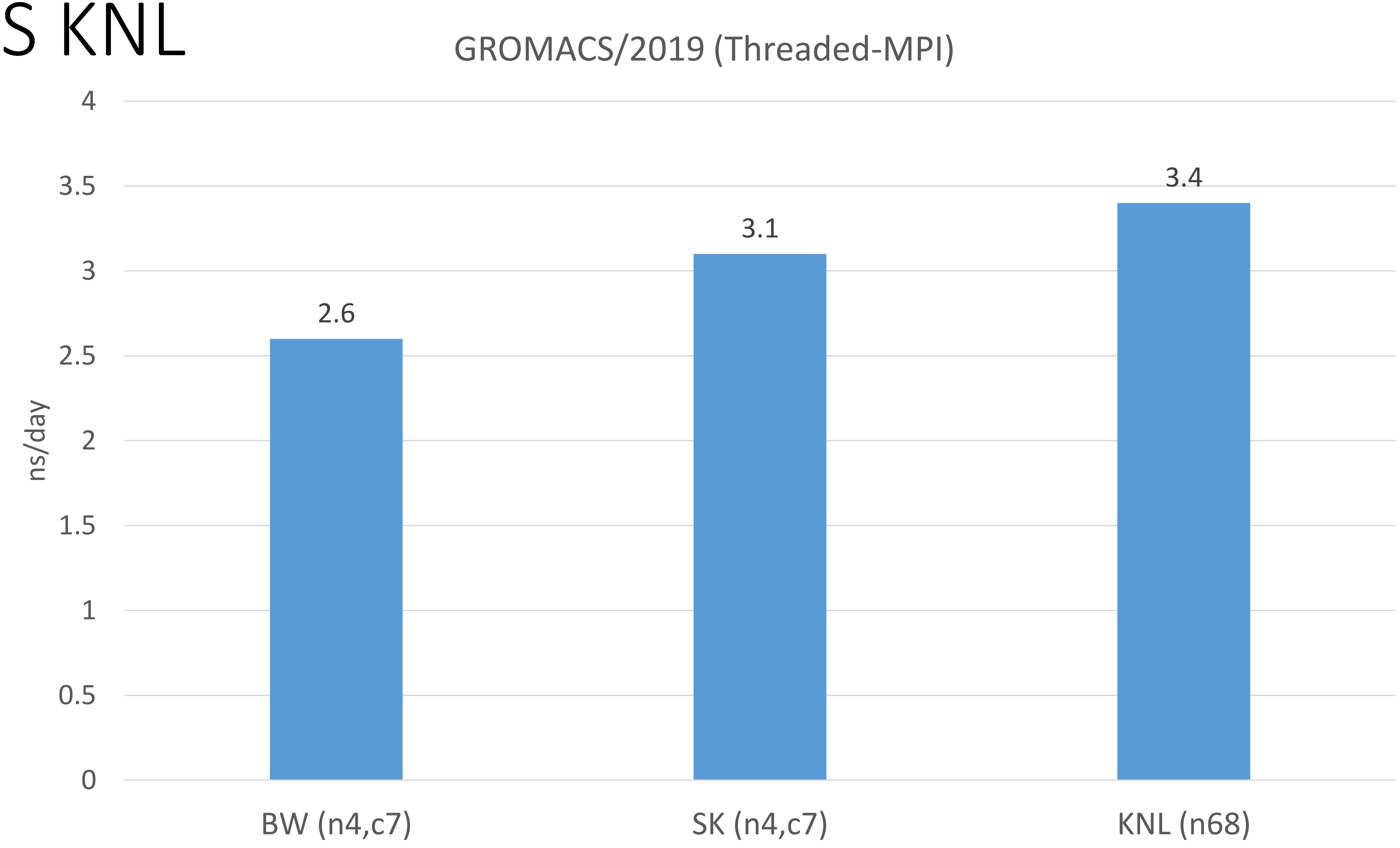
```
#!/bin/bash
#SBATCH -A project_ID
#SBATCH -t 00:50:00
#SBATCH -N 1
#SBATCH -n 68
#SBATCH -p knl
#SBATCH --constraint=cache,quad
#SBATCH --exclusive

ml GCC/7.3.0-2.30 OpenMPI/3.1.1
ml GROMACS/2018.3

export OMP_NUM_THREADS=2
gmx mdrun -ntmpi 68 -npme 18 -ntomp 2 -pin on -pinoffset 0 -pinstride 2 -dlb auto -v -deffnm step4.1_eq
```

GROMACS KNL

- Login to kebnekaise-knl.hpc2n.umu.se to check the GROMACS modules available and their dependencies.
- Submit your script either from the KNL or from the standard login nodes
- KNL queue is most of the time available compared to GPU one

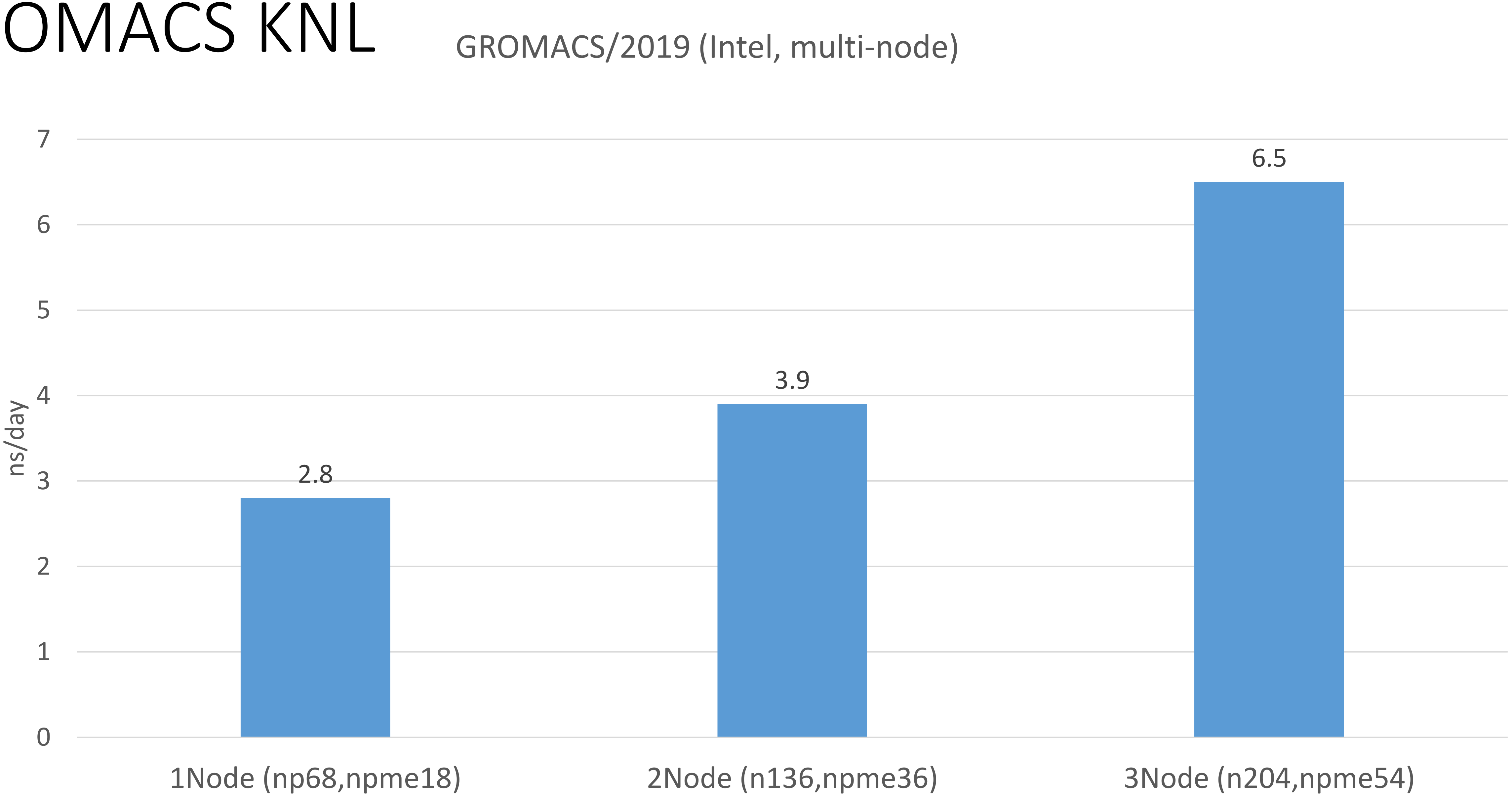
GROMACS KNL

2,136,412 atoms
ts = 4fs
It uses virtual sites
cutoff radii = 1.0nm



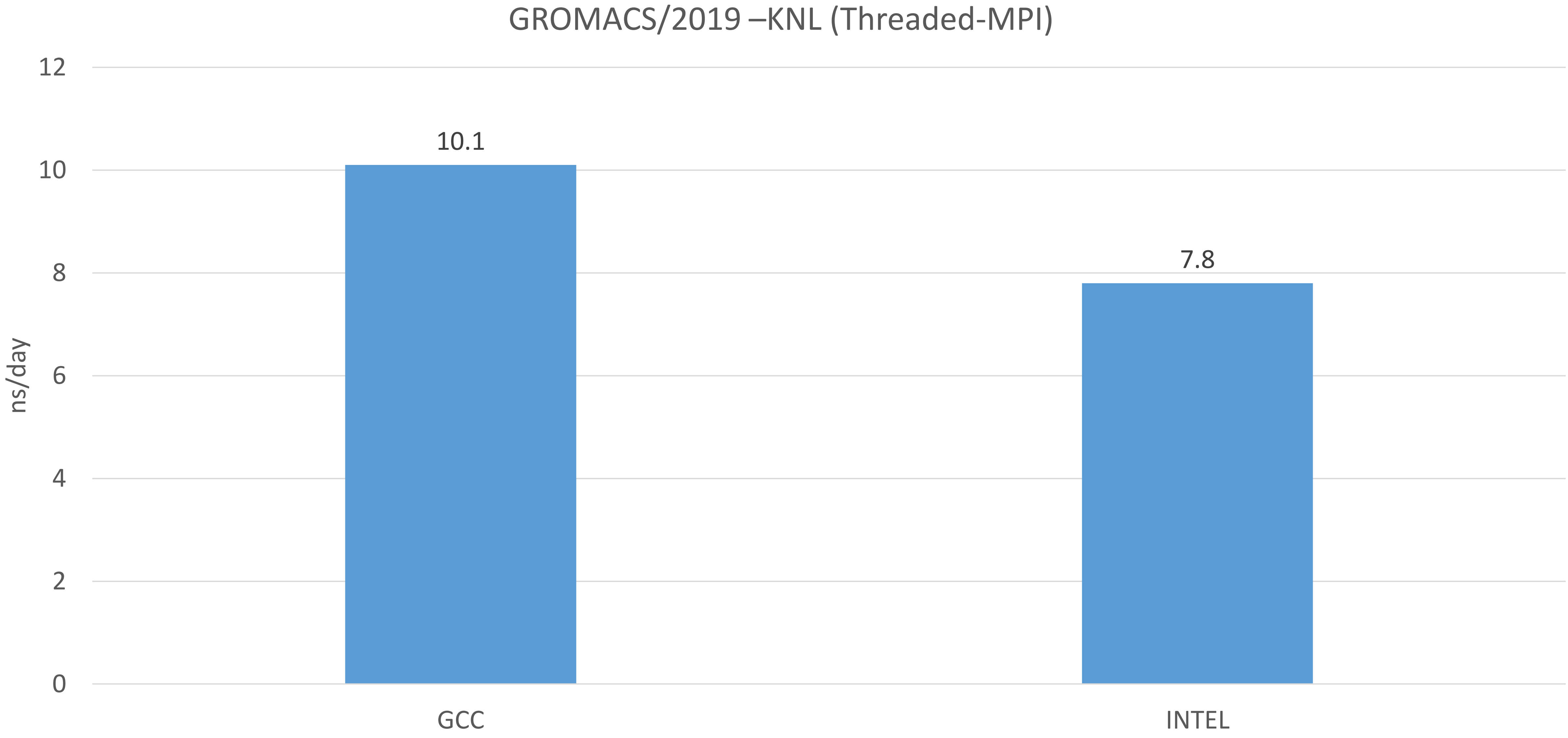
Benchmark (2M atoms) from: https://www.mpibpc.mpg.de/grubmueller/bench

GROMACS KNL



Benchmark (2M atoms) from: https://www.mpibpc.mpg.de/grubmueller/bench

GROMACS (toolchain effects)



GROMACS (single node, K80)

- (-n2,-c14) srun gmx_mpi mdrun -ntomp 14 -dlb yes will use 2 GPUs engines

```
Using 2 MPI processes
Using 14 OpenMP threads per MPI process

On host b-cn1309.hpc2n.umu.se 2 GPUs auto-selected for this run.
Mapping of GPU IDs to the 2 GPU tasks in the 2 ranks on this node:
  PP:0,PP:1
```

- (-n4,-c7) srun gmx_mpi mdrun -ntomp 7 -dlb yes will use 4 GPUs engines

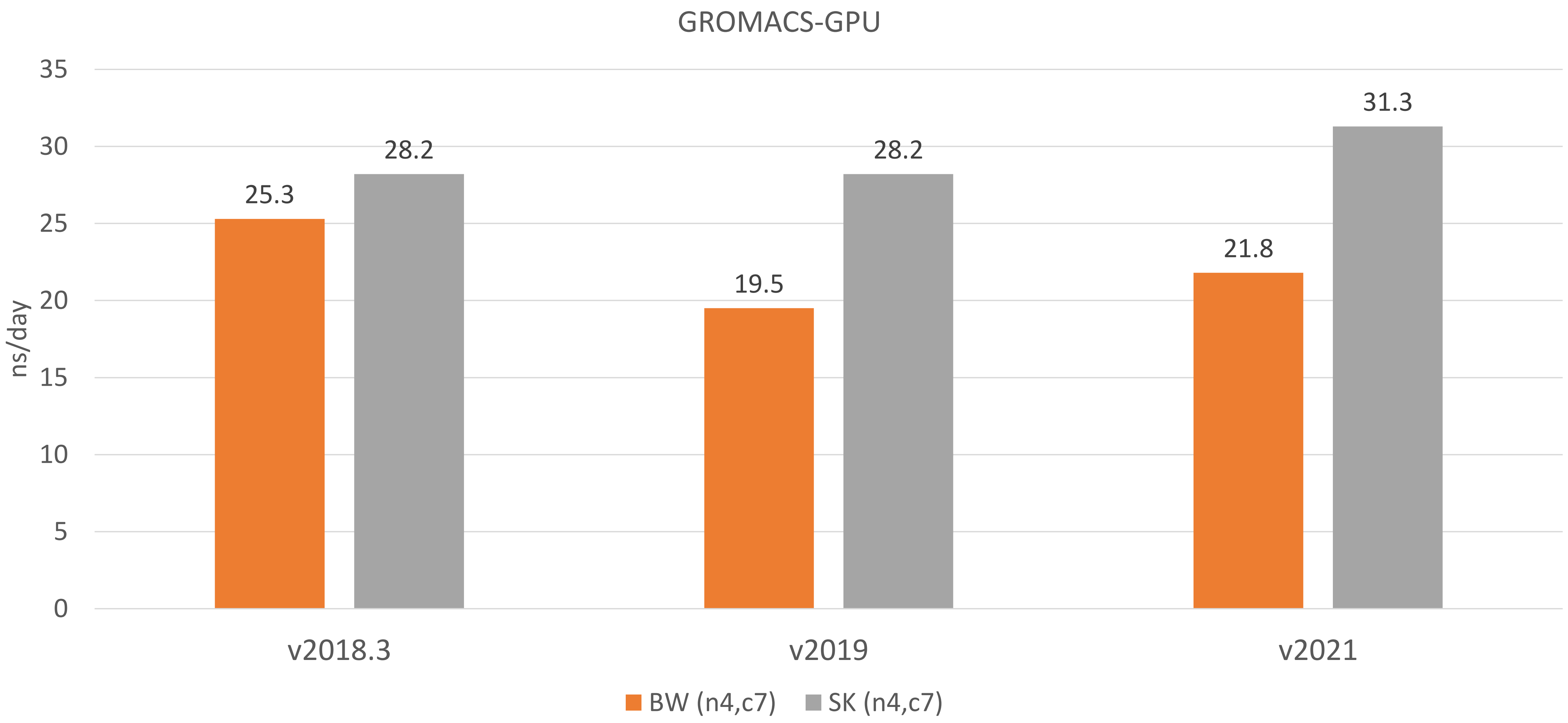
```
Using 4 MPI processes
Using 7 OpenMP threads per MPI process

On host b-cn1309.hpc2n.umu.se 4 GPUs auto-selected for this run.
Mapping of GPU IDs to the 4 GPU tasks in the 4 ranks on this node:
  PP:0,PP:1,PP:2,PP:3
```

GROMACS (single node, K80)

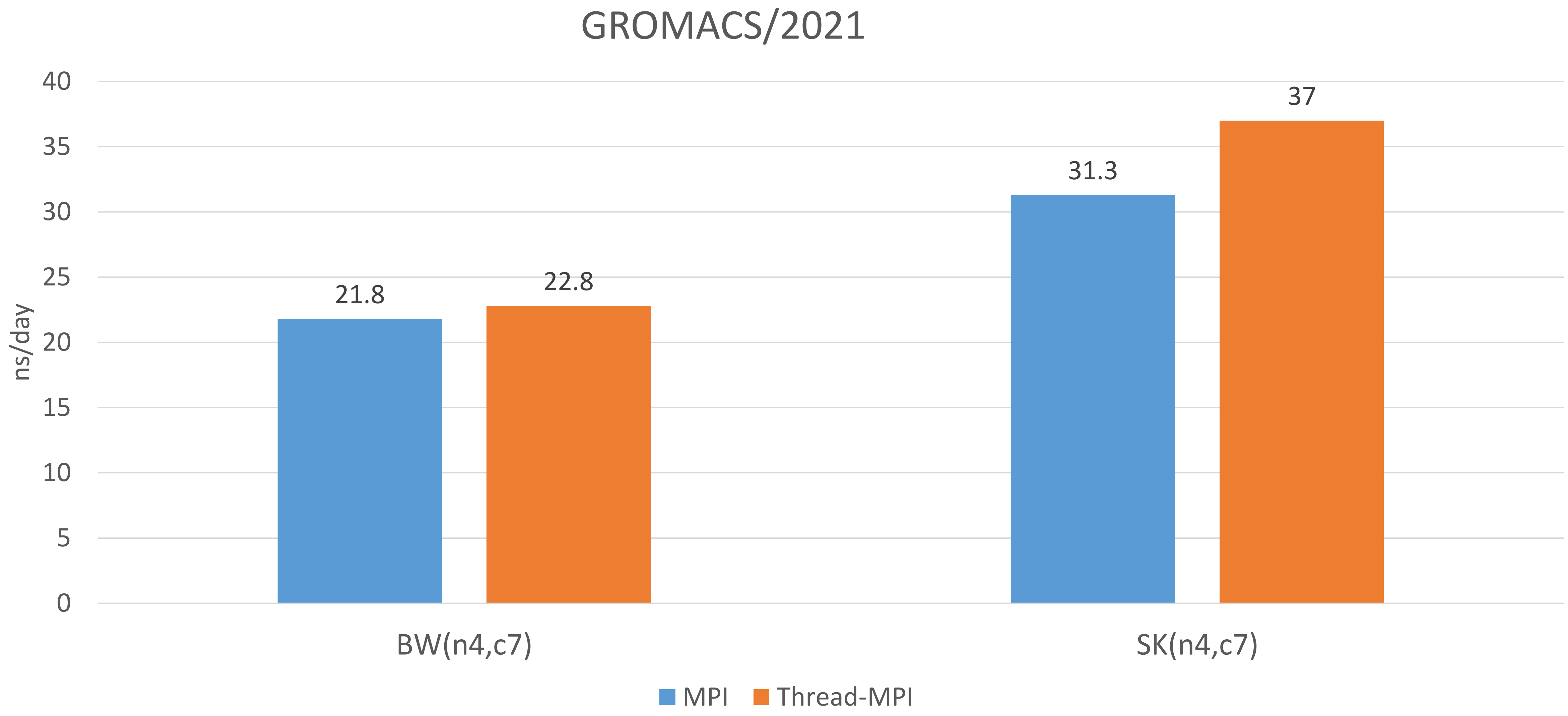
- (-n4,-c7) gmx mdrun -ntmpi 4 -ntomp 7 -dlb yes will use 4 GPUs engines

```
Using 4 MPI threads
Using 7 OpenMP threads per tMPI thread

On host b-cn1105.hpc2n.umu.se 4 GPUs auto-selected for this run.
Mapping of GPU IDs to the 4 GPU tasks in the 4 ranks on this node:
  PP:0,PP:1,PP:2,PP:3
PP tasks will do (non-perturbed) short-ranged and most bonded interactions
on the GPU
```

GROMACS (single node)



GROMACS (single node)



GROMACS (single node-offload)

- (-n4,-c7) srun gmx_mpi mdrun -ntomp 7 -dlb yes will use 4 GPUs:

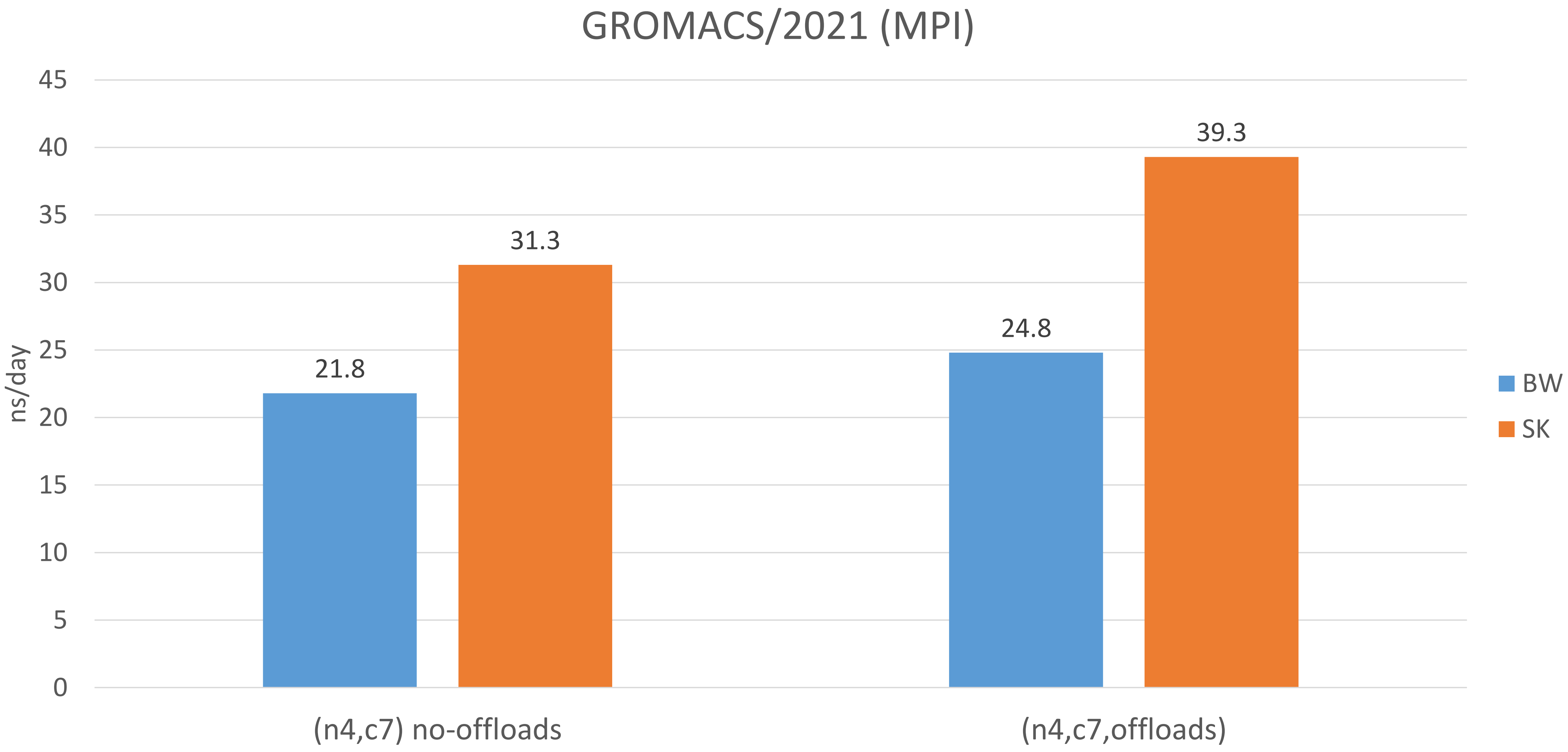
```
Using 4 MPI processes
Using 7 OpenMP threads per MPI process

On host b-cn1309.hpc2n.umu.se 4 GPUs auto-selected for this run.
Mapping of GPU IDs to the 4 GPU tasks in the 4 ranks on this node:
 PP:0,PP:1,PP:2,PP:3
```

- (-n4,-c7) gmx mdrun -gputasks 0123 -nb gpu -pme gpu -npme 1 -ntmpi 4 -dlb yes will use 4 GPUs:

npme must be 1

```
Using 4 MPI threads
Using 7 OpenMP threads per tMPI thread

On host b-cn1102.hpc2n.umu.se 4 GPUs user-selected for this run.
Mapping of GPU IDs to the 4 GPU tasks in the 4 ranks on this node:
 PP:0,PP:1,PP:2,PME:3
```

GROMACS (single node-offload)



GROMACS (multi node-offload)

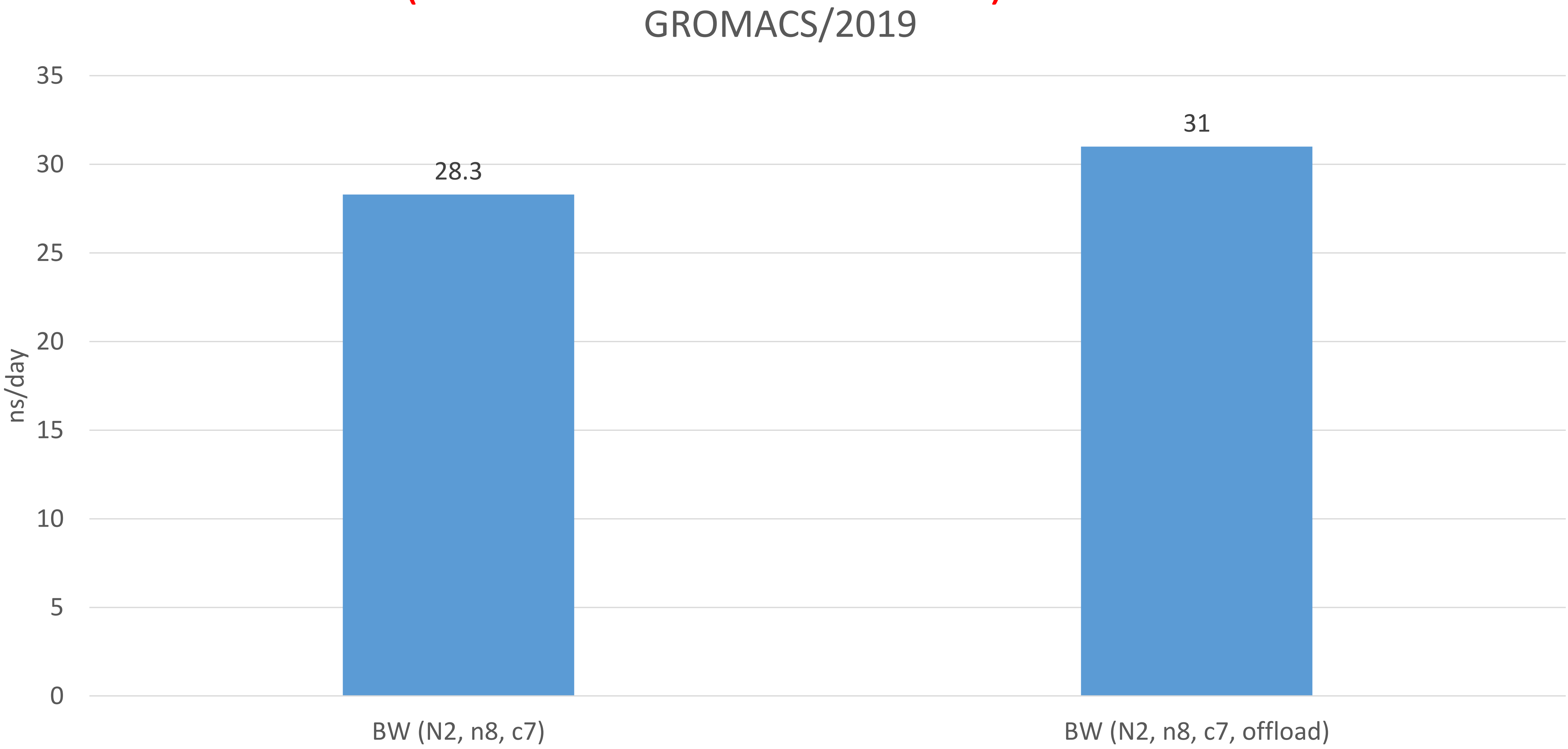
- (-N2,-n8,-c7) srun gmx_mpi mdrun -nb gpu -pme gpu -npme 1 -ntomp 7 -dlb yes will use 4 GPUs:

```
Using 7 OpenMP threads per MPI process

On host b-cn1106.hpc2n.umu.se 4 GPUs user-selected for this run.
Mapping of GPU IDs to the 4 GPU tasks in the 4 ranks on this node:
  PP:0,PP:1,PP:2,PP:3
PP tasks will do (non-perturbed) short-ranged interactions on the GPU
PME tasks will do all aspects on the GPU
```

- There are some limitations regarding the tasks that can be offloaded, please check:

  http://manual.gromacs.org/current/user-guide/mdrun-performance.html

GROMACS (multi node-offload)



GROMACS

- PLUMED, threaded MPI version is not supported.

Instead of:

```
gmx mdrun –ntmpi X
```

Use:

```
mpirun gmx_mpi …
```

GROMACS

- Additional information:

Recently, GROMACS 2021 added new features for offloading more tasks to the GPU, for instance bonded interactions (-bonded gpu) and updates (-update gpu). One can also move hard parallelizable PME parts to cpu (-pmefft cpu)

Resources

Manual for the current version:

https://manual.gromacs.org/current/user-guide/mdrun-performance.html

ENCCS information

https://enccs.github.io/gromacs-gpu-performance/md-algorithm/

GROMACS

Resources

GROMACS tutorials:

http://www.mdtutorials.com/gmx/

BIOEXCEL

https://bioexcel.eu/

LAMMPS (MPI)

```
#!/bin/bash
#SBATCH -A staff
#Asking for 10 min.
#SBATCH -t 02:10:00
#Number of nodes
#SBATCH -N 1
#Ask for 28 processes
#SBATCH -n 28
#SBATCH --exclusive

#Load modules necessary for running LAMMPS
ml GCC/8.3.0  OpenMPI/3.1.4
ml LAMMPS/3Mar2020-Python-3.7.4-kokkos

#Execute LAMMPS
srun lmp -in step4.1_equilibration.inp
```

LAMMPS (OpenMP)

```
#!/bin/bash
#SBATCH -A staff
#Asking for 10 min.
#SBATCH -t 02:10:00
#Number of nodes
#SBATCH -N 1
#Ask for 28 processes
#SBATCH -n 14
#SBATCH -c 2
#SBATCH --exclusive

#Load modules necessary for running LAMMPS
ml GCC/8.3.0  OpenMPI/3.1.4
ml LAMMPS/3Mar2020-Python-3.7.4-kokkos
export OMP_NUM_THREADS=2
#Execute LAMMPS
srun lmp -in step4.1_equilibration.inp
```

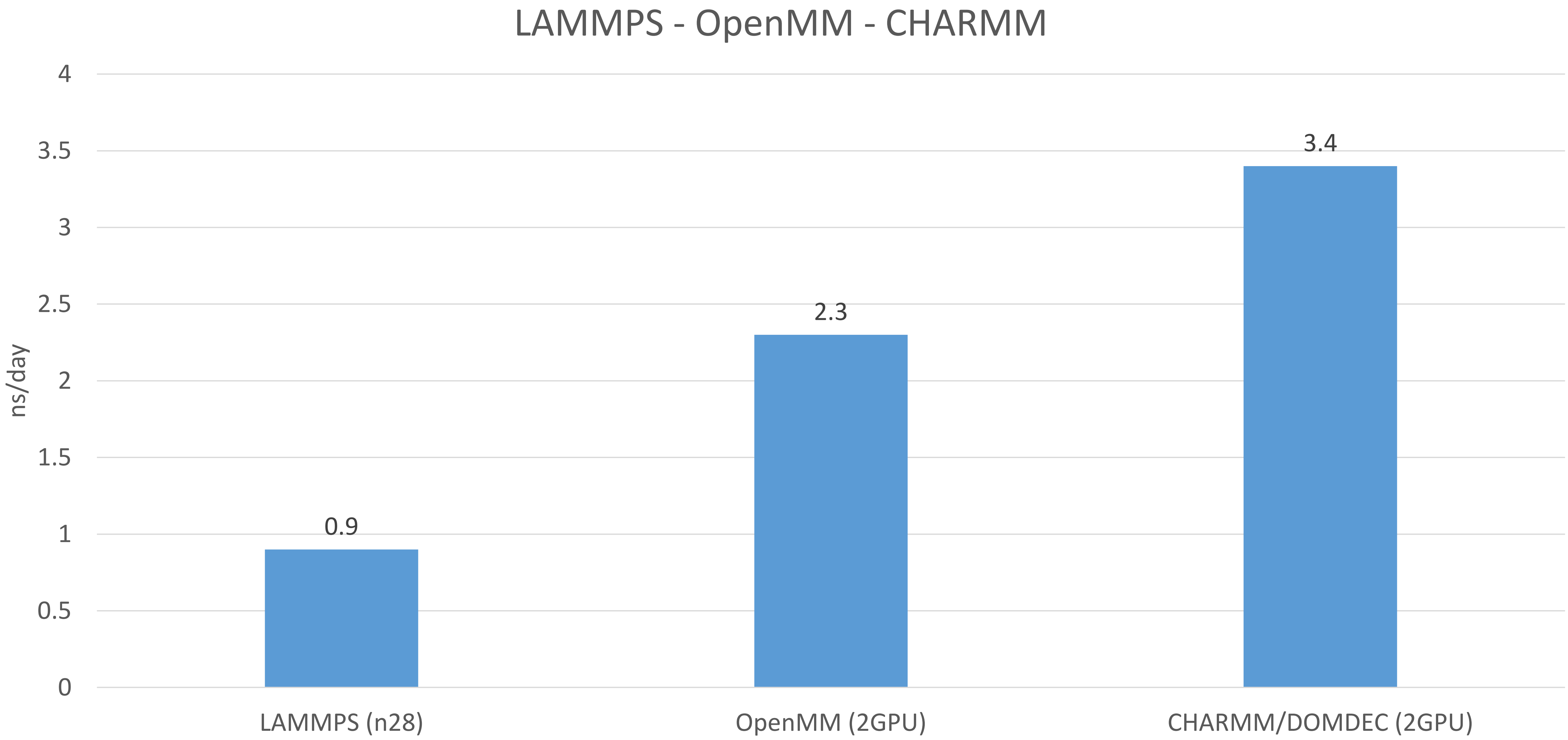
~3x slower than MPI only version

LAMMPS

Resources

LAMMPS tutorials
https://lammps.sandia.gov/tutorials.html

LAMMPS - OpenMM - CHARMM



Scratch directory

- If the program writes frequently data, you can get an additional speed up by using the local scratch directory:

```
parent=/proj/nobackup/projdir/somedir
rsync -avh $parent /scratch

cd /scratch/somedir

namd2 +p 28 +setcpuaffinity input.inp > output.dat

rsync -avh /scratch/somedir/. $parent/.

rm -rf /scratch/somedir
```

~10-15% speedup

Kebnekaise, standard nodes: 171 GB
Kebnekaise, GPU nodes: 171 GB
Kebnekaise, Largemem nodes: 352 GB
(a few of them have 391 GB)

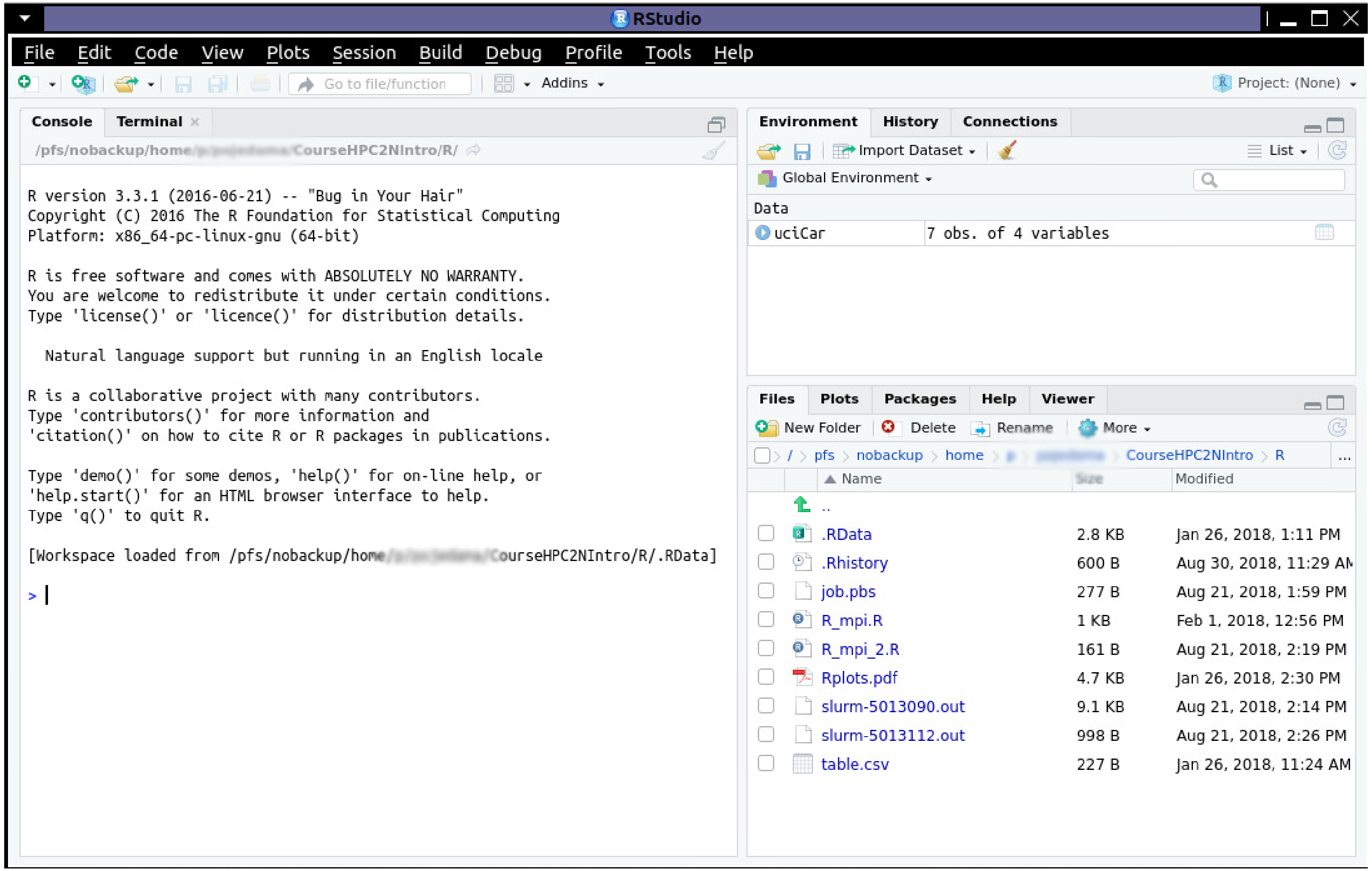
Plugins/Tools

Note: not all the tools referenced here are installed on our systems. It is indicated with the labels: I=installed, MI=manually installed

R/Rstudio (I)

$ml icc/2017.1.132-GCC-6.3.0-2.27 impi/2017.1.132 ifort/2017.1.132-GCC-6.3.0-2.27

$ml R/3.3.1
$rstudio

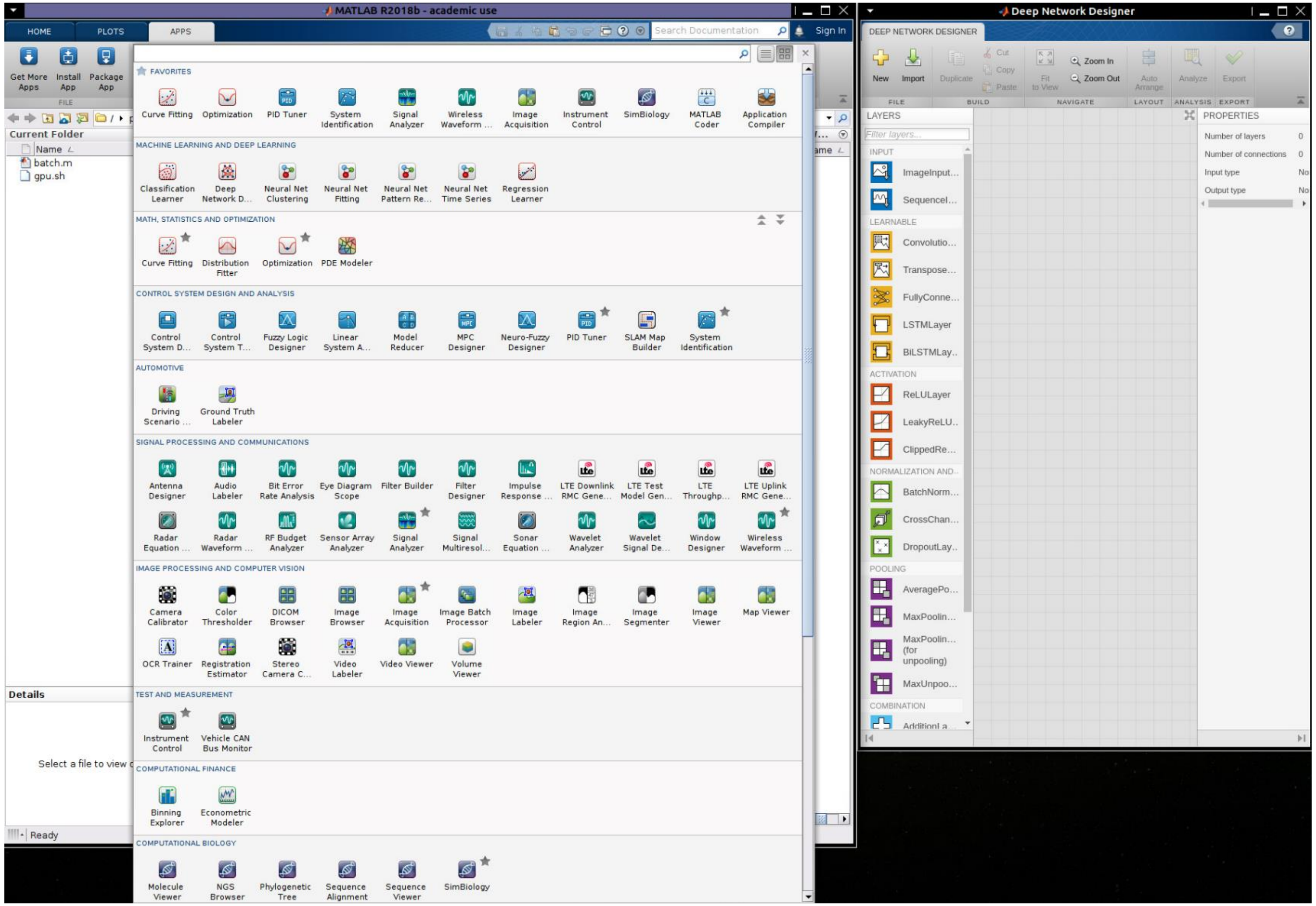


```
/pfs/nobackup/home/[redacted]/CourseHPC2NIntro/R/

R version 3.3.1 (2016-06-21) -- "Bug in Your Hair"
Copyright (C) 2016 The R Foundation for Statistical Computing
Platform: x86_64-pc-linux-gnu (64-bit)

R is free software and comes with ABSOLUTELY NO WARRANTY.
You are welcome to redistribute it under certain conditions.
Type 'license()' or 'licence()' for distribution details.

  Natural language support but running in an English locale

R is a collaborative project with many contributors.
Type 'contributors()' for more information and
'citation()' on how to cite R or R packages in publications.

Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.

[Workspace loaded from /pfs/nobackup/home[redacted]CourseHPC2NIntro/R/.RData]

> |
```

```
Data
uciCar        7 obs. of 4 variables
```

```
/ > pfs > nobackup > home > [redacted] > CourseHPC2NIntro > R

  Name                 Size     Modified
  ..
□ .RData               2.8 KB   Jan 26, 2018, 1:11 PM
□ .Rhistory            600 B    Aug 30, 2018, 11:29 AM
□ job.pbs              277 B    Aug 21, 2018, 1:59 PM
□ R_mpi.R              1 KB     Feb 1, 2018, 12:56 PM
□ R_mpi_2.R            161 B    Aug 21, 2018, 2:19 PM
□ Rplots.pdf           4.7 KB   Jan 26, 2018, 2:30 PM
□ slurm-5013090.out    9.1 KB   Aug 21, 2018, 2:14 PM
□ slurm-5013112.out    998 B    Aug 21, 2018, 2:26 PM
□ table.csv            227 B    Jan 26, 2018, 11:24 AM
```

MATLAB (I)



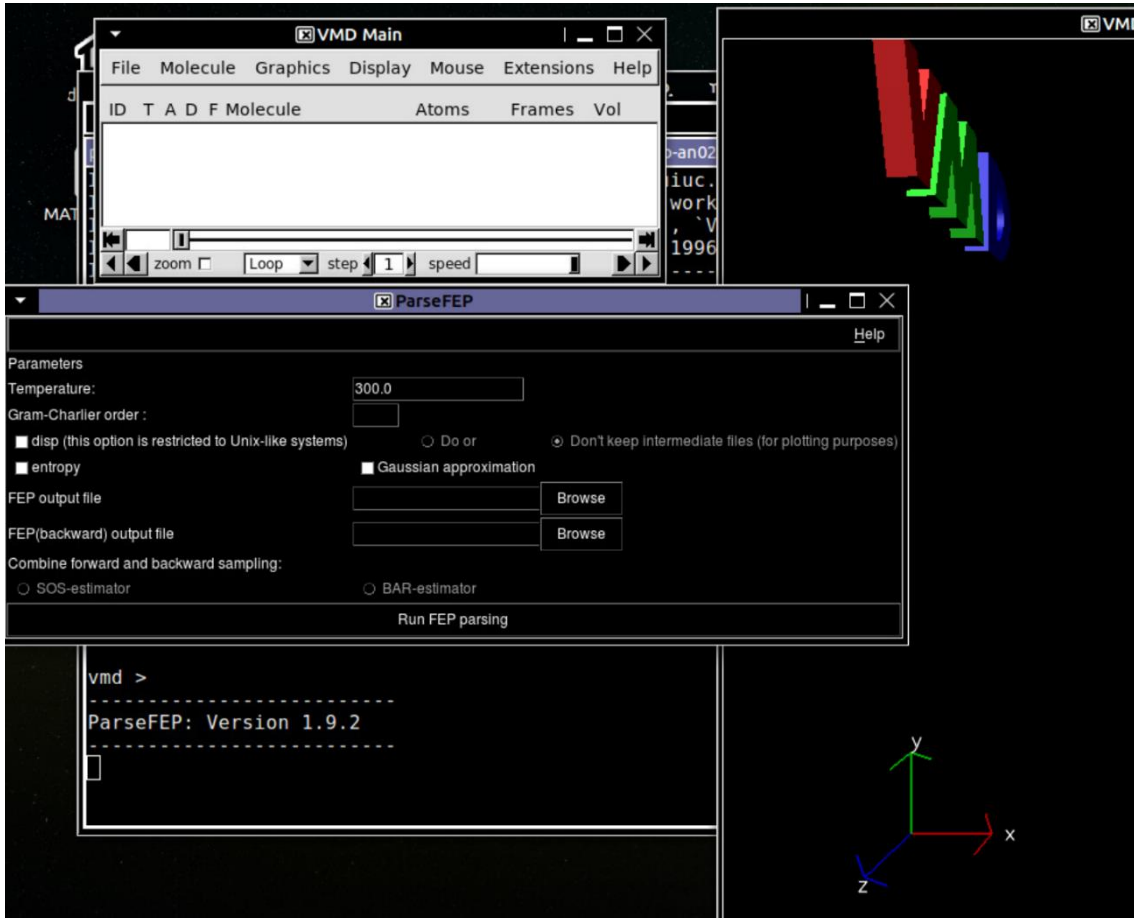
$ml MATLAB/2018b

Includes improved tools for Machine Learning and Deep Learning

PRL, 120, 143001 (2018)

Further information: https://www.hpc2n.umu.se/resources/software/matlab

Alchemical simulations (I)



Parameters

Temperature: 300.0

Gram-Charlier order :

□ disp (this option is restricted to Unix-like systems) ○ Do or ● Don't keep intermediate files (for plotting purposes)

□ entropy □ Gaussian approximation

FEP output file

FEP(backward) output file

Combine forward and backward sampling:

○ SOS-estimator ○ BAR-estimator

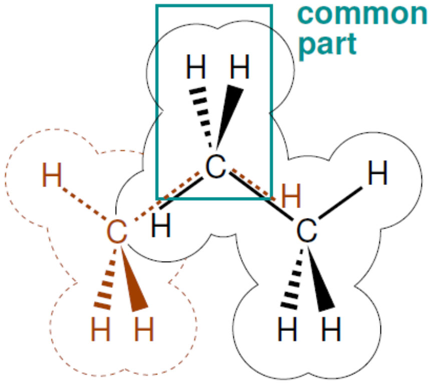
```
vmd >
--------------------------
ParseFEP: Version 1.9.2
--------------------------
```

parseFEP in VMD software

$$H(\lambda) = \lambda H_B + (1 - \lambda) H_A$$

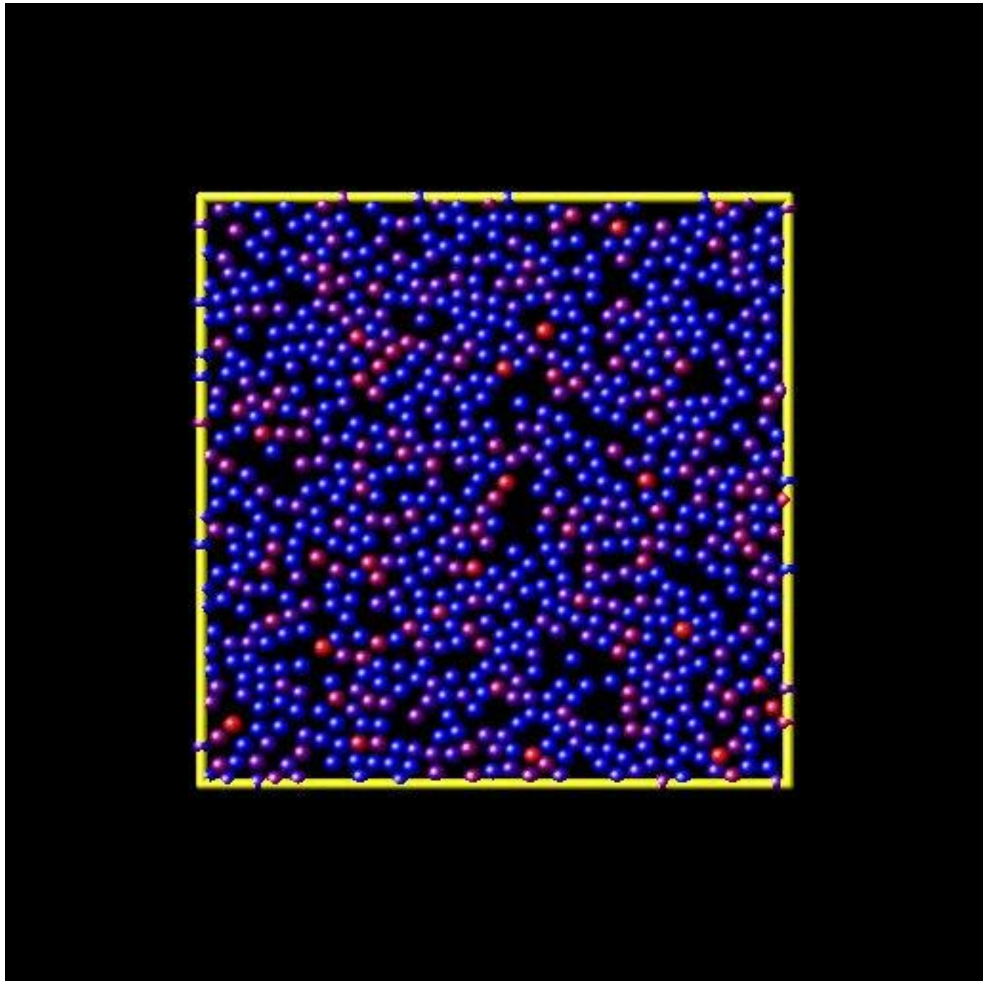
$$\Delta G = G_B - G_A = \sum_{\lambda=0}^{1} -RTln\left\langle e^{-\Delta H'/RT}\right\rangle_{\lambda}$$

Chem. Rev., 93, 2395-1417 (1993)



Dual topology. Figure taken from: http://www.ks.uiuc.edu/Training/Tutorials/namd/FEP/tutorial-FEP.pdf

NEMD-2D (I)



Simulation performed using LAMMPS

```
pair_style lj/cut ${rc}

# shear rate defined relative to perpendicular dimension

variable   xyrate equal ${srate}/ly

fix                  1 all nvt/sllod temp $t $t 0.1
fix                  2 all deform 1 xy erate ${xyrate} remap v
```

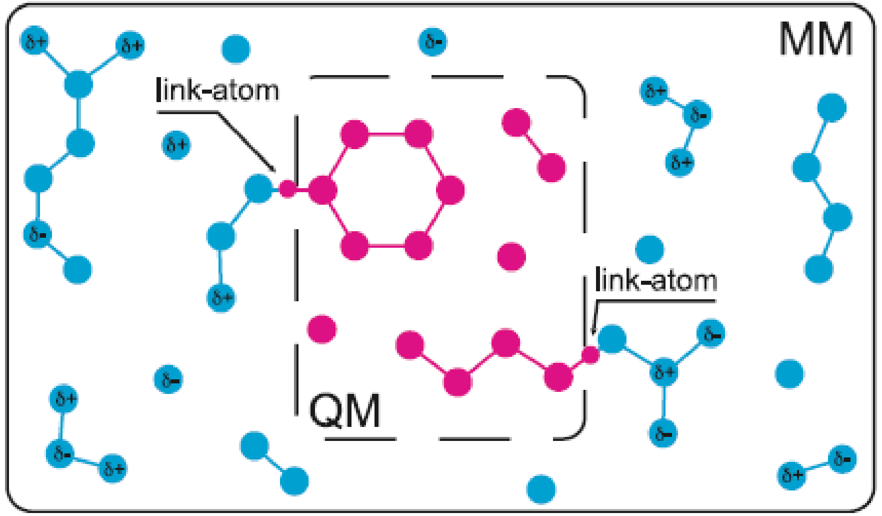
More information:
https://github.com/lammps/lammps/tree/master/examples/VISCOSITY

Similar NEMD simulations can be performed with GROMACS:
Mol. Sim., 36, 560-567 (2010).

QM/MM simulations

- CHARMM SQM (MI)

```
!Topology and coordinates files

!Define the  QM region
define subs sele segid mnp  show end

!Specify the QM method
mndo remo sele subs show end -
GLNK sele none show end amd char -3 -
switched  DXLBomd NORD 9 NSTEpSCF 7

!Perform the dynamics
dynamics cpt leap restart time 0.0005 nstep 40000 …
```



Adapted from Methods in Mol. Biology, vol. 924.
G. Groenhof.

QM/MM simulations

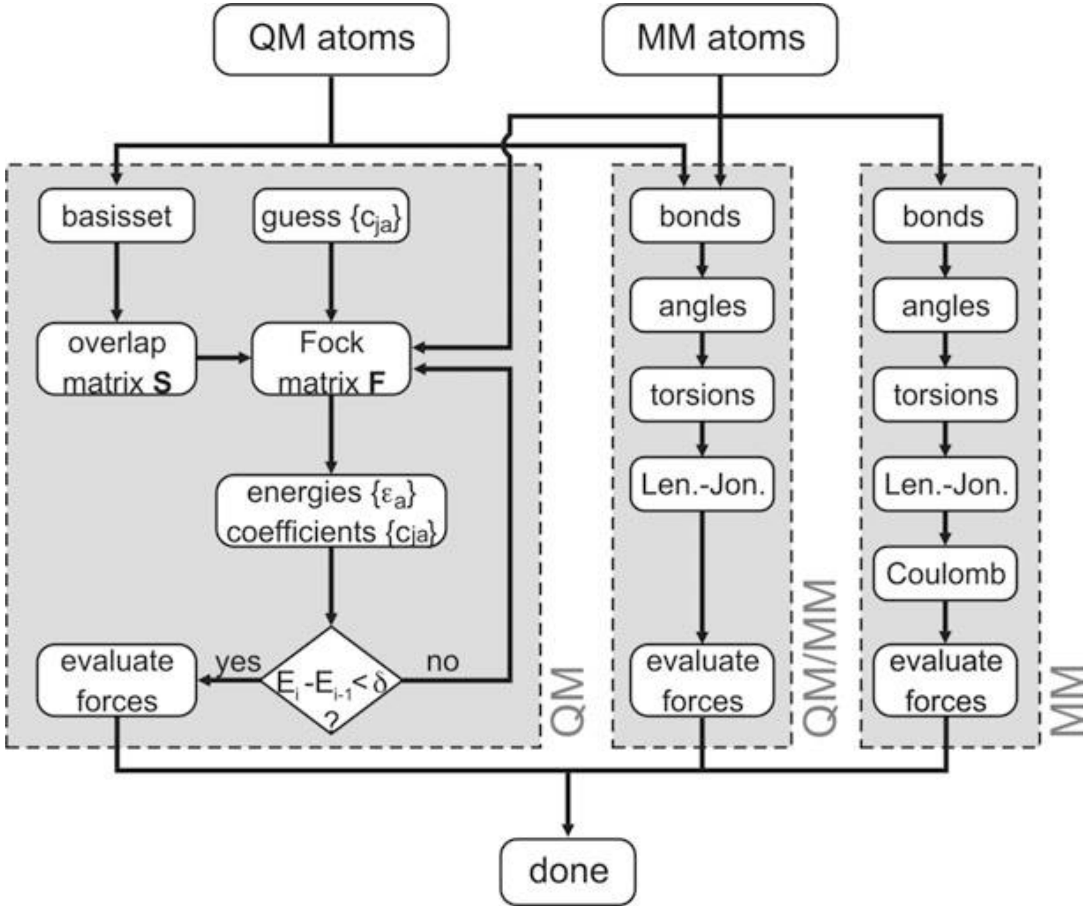
- CHARMM SQM (MI)

!Topology and coordinates files

!Define the QM region
define subs sele segid mnp show end

!Specify the QM method
mndo remo sele subs show end -
GLNK sele none show end amd char -3 -
switched DXLBomd NORD 9 NSTEpSCF 7

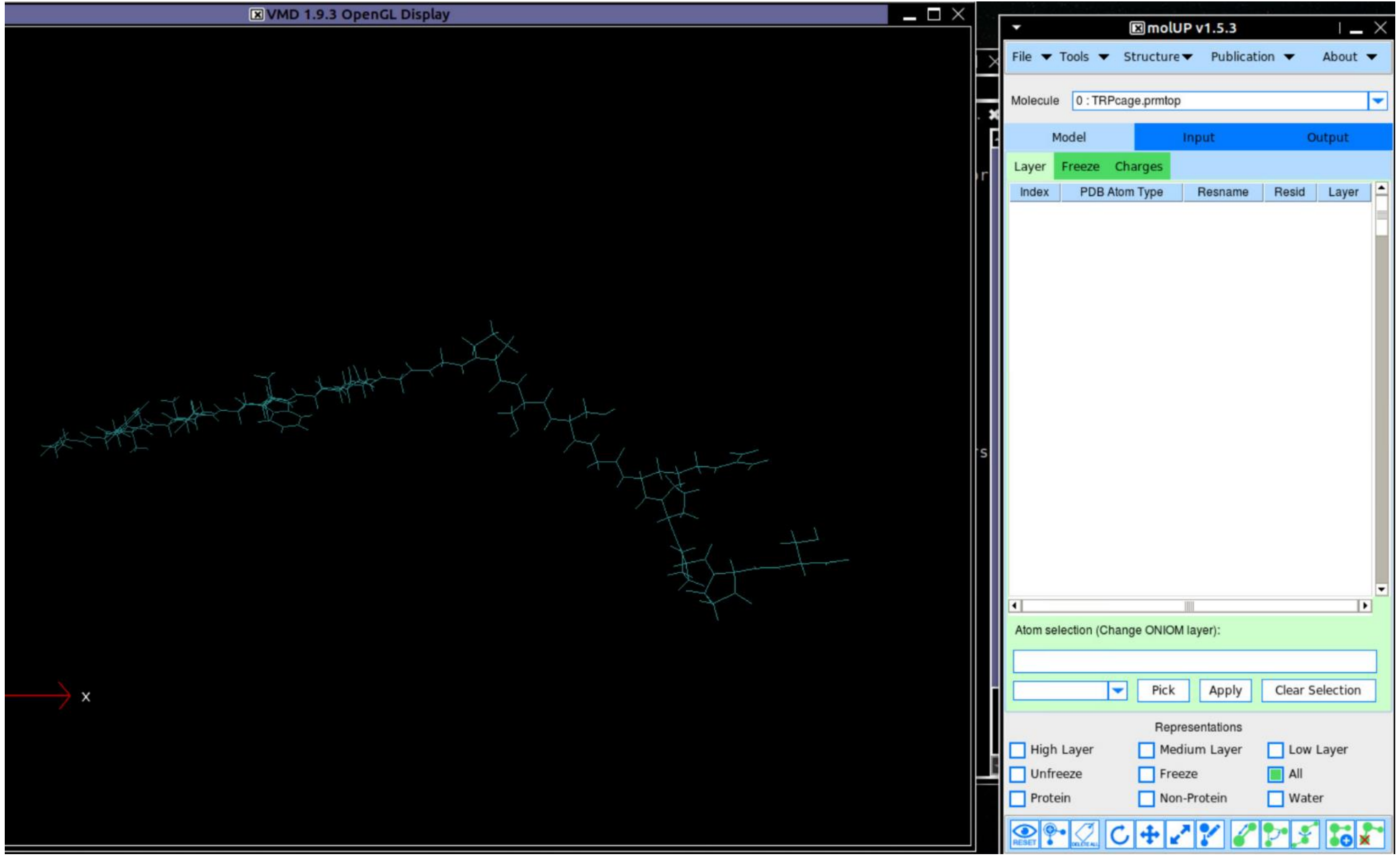
!Perform the dynamics
dynamics cpt leap restart time 0.0005 nstep 40000 …



Adapted from Methods in Mol. Biology, vol. 924. G. Groenhof.

QM/MM simulations

- CHARMM SQM
- molUP, (Amber, JCC, 39, 1344-1353, 2018) (MI)



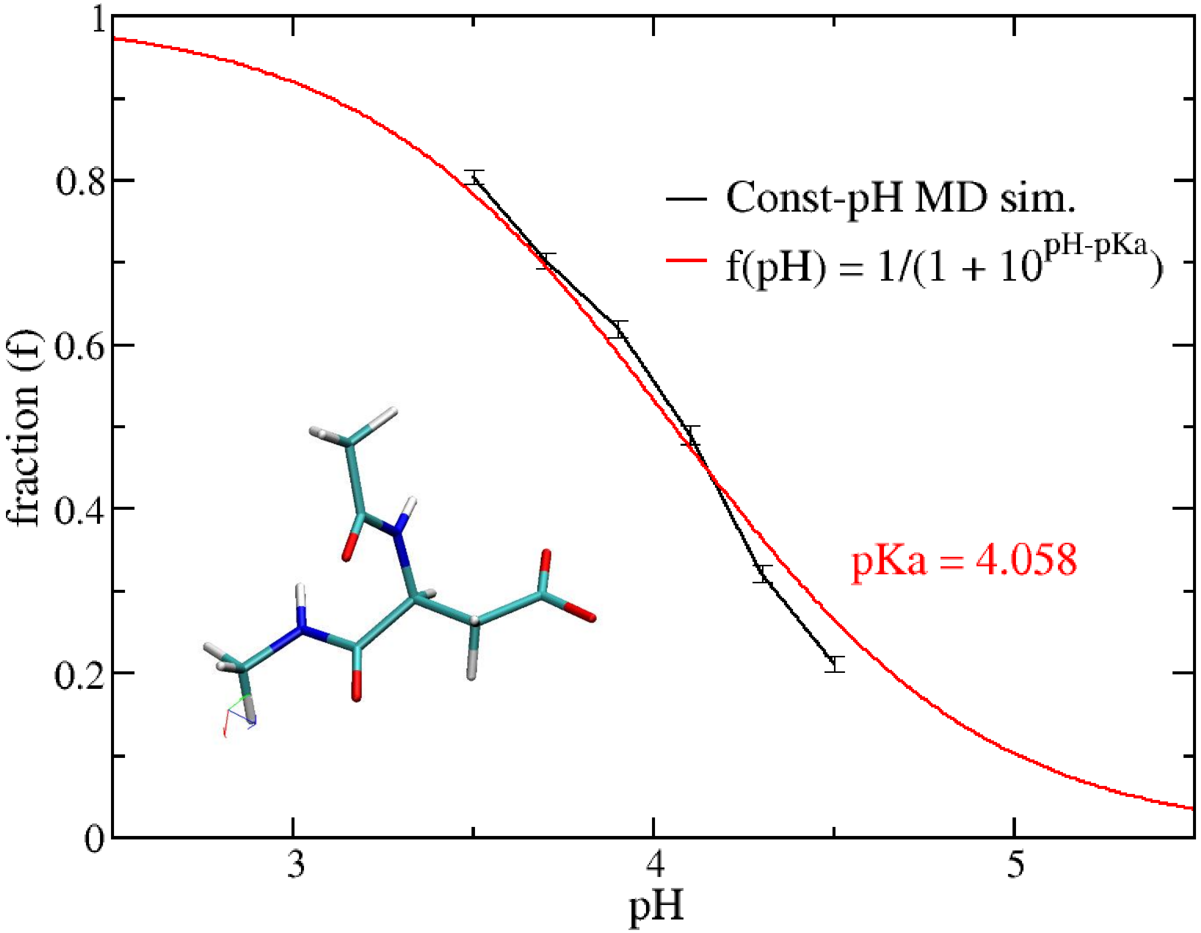
Molecule 0 : TRPcage.prmtop

Atom selection (Change ONIOM layer):

□ High Layer □ Medium Layer □ Low Layer
□ Unfreeze □ Freeze ☑ All
□ Protein □ Non-Protein □ Water

molUP plugin for QM/MM simulations in VMD

Constant pH simulation (I)



NAMD config file taken from:
http://www.ks.uiuc.edu/Training/Tutorials/
Method described in: JCTC, 13, 5933-5944 (2017)
http://ambermd.org/tutorials/

```
source ../../lib/namdcph/namdcph.tcl

…

parameters $toppar_dir/par_all36_solvent.prm
# Load constant-pH specific topology files
cphConfigFile $toppar_dir/conf_cph36_prot.json
topology      $toppar_dir/top_cph36_prot.rtf

# We will be running multiple pH values sorted into their own directories, but
# otherwise using the same naming scheme.
set pH 3.5
pH $pH
outputname      $pH/ace_asp_nme_prod0
cphMDBasename     $pH/namdcph.md
cphSwitchBasename $pH/namdcph.sw

# With the current settings this implies 1 ps between switching attempts,
# which will be 15 ps in length.
#
cphNumstepsPerSwitch 7500
cphRun 500 5
```

Constant pH simulation (I)

- Recent progress in this field, Cruzeiro et. al, JCP, 149, 072338 (2018), *Redox potential replica exchange molecular dynamics at constant pH in AMBER: Implementation and validation*

Analysis

- StreaMD: Advanced analysis of molecular dynamics using R, JCC, 39, 1666 (2018). (MI)
- http://thegrantlab.org/bio3d/tutorials/normal-mode-analysis (MI)
- http://www.ks.uiuc.edu/Training/Tutorials/
- https://github.com/rjdkmr/do_x3dna DNA structural analysis (GROMACS) (MI)

Validity test in MD

RESEARCH ARTICLE

Testing for physical validity in molecular simulations

Pascal T. Merz, Michael R. Shirts*

PLOS ONE (2018)

Suggestions

- Check if the software version you are trying is MPI (-n), OpenMP (-c), or hybrid (-n -c). Also, if you are using a GPU version.
- Is the cutoff radius for long-range interactions appropriate? PME?
- Could KNL nodes speed up your workflow?
- Keep your .bashrc file clean
- Upon asking a question to the support team: Make a folder with the case which displays the issue. Including all relevant files would be useful.
- Don’t forget to cite HPC2N and SNIC when publishing.
- Monitor your simulation on the fly with the command: “job-usage Job_ID”

Terminology

- BW: Broadwell nodes
- SK: Skylake nodes
- KNL: Knights Landing nodes
- MTS: Multiple Time Step algorithm