Applications' usage in HPC2N

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Why do we need HPC?

Scientific codes use loops extensively:

```
do j=1,N
      do i=1,N
        do k=1,N
           p(i,j) = p(i,j) + v1(i,k)* v2(k,j)
        enddo
      enddo
enddo
```

Heavy loops

MD, QM, CFD, …

```
!$omp parallel do private(i,j,k) shared(p,v1,v2) collapse(2)
    do j=1,N
      do i=1,N
        s=0.0d0
        do k=1,N
           s = s + v1(i,k)* v2(k,j)
        enddo
        p(i,j) = s
      enddo
    enddo
!$omp end parallel do
```

Parallelized loops

Processes communication

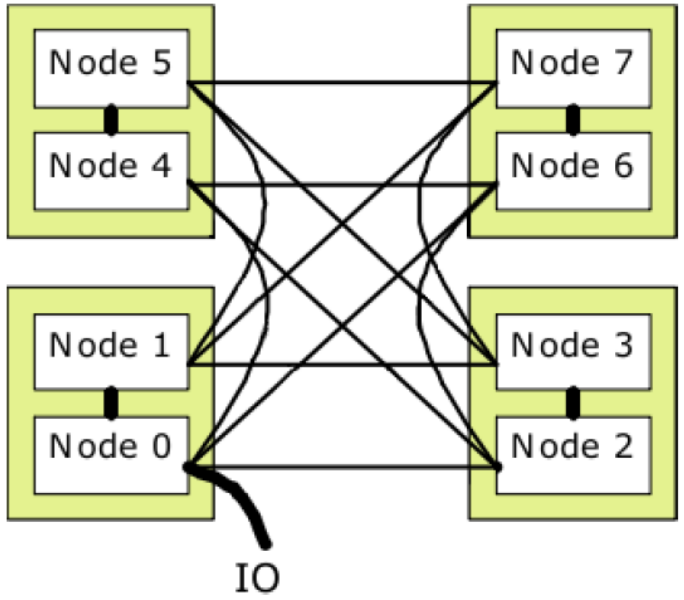


Figure : Nodes.

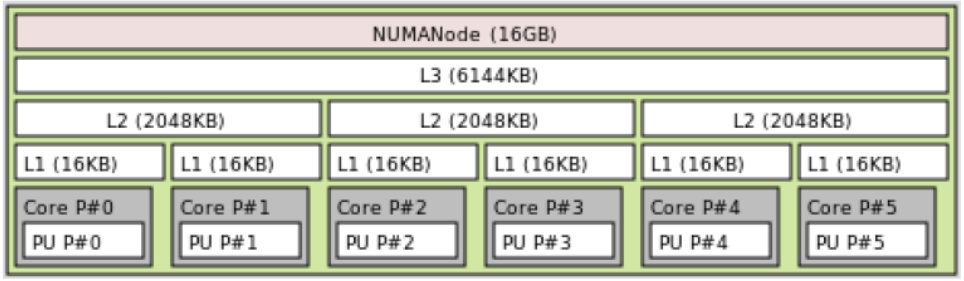
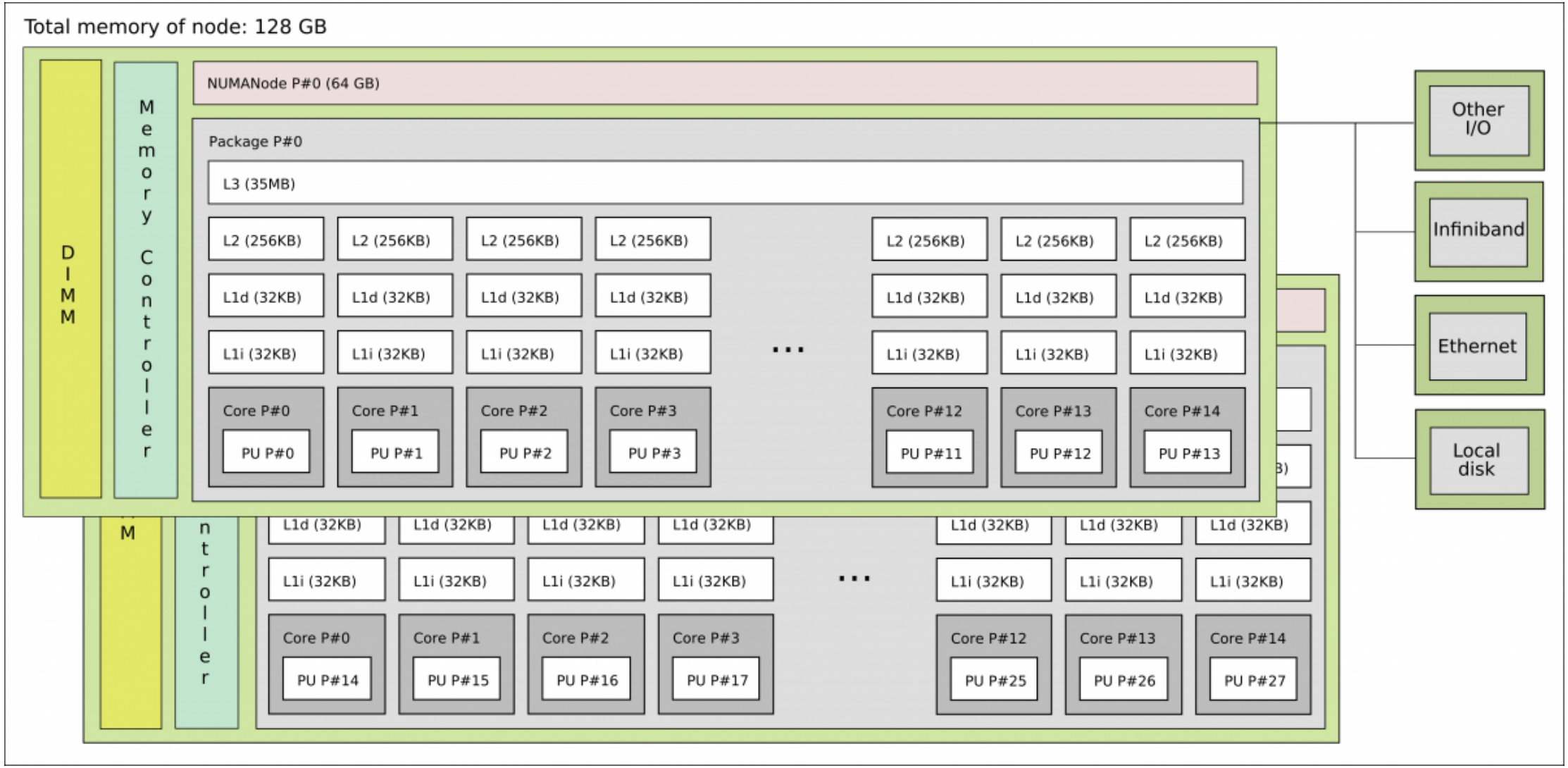


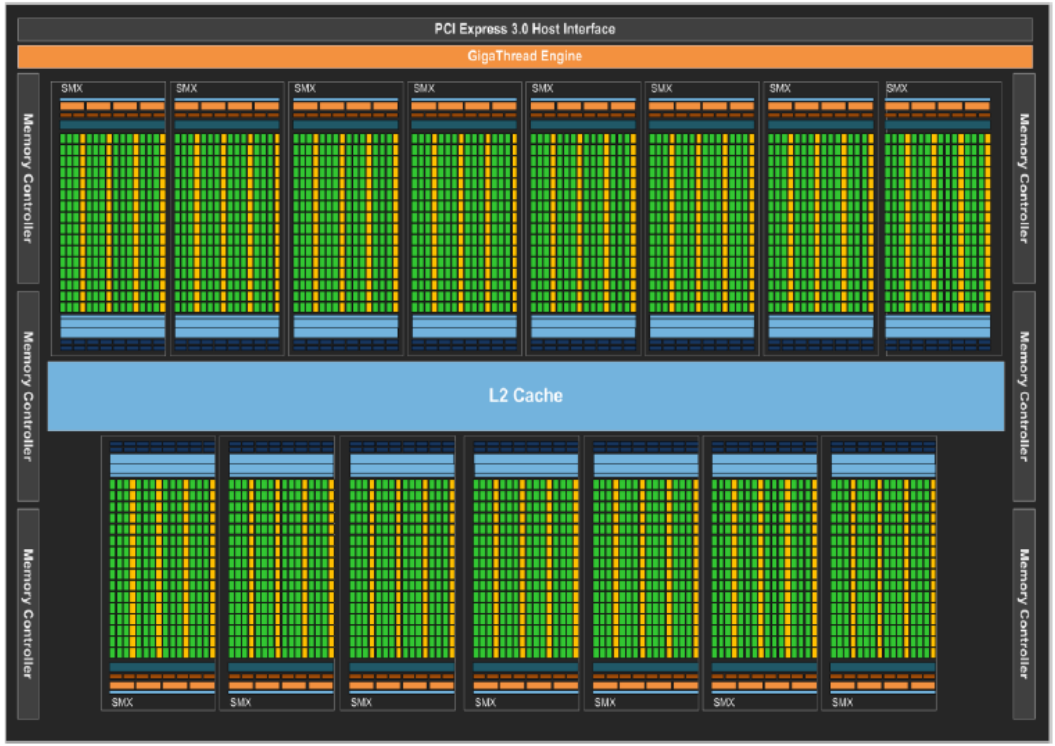
Figure : NUMA machine.

$$T_p = \frac{T_s}{P} + T_{comm}$$

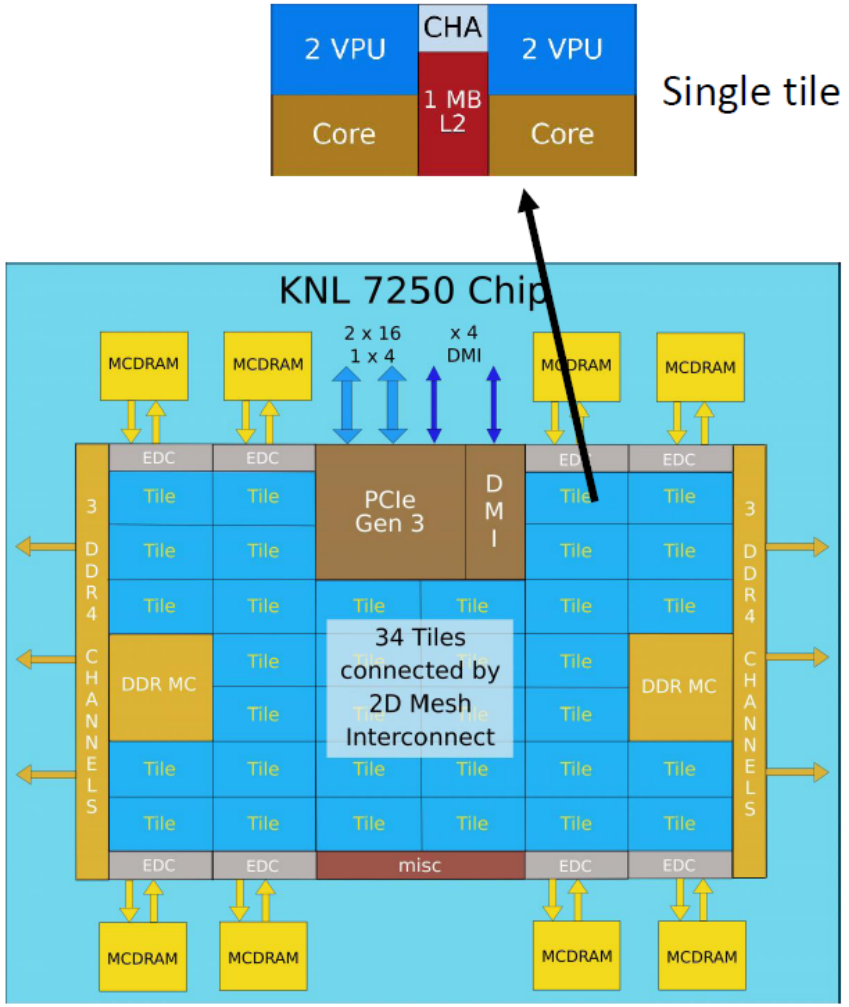
Broadwell node on Kebnekaise



Accelerators



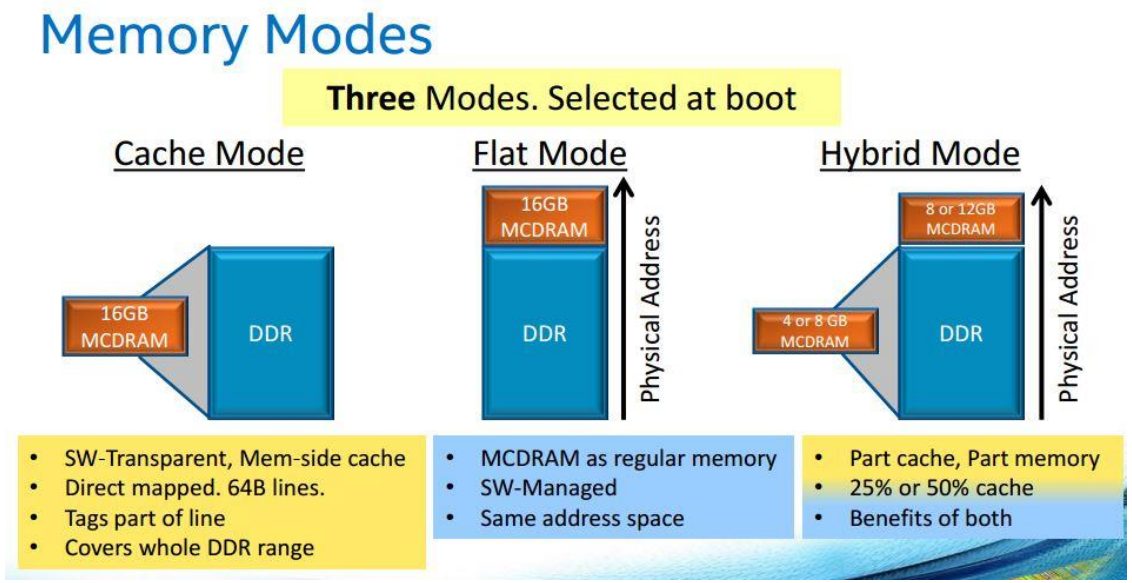
GPU showing the independent units Streaming Multiprocessors (SM).

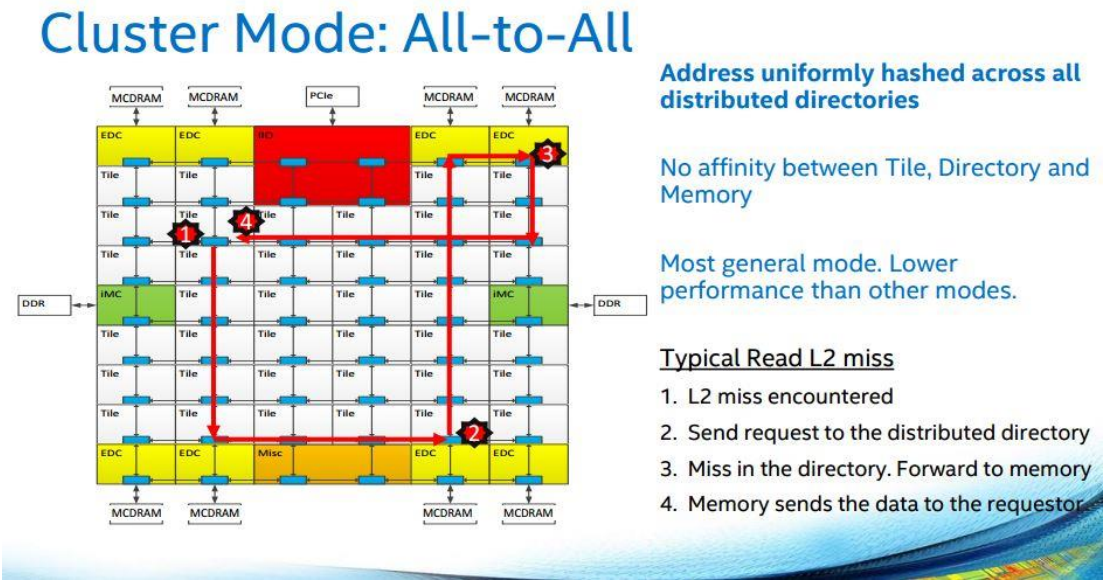


KNL, composed of several Tiles

$$Z(i) = A*X(i) + Y(i) \quad \text{(Vector Op.)}$$

KNL





#SBATCH --constraint=a2a,cache

#SBATCH --gres=hbm:4G

Credits: PRACE Best practice KNL (2017)

KNL Thread affinity

There are physical 68 cores with 4 hyperthreads on each.

Credits: Intel

Bind the threads by using OpenMP env. var.

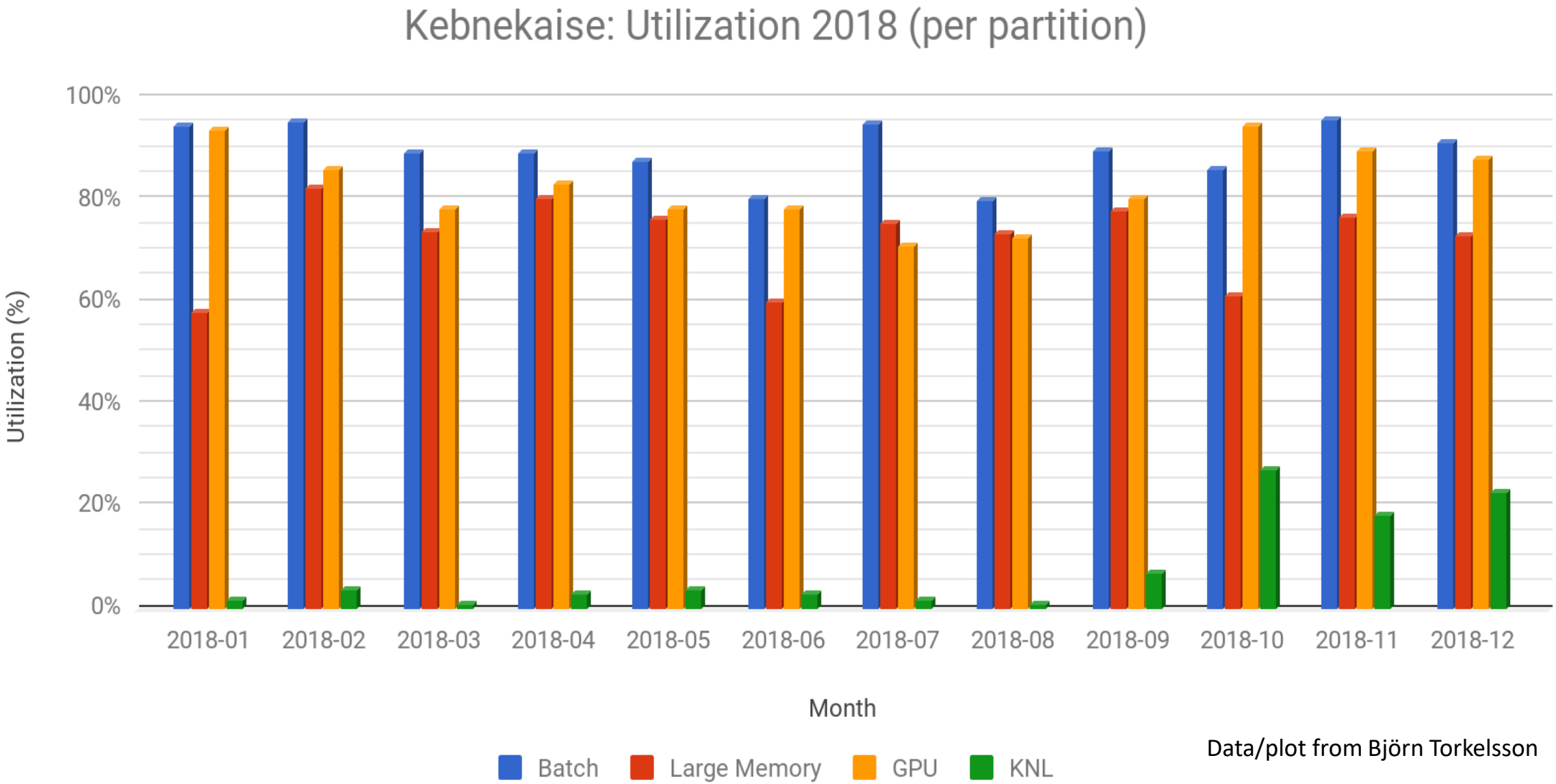
```
export OMP_NUM_THREADS=4
export OMP_PROC_BIND=spread
export OMP_PLACES=cores
```

```
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)
```



Data/plot from Björn Torkelsson

Tuning your own Applications

<no current project> - Intel VTune Amplifier@b-cn1203.hpc2n.umu.se

Welcome | profile

Basic Hotspots — Hotspots by CPU Usage viewpoint (change)

INTEL VTUNE AMPLIFIER XE 2017

Collection Log | Analysis Target | Analysis Type | Summary | Bottom-up | Caller/Callee | Top-down Tree | Platform

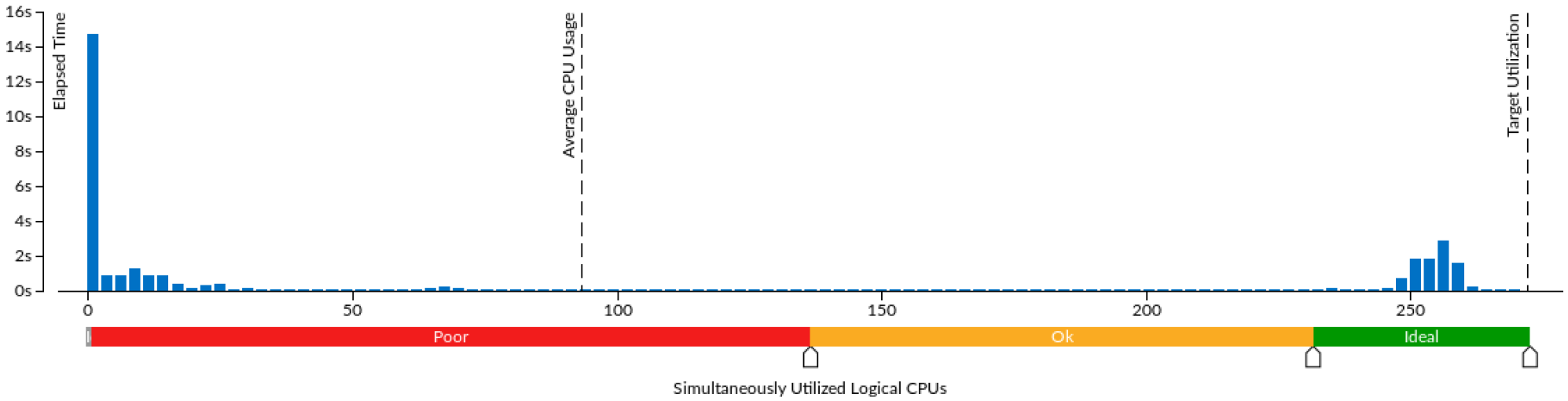
Top Hotspots

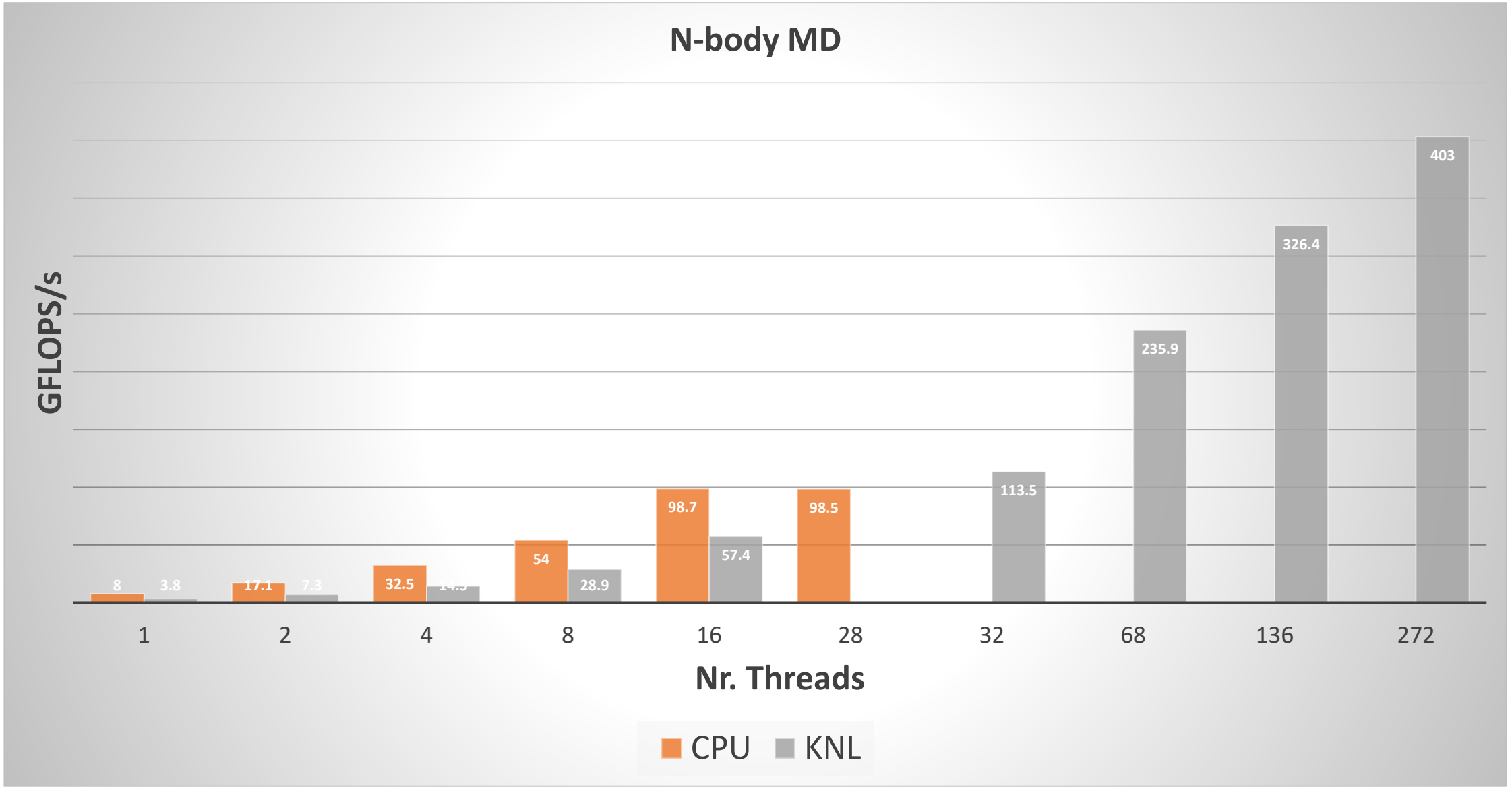
This section lists the most active functions in your application. Optimizing these hotspot functions typically results in improving overall application performance.

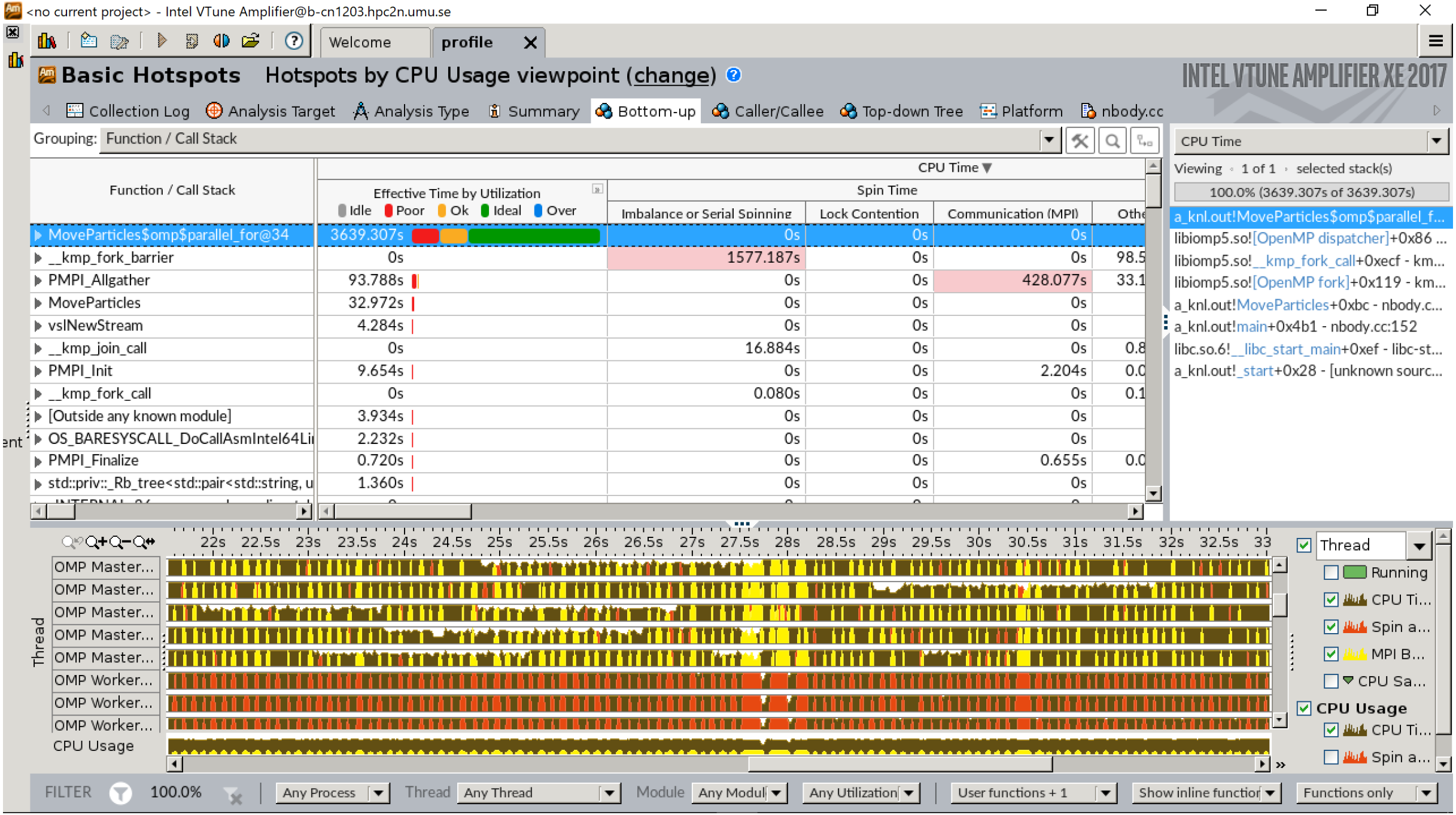
Function	Module	CPU Time
MoveParticlesompparallel_for@34	a_knl.out	3639.307s
__kmp_fork_barrier	libiomp5.so	1675.892s
PMPI_Allgather	libmpi.so.12	555.005s
MoveParticles	a_knl.out	32.972s
vslNewStream	libmkl_intel_lp64.so	24.794s
[Others]		57.713s

CPU Usage Histogram

This histogram displays a percentage of the wall time the specific number of CPUs were running simultaneously. Spin and Overhead time adds to the Idle CPU usage value.

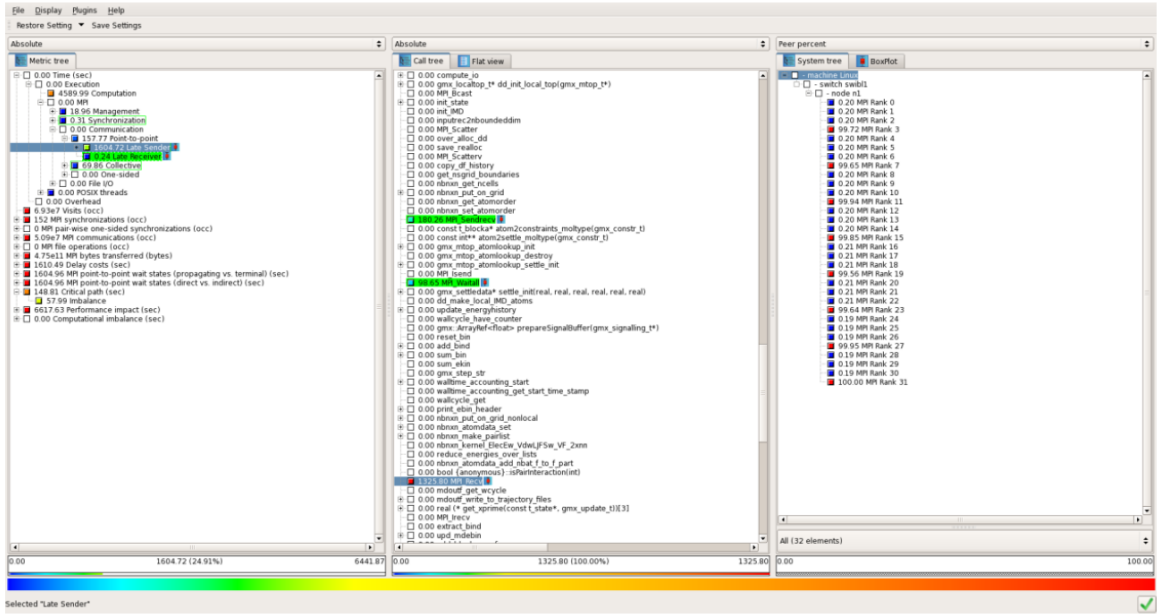


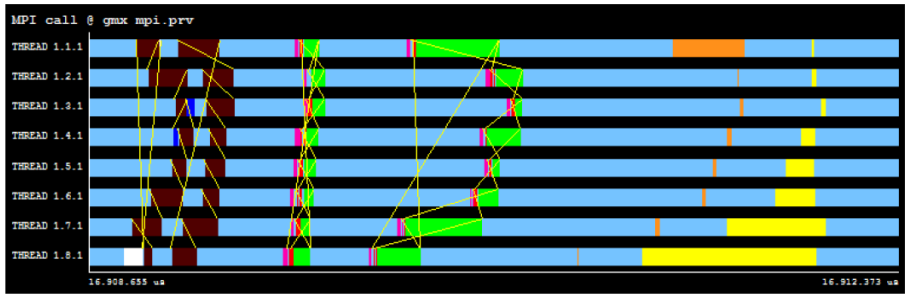

N-body MD
GFLOPS/s
8
3.8
17.1
7.3
32.5
54
28.9
98.7
57.4
98.5
113.5
235.9
326.4
403
1
2
4
8
16
28
32
68
136
272
Nr. Threads
CPU
KNL


<no current project> - Intel VTune Amplifier@b-cn1203.hpc2n.umu.se
Welcome
profile
Basic Hotspots
Hotspots by CPU Usage viewpoint (change)
INTEL VTUNE AMPLIFIER XE 2017
Collection Log
Analysis Target
Analysis Type
Summary
Bottom-up
Caller/Callee
Top-down Tree
Platform
nbody.cc
Grouping: Function / Call Stack
CPU Time
Viewing 1 of 1 selected stack(s)
100.0% (3639.307s of 3639.307s)
Function / Call Stack
CPU Time
Effective Time by Utilization
Idle Poor Ok Ideal Over
Spin Time
Imbalance or Serial Spinning
Lock Contention
Communication (MPI)
MovePartilesompparallel_for@34 3639.307s 0s 0s 0s
__kmp_fork_barrier 0s 1577.187s 0s 0s
PMPI_Allgather 93.788s 0s 0s 428.077s
MoveParticles 32.972s 0s 0s 0s
vslNewStream 4.284s 0s 0s 0s
__kmp_join_call 0s 16.884s 0s 0s
PMPI_Init 9.654s 0s 0s 2.204s
__kmp_fork_call 0s 0.080s 0s 0s
[Outside any known module] 3.934s 0s 0s 0s
OS_BARESYSCALL_DoCallAsmIntel64Li 2.232s 0s 0s 0s
PMPI_Finalize 0.720s 0s 0s 0.655s
std::priv::_Rb_tree<std::pair<std::string, u 1.360s 0s 0s 0s
a_knl.out!MoveParticlesompparallel_f...
libiomp5.so![OpenMP dispatcher]+0x86 ...
libiomp5.so!__kmp_fork_call+0xecf - km...
libiomp5.so![OpenMP fork]+0x119 - km...
a_knl.out!MoveParticles+0xbc - nbody.c...
a_knl.out!main+0x4b1 - nbody.cc:152
libc.so.6!__libc_start_main+0xef - libc-st...
a_knl.out!_start+0x28 - [unknown sourc...
22s 22.5s 23s 23.5s 24s 24.5s 25s 25.5s 26s 26.5s 27s 27.5s 28s 28.5s 29s 29.5s 30s 30.5s 31s 31.5s 32s 32.5s 33
Thread
OMP Master...
OMP Master...
OMP Master...
OMP Master...
OMP Master...
OMP Worker...
OMP Worker...
OMP Worker...
CPU Usage
Thread
Running
CPU Ti...
Spin a...
MPI B...
CPU Sa...
CPU Usage
CPU Ti...
Spin a...
FILTER 100.0%
Any Process
Thread Any Thread
Module Any Modul
Any Utilization
User functions + 1
Show inline functior
Functions only

Profiling Tools at HPC2N

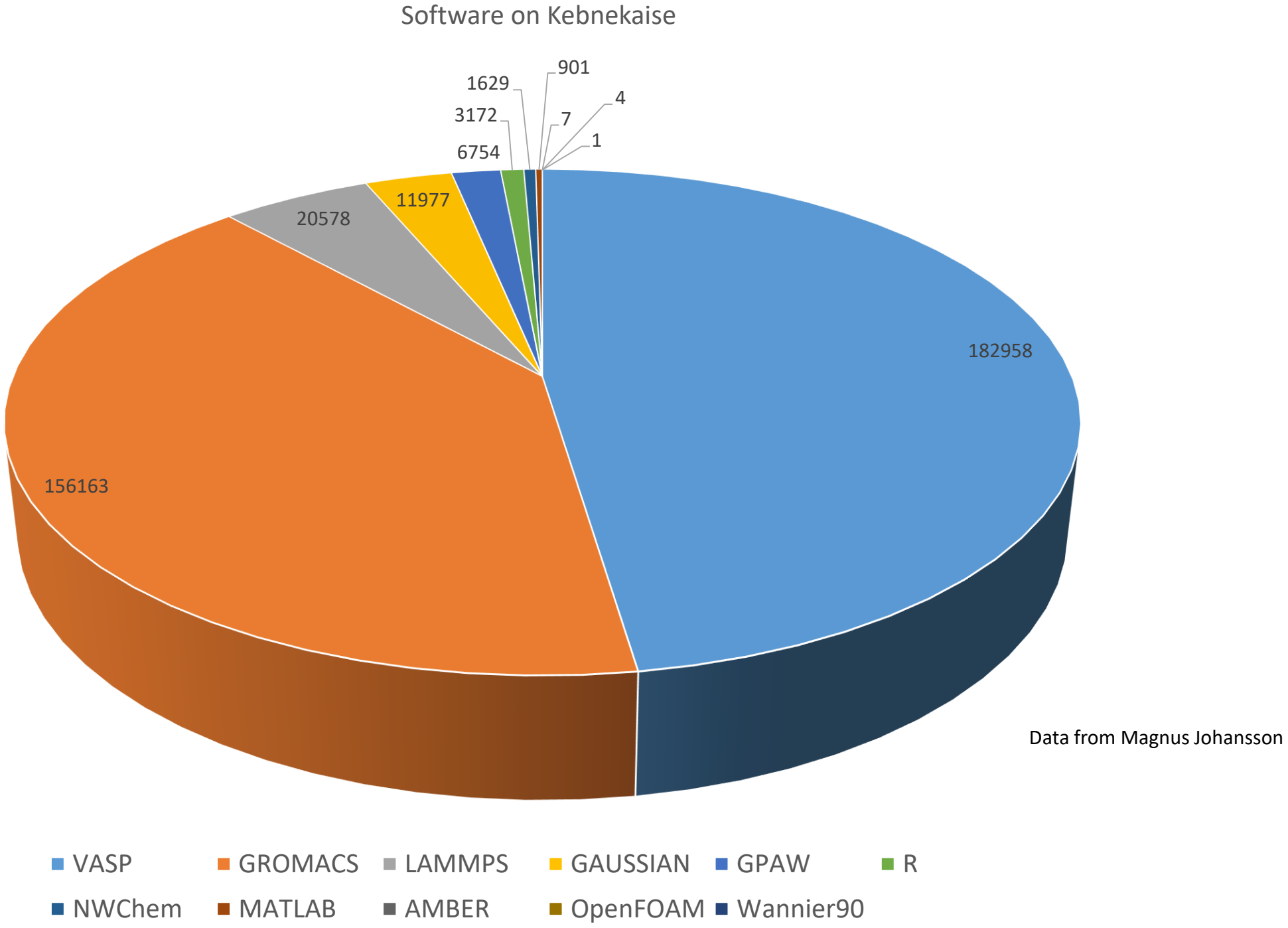
- Intel Vtune, Intel Inspector
- SCALASCA, Score-P, Cube
- Extrae/Paraver
- Allinea DDT
- Application Expert support on demand



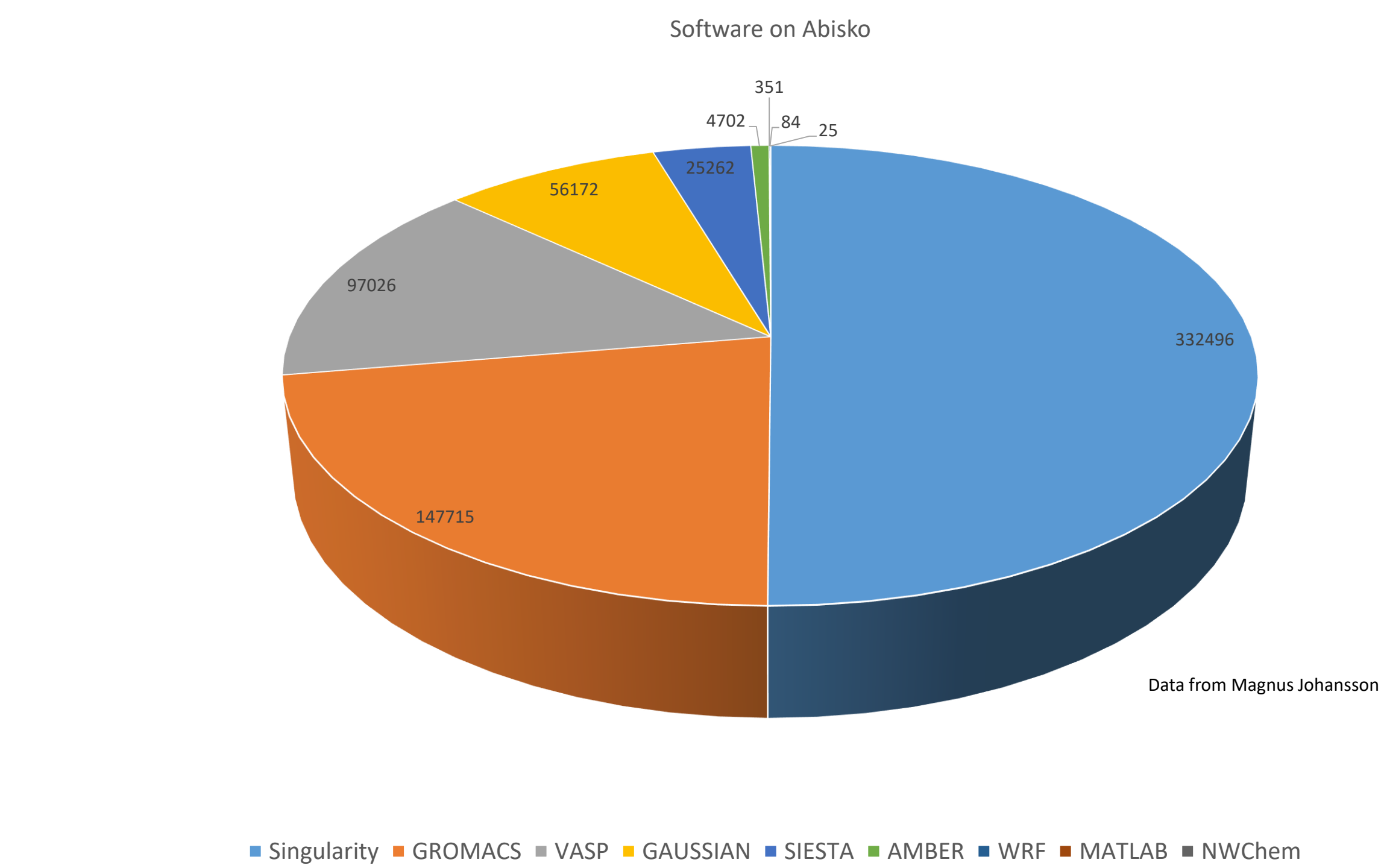


J. Eriksson, P. Ojeda, T. Ponweiser, T. Steinreicher (2017)

Applications



Data from Magnus Johansson


Software on Abisko
351
4702
84
25
25262
56172
97026
332496
147715
Data from Magnus Johansson
Singularity
GROMACS
VASP
GAUSSIAN
SIESTA
AMBER
WRF
MATLAB
NWChem

R/Rstudio

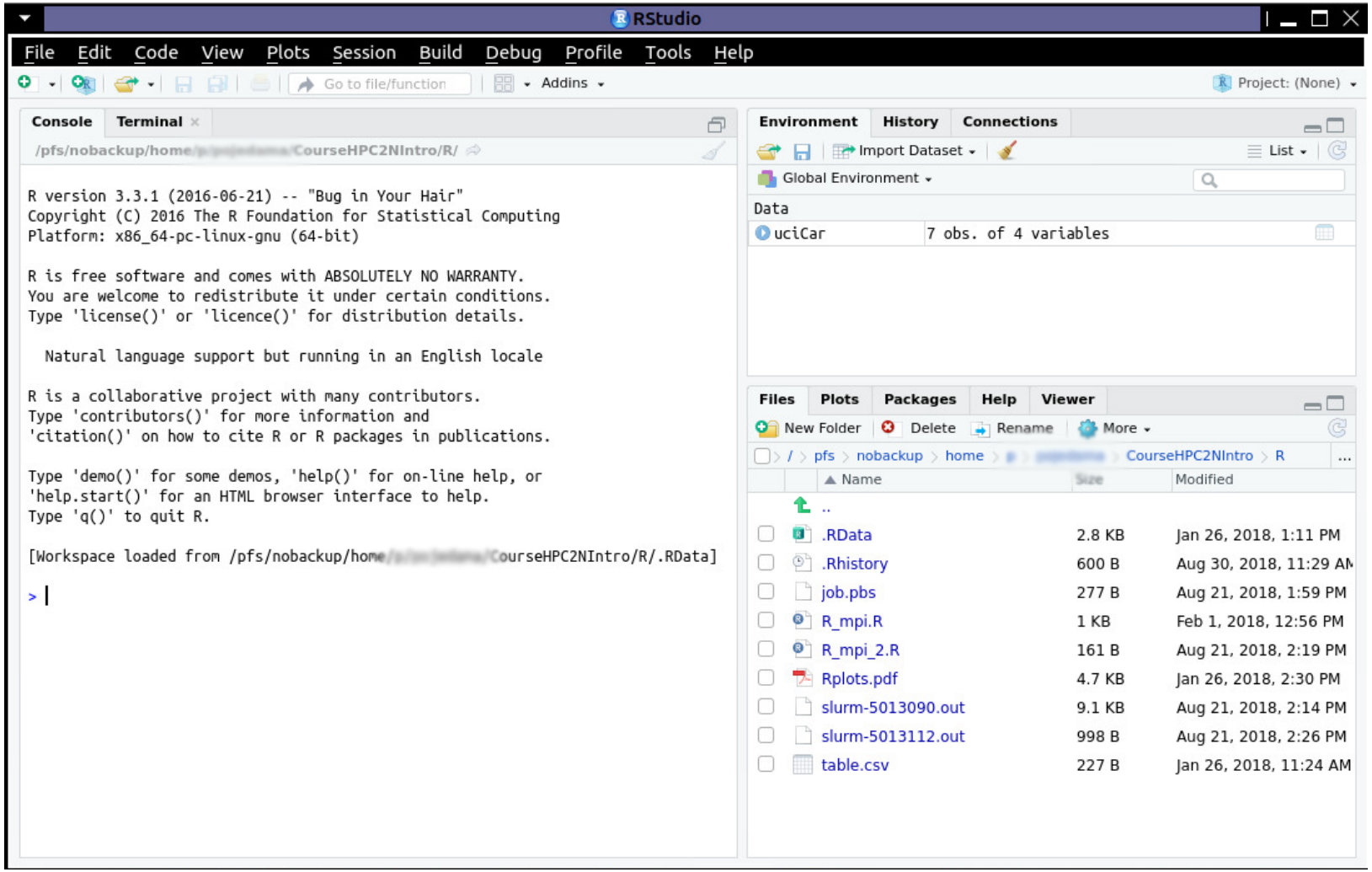
$ml icc/2017.1.132-GCC-6.3.0-2.27 impi/2017.1.132 ifort/2017.1.132-GCC-6.3.0-2.27

$ml R/3.3.1
$rstudio

Rstudio will use the loaded R version

Please use the GUI just for lightweight tasks, otherwise use the batch queues.

Heavy jobs will be cancelled!



R/Rstudio

Installing packages

In case you need to install some R package that is not included in the installed R version, you need to follow this guideline:

https://www.hpc2n.umu.se/resources/software/user_installed/r

Otherwise, the batch system won't have access to the manually installed packages.

R serial job

```
#!/bin/bash
### SNAC project number, enter your own
#SBATCH -A SNICXXXX-YY-ZZ
# Asking for one core
#SBATCH -n 1
#SBATCH --time=00:10:00

ml icc/2017.1.132-GCC-6.3.0-2.27
ml ifort/2017.1.132-GCC-6.3.0-2.27
ml impi/2017.1.132
ml R/3.3.1

R --no-save --quiet < input.R > Rexample.out
```

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

R parallel job (Rmpi)

File: Rmpi.R

```
library("Rmpi")
mpi.spawn.Rslaves(nslaves=5)

x <- c(10,20,30,40,50)
mpi.apply(x,runif)

# Close down the MPI processes and quit R
mpi.close.Rslaves()
mpi.finalize()
```

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

```
#!/bin/bash
#SBATCH -A project_ID
#Asking for 10 min.
#SBATCH -t 00:10:00
#SBATCH -N 1
#SBATCH -n 6

export OMPI_MCA_mpi_warn_on_fork=0

ml GCC/6.4.0-2.28 OpenMPI/2.1.2
ml R/3.4.4-X11-20180131

R -q --slave -f Rmpi.R
```

R parallel job (doParallel)

```
#!/bin/bash
#SBATCH -A project_ID
#Asking for 10 min.
#SBATCH -t 00:10:00
##SBATCH -N 1
#SBATCH -n 8
##SBATCH --exclusive

ml GCC/6.4.0-2.28 OpenMPI/2.1.2
ml R/3.4.4-X11-20180131

R -q --slave -f doParallel_ML.R
```

doParallel_ML.R

```
library(doParallel)
registerDoParallel(cores=8)
getDoParWorkers()

library(caret)
library(MASS)
library(klaR)
library(nnet)
library(e1071)
library(rpart)
```

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

R parallel job (doParallel)

```
#!/bin/bash
#SBATCH -A project_ID
#Asking for 10 min.
#SBATCH -t 00:10:00
##SBATCH -N 1
#SBATCH -n 8
##SBATCH --exclusive

ml GCC/6.4.0-2.28 OpenMPI/2.1.2
ml R/3.4.4-X11-20180131

R -q --slave -f doParallel_ML.R
```

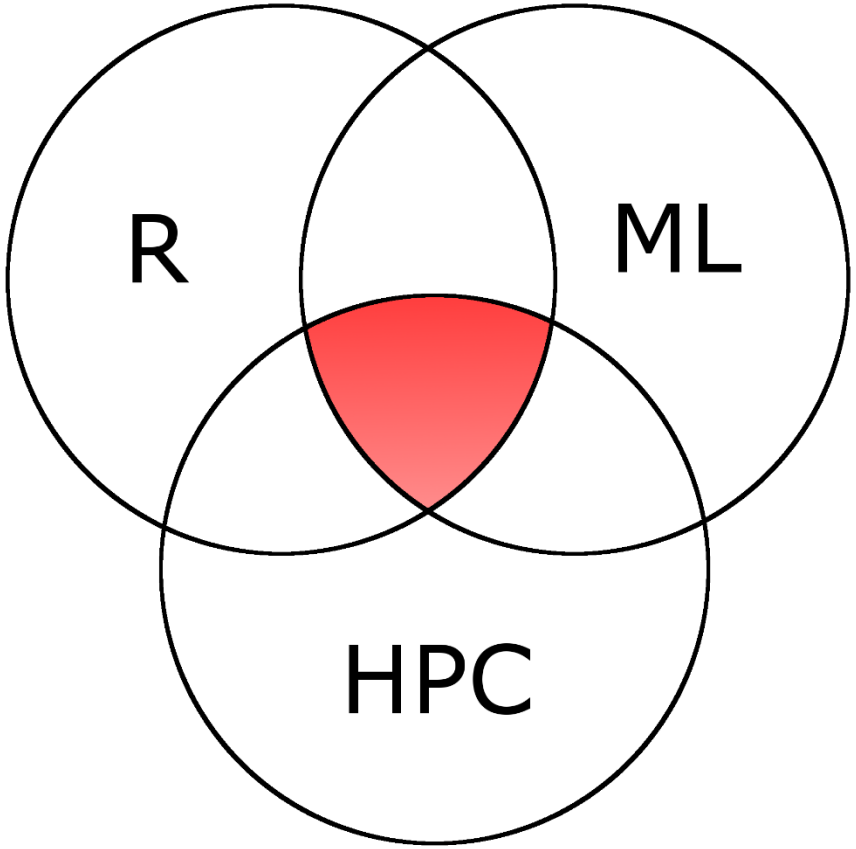
doParallel_ML.R

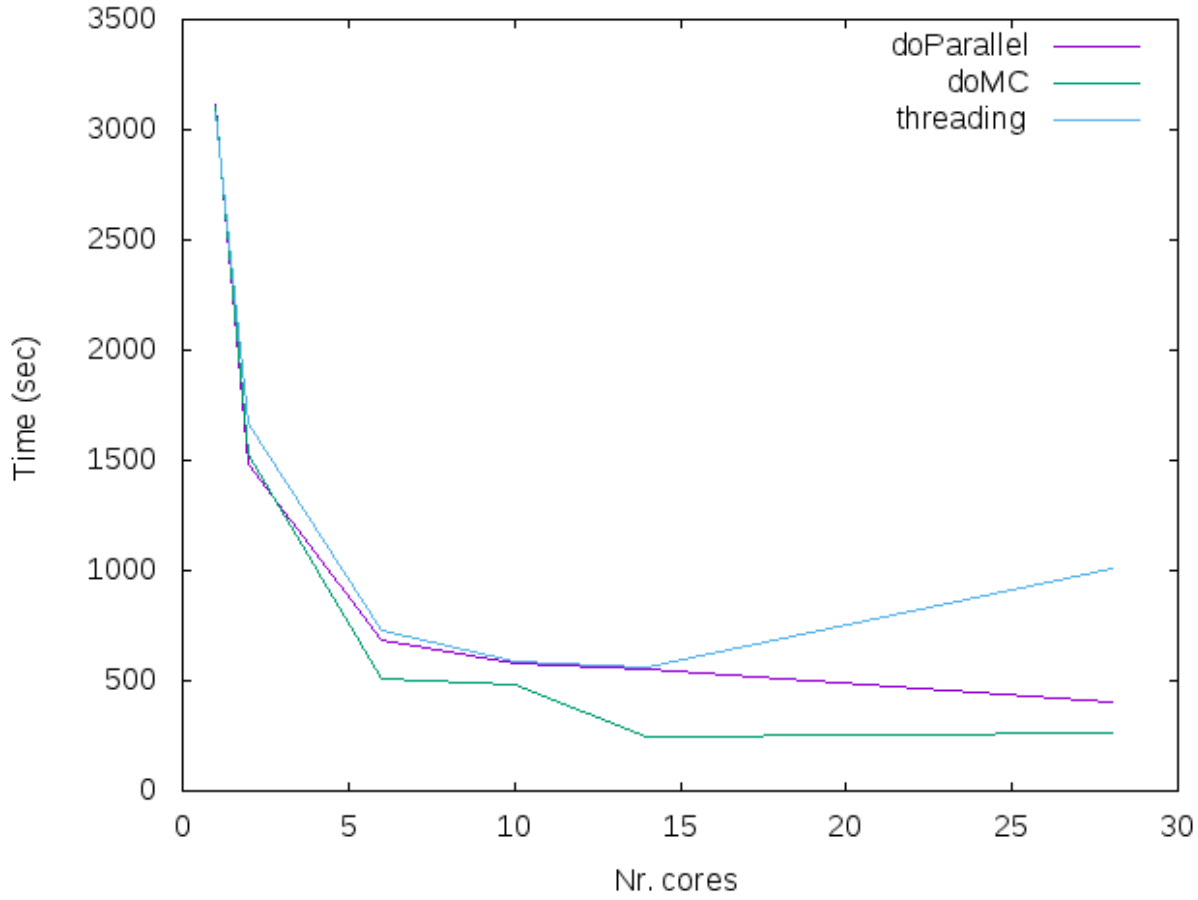
```
#Serial mode
sr <- foreach(1:runs, .combine = rbind) %do% evaluation()

#Parallel mode
pr <- foreach(1:runs, .combine = rbind) %dopar% evaluation()
```

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

R machine learning

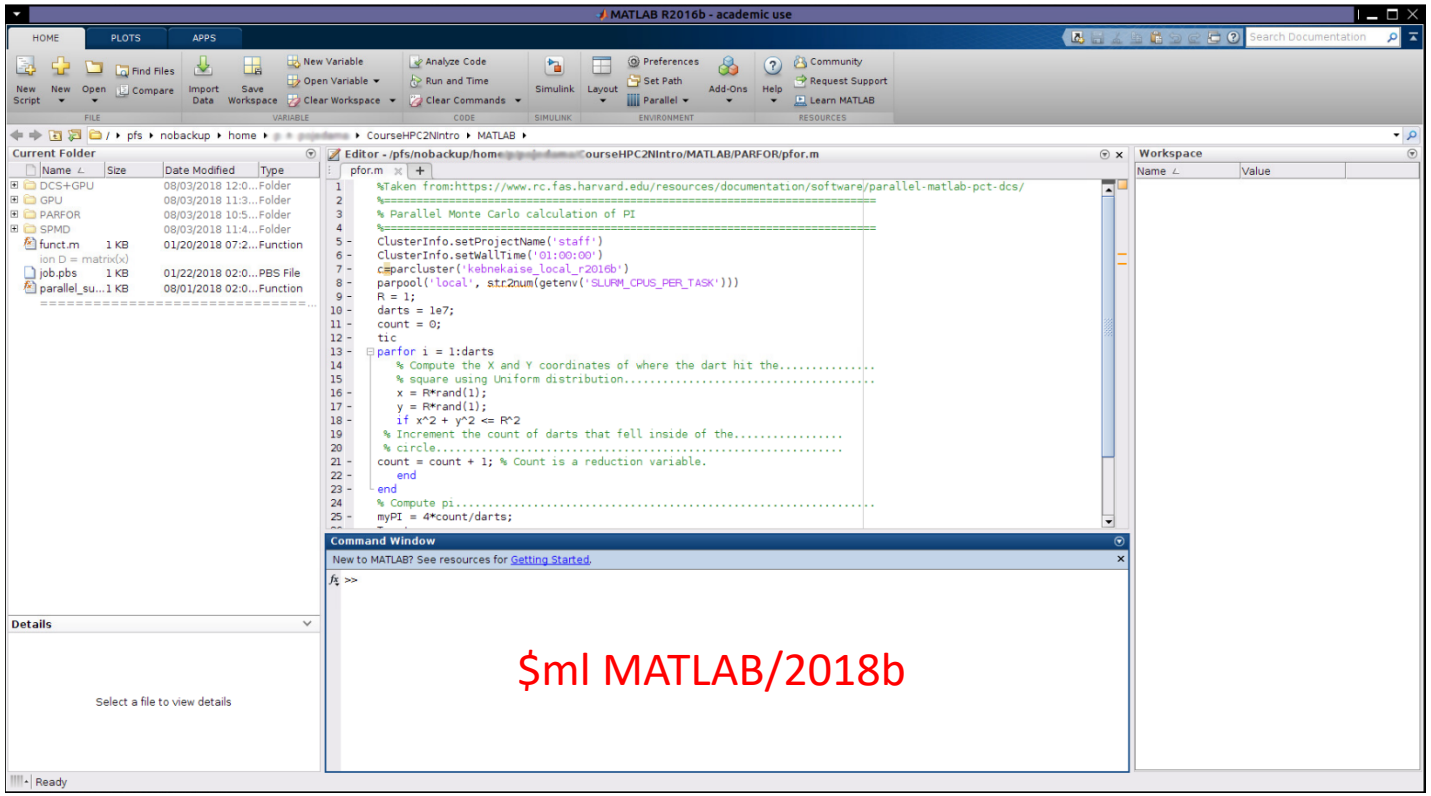
Example: Boosted classification model using “xgboost” (7 tunning parameters). Using R package on Kebnekaise (details: http://appliedpredictivemodeling.com/blog/2018/1/17/parallel-processing).





MATLAB

One needs to configure MATLAB the first time one uses it:
*MATLAB 2018b and later
(https://www.hpc2n.umu.se/resources/software/matlab)
(https://www.hpc2n.umu.se/resources/software/configure-matlab-2018)



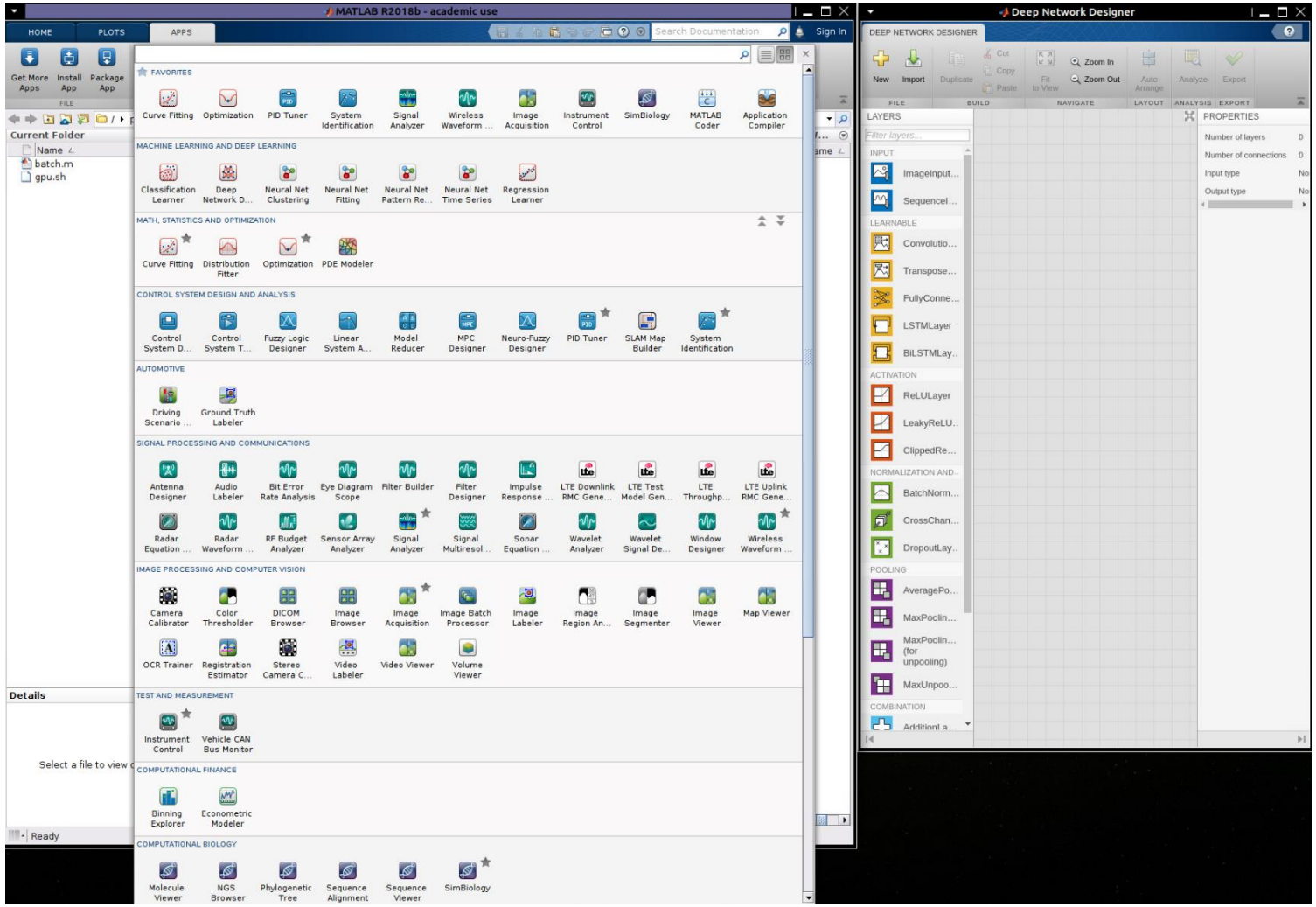
Please use the GUI just for lightweight tasks, otherwise use the batch queues.

Heavy jobs will be cancelled!

Start Matlab with:
matlab -singleCompThread

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

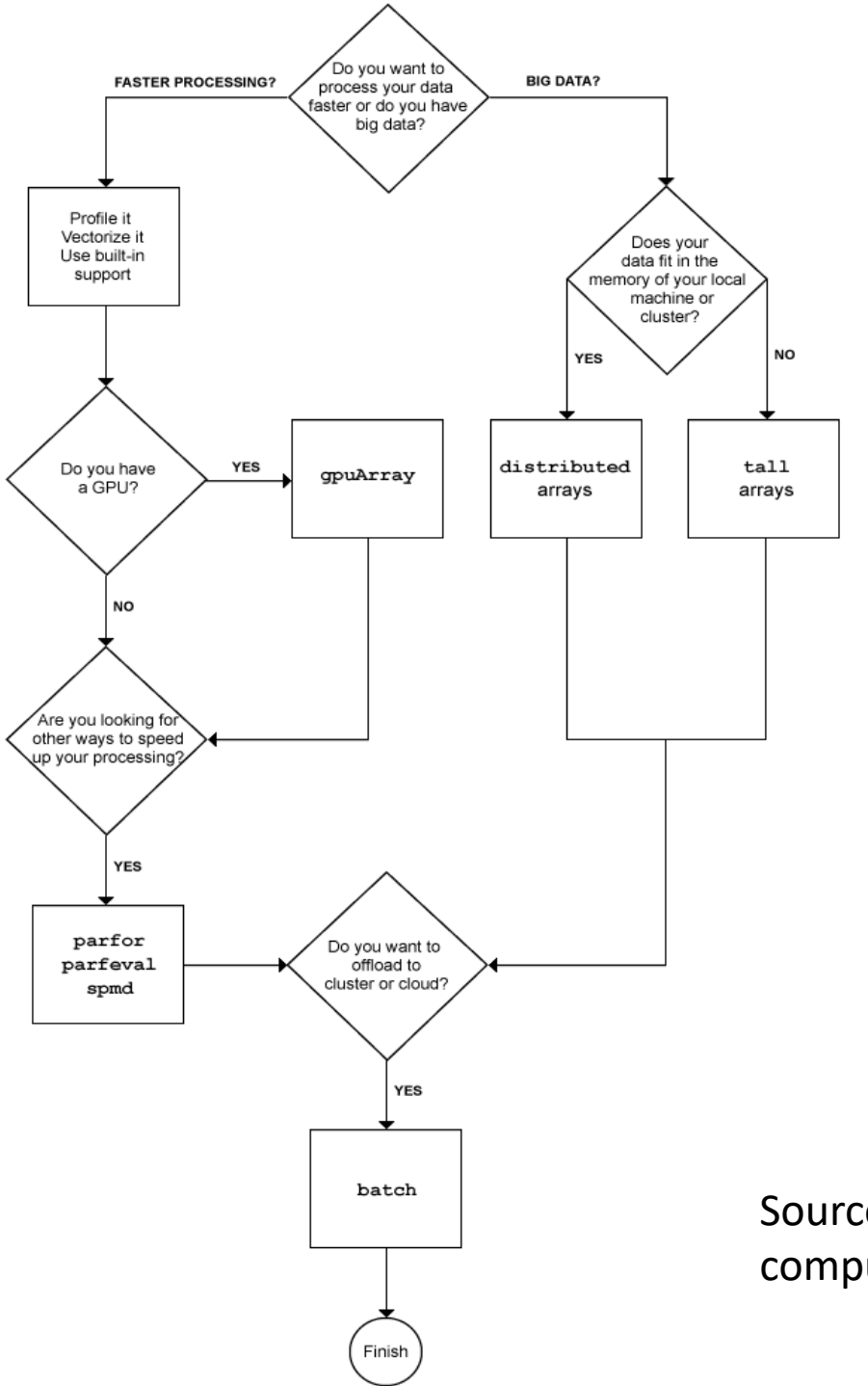
MATLAB



$ml MATLAB/2018b

Includes improved tools for Machine Learning and Deep Learning

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



Parallel computing tools in MATLAB

Source: https://se.mathworks.com/help/parallel-computing/choosing-a-parallel-computing-solution.html

MATLAB

- Parallel Computing Toolbox (PCT)
  - Parfor loops
  - Single Program Multiple Data, Labs are used to solve a task

- Distributed Computing Server (DCS)

Serial job

File name: funct.m

```
function D

format long
A1 = rand(10000,10000);
tic;
B1 = fft(A1);
time1 = toc;

filename = 'log.out';
mid=fopen(filename,'w');
fprintf(mid,'Time = %16.12f\n',time1);
fclose(mid);
```

```
#!/bin/bash
#SBATCH -A project_ID
#Asking for 10 min.
#SBATCH -t 00:10:00
#SBATCH -n 1
#SBATCH -p batch
#Load modules necessary for running MATLAB
ml MATLAB/2019b.Update2

srun matlab -nodisplay -singleCompThread -r
"funct;exit" > out.log

exit 0
```

Parfor

File name: pfor.m

```
parpool('local', str2num(getenv('SLURM_CPUS_PER_TASK')))
parfor i = 1:darts
x = rand(1);
y = rand(1);
  if x^2 + y^2 <= R^2
   count = count + 1; % reduction variable.
  end
end
```

Batch script:

```
#SBATCH -c 4
#SBATCH -p batch
#Load modules necessary for running MATLAB
ml MATLAB/2019b.Update2

srun matlab –nodisplay -r "pfor"
```

Timing

Nr. Workers	Time(sec)
1	26.43
2	17.17
3	11.82
4	7.71
28	1.82

Source: https://www.rc.fas.harvard.edu/resources/documentation/software/parallel-matlab-pct-dcs/

SPMD

File: spmdex.m

```
parpool('local', str2num(getenv('SLURM_CPUS_PER_TASK')))
% The expression that we wish to integrate:
f = @(x) 4./(1 + x.^2);
spmd
  % Choose a range over which to integrate based on my unique index:
  range_start     = (labindex - 1) / numlabs;
  range_end       = labindex / numlabs;
  % Calculate my portion of the overall integral
  my_integral     = quadl( f, range_start, range_end );
  % Aggregate the result by adding together each value of ?my_integral?
  total_integral  = gplus( my_integral );
end
total_int = total_integral{1};
fprintf('The computed value of pi is %8.7f.n',total_int);
delete(gcp);
```

```
#!/bin/bash
#SBATCH -A staff
#Asking for 10 min.
#SBATCH -t 00:10:00
#SBATCH -c 4
#SBATCH -p batch
#Load modules necessary for MATLAB
ml MATLAB/2019b.Update2


srun matlab -nodisplay -r "spmdex" > out.log
```

Source: https://se.mathworks.com/company/newsletters/articles/solving-large-scale-linear-algebra-problems-using-spmd-and-distributed-arrays.html

MATLAB+GPU

On the MATLAB GUI:

```
c = parcluster;
ClusterInfo.setProjectName('staff');
ClusterInfo.setWallTime('00:10:00');
% Tell the scheduler that you want to use the GPUs
ClusterInfo.setUseGpu(true)
% number of GPUs per node to use
ClusterInfo.setGpusPerNode(2)
ClusterInfo.setUserDefinedOptions('--gres=gpu:k80:2,mps')
%gpuDevice

j = c.batch(@parallelex, 1, {1}, 'pool', 2);
```

File: parallelex.m

```
function speedUp = parallel(x)
format long
A1 = rand(10000,10000);
tic;
B1 = fft(A1);
time1 = toc;


A2 = gpuArray(A1);
tic;
B2 = fft(A2);
time2 = toc;

speedUp = time1/time2;
end
```

MATLAB+GPU

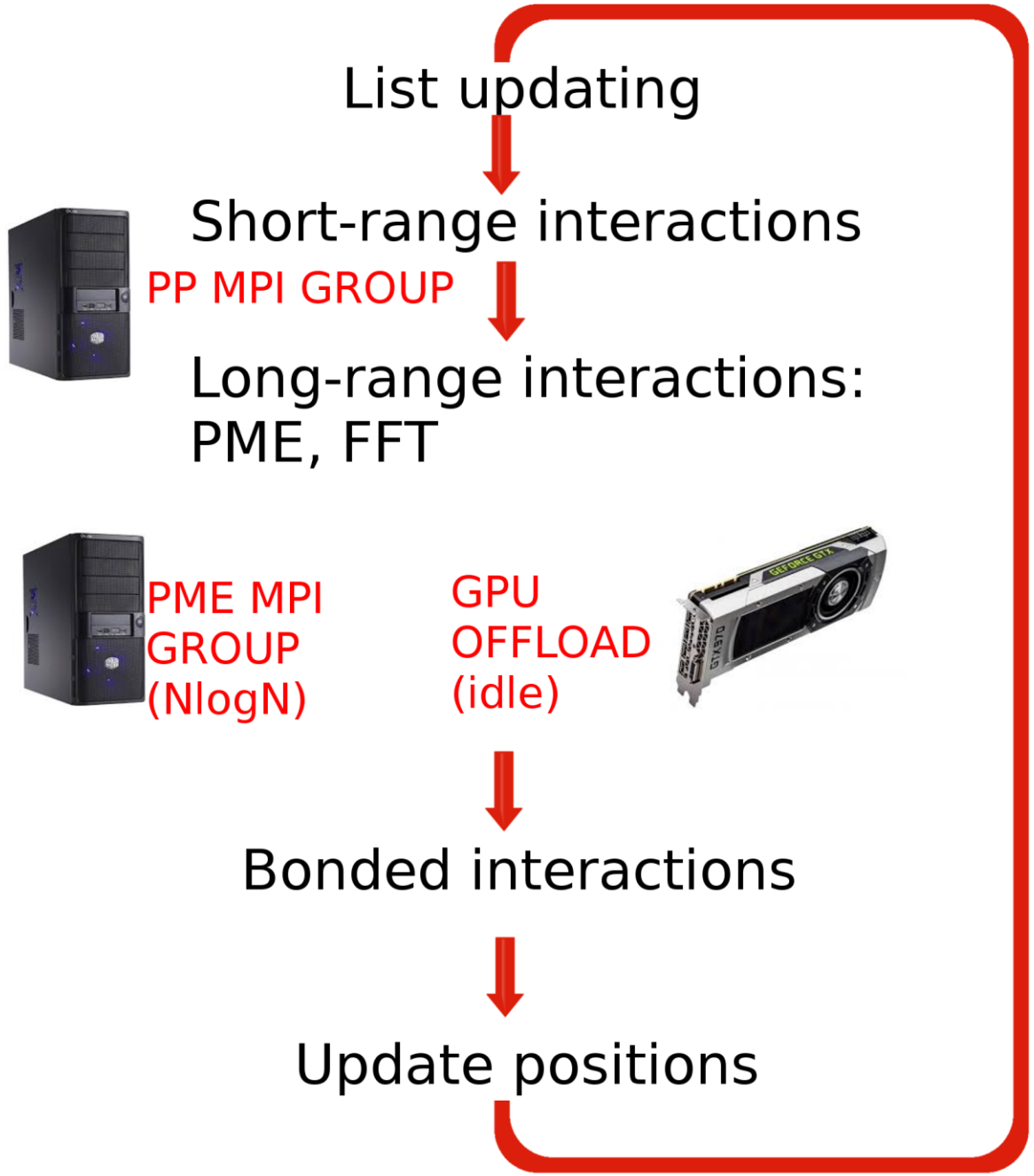
Using a batch file: gpu.sh

```
#!/bin/bash
#SBATCH -A staff
#Asking for 10 min.
#SBATCH -t 00:10:00
#SBATCH -N 1
#SBATCH -n 1
#SBATCH --gres=gpu:k80:2
#SBATCH -p batch
#SBATCH --exclusive
#Load modules necessary for running MATLAB
ml MATLAB/2019b.Update2
srun matlab -nodisplay -singleCompThread -r "parallelex" > test_parallel.log
```

File: parallelex.m

```
function speedUp = parallel(x)
format long
A1 = rand(10000,10000);
tic;
B1 = fft(A1);
time1 = toc;


A2 = gpuArray(A1);
tic;
B2 = fft(A2);
time2 = toc;

speedUp = time1/time2;
end
```

MD Codes


List updating
Short-range interactions
PP MPI GROUP
Long-range interactions:
PME, FFT
PME MPI
GROUP
(NlogN)
GPU
OFFLOAD
(idle)
Bonded interactions
Update positions

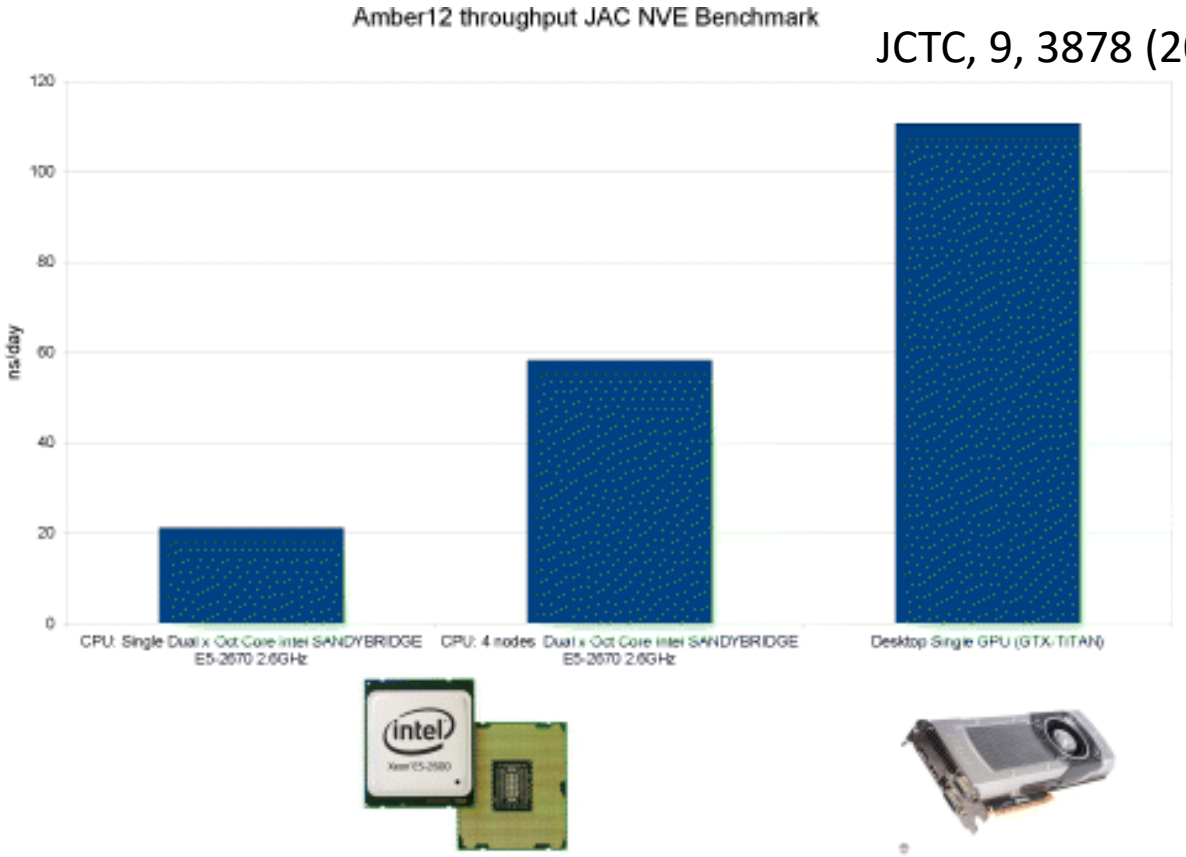
Benchmark

- Solvated protein
- 158945 atoms
- 1.2 nm cutoff radius
- 1 fs time step
- PME for electrostatics

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)


```
module load icc/2017.1.132-GCC-5.4.0-2.26  CUDA/8.0.44
impi/2017.1.132
module load ifort/2017.1.132-GCC-5.4.0-2.26  CUDA/8.0.44
ml Amber/16-AmberTools-16-patchlevel-20-7-hpc2n
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, …):

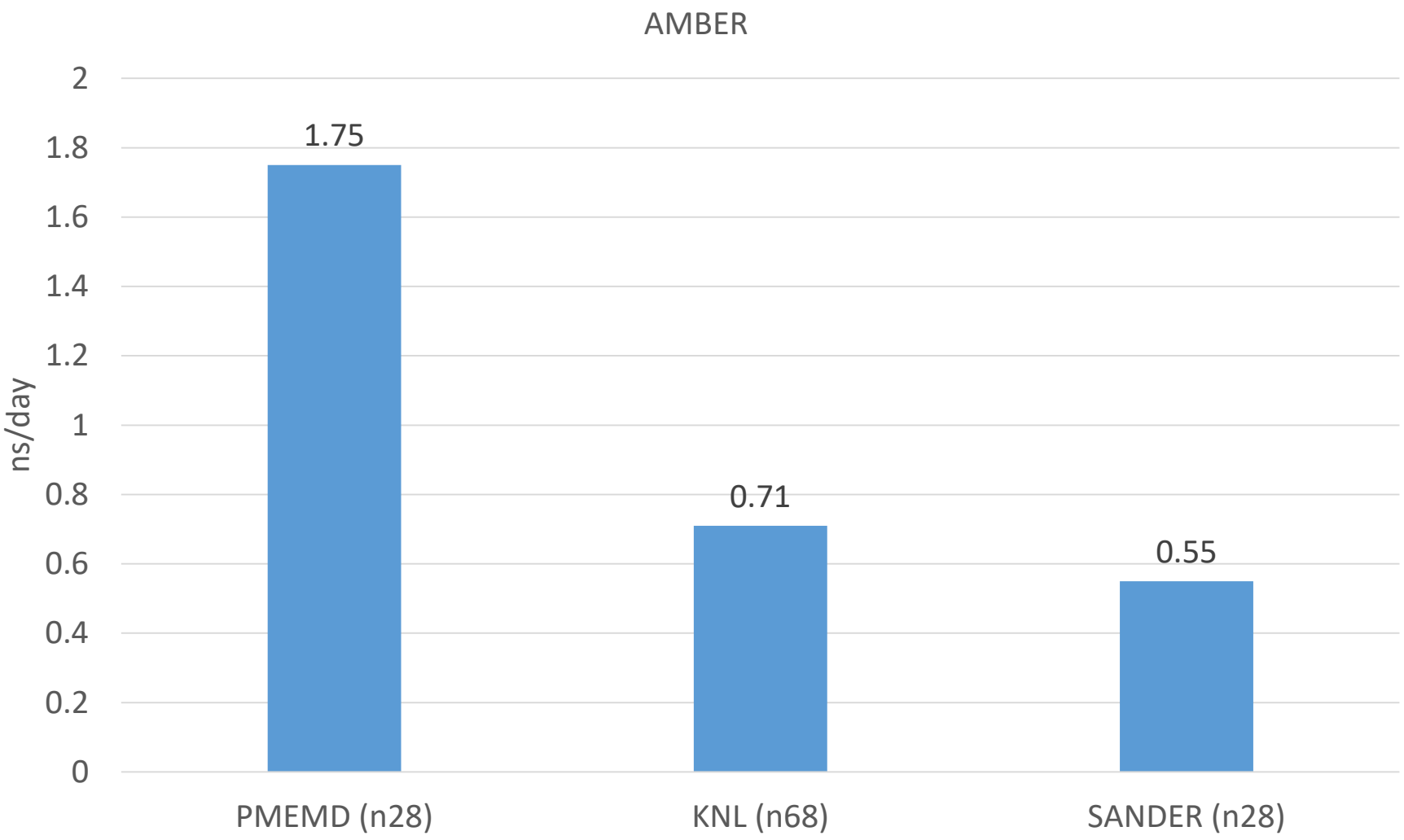
Load the modules:

$ml icc/2017.4.196-GCC-6.4.0-2.28 ifort/2017.4.196-GCC-6.4.0-2.28 impi/2017.3.196
$ml Amber/16-AmberTools-17-patchlevel-8-12

On the command line:

$tleap, antechamber, cpptraj, …

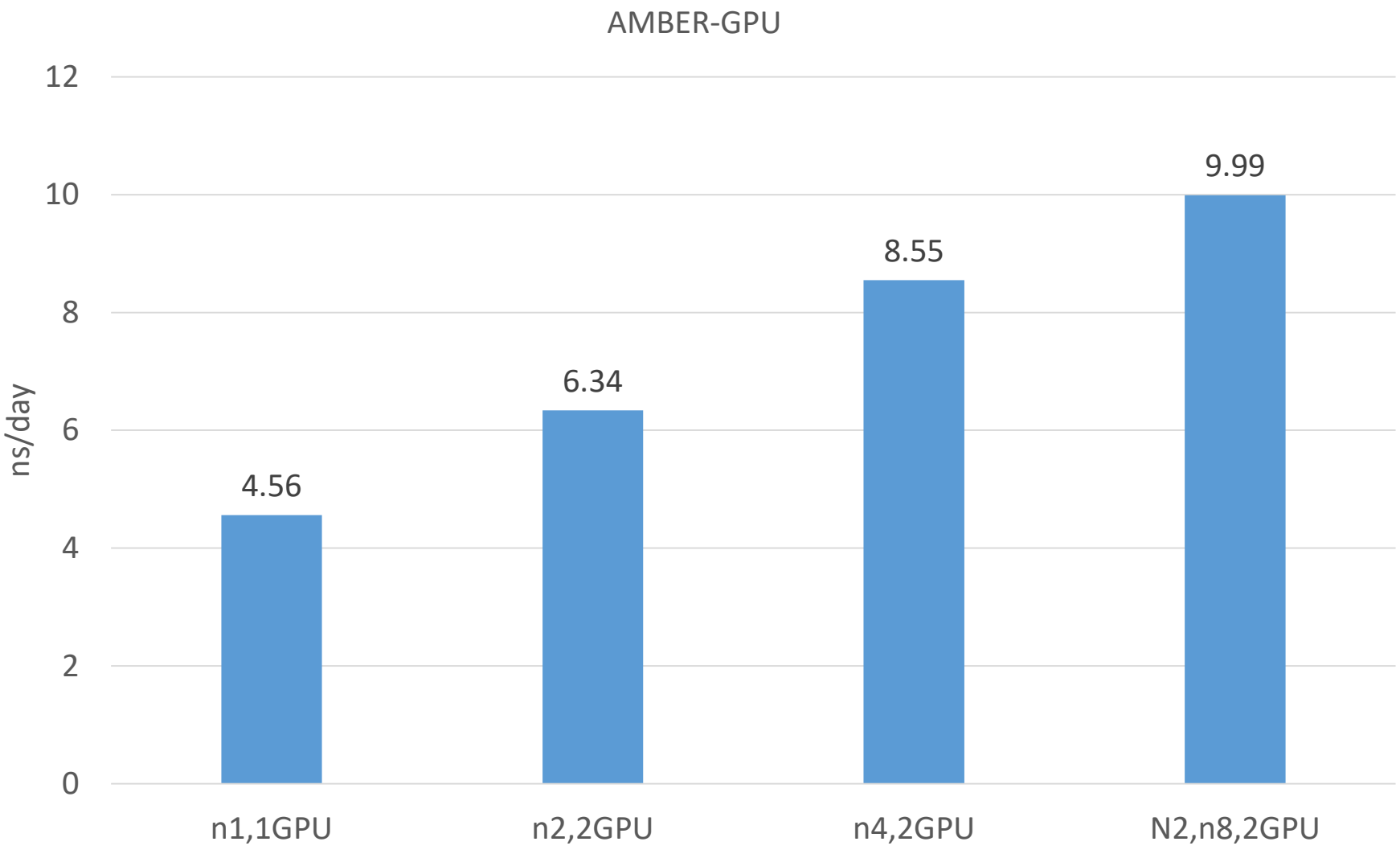
AMBER


AMBER
ns/day
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
1.75
0.71
0.55
PMEMD (n28)
KNL (n68)
SANDER (n28)

AMBER

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

Notice that, the remaining CPUs are not used.



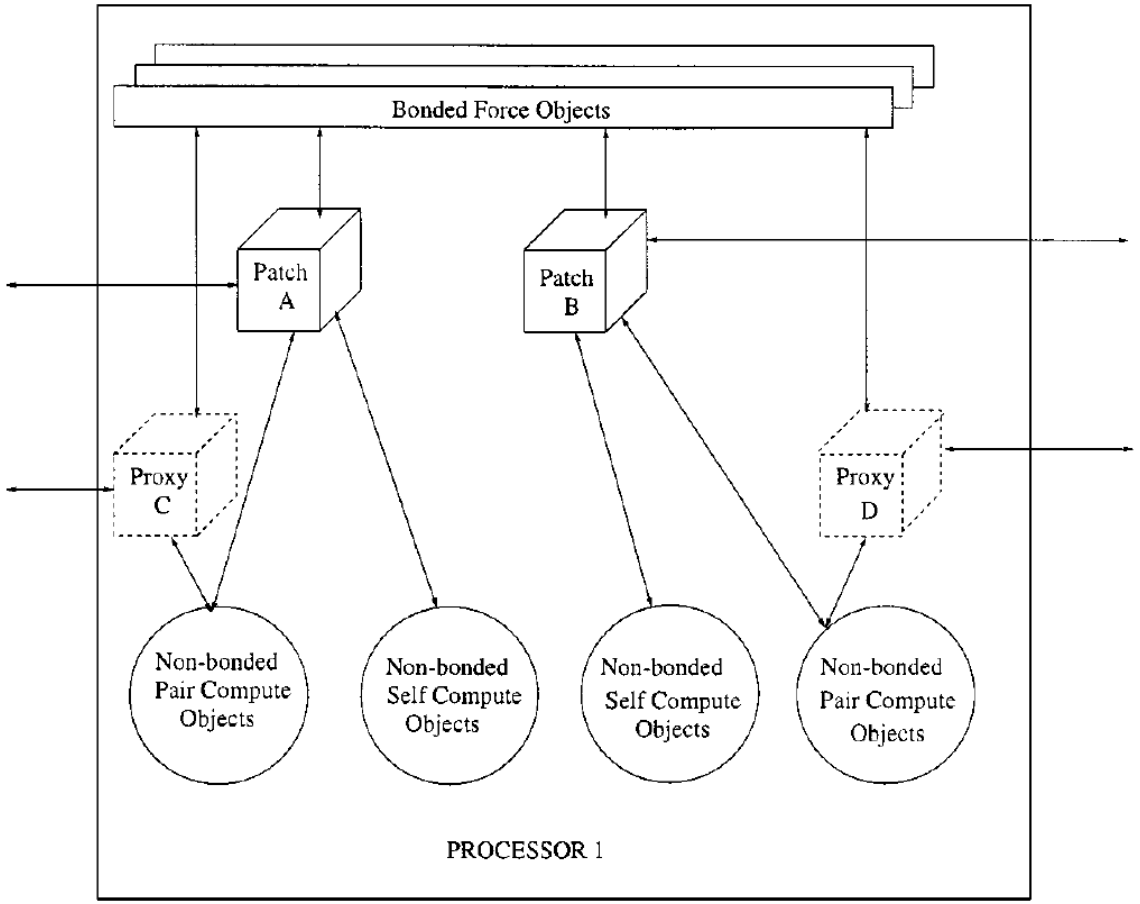
Comment on the CUDA version

- AMBER-CUDA does all computations on the GPUs. Thus, the remaining cores remain idle. One can use those cores by launching an additional MPI simulation:

```
#!/bin/bash
#SBATCH -N 1
#SBATCH -n 28
#SBATCH --gres=gpu:k80:2
#Load the AMBER-CUDA version

export init="step3_charmm2amber"
export pstep="step4.0_minimization"
export istep="step4.1_equilibration"
mpirun -np 4 pmemd.cuda.MPI -O -i ${istep}.mdin -p ${init}.parm7 -c ${pstep}.rst7 -o ${istep}.mdout -r ${istep}.rst7 -inf
${istep}.mdinfo -ref ${init}.rst7 -x ${istep}.nc &

export istep2="step4.1_equilibration_parall"
mpirun -np 24 pmemd.MPI -O -i ${istep2}.mdin -p ${init}.parm7 -c ${pstep}.rst7 -o ${istep2}.mdout -r ${istep2}.rst7 -inf
${istep2}.mdinfo -ref ${init}.rst7 -x ${istep2}.nc &

wait
```

NAMD

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



JCC, 151, 283 (1999)

NAMD (SMP)

```
#!/bin/bash
#SBATCH -A staff
#Asking for 10 min.
#SBATCH -t 00:50:00
#Number of nodes
#SBATCH -N 1
#Ask for 28 processes
#SBATCH -n 28
#SBATCH --exclusive
#Load modules necessary for running NAMD
module add icc/2017.1.132-GCC-6.3.0-2.27 impi/2017.1.132
module add NAMD/2.12-nompi
#Execute NAMD
namd2 +p 28 +setcpuaffinity step4_equilibration.inp > output_smp.dat
```

NAMD (GPU) (single node)

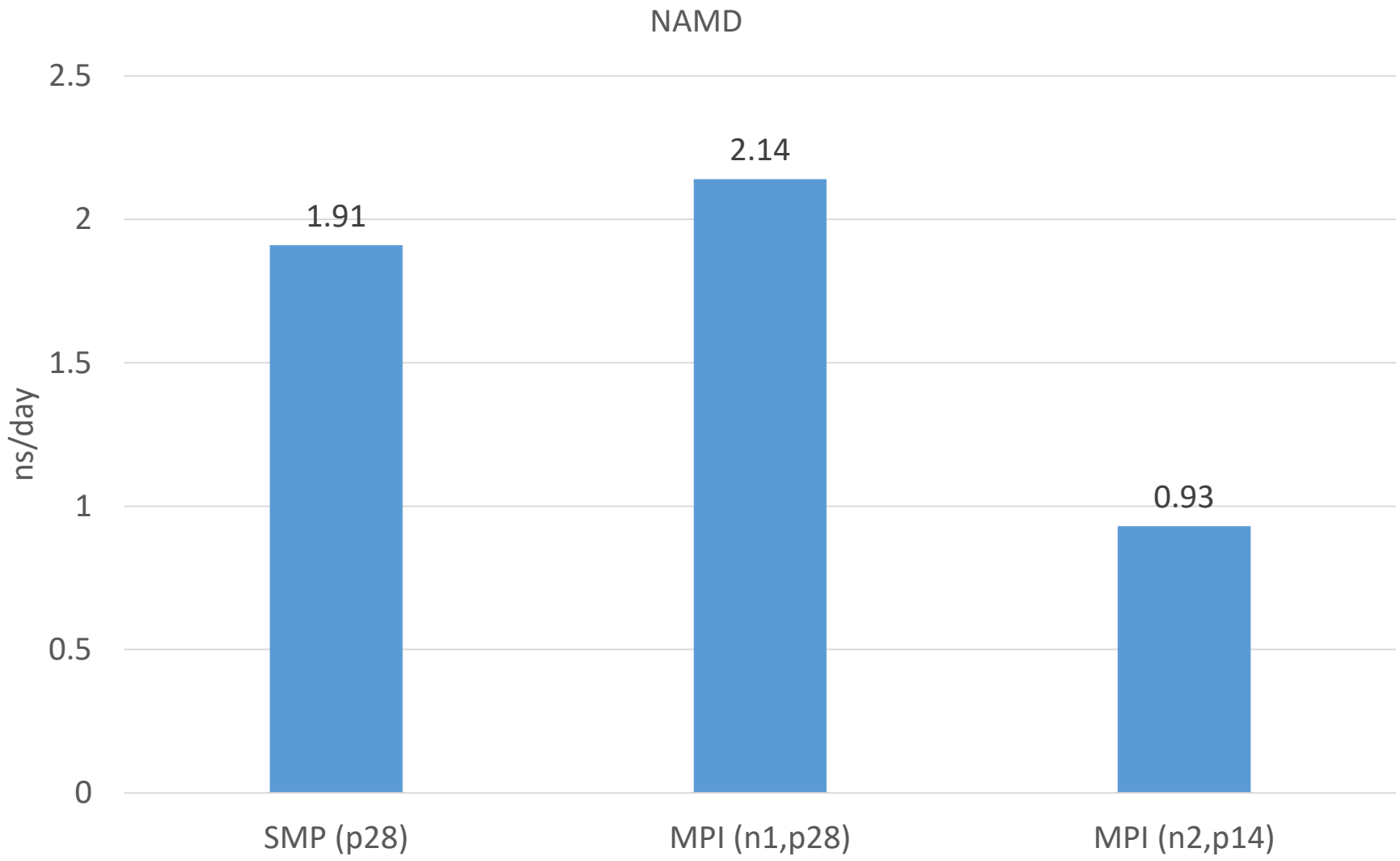
```
#!/bin/bash
#SBATCH -A staff
#SBATCH -t 00:50:00
#SBATCH -N 1
#SBATCH -n 28
#SBATCH –exclusive
#Ask for 2 GPU cards
#SBATCH --gres=gpu:k80:2
#Load modules necessary for running NAMD
module add GCC/5.4.0-2.26  CUDA/8.0.61_375.26  OpenMPI/2.0.2
module add NAMD/2.12-nompi
#Execute NAMD
namd2 +p 28 +setcpuaffinity step4_equilibration.inp > output_smp.dat
```

NAMD

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

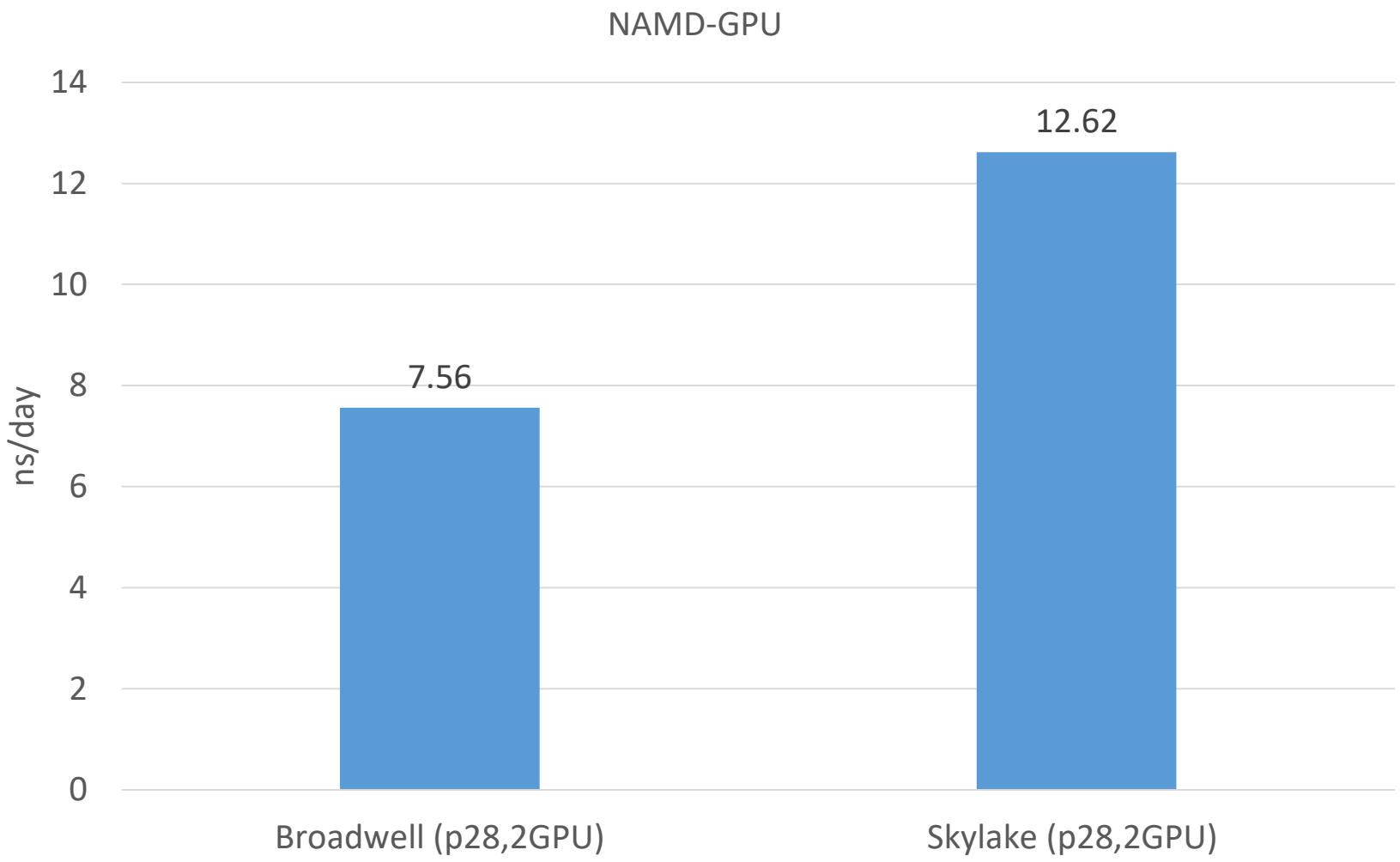
NAMD

Use the +setcpuaffinity flag for a 10% speedup



NAMD

With the new Volta GPU cards one can speed up the simulation by 1.66x



GROMACS

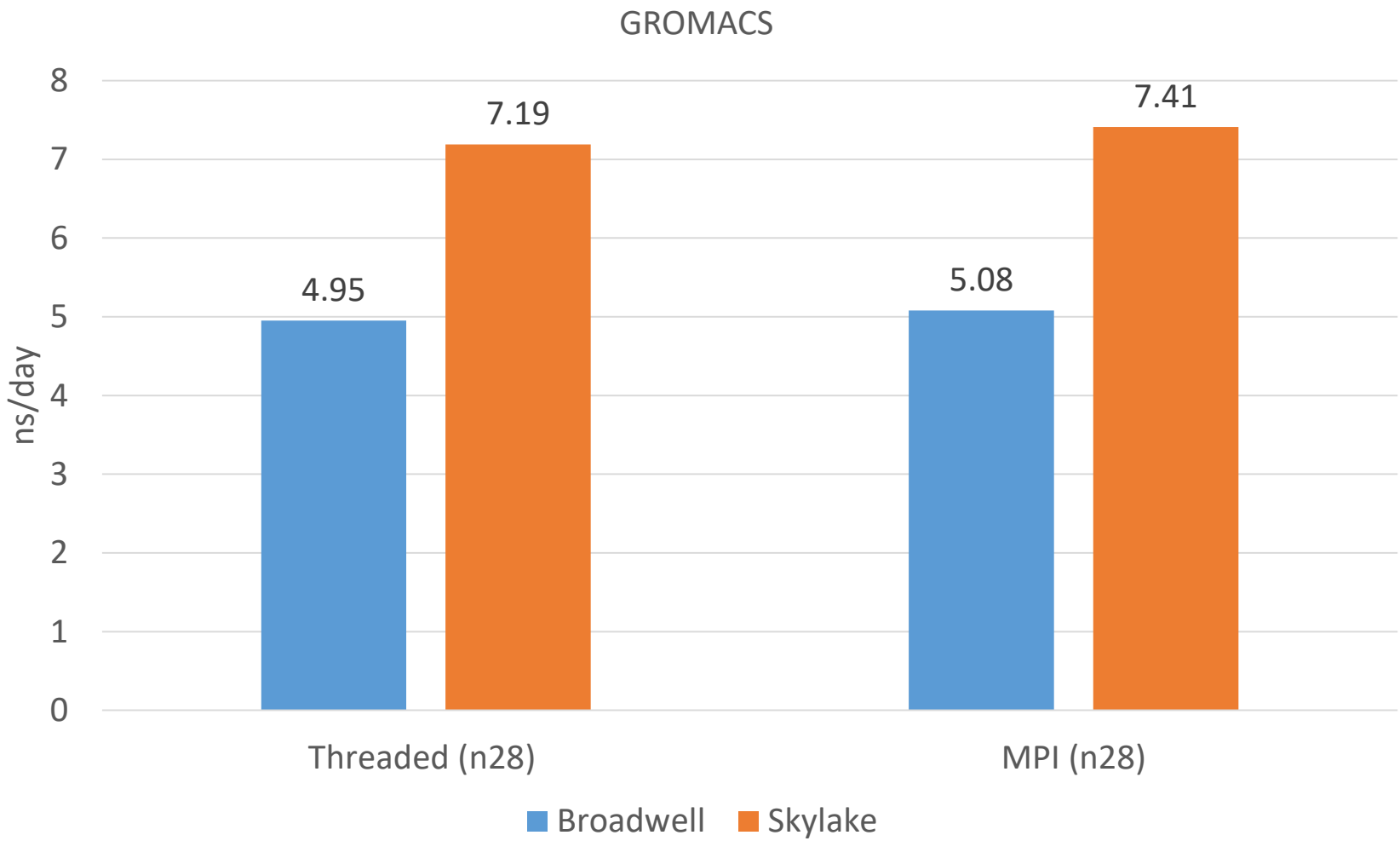
```
#SBATCH -n 4
#SBATCH -c 7
# Asking for 2 GPUs
#SBATCH --gres=gpu:k80:2
#SBATCH -p batch

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

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

srun -n $SLURM_NTASKS 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

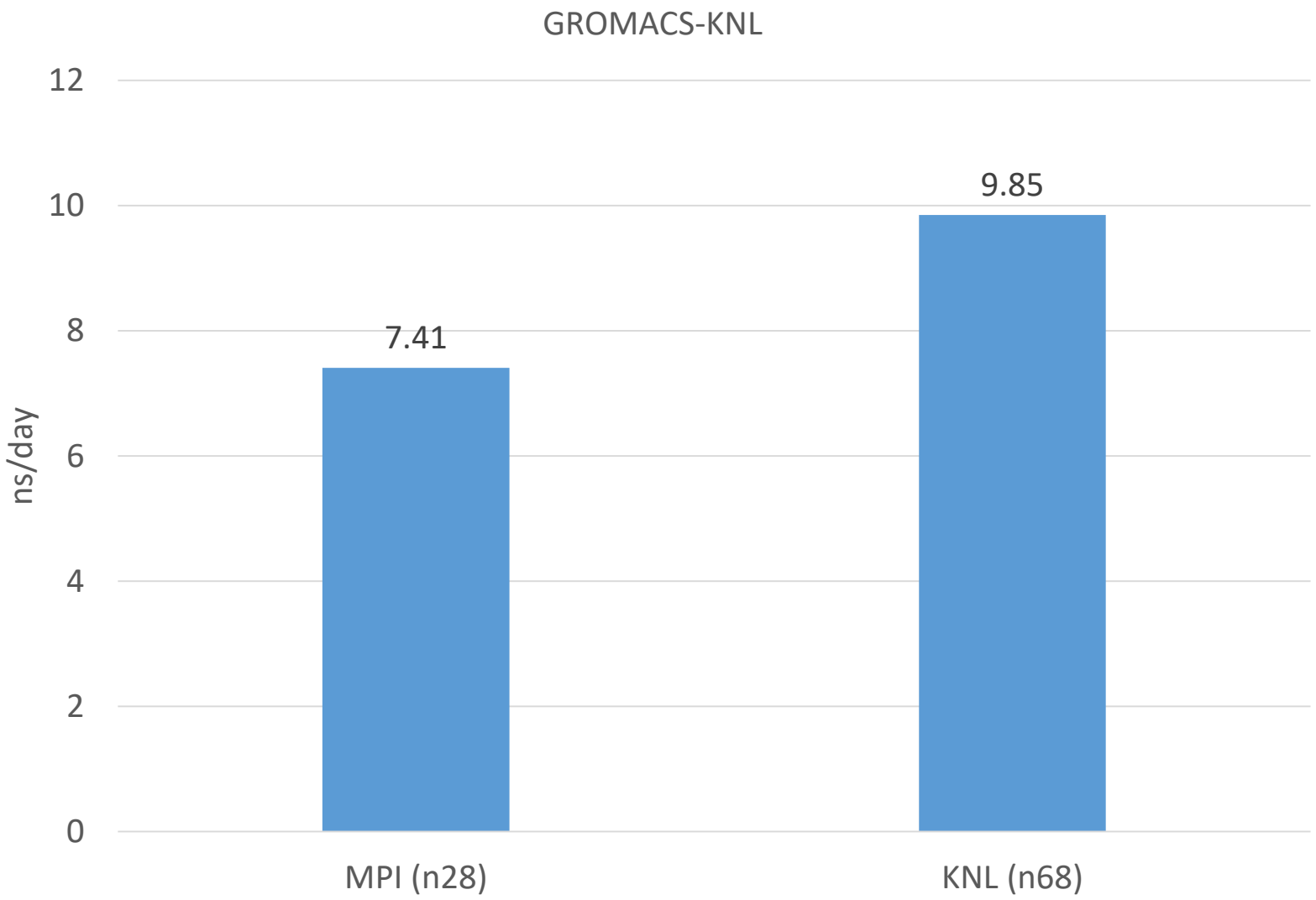

GROMACS
ns/day
8
7
6
5
4
3
2
1
0
4.95
7.19
5.08
7.41
Threaded (n28)
MPI (n28)
Broadwell
Skylake

GROMACS KNL

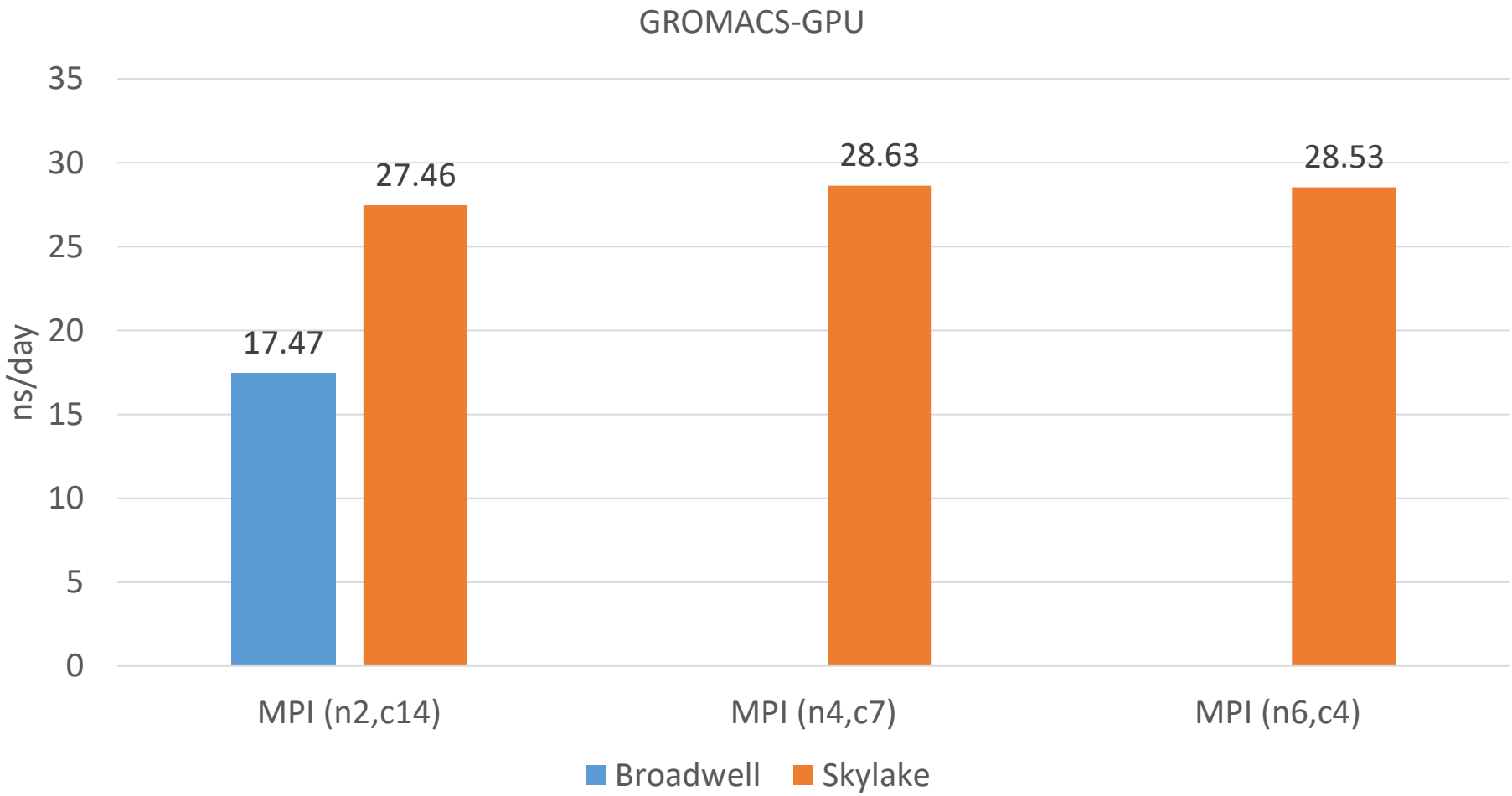
```
#!/bin/bash
#SBATCH -A project_ID
#SBATCH -t 00:50:00
#SBATCH -N 1
#SBATCH -n 68
#SBATCH -p knl
#SBATCH --constraint=cache,quad
#SBATCH --exclusive

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_equilibration
```

GROMACS KNL

- Login to kebnekaise-knl.hpc2n.umu.se and submit your script from there
- KNL queue is most of the time available compared to GPU one



GROMACS


GROMACS-GPU
35
30
25
20
15
10
5
0
ns/day
17.47
27.46
28.63
28.53
MPI (n2,c14)
MPI (n4,c7)
MPI (n6,c4)
Broadwell
Skylake

GROMACS

- PLUMED, threaded MPI version is not supported.

Instead of:

gmx mdrun –ntmpi X

Use:

mpirun gmx_mpi …

- Avoid writing energies

- Offloading features starting from 2018 version

https://www.hpc2n.umu.se/events/courses/md-course-spring-2019

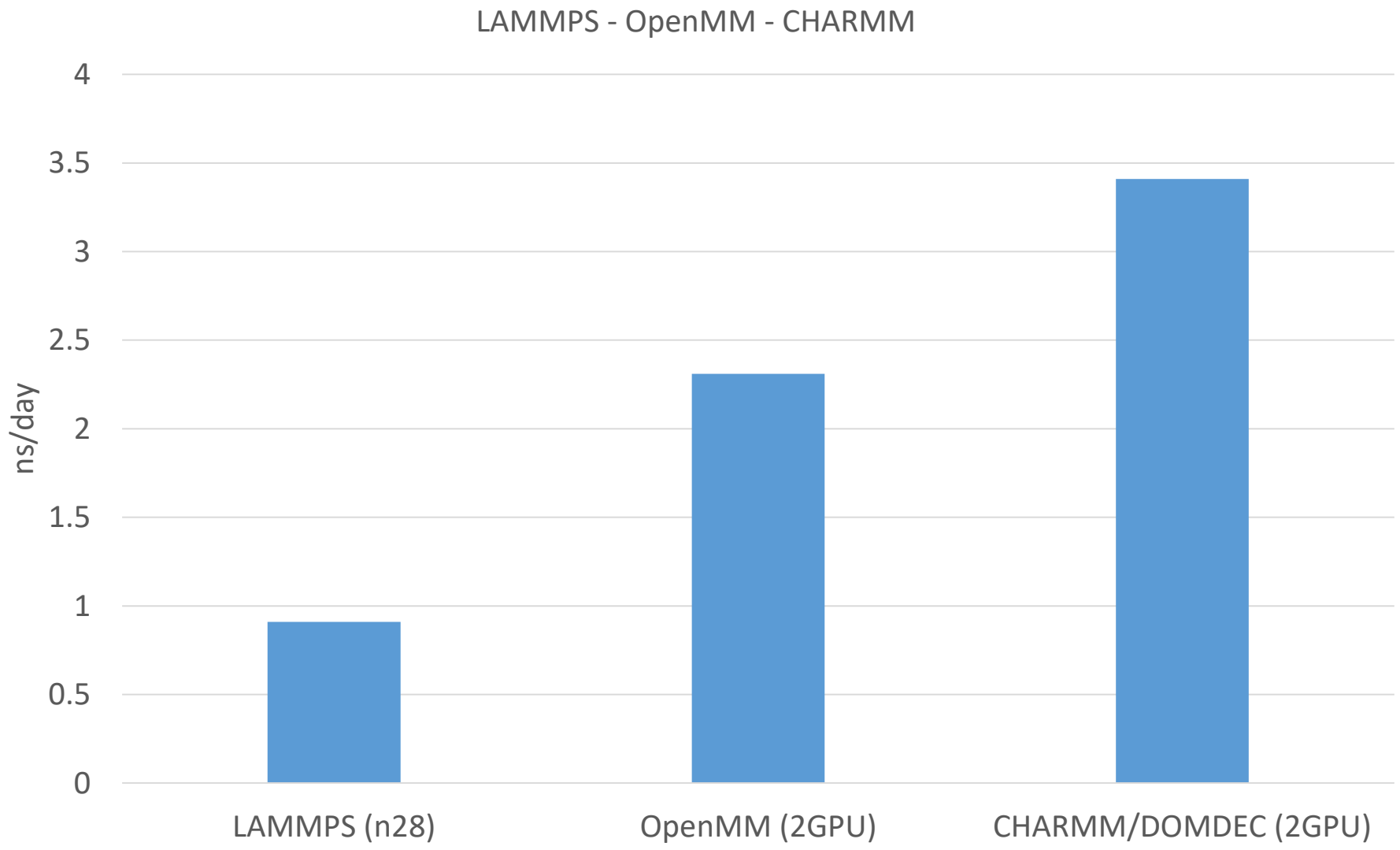
LAMMPS (MPI)

```
#!/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

#Load modules necessary for running LAMMPS
module load icc/2017.1.132-GCC-6.3.0-2.27 ifort/2017.1.132-GCC-6.3.0-2.27
impi/2017.1.132
module load LAMMPS/31Mar17

#Execute LAMMPS
srun lmp_intel_cpu -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

#Load modules necessary for running LAMMPS
module load icc/2017.1.132-GCC-6.3.0-2.27 ifort/2017.1.132-GCC-6.3.0-2.27
impi/2017.1.132
module load LAMMPS/31Mar17
export OMP_NUM_THREADS=2
#Execute LAMMPS
srun lmp_intel_cpu -in step4.1_equilibration.inp
```

LAMMPS - OpenMM - CHARMM



Scratch directory

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

```
rm -rf /scratch/test
export parent=/pfs/nobackup/home/u/username/benchmarks/
mkdir /scratch/test
rsync -avzh $parent/ /scratch/test/

cd /scratch/test

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

cd $parent
rsync -avzh /scratch/test/ $parent/

rm -rf /scratch/test
```

~10-15% speedup

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

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 your simulation scaling properly?
- Is the cutoff radius for long-range interactions appropriate? PME (gmx tune_pme for GROMACS)?

Tensorflow

```
#!/usr/share/python

import tensorflow as tf
hello = tf.constant('Hello, TensorFlow!')
sess = tf.Session()
print(sess.run(hello))
```

```
#!/bin/bash
#SBATCH -A staff
#SBATCH -t 00:50:00
#SBATCH -N 1
#SBATCH --exclusive
#SBATCH --gres=gpu:k80:2

ml icc/2017.1.132-GCC-5.4.0-2.26
ml ifort/2017.1.132-GCC-5.4.0-2.26
mlCUDA/8.0.44  impi/2017.1.132
ml Python/3.6.1
ml Tensorflow/1.3.0-Python-3.6.1
python tensor.py
```

```
name: Tesla K80
major: 3 minor: 7 memoryClockRate (GHz) 0.8235
pciBusID 0000:0f:00.0
Total memory: 11.17GiB
Free memory: 11.10GiB
2017-12-05 17:13:03.555397: W
Found device 1 with properties:
name: Tesla K80
>>> print(sess.run(hello))
b'Hello, TensorFlow!'
```

Tensorflow

```
#!/usr/share/python
import tensorflow as tf

#Parameters
W = tf.Variable([.3],tf.float32)
b = tf.Variable([-.3],tf.float32)
#Input and output
x = tf.placeholder(tf.float32)
linear_model = W*x+b
y = tf.placeholder(tf.float32)

#Loss
square_delta = tf.square(linear_model-y)
loss = tf.reduce_sum(square_delta)
#Optimize
optimizer = tf.train.GradientDescentOptimizer(0.01)
train = optimizer.minimize(loss)

init = tf.global_variables_initializer()
sess = tf.Session()
sess.run(init)

for i in range (1000):
   sess.run(train,{x:[1,2,3,4],y:[0,-1,-2,-3]})

print(sess.run([W,b]))
```

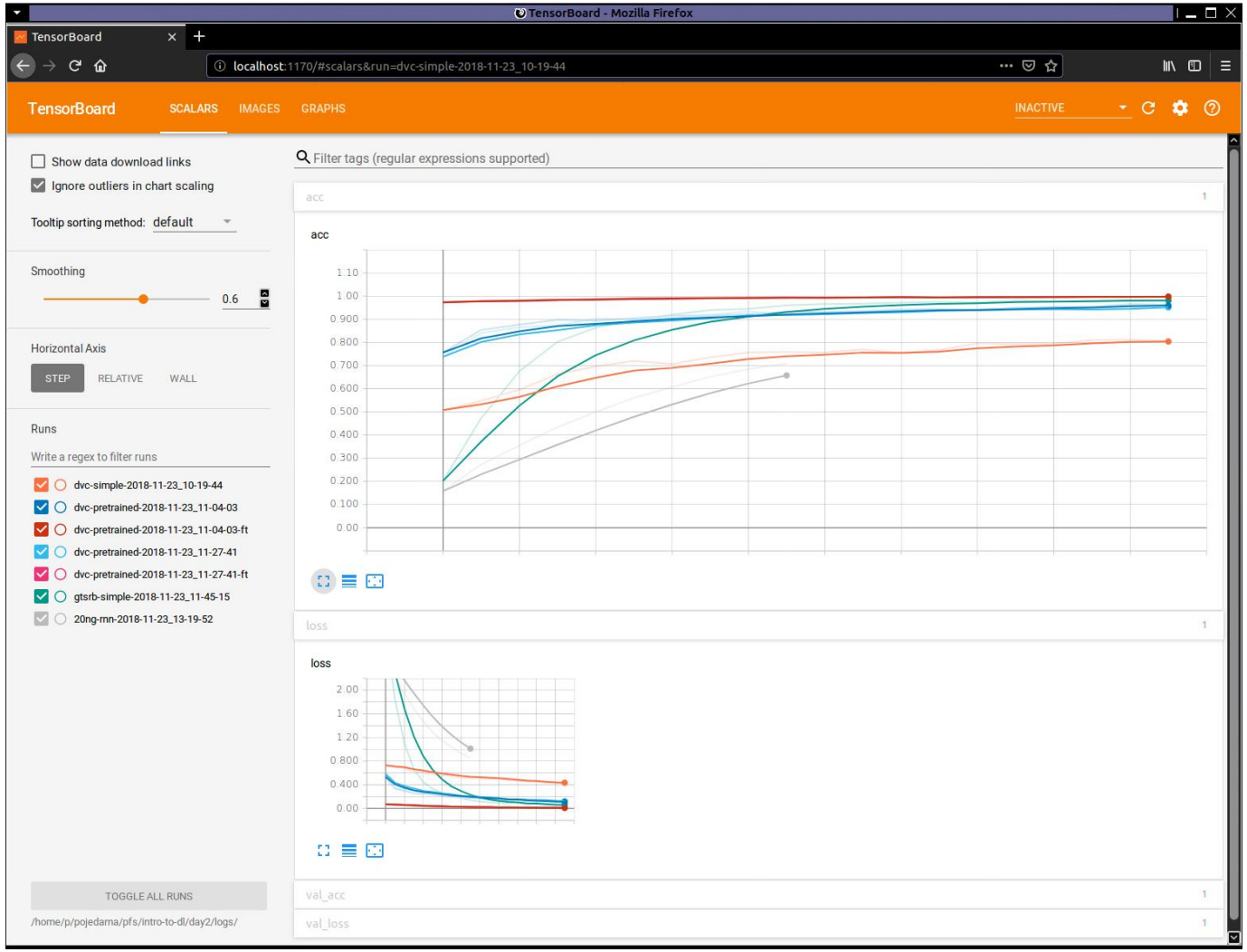
Computing the loss

name: Quadro K6000
major: 3 minor: 5 memoryClockRate (GHz) 0.9015
pciBusID 0000:06:00.0
Total memory: 11.92GiB
Free memory: 11.82GiB
Creating TensorFlow device (/gpu:0) -> (device: 0, name: Quadro K6000, pci bus id: 0000:06:00.0)

[array([-0.9999969], dtype=float32), array([0.99999082], dtype=float32)]

Tensorflow+Tensorboard

```
module load GCC/7.3.0-2.30  CUDA/9.2.88  OpenMPI/3.1.1     #On the command line execute these instructions
module load TensorFlow/1.10.1-Python-2.7.15 Keras/2.2.2-Python-2.7.15
tensorboard --logdir=/home/p/<path-to-directory>/logs --port=1170
```



To monitor the behavior of you jobs open a web browser and type:

localhost:1170

GAUSSIAN+GPU

Initial input file:

```
$more input_bk.com
%chk=geom_optim.chk
%mem=16GB
#UB3LYP/6-31+G(d) OPT=(ModRedun) SCF=(MaxCycle=256) pop=none NoSymm

45 atoms structure, RESP

+5 15
O       3.744336        -1.126487       6.111505
P       2.893853        -1.251776       4.246949
O       4.150424        -3.154051       4.078061
```

Corrected input file:

```
$more input.com
%cpu=0,1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27
%gpucpu=0-3=0,7,14,21
%chk=geom_optim.chk
%mem=16GB
#UB3LYP/6-31+G(d) OPT=(ModRedun) SCF=(MaxCycle=256) pop=none NoSymm
```

```
#!/bin/bash
#SBATCH -A staff
#SBATCH -N 1
#SBATCH -c 28
#SBATCH --exclusive
#SBATCH --gres=gpu:k80:2
#SBATCH --time=00:10:00

module add gaussian/16.A.03-AVX2
# Assume that the job file are located
g16.set-cpu+gpu-list input.com
time g16 input
```

Integral=(FineGrid,Acc2E=10) Constants=2006

VASP

Batch script:

#SBATCH -c 10 (number of cores per task)
#SBATCH -n 1 (number of tasks)

ml ifort/2017.1.132-GCC-6.3.0-2.27 OpenMPI/2.0.2
ml NWChem/6.6.revision27746-2015-10-20-Python-2.7.12

mpirun -n 10 nwchem input.nw (this script will fail)

VASP

Batch script:

#SBATCH -c 1 (number of cores per task)
#SBATCH -n 10 (number of tasks)

ml ifort/2017.1.132-GCC-6.3.0-2.27 OpenMPI/2.0.2
ml NWChem/6.6.revision27746-2015-10-20-Python-2.7.12

mpirun -n 10 nwchem input.nw (this script is correct!)

Suggestions

- One common issue with Comp. Chem. Software is related to the available memory. A possible solution is to request a larger number of cpus (with –n or –c in SLURM) but make use of less than that number.

Final comments

- 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 number of cores/nodes you request optimal? Trying a short simulation could help.
- Is your simulation scaling well?
- Could KNL nodes speed up your workflow?
- Use job-usage script on the command line

Final comments

- 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.
- Avoid using SLURM batch scripts from other centers, use those provided in our web site.
- Don’t load modules in your *.bashrc* file, this can caused troubles with software.
- Don’t forget to cite HPC2N and the SNIC project upon publishing.