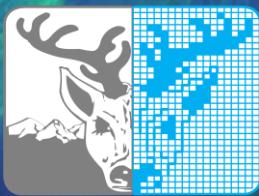


# High Performance Computing Center North (HPC2N)

Pedro Ojeda-May

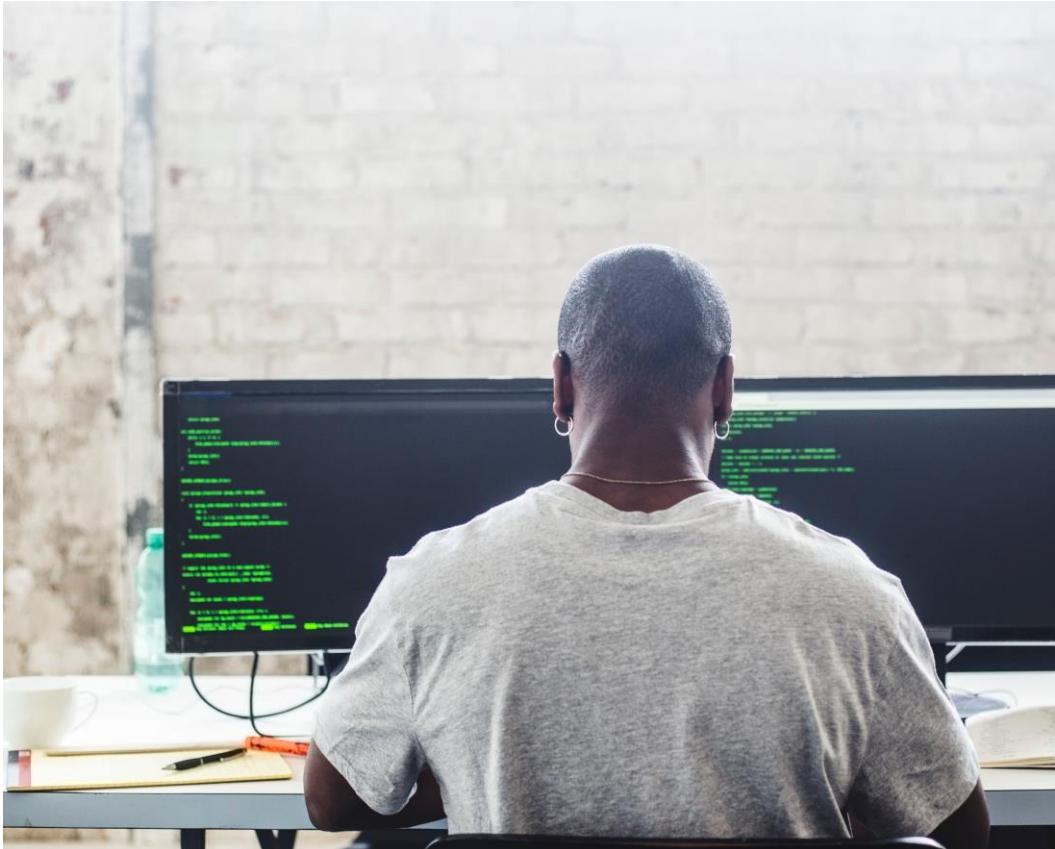


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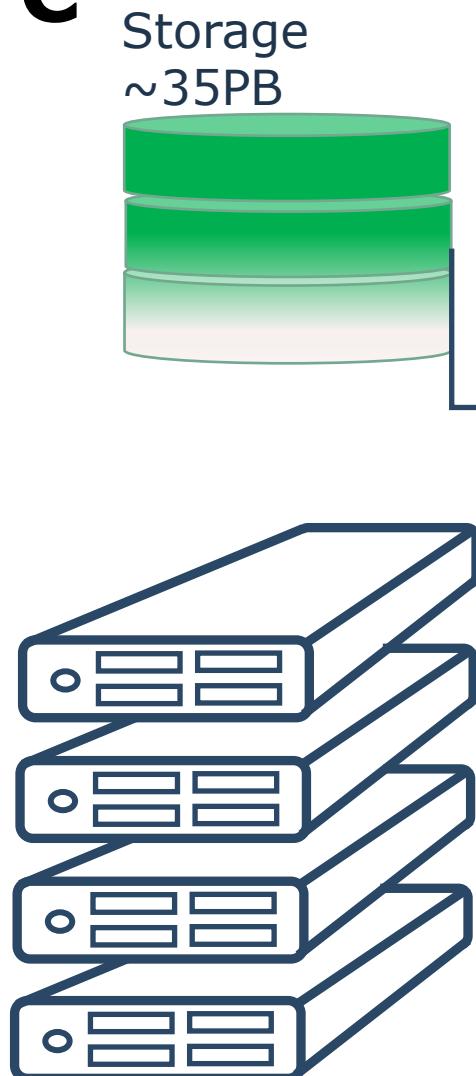
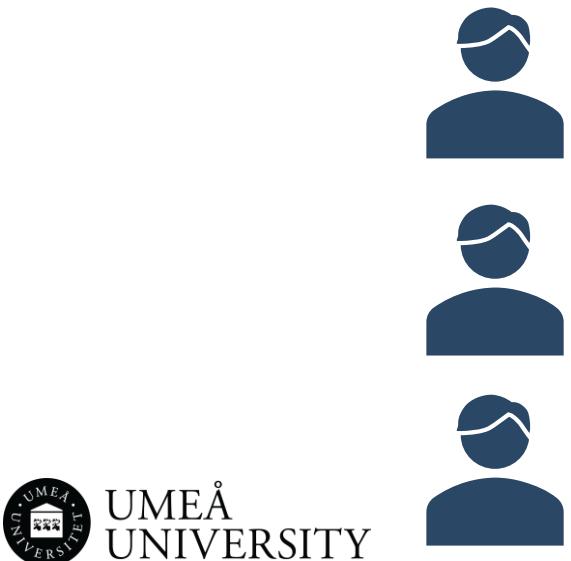
# HPC2N in a nutshell

- HPC2N is a local/regional resource for researchers at HPC2N's partners (IRF, LTU, Mittuniversitetet, SLU and UmU)  
*The local project/resources are independent of the national ones*
- Director of HPC2N: Prof. Paolo Bientinesi at Computing Science Dept.
- Training courses: Molecular Dynamics, QM/MM, Git, R, ML, MPI, OpenMP, Containers (Singularity/Aptainer)
- General support (ticket system)
- Advanced support, specific questions from researchers

# Workflow on a PC

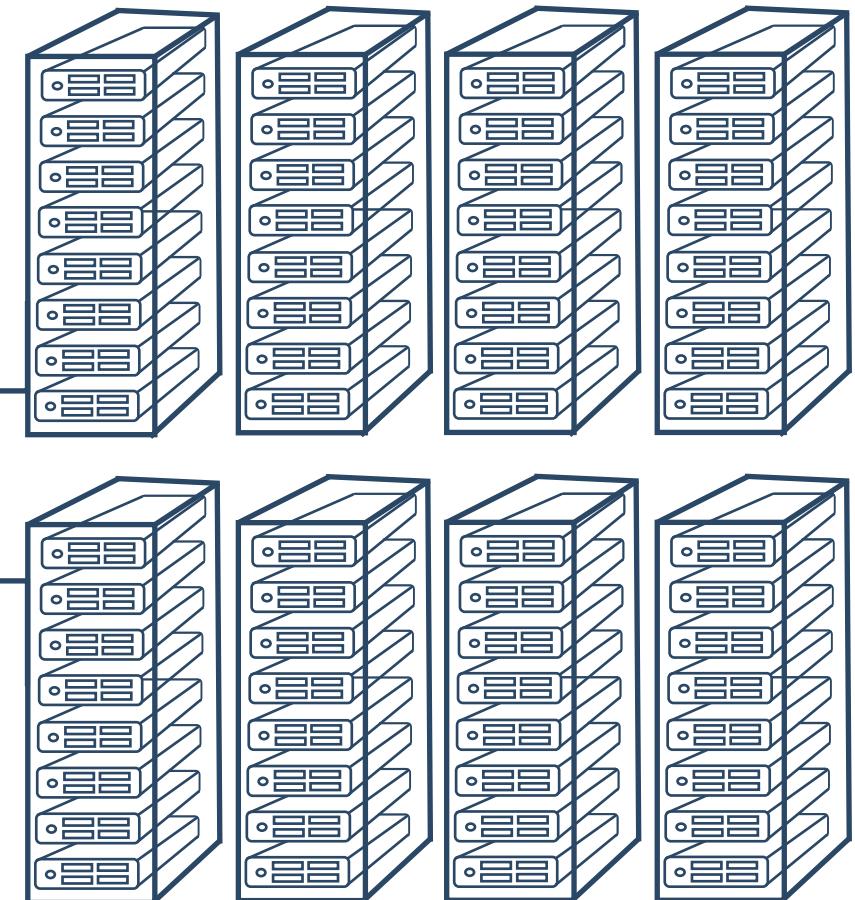


# Workflow in HPC



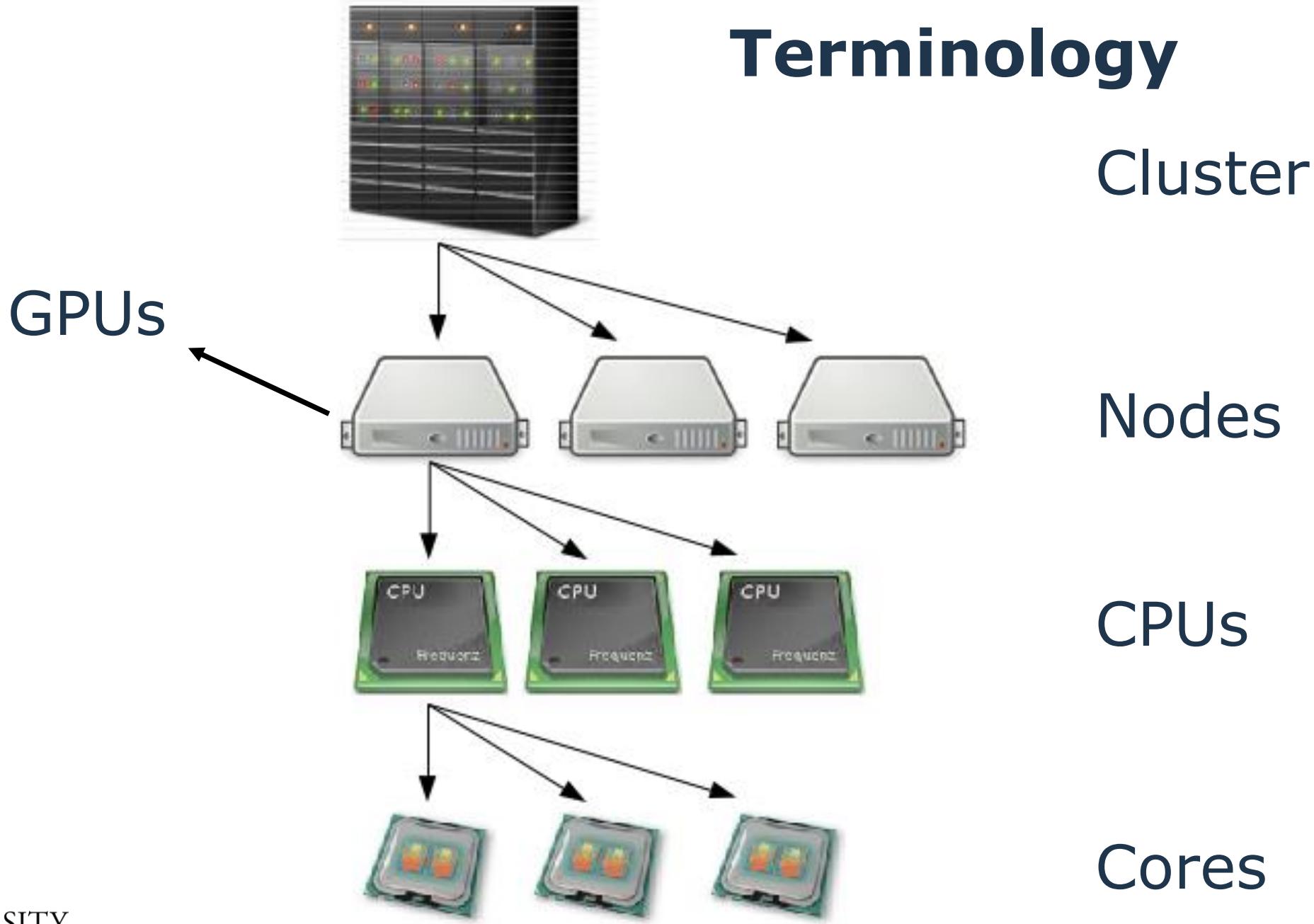
logging nodes

Linux



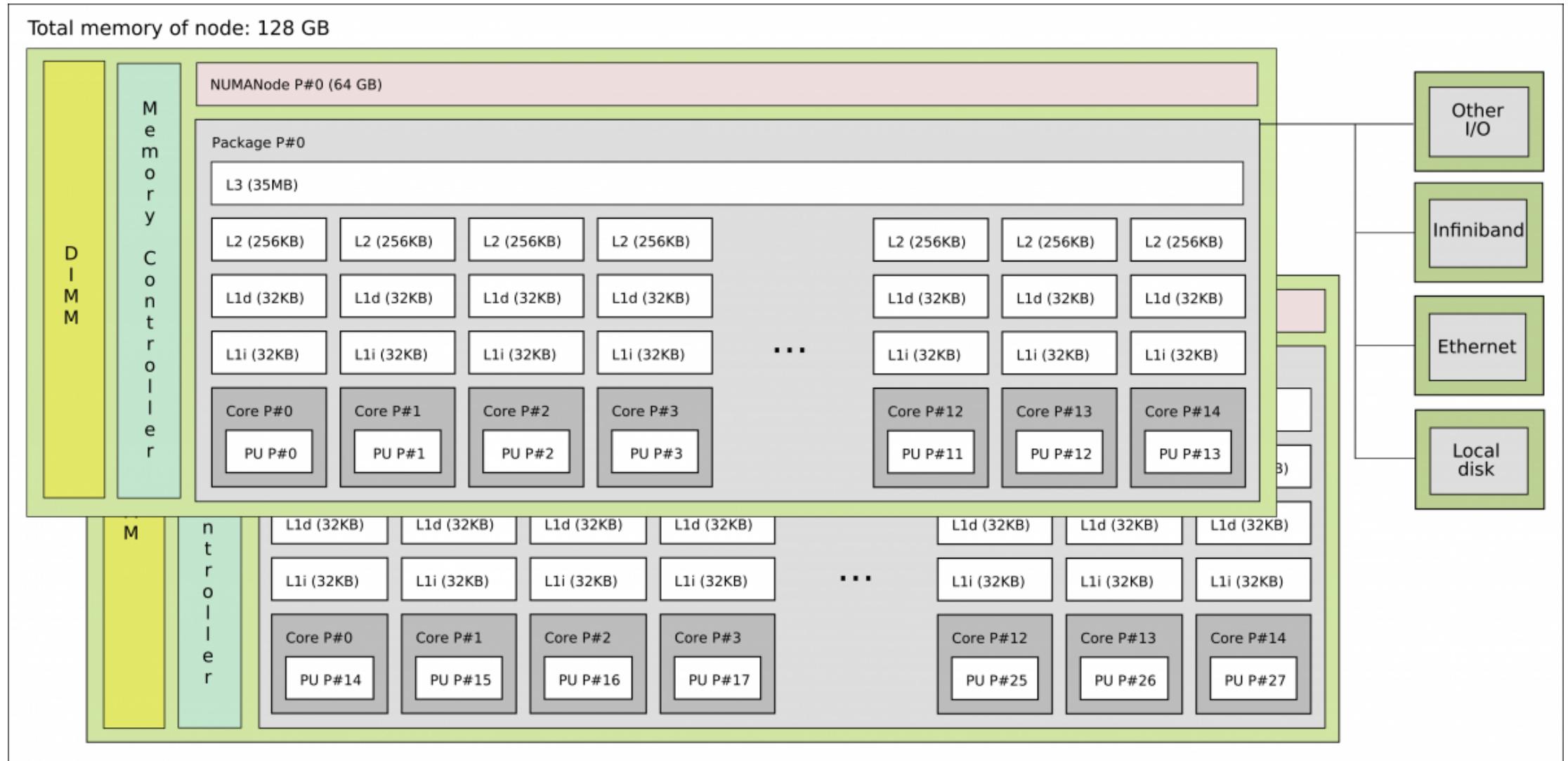
~550 computing nodes

# Terminology



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# Broadwell node on Kebnekaise



# GPU nodes on Kebnekaise



# GPU nodes on Kebnekaise

- V100 (NVIDIA)
- A100 (NVIDIA)            Login: kebnekaise-amd,  
Thinlinc: kebnekaise-amd-tl

# Parallelization techniques

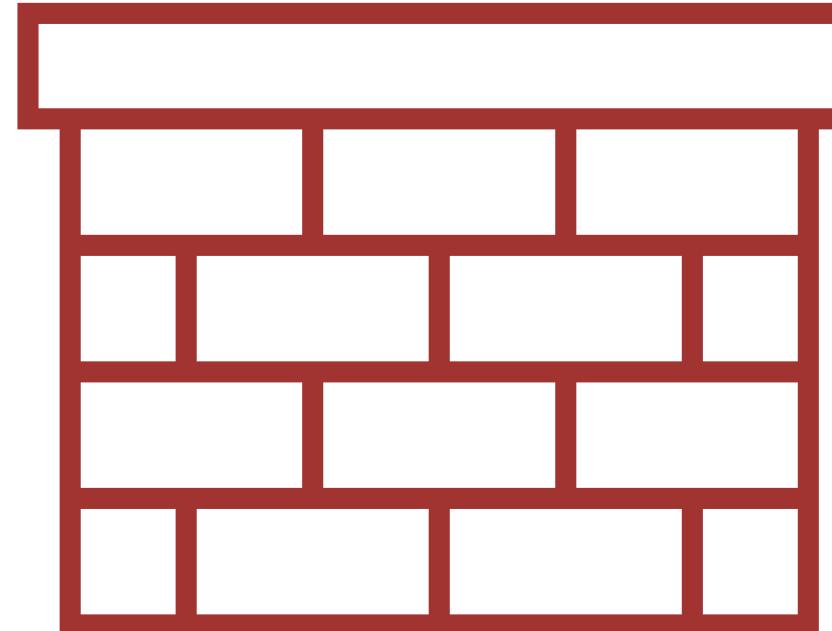
Speedup =  $(1 \text{ day})/(0.5 \text{ day}) = 2$



1 day



0.5 day



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# Parallelization techniques



# Metrics for performance

Nr. cores (n)	Time (min)	Speedup (S)	dS/dn
1	19.5	1	-
2	10.8	1.80	0.80
4	5.5	3.54	0.86
8	2.8	6.96	0.85
16	1.5	13	0.75
32	0.9	21.66	0.54
48	0.9	21.66	0

Timing results of a AMBER simulation.

$$S(x \text{ cores}) = \text{Time}(1 \text{ core})/\text{Time}(x \text{ cores})$$

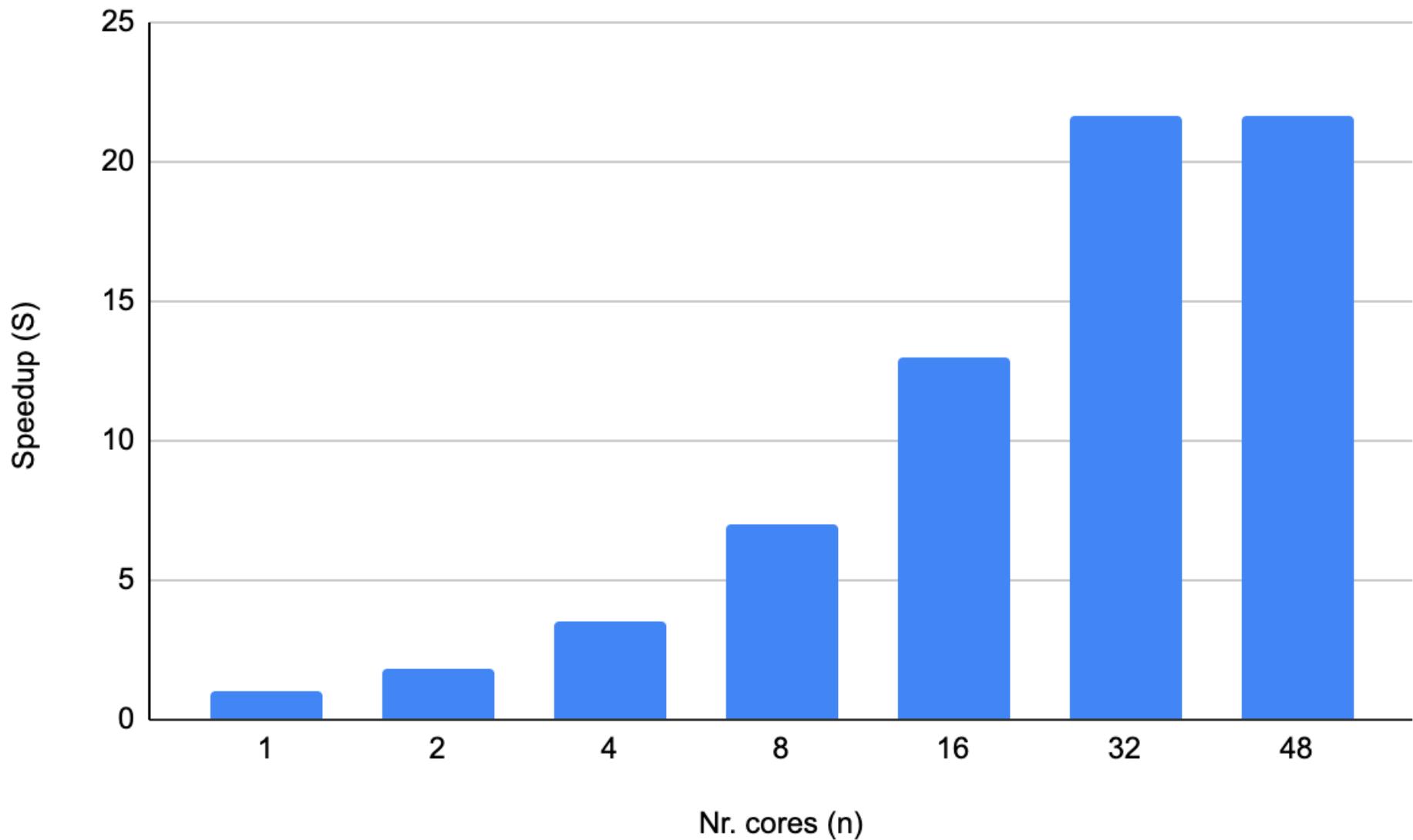
Example:

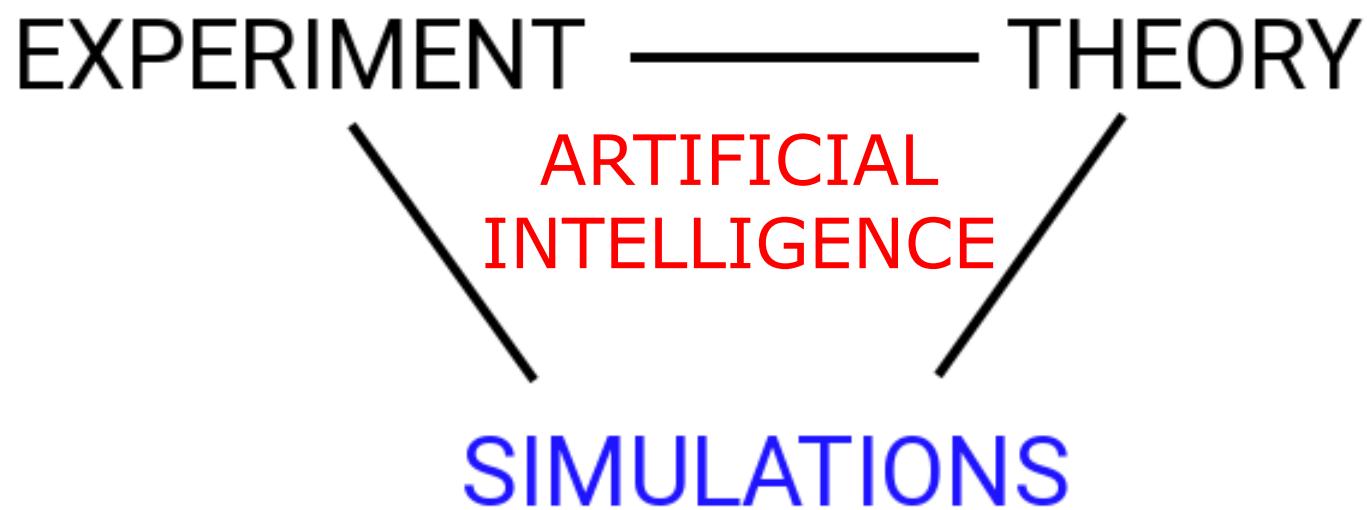
$$S(2 \text{ cores}) = 19.5 \text{ min}/10.8 = 1.8$$

Derivative example

$$\frac{\partial S}{\partial n} |_{n=32} = (21.66 - 13) / (32 - 16) = 0.54$$

Results from  
MD simulations  
with AMBER





## The Nobel Prize in Chemistry 2013



Photo: A. Mahmoud  
Martin Karplus  
Prize share: 1/3



Photo: A. Mahmoud  
Michael Levitt  
Prize share: 1/3



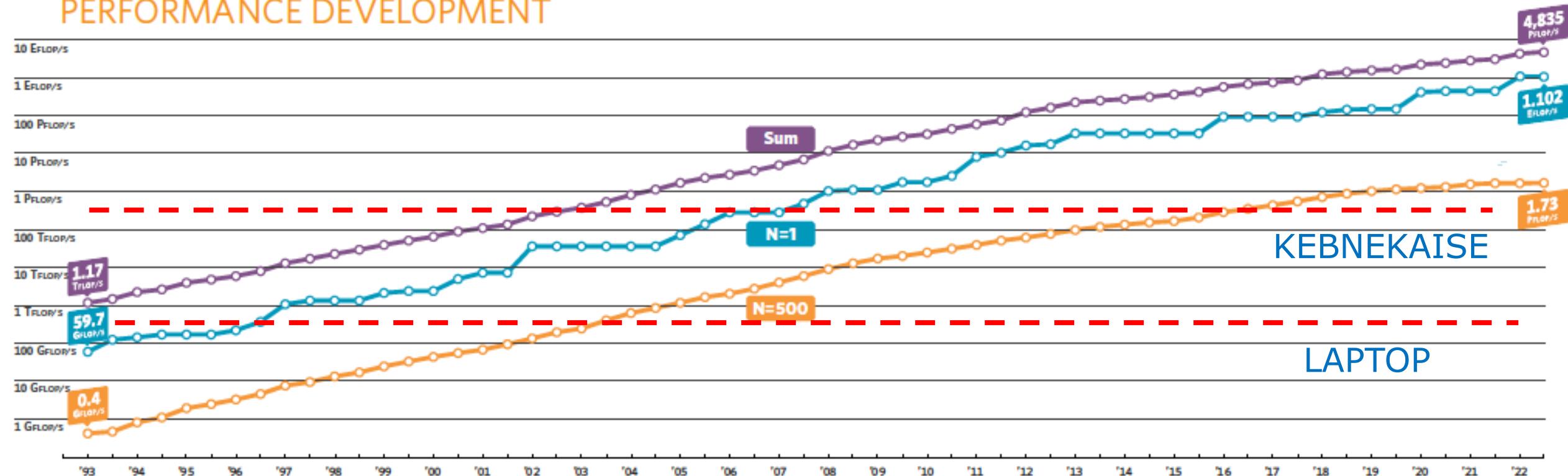
Photo: A. Mahmoud  
Arieh Warshel  
Prize share: 1/3

The Nobel Prize in Chemistry 2013 was awarded jointly to Martin Karplus, Michael Levitt and Arieh Warshel *"for the development of multiscale models for complex chemical systems"*.

<https://www.nobelprize.org/prizes/chemistry/2013/summary/>

# Top 500 list

## PERFORMANCE DEVELOPMENT



# Job scheduler (SLURM)



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# Software management

We use **EasyBuild** and **Lmod** to install and manage software, respectively.

If you are interested in some package whose name contains some **\*string\***, you can see if that package is already installed by typing:

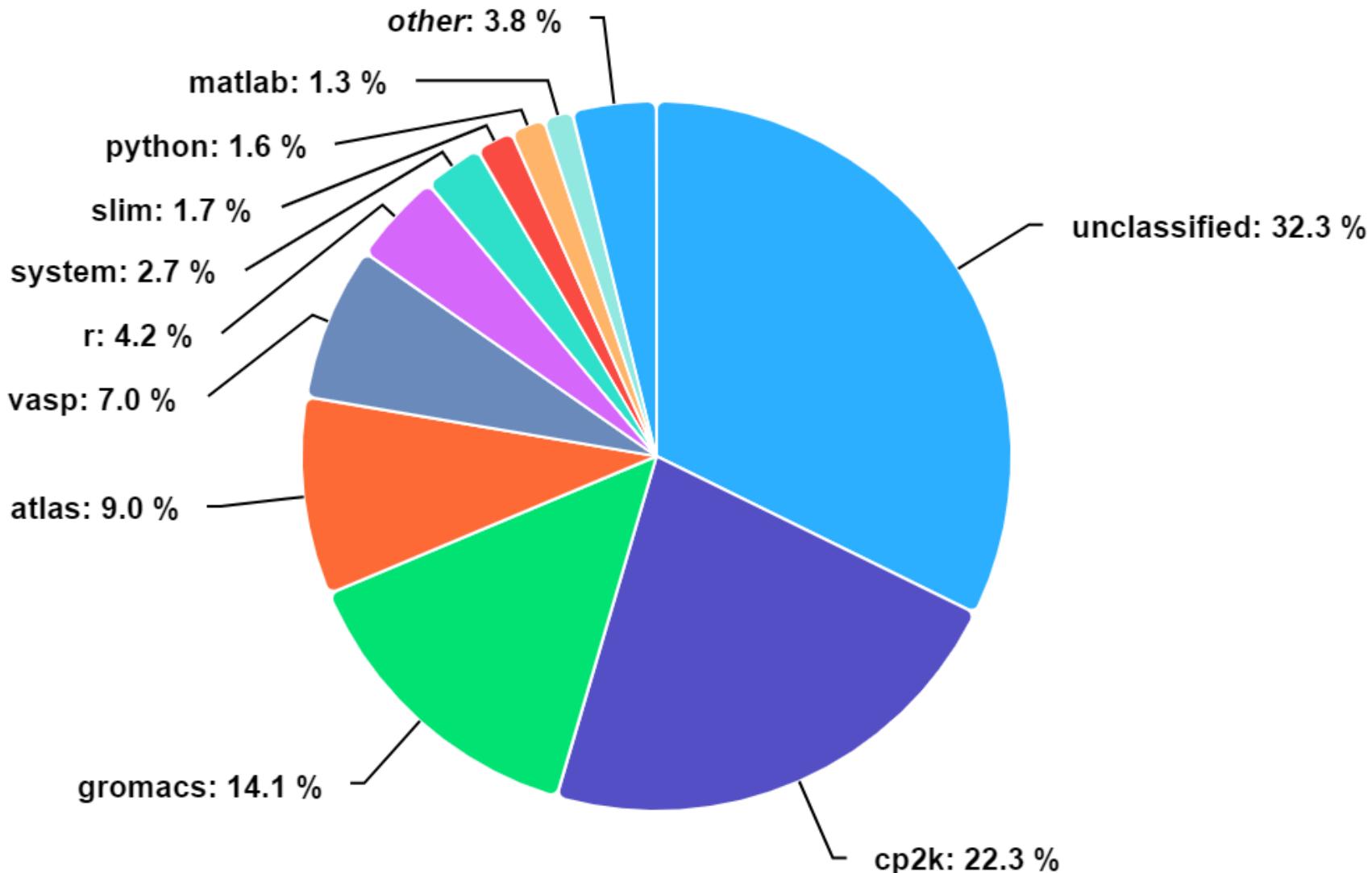
```
module spider *string*
```

Here, you will see all the modules that need to be loaded prior to using this package. You can load the modules with

```
module load *package*
```

# Core hour usage per software for Kebnekaise @ HPC2N

Period: 2023-01-01 - 2023-09-01



Software   www.hpc2n.umu.se	
Search	
<a href="#">FDTD_Solutions (Lumerical)</a>	High performance FDTD-method Maxwell solver for the design, analysis and optimization of nanophotonic devices, processes and materials.  External info: <a href="#">↗</a>
<a href="#">galamost</a>	GALAMOST is a versatile molecular simulation package which is designed to fully utilize computational power of graphics processing units (GPUs). It is developed specially for coarse-graining simulations of polymeric systems by including some latest techniques  External info: <a href="#">↗</a>
<a href="#">GAMESS-US</a>	The General Atomic and Molecular Electronic Structure System (GAMESS) is a general ab initio quantum chemistry package.  External info: <a href="#">↗</a>
<a href="#">Gaussian</a>	Gaussian provides state-of-the-art capabilities for electronic structure modeling.  External info: <a href="#">↗</a>
<a href="#">GPAW</a>	GPAW is a density-functional theory (DFT) Python code based on the projector-augmented wave (PAW) method and the atomic simulation environment (ASE).  External info: <a href="#">↗</a>
<a href="#">Gromacs</a>	A molecular dynamics package primarily designed for biomolecular systems such as proteins and lipids. It is a free software.  External info: <a href="#">↗</a>
<a href="#">HDF5</a>	HDF5 is a data model, library, and file format for storing and managing data.  External info: <a href="#">↗</a>
<a href="#">hwloc</a>	The Portable Hardware Locality (hwloc) software package provides a portable abstraction (across OS, versions, architectures, ...) of the hierarchical topology of modern architectures, including NUMA memory nodes, sockets, shared caches, cores and simultaneous multithreading. It also gathers various system attributes such as cache and memory information as well as the locality of I/O devices such as network

# **Application's usage**



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# R/Rstudio

\$ml dependencies\_of\_R

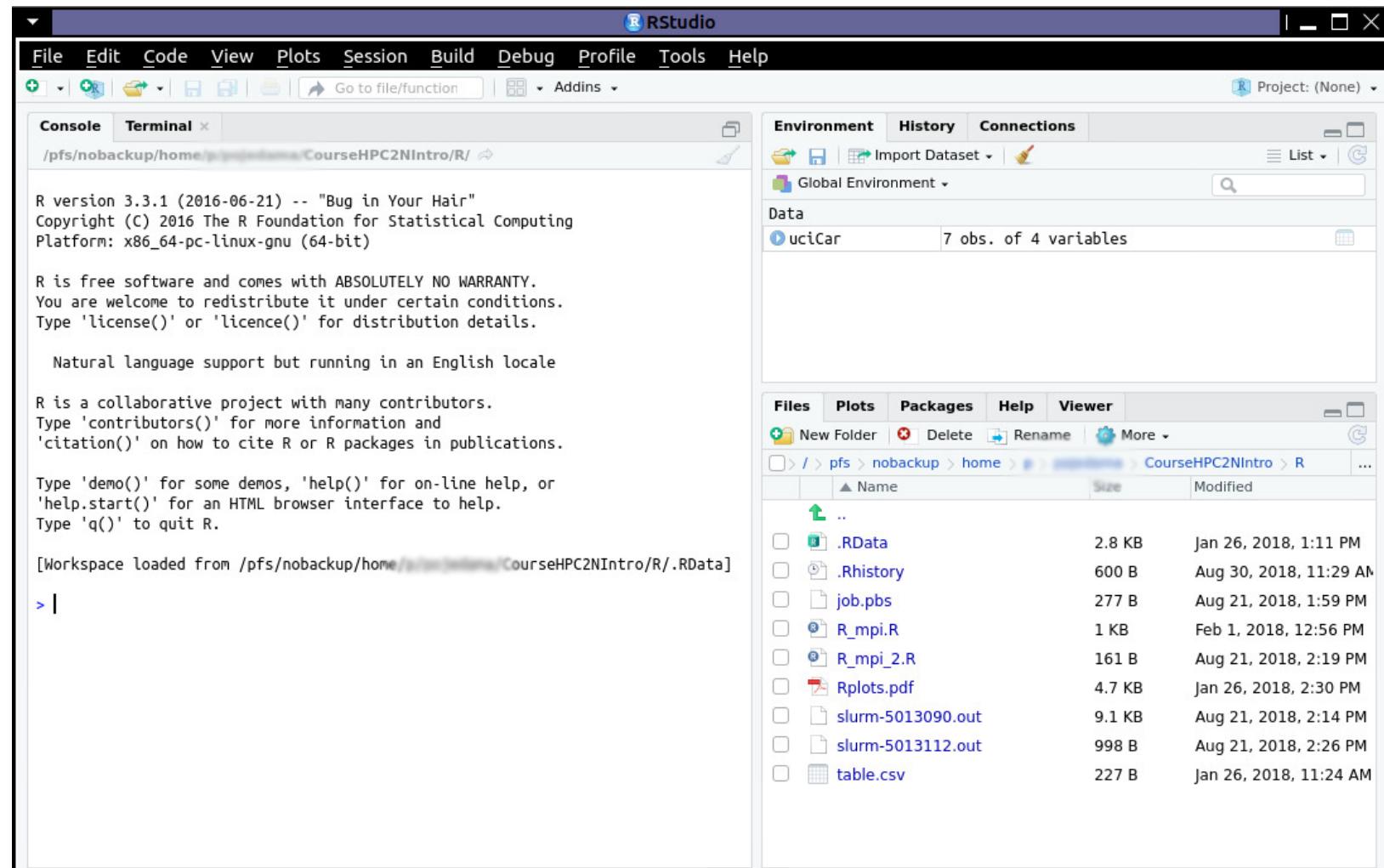
\$ml R/version

\$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](https://www.hpc2n.umu.se/resources/software/user_installed/r)



# R serial job

```
#!/bin/bash
### SNAC project number, enter your own
#SBATCH -A hpc2n202X-XYZ
# Asking for one core
#SBATCH -n 1
#SBATCH --time=00:10:00

ml dependencies_of_R
ml R/version

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

# 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()
```

```
#!/bin/bash
#SBATCH -A hpc2n202X-XYZ
#Asking for 10 min.
#SBATCH -t 00:10:00
#SBATCH -n 6

export OMPI_MCA_mpi_warn_on_fork=0
ml dependencies_of_R
ml R/version

R --no-save --quiet -f Rmpi.R
```

# R parallel job (doParallel)

```
#!/bin/bash
#SBATCH -A hpc2n202X-XYZ
#Asking for 10 min.
#SBATCH -t 00:10:00
#SBATCH -n 8

ml dependencies_of_R
ml R/version

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

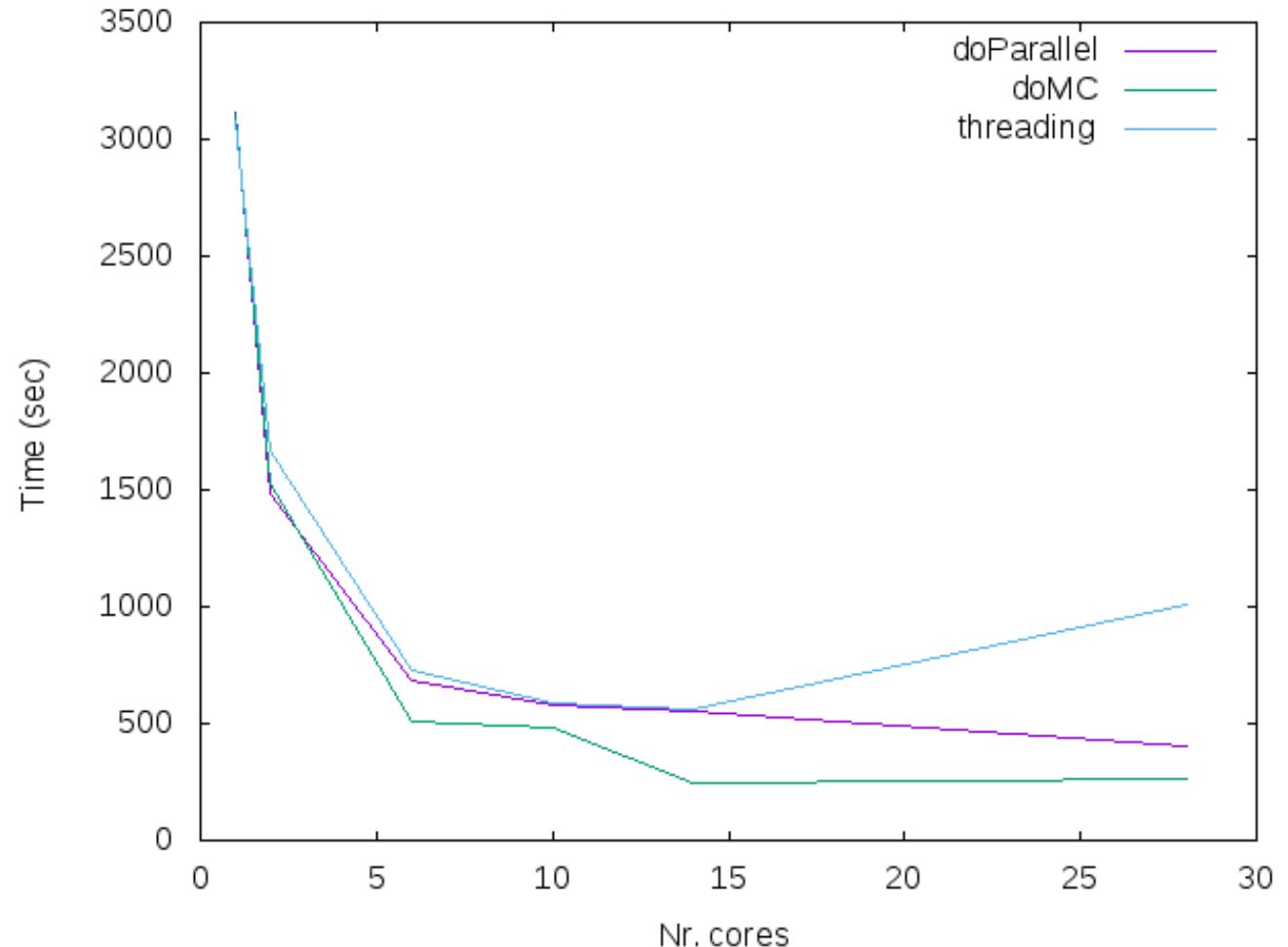
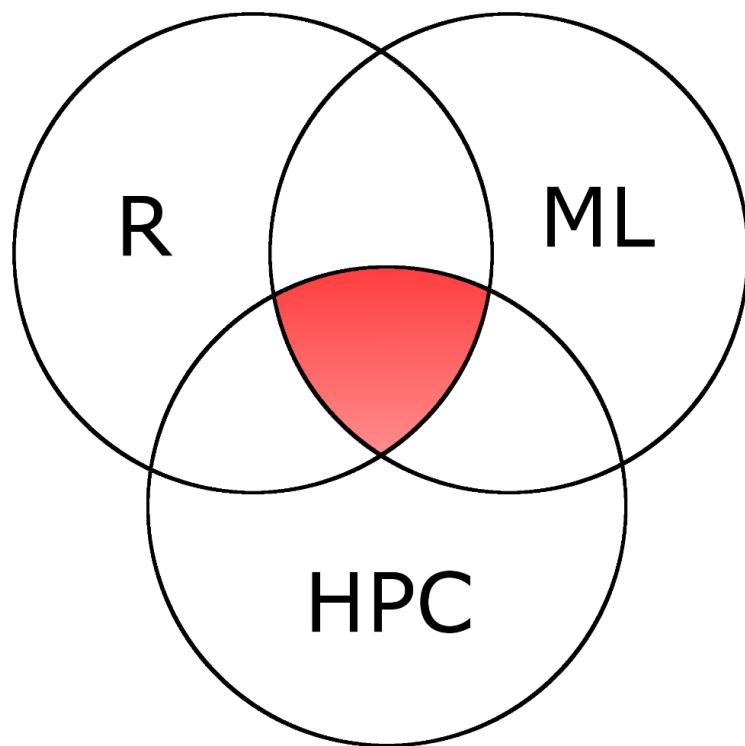
doParallel\_ML.R

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

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

# R Machine Learning job

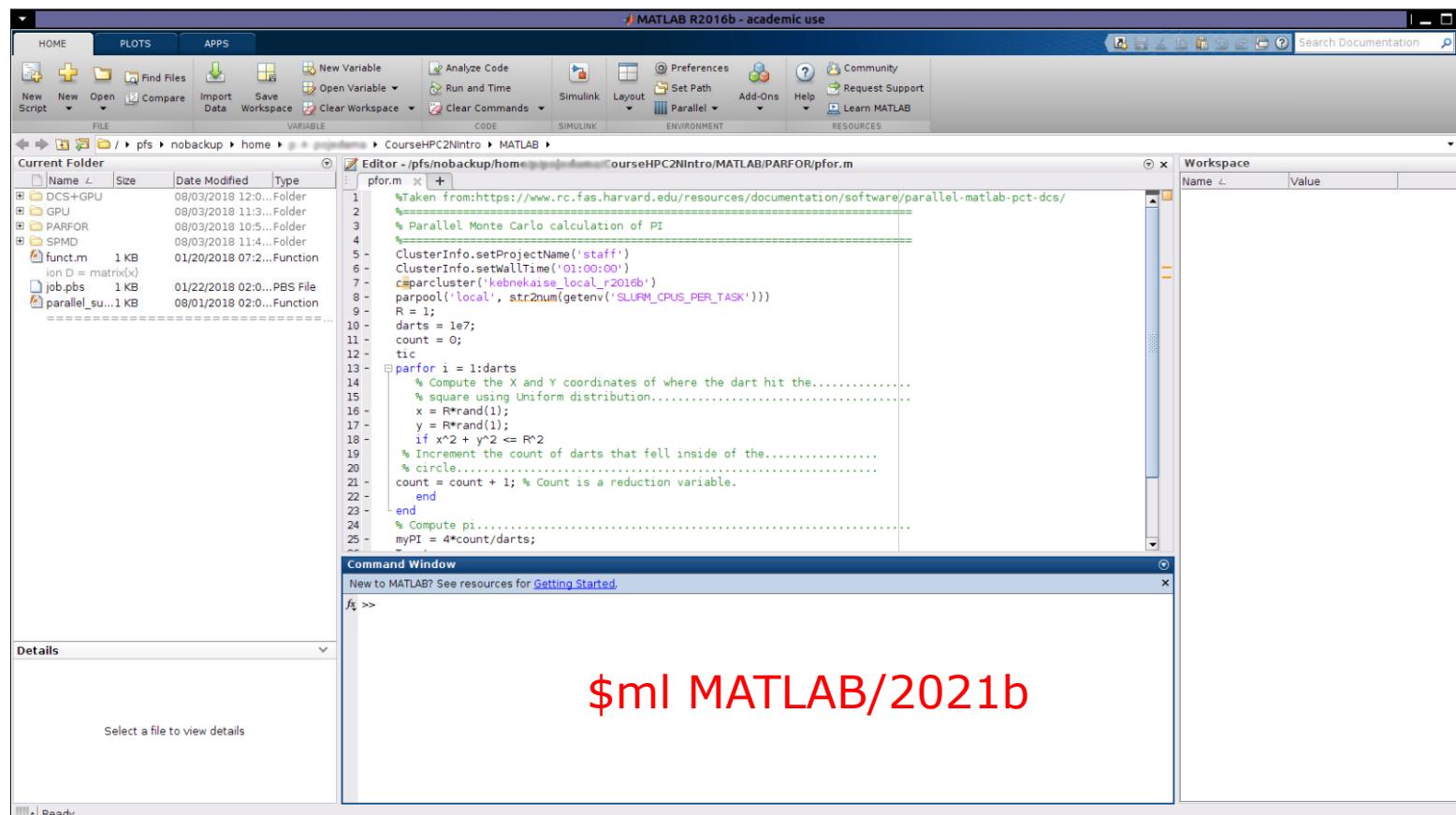
Example: Boosted classification model using “**xgboost**” (7 tuning parameters). Further details: <http://appliedpredictivemodeling.com/blog/2018/1/17/parallel-processing>.



# MATLAB

One needs to configure MATLAB the first time one uses it:

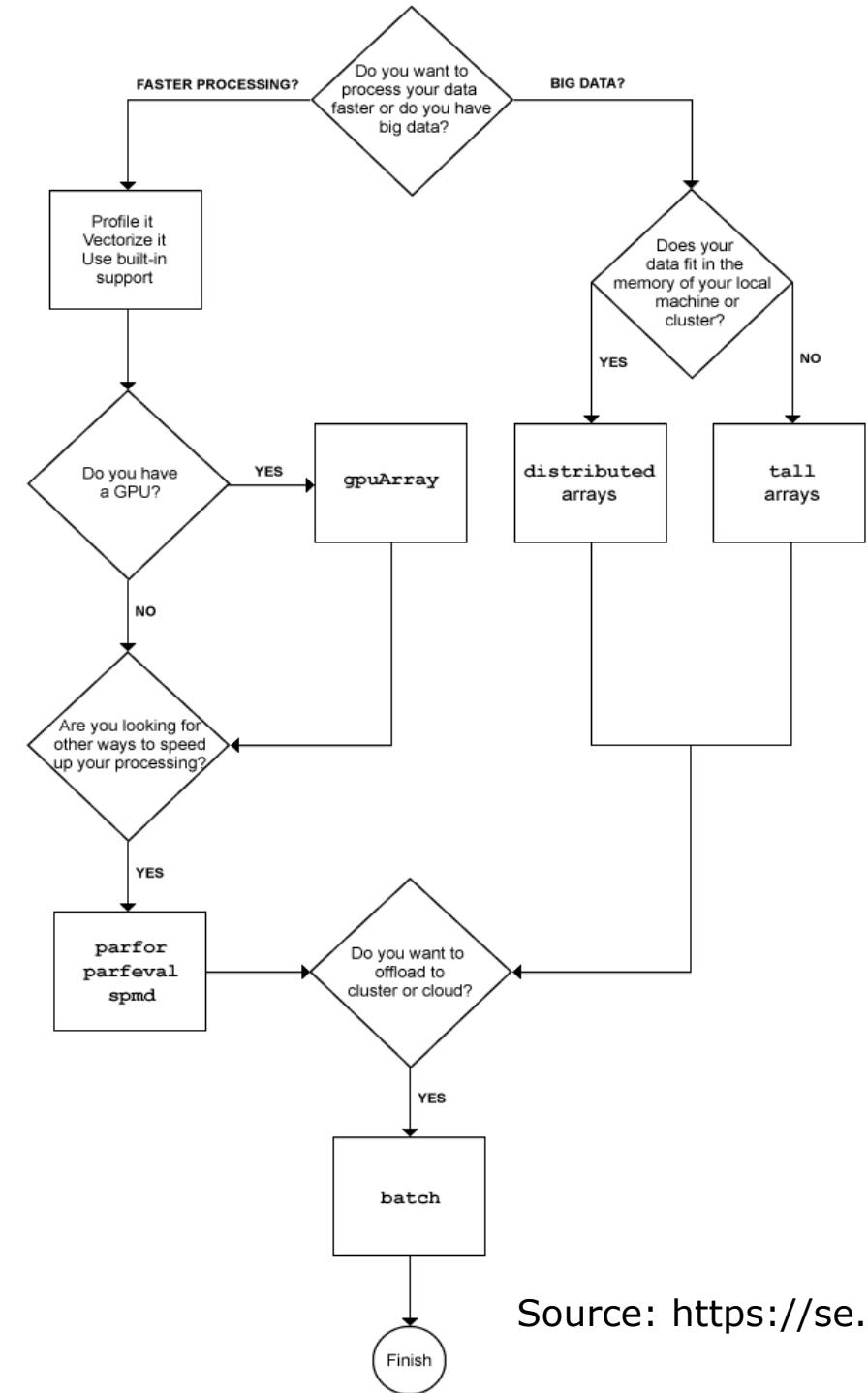
( <https://www.hpc2n.umu.se/resources/software/configure-matlab-2018> )



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

Heavy jobs will be cancelled!

Start Matlab with:  
matlab -singleCompThread



# MATLAB Parallel computing tools

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

# 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 hpc2n202X-XYZ  
#Asking for 10 min.  
#SBATCH -t 00:10:00  
#SBATCH -n 1  
#SBATCH -p batch  
  
#Load modules necessary for running  
MATLAB  
ml MATLAB/2021b  
  
srun matlab -nodisplay -  
singleCompThread -r "funct;exit" >  
out.log
```



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# Parfor

```
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
```

File name: pfor.m

Batch script:

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

```
srun matlab -nodisplay -r "pfor"
```

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

# GPU jobs

On the MATLAB GUI:

```
c=parcluster('kebnekaise')

% submit the job to the queue
j = c.batch(@parallelex, 1, {})

% Wait for the job to finish.
j.wait

% Fetch the result after the job has finished
j.fetchOutputs{ : }
```

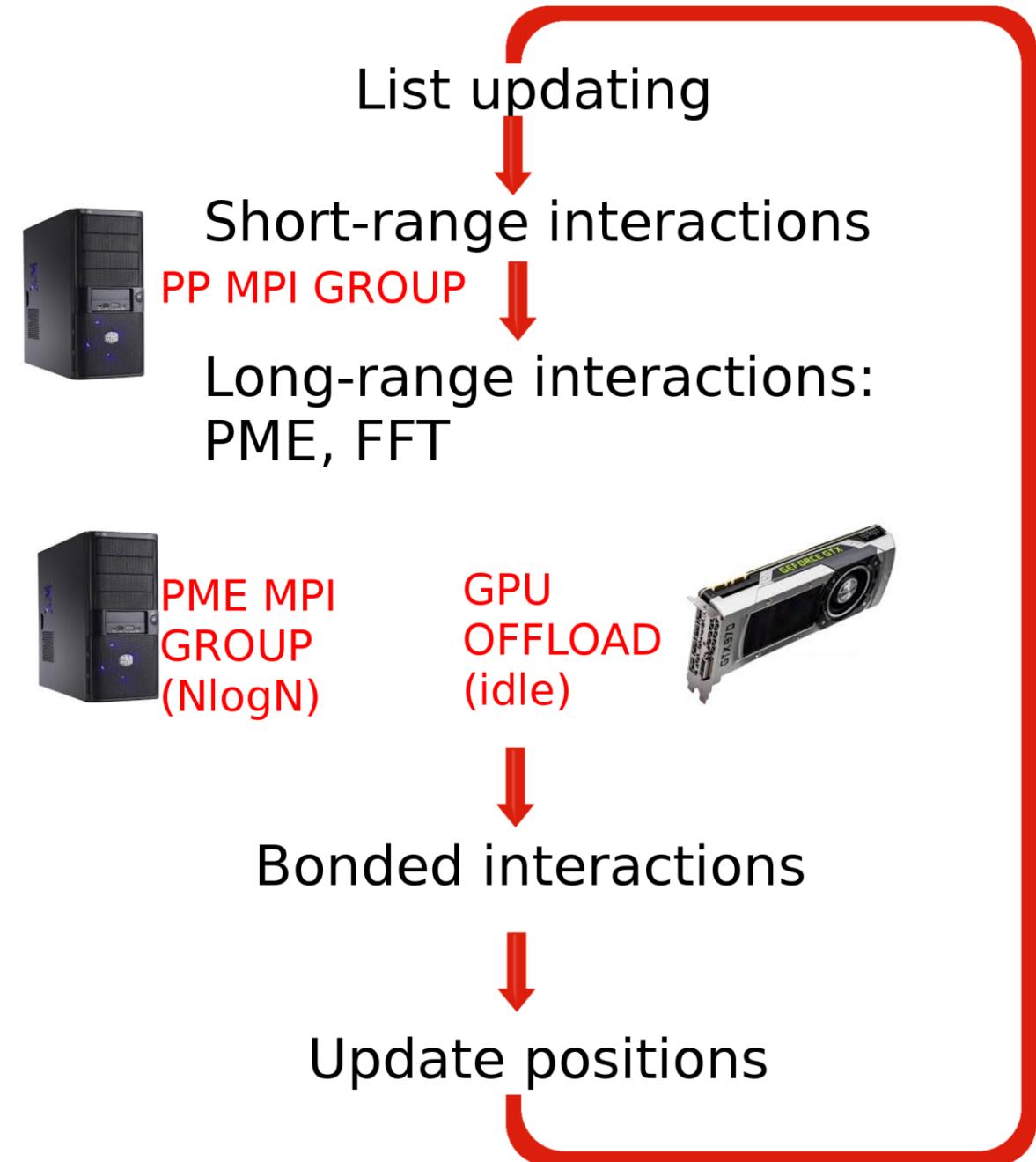
File: parallelex.m

```
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
```

# N-body Dynamics



# Benchmark

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

# AMBER

- Collection of independent routines
- It uses Sander/PMEMD for solving the Newton's equations
- It offers a robust set of analysis tools
- Resources: <https://ambermd.org/>

```
# module load dependencies_of_amber
ml Amber/version
srun pmemd.MPI -O -i input.mdin
srun pmemd.cuda.MPI -O -I input.mdin
```

# AMBER Tools

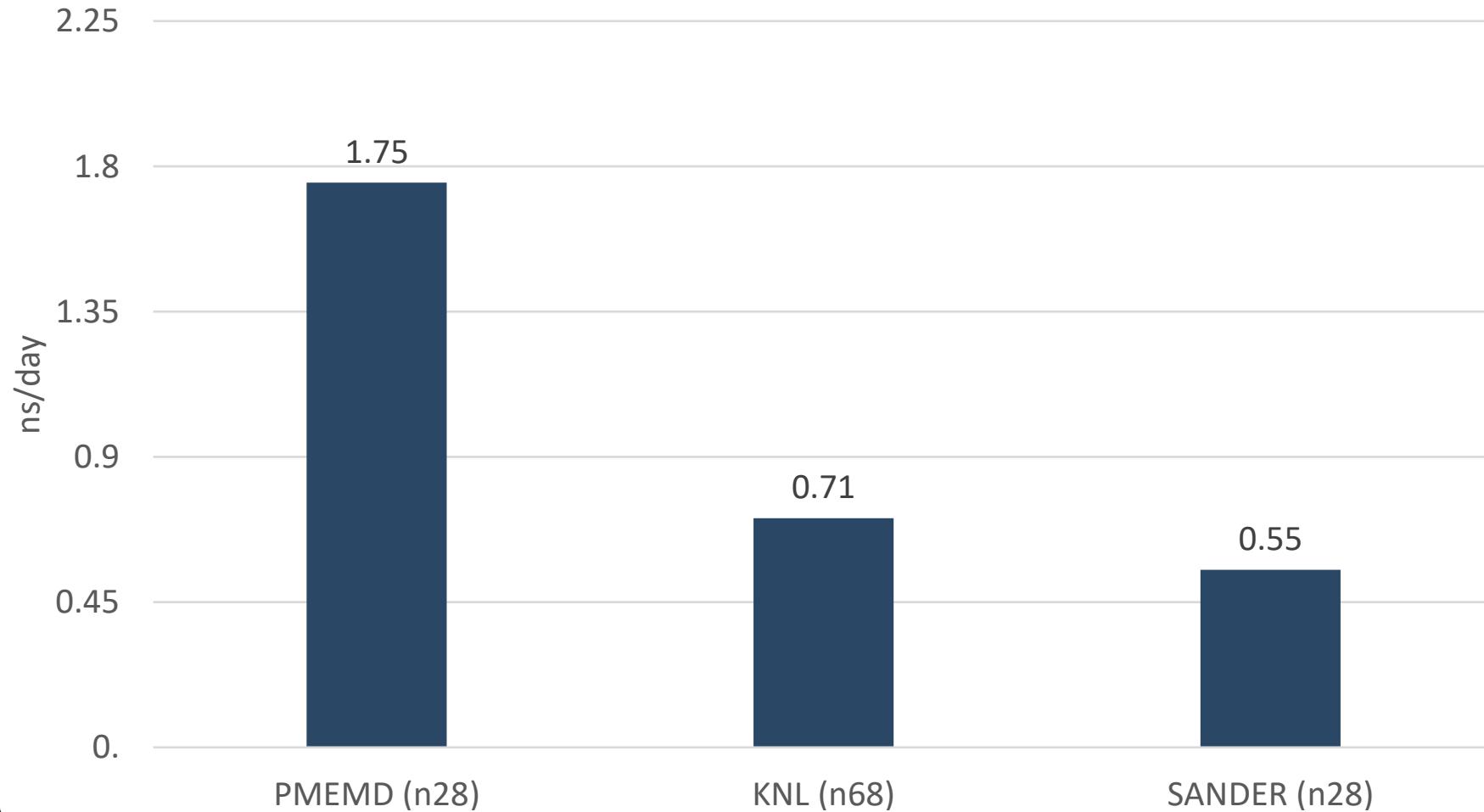
- For setting up a simulation (initial structure, solvation, ions, ...):

On the command line:

\$tleap, antechamber, cpptraj, ...

# AMBER

AMBER

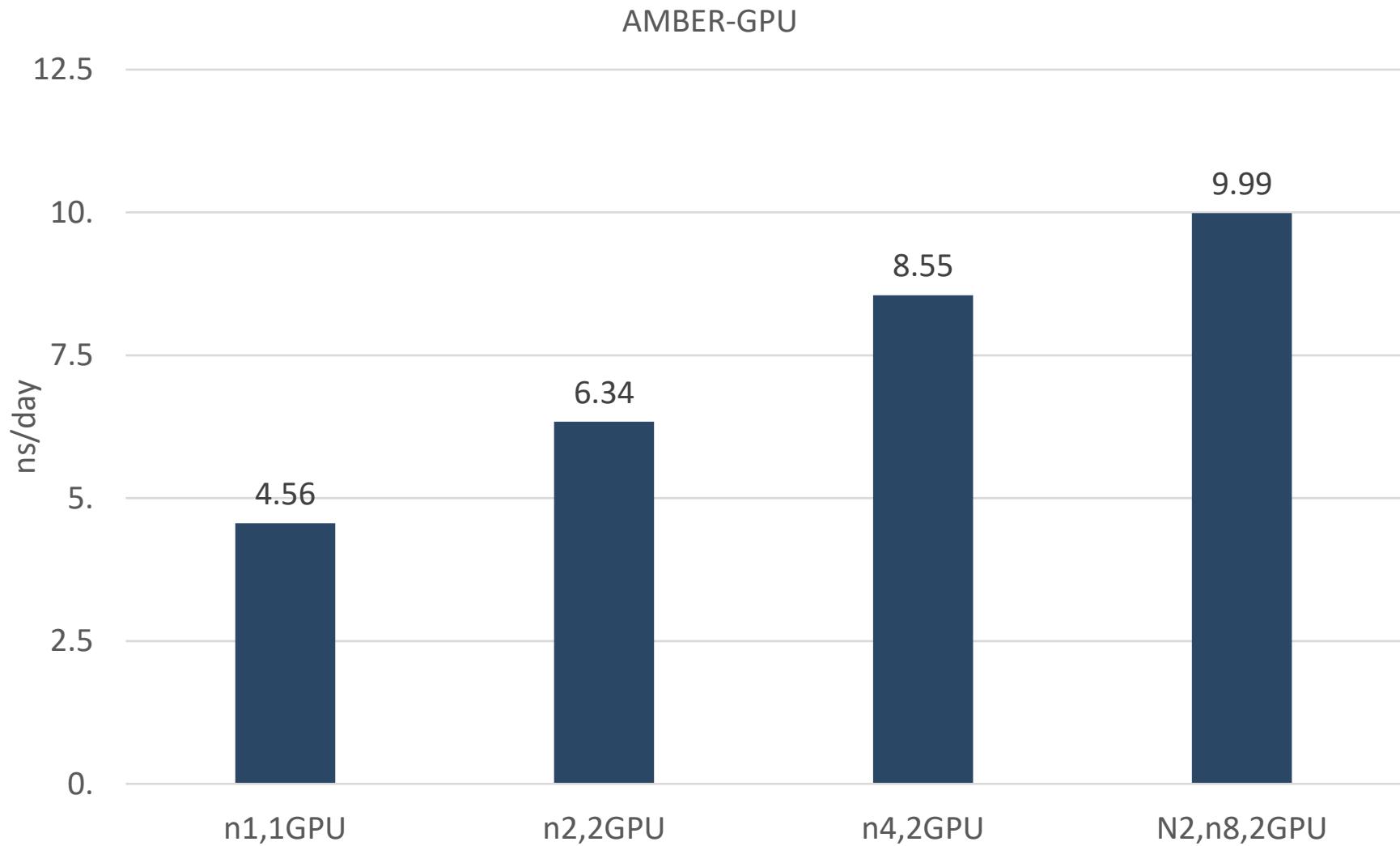


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# AMBER

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

Notice that, the  
remaining CPUs  
are not used.



# NAMD

- Based on charm++ communication protocol
- Versions: single node, multi-node, and GPU
- Highly scalable
- Resources: <https://www.ks.uiuc.edu/Research/namd/>

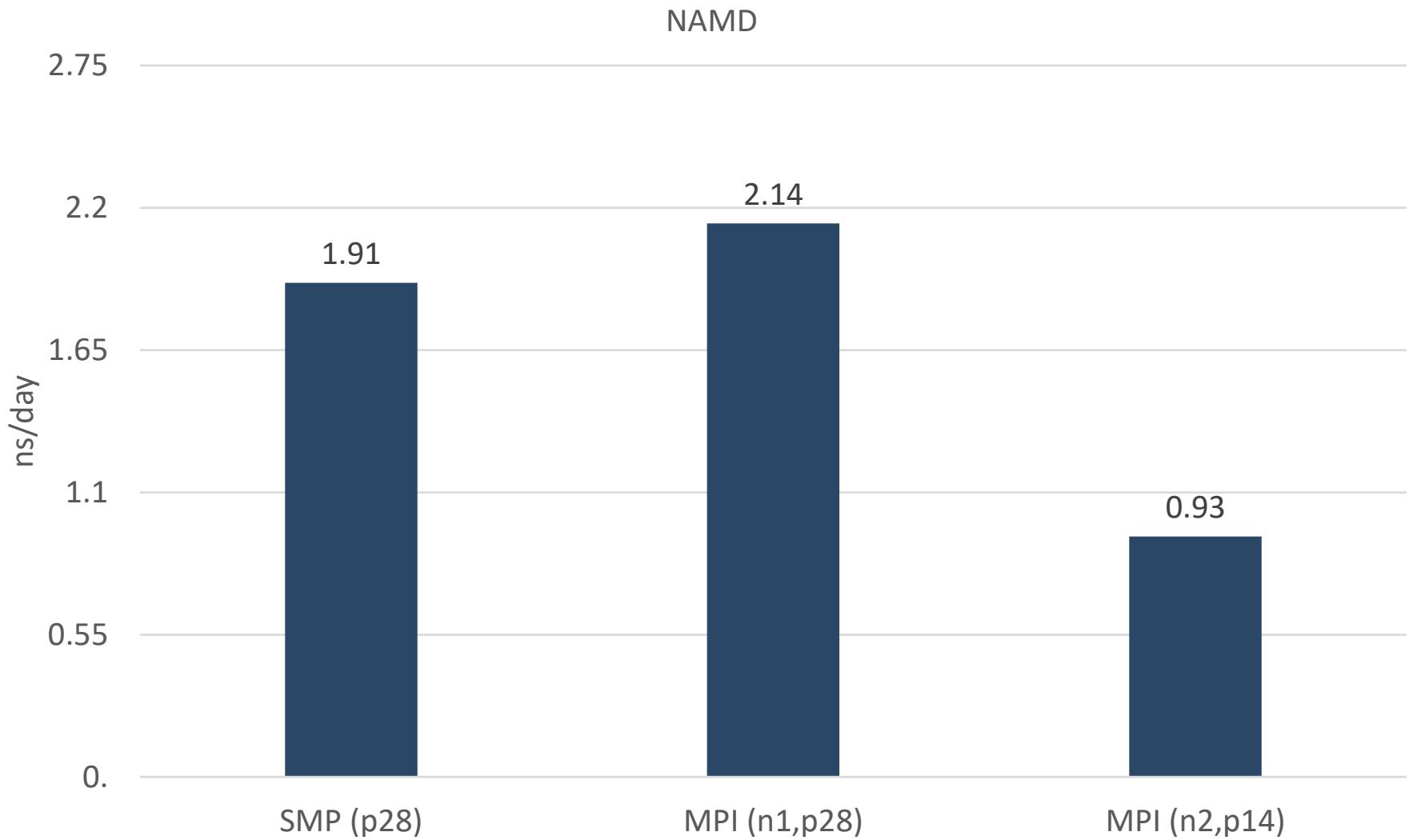
# NAMD GPU

```
#!/bin/bash
#SBATCH -A staff
#SBATCH -t 00:50:00
#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 step4_equilibration.inp > output.dat
```

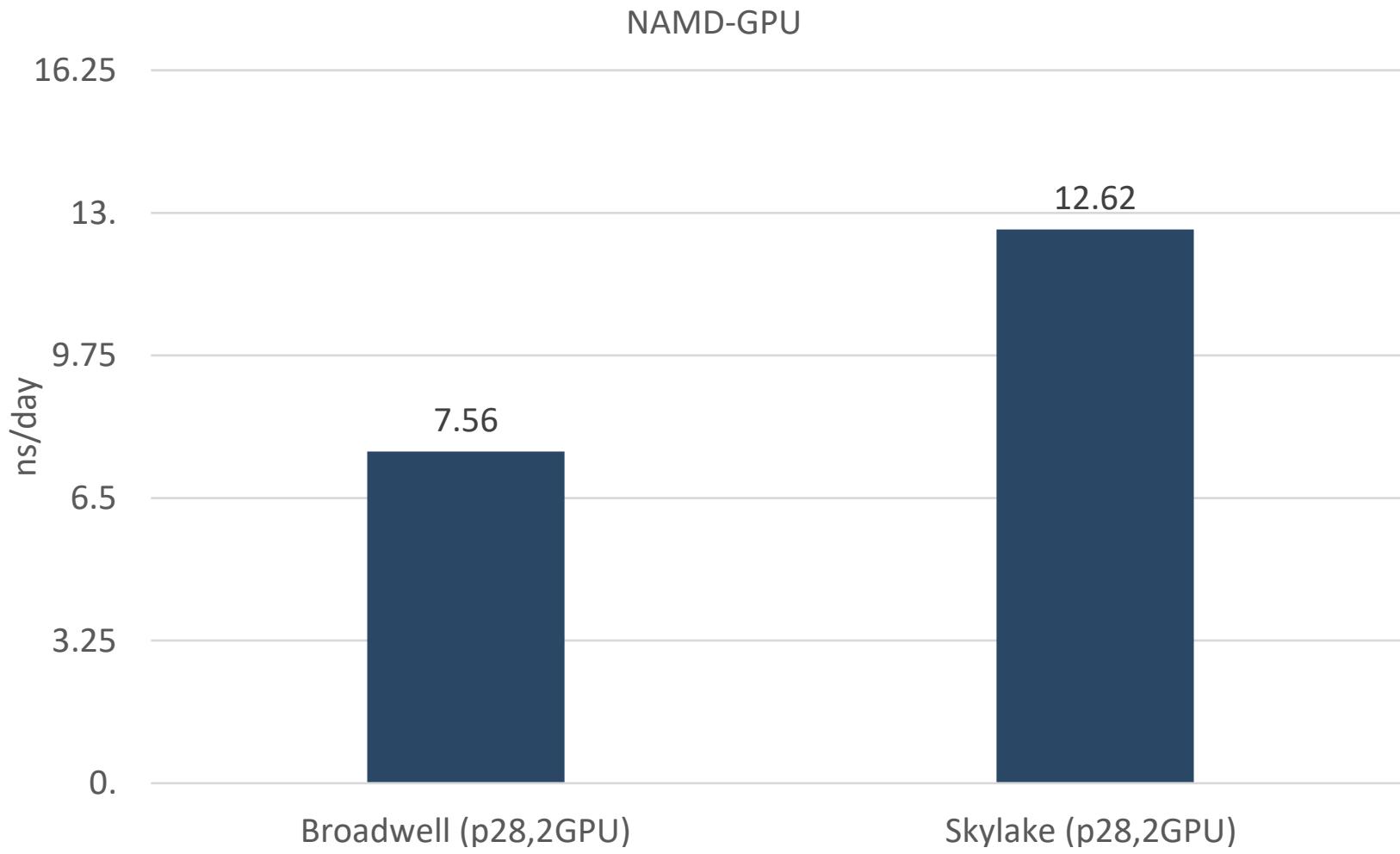
# NAMD

Use the  
**+setcpuaffinity** flag  
for a 10% speedup



# NAMD

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



# GROMACS

- Resources:
  - <https://www.gromacs.org/index.html> (website)
  - <https://gromacs.bioexcel.eu/top?period=monthly> (forum)

# GROMACS

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

ml dependencies_of_gromacs
ml GROMACS/version

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

# GROMACS

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:

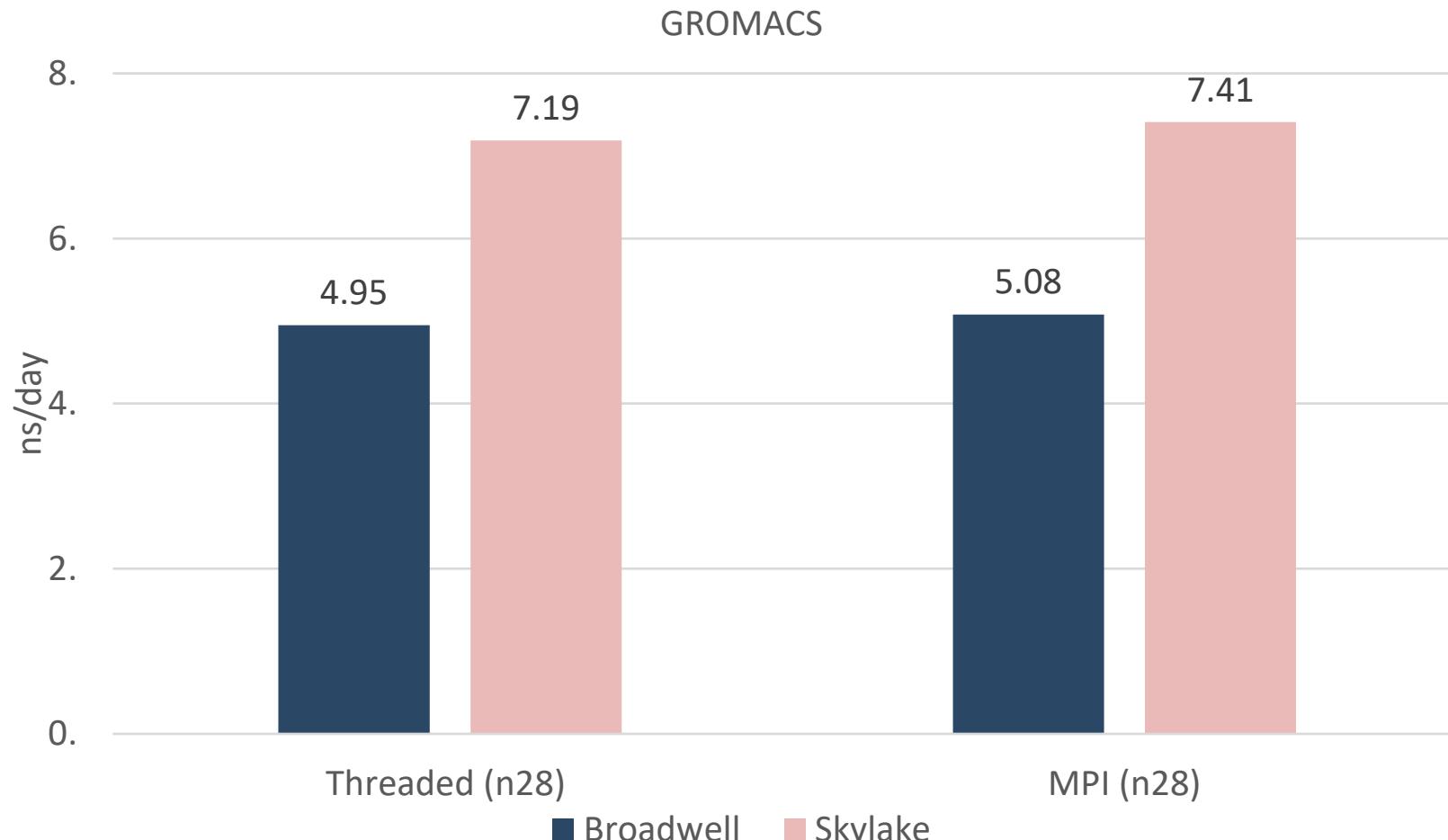
Line	tpr	PME ranks	Gcycles	Av.	Std.dev.	ns/day	PME/f	DD grid
0	0	0	4397.181	133.917	57.257	-	4	1 1
1	0	-1( 0)	4390.500	99.855	57.329	-	4	1 1

---

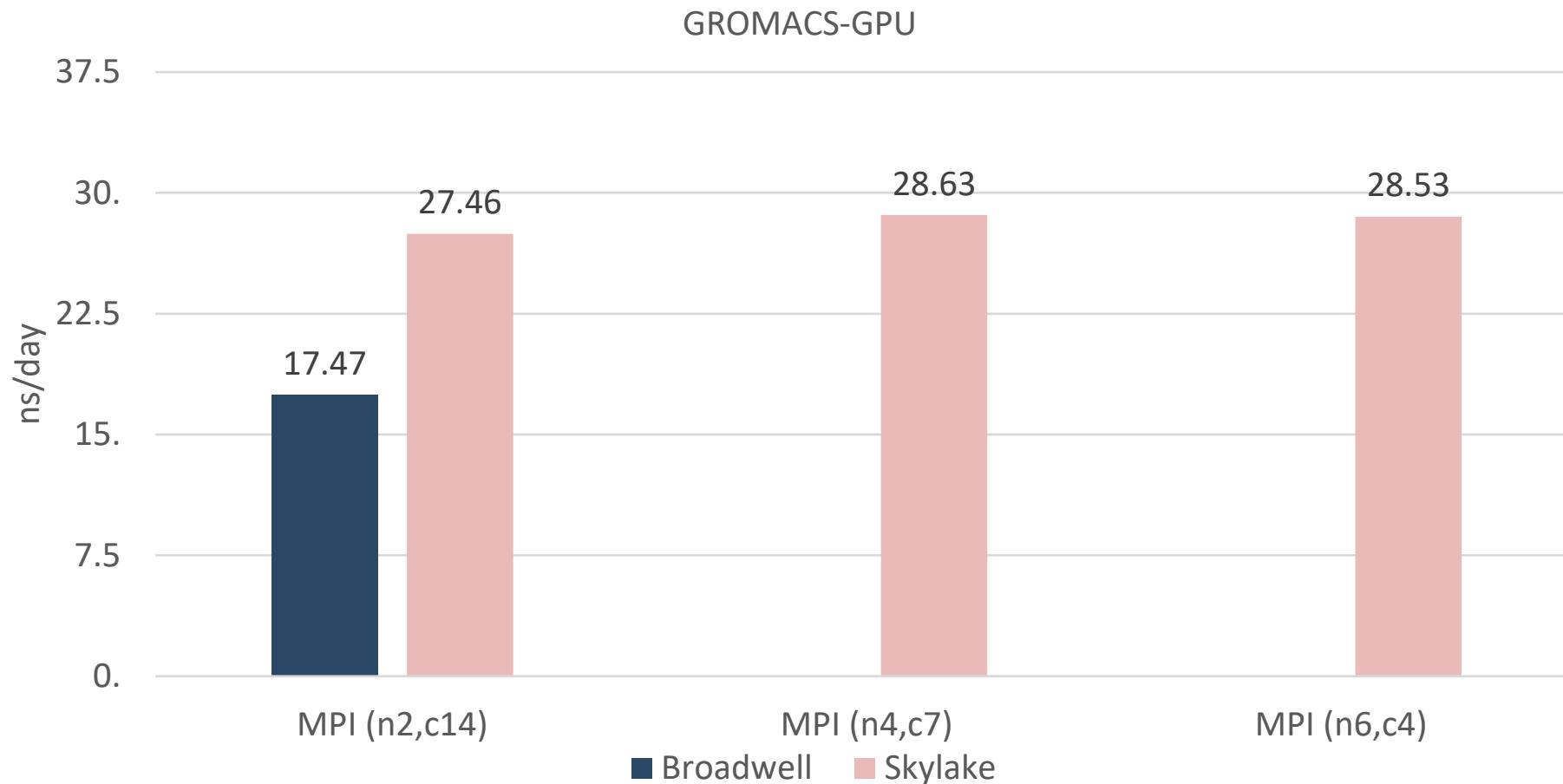
Best performance was achieved with the automatic number of PME ranks (see line 1)  
Please use this command line to launch the simulation:

mpirun -np 4 gmx\_mpi mdrun -npme -1 -s npt.tpr -ntomp 7 -dlb yes

# GROMACS



# GROMACS



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# 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

# LAMMPS

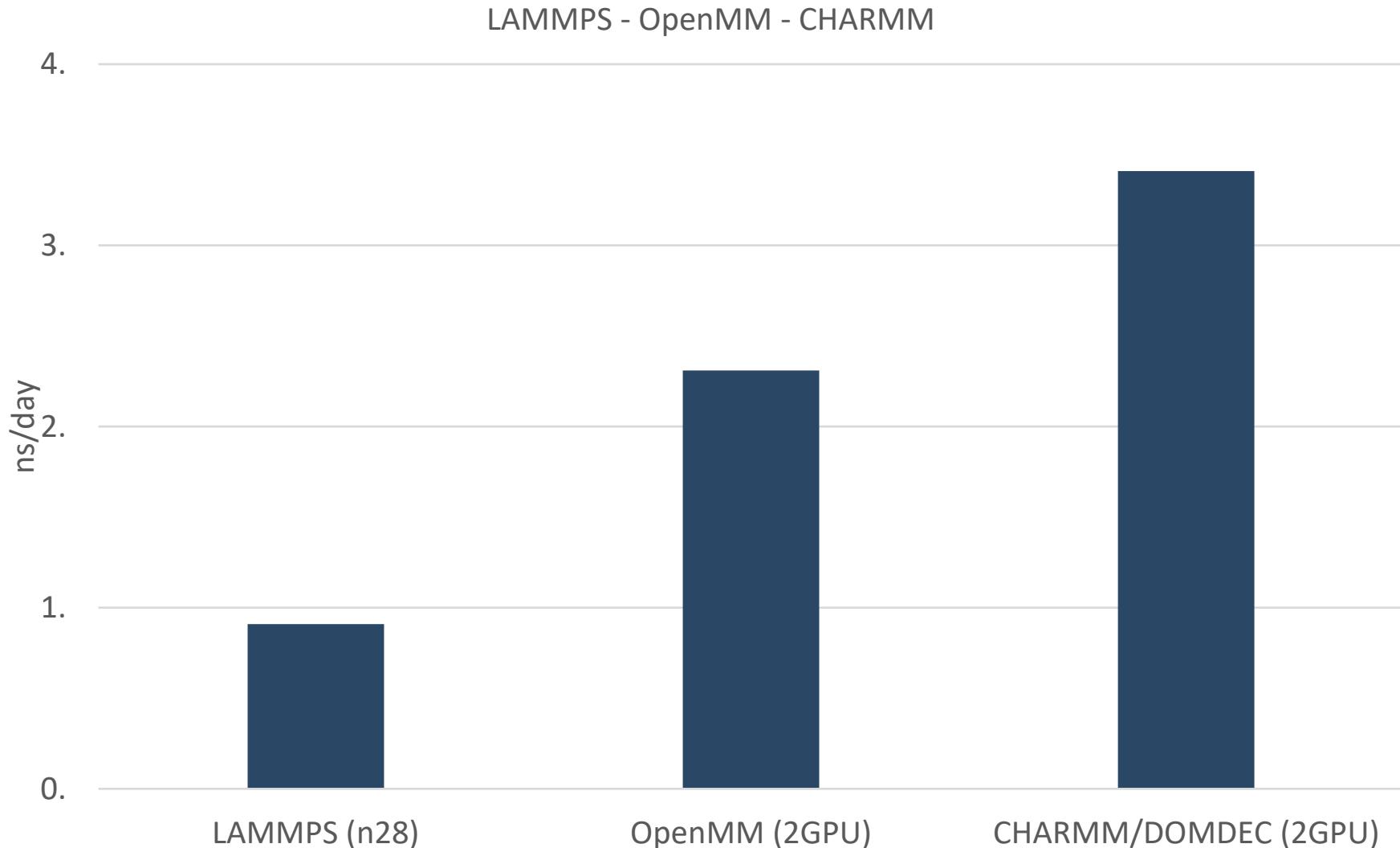
```
#!/bin/bash
#SBATCH -A staff
#Asking for 10 min.
#SBATCH -t 02:10:00
#Ask for 28 processes
#SBATCH -n 28

#Load modules necessary for running LAMMPS
module load LAMMPS/version

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



# LAMMPS-OpenMM-CHARMM



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# 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 dependencies_of_Tensorflow
ml Tensorflow/version
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

```
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

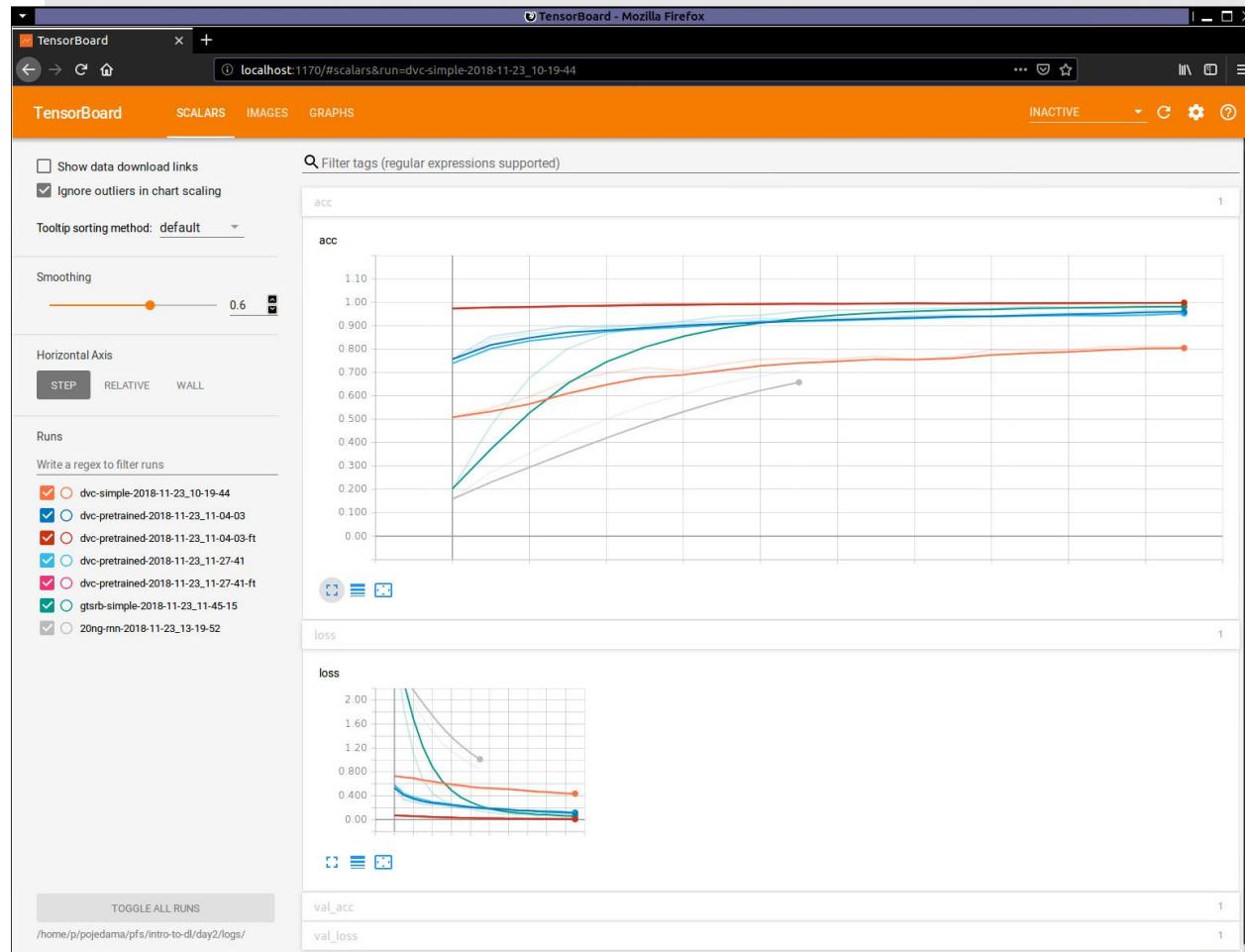
name: Quadro K6000  
major: 3 minor: 5 memoryClockRate (GHz) 0.9015  
pciBusID 0000:06:00.0  
Total memory: 11.92GiB  
Free memory: 11.82GiB  
**Creating TensorFlow device (/gpu:0) -> (device: 0, name: Quadro K6000, pci bus id: 0000:06:00.0)**

[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 your jobs open a web browser and type:

`localhost:1170`

# Gaussian

## 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
```

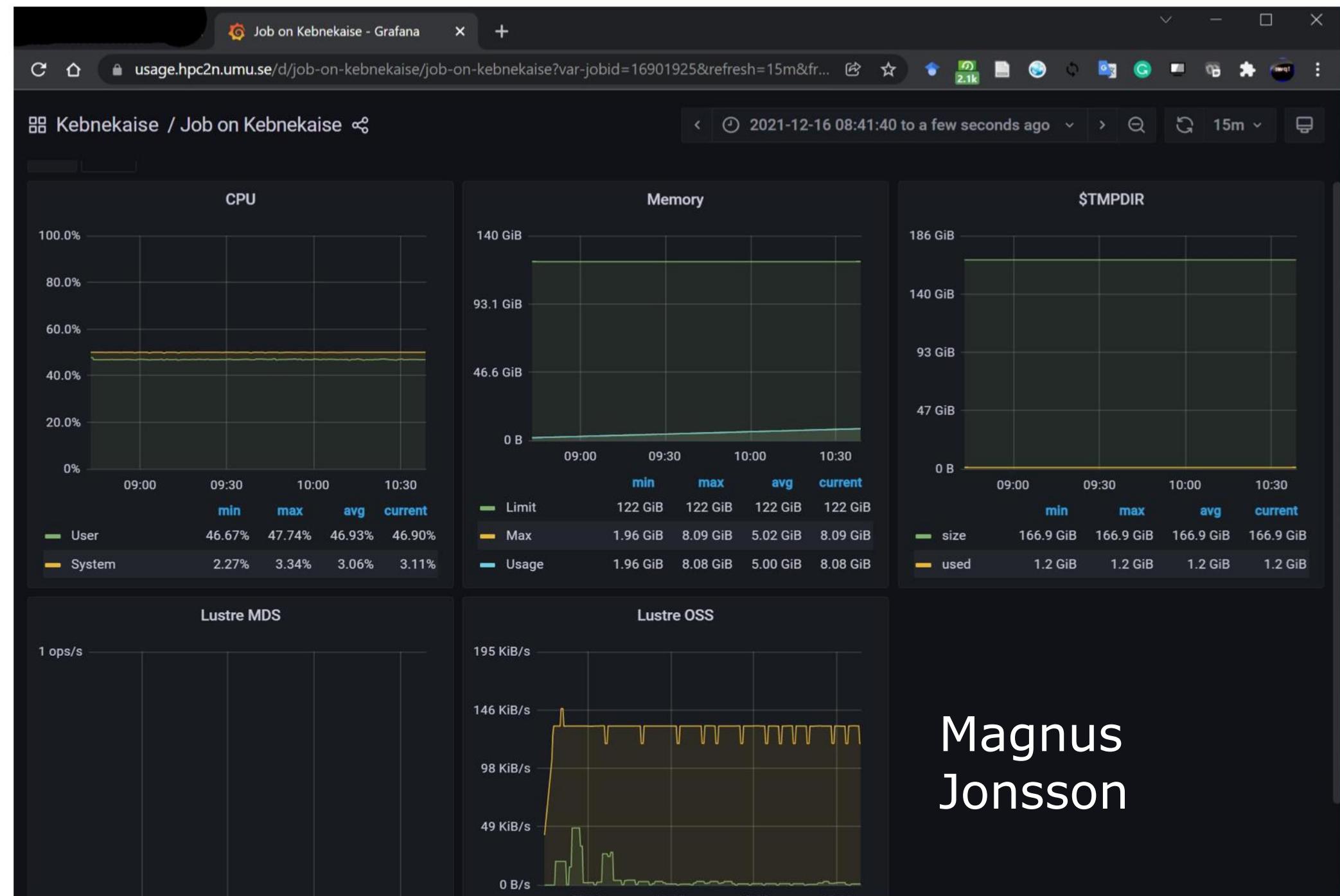
```
#!/bin/bash
#SBATCH -A staff
#SBATCH -N 1
#SBATCH -c 28
#SBATCH --exclusive
#SBATCH --gres=gpu:k80:2
#SBATCH --time=00:10:00

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**

# 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?
- Use **job-usage** script on the command line, this will allow you to monitor the resources usage in your local browser

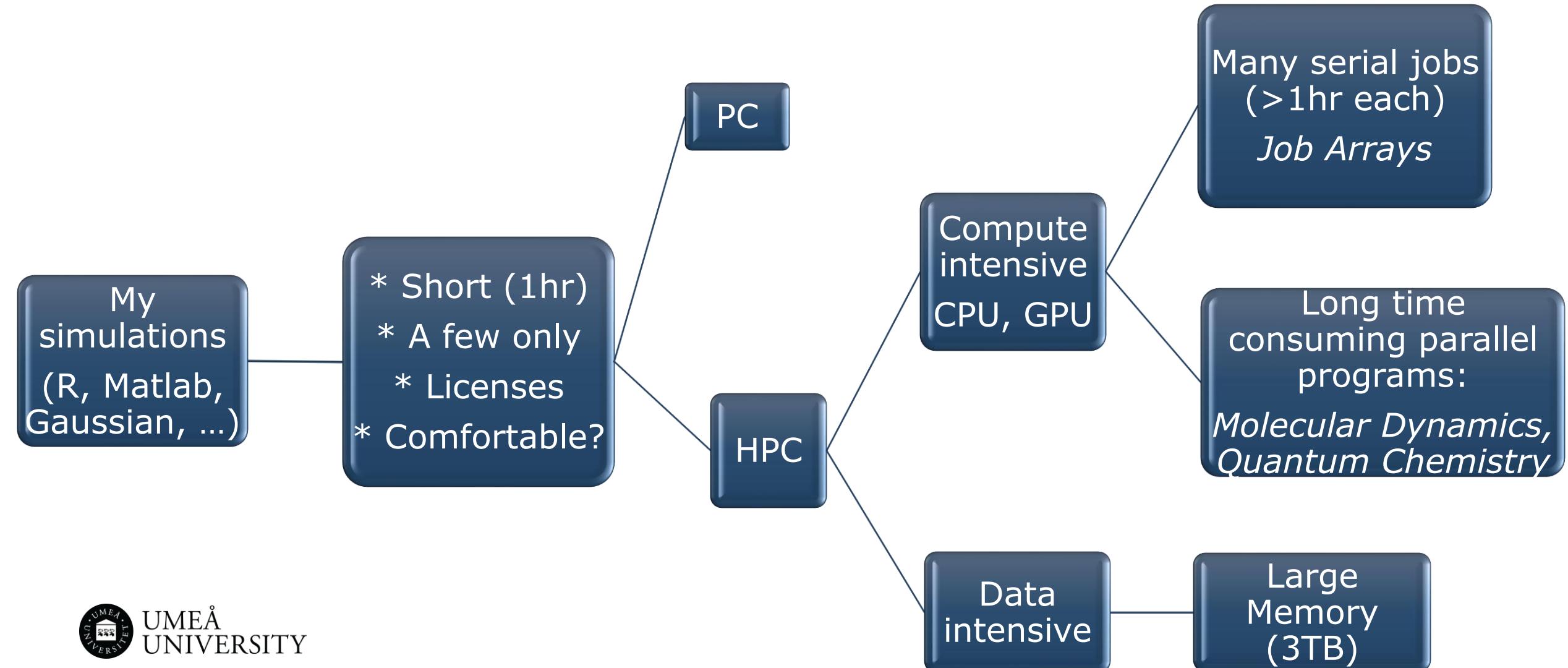


Magnus  
Jonsson

# 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.**
- Keep the topics of the support tickets independent (one ticket per case)
- 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 cause troubles with software.
- Don't forget to cite HPC2N upon publishing.

# Why/when to use HPC?



# HPC2N success stories

*Clinical Infectious Diseases*  
MAJOR ARTICLE



## Managing Coronavirus Disease 2019 Spread With Voluntary Public Health Measures: Sweden as a Case Study for Pandemic Control

Shina C. L. Kamerlin<sup>1</sup> and Peter M. Kasson<sup>2,3,□</sup>

<sup>1</sup>Science for Life Laboratory, Department of Chemistry–BMC, Uppsala University, Uppsala, Sweden, <sup>2</sup>Science for Life Laboratory, Department of Cell and Molecular Biology, Uppsala University, Uppsala, Sweden, and <sup>3</sup>Departments of Molecular Physiology and Biomedical Engineering, University of Virginia, Charlottesville, Virginia, USA



# HPC2N success stories

## Mechanistic Basis for a Connection between the Catalytic Step and Slow Opening Dynamics of Adenylate Kinase

Beata Dulko-Smith, Pedro Ojeda-May, Jörgen Ådén, Magnus Wolf-Watz, and Kwangho Nam\*



Cite This: *J. Chem. Inf. Model.* 2023, 63, 1556–1569



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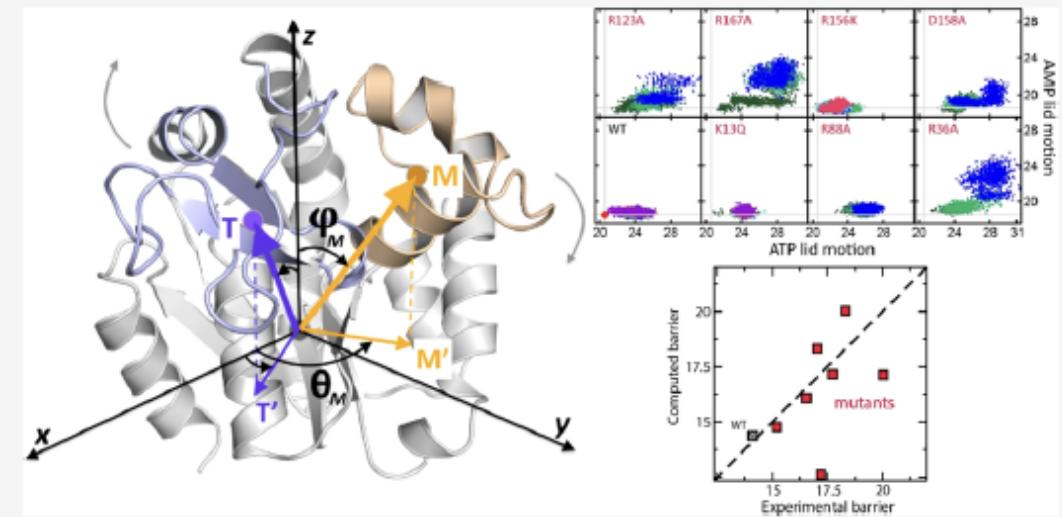
ACCESS |

Metrics & More

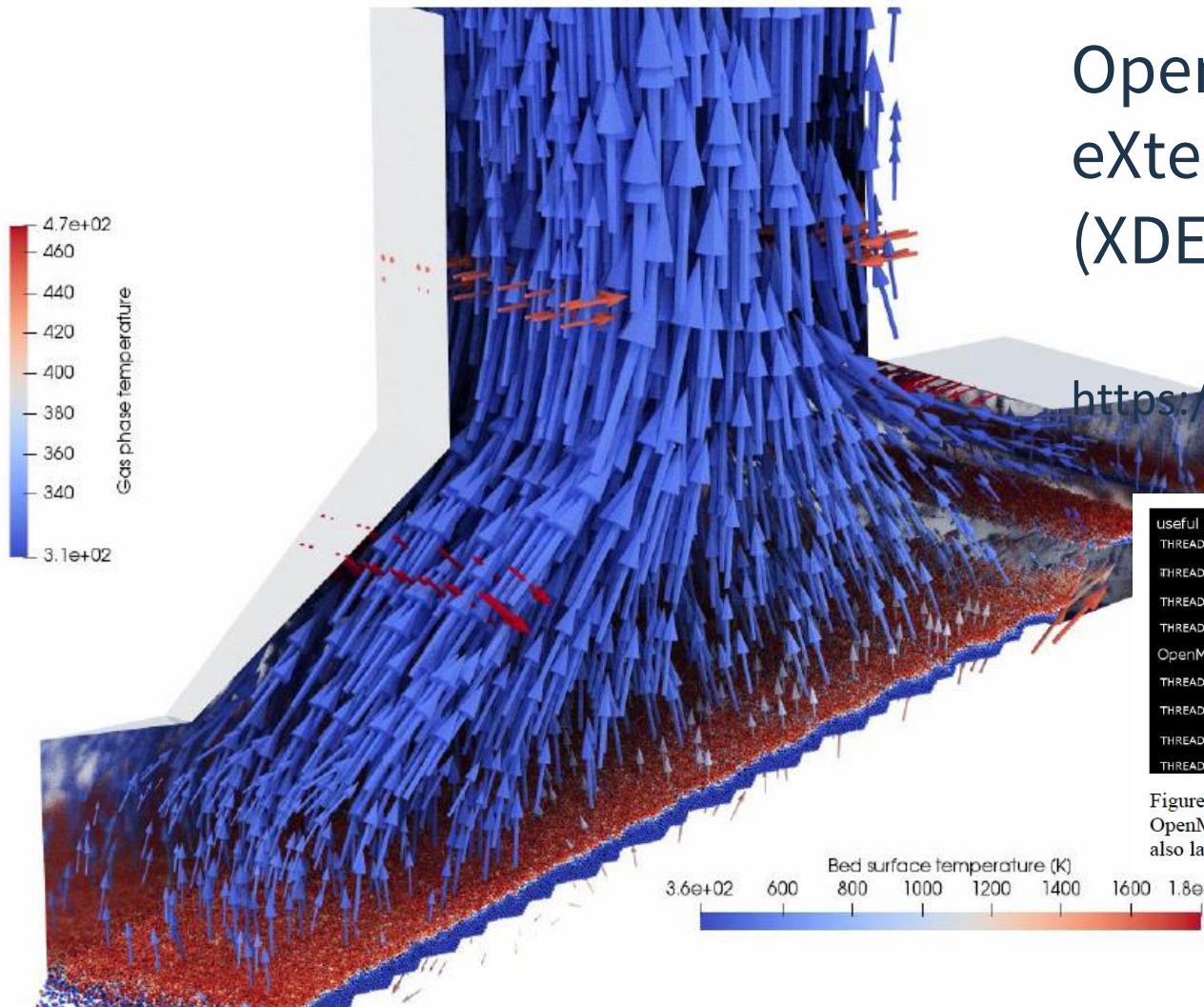
Article Recommendations

SI Supporting Information

**ABSTRACT:** *Escherichia coli* adenylate kinase (AdK) is a small, monomeric enzyme that synchronizes the catalytic step with the enzyme's conformational dynamics to optimize a phosphoryl transfer reaction and the subsequent release of the product. Guided by experimental measurements of low catalytic activity in seven single-point mutation AdK variants (K13Q, R36A, R88A, R123A, R156K, R167A, and D158A), we utilized classical mechanical simulations to probe mutant dynamics linked to product release, and quantum mechanical and molecular mechanical calculations to compute a free energy barrier for the catalytic event. The goal was to establish a mechanistic connection between the two activities.



# HPC2N success stories



OpenMP optimisation of the eXtended Discrete Element Method (XDEM)

<https://prace-ri.eu/wp-content/uploads/WP298.pdf>

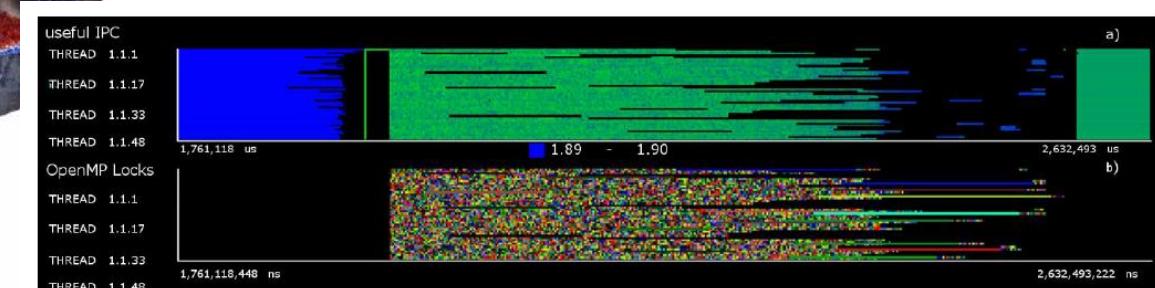
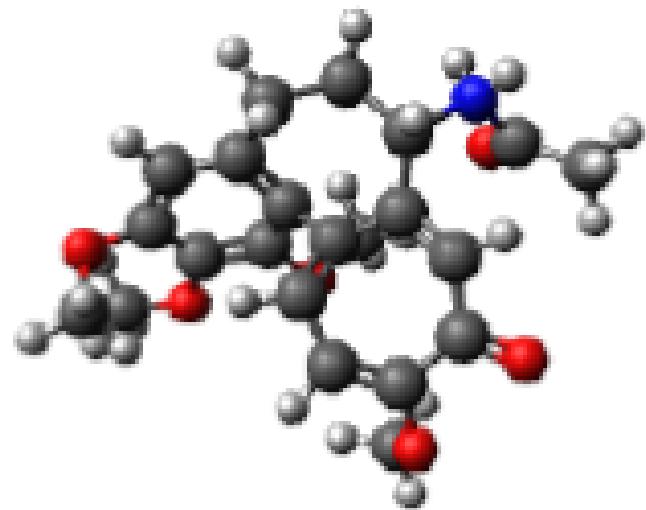


Figure 2. Initial profiling analysis with Extrae/Paraver showing the useful Instructions per Clock cycle (IPC) (a) and the OpenMP locks (b) for a cut region of the collected trace. In (a), blue colour represents high while green low IPC. There were also large waiting time regions in black. In (b) the addresses of memory for the locks are displayed with different colours.

Figure 1. Biomass3D test case showing the fuel bed and gas phase, temperature scales are provided in the boxes

# HPC2N success stories

Dr. Christine Gallampois



Collision Cross Sections



$$\Omega_{av} = \frac{1}{4\pi^2} \int_0^{2\pi} d\theta \int_0^\pi d\varphi \sin \varphi \int_0^{2\pi} d\gamma \int_0^\infty db 2b (1 - \cos \chi(\theta, \varphi, \gamma, b))$$

# Reaching out

- Website: <https://www.hpc2n.umu.se/>
- General questions: [info@hpc2n.umu.se](mailto:info@hpc2n.umu.se)
- For questions related to Kebnekaise for instance, software, hardware, login, projects: [support@hpc2n.umu.se](mailto:support@hpc2n.umu.se)
- YouTube channel: <https://www.youtube.com/user/HPC2N>
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