Useful examples

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February 20, 2017

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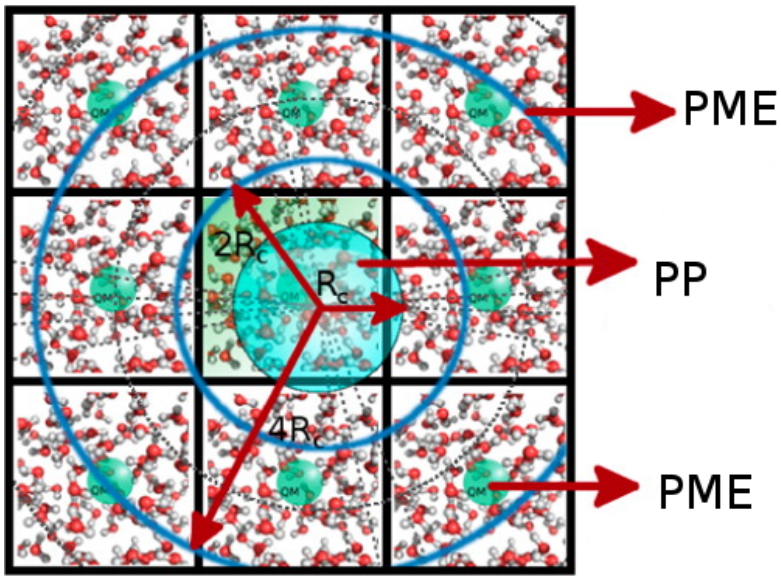
Long-range interactions



adapted from JCTC,10,134 (2014)

- particle-particle interactions are solved in real space (80%)
- PME contribution is solved in reciprocal space (20%)

GROMACS

```
$module spider gromacs
----------------------------------------------------------
  GROMACS:
----------------------------------------------------------
    Description:
      GROMACS is a versatile package to perform molecular
      systems with hundreds to millions of particles. -

     Versions:
        GROMACS/5.1.4-hybrid
        GROMACS/5.1.4-mt
        GROMACS/2016-hybrid
        GROMACS/2016-mt

----------------------------------------------------------
  For detailed information about a specific "GROMACS"
  For example:
```

GROMACS

```
$module spider GROMACS/2016-hybrid
----------------------------------------------------------
  GROMACS: GROMACS/2016-hybrid
----------------------------------------------------------
 Description:
   GROMACS is a versatile package to ...
   Homepage: http://www.gromacs.org

   You will need to load all module(s) on any one of
   the lines below before the "GROMACS/2016-hybrid" ...

   GCC/5.4.0-2.26  CUDA/8.0.44  OpenMPI/2.0.1
   GCC/6.2.0-2.27  OpenMPI/2.0.1
```

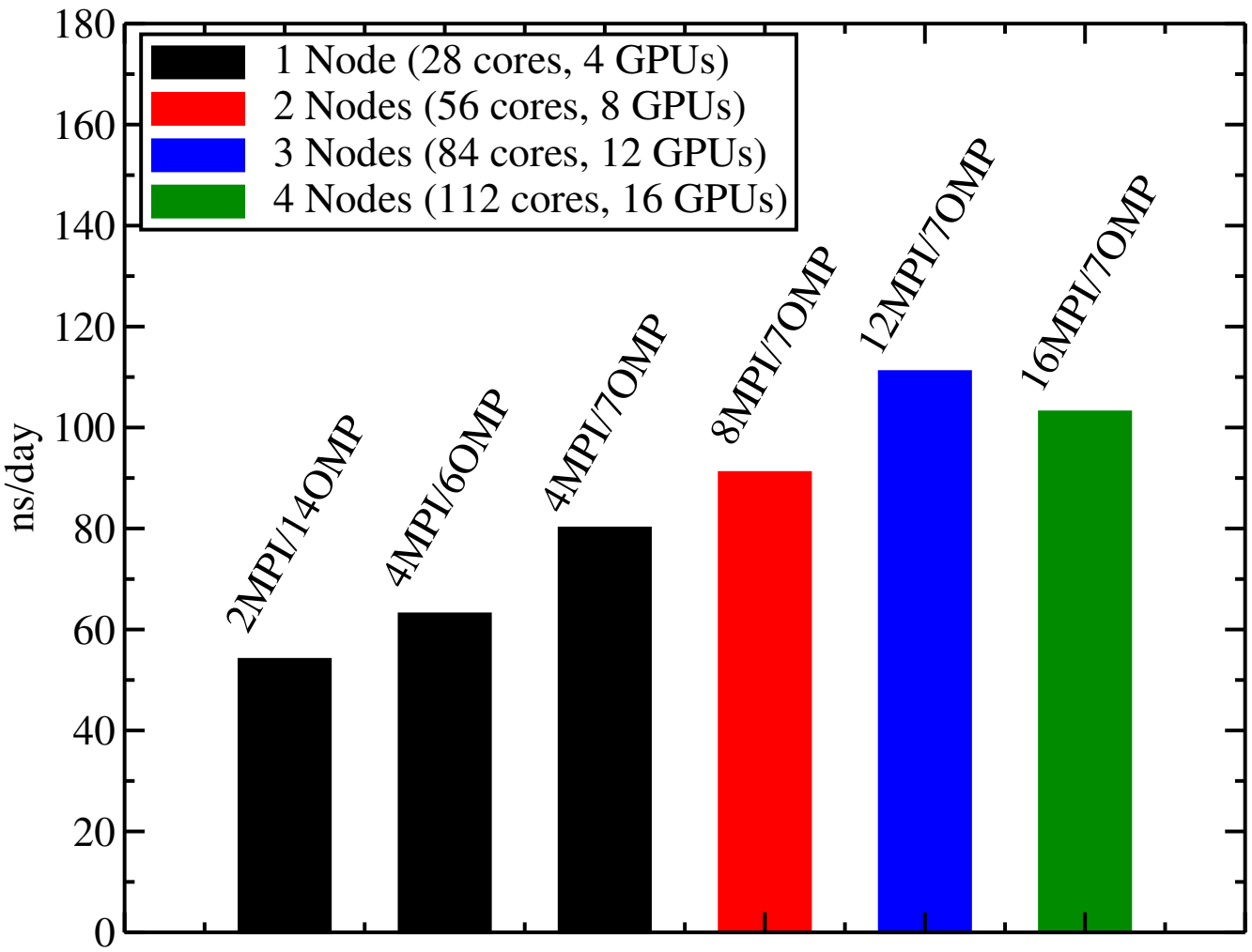
GROMACS batch script

```
#!/bin/bash
#SBATCH -A ~SNICYYYY-XX-NN
#SBATCH -J G2016-gpu
#SBATCH -t 01:00:00
#SBATCH -n 12
#SBATCH -c 7
#SBATCH --gres=gpu:k80:2
#SBATCH -p batch
module add CUDA/8.0.44   GCC/5.4.0-2.26
module add OpenMPI/2.0.1 GROMACS/2016-hybrid
mdargs="-ntomp $SLURM_CPUS_PER_TASK"
mpirun -np $SLURM_NTASKS gmx_mpi mdrun $mdargs \
-dlb yes  -v -deffnm npt
```

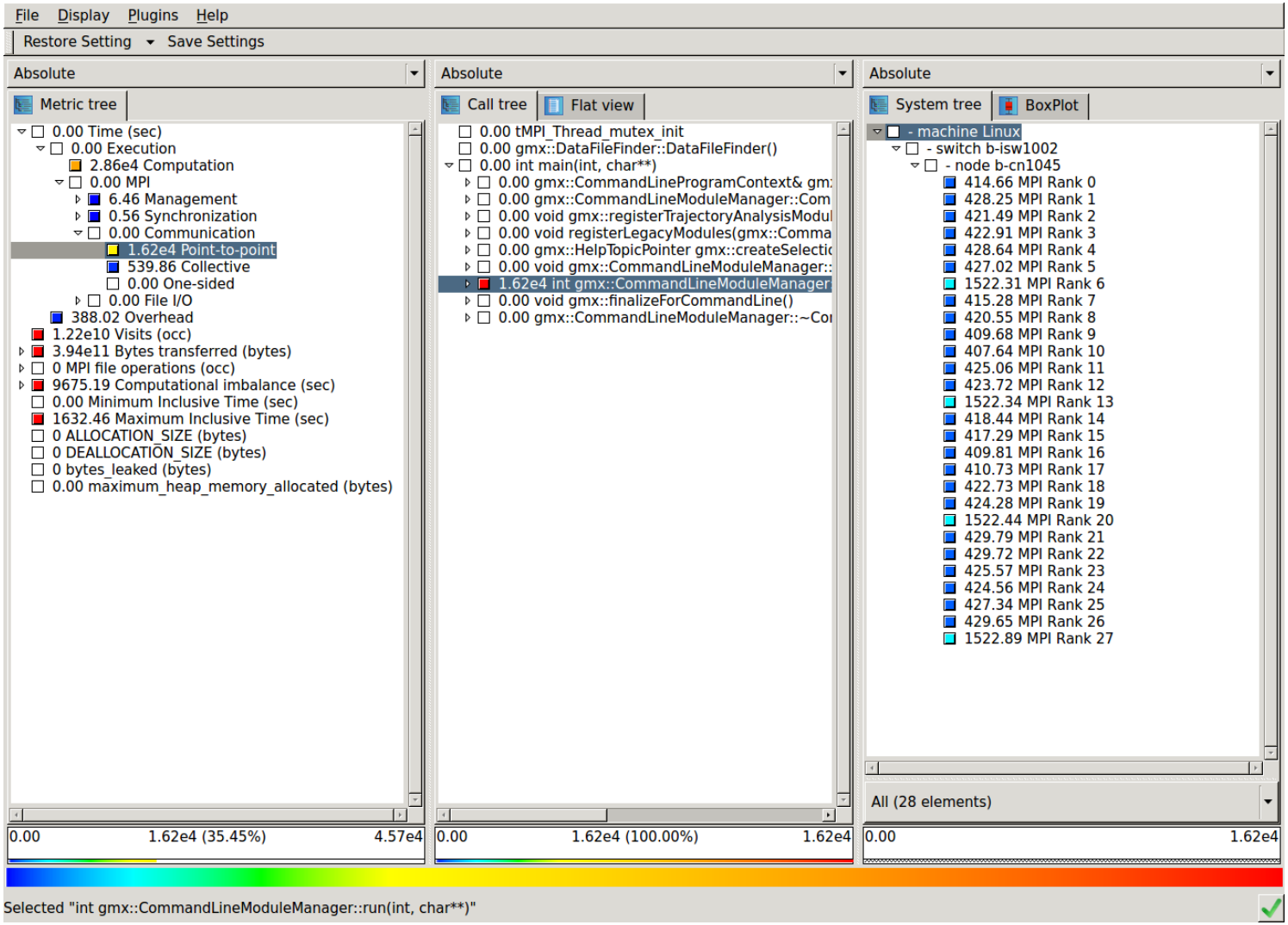
GROMACS output

```
Running on 3 nodes with total 84 cores,
84 logical cores, 12 compatible GPUs
  Cores per node:            28
  Logical cores per node:    28
  Compatible GPUs per node:  4
  All nodes have identical type(s) of GPUs
```

GROMACS performance 100K atoms



Profiling Tools SCALASCA/GROMACS



DOMDEC CHARMM

```
module add GCCcore/5.4.0
module add GCC/5.4.0-2.26
module add CUDA/8.0.44

./install.com gnu M fftw  domdec_gpu
```

DOMDEC CHARMM

```
<domdec_dr_common> No direct/recip split, using all nodes c
Number of CUDA devices found 4
Using CUDA driver version 8000
Using CUDA runtime version 8000
Node 0 uses CUDA device 3 Tesla K80 with CUDA_ARCH 350
Intel CPU | Using CUDA version of non-bonded force loops ar
Initializing DOMDEC with NDIR =   1  1  1
Number of threads per MPI node =  28
Dynamic Load Balancing disabled
Splitting recip cores into (y by z):   1 by    1
```

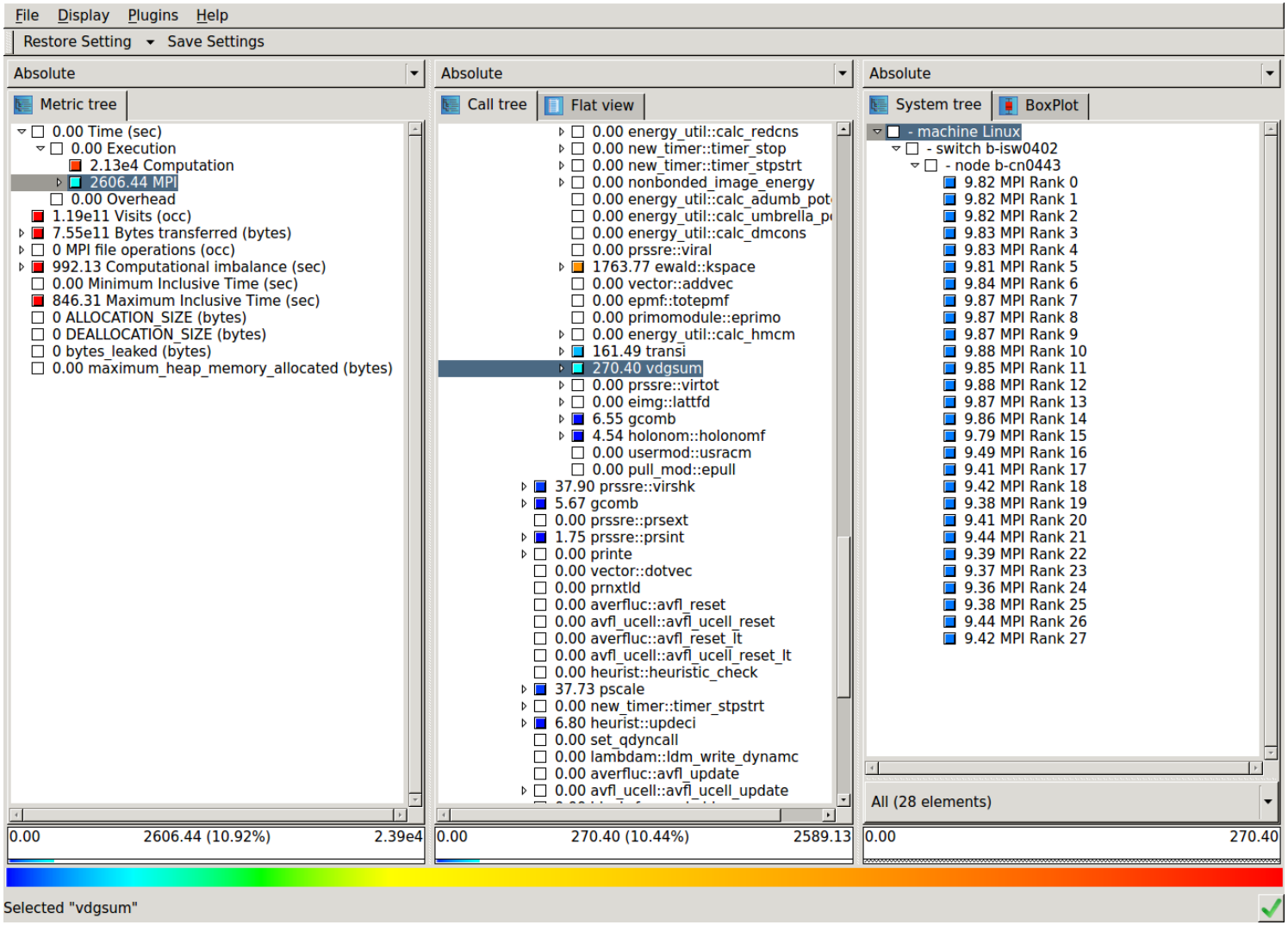
batch script DOMDEC CHARMM

```
#!/bin/bash
#SBATCH -A staff
#SBATCH -J G2016-gpu
#SBATCH -t 12:00:00
#SBATCH -n 1          ##number of mpis
#SBATCH -c 28          ##number of openmp threads
#SBATCH --gres=gpu:k80:2
#SBATCH -p batch

module add GCCcore/5.4.0 GCC/5.4.0-2.26 CUDA/8.0.44

mpirun -np $SLURM_NTASKS -x OMP_NUM_THREADS=28 \
 --bind-to none /home/p/pojedama/pfs/c42a1/ \
exec/gnu_M/charmm < m.inp > out.dat
```

Profiling Tools SCALASCA/CHARMM



batch script GAUSSIAN

```
#!/bin/bash
#SBATCH -A staff
#SBATCH --error=structure.err
#SBATCH --output=structure.out
#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 in the submit direct
g16.set-cpu+gpu-list input.com
```

GAUSSIAN on GPUs

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

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
```