HOOMD-blue - Scalable Molecular Dynamics and Monte Carlo

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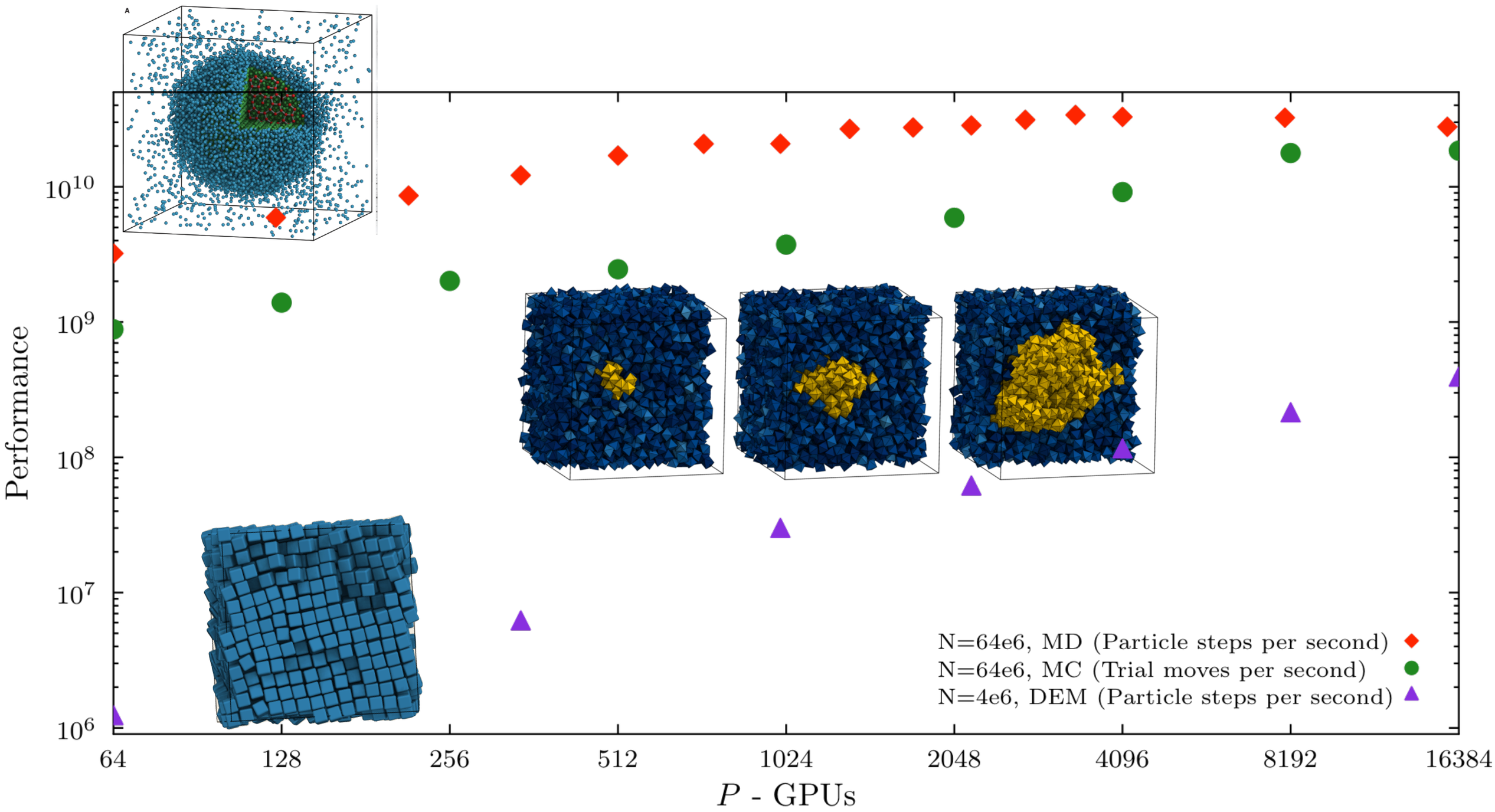
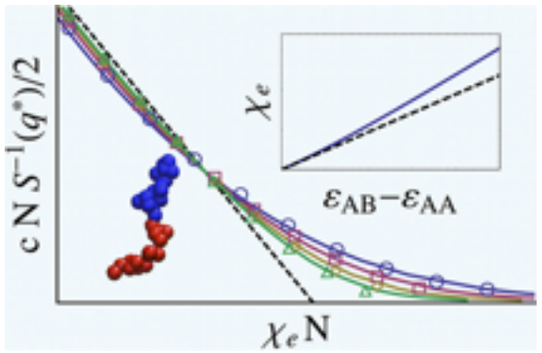
Glotzer Group, Chemical Engineering, University of Michigan

Blue Waters Symposium, Sun River, OR 05/12/2015

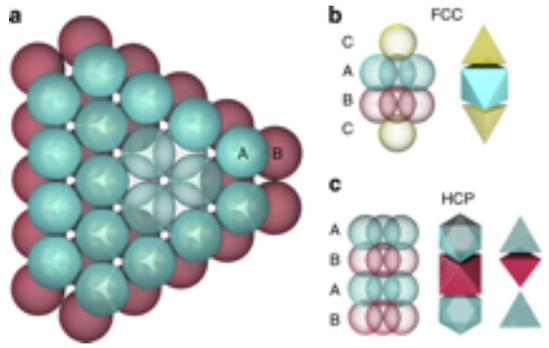
Scaling on OLCF Cray XK7



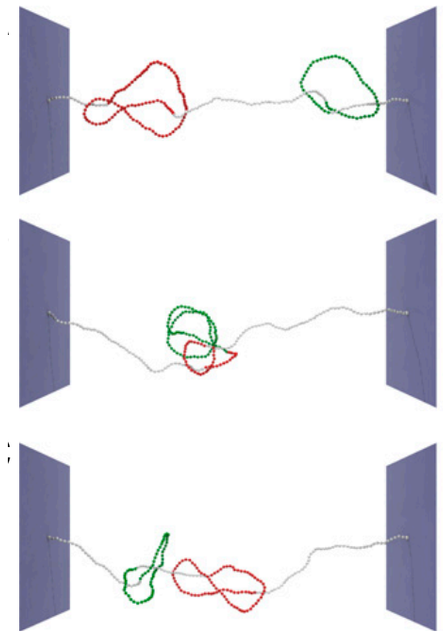
Applications of HOOMD-blue



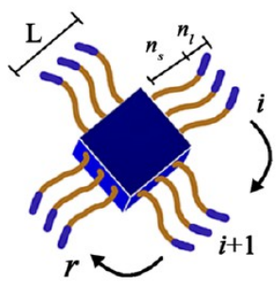
Glaser et al. Macromolecules 2014



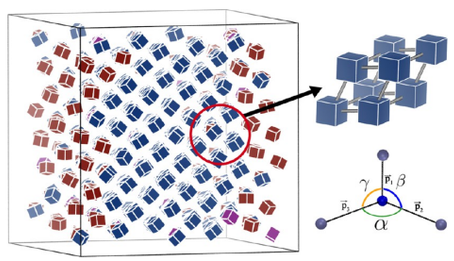
Mahynsk, A. Nat. Comm. 2014



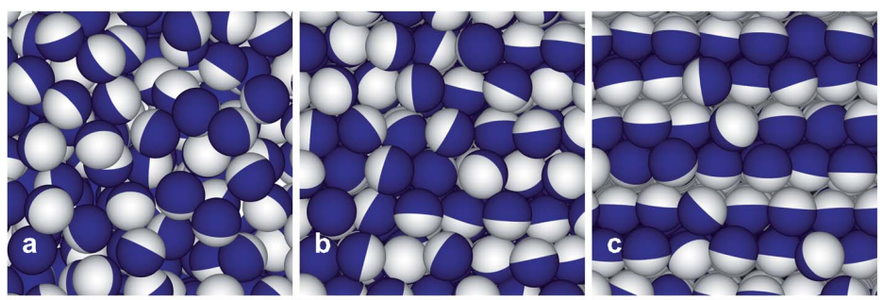
Trefz, B. et al. PNAS 2014

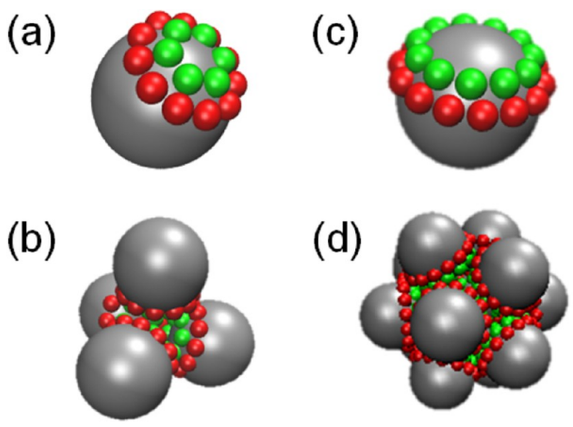


Knorowski, C. and Travesset, A. JACS 2014

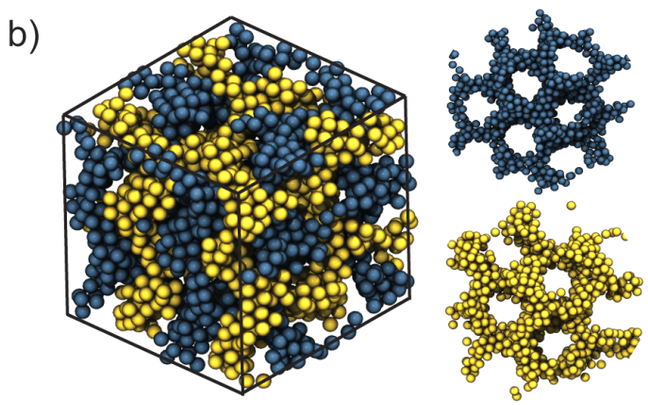


Beltran-Villegas et al. Soft Matter 2014

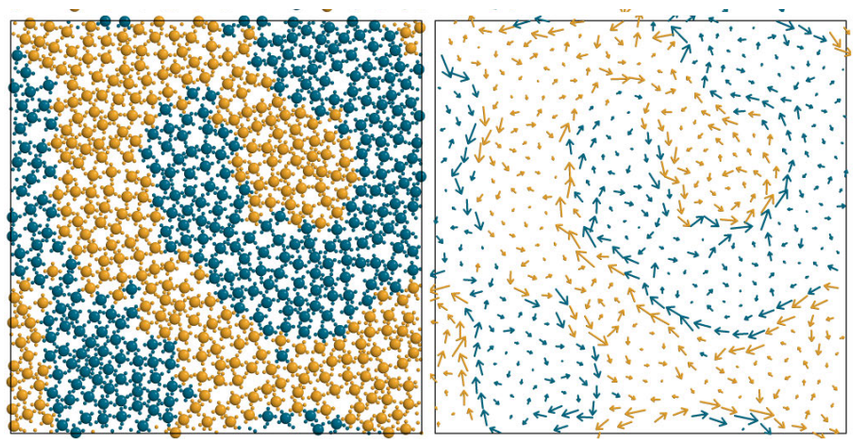




Long, A.W. and Ferguson, A.L. J. Phys. Chem. B 2014



Marson, R. L. et al. Nano Lett. 2014

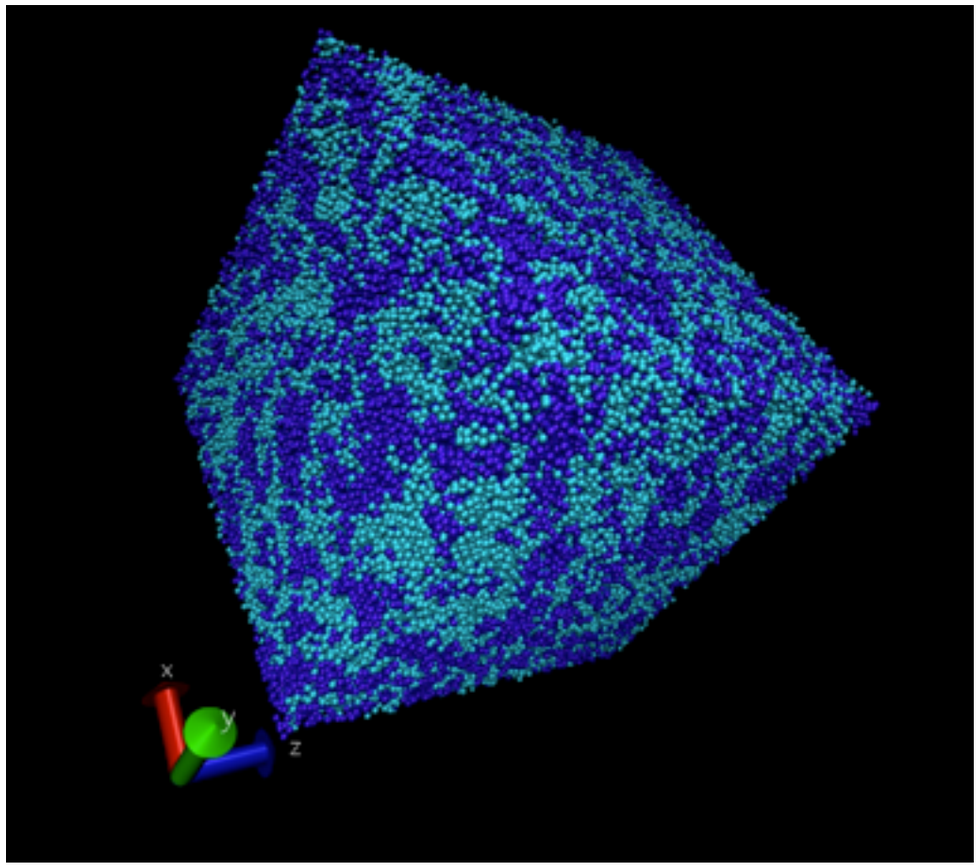


Nguyen et al. Phys Rev. Lett. 2014

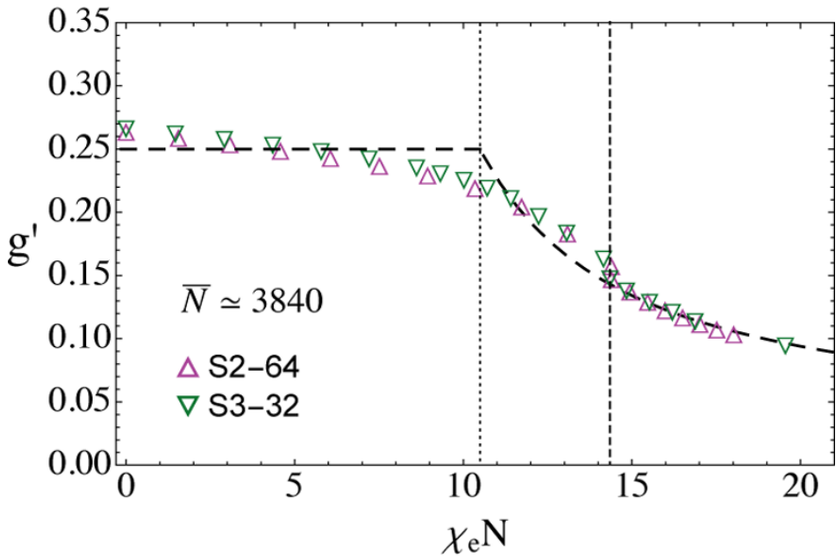
>100 peer-reviewed publications using HOOMD-blue as of May 2015

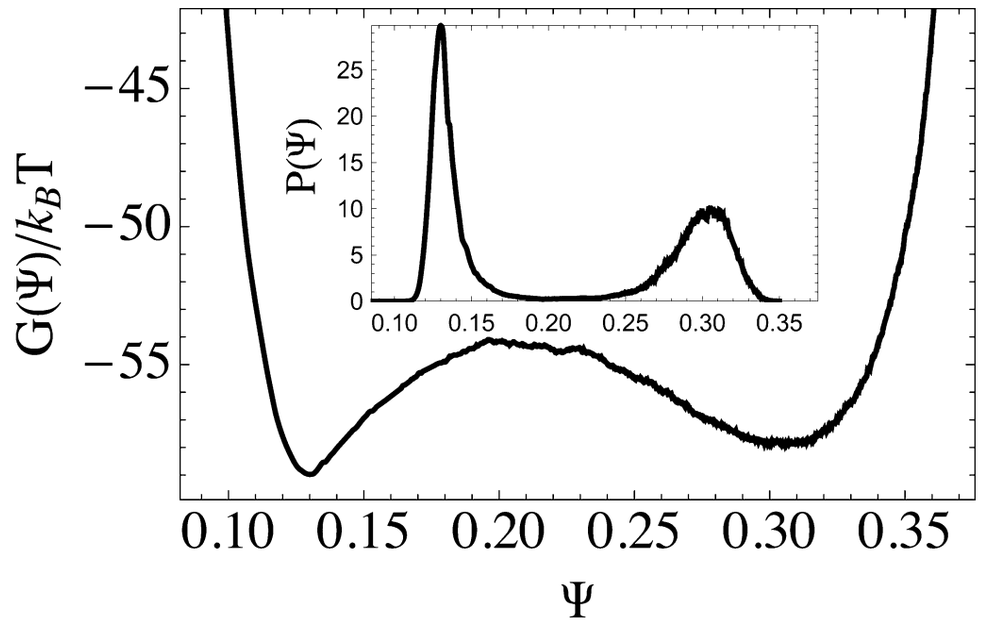
http://codeblue.umich.edu/hoomd-blue/publications.html

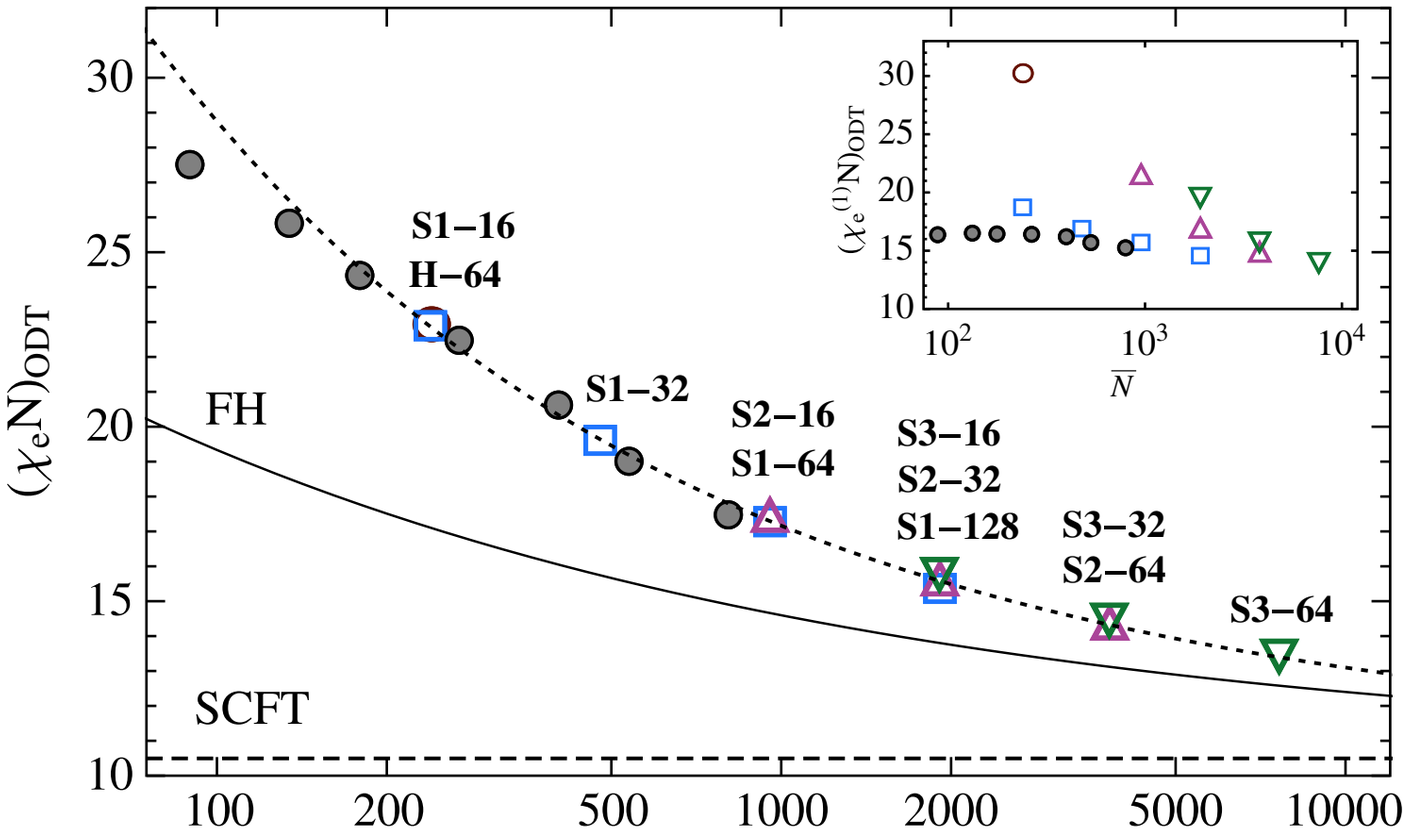
Universality of Block Copolymer Melts



AB Diblock copolymer melt



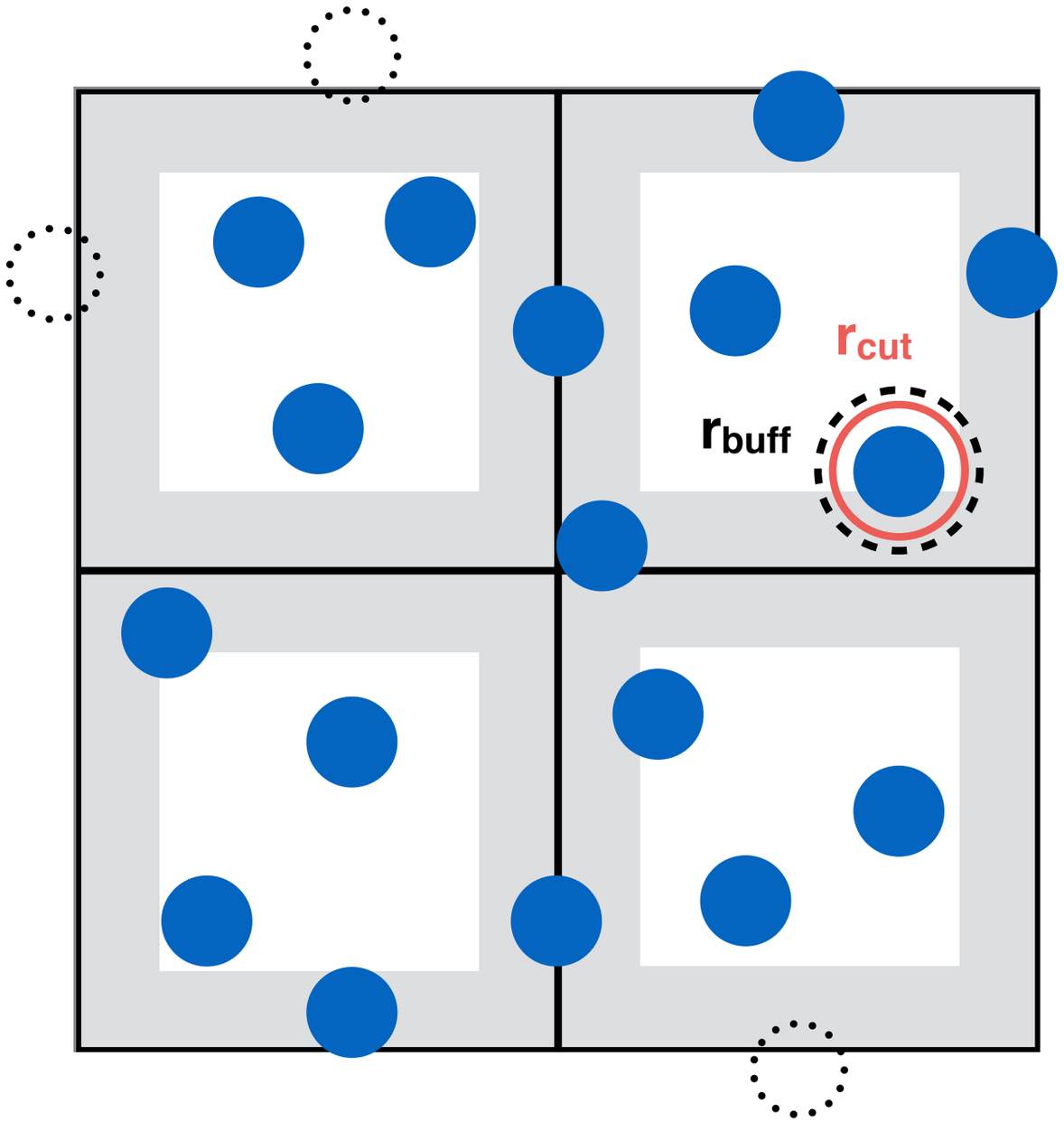




Glaser, J., Medapuram, P., Beardsley, T. M., Matsen, M. W., & Morse, D. C. *PRL*, **113**, 068302 (2014)

Medapuram P., Glaser J., Morse D. C. Macromolecules 2015, **48**, 819-839.

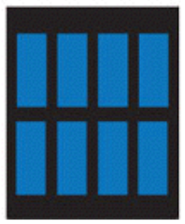
Spatial domain decomposition



- Particles can **leave** and **enter** domains under periodic boundary conditions
- **Ghost** particles required for force computation
- **Update** positions of ghost particles every time step

Scaling bottlenecks in spatial domain decomposition

4-12 cores

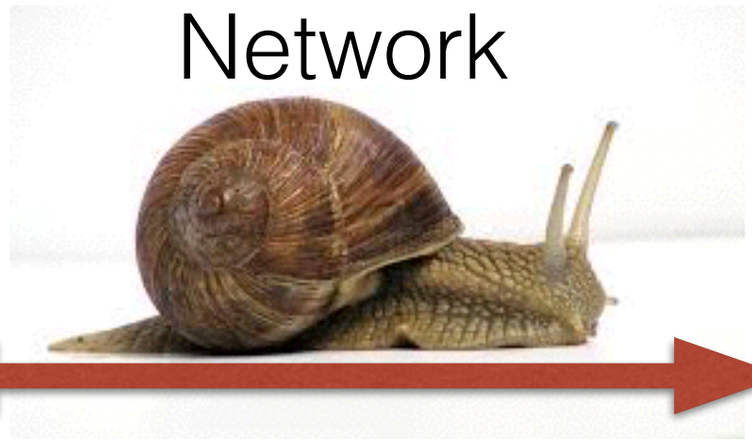


6 GB/s

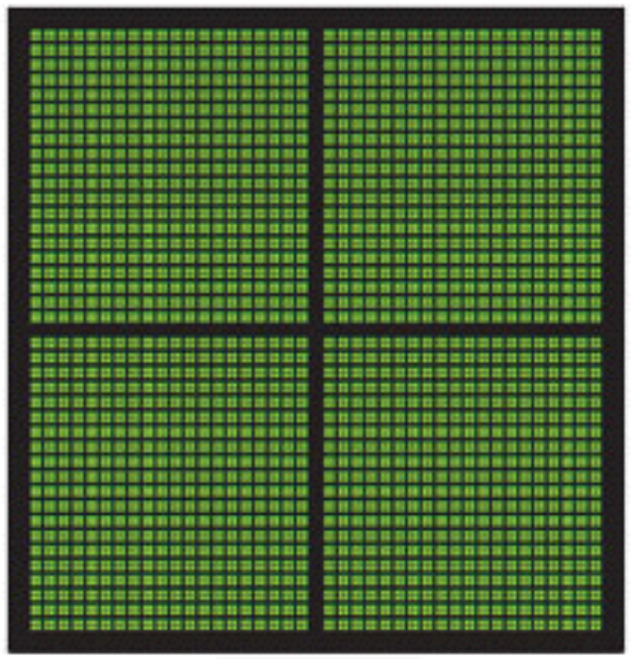
CPU

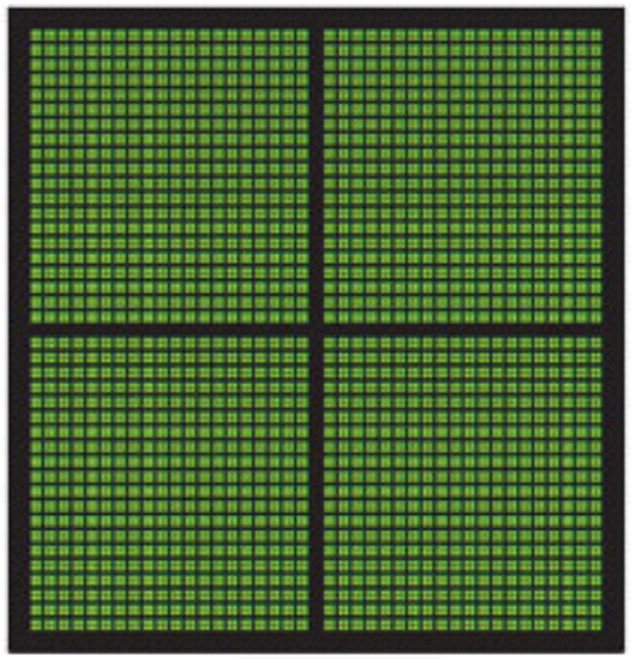
CPU

Network



6 GB/s



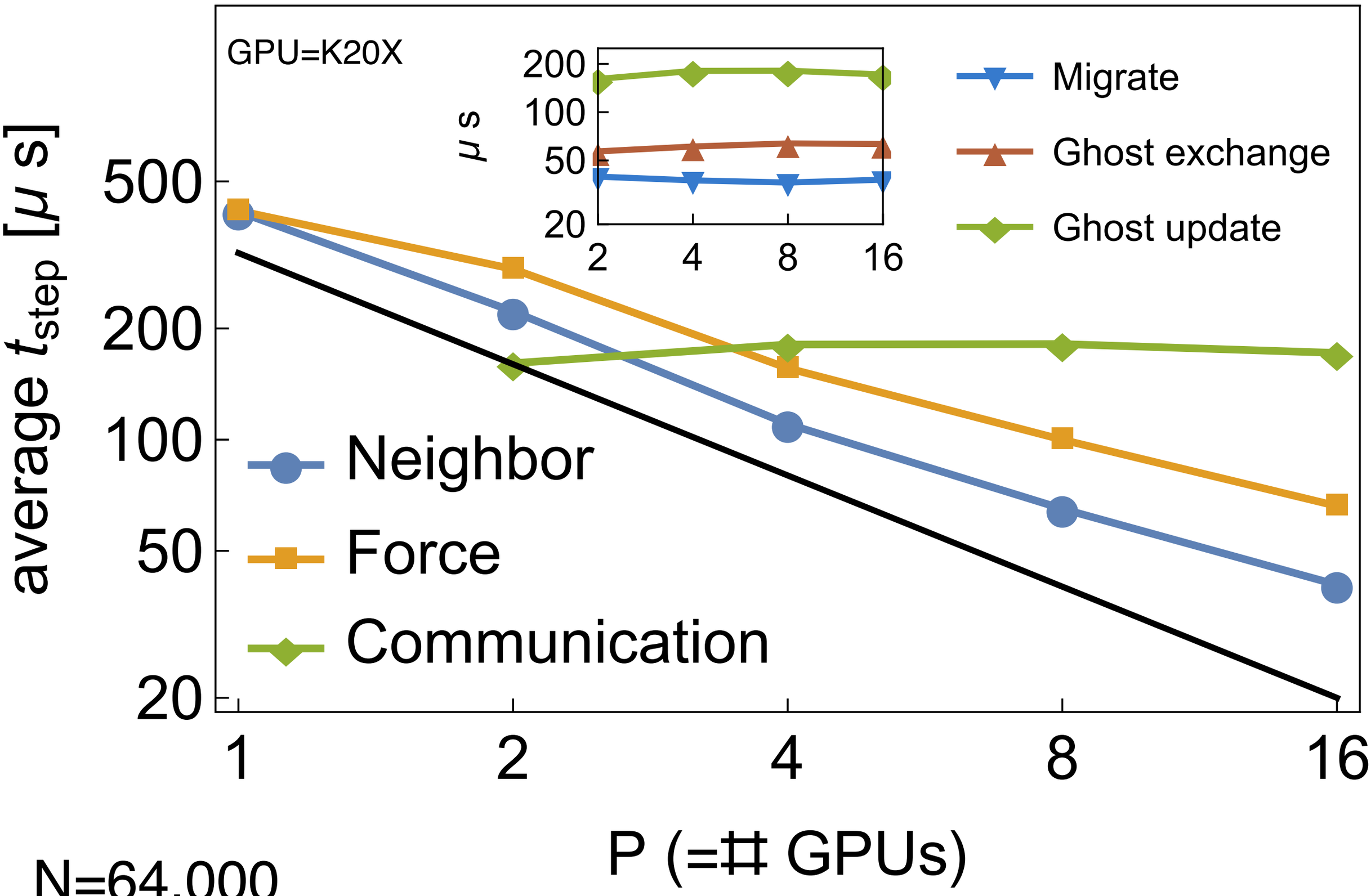


GPU

GPU

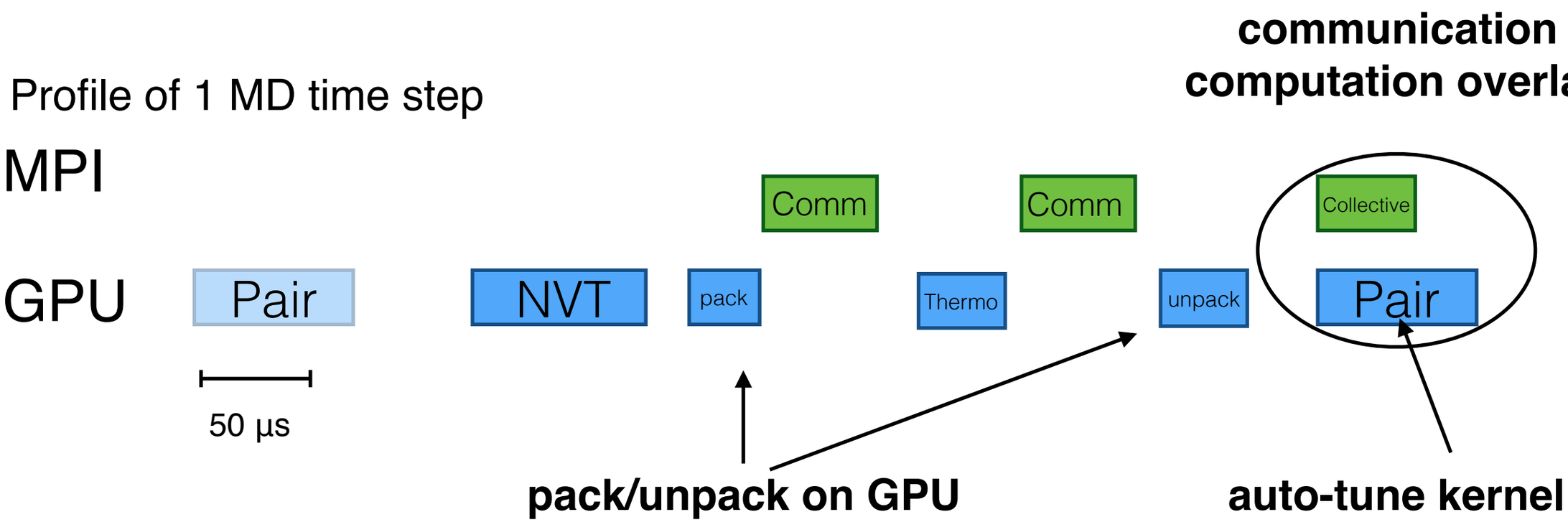
1000’s of cores

Compute vs. Communication



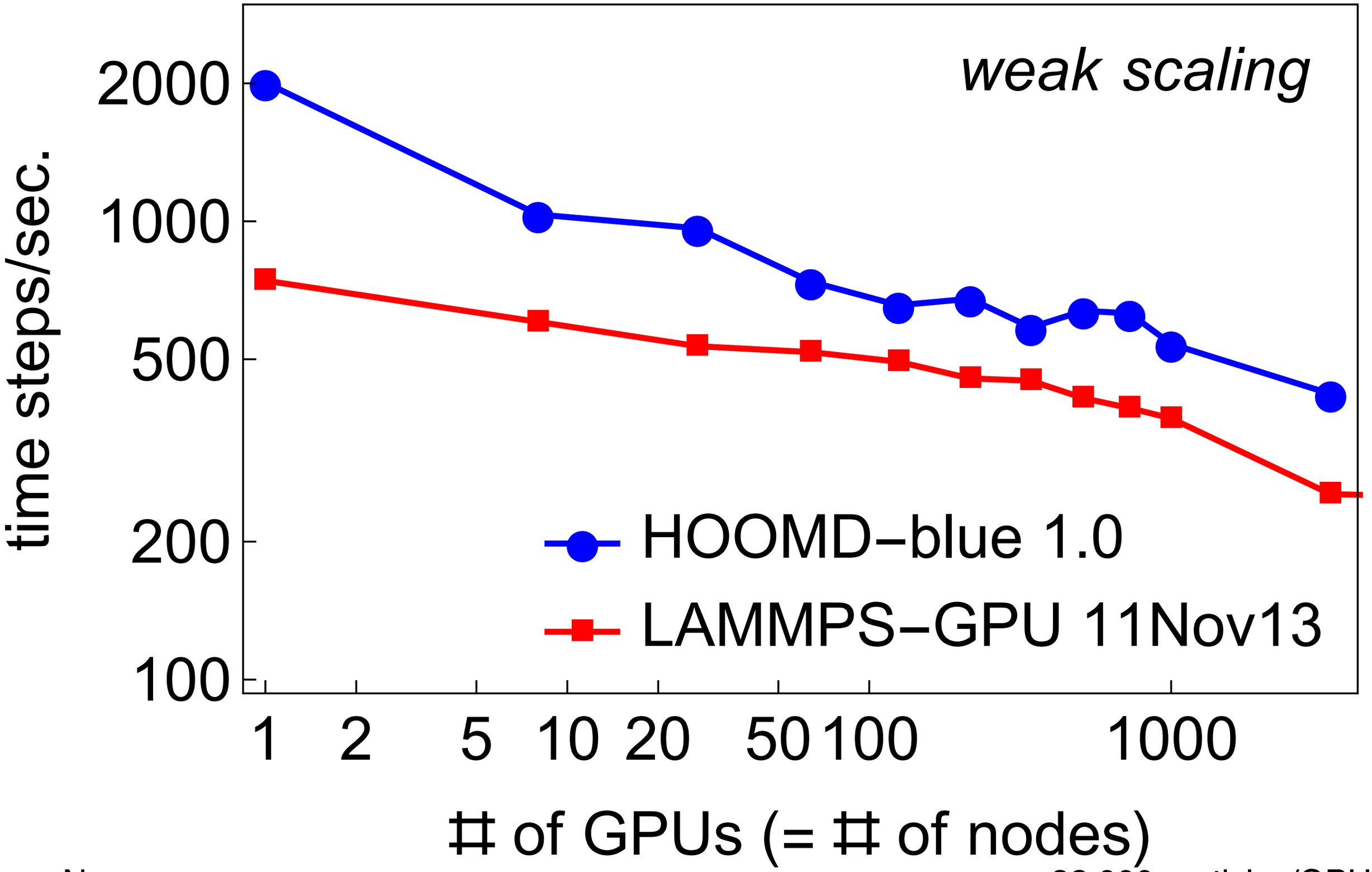
N=64,000

Optimization of the communication algorithm



- **Device-resident** data
- **Autotune** kernels
- **Overlap** synchronization with computation

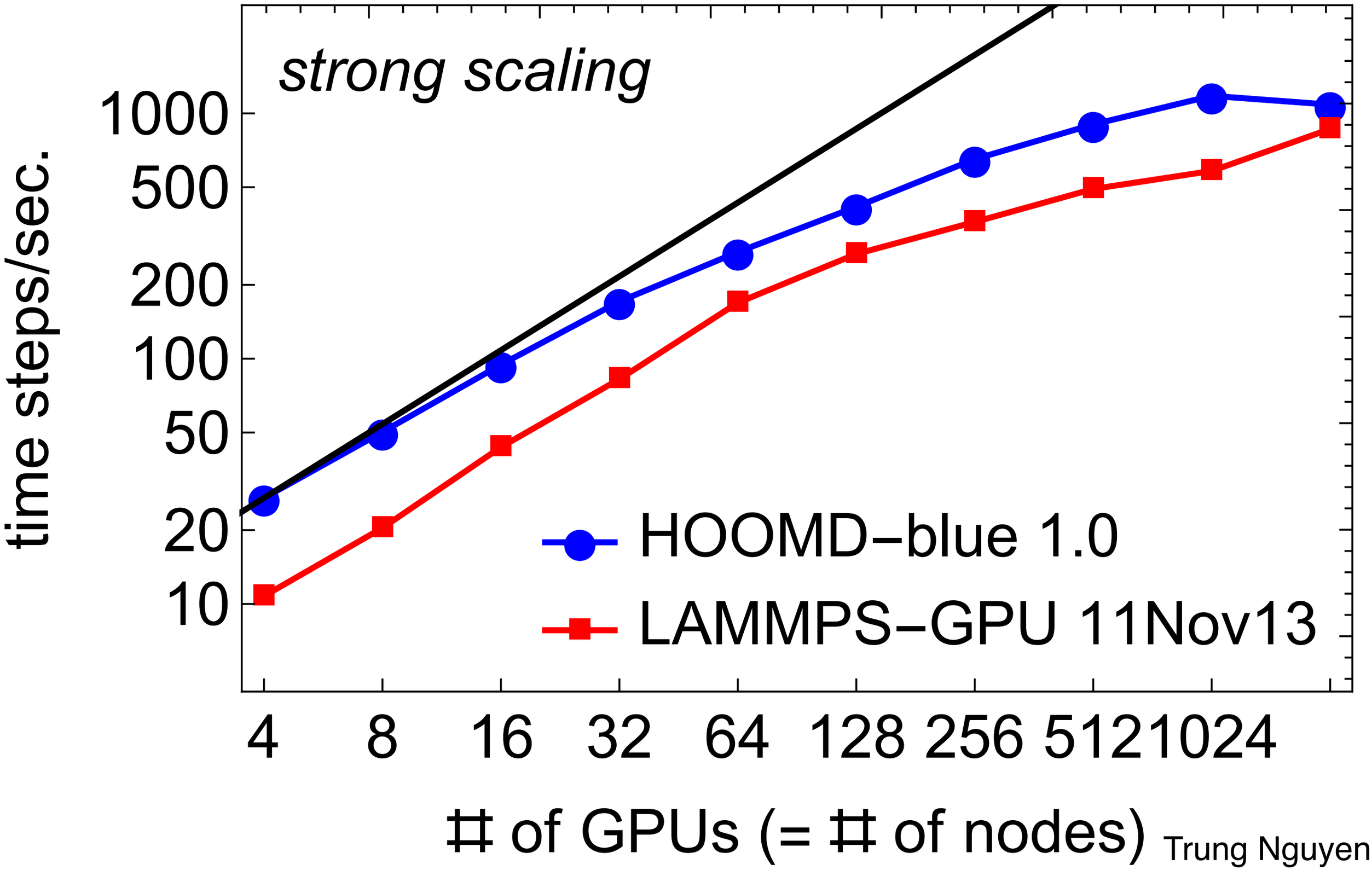
Weak scaling up to 108,000,000 particles



Trung Nguyen

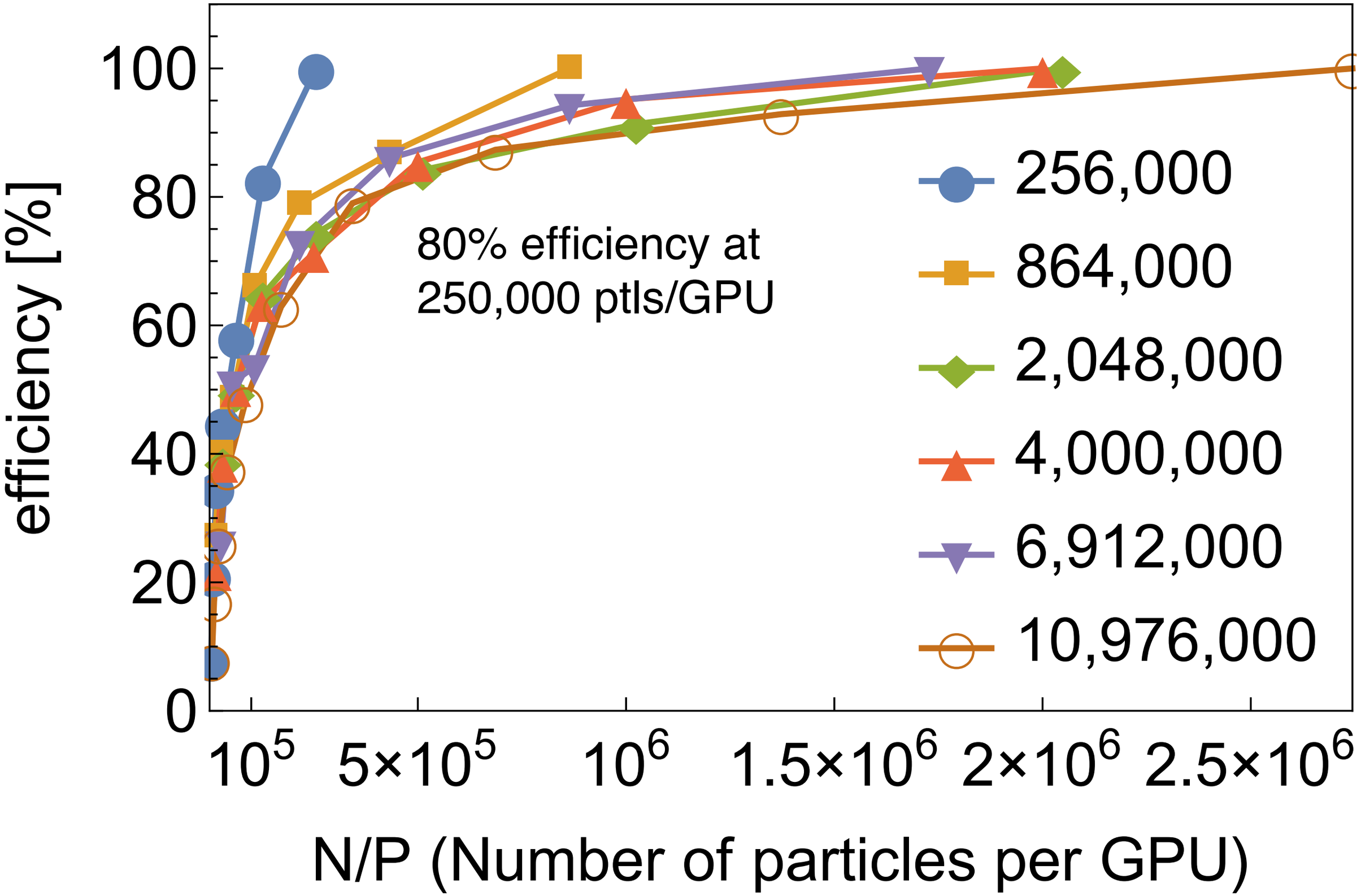
32,000 particles/GPU

Strong Scaling of a LJ Liquid (N=10,976,000)

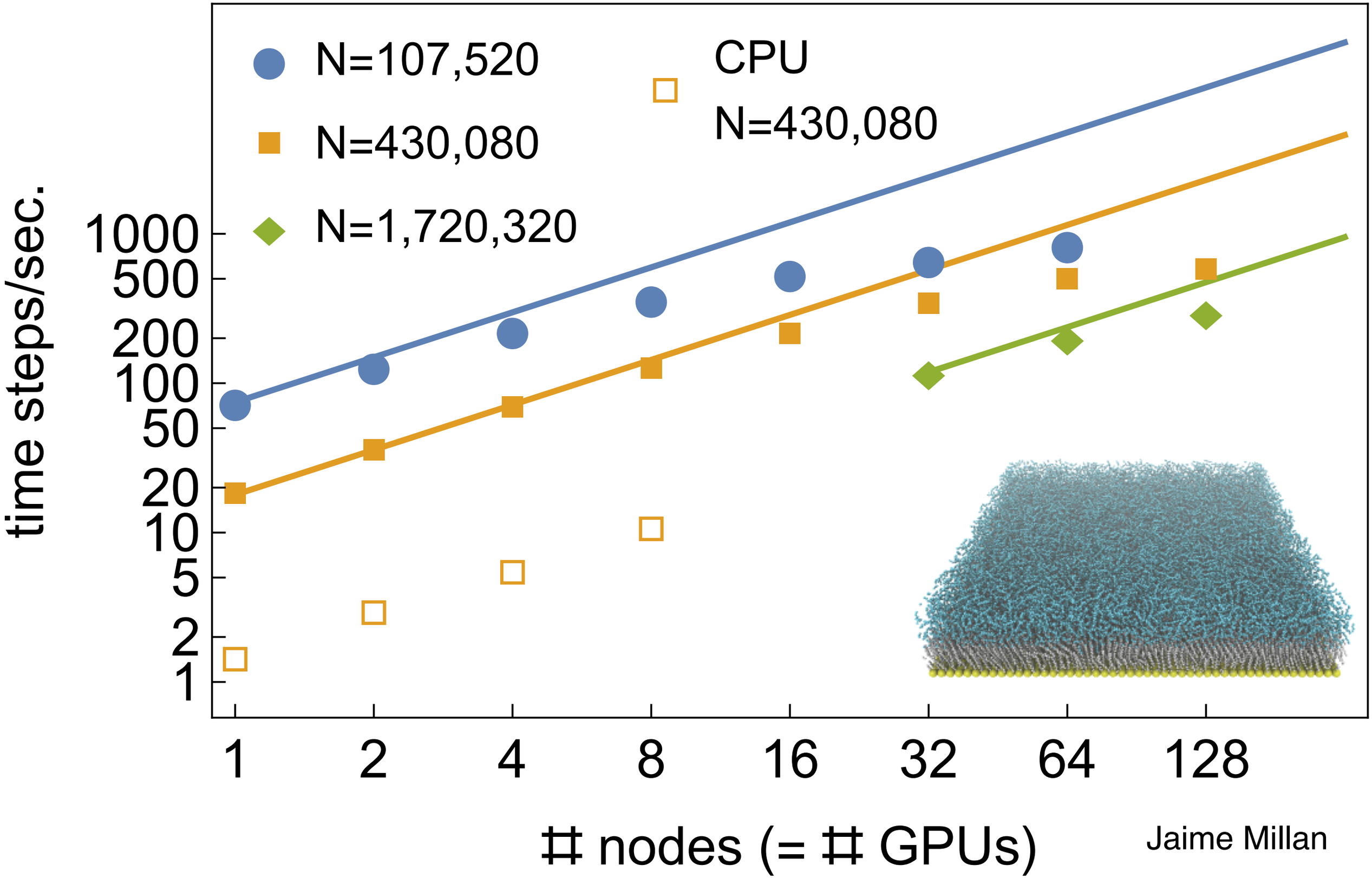


Trung Nguyen

Strong Scaling Efficiency

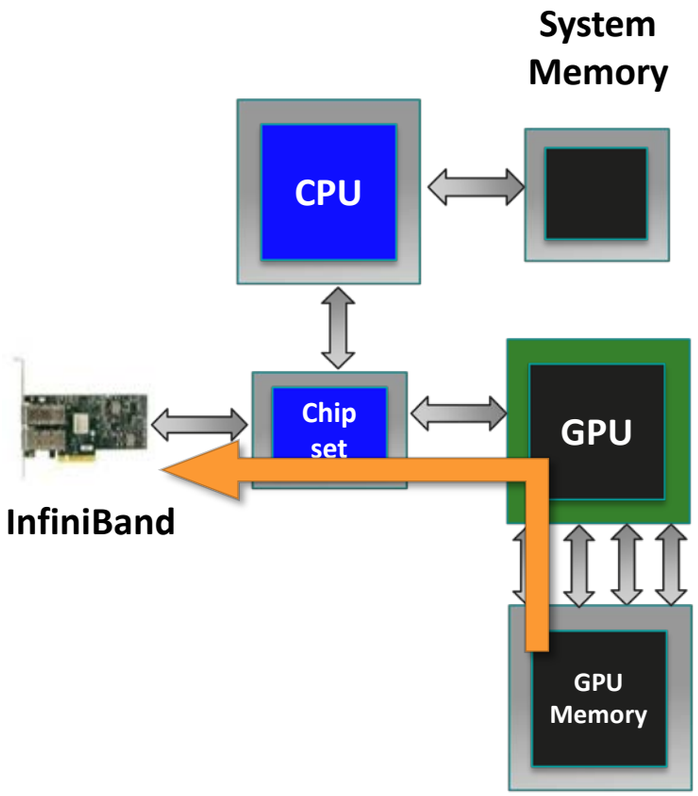


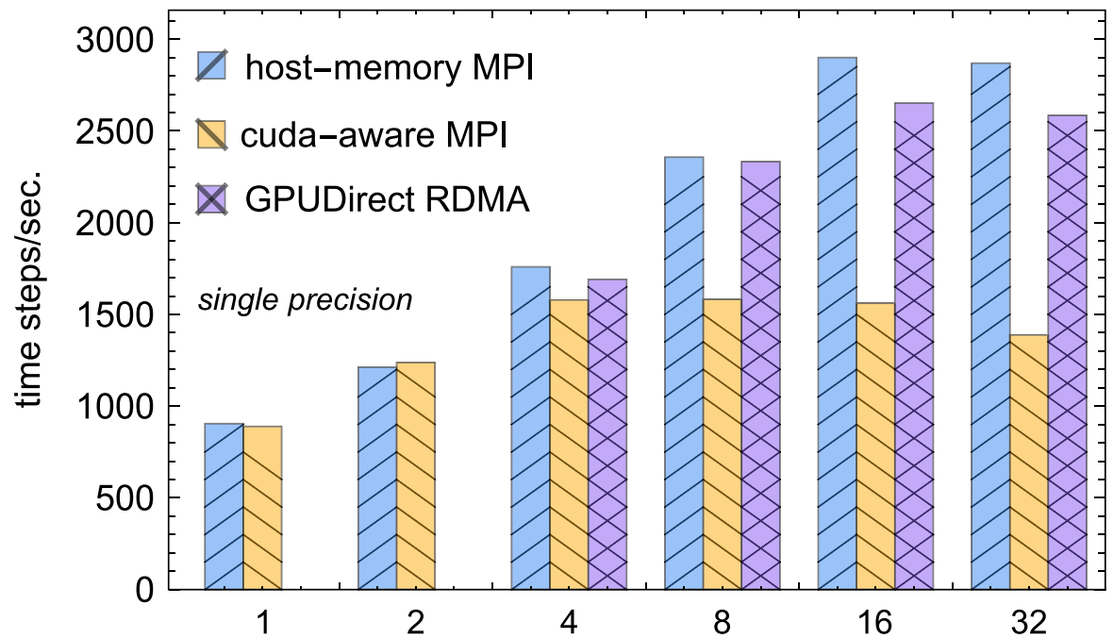
Polymer Brush Scaling

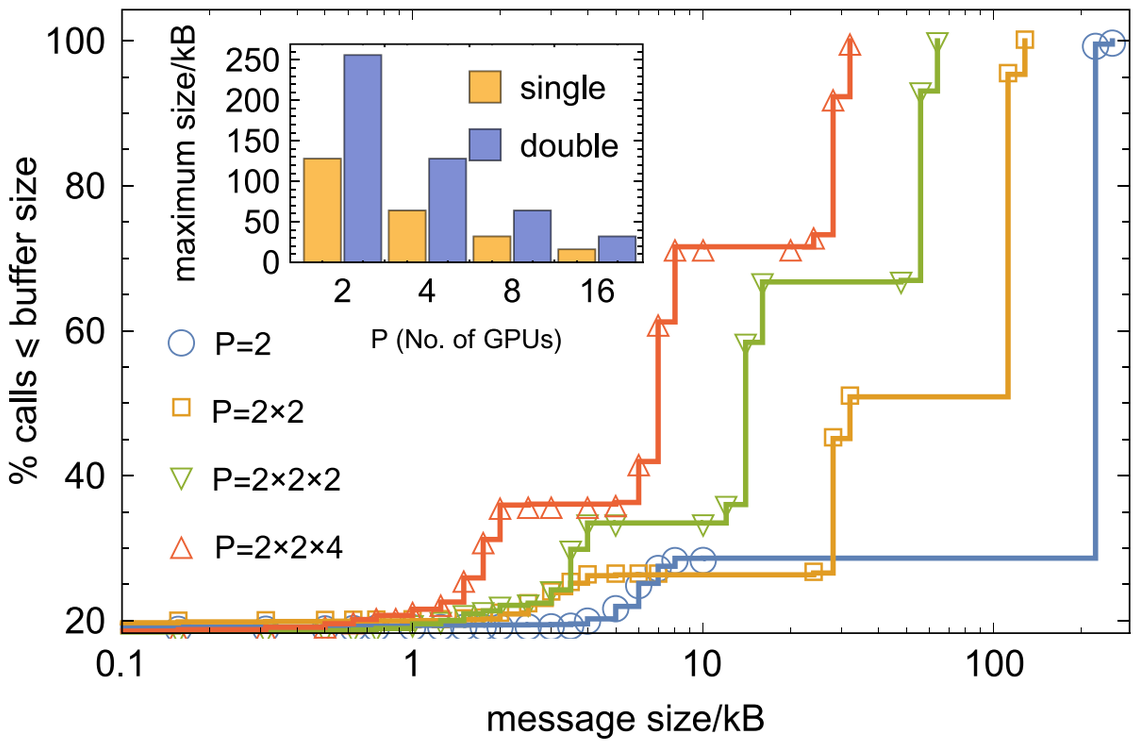


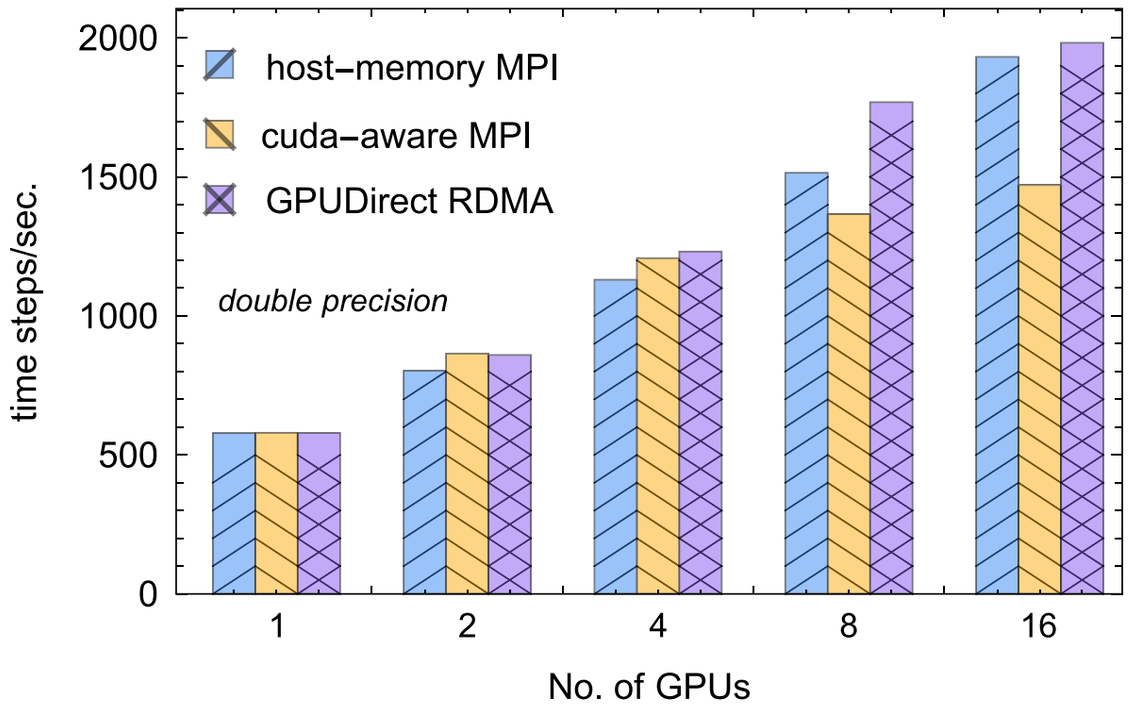
Jaime Millan

GPUDirect RDMA on Wilkes



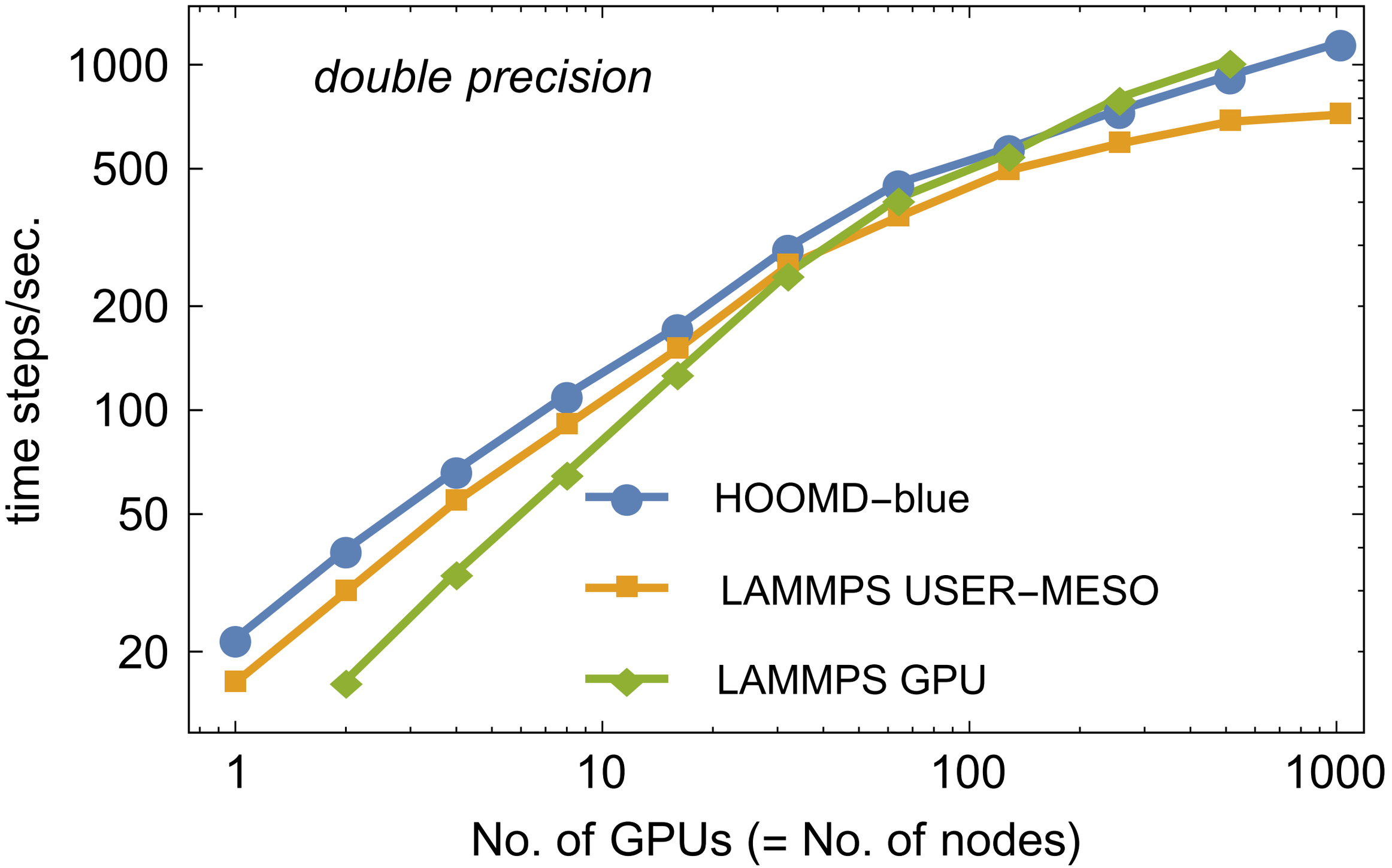






Pak Lui, Filippo Spiga, Rong Shi

Dissipative Particle Dynamics on Blue Waters and Titan



Summary - Molecular Dynamics

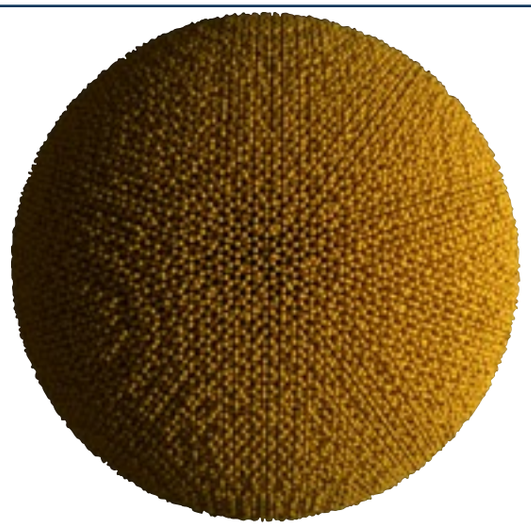
- **Multi-GPU** support in **HOOMD 1.0** enables large-scale MD using spatial domain decomposition

- **Strong Scaling** extends to 1000's of GPUs, and to more complex systems

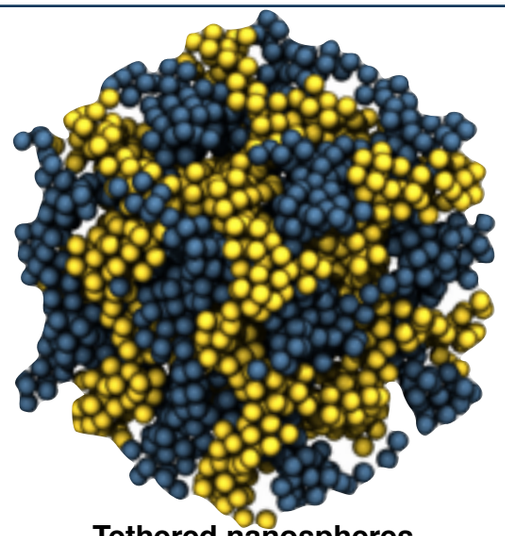
- **GPUDirect RDMA** is a promising technology, although strong scaling is ultimately limited by PCIe and kernel launch latency

Glaser J., Nguyen T.D., Anderson J.A. et al.
Strong scaling of general-purpose molecular dynamics simulations on GPUs.
Comput. Phys. Commun. **192**, pp. 97-107 (2015)
doi:10.1016/j.cpc.2015.02.028.

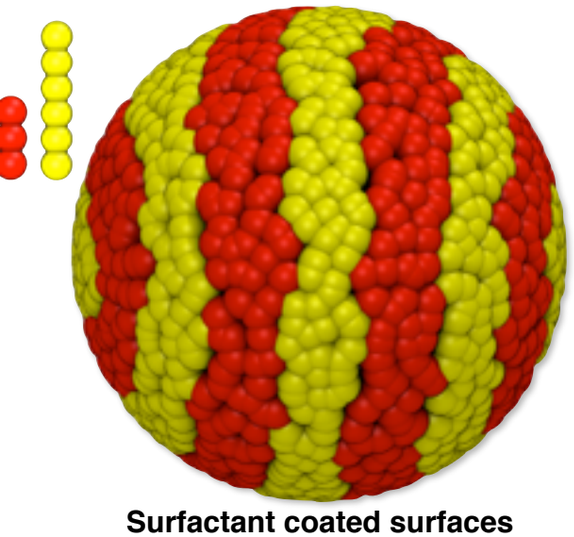
Molecular dynamics



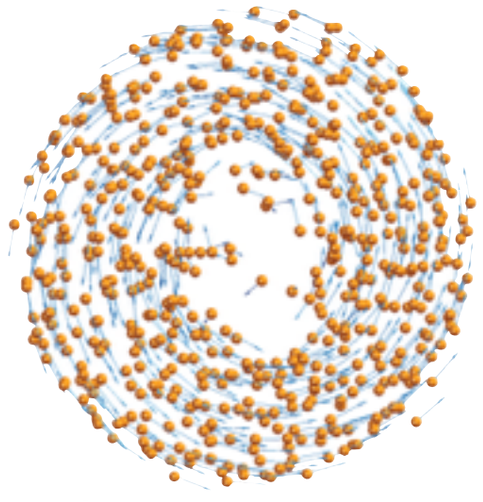
Quasicrystal growth
Molecular Dynamics
Engel M. et al., *Nature Materials* (in press)



Tethered nanospheres
Langevin dynamics
Marson, R, *Nano Letters* **14**, 4, 2014

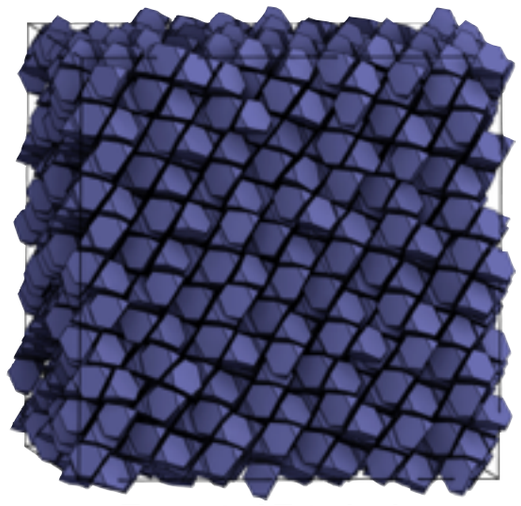


Surfactant coated surfaces
Dissipative particle dynamics
Pons-Siepermann, I. C., *Soft* matter **6** 3919 (2012)

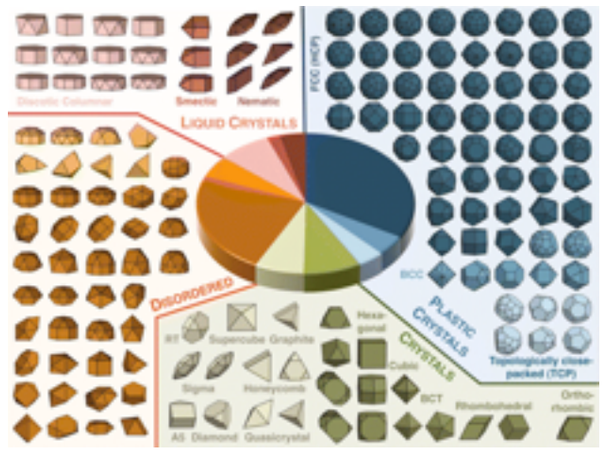


Self-propelled colloids
Non-equilibrium MD
Nguyen N., *Phys Rev E* **86** 1, 2012

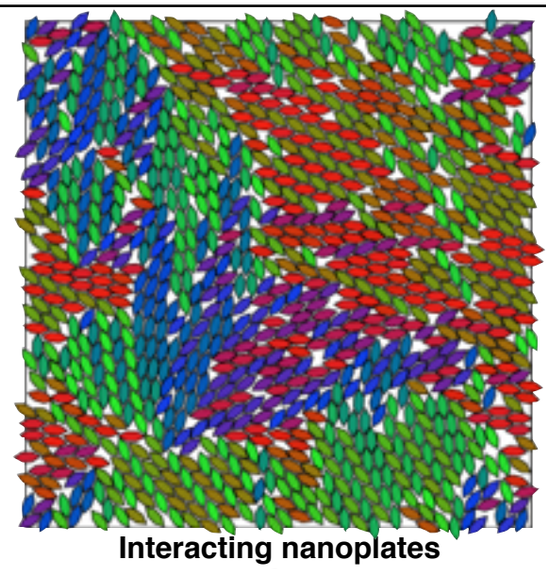
Monte Carlo



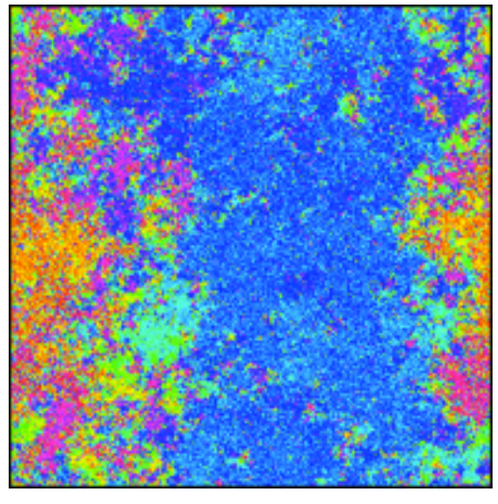
Truncated Tetrahedra
Hard particle MC
Damasceno, P. F. et al., *ACS Nano* **6**, 609 (2012)



Arbitrary polyhedra
Hard particle MC
Damasceno, P. F. et al., *Science* **337**, 453 (2012)

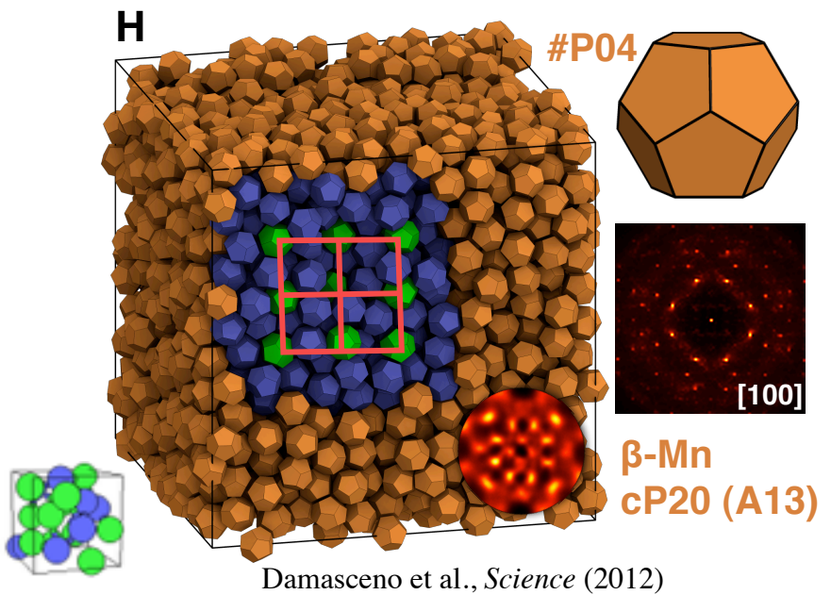


Interacting nanoplates
Hard particle MC with interactions
Ye X. et al., *Nature Chemistry* **cover article** (2013)

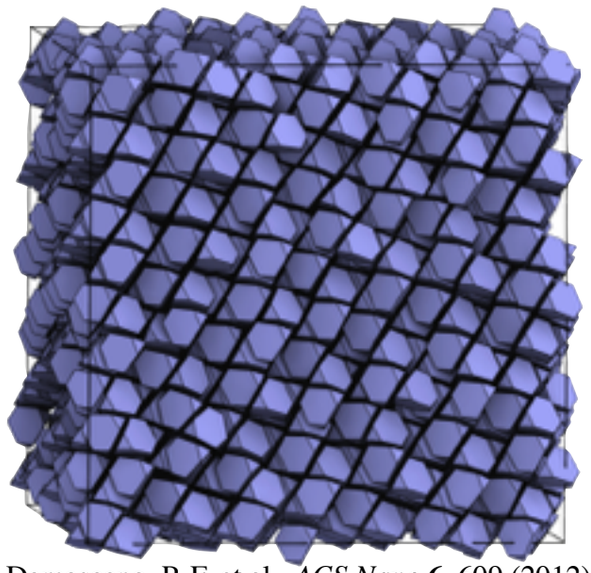


Hard disks - hexatic
Hard particle MC
Engel M. et al., PRE **87**, 042134 (2013)

Hard particle Monte Carlo

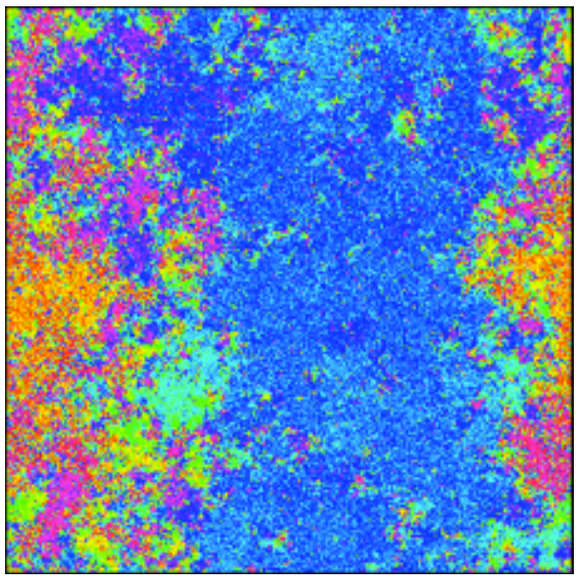


Damasceno et al., *Science* (2012)



Damasceno, P. F. et al., *ACS Nano* **6**, 609 (2012)

Damasceno et al., *Science* (2012)

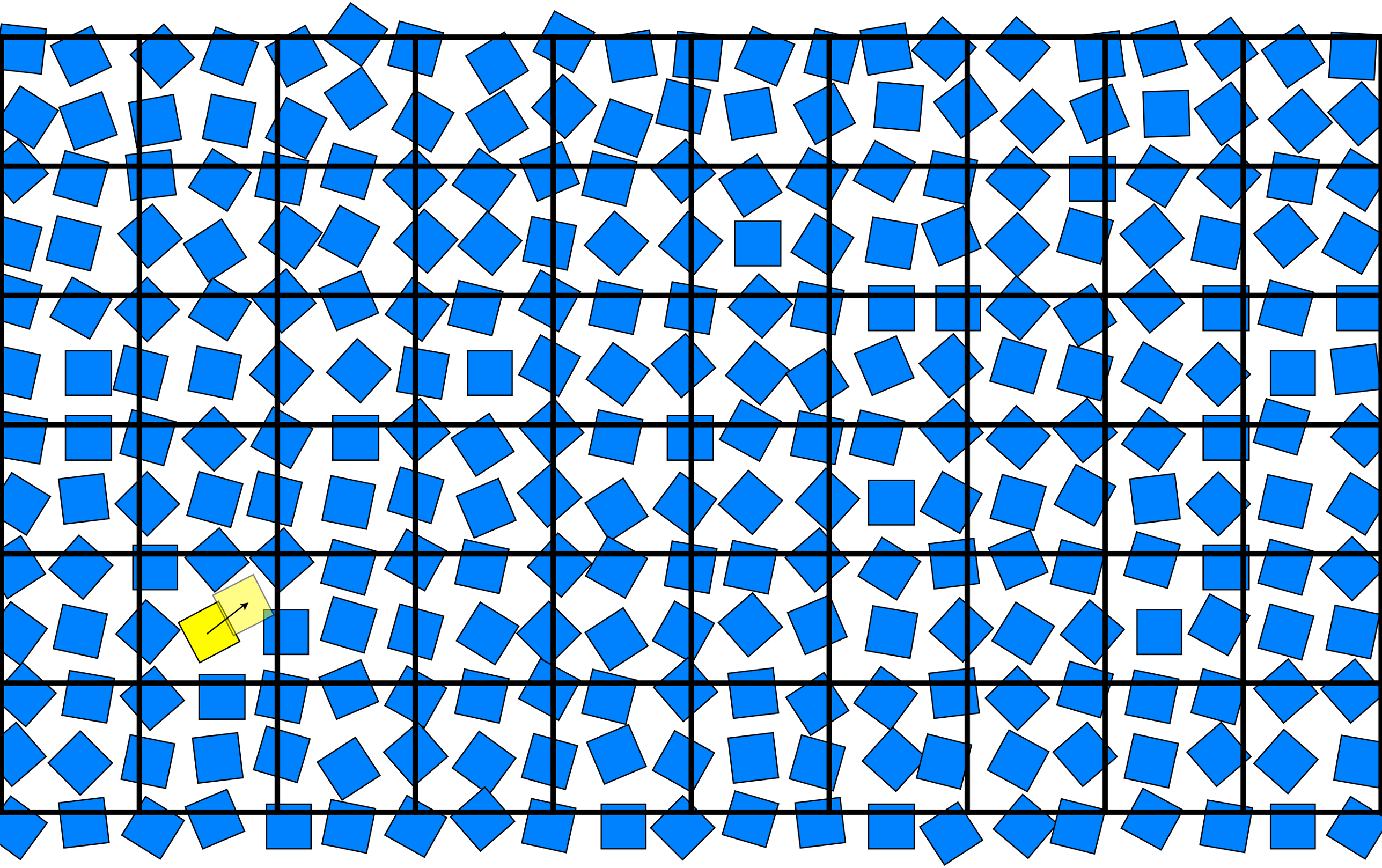


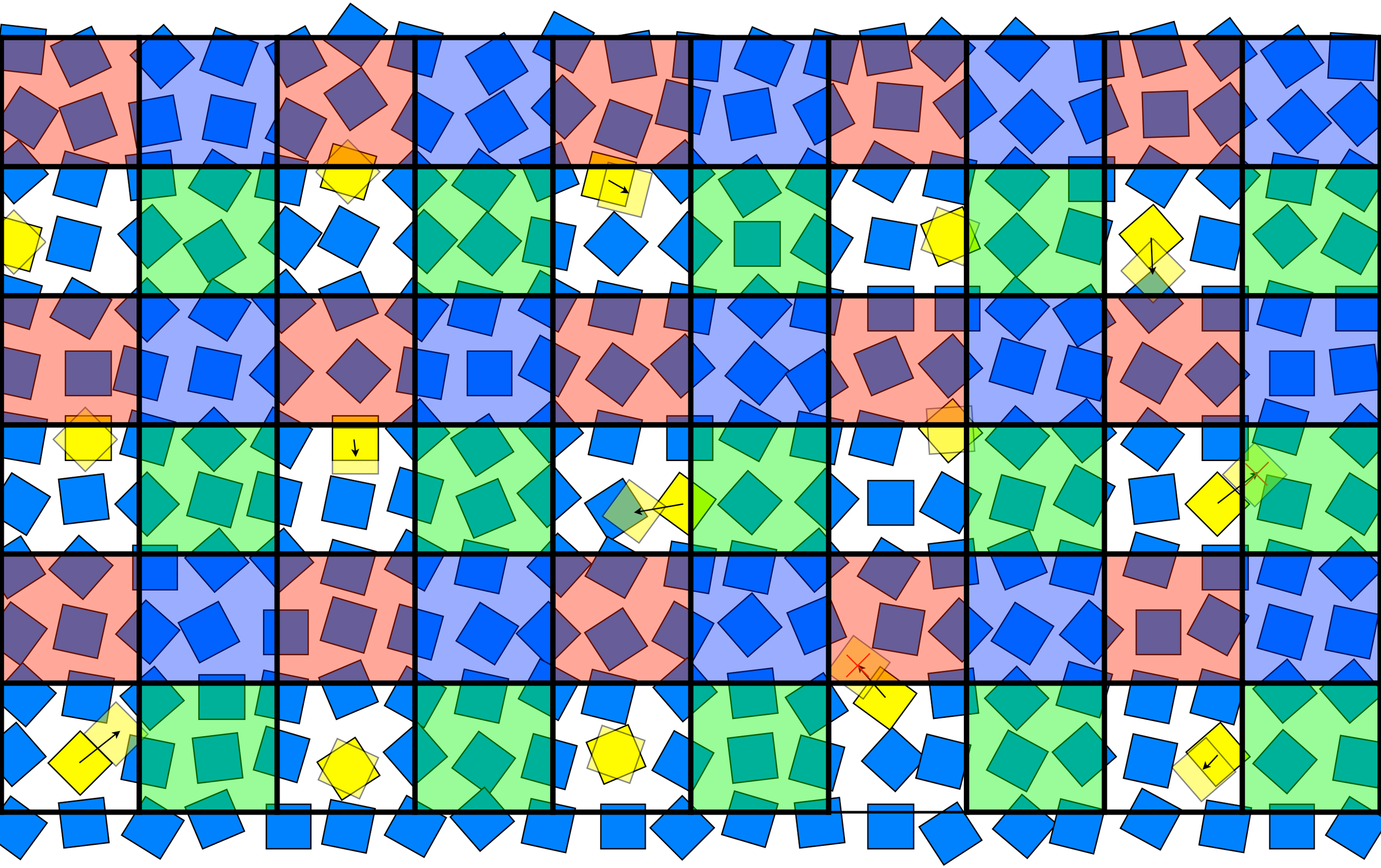
Engel M. et al., PRE **87**, 042134 (2013)

- Hard Particle Monte Carlo plugin for HOOMD-blue
- 2D Shapes
  - Disk
  - Convex (Sphero)polygon
  - Concave polygon
  - Ellipse
- 3D Shapes
  - Sphere
  - Ellipsoid
  - Convex (Sphero)polyhedon
- NVT and NPT ensembles
- Frenkel-Ladd free energy
- Parallel execution on a single GPU
- Domain decomposition across multiple nodes (CPUs or GPUs)

Easy and flexible to use

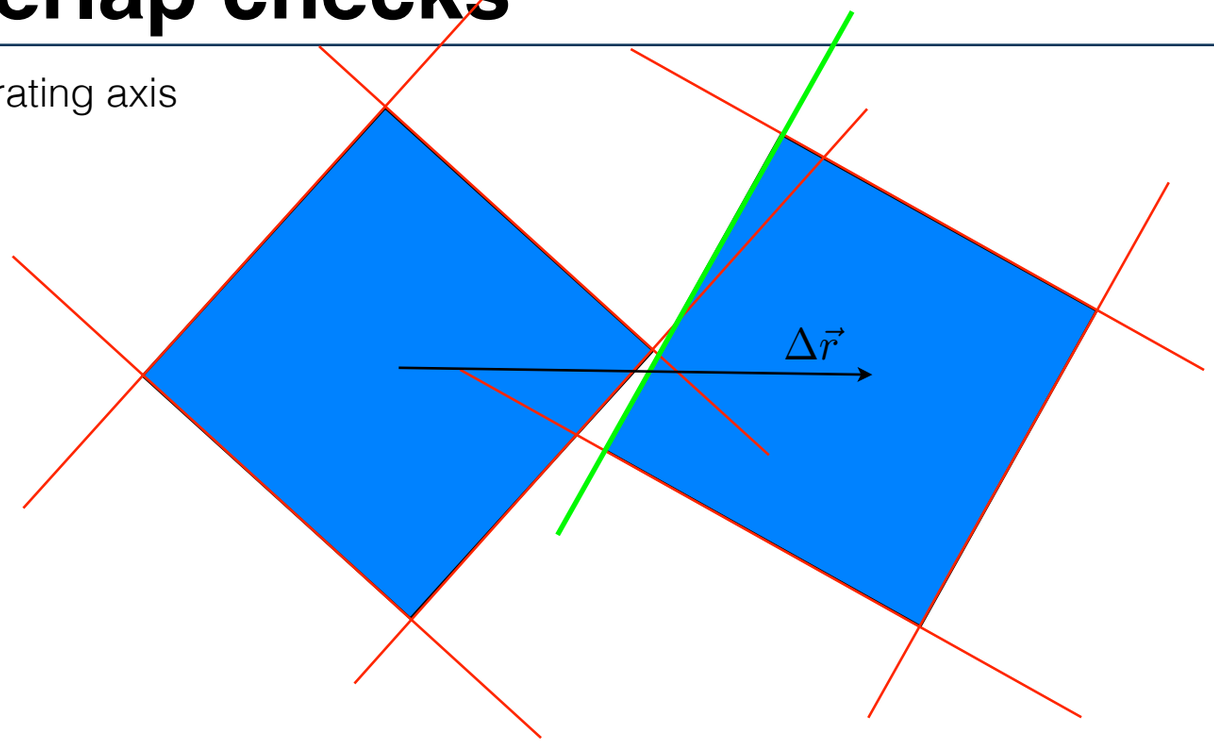
```
from hoomd_script import *
from hoomd_plugins import hpmc

init.read_xml(filename='init.xml')

mc = hpmc.integrate.convex_polygon(seed=10, d=0.25, a=0.3);
mc.shape_param.set('A', vertices=[(-0.5, -0.5), (0.5, -0.5),
                                  (0.5, 0.5), (-0.5, 0.5)]);

run(10e3)
```





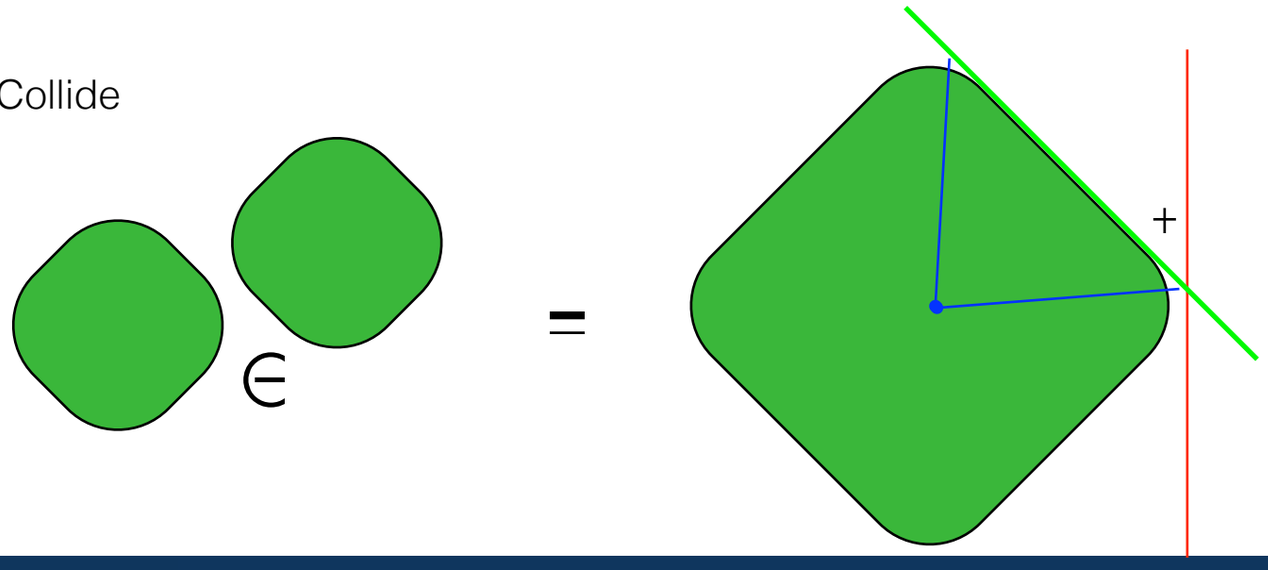
Overlap checks

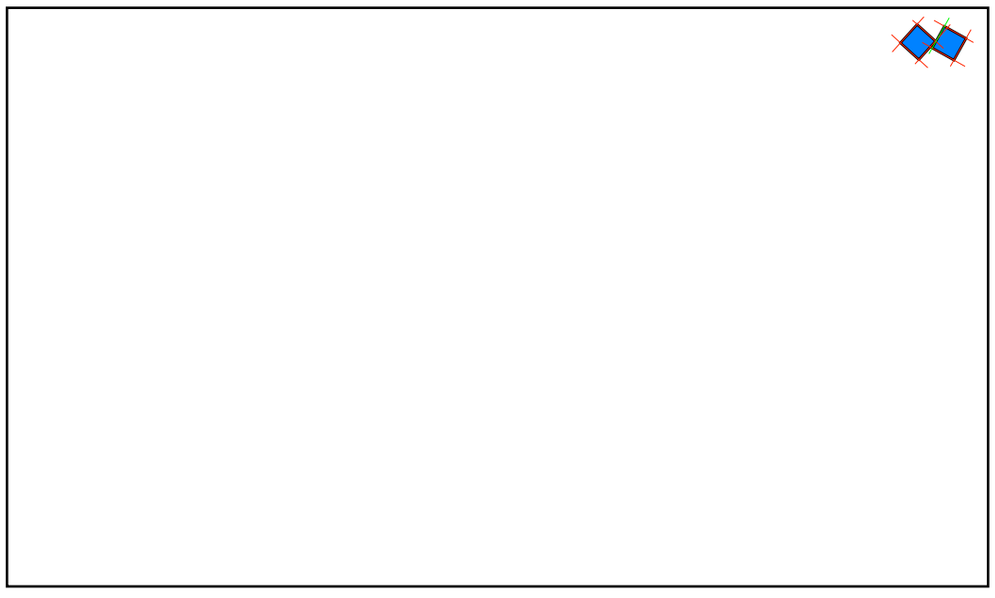
Separating axis



- Disk/sphere - trivial
- Convex polygons - separating axis
- Concave polygons - brute force
- Spheropolygons - XenoCollide/GJK
- Convex polyhedra - XenoCollide/GJK
- Ellipsoid / Ellipse: Matrix method
- Compute delta in double, convert to single for expensive overlap check

XenoCollide

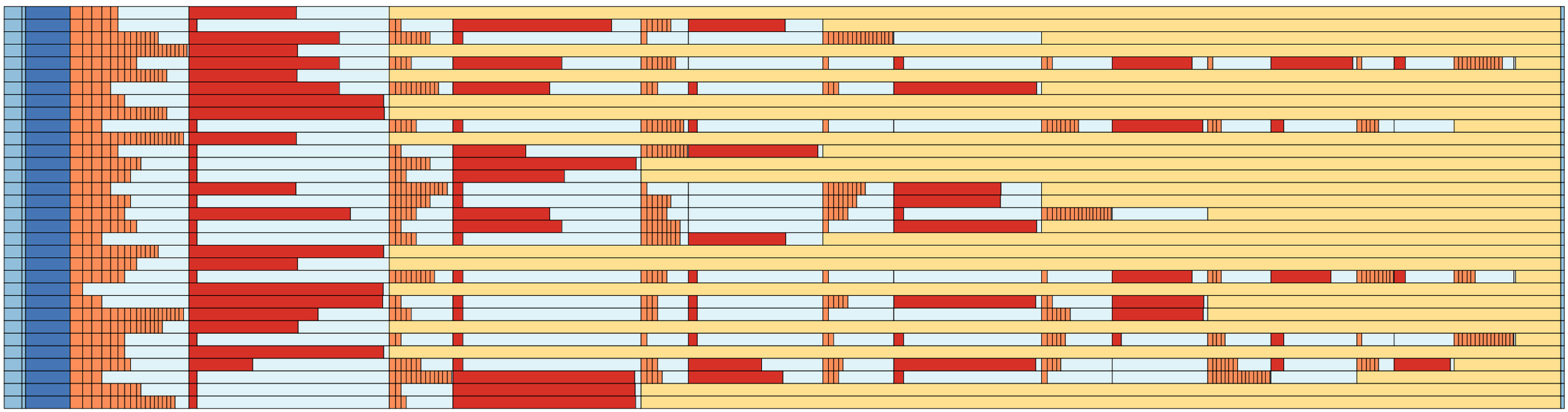




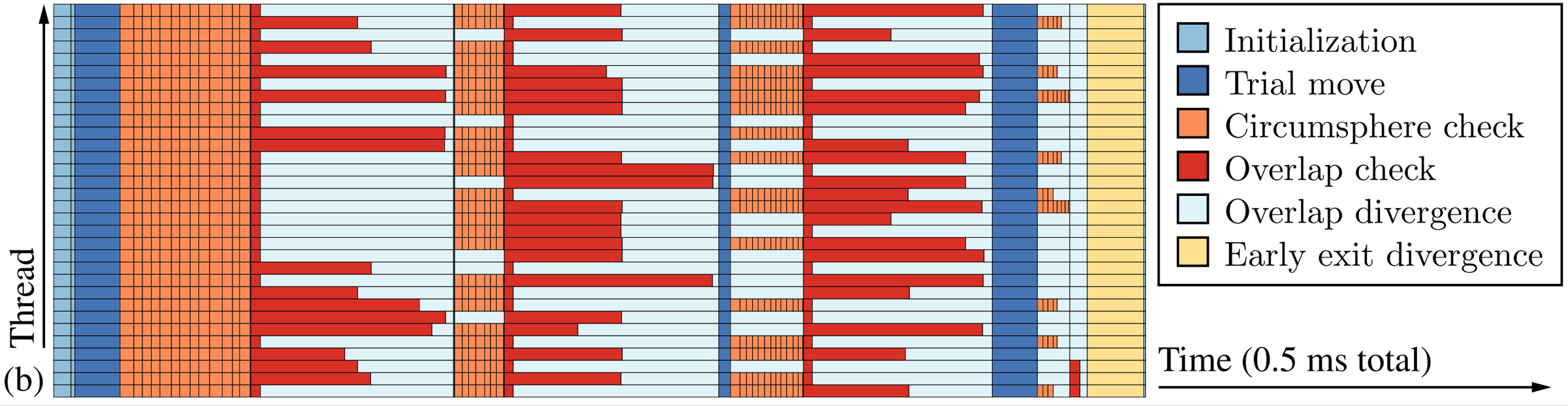
1001.842 - 1000.967 = 0.875

Divergence

(a)

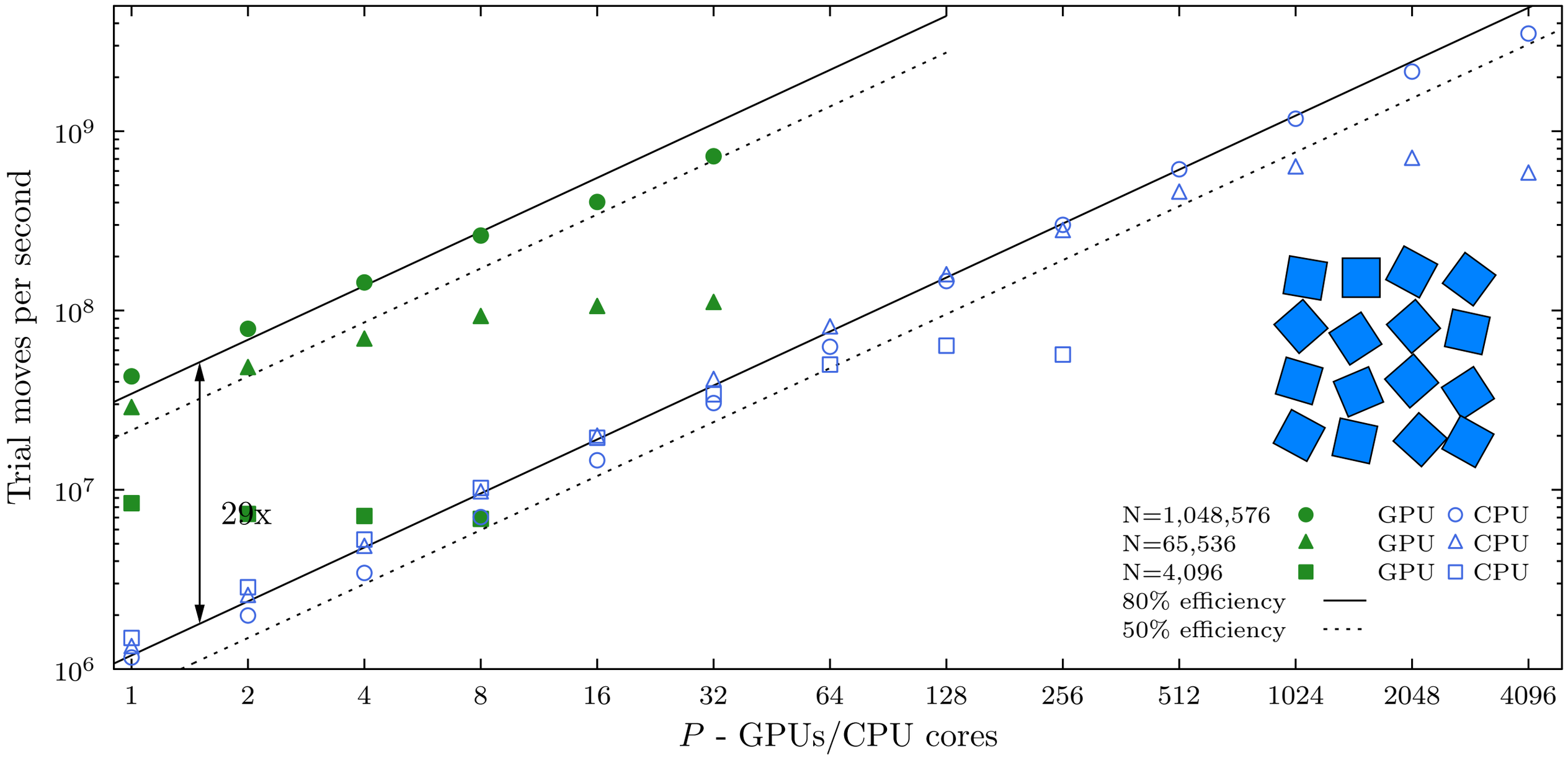


(b)



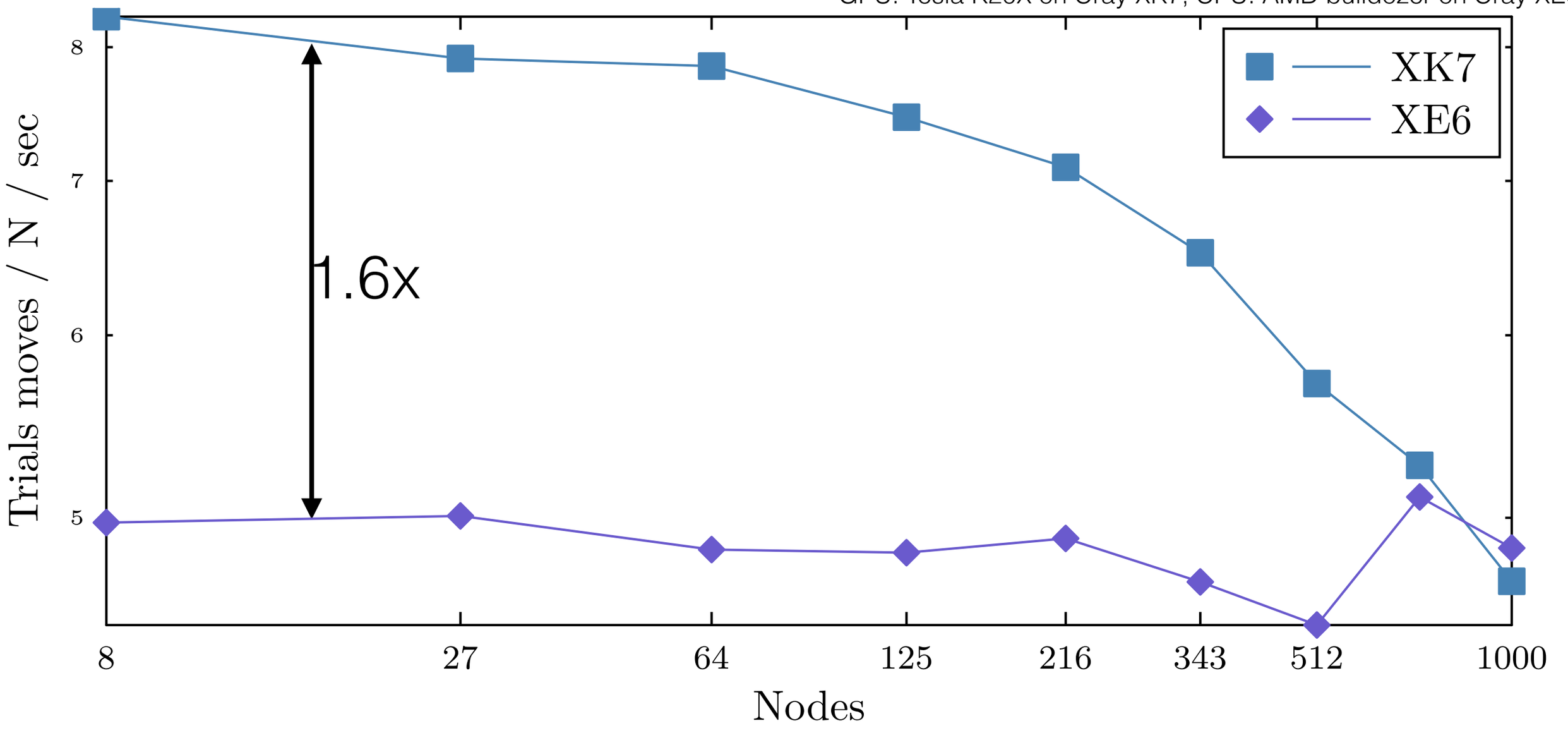
Strong scaling - squares

GPU: Tesla K20X, CPU: Xeon E5-2680 (XSEDE Stampede)



Weak scaling - truncated octahedra (3D)

GPU: Tesla K20X on Cray XK7, CPU: AMD bulldozer on Cray XE6



Questions?

HOOMD-blue: http://codeblue.umich.edu/hoomd-blue
Monte Carlo code not yet publicly available.

- It will eventually be released open-source as part of HOOMD-blue
- Paper on hard disks: Anderson, J. A. et al., JCP **254**, 27-38 (2013)
- Paper on 3D, anisotropic shapes, multi-GPU: *coming soon*

Funding / Resources

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