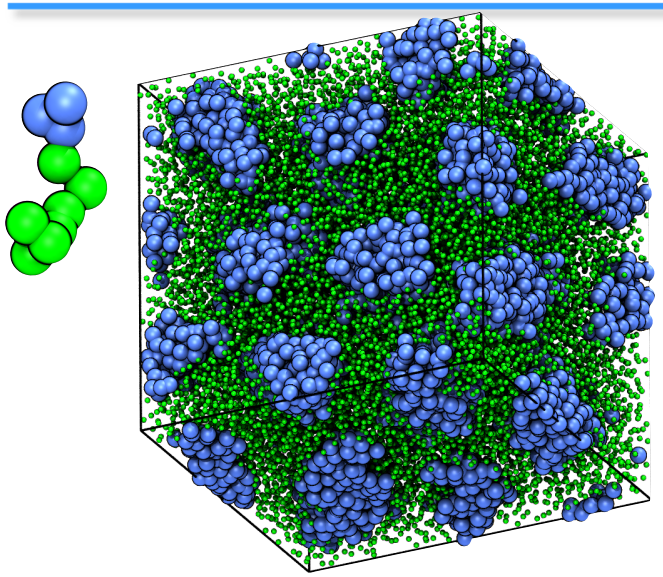
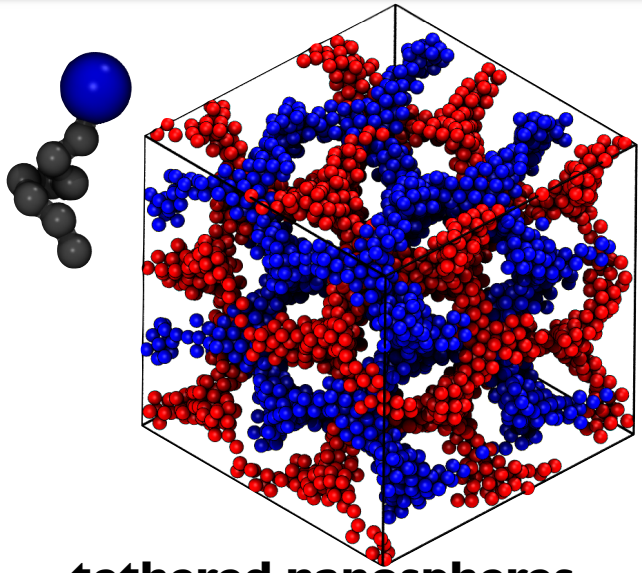
Simulating nano-materials, polymers, and complex fluids on GPUs with HOOMD-blue

Joshua A. Anderson

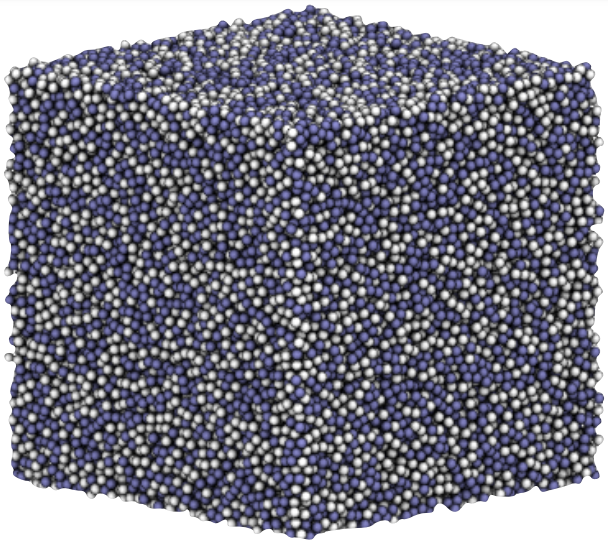
Examples



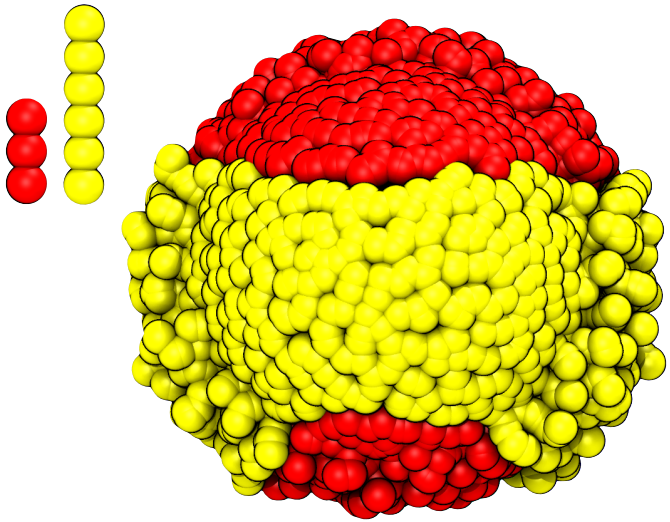
polymer systems
Dissipative Particle Dynamics (DPD)



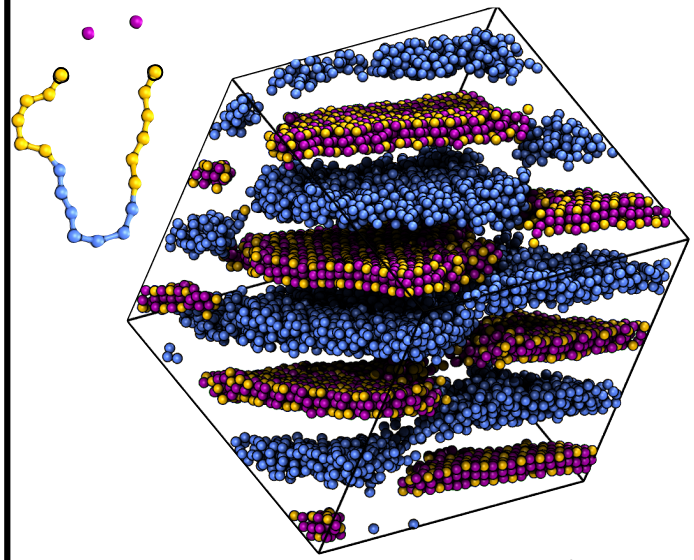
tethered nanospheres
Brownian Dynamics



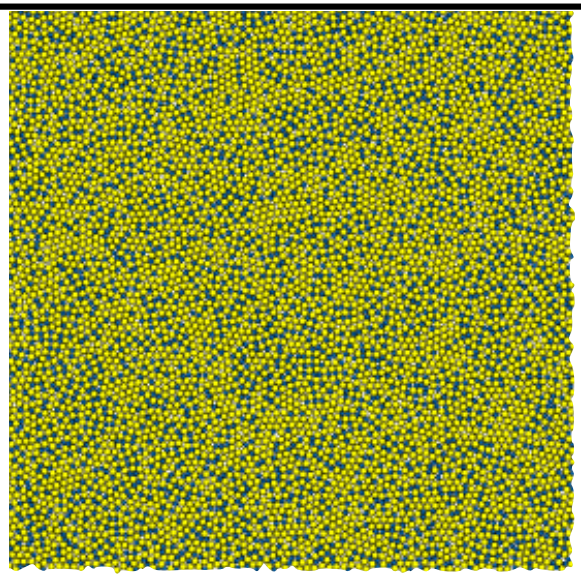
supercooled liquids
Molecular Dynamics



surfactant coated surfaces
DPD with constraints



polymer nanocomposites
coarse-grained Molecular Dynamics



supercooled liquids
2D Molecular Dynamics

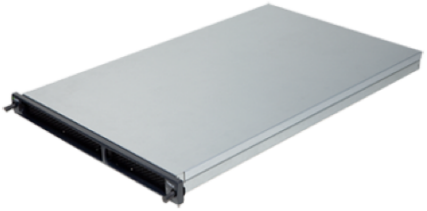
GPU Specifications

Desktop

GTX 480

480 Processor elements
1.3 TFLOPS single precision
158 GFLOPS double precision
177 GB/s memory bandwidth
1.5 GB memory

Data center



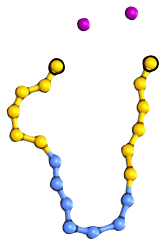
Tesla S2050

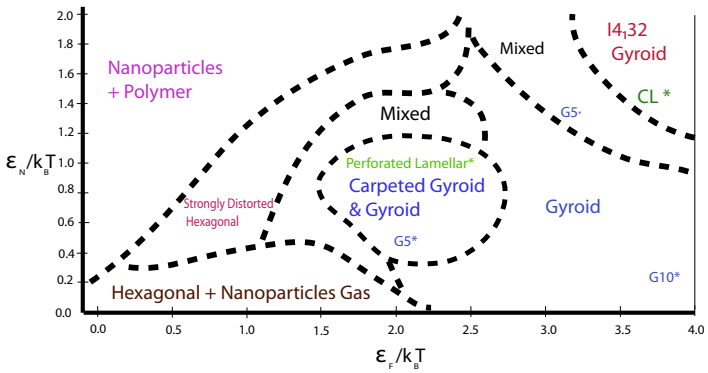
448 (*x4*) Processor elements
1.03 (*x4*) TFLOPS single precision
515 (*x4*) GFLOPS double precision
144 (*x4*) GB/s memory bandwidth
3 (*x4*) GB memory

Benefits of GPU computing

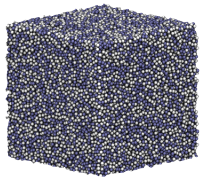
Papers with CPU jobs...

run thousands of serial jobs - often **one month** of CPU time for each

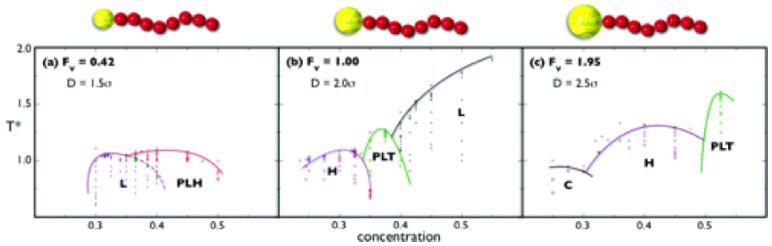




compute a phase diagram for one polymer architecture



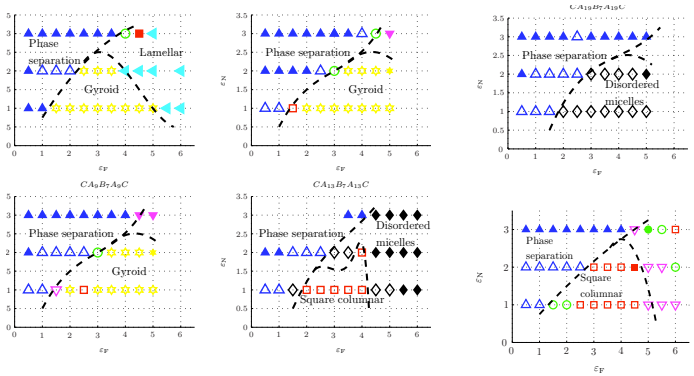
study one supercooled liquid model



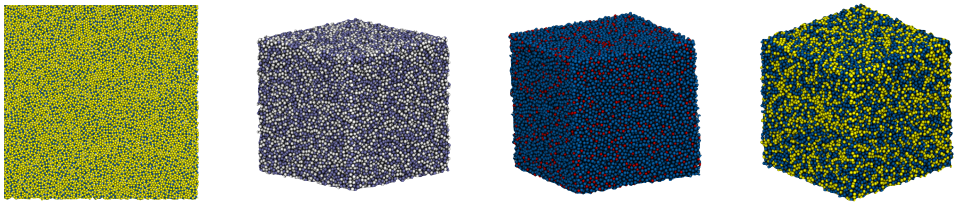
study three monodisperse tethered nanospheres

Papers with GPU jobs...

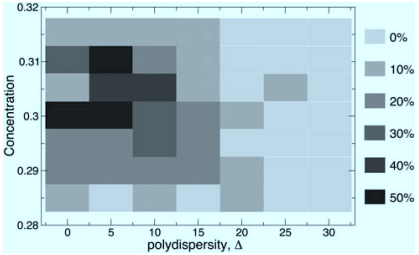
run thousands of single GPU jobs - **one day** of GPU time for each



compute phase diagrams for six polymer architectures



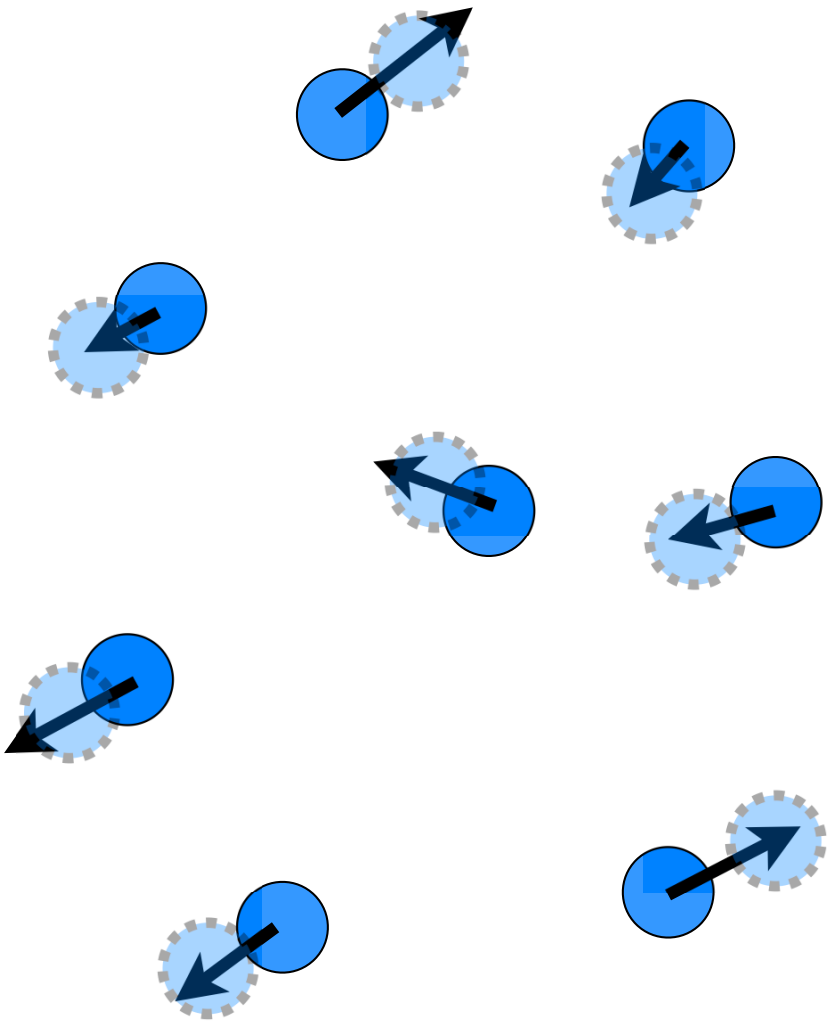
provide an in-depth comparison of four different models



490 jobs just for one figure!

study the effects of of varying polydispersity

Method overview



$$\vec{r}_i(t)$$
$$\vec{v}_i(t)$$

$\downarrow$

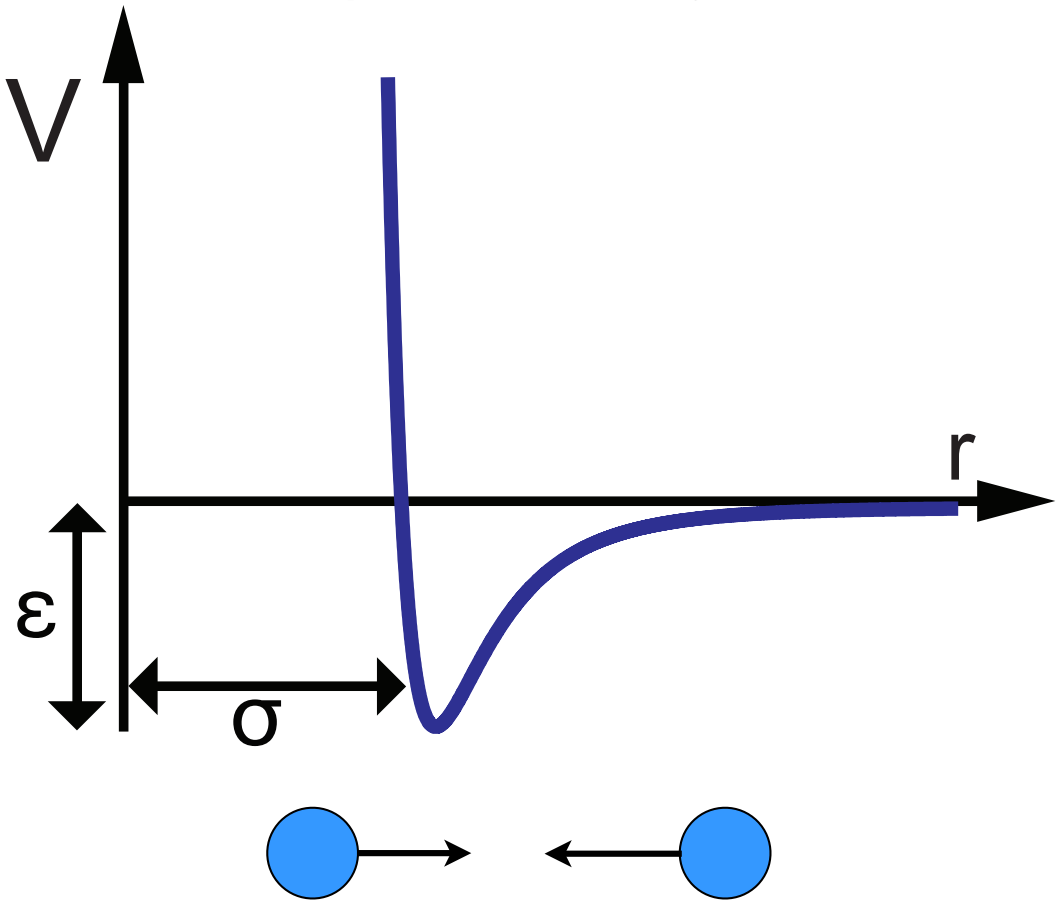
Calculate accelerations

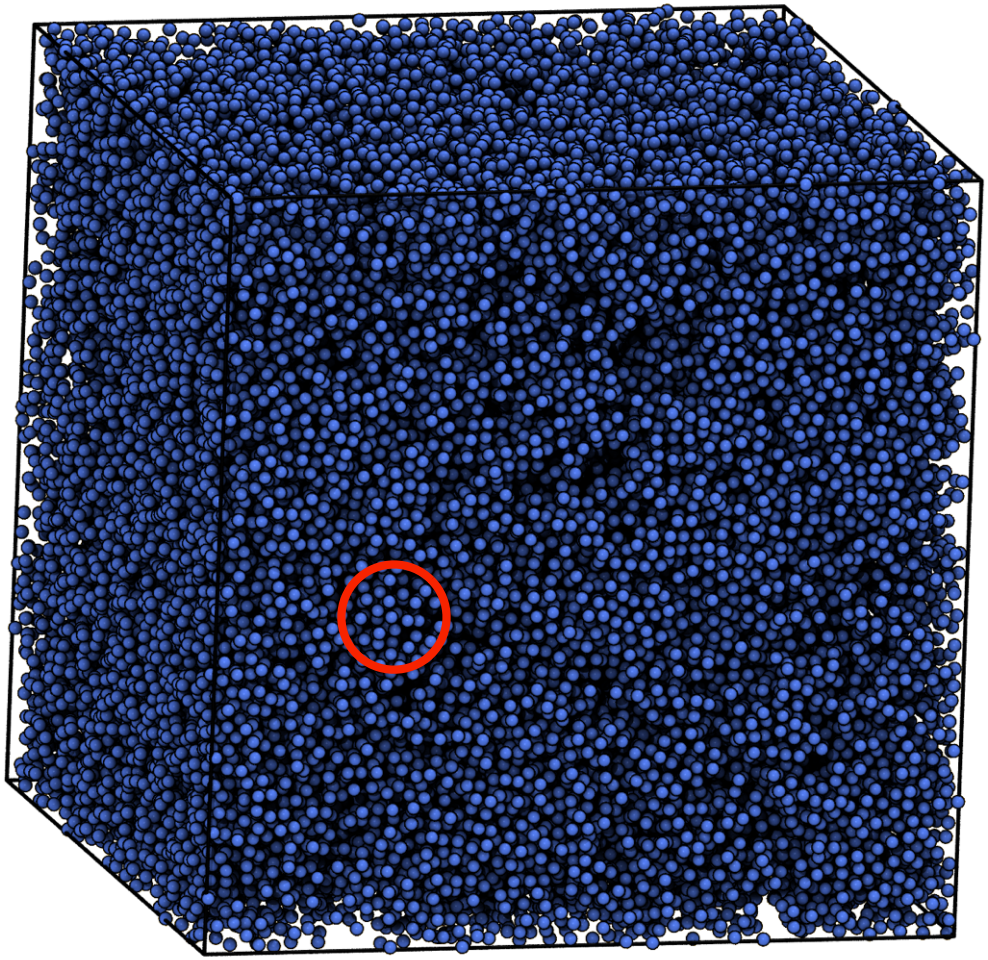
$\downarrow$

$$\vec{r}_i(t+\delta t)$$
$$\vec{v}_i(t+\delta t)$$

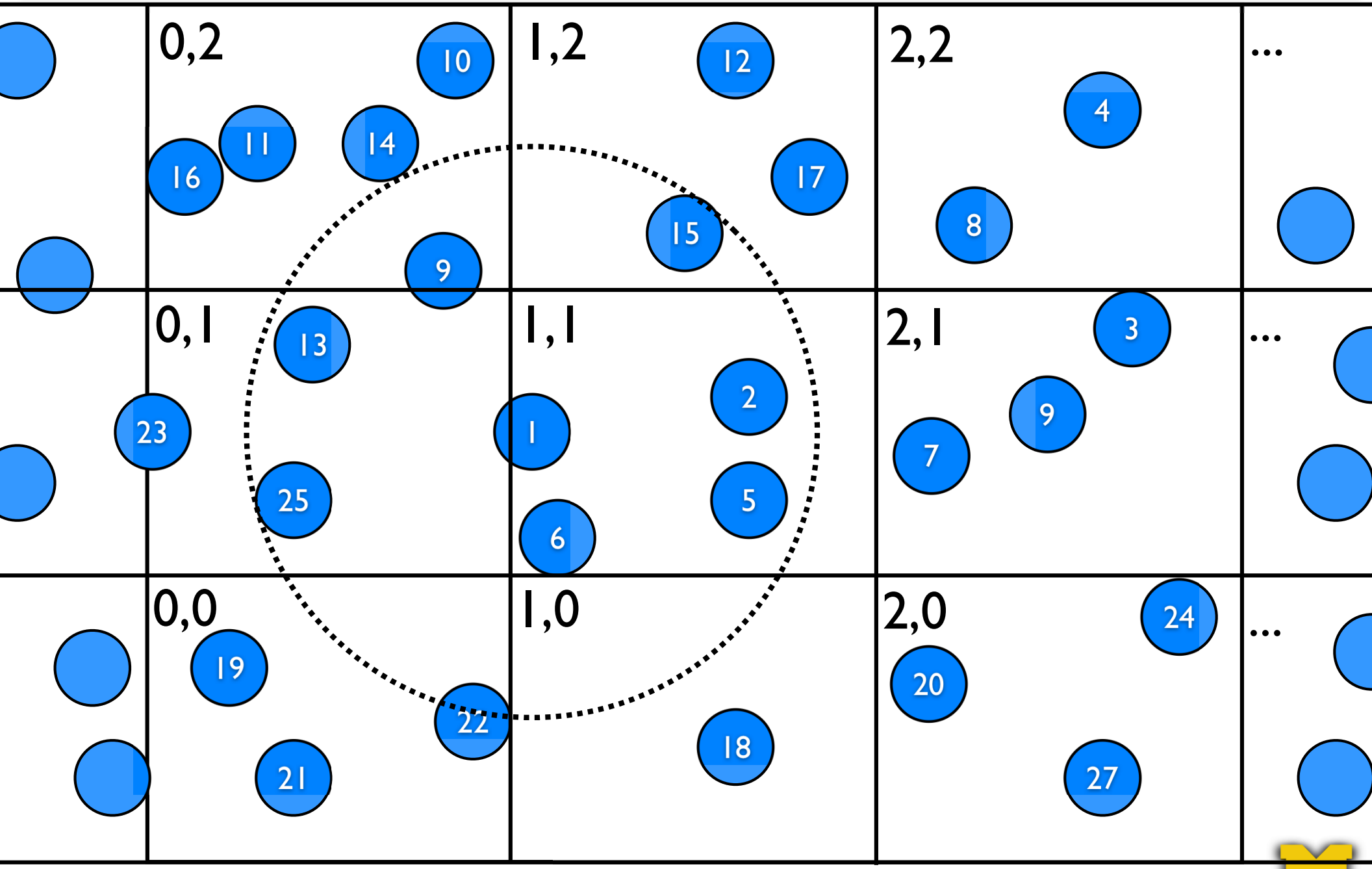
Pair potential

Example - Lennard-Jones

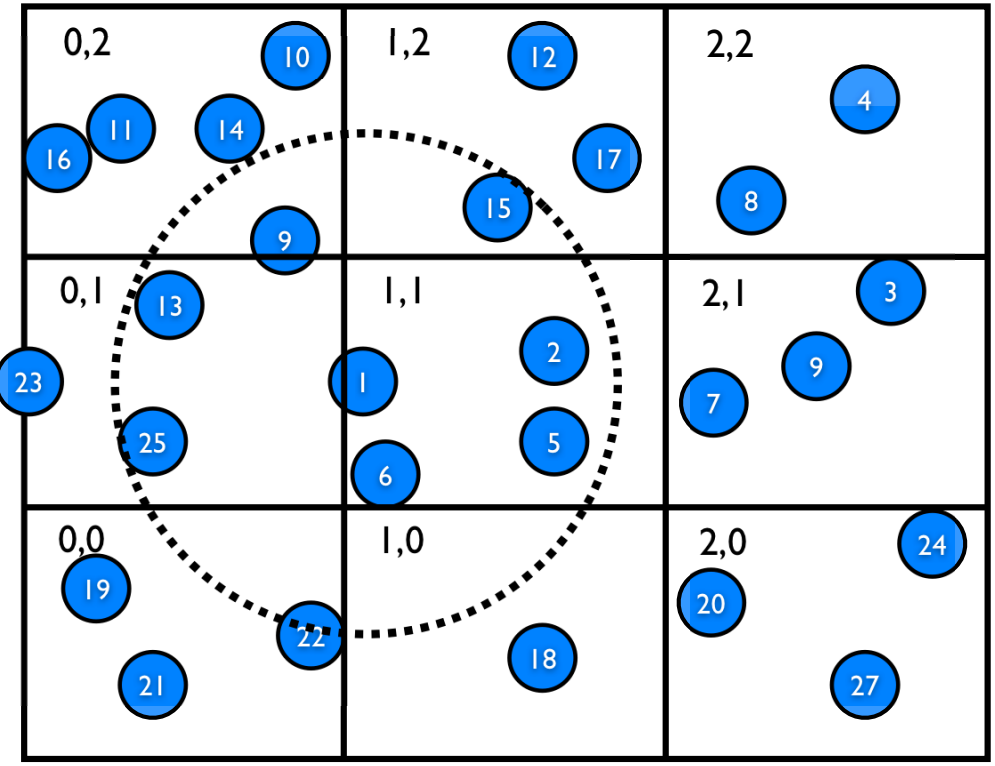




Cell list


0,2
10
11
14
16
9
1,2
12
17
15
2,2
4
8
...
0,1
13
23
25
1,1
2
1
5
6
2,1
3
9
7
...
0,0
19
22
21
1,0
18
2,0
24
20
27
...

Generating the cell list

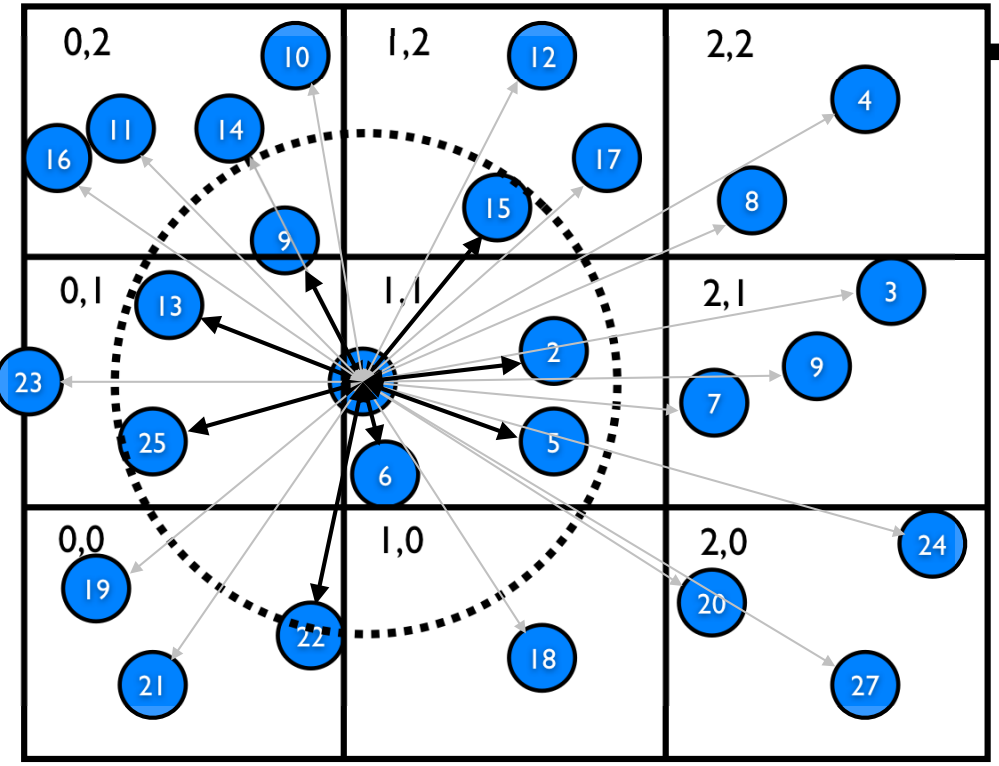



```
for each particle i in parallel
  load position pos[i]
  compute cell index ci
  cur_size = atomicInc length[ci]
  write (ci, pos[i]) to
    cell_list[ci][cur_size]
```

	Length	Cell list				
0,0	3	19	21	22		
1,0	1	18				
2,0	3	20	24	27		
0,1	3	23	25	13		
1,1	4	**1**	6	**2**	**5**	
2,1	3	7	9	**3**		
0,2	5	16	11	14	10	9
1,2	3	12	15	17		
2,2	2	8	**4**			

• • •

Creating the neighbor list



1	2	3	4	5
25	1	7	3	18
13	6	9	8	20
6	5	8	...	1
2	7	4		2
5	15	...		6
9	17			7
15				15

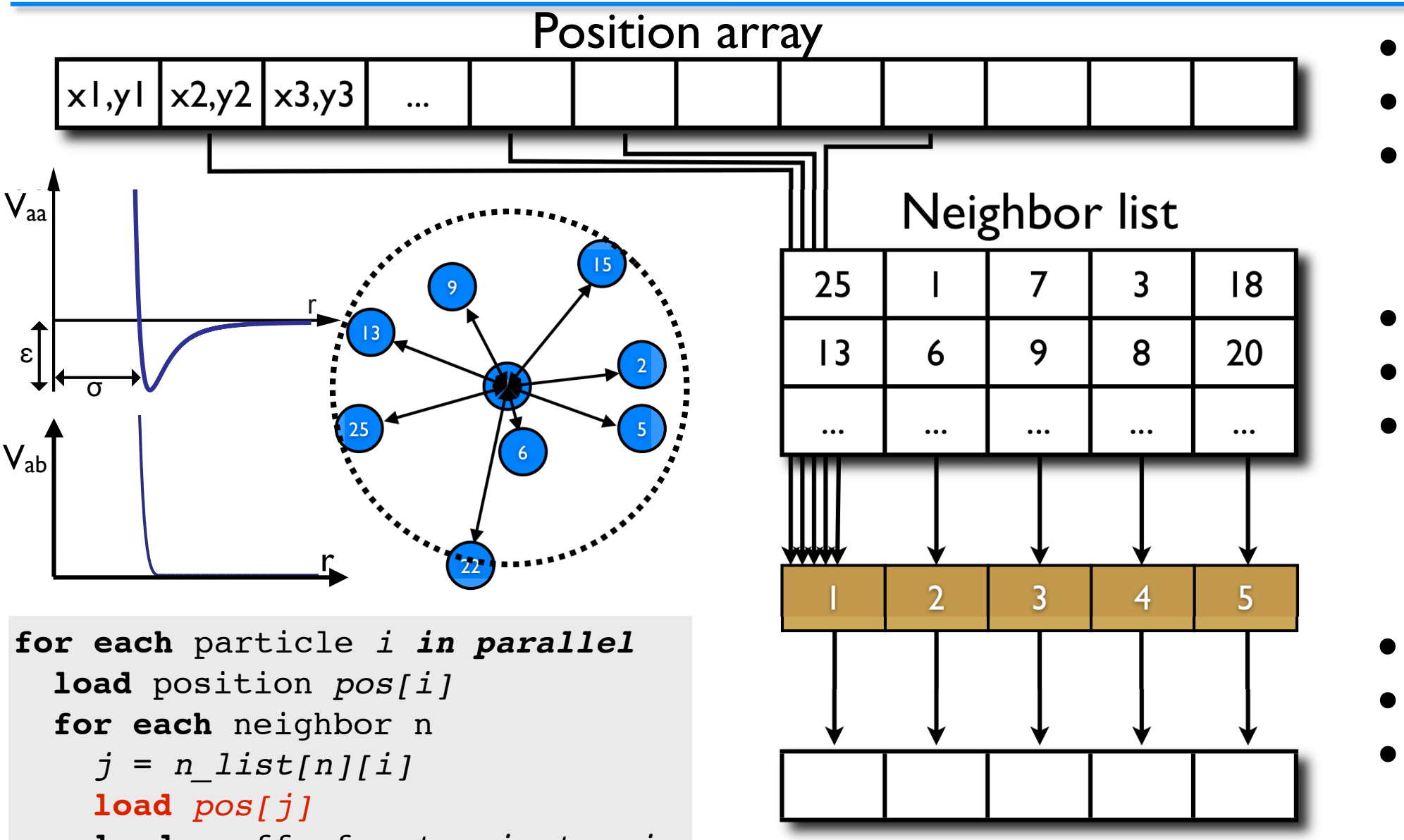
Neighbor list

7	6	...	...	7

Num Neighbors

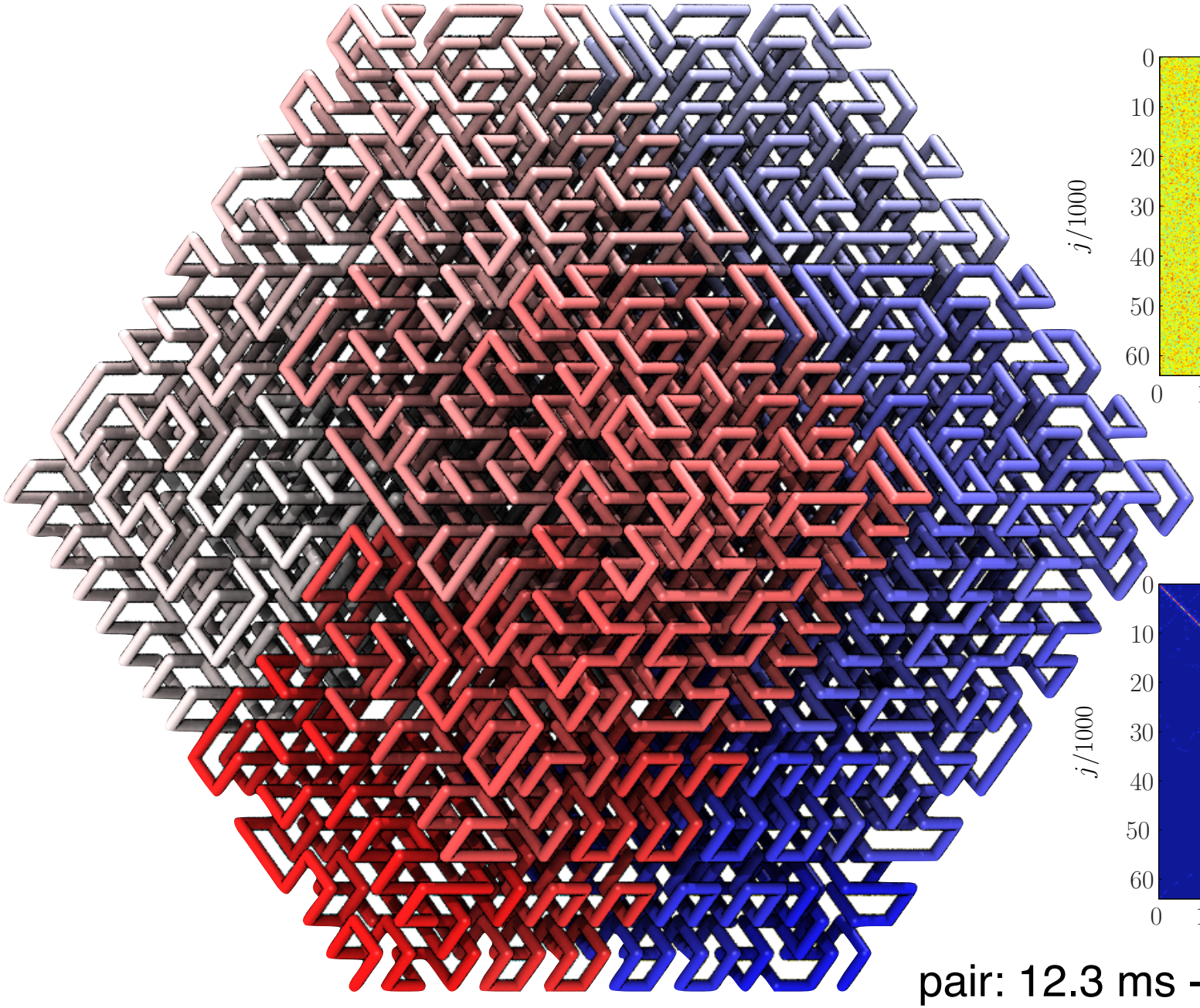
```
for each particle i in parallel
  load position pos[i]
  compute cell index ci
  for each nearby cell cn
     for each particle p in cn
        load cell_list[cn][p]
        if distance < rcut
          append to n_list[][i]
```

Computing pair forces

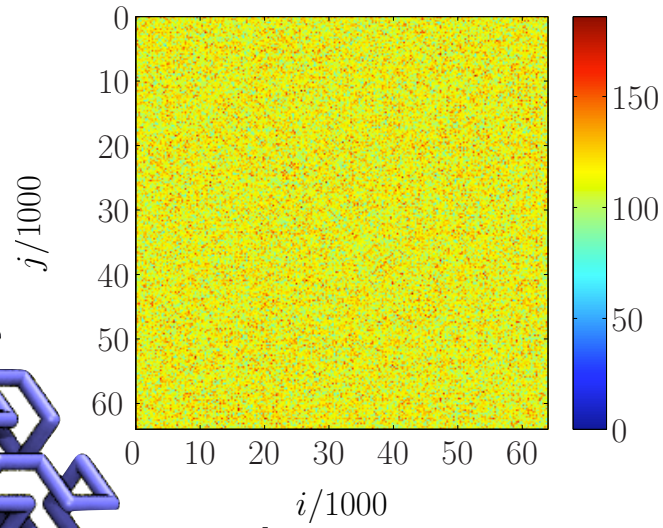



```
for each particle i in parallel
  load position pos[i]
  for each neighbor n
    j = n_list[n][i]
    load pos[j]
    load coeffs for typei, typej
    compute interaction i,j
  write total interaction on i
```

Spatial sorting reorders particles

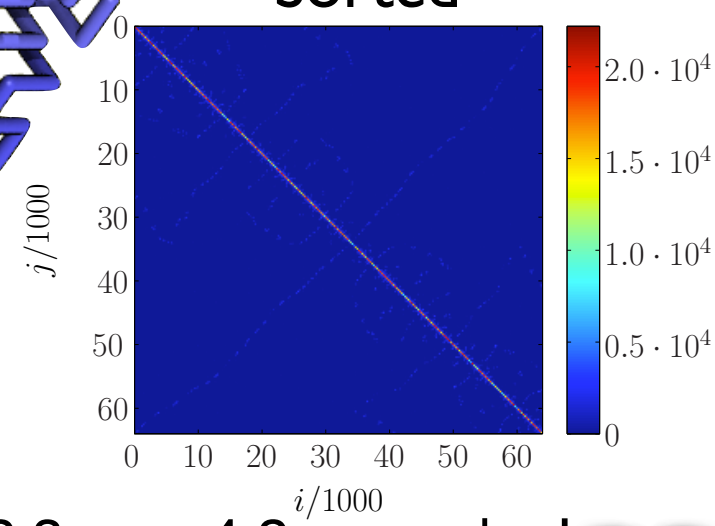


Random



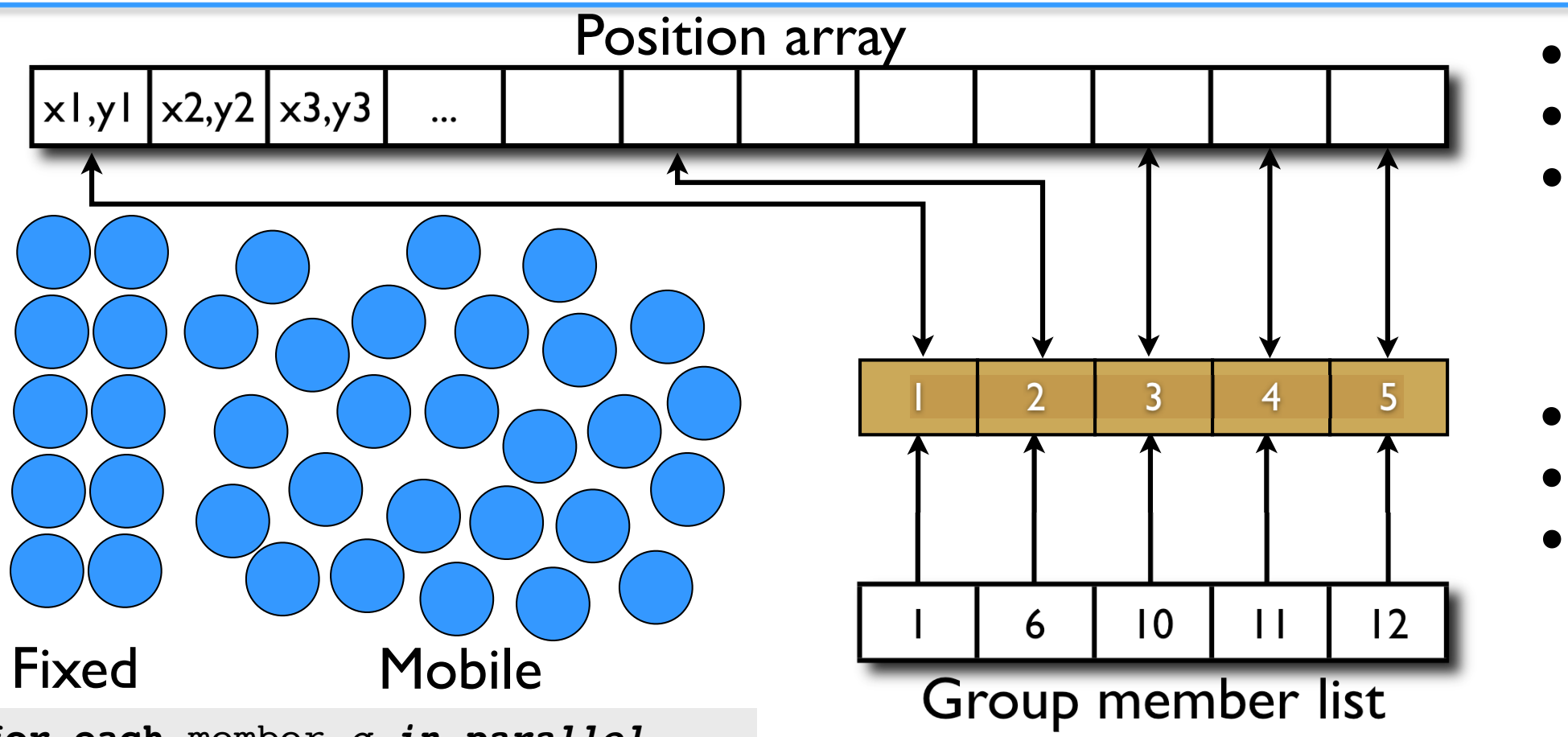
pair: 50.4 ms

Sorted



pair: 12.3 ms - 4.2x speedup!

Flexible integration




```
for each member g in parallel
  i = load group_idx[g]
  load pos[j]
  load vel[j]
  load force[j]
  compute updated quantities
  write pos[j]
  write vel[j]
```

Notes

- Member list is maintained in a sorted order
- This reduces the number of wasted memory transactions

Feature sheet

Integration
- NVT (Nosé-Hoover)
- NPT
- Brownian Dynamics
- Dissipative Particle Dynamics
- NVE
- FIRE energy minimization

Bond forces
- harmonic
- FENE

Angle forces
- harmonic
- CGCMM

Dihedral/Improper forces
- harmonic

Simulation types
- 2D and 3D
- Replica exchange (via script)

Snapshot formats
- MOL2
- DCD
- PDB
- XML

Pair forces
- Lennard Jones
- Gaussian
- CGCMM
- Morse
- Arbitrary table
- Yukawa
- PPPM (*in development*)

Many-body forces
- EAM (*in development*)

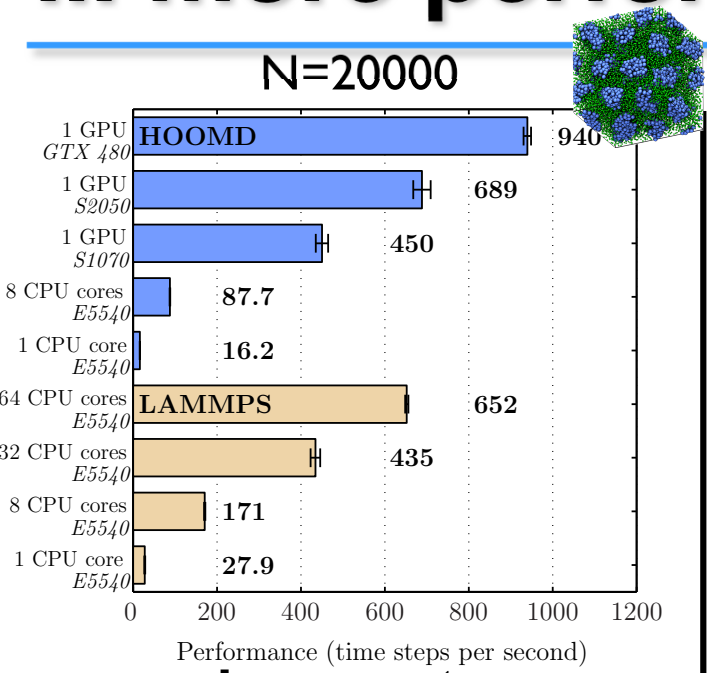
Hardware support
- All recent NVIDIA GPUs
- Multi-core CPUs via OpenMP

Script example

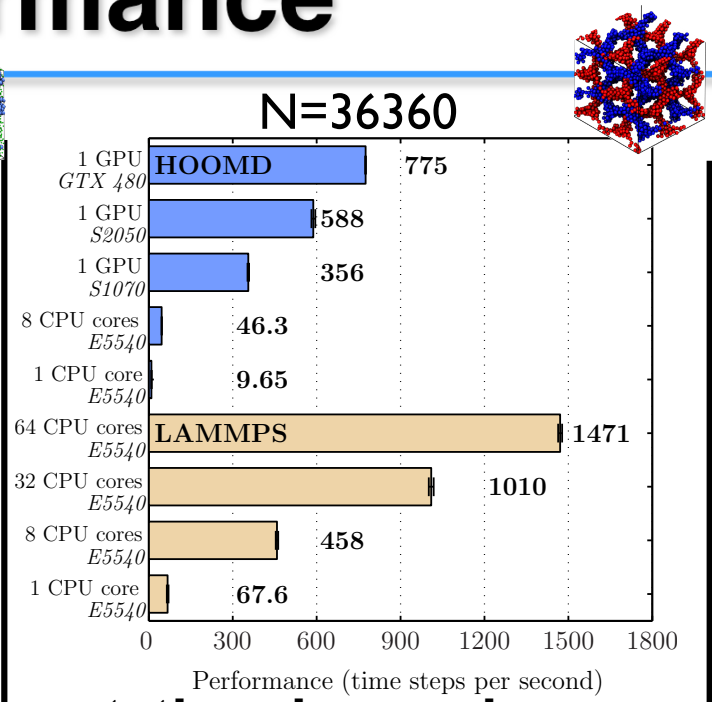
Documentation online: http://codeblue.umich.edu/hoomd-blue/doc

```
from hoomd_script import *

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

lj = pair.lj(r_cut=2.5)
lj.pair_coeff.set('A', 'A', epsilon=1.0,
                            sigma=1.0)

integrate.mode_standard(dt=0.005)
integrate.nvt(T=1.2, tau=0.5)

run(10e3)
```

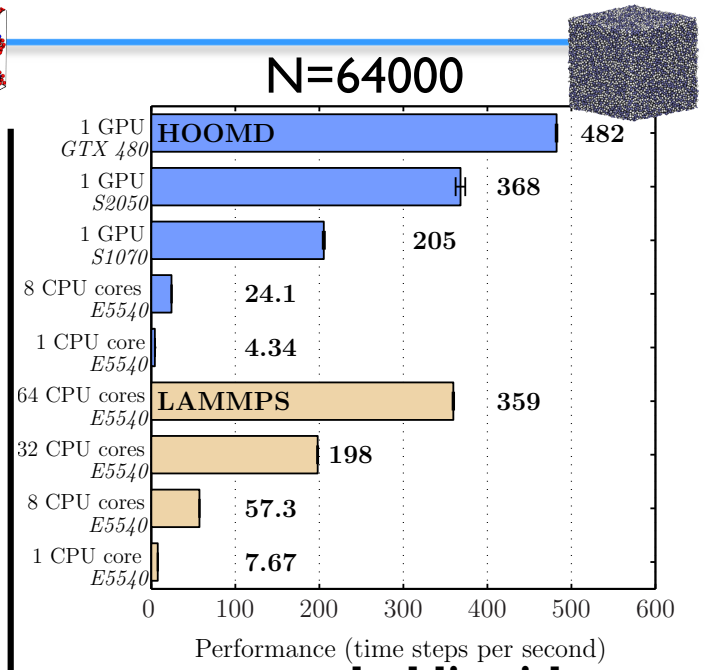
... more performance



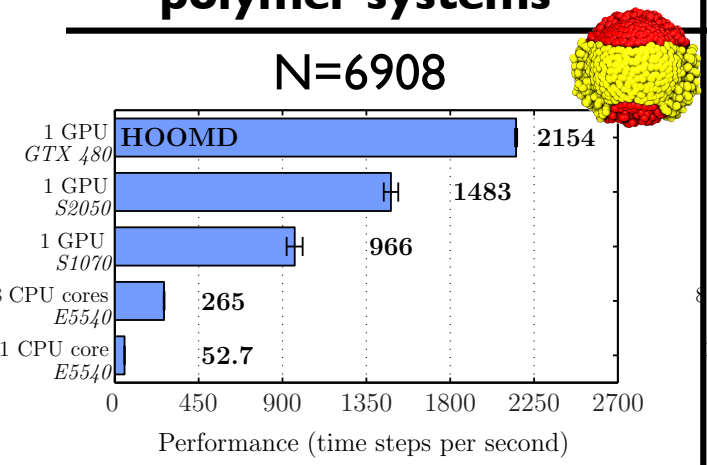
polymer systems



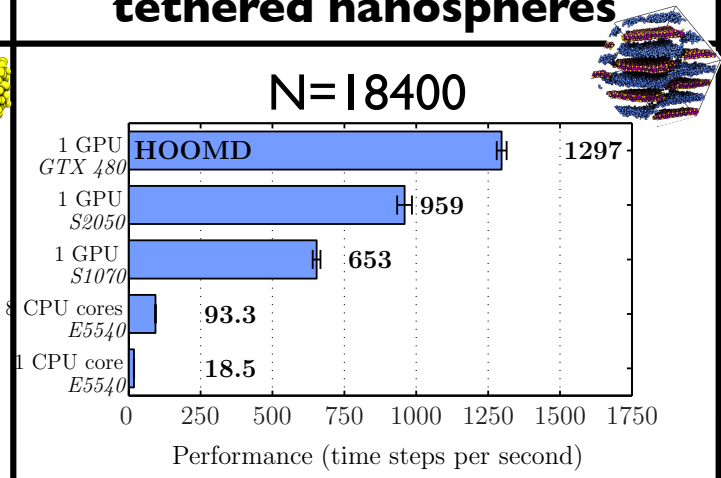
tethered nanospheres



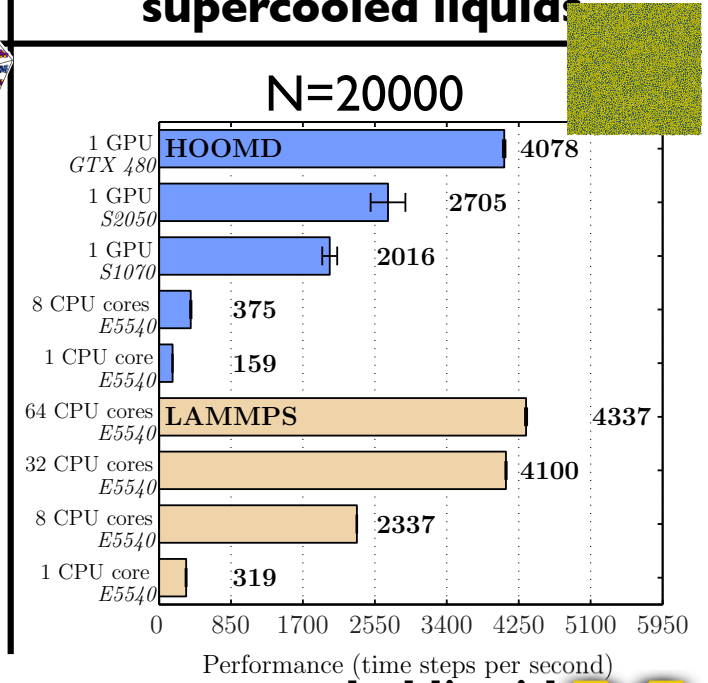
supercooled liquids



surfactant coated surfaces



polymer nanocomposites



supercooled liquids

Acknowledgements

HOOMD-blue is open source!

- Contributions from around the world
  - Joshua Anderson, Aaron Keys, Trung Dac Nguyen, Carolyn Phillips (University of Michigan)
  - Rastko Sknepnek (Northwestern)
  - Alex Travesset (Iowa State University)
  - Axel Kohlmeyer, David Lebard, and Ben Levine (Temple)
  - Igor Morozov, Kazennov Andrey, Bystriy Roman (Russian Academy of Sciences)