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Petascale Multiscale Simulations of Biomolecular Systems

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About me

- Background: experimental guy in grad school (LSCM, drug delivery) – I seem to have become a theoretical chemist. I'm as confused as anyone regarding how *that* happened.

- **Argonne National Labs / University of Chicago**

- Talk is about a side project I've been working on amongst my usual day-to-day activities; it's at an early stage!

- **This is a via a PRAC sub-award**

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Molecular dynamics

MD (classical) numerically integrates molecular equations of motion:

$$\boldsymbol{F = ma}$$

- One or more atoms, linked by springs
- Typically, also special springs to maintain structure (angles formed between 3 atoms etc)
- Interactions between molecules are distance dependent (get weaker with distance)
- **“True” atomic level-of-detail is computationally expensive!**

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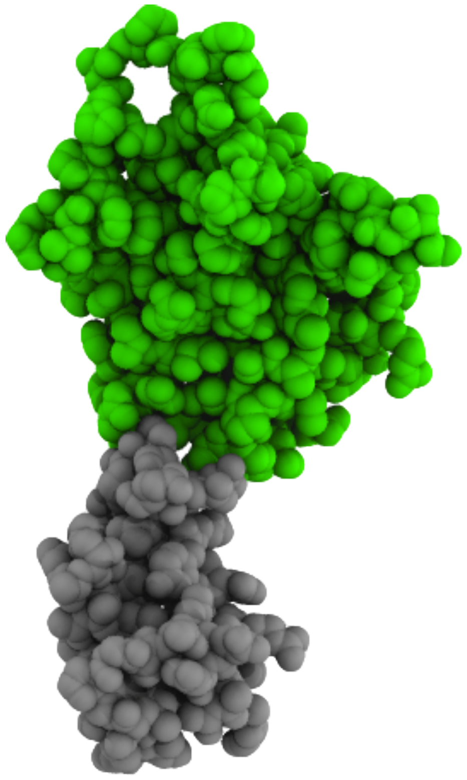
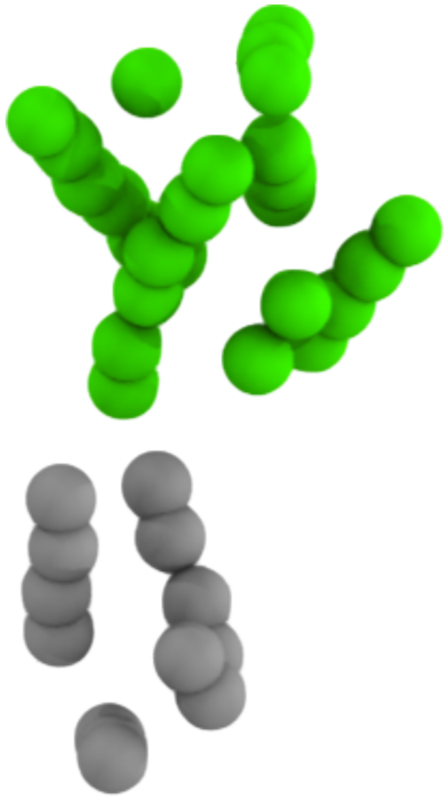
“Coarse graining” (CG)



Make the model simpler, while maintaining the essential behaviours!



Atomic model

CG model

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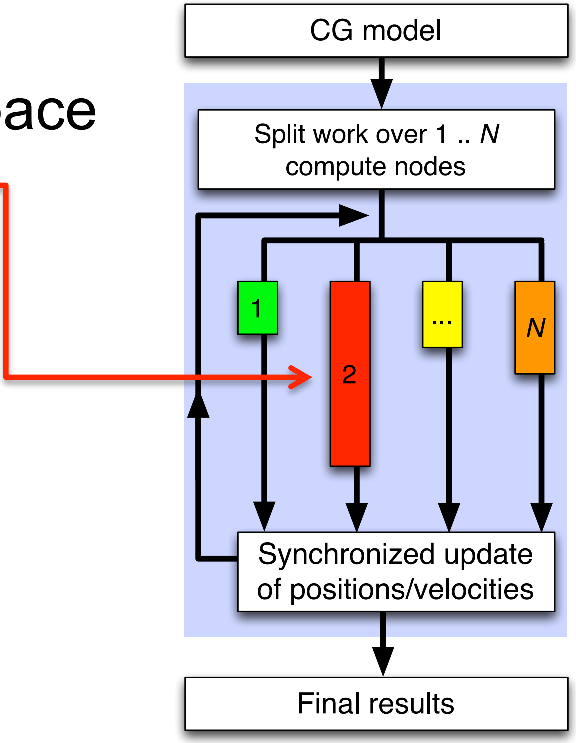
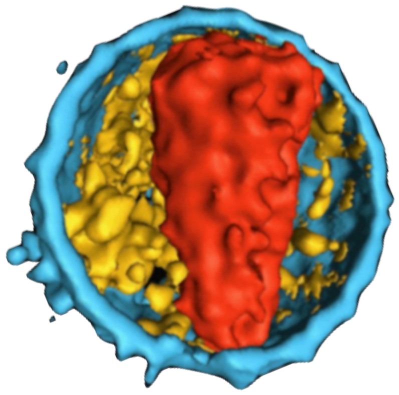
CG-MD problems

Implicit solvent for large scale ultra-CG: introduces large, dynamic areas of low particle density:

- *Load balancing*: MD simulation proceeds at pace of **slowest node**


CG model
Split work over 1 .. *N* compute nodes
1
2
...
N
Synchronized update of positions/velocities
Final results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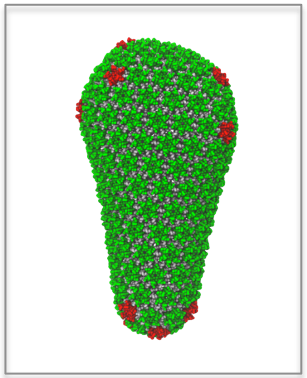
Ultra-CG model

- *Memory requirements*: memory needed even for empty regions of simulation

[1]Tom Goddard 2009, UCSF

CG-MD problems

A new MD code for multiscale CG:

- **Dynamic sparse data** representations (removes memory barriers for very large systems)

- **Load balancing** via Hilbert space filling curves (better use of supercomputing resources)

End goal: enable highly dynamic CG-MD simulations at a **cellular scale**!

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“Sparse” data

Two fundamentally different approaches vs standard MD:

- No global bonding topology – topology is local and *implicit*, allows significant dynamic runtime changes (add/remove/modify molecules etc)

- Reduced “link cell” memory requirements

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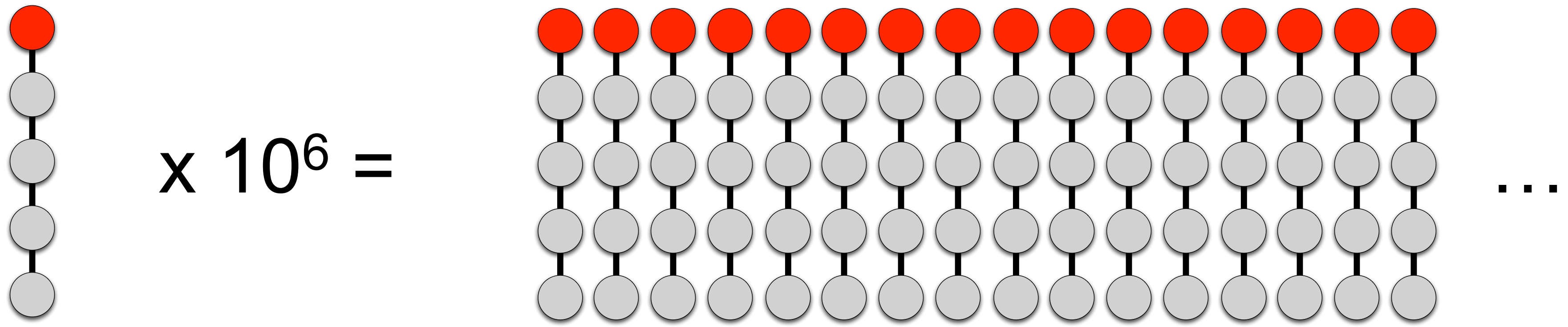
"Sparse" data



1M CG lipids = **~240 megabytes** of disk space in LAMMPS for bonding topology*: *but the same information is repeated for all lipids!*

New CG code needs **364 *bytes***. *Always*. One single "template" lipid structure, local topology calculated dynamically

*4 bonds + 3 angles

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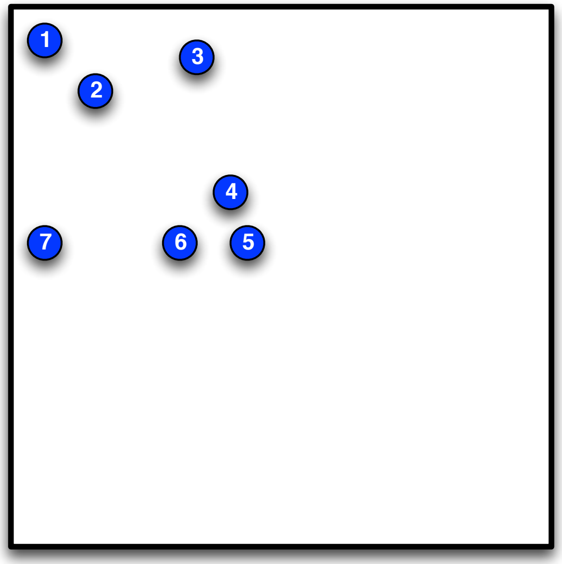
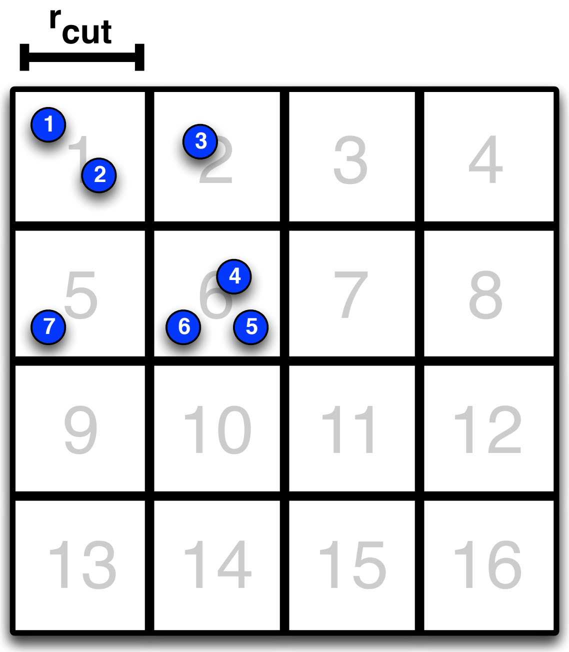
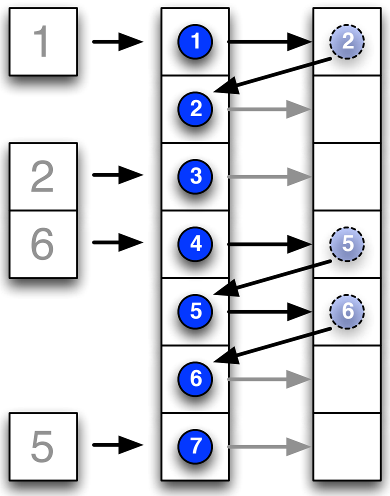
“Sparse” data



System



Divide into cells of size r_{cut}



Linked list of atoms in each “link cell”

“Link cell” algorithm used behind the scenes in MD – fast calculation of nonbonded interactions, but …

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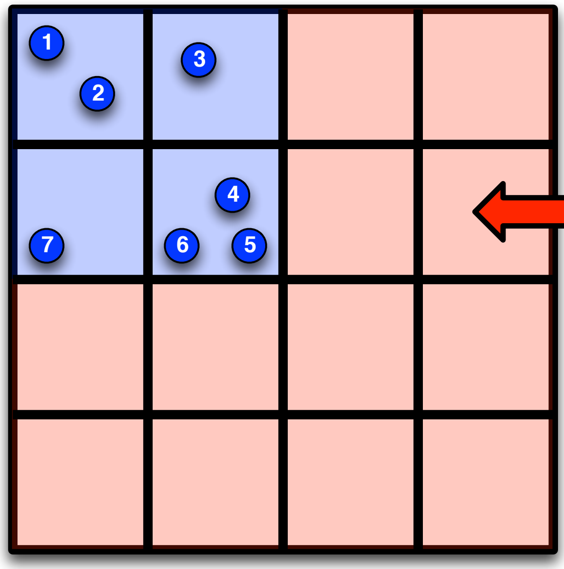
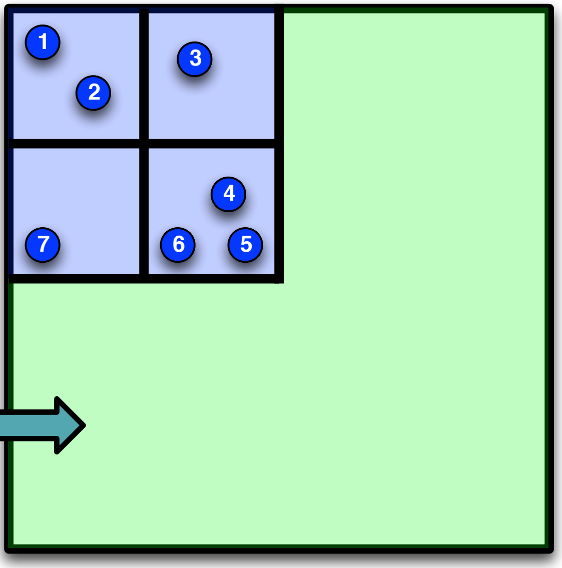
“Sparse” data

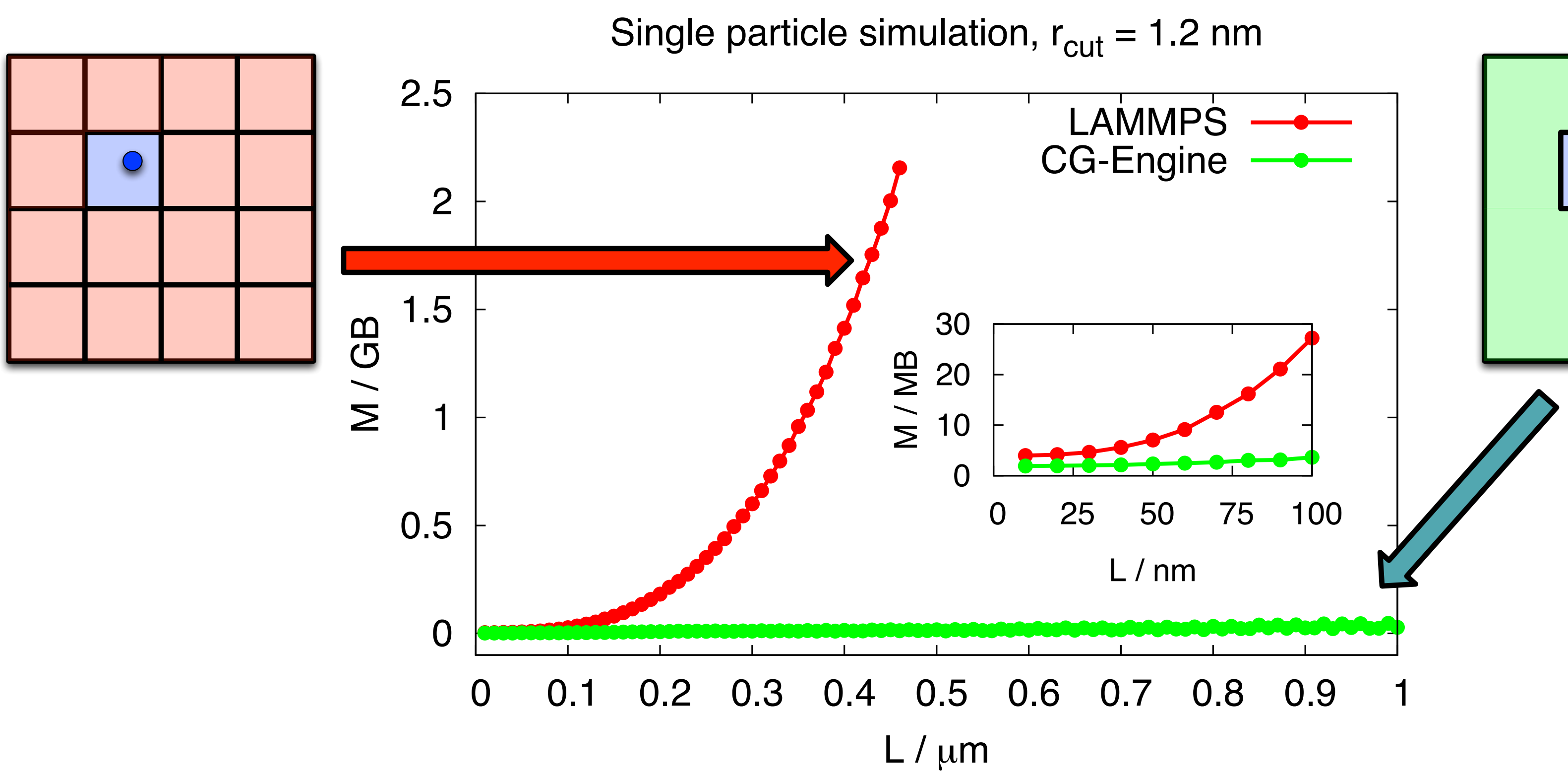


… conventional link cell algorithm: red cells require memory, even when empty!



CG-MD “sparse” link cells: green region requires no memory if empty!

“Sparse” data



Trivial example: **single particle** in large volume uses *huge* amounts of memory – yet the simulation is basically empty!

New CG code is much better behaved.

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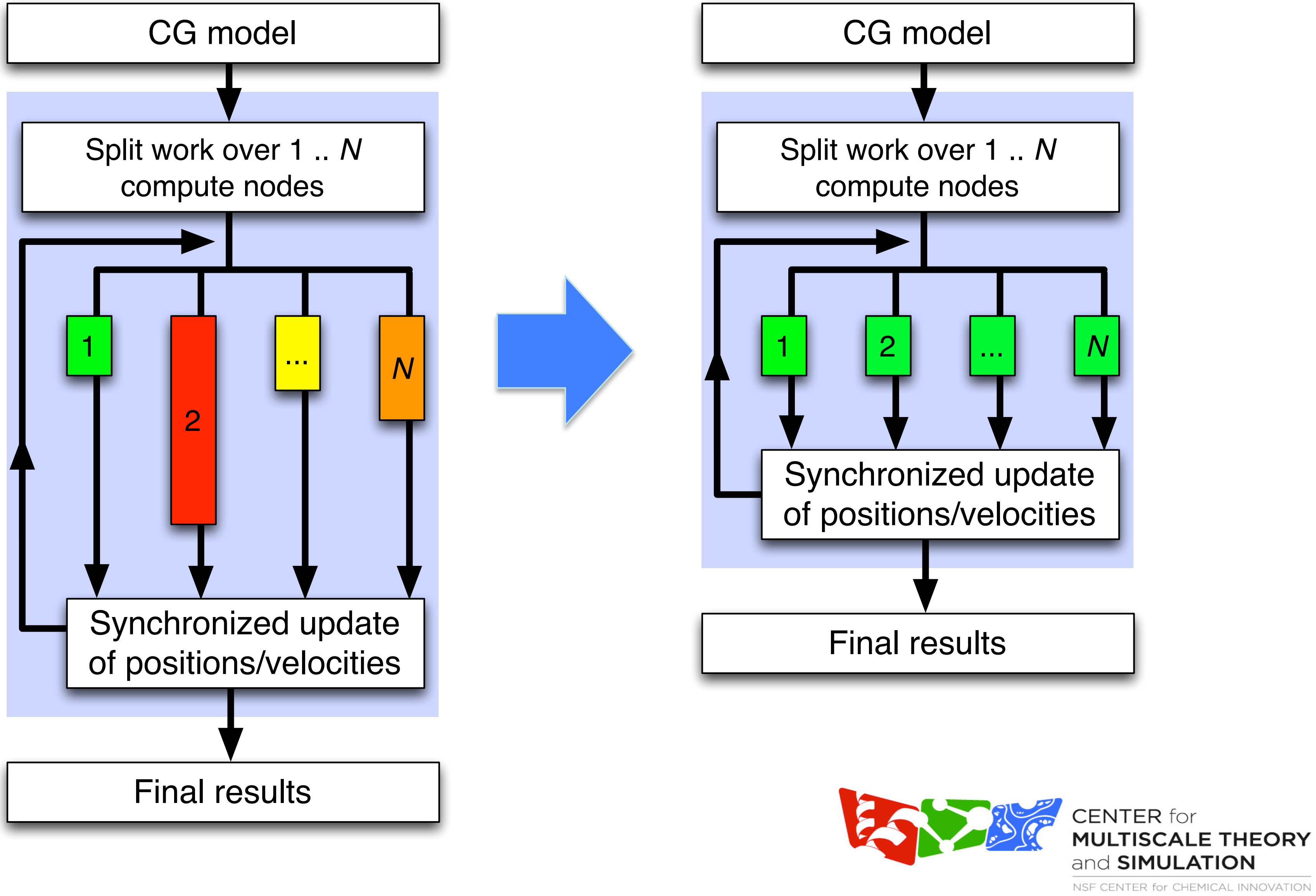
Load balancing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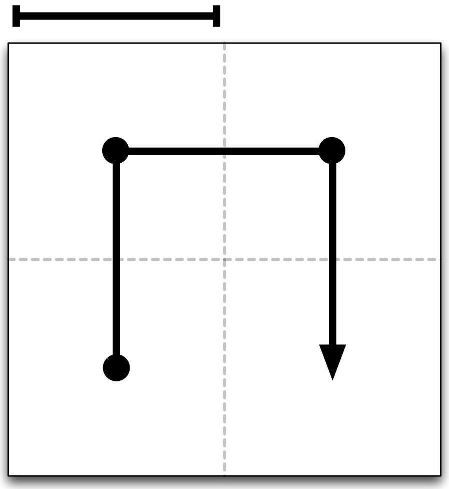
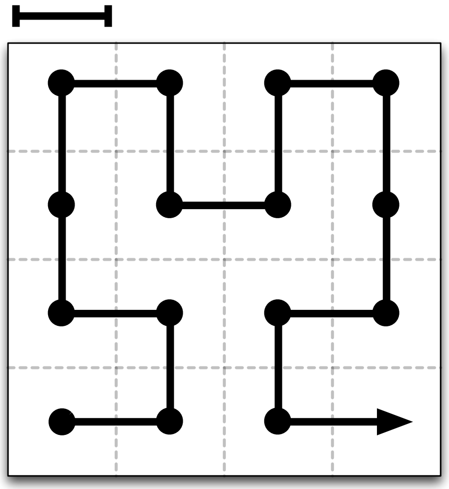
Load balancing

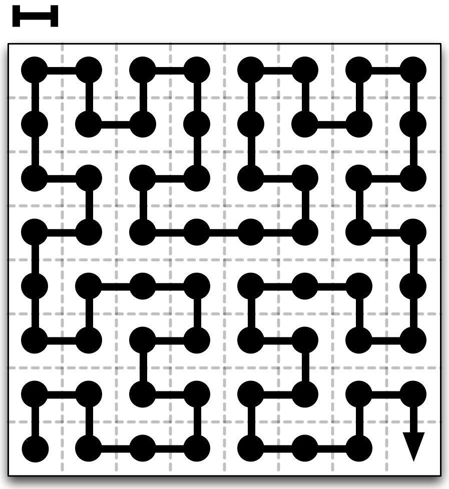
The space filling Hilbert curve



1st order



2nd order



3rd order

Useful properties:

- **Space filling** (high resolution where needed)
- **Dynamic generation** (no precalculation)
- **Locality** (adjacent SFC "indices" also local in the original 2D/3D Cartesian space)

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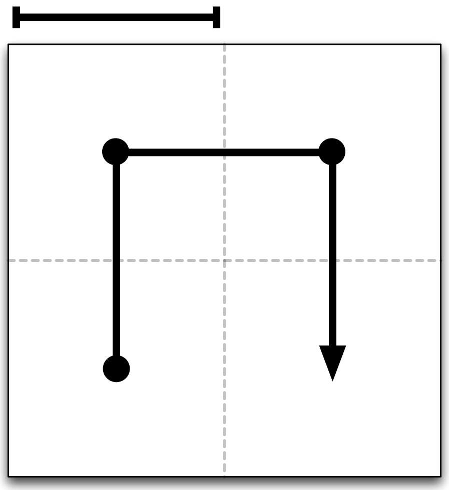
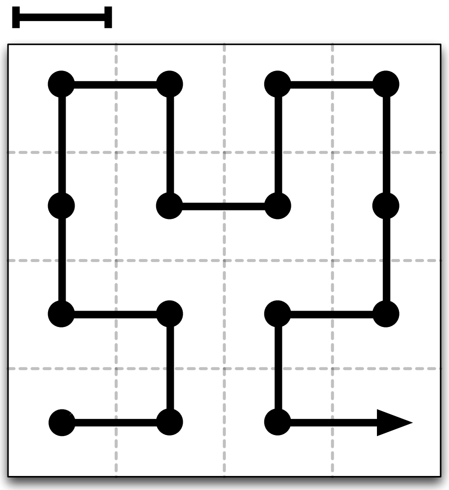
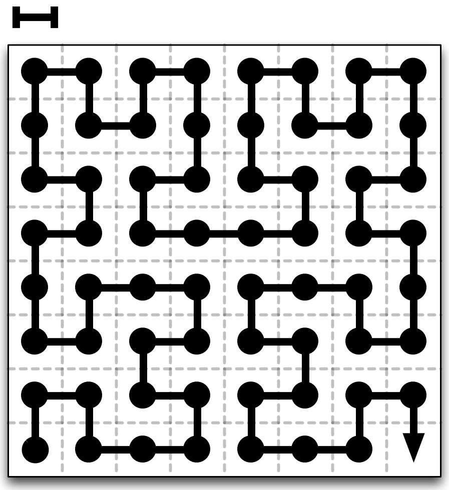
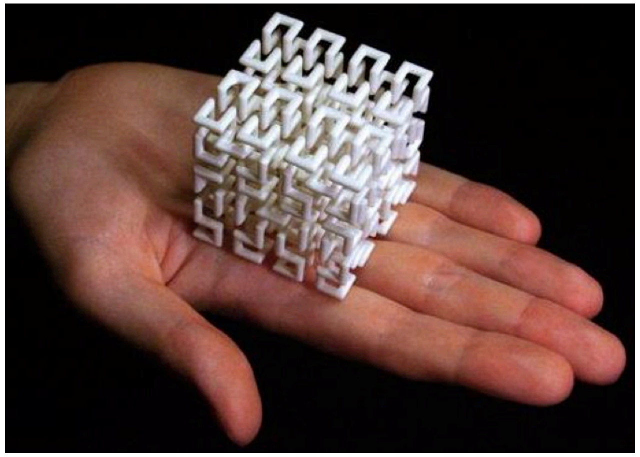
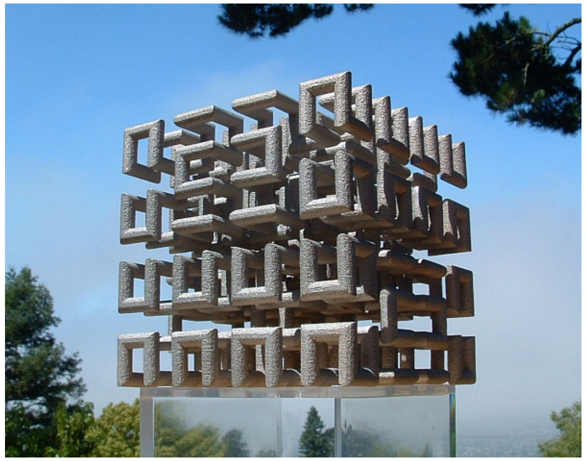
Load balancing











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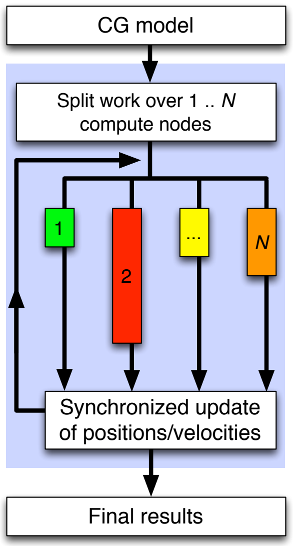
Load balancing

Example: 16 particle simulation run with four CPUs: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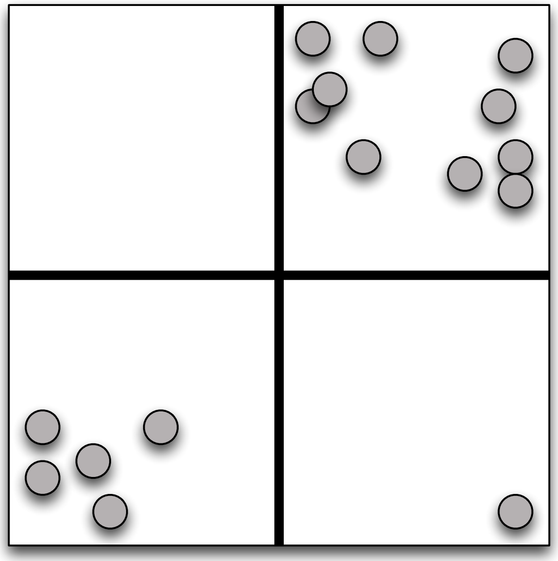

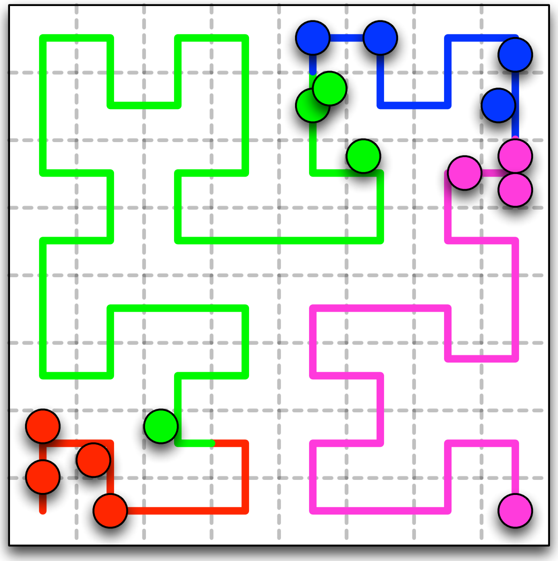

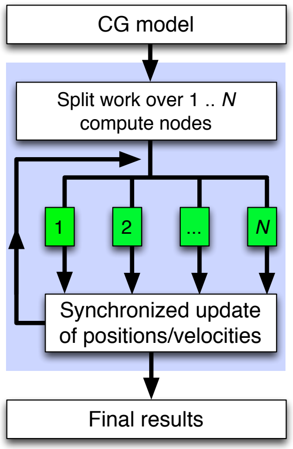
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Naïve, uniform spatial decomposition

Hilbert curve spatial decomposition

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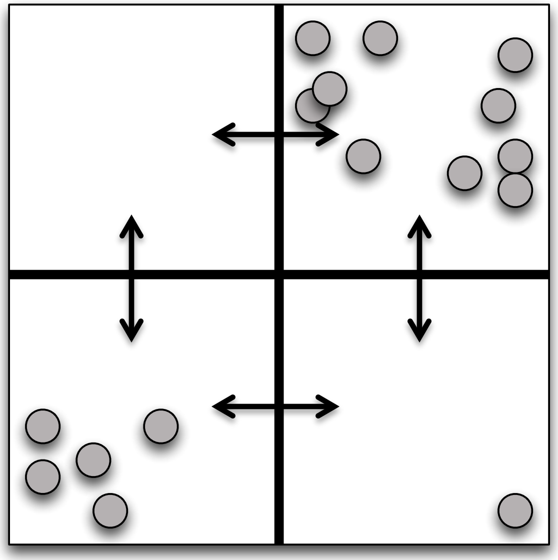
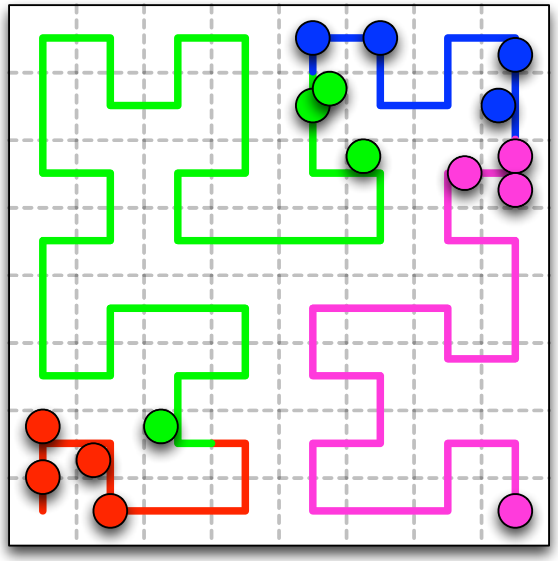
Load balancing

Who do we need to talk to?



Conventional: easy! We have up, down, left, right … etc



Hilbert curve: Irregular, boundaries between domains not simple

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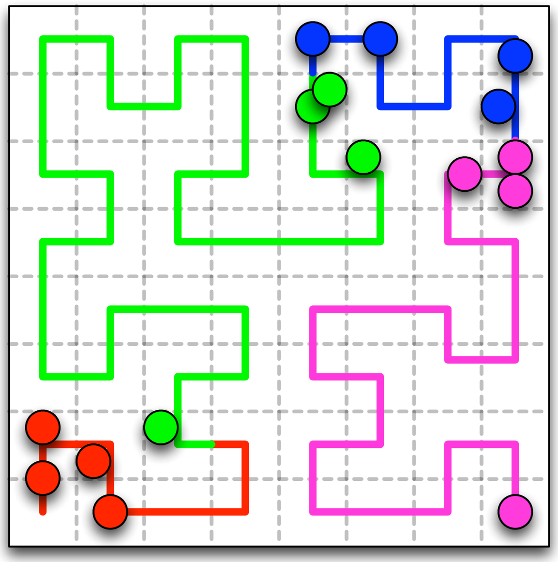
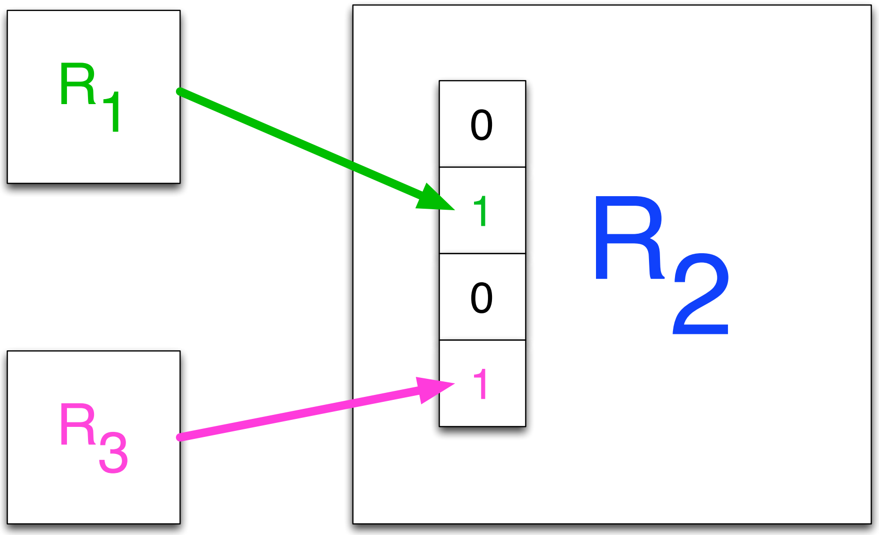
Load balancing

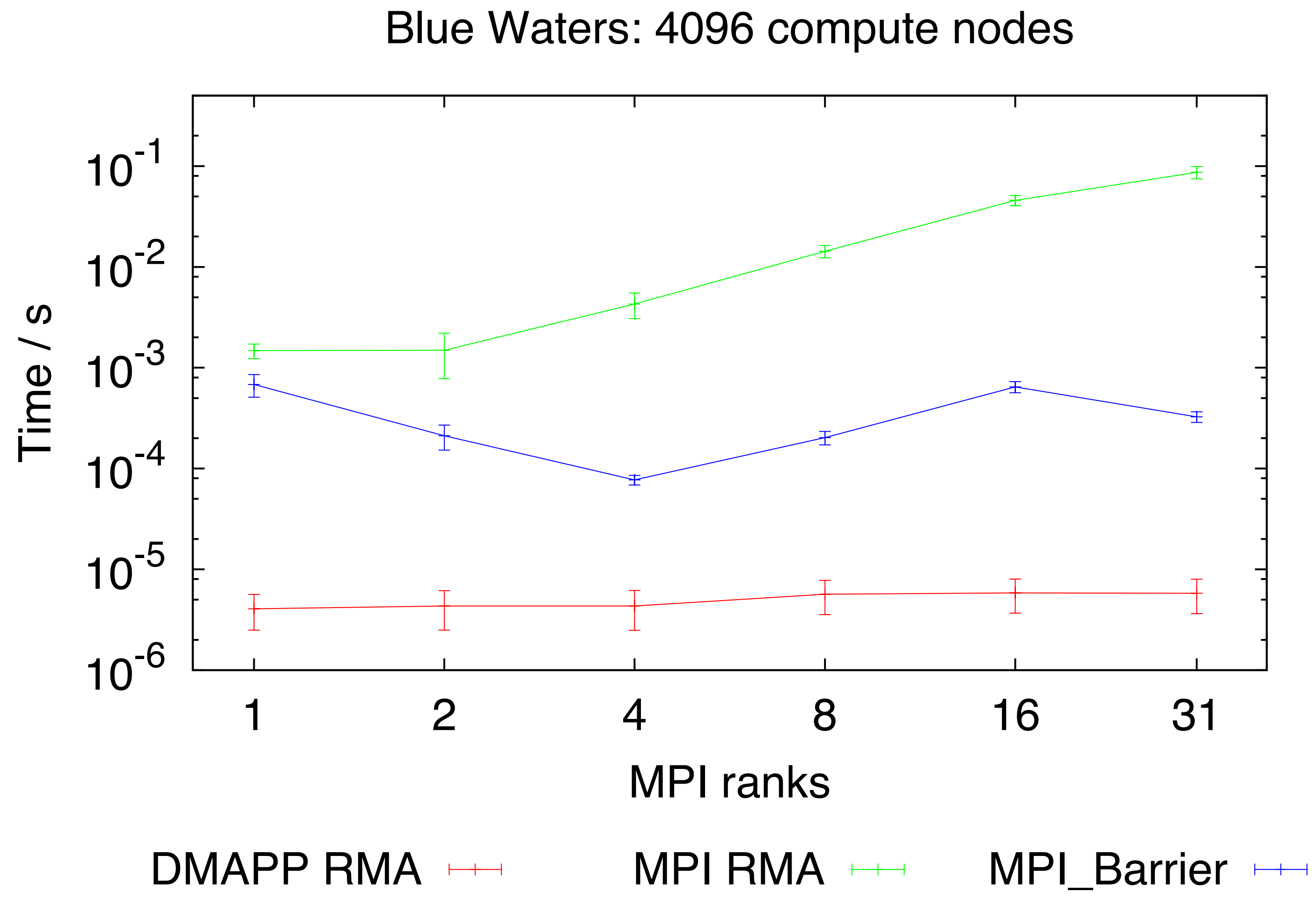
Who do we need to talk to? *MPI_Allreduce* etc slow.





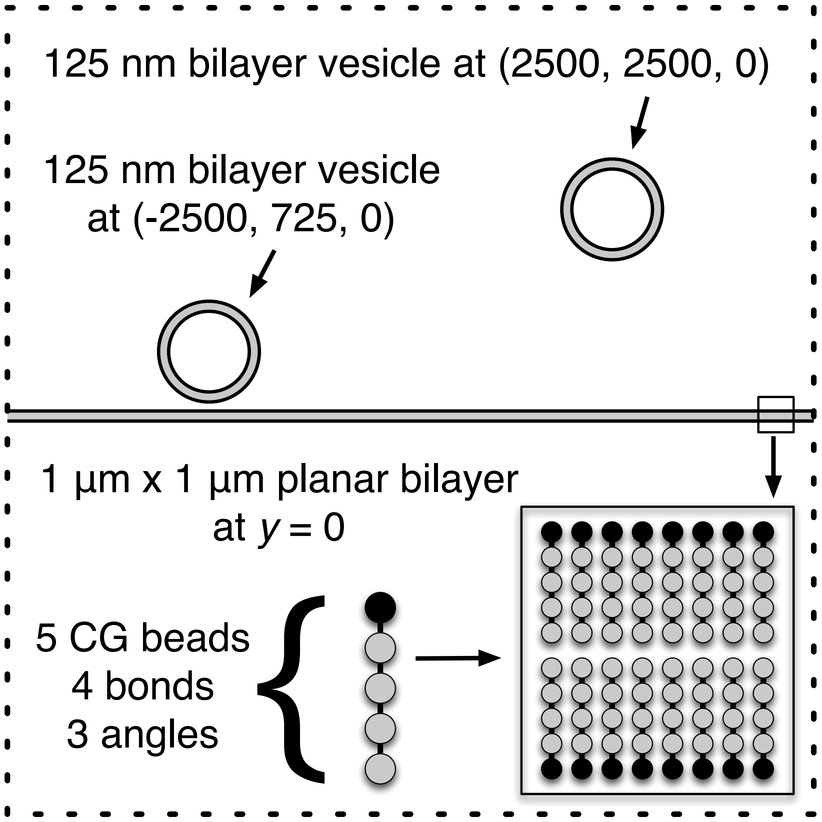
MPI's *Remote Memory Access* (RMA) to the rescue!

Load balancing

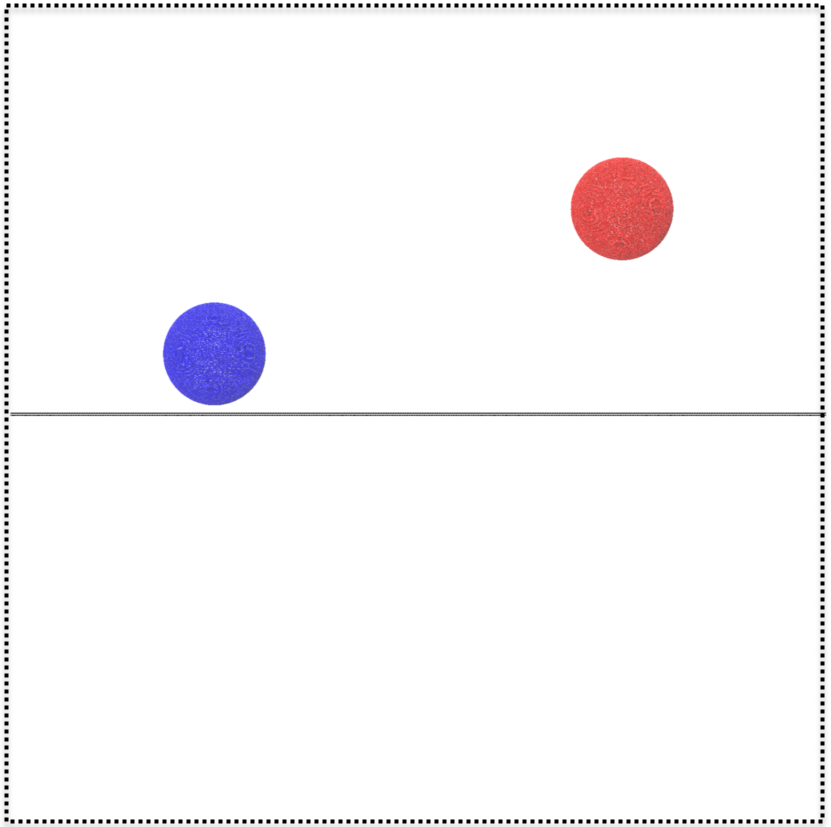


… or maybe not. I used DMAPP!

Example test system



125 nm bilayer vesicle at (2500, 2500, 0)
125 nm bilayer vesicle at (-2500, 725, 0)
1 μm x 1 μm planar bilayer at $y = 0$
5 CG beads
4 bonds
3 angles



Quite small (~15M particles), ***extremely*** heterogeneous density

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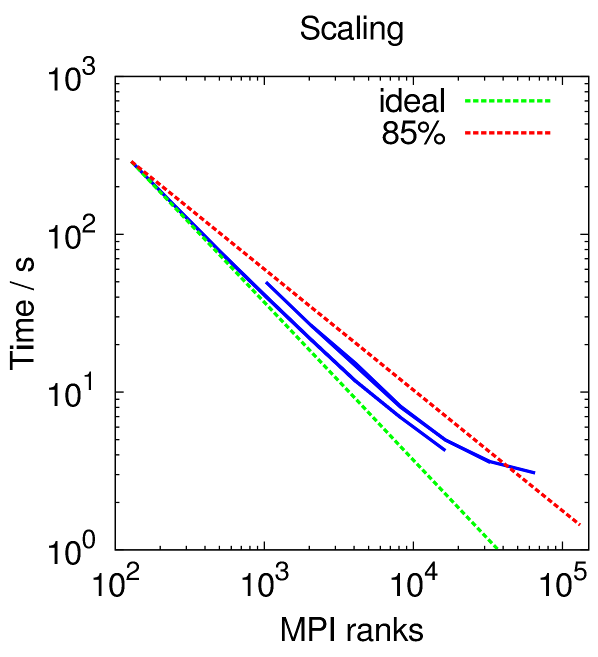
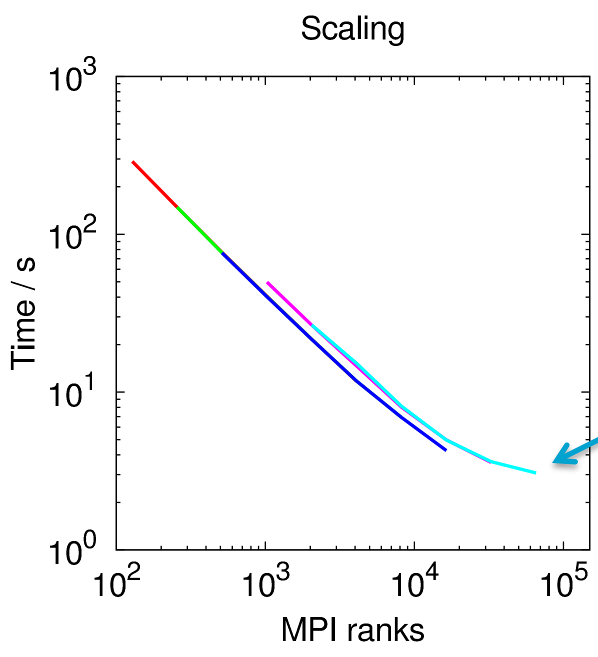
Example test system





238 particles per rank, ~3 ms per MD timestep

128, 256, … 4096 compute nodes with 1, 2, 4, 8, 16 ranks per node. *Why does it stop scaling?*

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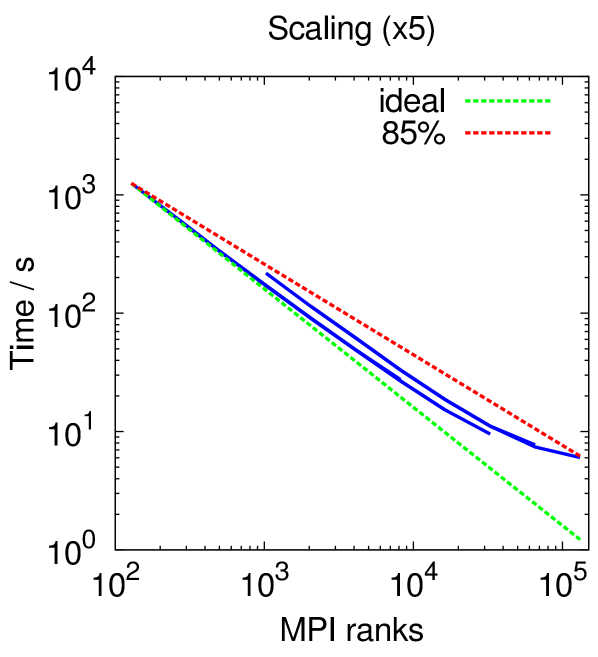
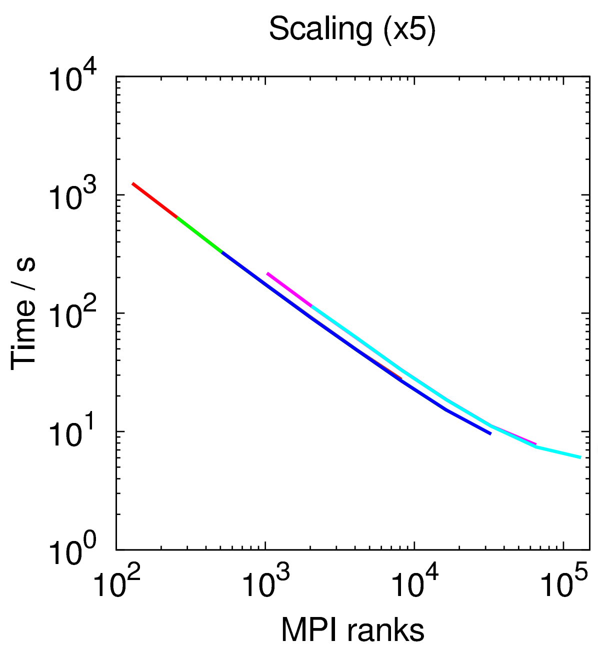
Example test system

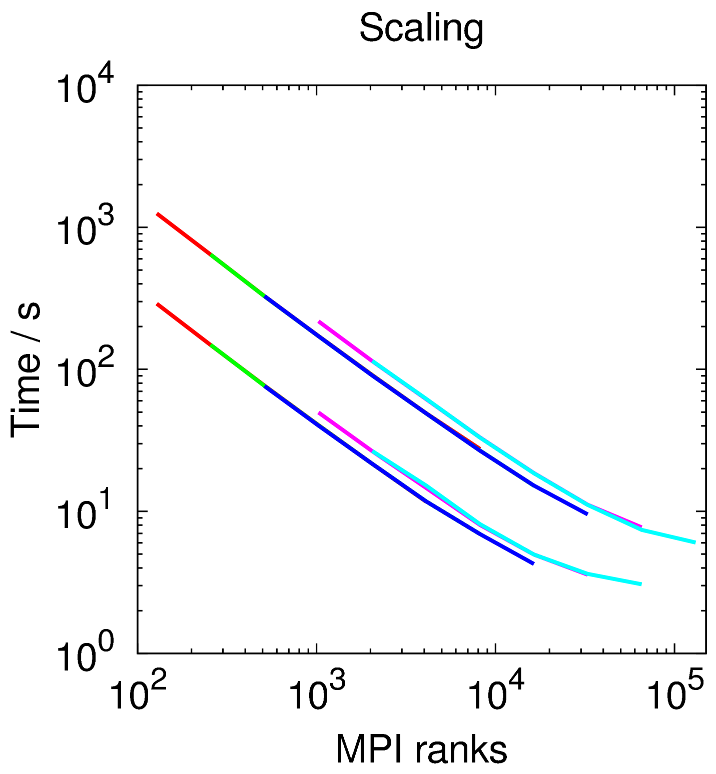




119 particles per rank, ~6 ms per MD timestep

Repeat force calculation x5 at each timestep: different scaling characteristics! *It's not the load balancer!*

Example test system



Not simply the same graph shifted up/down; so what's the problem? *It's not due to an MPI collective!*

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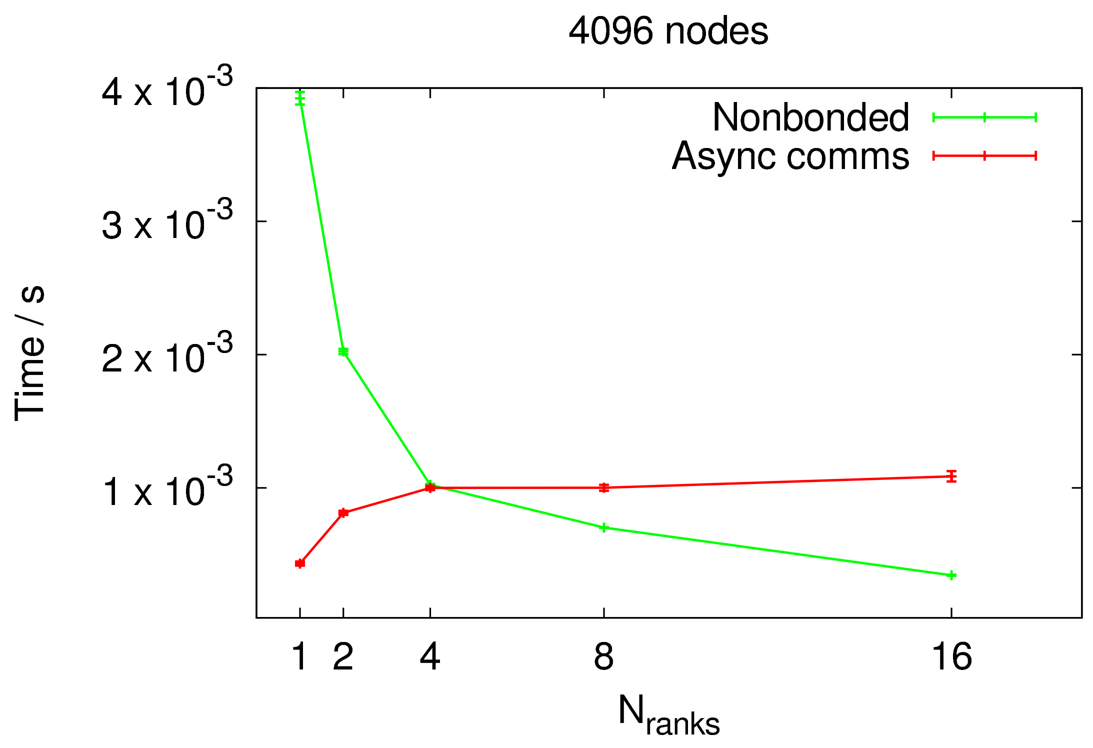
Example test system



Problem is MPI's asynchronous point-to-point calls (irecv, isend) – they can't keep up! DMAPP again?

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Summary

- Designed & implemented a custom MD code for large-scale, very dynamic CG simulations:
    - Very memory efficient
    - Load balances well
    - “Simple” & relatively friendly; < 5K lines of C++ with vanilla MPI (except for a few lines of DMAPP RMA code)

- Performance is very promising, despite unoptimised state

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Thanks to …

- NSF
- Prof. Greg Voth & the group
- Blue Waters staff, particularly:
  - Robert Brunner (long-suffering point-of-contact)
  - Kalyana Chadalavada

- jgrime@uchicago.edu - **comments and advice are very welcome!**

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