High Performance Computing: Tools and Applications

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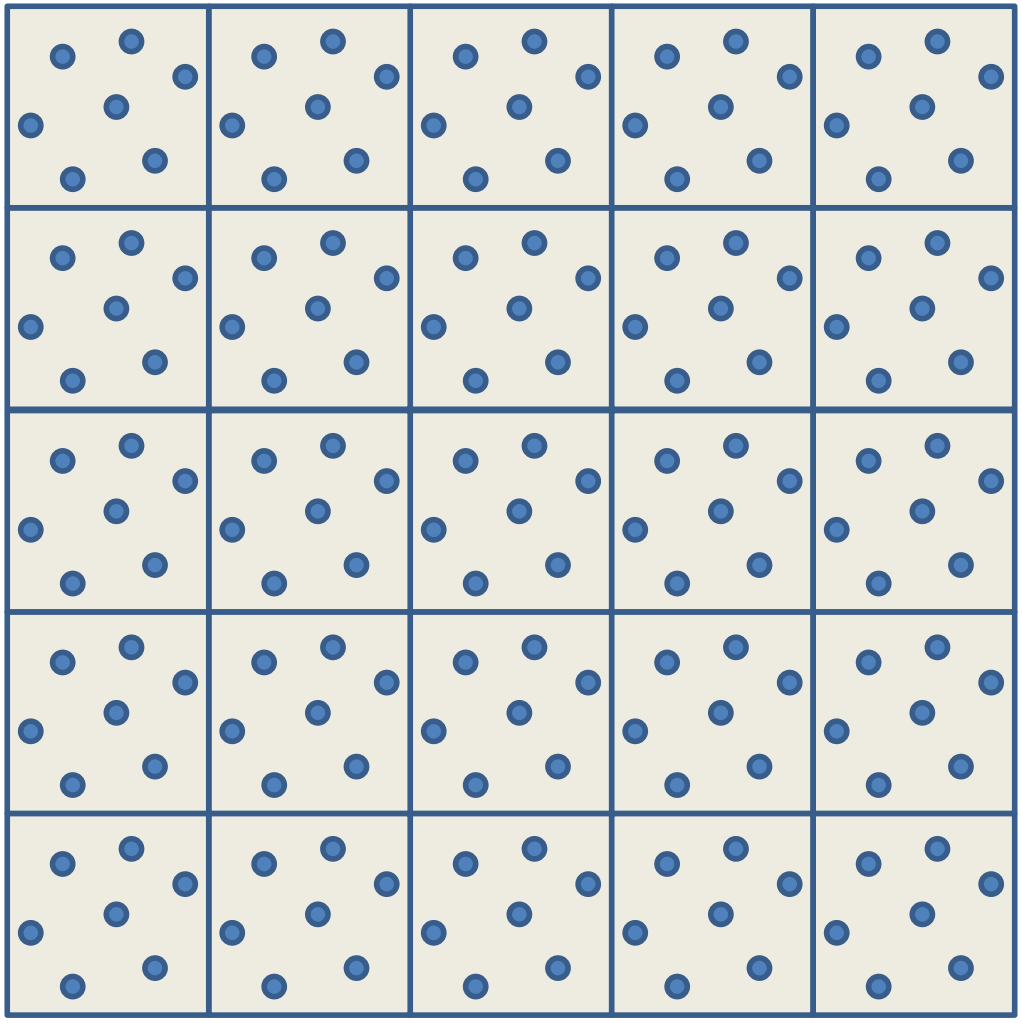
Lecture 5

Brownian dynamics with periodic boundary conditions

Simulate an *infinite* system of particles using a periodic simulation box with a fixed number of particles



Brownian dynamics with periodic boundary conditions

- When a particle exits the box, an *image* of the particle enters the box
- We only need to keep track of one of these two particles
  - keep track of the original particle that left the box
  - since we need to measure how far it has moved
  - do not need to “wrap” that particle’s positions back into the box
- However, when computing distances to see if particles overlap, we need to consider all possible images of all particles
  - when computing the distance between a particle and another particle and all its images, convert that distance to the smallest distance
  - this is handled by:

```
dx = remainder(ri[0]-rj[0], L);
dy = remainder(ri[1]-rj[1], L);
dz = remainder(ri[2]-rj[2], L);
```

Mean squared displacement (MSD)

In 3D, the mean square displacement of particles is

$$\langle r^2 \rangle = 6Dt$$

where t is the time interval during which particles are moving, and D is the diffusion constant.

"Displacement" is used to mean the *magnitude* of the displacement; not the cumulative distance moved (which is linear in t)

Therefore the diffusion constant can be computed as follows:

- Consider the graph of the mean of the *square* of the displacement for each t (note, this is different from the square root of the average displacement)
- This graph is expected to be linear in t (except for very small t in some cases)
- The slope of this line divided by 6 is D

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  - Solve for L in $\frac{4}{3}\pi a^3 n = \phi L^3$
- Different volume fractions will lead to different diffusion constants D

Notes on assignment submissions

- No need to make *pull requests*
- Executables and objects are normally not checked into the repository
- Do not use tabs in your source files
  - My editor generally doesn't map tabs to the same number of spaces as your editor; therefore we don't see your source the way you intended
  - Use your editor settings to change tabs to spaces

HPC Algorithms

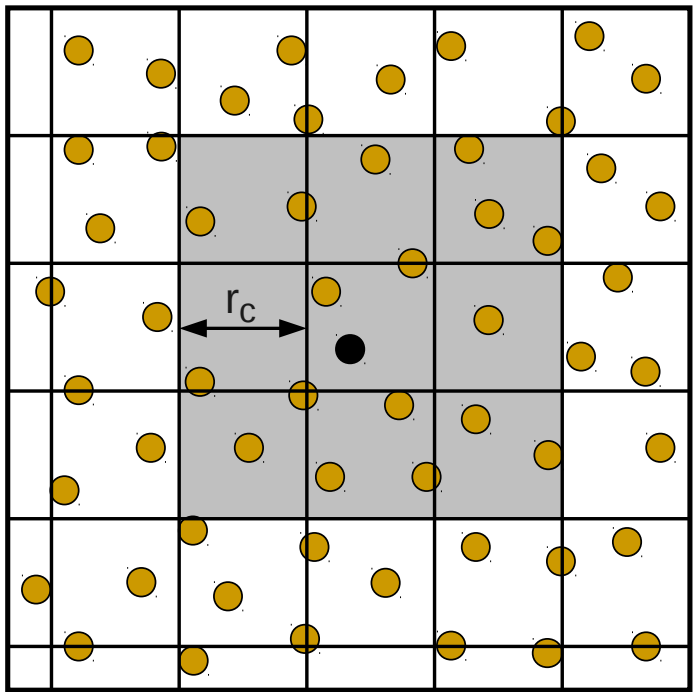
- In HPC research, use of good algorithms is just as important as good parallel implementations
- Usually, the best sequential algorithms are not the best parallel algorithms, and the best parallel algorithms can be very complicated

Computing steric repulsions

- For n particles, there are $n(n+1)/2$ possible interactions
- How to reduce the complexity to $O(n)$?

Cell lists

- Divide space into a set of cells, with cell width $\geq r_c$, where $r_c = 2$ in our case
- Particle *i* interacts only with particles in its own cell and its neighboring cells
- One sweep through all the particles is used to construct the *cell list* data structure (list of particles in each cell)
- When particles move, the cell list data structure must be reconstructed



Interesting optimization for cell lists

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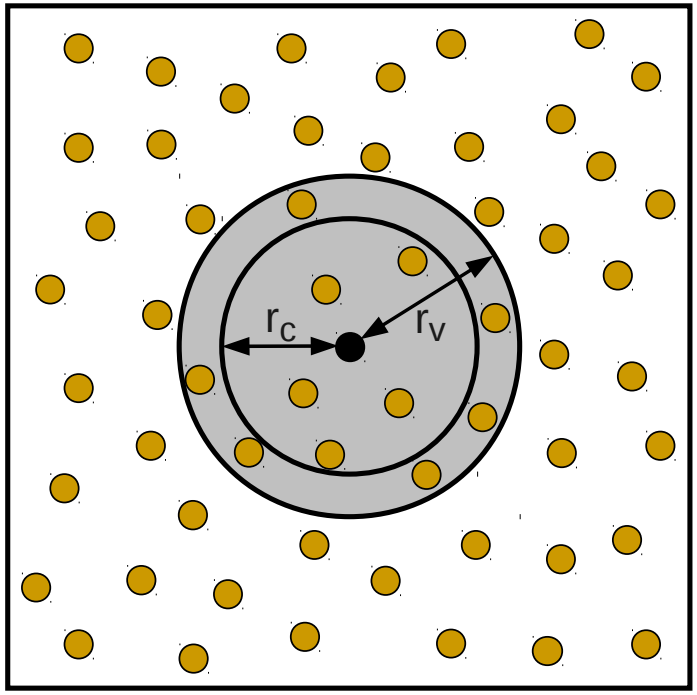
- Make the cells slightly larger, so that they can be reused for many time steps (or use cells that are one layer beyond the immediate neighbor cells)
- How can we optimize to exploit Newton's third law, i.e., don't compute equal and opposite interactions?
- Traversing *all* the particles to construct the cell lists can be expensive

Neighbor list method

- Exploits the idea that particles are moving slowly
- Each particle maintains a list of neighbors within a cutoff of $r_v > r_c$
- The neighbor list can be reused for a given number of time steps, in which it could be guaranteed that an particle beyond r_v does not move closer than r_c
- How to exploit Newton's third law?



How do we construct the neighbor list?

- Naive: $O(n^2)$
- Better: use cell lists whenever the neighbor lists must be reconstructed
  - this is the strategy of many particle codes

Sequential `interactions.c` code for cell lists

Code will be in the repo `ex05` directory.

Exercise 5

- Integrate the (sequential) `interactions` function into your Brownian dynamics code; you are free to make any modifications
- Compare the performance between your Exercise 4 code and your code using the `interactions` function
- Submit your results in the `ex05` directory, including
  - `ex05.c` or `ex05.cpp` source file and `makefile`
  - `ex05.pdf` report with performance comparison
- *Due 10 pm, Wed., Sept. 7*
- We are working toward a parallel version of the interactions function for mini-project 1.