N-Body System - LJMD

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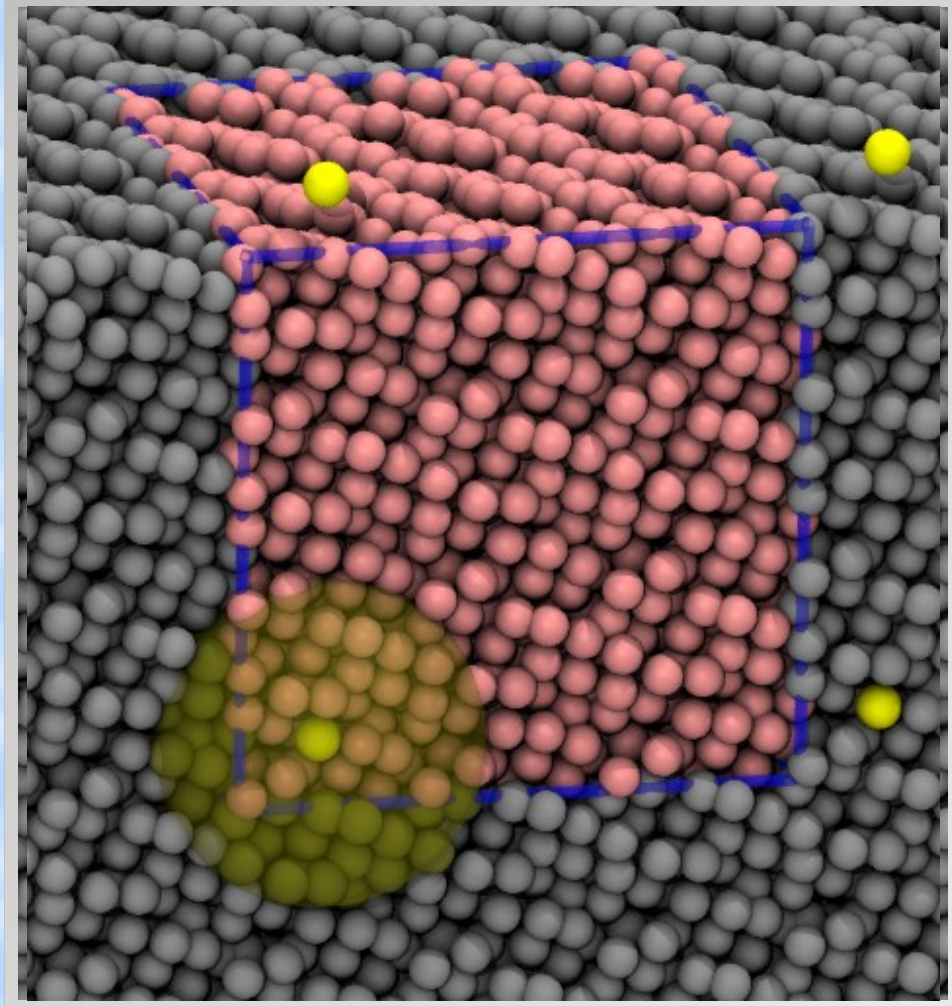
A Model for Liquid Argon



- Cubic box of particles with a Lennard-Jones type pairwise additive interaction potential

$$U(r)=\sum_{i,j}\begin{cases}4\epsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12}-\left(\frac{\sigma}{r_{ij}}\right)^{6}\right], & r_{ij}<r_c\\ 0, & r_{ij}\geq r_c\end{cases}$$

- Periodic boundary conditions to avoid surface effects

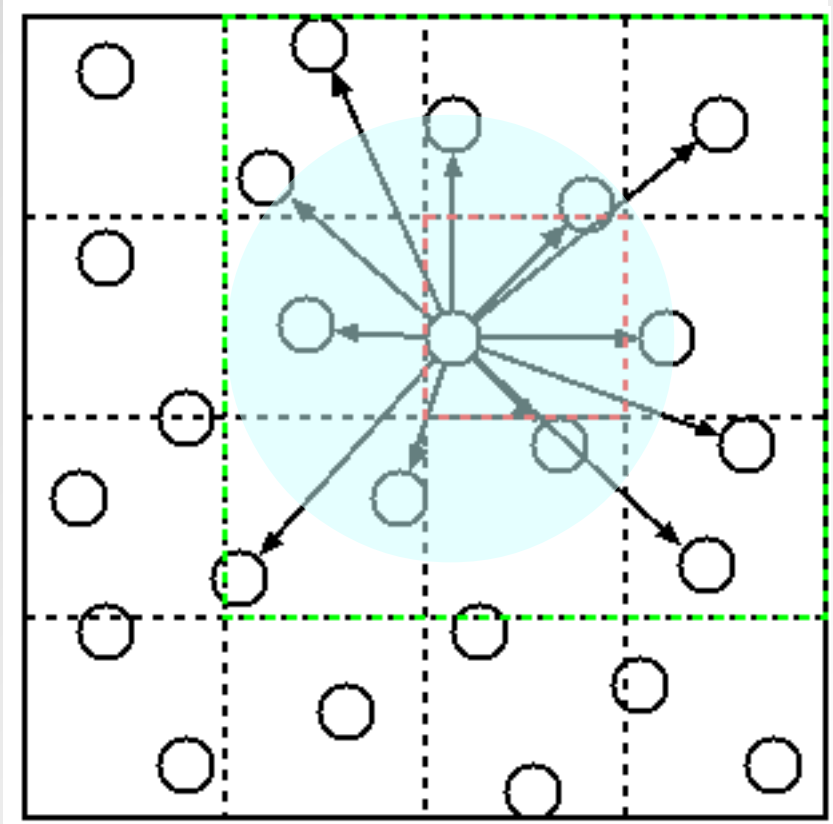
Does the Program Do?

1. Read in parameters and initial status and compute what is missing (e.g. accelerations)
2. Integrate Equations of motion with a velocity verlet integrator for a given number of steps
   a) Propagate all velocities for half a step
   b) Propagate all positions for a full step
   c) Compute forces on all atoms to get accelerations
   d) Propagate all velocities for half a step
   e) Output intermediate results, if needed

Making it Scale with System Size

- Lets look at the force compute algorithm: We compute all distances between all pairs
- But for larger systems not all pairs contribute and our effort is $O(N^2)$
- So we need a way to avoid looking at pairs that are too far away

  => Sort atoms into cell lists, which is O(N)



LJMD Project Tasks

- Refactor the project where most of the code is written in python and only time critical code in C
- Add an interface to matplotlib to support graphical monitoring of the simulation progress - optionally add GUI to enter run time flags
- Add capability to have multiple atom types with per-type masses and per type-pair parameters
- Add an option to use a Morse potential
- Add an option to apply a thermostat method