Assignment II: DUE 04/26/2019

We now consider our variables vectors, $\bar{r}, \bar{v}, \bar{U}, \bar{F}$ such that the equation of motion reads

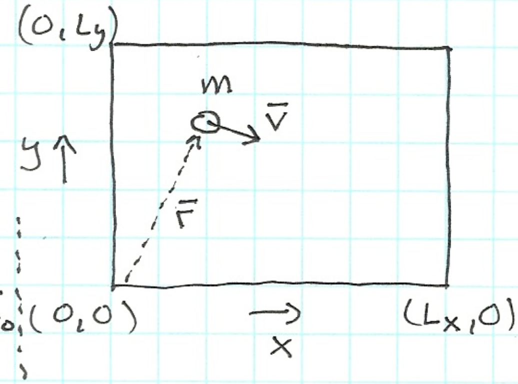
$$m\dot{\bar{v}} = \bar{f} \quad , \quad \bar{r} = \begin{pmatrix} x \\ y \end{pmatrix} \quad , \quad \bar{v} = \dot{\bar{r}}$$

with

$$\bar{f} = -\nabla U(\bar{r}) = -\begin{pmatrix} \partial/\partial x \\ \partial/\partial y \end{pmatrix} U(\bar{r})$$

Where $U(\bar{r})$ is a Potential energy surface. Time dependence can be included in $\bar{f}$ as well.

We wish to simulate a particle confined in a box with repulsive boundaries. The particle interacts with the walls according to the potential



$$U_W(s) = E_0\left\{\left(\frac{r_0}{s}\right)^{12} - 2\left(\frac{r_0}{s}\right)^{6}\right\} + E_0$$

For $|s| < r_0$ and $U_W(s) = 0$ for $|s| \geq r_0$. s is the distance (orthogonal) to the wall. Thus, the particle experiences four such interactions.

Assuming that $\bar{r} = \begin{pmatrix} x \\ y \end{pmatrix}$ is already normalized to r_0, normalizing energy to E_0, and time to t_0, such that m is normalized to m_0 (m is now unitless), make the particle bounce around in the box with parameters

$m = 1, \; L_x = L_y = 20$

with initial conditions (normalized)

$(x^0, y^0) = \bar{r}^0 = (5, 5)$ and $(v_x^0, v_y^0) = \bar{v}^0 = (2, 3)$

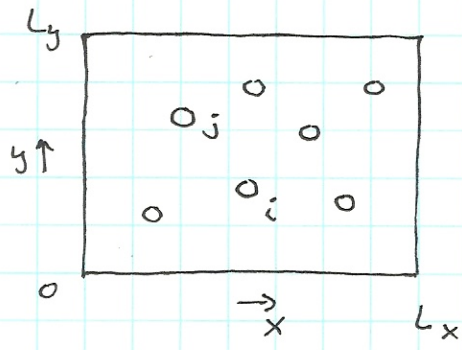
Calculate and display a trace of the particles' motion as it is making a reasonable number of collisions with each of the walls.

Calculate the potential and kinetic energies as a function of time (for both kinetic energies), and likewise calculate the total energy as a function of time.

Do the above for different time step sizes, and comment on the stability limit.

Change $\bar{v}^0$ to $\bar{v}^0 = (4, 6)$ and do all of the above. How does accuracy of energy and time step stability change with $\bar{v}^0$?

We now define the same box, but put more particles in it.



Each particle has an equation of motion

$$m_i \bar{v}_i = \bar{F}_i \quad , \quad i = 1, 2, \ldots, N$$

(N particles).

In addition to interacting with the wall, these particles interact with each other through

$$U_{LJ}(r_{ij}) = -E_0 \left\{ \left(\frac{r_0}{|r_{ij}|}\right)^{12} - 2\left(\frac{r_0}{|r_{ij}|}\right)^{6} \right\}$$

where $r_{ij} = |\bar{r}_i - \bar{r}_j|$

With the same normalization as above, start N particles in a box (the same box) such that the particles are initially separated by at least r_0, both from the walls and from each other.

Validate visually that the dynamics looks reasonable.

Calculate potential, kinetic (both), and total energy averages of the system as a function of time -- Energies per particle.

Calculate both spatial and temporal averages of the energies per particle as well. For example, Potential energy average ~~over time is~~ : per particle:

$$\langle E_p^n \rangle_i = \frac{1}{N} \left\{ \sum_{i=1}^{N} \sum_{j>i}^{N} U(r_{ij}^n) + \sum_{i=1}^{N} U_w(r_i^n) \right\}$$

all four walls

Whereas the potential energy average per particle over time is

$$\langle E_p^n \rangle = \frac{1}{M} \sum_{n=1}^{M} \langle E_p^n \rangle_i$$

Plot the Energy averages over time as a function of time step and as a function of initial energy of your initial condition.

Comment on the stability of the time step.

Use $N = 20$ and simulate enough time steps in order to obtain robust statistics (good averages) in $\langle E_p^n \rangle$, $\langle E_k^n \rangle$ (both velocities), $\langle E_t^n \rangle$ (total energy).

Attach plots and code listing.