Project assignment 2

KEM 342

Project teams:

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Part 1

- Put the harmonic oscillator in 3D
- Show:

$$H = E = T(\vec{p}^N) + U(\vec{r}^N) = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + U(\vec{r}^N) = \sum_{i=1}^{N} \frac{m_i \dot{r}_i^2}{2} + U(\vec{r}^N)$$

$$P_l = \sum_{i=1}^{N} m_i \hat{l} \cdot \dot{\vec{r}} \qquad l = x, y, z \qquad \vec{L} = \sum_{i=1}^{N} \vec{r}_i \times \vec{p}_i = \sum_{i=1}^{N} \vec{r}_i \times m_i \vec{v}_i$$

Part 2

- Back to 2 D
- Put on periodic boundary conditions in the x and y axes
- Simulate many harmonic oscillators each ball starting with random velocity
- First have them not interacting: use visualization to show that the periodic boundary conditions are working
- Now have all the balls interact with the balls in different ”molecules” through Lennard-jones interactions
- You have the LJ parameters σ and ε and you have the bond parameters U and bond length, the size of the system (periodic boundary conditions) number of ”molecules” and the timestep as parameters
    1. Find initial condition and range of these parameters where the simulation is stable

    HINT: start in position with balls not too close together

    1. Show that total energy is conserved
    2. Bonus: Remove periodic boundary conditions and show that the total linear and angular momentum are conserved

Part 3

- Remove the bonds: just Lennard-Jones balls in 2D
- Show that when the energy is minimized they form a triangular lattice in 2D
- Visualize this energy minimization

Part 4: something for the scientists on the team to do while the programmers are coding ☺

- Consider just the parameters available in this model
- i.e. parameters σ and ε, bond parameters U and bond length, the size of the system (periodic boundary conditions) number of ”molecules” and the timestep
- Three dimensions instead of two of course
- What real systems can you simulate with this model?
- For these systems, what would the values be for each parameter?
- This requires a literature search…
- What would the system size in REAL units be?
- What would the timestep in REAL units be?
- What REAL density range can you simulate from what you determined in part 2?
- Explain why, for these systems, this paradigm can effectively model this system. What approximations are being made?
- Hint: no partial charges on atoms or angle or dihedral potentials available and you dont have to use every parameter hint-hint: with or without the bond