Week Five Phy-480

Lewis

September 2025

1. Structuring a Python Code for MD Simulations

Below you will find the Python code structured to carry out molecular dynamics simulations of a cloud of electrons in free space using the velocity Verlet algorithm.

1. **Initialization:**
   - Define constants
   - Initialize particle positions $\vec{r}_i(0)$ randomly in a region.
   - Initialize velocities $\vec{v}_i(0)$.
   - Initialize accelerations $\vec{a}_i(0)$.
2. **Force Calculation:**
   - Compute pairwise Coulomb forces between particles:

$$\vec{F}_{ij} = k_C \frac{e^2 \vec{r}_{ij}}{|\vec{r}_{ij}|^3}$$

   - Sum over j for each particle i.
3. **Time Integration (Velocity Verlet):**

$$\vec{r}_i(t+\delta t) = \vec{r}_i(t) + \delta t \vec{v}_i(t) + \frac{\delta t^2}{2m}\vec{F}_i(t),$$
$$\vec{v}_i(t+\delta t) = \vec{v}_i(t) + \frac{\delta t}{2m}\Big(\vec{F}_i(t) + \vec{F}_i(t+\delta t)\Big).$$

4. **Loop Over Timesteps:**
   - Update positions.
   - Recompute forces.
   - Update velocities.

- Save positions, velocities, and energies for analysis.

5. **Output and Analysis:**
   - Track kinetic, potential, and total energies.
   - Monitor conserved quantities and system behavior.

2. Mechanical Energy in an Electron Cloud

In an electron cloud in free space:

- There are no external forces on the system as a whole. By Newton's third law, internal forces cancel out in pairs. Which would mean that the **center of mass** of the system moves with constant velocity. If initially at rest, the center of mass must be fixed.
- The **total mechanical energy** of the system consists of the sum of kinetic and potential energies:

$$E_{\text{tot}} = \sum_i \frac{1}{2} m v_i^2 + \sum_{i<j} \frac{k_C e^2}{r_{ij}}.$$

- The total energy is conserved because there are no external forces.

Thus, the system's energy remains constant, and the COM motion is uniform.

3. Velocity Distribution and Temperature in Expanding Clouds

In an MD simulation of an expanding electron cloud in a micro-canonical ensemble:

- The system is far from equilibrium. Therefore, the **velocity distribution does not immediately follow Maxwell-Boltzmann statistics**.
- Over time, if collisions randomize velocities sufficiently, the distribution may relax toward a Maxwell-Boltzmann form, but during expansion, it typically deviates.
- The **concept of temperature** becomes less clear. Temperature is well-defined in equilibrium ensembles, but here, one can only assign an "effective temperature" based on average kinetic energy:

$$k_B T_{\text{eff}} \sim \frac{2}{3N} \sum_i \frac{1}{2} m v_i^2.$$

Thus, while temperature has limited meaning in far-from-equilibrium conditions, the velocity distribution can still provide insight into the system's dynamics.