Evaluating Glass Forming Compounds via NVE Ensemble Molecular Dynamics Simulation

Background and Methodology for PHYS338 Final Project

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Motivation and Project Goals

- **Why study glass formers?** They exhibit complex, non-crystalline behavior and unique energy dynamics that are critical to understanding material properties.
- **Role of MD:** Molecular Dynamics (MD) simulations allow us to explore microscopic structural and dynamic phenomena.
- **Project Aim:** Use an NVE ensemble to preserve energy conservation while analyzing diffusion and structure in glass forming compounds.

Molecular Dynamics Formulation

- From Newton's second law:

$$\mathbf{F}_i = m_i \frac{d^2\mathbf{r}_i}{dt^2}.$$

- The force is obtained from the interatomic potential $U(\mathbf{r})$:

$$\mathbf{F}_i = -\nabla_i U(\mathbf{r}_i).$$

Lennard-Jones Potential

- A simple yet widely used model for interatomic interactions:

$$U(r_{ij}) = 4\epsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right].$$

where:

  - ϵ is the depth of the potential well.
  - σ is the finite distance at which the inter-particle potential is zero.
  - r_{ij} is the distance between particles i and j.
  - The equilibrium separation is at $r_{ij} = 2^{1/6}\sigma$.

Kob-Andersen Model

- An extension of the Lennard-Jones model tailored for binary mixtures.
- For particle types $\alpha, \beta \in \{A, B\}$ in an 80:20 A:B mixture:

$$U_{ij} = U_{\alpha\beta}(r_{ij}) = 4\epsilon_{\alpha\beta} \left[\left(\frac{\sigma_{\alpha\beta}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{\alpha\beta}}{r_{ij}} \right)^{6} \right].$$

- This adjustment captures additional anharmonic effects relevant to glass formation.

Velocity-Verlet Algorithm

To update positions and velocities, we use the Velocity-Verlet algorithm:

$$\mathbf{r}_i(t + \Delta t) = \mathbf{r}_i(t) + \mathbf{v}_i(t)\Delta t + \frac{1}{2}\mathbf{a}_i(t)\Delta t^2, \tag{1}$$

$$\mathbf{v}_i(t + \Delta t) = \mathbf{v}_i(t) + \frac{1}{2}\left[\mathbf{a}_i(t) + \mathbf{a}_i(t + \Delta t)\right]\Delta t. \tag{2}$$

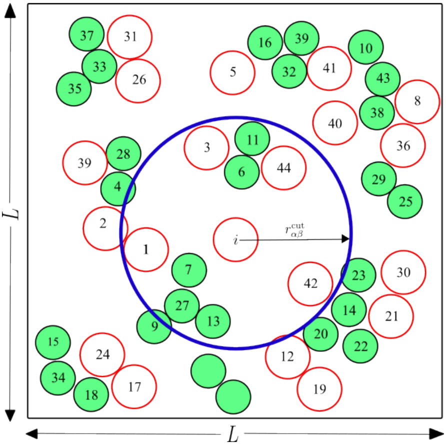
- **Benefits:** Time-reversible, stable, and energy conserving.
- **Ensemble:** NVE ensures constant total energy during simulation.

Periodic Boundary Conditions

- **Purpose:** Mimic an infinite system by wrapping particles into a simulation box.
- **Minimum Image Convention:**

$$r_{ij} = \min_{n \in \{-1,0,1\}^3} |\mathbf{r}_j - \mathbf{r}_i - \mathbf{L} \cdot \mathbf{n}|$$

- A cutoff radius $r_{cut} \approx 2.5\sigma$ is applied to reduce computation.
- To avoid discontinuities, define U_{ij}^{cut} at r_{cut}:



$$U_{ij}^{\text{cut}} = \begin{cases} U_{\alpha\beta}(r_{ij}) - U_{\alpha\beta}(r_{\alpha\beta}^{\text{cut}}) & r_{ij} < r_{\alpha\beta}^{\text{cut}} \\ 0 & \text{otherwise} \end{cases}$$

Analysis Techniques

- **Radial Distribution Function (RDF):** Measures local structural order and describes the probability of finding a particle at a distance r from another reference particle.

$$g_{\alpha\alpha}(r) = \frac{V}{N_\alpha(N_\alpha - 1)} \left\langle \sum_{i=1}^{N_\alpha} \sum_{\substack{j=1 \\ j\neq i}}^{N_\alpha} \delta\Big(r - |\mathbf{r}_i - \mathbf{r}_j|\Big) \right\rangle.$$

  where the Dirac delta function $\delta(r - |\mathbf{r_i} - \mathbf{r_j}|)$ ensures that only particles at a distance r contribute to the sum.

- **Mean Square Displacement (MSD):** Quantifies diffusion by tracking particle displacement over time.

Conclusions & Future Directions

- MD simulations provide valuable microscopic insight into glass forming compounds.
- The NVE ensemble effectively conserves energy, making it ideal for studying diffusion and energy dynamics.
- **Future Directions:**
  - Incorporate advanced analysis techniques to further probe dynamic properties.
  - Explore different binary mixtures to understand their impact on glass formation.