**1. What is Mean Square Displacement (MSD)?**

**Physical Explanation:**

* MSD is a measure used to quantify the spatial extent of an object's movement as a function of time. In the context of polymers, it helps us understand how a monomer or the centre of mass of a polymer chain moves through space over time.

**Mathematical Expression:**

* The MSD is defined as: MSD(*t*)=⟨∣*r*(*t*)−*r*(0)∣^2⟩ where *r*(*t*) is the position of a monomer at time *t*, *r*(0) is its initial position, and the brackets ⟨⟩ denote an average over time and monomers.

**Effect of Polymer Properties**:

* Study how the MSD changes with different polymer properties such as chain length, stiffness, and interaction potentials.

**External Forces and Constraints**:

* Analyze how the MSD is affected by external forces, obstacles, or confinement.

**3. Calculating MSD in Simulations:**

**a. Single Polymer Dynamics:**

* Track the motion of a single monomer or the center of mass of a polymer chain.

**b. Multiple Polymers:**

* Track the motion of monomers in a system of multiple interacting polymers.
* Calculate the average MSD over all monomers.

**4. Different Diffusion Regimes:**

1. **Normal (Brownian) Diffusion:**
   * MSD vs Time Relation: *MSD*(*t*)∝*t*
   * Interpretation: In normal diffusion, particles move randomly and independently. The MSD is linear with time, indicating that the particle is exploring the space at a constant rate.
2. **Subdiffusion:**
   * MSD vs Time Relation: *MSD*(*t*)∝*t^α, where* 0<*α*<1
   * It occurs when the particle's movement is hindered or slowed down, for example, due to obstacles or a viscoelastic medium. The MSD grows slower than linearly with time.
   * Example: Movement of particles in a crowded cellular environment.
3. **Superdiffusion:**
   * MSD vs Time Relation *MSD*(*t*)∝*t^α*, where a >1
   * Superdiffusion occurs when particles have a tendency to move in the same direction for extended periods, leading to faster exploration of space. The MSD grows faster than linearly with time.
   * Example: Movement of predators tracking prey.
4. **Ballistic Motion:**
   * MSD vs Time Relation: *MSD*(*t*)∝*t^2*
   * Interpretation: In ballistic motion, particles move in a straight line with constant velocity. The MSD grows quadratically with time.
   * Example: A thrown projectile in a vacuum.