Multiscale Modelling course (MTEK0033)

Projects Brownian Dynamics

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Brownian Dynamics Projects

Overview of the Project Suite

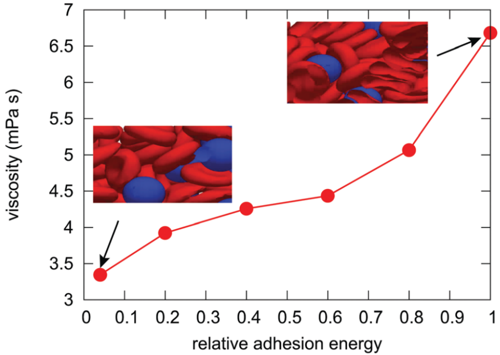
Objective: This project suite introduces students to equilibrium and non-equilibrium phenomena in soft-matter systems using **Brownian Dynamics (BD)** simulations.

Key physical themes:

- Transport coefficients and rheology
- Polymer translocation derived by heterogeneous environments
- Phase coexistence and interfacial phenomena
- Mechanical properties of Nano-Materials and the environmental effect
- Molecular relaxation and thermostatting strategies

Transport Properties

Project I: Viscosity and Shear Flow



Example reference: Viscosity measurements in red blood cells using simulations.

Focus:

- Measurement of shear viscosity in soft-matter systems
- Comparison of equilibrium and non-equilibrium approaches
- Shear generation via Muller-Plathe method

Project I: Viscosity and Shear Flow

Methods employed:

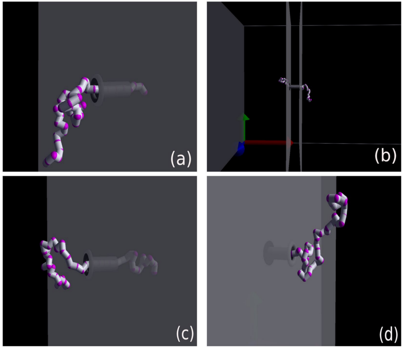
- Green-Kubo stress autocorrelation method
- Muller-Plathe momentum exchange method

Key outcomes:

- Consistency and limitations of different viscosity estimators
- Role of boundaries and velocity profiles

Passive driven Motion in Confinement

Project II: Polymer Translocation in Non-Additive Binary Mixtures



Example reference: DNA translocation through a membrane.

Focus:

- Stochastic polymer translocation through a nanopore
- Role of non-additive interactions in binary mixtures
- Transport induced by environmental and thermal asymmetry

Project II: Polymer Translocation in Non-Additive Binary Mixtures

Methods employed:

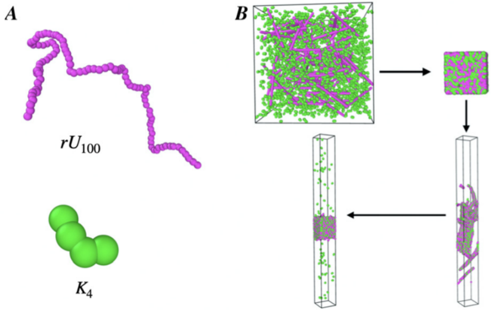
- Directional transport without external forcing using non-additivity properties
- Directional transport using temperature gradient

Key Outcomes:

- Non-additive interactions across a membrane
- Effect of temperature gradients and entropic driving forces

Phase properties in Multi-component System

Project III: Phase separation in a Contaminated Fluid



Example reference: Modeling of stiff RNA strands and phase-separated environments.

Focus:

- Liquid-vapor phase coexistence and interfacial structure
- Slab simulations and density profile analysis
- Effect of contaminants on coexistence and critical behavior

Project III: Phase separation in a Contaminated Fluid

Method employed:

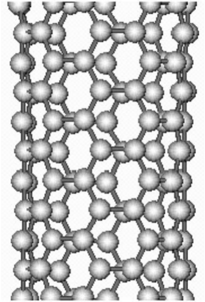
- Slab simulation method
- Density Profile computation

Key Outcomes:

- Temperature dependence of interfacial width
- Qualitative connection to surface tension

Study of Mechanical Properties

Project IV: Tensile Deformation and Environmental Effects in Carbon Nanotubes



Example reference: Mechanical property estimation from geometric deformation measures.

Focus:

- Tensile deformation and mechanical response in simulations
- Effect of environmental and interaction parameters on material strength
- Stress-strain relations and failure mechanisms

Project IV: Tensile Deformation and Environmental Effects in Carbon Nanotubes

Method employed:

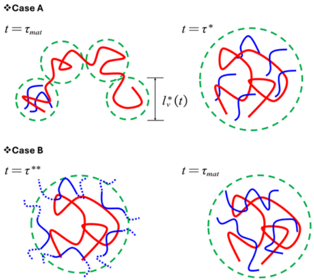
- Using external force to stress the CNT
- Analyzing stress-strain curve

Key Outcomes:

- Stabilizing the structures by tuning the forces at microscopic level
- Testing the stability of the materials
- Environmental effects on materials

Relaxation Dynamics, and Tracer Motion

Project V: Relaxation Dynamics, Thermostats, and Tracer Motion



Example reference: Diffusion of tracer particles (red) in a polymer matrix (blue).

Focus:

- Velocity autocorrelation functions in NVE simulations
- Estimation of relaxation times and friction coefficients
- Validation of Brownian motion using tracer particles
- Comparison between full-particle and tracer-only dynamics

Project V: Relaxation Dynamics, Thermostats, and Tracer Motion

Method employed:

- Applying NVE to calculate the dynamics
- Verify the Brownian motion using Langevin equation of motion

Key Outcomes:

- Microscopic forces leading to the resultant random motion
- Setting up correct dynamics in the colloidal system

Unified Physical Picture

Takeaway: Brownian Dynamics provides a unified framework for studying transport, translocation, phase behavior, mechanical properties, and relaxation phenomena in complex soft-matter systems across a wide range of length scales.

Future Aspects and Extensions

- Hydrodynamic interactions and long-range correlations
- Active polymers and driven translocation
- Frequency-dependent and viscoelastic transport
- Coupling BD with DPD, MPCD, or atomistic MD
- Extension to three-dimensional and multiscale systems

References

Image Page 2 Antonio Perazzo et al. (2022). **"The effect of rigid cells on blood viscosity: linking rheology and sickle cell anemia".** In: *Soft Matter* 18 (3), pp. 554–565

Image Page 5 Mohammadreza Niknam Hamidabad and Rouhollah Haji Abdolvahab (2019). **"Translocation through a narrow pore under a pulling force".** In: *Scientific Reports* 9.1, p. 17885

Image Page 8 Isha Malhotra and Davit A Potoyan (2023). **"Re-entrant transitions of locally stiff RNA chains in the presence of polycations leads to gelated architectures".** In: *Soft Matter* 19 (29), pp. 5622–5629

References

Image Page 11 Tantrakarn Natsuki, K Tantrakarn, and MJAPA Endo (2004). **"Effects of carbon nanotube structures on mechanical properties".** In: *Applied Physics A* 79.1, pp. 117–124

Image Page 14 Nuofei Jiang (2026). **"Diffusion of a Polymer Tracer in an Unentangled Matrix".** In: *Macromolecules* 59.1, pp. 587–600