Particle-Based Simulations — Assignment 3 (2025)

Dissipative Particle Dynamics (DPD)

Context and goals

In this assignment you will study the mesoscopic particle-based simulation technique called Dissipative Particle Dynamics (DPD). You will modify the Molecular Dynamics (MD) code from the previous assignment to implement DPD and simulate polymeric liquids. The paper by Groot and Warren (J. Chem. Phys. 107, 4423 (1997)) serves as the reference for implementation, verification, and validation.

Units in DPD

- The unit of length is the cutoff distance of the DPD interactions, r_c.
- The unit of mass is the DPD particle mass, m.
- The unit of energy is kT.

Tasks

A. Implementing the DPD Method

Start from the MD code provided in `PBS-MD.zip`. The overall structure of the DPD code is similar to MD. Continue using the velocity-Verlet algorithm (equivalent to Eq. (9) in Groot and Warren with $\lambda = 1/2$).

A1) Replace the Lennard-Jones interactions by the DPD pairwise forces as described in Eqs. (2–4) of Groot and Warren:

- Conservative force $\mathbf{F}_C$
- Dissipative force $\mathbf{F}_D$
- Random force $\mathbf{F}_R$

Use $\gamma = 4.5$ and $\sigma = 3$, linked via Eq. (5). For the random force, use ζ_{ij} with mean zero and variance 1. Uniformly distributed numbers from $[-\sqrt{3}, \sqrt{3}]$ are acceptable.

A2) Adapt the code to bead–spring chains of length N. The spring force between bonded beads is

$$\mathbf{f}_{ij} = -C\mathbf{r}_{ij}, \qquad C = 2kTr_c^{-2}.$$

Ensure that 1–2 and 1–3 bonded pairs are included in the non-bonded interactions by setting `exclude_12_nb` and `exclude_13_nb` to zero.

A3) **Radial Distribution Function:** Implement functions to calculate the radial distribution function, $g(r)$, on-the-fly during the simulation.

B. Verification for Monomers ($N = 1$)

B1) **Energy conservation:** Derive an expression for the potential energy from the conservative pair-forces. Disable dissipative and random interactions and verify conservation of total energy.

B2) **Ideal gas structure:** Disable conservative interactions while keeping dissipative and random interactions. Show that the system exhibits the equilibrium structure of an ideal gas.

B3) **Velocity statistics:** Verify that the velocity distribution matches the imposed temperature.

C. Validation for Monomers ($N = 1$)

C1) **Radial distribution function:** Reproduce the RDF shown in Fig. 2 of Groot and Warren.

C2) **Binary mixture:** Reproduce phase separation as in Fig. 6, using the parameters given in the caption.

C3) **Measuring the χ-parameter:** Measure χ with Eq. (18) and reproduce the results of Fig. 7 for varying a_{AB} at $\rho = 3$.

D. Validation for Chains ($N > 1$)

D1) **Snapshots:** Provide a snapshot of equilibrated bead–spring chains with $N = 4$.

D2) **Two-phase simulations:** Perform simulations for $N = 2$, 4, and 8. Provide plots similar to Fig. 6 for these cases.

D3) **χ-parameter for chains:** Measure χ and compare with Eq. (27) and Fig. 8.

Deliverables

1. Report (PDF, max 8 pages + appendix) with methods, parameter settings, verification/-validation plots, and a concise *lessons learned* box reflecting on the DPD implementation and observations.

2. Code archive (zip) with modified `.c` and `.h` files, and a `README.md`. No binaries.