A Coarse-Graining Procedure for Mapping Atomistic Models
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Motivation

Continuum mechanics: efficient but inadequate at nano scales.
Molecular dynamics: accurate but computationally expensive.
Goal: to develop effective hybrid computational methods for nano-scale flows.
Key issue: to determine whether an intermediate mesoscale description is required.

Model

Atomic model: \( N = 1000, \rho/\text{number density} = 0.8, r_{\text{cut}} = 2.5\sigma \) and Lennard-Jones (LJ) potential.

\[ U(r) = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} \right] \]

CG model: \( N = N/100 \)

Coarse-grained (CG) model should preserve the thermodynamic and dynamic properties of the detailed atomistic system.

Method

Iterative Boltzmann inversion: construct an effective pairwise potential for the CG model that reproduces the radial distribution function, \( g(r) \), of the detailed atomistic system.[1]

\[ U_c = -k_B T \ln g_{\text{max}}(r) \]

Pressure matching: put pressure constraint on the effective potential through an optimization procedure.

Objective function

\[ f(U) = \frac{1}{2} \int \left( \ln \frac{g(r) U}{g_{\text{max}}(r)} - \frac{\epsilon}{2r^6} \right)^2 dr + \alpha \left( \frac{P_{\text{target}}}{P_{\text{max}}} - 1 \right)^2 \]

Steepest decent algorithm

\[ U_{i+1} = U_i - \alpha \frac{\partial f}{\partial U} \]

After matching the pressure

\[ \text{The attractive part of the potential is recovered. Now the potentials are more similar qualitatively.} \]

\[ \text{Pressure matching acts mainly on the long-range potential.} \]

\[ \text{Pressure is very sensitive to the potential, unlike } g(r). \]

\[ \text{Long-ranged interactions are important in high CG level case.} \]

The cutoff needs to be extended to recover \( g(r) \) and pressure.

Dissipative Particle Dynamics thermostat (DPD)

Galilean-invariant thermostat

- the dissipative force term mimics the friction between particles and dissipates energy.

- The cutoff should be optimized based on the computational efficiency.

Results and Discussion

Effective potentials for various CG levels

Potential of mean force is a good initial guess for high CG level case.

0% CG case doesn’t reproduce the LJ potential \((r_{\text{cut}} = 2.5)\) since we start with a longer-ranged interaction \((r_{\text{cut}} = L/2 \approx 3.4)\).

Convergence test[1]

The potential is closer to the LJ potential when \( r_{\text{cut}} \) is reduced to 2.5.

the structure of a dense LJ \((\rho \approx 0.65)\) system is mainly determined by the repulsive part of the potential.[4]

References