Refs: Ch. 17 in f+s

Length and Time Scales

- macroscopic -
  - quark elements,
  - fluid mechanics
- Mesoscale
  - OPD, lattice Boltzmann
- Atomscale
  - MD, MC
- Electonic
  - Structure
  - Ab initio

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<td>(cm)</td>
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* Separate or hybrid simulations?
* Mechanism for linking different scales?

Renormalization group transformations

for exact correspondence, need more complex, longer-range interactions, multiple states
Certain properties can be made invariant under the transformation—e.g., end-to-end distance for 3D
\[ \frac{\text{diameter}}{\text{bond}} \leq 0.55 \]

Combine two beads into one

General criteria used for coarse-graining:
* Structure (gcr) \{ commonly used
* Forces / potential
* Thermodynamics (e.g., phase behavior) \rightarrow hard!

Polystyrene


Klein group model for DMPC lipid (dimyristophosphatidylcholine)
Structure matching from

(a) Iterative Boltzmann
inversion of distribution functions

\[ w(r) = -\ln(g(r)) \]

(b) Reverse Monte Carlo
Perform perturbation on intermolecular potential model parameters, accept/reject based on reproduction of desired structure

Issues with static coarse-graining

* Interactions are state dependent (change with density, temperature, composition in a mixture etc.)

* Properties not taken into account while coarse-graining are not well reproduced

* Thermodynamics / phase transitions usually not well represented
Dynamics

Coarse-grained models have intrinsically faster dynamics than their atomistic counterparts:
(Smaller interactions, lower barriers)

Reverse Mapping

To address detailed structural questions over long time scales (e.g., for interpreting NMR data)

Atomistic Structure \rightarrow \text{Coarse-grained long simulation} \rightarrow \text{Atomistic Structure}

\text{reverse mapping}
Dissipative Particle Dynamics

Essentially Molecular/Brownian Dynamics with a very soft potential


\[
\text{Total force} = \sum_{j \neq i} \left( F_{\text{cons}} (\vec{r}_{ij}) + F_{\text{dis}} (\vec{r}_{ij}, \vec{V}_{ij}) \right) + F_{\text{random}} (\vec{r}_{ij})
\]

\[
F_{\text{dis}} (\vec{r}_{ij}, \vec{V}_{ij}) = -\gamma w^{0}(r_{ij})(\vec{V}_{ij} \cdot \vec{r}_{ij}) \vec{r}_{ij}
\]

\[
F_{\text{random}} (\vec{r}_{ij}) = \sigma w^{2}(r_{ij}) \vec{z}_{ij} \vec{r}_{ij}
\]

Conservative Force \[ F_{\text{cons}} \]

Dissipative Force \[ F_{\text{dis}} \]

Random Force \[ F_{\text{random}} \]
In order for the configurations of the system to appear with the correct Boltzmann weight, the following condition must be satisfied:

\[
W^0(r_{ij}) = \left[ W^2(r_{ij}) \right]^2 \quad \text{often used: } (1-r^2)^2 r < 1 \]
\[
W^0(r_{ij}) = \begin{cases} 
0 & r > 1 
\end{cases}
\]

\( \sigma \) and \( \sigma^2 \) are related to the temperature:

\[
\sigma^2 = 2k_B T \delta
\]

DPD is similar to Brownian Dynamics, but unlike BD, DPD is frictional (dissipative) and random forces conserve momentum →

DPD obeys "hydrodynamic" (Navier-Stokes) behavior at long time and length scales

Soft, penetrable spheres → "blobs" of fluid

Much larger time steps can be used with respect to e.g. LJ simulations

Implementation issues

I. Integration method: forces on a particle depend on its velocity

\[ v(t+\Delta t/2) = v(t-\Delta t/2) + \Delta t \frac{F(t)}{m} \]

\[ r(t+\Delta t) = r(t) + \Delta t \cdot v(t+\Delta t/2) \]

In DPD, force at time \( t \) depends on velocities at time \( t - \Delta t \) approximate \( v(t) \) as

\[ v(t) = \frac{v(t+\Delta t/2) + v(t-\Delta t/2)}{2} \]

(2) implies that in (1) \( v(t+\Delta t/2) \) appears on both sides of the equation \( \rightarrow \) solve self-consistently by iteration.

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Fig. 1. – Comparison of the equilibrium properties of an ideal 2D DPD gas with the self-consistent and the Euler algorithms, for \( \sigma=1.5, \gamma=1, n = 25, L = 10r_c, r_c = 4 \). a) Measured and imposed temperature; \( t \) is the time in units of \( r_c \cdot m/(2k_B T) \). b) Radial distribution function.