Dissipative Particle Dynamics: Foundation, Evolution and Applications

Lecture 4: DPD in soft matter and polymeric applications

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Outline

- Dissipative Particle Dynamics (DPD)

- Applications:
  - Fluid Flow
    - Boundary conditions
    - Triple-Decker: MD - DPD - NS
  - Blood Flow
  - Amphiphilic Self-assembly

- Future of DPD
Dissipative Particle Dynamics (DPD)

• Stochastic simulation approach for simple and complex fluids.

• Mesoscale approach to simulate soft matter.

• Conserve momentum locally & preserve hydrodynamics.

• Access to longer time and length scales than are possible using conventional MD simulations.
Simulations with DPD

- Applying appropriate boundary conditions, so we can simulate problems of interest.
- A choice for the inter-particle forces, so we can model materials of interest.
- DPD has been applied to model a diverse range of systems:
  - Fluid flow (pipes, porous media)
  - Complex fluids (Colloidal suspension, blood)
  - Self-assembly (polymers, lipids, surfactants, nanoparticles)
  - Phase phenomena (polymer melts, dynamic wetting)
Fluid flow

The development of velocity profiles in Poiseuille flow
Boundary Conditions in DPD

- Lees-Edwards boundary conditions can be used to simulate an infinite but periodic system under shear.
- Revenga et al. (1998) created a solid boundary by freezing the particles on the boundary of solid object; no repulsion between the particles was used.
- Willemsen et al. (2000) used layers of ghost particles to generate no-slip boundary conditions.
- Pivkin & Karniadakis (2005) proposed new wall-fluid interaction forces.
Boundary conditions in DPD

Frozen wall boundary condition

- Fluid in between parallel walls
- Walls are simulated by freezing DPD particles
- Flow induced by external body force

Bounce forward reflection

Bounce back reflection
Boundary conditions in DPD

No-slip boundary condition

Poiseuille flow results

\[ F_w = a_e \left( 0.0303n_w^2 + 0.5617n_w - 0.8536 \right) \]

Boundary conditions in DPD

Adaptive boundary condition

Iteratively adjust the wall repulsion force in each bin based on the averaged density values.

Pivkin & Karniadakis, PRL, 2006
Boundary conditions in DPD

Polymer translocation

No-slip B.C. + Adaptive B.C.

velocity vector field
Boundary conditions in DPD

Polymer translocation

Translocation of polymer in single-file conformations

Translocation of polymer in double-folded conformations

Macro-Meso-Micro Coupling

NS + DPD + MD
Triple-Decker Algorithm

- Atomistic - Mesoscopic - Continuum Coupling
- Efficient time and space decoupling
- Subdomains are integrated independently and are coupled through the boundary conditions every time $\tau$

Communications among domains


Triple-Decker Algorithm

Step 1
1) Integrate MD domain during time $\tau$
2) Obtain BCs for DPD domain

Step 2
1) Integrate DPD domain during time $\tau$
2) Obtain BCs for MD and NS domains

Step 3
1) Integrate NS domain during time $\tau$
2) Extract BCs for DPD domain

MD

DPD

NS
Algorithm validation: 1D flows

Couette flow

Poiseuille flow

Square cavity flow

Square cavity, upper wall is moving to the right

Blood flow

Modeling human blood flow in health and disease
Red Blood Cells

50-100 nm spectrin length between junctions
27000 - 40000 of junctions per RBC
General Spectrin-level and Multiscale RBC Models

- RBCs are immersed into the DPD fluid
- The RBC particles interact with fluid particles through DPD forces
- Temperature is controlled using DPD thermostat

1. Pivkin & Karniadakis, PRL, 2008;
Triangular mesh:
- each vertex - a DPD particle
- each edge - a viscoelastic spring

\[ U_{POW-WLC}(x) = \frac{k_p}{(n-1)x^{n-1}} \]

- bending resistance of lipid bilayer

\[ U_{BEND}(\theta_{\alpha\beta}) = k_b \left[ 1 - \cos(\theta_{\alpha\beta} - \theta_0) \right] \]

- shear resistance of cytoskeleton

Multiscale RBC model

Triangular mesh:

- constant surface area

\[ U_{\text{AREA}}(A) = \frac{k_A (A - A_0^{\text{tot}})^2}{2A_0^{\text{tot}}} + \sum_{j=1}^{N_f} \frac{k_d (A_j - A_0)^2}{2A_0} \]

- constant volume

\[ U_{\text{VOLUME}}(V) = \frac{k_V (V - V_0^{\text{tot}})^2}{2V_0^{\text{tot}}} \]

Spectrin-level/Coarse RBC Representation

The membrane macroscopic elastic properties are found analytically for all representations: from spectrin-level to coarse-level.

Pivkin & Karniadakis, PRL, 2008
MS-RBC mechanics: healthy

\[ \mu_0 = 6.3 \times 10^{-6} \frac{N}{m} \]

\[ Y = 18.9 \times 10^{-6} \frac{N}{m} \]

\[ k_c = 2.4 \times 10^{-19} J \]

Experiment - Suresh et al., *Acta Biomaterialia*, 1:15-30, 2005
RBC dynamics in shear flow
RBC dynamics in Poiseuille flow

\[ D = 9 \, \mu m \] - tube diameter

\[ C = 0.05 \] - RBC volume fraction
RBC dynamics in Poiseuille flow

\[
\overline{U} = \frac{\int v(r) dA}{A}
\]

\[
g_{mn} = \frac{1}{N} \sum_i \left( r^i_m - r^{CM}_m \right) \left( r^i_n - r^{CM}_n \right)
\]

- gyration tensor

![Graph showing RBC dynamics with various parameters](image)
Prediction of Human Blood Viscosity In Silico

Fedosov, Pan, Caswell, Gompper & Karniadakis, PNAS, 2011
Vaso-occlusion in sickle cell disease

Pipe flow (SS2 + SS4)

Deformable SS2 cells adherent to post capillary

Trap rigid SS4 cells (mostly Irreversible sickle cells)

Blood occlusion in post capillary

Lei & Karniadakis, PNAS, 2013
Amphiphilic self-assembly

Self-assembled vesicles from 128M particle simulations
Amphiphilic self-assembly

Amphiphilic molecule

Hydrophilic + Hydrophobic

Micelle

hydrophilic head    hydrophobic tail

Vesicle
Amphiphilic self-assembly

DPD repulsion parameter

\[ a_{ij} = a_{ii} + \Delta a \]

Hydrophilic and hydrophobic molecules need differences in the repulsion parameters otherwise they would mix.

How do we define ‘not mixing’ and separation?

Phase separation: mean-field theory

\[ \chi N < 10.5 \quad \text{homogeneous or disordered system} \]

\[ \chi N \approx 10.5 \quad \text{weak segregation demixing} \]

\[ \chi N \gg 10.5 \quad \text{strong segregation demixing} \]

\[ \frac{\chi N k_B T}{\Delta a} = 0.306 N \quad \text{[Groot & Warren (1997)]} \]
Amphiphilic self-assembly

DPD model

A: hydrophilic
B: hydrophobic
S: solvent

Particle density: $\rho = 5$; Polymer length: $N = 7$

DPD parameters

Two alike particles
($A-A$, $B-B$, $S-S$, $A-S$)

$$a_{ii} = 75 \frac{k_B T}{\rho r_c^4}$$

Two unlike particles
($A-B$, $B-S$)

$$a_{ij} = a_{ii} + \Delta a$$

$$\chi N k_B T \frac{\Delta a}{\chi N} \approx 32.1$$

($\chi N$ strong segregation regime)

$$a_{ij} = 120$$
Amphiphilic self-assembly

Repulsive parameters:

\[
\begin{pmatrix}
A & B & S \\
A & 15 & 120 & 15 \\
B & 120 & 15 & 120 \\
S & 15 & 120 & 15 \\
\end{pmatrix}
\]

A: hydrophilic
B: hydrophobic
S: solvent

Self-assembled microstructures:

spherical micelle  slice  vesicle  slice

Li, Tang, Liang & Karniadakis, Chem Commun, 2014
Chirality controls molecular self-assembly

HbS molecule (MW: ~ 67,000 Da)

HbS polymerizes into filaments

Polymer fiber

Coarse-graining

Hydrophilic
Hydrophobic

Sickle hemoglobin (HbS)
Chirality controls molecular self-assembly

DPD interactions:

\[ V_{\text{tot}} = V_{\text{bonded}} + V_{\text{nonbonded}} = (V_{\text{str}} + V_{\text{bend}} + V_{\text{tors}}) + (V_{\text{vdw}} + V_{\text{es}} + \ldots) \]

Bonded interactions:

**Hookean spring interaction:**

\[ V_{\text{str}} = k_{\text{str}} (r - r_0)^2 \]  

**(a)** Control chain rigidity

**Bond-bending interaction:**

\[ V_{\text{bend}} = k_{\text{bend}} (\theta - \theta_0)^2 \]  

**(b1)** Describe chain chirality

**Bending FENE interaction:**

\[ F_{\text{FENE}} = k_{\text{BEND}} \left[ \frac{\theta - \theta_0}{1 - (\theta - \theta_0)/\Delta \theta_{\text{max}}} \right] \]  

**(c)**

Non-bonded interactions:

**Pairwise DPD conservative interaction:**

\[ V_{\text{non-bonded}} = -\frac{a_{ij}}{2} \left(1 - r_{ij}/r_c\right)^2 \]
Chirality controls molecular self-assembly

Elongated step-like fiber

Elongated sheet-like membrane

Li, Caswell & Karniadakis, Biophys. J., 2012
Summary

Dissipative Particle Dynamics is a powerful tool to

- treat boundary conditions in microchannel flows
- simulate the dynamic and rheological properties of simple and complex fluids
- understand the dynamic behavior of polymer and DNA chains
- model blood flow in health and disease
The future of DPD

- Multiscale modeling: MD - DPD - SDPD - SPH
- Complex fluids and complex geometries
- Parameterization development for simulating real fluids
- Structural models
References


References


