Dissipative Particle Dynamics: Foundation, Evolution and Applications

Lecture 3: New methods beyond traditional DPD

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The CRUNCH group: www.cfm.brown.edu/crunch
Outline

1. Single Particle DPD
   Particle size: mono-size $\rightarrow$ multi-size

2. Many-body DPD
   Quadratic EOS $\rightarrow$ Higher-order EOS

3. Energy conservative DPD
   Isothermal system $\rightarrow$ Non-isothermal system

4. Smoothed DPD
   Bottom-up approach $\rightarrow$ Top-down approach

5. Other DPD models
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5. Other DPD models
Successful DPD applications using mono-size particles

Application 1: Polymer drops in a shear flow

N = 2096

Application 2: Flow around spheres

N = 452
Successful DPD applications using mono-size particles

Application 3: Dynamic of colloids in electric fields

Application 4: Accurate Modeling of Red Blood Cells
Disadvantage of using mono-size particles

Problem: DPD simulation using mono-size particles is still too expensive for some cases such as modeling of many colloids or many RBCs.

Solution: Multi-size particles.
— Single Particle DPD model

N = 452
Many colloids

www.teunvissers.nl
N = 27344
Many RBCs
Single Particle DPD model

**DPD Generalization:**

Extra requirements:

- Should be easy to be implemented!
- Should be a generalization of DPD!

Single Particle DPD model

Equations of Motion:

\[ \dot{r}_i = v_i \]

\[ \dot{v}_i = -\frac{1}{m_j \neq i} \sum_j F_{ij} \]

\[ \dot{\Omega}_i = -\frac{1}{I_j \neq i} \sum_j T_{ij} \]

\[ F_i = \sum_j F_{ij} \]

\[ T_i = -\sum_j \lambda_{ij} r_{ij} \times F_{ij} \]

\[ \lambda_{ij} = \frac{R_i}{R_i + R_j} \]

\[ \lambda_{ij} = 1/2 \quad \text{when} \quad R_i = R_j \]

\[ F_{ij} = F_{ij}^C + F_{ij}^T + F_{ij}^R + \tilde{F}_{ij} \]

Conservative force

\[ F_{ij}^C = -V'(r_{ij})e_{ij} \]

Translational force

\[ F_{ij}^T = -\gamma_{ij} m \Gamma_{ij} \cdot v_{ij} \]

Rotational force

\[ F_{ij}^R = -\gamma_{ij} m \Gamma_{ij} \cdot \left[ r_{ij} \times (\lambda_{ij} \Omega_i + \lambda_{ji} \Omega_j) \right] \]

Random force

\[ \tilde{F}_{ij} dt = (2k_B T \gamma_{ij} m)^{1/2} \left[ \widetilde{A}(r_{ij}) d\mathbf{W}_{ij}^S + \widetilde{B}(r_{ij}) \frac{1}{d} tr[d\mathbf{W}_{ij}] \mathbf{1} + \widetilde{C}(r_{ij}) d\mathbf{W}_{ij}^A \right] \cdot e_{ij} \]

\[ \Gamma_{ij} = A(r_{ij}) \mathbf{1} + B(r_{ij}) e_{ij} e_{ij} \quad \text{is weighting matrix} \]

Examples of Single Particle DPD

**Rheology in Colloidal Suspensions:**

**Colloid transport in porous media:**

Relative viscosity vs $Pe$ number:

Colloid transport surrounding a single collector:

Colloid transport in a polysized porous medium:
Examples of Single Particle DPD

Flow around a circular cylinder:

Velocity vector:

Velocity and density profiles across the cylinder:

Comparison of drag coefficients:

<table>
<thead>
<tr>
<th>Re</th>
<th>Experiment</th>
<th>DPD</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>2.93</td>
<td>2.99</td>
</tr>
<tr>
<td>20</td>
<td>2.08</td>
<td>2.14</td>
</tr>
<tr>
<td>30</td>
<td>1.76</td>
<td>1.74</td>
</tr>
<tr>
<td>40</td>
<td>1.58</td>
<td>1.66</td>
</tr>
</tbody>
</table>
Examples of Single Particle DPD

Low-dimensional model for the red blood cell:

RBC shapes at various stretching forces:

RBCs in a channel with a geometrical constriction:

Aggregation of RBCs under shear:
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1. **Single Particle DPD**
   Particle size: mono-size → multi-size

2. **Many-body DPD**
   Quadratic EOS → Higher-order EOS

3. **Energy conservative DPD**
   Isothermal system → Non-isothermal system

4. **Smoothed DPD**
   Bottom-up approach → Top-down approach

5. **Other DPD models**
Equation of State (EOS) of traditional DPD

\[
P = \rho k_B T + \frac{1}{3V} \left\langle \sum_i r_i \cdot F_i \right\rangle \\
= \rho k_B T + \frac{1}{3V} \left\langle \sum_i \sum_{j>i} r_{ij} \cdot F_{ij}^C \right\rangle \\
= \rho k_B T + \frac{2\pi}{3} \rho^2 \int_0^1 r F^C(r) g(r) r^2 dr \\
F^C(r) = a(1 - r)
\]

\[
P = \rho k_B T + \lambda \cdot a \rho^2
\]

Making conservative force density dependent

The quadratic EOS is monotonic and has no van der Waals loop. It cannot produce liquid-vapor coexistence.

EOS needs high order terms of $\rho$ to model liquid-vapor coexistence.

EOS with high order terms:

<table>
<thead>
<tr>
<th></th>
<th>Traditional DPD</th>
<th>Many-body DPD</th>
</tr>
</thead>
<tbody>
<tr>
<td>Force $F_{ij}^C$</td>
<td>$a \cdot \omega_C (r_{ij}) e_{ij}$</td>
<td>$\frac{1}{2} \left(a(\rho_i) + a(\rho_j)\right) \cdot \omega_C (r_{ij}) e_{ij}$</td>
</tr>
<tr>
<td>EOS $P$</td>
<td>$\rho k_B T + \lambda a \rho^2$</td>
<td>$\rho k_B T + \lambda a(\rho) \rho^2$</td>
</tr>
</tbody>
</table>

Making conservative force density dependent

A common choice:

\[ F^C_{ij} = a \cdot (\rho_i + \rho_j) \cdot \omega_a (r_{ij}) e_{ij} + b \cdot \omega_b (r_{ij}) e_{ij} \]


Other approach:

\[ F^C = \nabla \left( k_B T \ln (1 - b \cdot \rho) + a \cdot \rho \right) + \kappa \nabla \nabla^2 \rho \]

Examples of Many-body DPD

Free oscillation of a droplet:

Nano-Jet:

Droplets wetting microchannels:
Examples of Many-body DPD

Forced Water-Oil movement in capillary:

Calibration of the solid-liquid interaction parameter $A_{SL}$ related to the static contact angle $\theta_0$:

Two different modes of the water-oil displacement:
Examples of Many-body DPD

Flow with wetting in microchannel network:
Examples of Many-body DPD

Electrowetting of a droplet:

Low frequency mode

High frequency mode

Hydrodynamic flow in the droplet

DC

AC

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5. Other DPD models
Energy is not conserved in traditional DPD

Equations of DPD:

\[ F_{ij}^C = a \omega_C (r_{ij}) e_{ij} \]
\[ F_{ij}^D = -\gamma \omega_D (r_{ij}) (e_{ij} \cdot v_{ij}) e_{ij} \]
\[ F_{ij}^R = \sigma \omega_R (r_{ij}) \zeta_{ij} dt^{-1/2} e_{ij} \]

\[ \omega_C (r) = 1 - r / r_c \]
\[ \omega_D (r) = 1 - r / r_c \]
\[ [w_R]^2 = w_D = (1 - r / r_c)^2 \]
\[ \sigma^2 = 2\gamma k_B T \]

DPD thermostat is good to maintain a constant temperature.

Limitation: (no energy equation)
It does not conserve the energy of the system. Thus, it is only valid for isothermal systems.
Energy-conserving DPD Model for non-isothermal fluid systems

Include the energy equation:

\[
\begin{align*}
\mathbf{F}^C_{ij} &= \alpha \omega^C (r_{ij}) \mathbf{e}_{ij} \\
\mathbf{F}^D_{ij} &= -\gamma \omega^D (r_{ij}) (\mathbf{e}_{ij} \cdot \mathbf{v}_{ij}) \mathbf{e}_{ij} \\
\mathbf{F}^R_{ij} &= \sigma \omega^R (r_{ij}) \zeta_{ij} dt^{-1/2} \mathbf{e}_{ij} \\
\omega^C (r) &= 1 - r / r_c \\
[w_R]^2 &= w_D = \left(1 - \frac{r}{r_c}\right)^S \\
\sigma_{ij}^2 &= \frac{4\gamma_{ij} k_B T_i \cdot T_j}{T_i + T_j}
\end{align*}
\]

\[C_v dT_i = \sum_{i \neq j} q_{ij}^{\text{cond}} dt + \sum_{i \neq j} q_{ij}^{\text{visc}} dt + \sum_{i \neq j} q_{ij}^{R} dt\]

- \(q_{ij}^{\text{cond}} = \sum_{j \neq i} k_{ij} w_{CT} (r_{ij}) \left(\frac{1}{T_i} - \frac{1}{T_j}\right)\)
- \(q_{ij}^{\text{visc}} = \frac{1}{2C_v} \sum_{j \neq i} \left(w_D (r_{ij}) \left[\gamma_{ij} (\mathbf{e}_{ij} \cdot \mathbf{v}_{ij})^2 - \left(\frac{\sigma_{ij}}{m}\right)^2\right] - \sigma_{ij} w_R (r_{ij}) (\mathbf{e}_{ij} \cdot \mathbf{v}_{ij}) \zeta_{ij}\right)\)
- \(q_{ij}^{R} = \sum_{j \neq i} \alpha_{ij} w_{RT} (r_{ij}) dt^{-1/2} \zeta_{ij}^e\)

\[w_{CT} (r_{ij}) = \left[w_{RT} (r_{ij})\right]^2 = \left(1 - \frac{r_{ij}}{r_{cut}}\right)^{S_T}\]

\[\alpha_{ij} = \sqrt{2k_B k_{ij}}, \quad k_{ij} = C_v \kappa (T_i + T_j)^2 \frac{r_{ij}}{r_{cut}}\]

Examples of Energy-conserving DPD

Natural convection heat transfer simulation:

Temperature isotherms and velocity field (solid lines: eDPD, dashed dotted lines: finite volume solutions):
Examples of Energy-conserving DPD

Heat conduction in nanocomposite:
— Qiao and He, Molecular Simulation, 2007.

Thermal conductivity enhancement by nanoparticles:

![Graph showing thermal conductivity enhancement with different alignments and particle volume fractions.]

- Horizontal alignment
- Vertical alignment
- Random packing

Graph showing the ratio of composite to matrix thermal conductivity ($k_{\text{composite}}/k_{\text{matrix}}$) with varying particle volume fractions ($\phi=4.8\%$).
Examples of Energy-conserving DPD

Natural convection in eccentric annulus:

Physical model:

Isotherms for $Ra = 4.59 \times 10^4$
and $Pr = 0.7$:

<table>
<thead>
<tr>
<th>eDPD</th>
<th>Experiment</th>
</tr>
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<tbody>
<tr>
<td>[Diagram]</td>
<td>[Diagram]</td>
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</table>
Examples of Energy-conserving DPD

Flow between Cold-Hot walls:

Temperature-dependent properties:

Coupling of flow and heat conduction:

![Graphs showing flow and temperature profiles](image)
An easy way to compute the thermal conductivity:

The heat conduction of a fluid is governed by

$$\rho C_v \frac{\partial T}{\partial t} = \eta \nabla^2 T + \rho q$$

For steady state

$$\lambda \nabla^2 T = -Q$$

$$\lambda = \frac{\eta}{\rho C_v}, \text{ and } Q = q/C_v$$

With a constant thermal diffusivity $\lambda$ the steady state solution

$$T(z) = \frac{Qz}{2\lambda} (d - |z|) + T_0$$

When $\lambda$ is temperature dependent:

$$\lambda(T_0) = \frac{1}{2} (\lambda_+ + \lambda_-)$$

$$= \frac{Q d^2}{16} \left( \frac{1}{T_{\max}} - \frac{1}{T_{\min}} \right)$$
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Mapping DPD units to Physical units

Bottom-up approach:
DPD is considered as coarse-graining of MD system

1. The mass of the DPD particle is $N_m$ times the mass of MD particle.

$$m_{DPD} = N_m \cdot m_{MD}$$

2. The cut-off radius is determined by equating mass densities of MD and DPD systems.

$$\frac{m_{DPD} \cdot \rho_{DPD}}{r_C^3} = \frac{m_{MD} \cdot \rho_{MD}}{\sigma^3}$$

3. The time scale is determined by insisting that the shear viscosities of the DPD and MD fluids are the same.

$$t_{DPD} = \frac{\nu_{DPD} \left( \frac{r_C}{\sigma} \right)^2}{\nu_{MD} \left( \frac{\sigma}{\sigma} \right)} t_{MD}$$
## DPD and Smoothed DPD

<table>
<thead>
<tr>
<th>Major difference</th>
<th>DPD</th>
<th>Smoothed DPD</th>
</tr>
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<tbody>
<tr>
<td>Bottom-up approach</td>
<td>Coarse-graining force field governing DPD particles</td>
<td>Top-down approach</td>
</tr>
<tr>
<td></td>
<td>Discretization of fluctuating Navier-Stokes equation</td>
<td></td>
</tr>
<tr>
<td>Inputs</td>
<td>Forms and coefficients for particle interactions, temperature, mesoscale heat friction</td>
<td>Equation of state, viscosity, temperature, thermal conductivity</td>
</tr>
<tr>
<td>Outputs</td>
<td>Equation of state, diffusivity, viscosity, thermal conductivity</td>
<td>As given</td>
</tr>
<tr>
<td>Advantages</td>
<td>1. No requirements in constitutive equation. 2. Good for complex materials and systems involving multicomponents.</td>
<td>Clear physical definition of parameters in Navier-Stokes equation</td>
</tr>
<tr>
<td>Disadvantages</td>
<td>1. No clear physical definition for the parameters. 2. Need to map DPD units to physical units based on output properties.</td>
<td>Must know the constitutive equation and properties of the system.</td>
</tr>
</tbody>
</table>
Equations of Smoothed DPD

Navier-Stokes equations in a Lagrangian framework:

\[
\frac{d\rho}{dt} = -\rho \nabla \cdot \mathbf{v}
\]

\[
\rho \frac{d\mathbf{v}}{dt} = -\nabla P + \eta \nabla^2 \mathbf{v} + \left( \zeta + \frac{\eta}{3} \right) \nabla \nabla \cdot \mathbf{v}
\]

\[
T \rho \frac{ds}{dt} = \phi + \kappa \nabla^2 T
\]

The transport coefficients are the shear and bulk viscosities \(\eta, \zeta\) and the thermal conductivity \(\kappa\). They are input parameters.

Discretize above equations using smoothed particle hydrodynamics (SPH) methodology, and introduce systematically thermal fluctuations via \textit{GENERIC} framework, then we have the governing equations of smoothed DPD:

\[
d\mathbf{r}_i = \mathbf{v}_i dt
\]

\[
md\mathbf{v}_i = \sum_j \left[ \frac{P_i}{d_i^2} + \frac{P_j}{d_j^2} \right] F_{ij} \mathbf{r}_{ij} dt - \sum_j (1 - d_{ij}) a_{ij} \mathbf{v}_{ij} dt - \sum_j (1 - d_{ij}) \left( \frac{a_{ij}}{3} + b_{ij} \right) \mathbf{e}_{ij} \mathbf{e}_{ij} \cdot \mathbf{v}_{ij} dt + md\tilde{\mathbf{v}}_i
\]

\[
T_i dS_i = \frac{1}{2} \sum_j \left( 1 - d_{ij} - \frac{T_j}{T_i + T_j} \frac{k_B}{C_i} \right) \left[ a_{ij} \mathbf{v}_{ij}^2 + \left( \frac{a_{ij}}{3} + b_{ij} \right) \mathbf{e}_{ij} \cdot \mathbf{v}_{ij} \right] dt - \frac{2k_B}{m} \sum_j \frac{T_i T_j}{T_i + T_j} \left( \frac{10}{3} a_{ij} + b_{ij} \right) dt
\]

\[
-2 \kappa \sum_j \frac{F_{ij}}{d_i d_j} T_{ij} dt - 2 \kappa \frac{k_B}{C_i} \sum_j \frac{F_{ij}}{d_i d_j} T_j dt + T_i d\tilde{S}_i.
\]

Examples of Smoothed DPD

Polymer chain in suspension:

Solvent:
Newtonian fluid

Polymer chain:
Finitely Extendable Nonlinear Elastic (FENE) springs

Scaling of the radius of gyration $R_G$ for several chain lengths:

Static structure factor $\tilde{S}(k) = S(k)/S(0)$ versus $R_G k$:

Polymer conformations under confinement:

Solvent:
Newtonian fluid

Polymer chain:
Finitely Extendable Nonlinear Elastic (FENE) springs

Examples of Smoothed DPD

Flow through porous media:

A colloidal particle near a rigid wall:

Model:
Periodic array of fixed circular/spherical objects

Three-dimensional dimensionless drag coefficient:

\[
\frac{F_{\text{drag}}}{6\pi\eta R_C V}
\]

Diffusion coefficients perpendicular and parallel to the wall:
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5. Other DPD models
Other DPD models

1. Low-mass DPD model for an approximation of incompressible fluids.

2. Spring model for colloids in suspension.

3. Anisotropic DPD particle (under development in CRUNCH group).
References


References


