Dissipative Particle Dynamics
Some Recent Developments

M. B. Liu (刘谋斌)
mbliu@pku.edu.cn

November 30, 2016

@NTU
1. Background
2. Recent developments in methodology
3. Micro drop dynamics with DPD
4. Multiphase flows with DPD
5. Complex fluids in micro channels
6. Modeling single cells with DPD
7. Conclusions
1. Background

1.1 Meso & multiple scale problems

- Cross section of a bilayer of lipid in water molecules
- Evolution of a polymer drop break-up
- Water droplets in oil

- Numerical methods based on continuum scale constitutive equations may not be valid when the dimension diminishes,

- Conventional MD is heavily restricted from practical applications due to the extremely small time scales (nanoseconds) and length scales (nanometers).

- How to increase computational ability:
  1. High performance computing with thousands of processors,
  2. New computational methods which can be realizable for bigger scales.
1. Background

1.2 Particle methods at different scales
1.3 General features of particle methods

- Individual particles are used to represent a volume of fluid that may vary in size, depending on the model, from a single atom/molecule (in MD), a small cluster of atoms or molecules (in DPD), to a macroscopic region in a continuum solid or fluid (in SPH).
- Masses are centered on particles.
- Particles move with local velocity of the fluid — Lagrangian nature.
- Forces are usually calculated from particle interactions either using an interaction potential (DPD) or some kind of weight function (SPH) with a cutoff distance.
1. Background

1.4 SPH – Methodology

History

- *Originally invented* for solving astrophysical problems in open space
- *Recently applied* to general fluid dynamic problems

Numerical approximation

- **Weight function (or smoothing function)**, $W$, centered on particles and describe continuous or discrete field function,
- **Kernel approximation**:

  $$ f_i \approx \int f(x)W_i(x)dx \quad f_{i, \alpha} \approx \int f(x)W_{i, \alpha}dx $$

- **Particle approximation**:

  $$ f_i \approx \sum_{j=1}^{N} f_j W_{ij} \frac{m_j}{\rho_j} \quad f_{i, \alpha} \approx \sum_{j=1}^{N} f_j W_{i, \alpha} \frac{m_j}{\rho_j} $$

SPH approximations in a two-dimensional space
1. Background

1.4 SPH – Applications

- Water discharge
- Injection flow
- Water exit
- Liquid sloshing
- Oil spill and boom movement
1. Background

1.4 SPH – Applications

UNDEX  
Shaped charge jet  
Explosive welding
1. Background

1.5 DPD-dissipative particle dynamics

a. Coarse-grained MD
b. A cluster of atoms/molecules
c. Soft interactions
d. Applications:
   - colloidal suspension
   - Surfactant
dilute polymer solutions
   - biological membranes
   - macromolecular movements

A model of lipid

Maximum time-step

\[ \Delta t_{\text{max}} \sim l \sqrt{\frac{m}{k_B T}} \]

2. DPD – Method development

2.1 Governing equations

\[
\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i, \quad \frac{d\mathbf{v}_i}{dt} = \mathbf{f}_i = \mathbf{f}_i^{\text{int}} + \mathbf{f}_i^{\text{ext}} \quad \mathbf{f}_i^{\text{int}} = \sum_{j \neq i} \mathbf{F}_{ij} = \sum_{j \neq i} \mathbf{F}_{ij}^C + \mathbf{F}_{ij}^D + \mathbf{F}_{ij}^R
\]

Conservative force

\[
\mathbf{F}_{ij}^C = a_{ij} w^C (r) \hat{\mathbf{r}}_{ij}
\]

Dissipative force

\[
\mathbf{F}_{ij}^D = -\gamma w^D (r) (\hat{\mathbf{r}}_{ij} \cdot \mathbf{v}_{ij}) \hat{\mathbf{r}}_{ij}
\]

Random force

\[
\mathbf{F}_{ij}^R = \sigma w^R (r) \xi_{ij} \hat{\mathbf{r}}_{ij}
\]

Fluctuation-Dissipation theorem

\[
w^D (r) = \left[ w^R (r) \right]^2, \quad \gamma = \frac{\sigma^2}{2k_B T}
\]
2. DPD – Method development

2.2 Constructing new DPD interaction

1. Conventional conservative weight function $W_c(r) = 1 - r$
   Corresponding potential $U(r) = 0.5 - (r - 0.5r^2)$

2. New conservative interaction potential

   $U(r) = AW_1(r) - BW_2(r) = AW_1(r, r_{c1}) - BW_2(r, r_{c2})$

   - $W(r)$: purely repulsive, $-W(r)$: purely attractive
   - U shape $\Leftarrow A, B, r_{c1}, r_{c2}$
   - Fluid properties $\Leftarrow U$ shape
   - It is feasible to model liquid/gas co-existing systems like multiphase fluid transport.
2. DPD – Method development

\[ U(r) = 18.75[2W_1(r, 0.8) - BW_2(r, 1.0)] \]

Different interaction parameters determines different fluid properties.

Surface tension
2. DPD – Method development

2.3 Treating complex solid boundary

1. Solid matrix

2. Solid boundary
   a. fluid boundary layer
   b. reflective/mirror BC
2. DPD – Method development

- Porous media
- Channel network

Flow geometry

Simulation setup

Examples

Liu M. B. et al., JCP, 2007

Liu MB et al., ACME, 2015
2. DPD – Method development

2.4 Modeling wetting phenomenon

The particle-particle interactions between fluid-solid and fluid-fluid determine the contact line dynamics and wetting behavior.

\[ U(r) = 18.75[2W_1(r, 0.8) - BW_2(r, 1.0)] \]

Different strength ratio leads to different wetting behaviors.
When modeling complex fluids (macromolecules like DNA), it is possible to use bead-chain model to simulate the interaction between chained particles.

The FENE (finitely extendible nonlinear elastic) model

\[ F_{ij}^S = \frac{H r_{ij}}{1 - \left( \frac{r_{ij}}{r_{\text{max}}} \right)^2} \]

Other models like worm-like chain (WLC) can further consider length and angle, and surface energy...
3. Micro drop dynamics with DPD

- Liquid drop and associated phenomena widely exist: ink-jet printing, enhanced oil recovery, soil erosion, and fuel injection atomization...

Water droplet on lotus leaf

Liquid drop stuck in a micro channel due to non-wetting effects

Water droplet on a caterpillar
3. Micro drop dynamics with DPD

Formation of liquid drop

Liquid drop oscillation

Evolution of axis
3. Micro drop dynamics with DPD

Head-on collision

Off-center collision
Dripping flow

Continuous flow $\rightarrow$ dripping flow $\rightarrow$ liquid drops
4. Multiphase flows with DPD

4.1 Two phase flow – Inverted Y channel

DPD VS VOF


Liu & Liu, WSPC, 2015
4. Multiphase flows with DPD

4.2 Two phase flow – channel network

DPD VS VOF、Experiment

Liu M. B. et al., *Phys Fluids*, 2007

Liu & Liu, WSPC, 2015
4. Multiphase flows with DPD

4.3 Two phase flow – Porous media


Liu & Liu, WSPC, 2015
5. Complex fluids in micro channels

- Micro-devices enable processing, analyzing, and delivering biochemical materials in a wide range of biomedical and biological applications.

- Micro-channels are the main field to deliver and control injected materials. By designing optimal structures of micro-channels or micro-channel networks, it is possible to efficiently control the injection process, either for simple fluids or complex fluids with macromolecules.

- In the device, DNA molecules were observed to undergo elongation, non-uniform shear and compression. Near the channel wall, high shear rates results in dramatic stretching of the molecules, and may also result in chain scission of the macromolecules.
5. Complex fluids in micro channels

5. Complex fluids in micro channels

Zhou, Liu, Chang, IMMIJ, 2013
6. Modeling single cells with DPD

- The study of the movement and deformation of single cells (in blood vessels) is important for understanding mechanical properties of cells.

- The changes in mechanical properties of cells may be closely related to severe cell diseases.

- Modern physiology medicine have established the relationship of mechanical changes between healthy and pathological cells.

- Differences of mechanical properties could be used to distinguish between normal and diseased cells.
6. Modeling single cells with DPD

- **Solid model:** Assuming the whole cell to be homogeneous without considering the distinct cortical layer. For large cell deformations, this model may not work.

- **Liquid drop model:** By treating the cell as a liquid drop, and liquid drop models can be used to model large cell deformation. For cell fast deformations, this model also may not work.

- **Compound drop model:** In order to consider the effects of the nucleus on cell deformation, the compound drop model was developed, which assumes the nucleus to be an encapsulated liquid drop.
6. Modeling single cells with DPD

DPD modeling of a cell and its environment

Constructing cell membrane
6. Modeling single cells with DPD

- The cell membrane structure is defined by a 2D triangular network on the spherical surface.
- Each link of triangular network is modeled by nonlinear WLC spring model.
- The force between membrane particles includes the elastic and viscous parts. The elastic part is characterized by an energy potential, given by

\[ U(\mathbf{r}_i) = U_{\text{plane}} + U_{\text{bending}} + U_{\text{area}} + U_{\text{volume}} \]
6. Modeling single cells with DPD

6.1 Biconcave cell (RBC)

- A red blood cell has a biconcave shape. All healthy mammalian RBCs (unstressed shapes) are disc-shaped (discocyte).

- The biconcave discocyte RBC has a flexible membrane with a high surface-to-volume ratio that facilitates large reversible elastic deformation of the RBC as it repeatedly passes through small capillaries to deliver oxygen to various parts of the body.

- The pathological RBCs are too stiff to deform sufficiently to traverse narrow capillaries.
6. Modeling single cells with DPD

6.1 Biconcave cell (RBC)

RBC stretching

force = 0 pN

Zhou, Liu, Chang, IJCM, 2016
6. Modeling single cells with DPD

6.1 Biconcave cell (RBC)

RBC stretching

- Force: 0 pN
- Force: 40 pN
- Force: 80 pN
- Force: 120 pN
- Force: 160 pN
- Force: 200 pN

Graph showing the effect of force on RBC diameter with DPD simulations and experimental data.
6. Modeling single cells with DPD

6.1 Biconcave cell (RBC)

RBCs in shear flows

Tumbling

Intermediate

Tank-treading
6. Modeling single cells with DPD

6.1 Biconcave cell (RBC)

RBCs in shear flows

\[ \dot{\gamma} = \{10, 30, 100\} \text{ s}^{-1} \]

- Tumbling
- Intermittent
- Tank-Treading

\[ \eta_m = 2.2 \times 10^{-2} \text{ Pa} \cdot \text{s} \]
\[ \eta_l = \eta_0 = 5.0 \times 10^{-3} \text{ Pa} \cdot \text{s} \]
6. Modeling single cells with DPD

6.1 Biconcave cell (RBC)

Multi-RBCs in Poiseuille flow in a tube

- Based on proper simulations of single RBCs with accurate mechanics, rheology and dynamics, more complicated situations can further be simulated. One of those situations is blood flow.
6. Modeling single cells with DPD

6.2 Spherical cells

Cell passing through channel

The deformation and dynamic response of a cell passing through a micro-channel can be used to investigate the mechanic, physical and biological features of a cell, and thus can be used to cell classification, separation, and disease diagnosis.
6. Modeling single cells with DPD

6.2 Spherical cells

Entry process of benign breast epithelial cells (MCF-10A)
6. Modeling single cells with DPD

6.2 Spherical cells

F.Y.Leong et al. Biomechanics and modeling in mechanobiology 10, 755766 (2011)
6. Modeling single cells with DPD

6.2 Spherical cells

Approaching (reduce speed) \(\rightarrow\) partially enter (\(v\rightarrow0\), long time duration) \(\rightarrow\) fully enter (acceleration-roughly constant) \(\rightarrow\) partially exit (accelerate suddenly \(\rightarrow\) reduce speed)

Cell displacement and deformation pattern

Cell displacement vs experimental data
7. Conclusions

1. As a meso-scale particle methods, DPD is attractive and more efficient than classic MD.

2. After modification or extension, the DPD method has been applied to different areas including drop dynamics, multiphase flows in complex geometries, and cell modeling.

3. DPD need further development:
   a. Interaction potential: for different materials/fluids?
   b. Coarse-graining: to what extent?
   c. Parameter matching: modeling parameter and physical ones?
   d. Multi-scale: possible coupling with or converting to MD or SPH?
   e. Others…
Thank You!