Dissipative Particle Dynamics
Some Recent Developments

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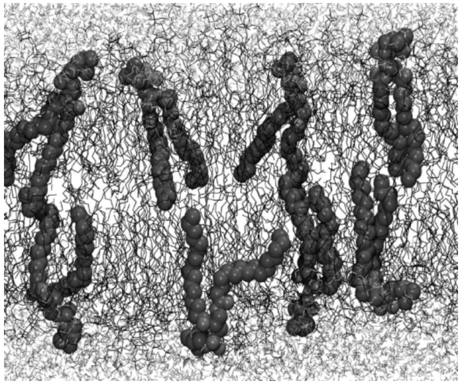
Outline

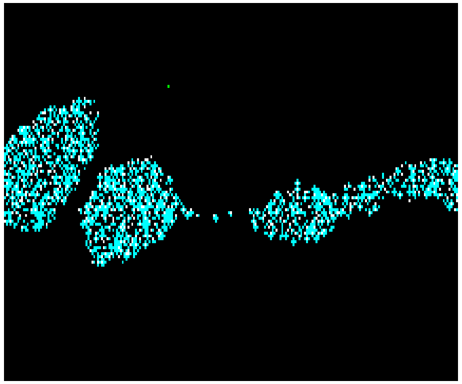
1. Background
2. Recent developments in methodology
3. Micro drop dynamics with DPD
4. Multiphase flows with DPD
5. Complex fluids in micro channels
6. Modeling single cells with DPD
7. Conclusions

1. Background

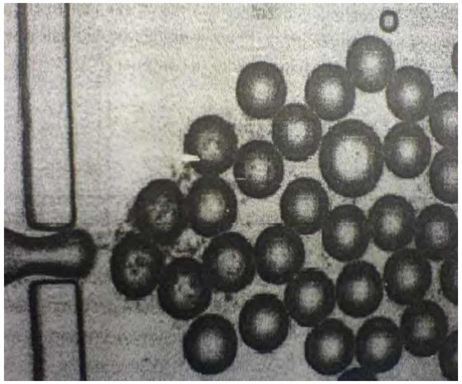
1.1 Meso & multiple scale problems



Cross section of a bilayer of lipid in water molecules



Evolution of a polymer drop break-up



Water droplets in oil

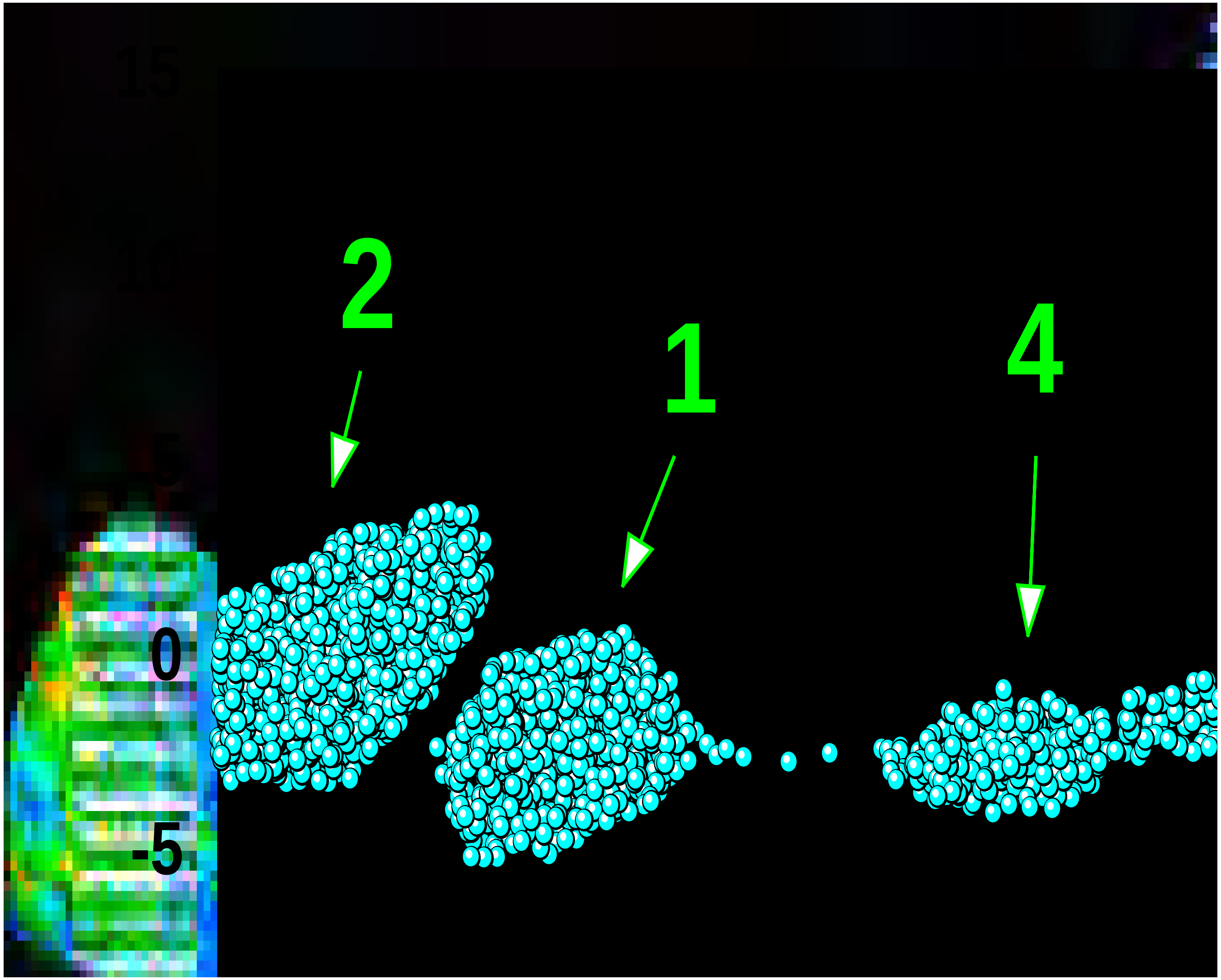
- Numerical methods based on continuum scale constitutive equations may not be valid when the dimension diminishes,
- Conventional MD is heavily restricted from practical applications due to the extremely small time scales (nanoseconds) and length scales (nanometers).
- How to increase computational 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. Background

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.**

Particle-Particle Interaction

1.4 SPH – Methodology

History

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

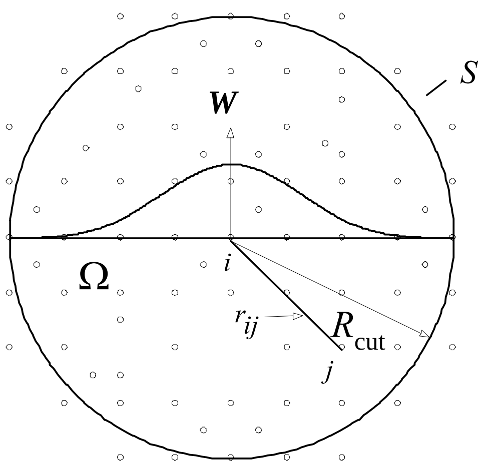
Numerical approximation

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

$$f_i \cong \int f(\mathbf{x}) W_i(\mathbf{x}) d\mathbf{x} \qquad f_{i,\alpha} \cong \int f(\mathbf{x}) W_{i,\alpha} d\mathbf{x}$$

- **Particle approximation:**

$$f_i \cong \sum_{j=1}^{N} f_j W_{ij}\, m_j / \rho_j \qquad f_{i,\alpha} \cong \sum_{j=1}^{N} f_j W_{i,\alpha}\, m_j / \rho_j$$

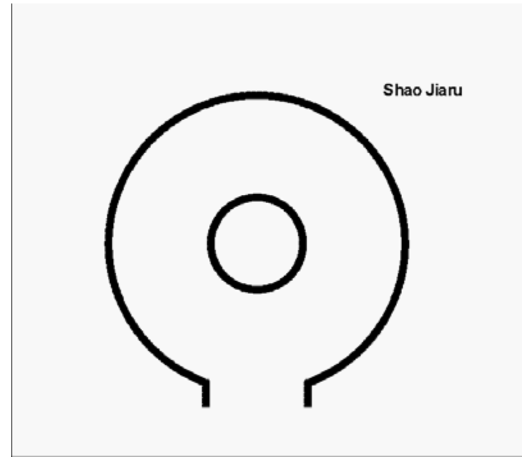


SPH approximations in a two-dimensional space

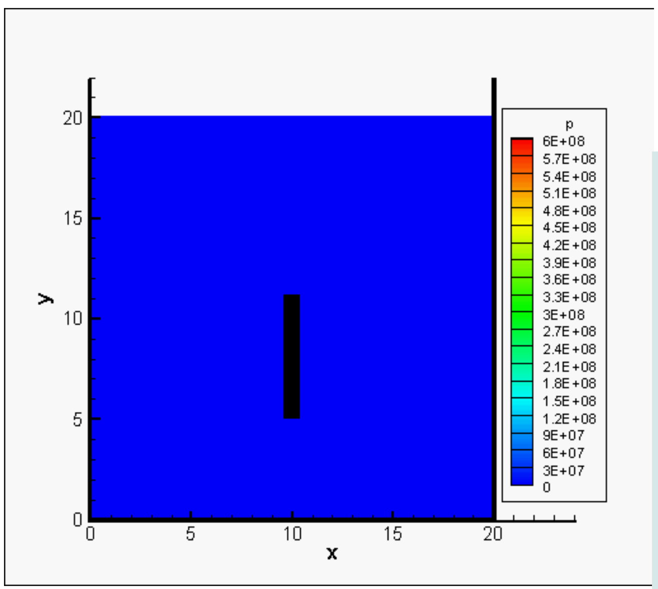
1. Background

1.4 SPH – Applications

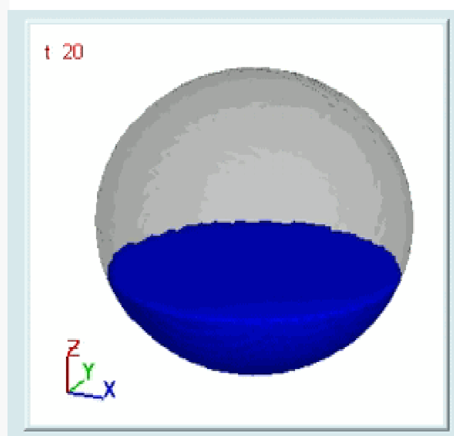
Water discharge



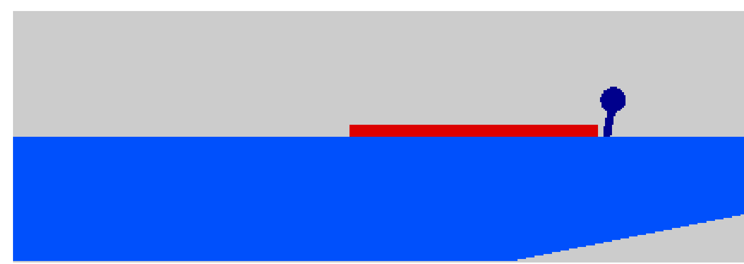
Injection flow



Water exit



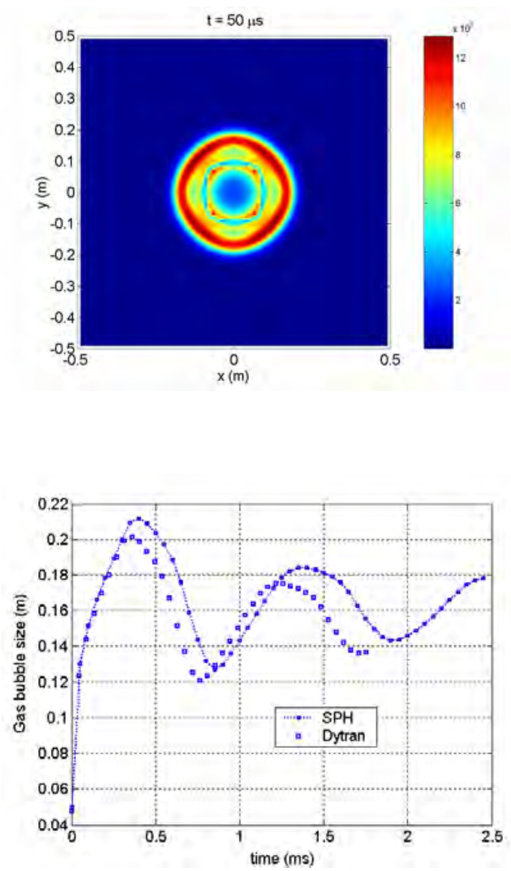
Liquid sloshing



Oil spill and boom movement

1. Background

1.4 SPH – Applications



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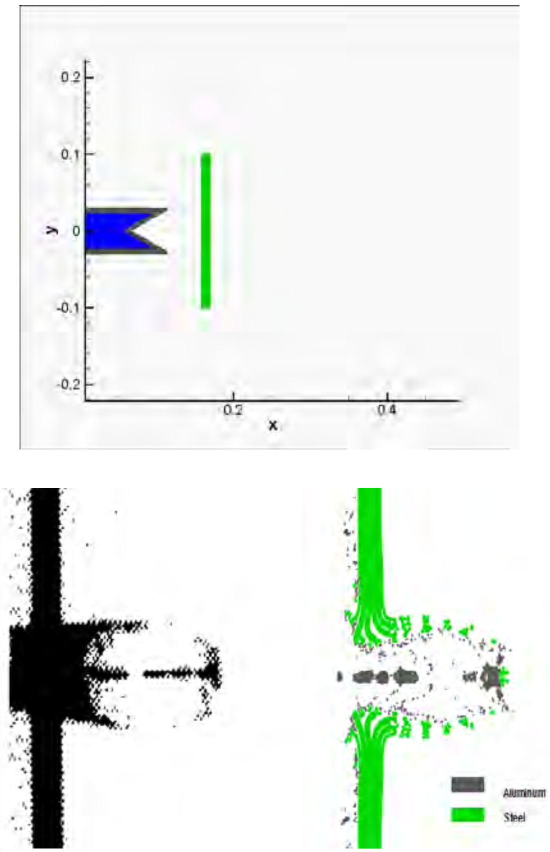
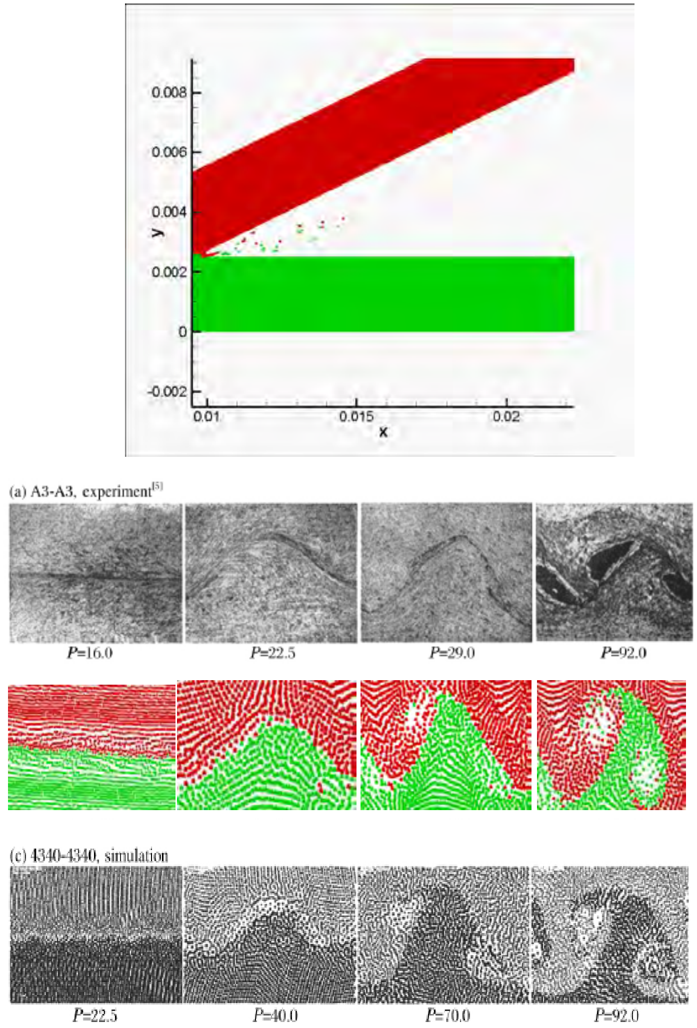


Shaped charge jet



Explosive welding

1. Background

1.5 DPD-dissipative particle dynamics

a. Coarse-grained MD

b. A cluster of atoms/molecules

c. Soft interactions

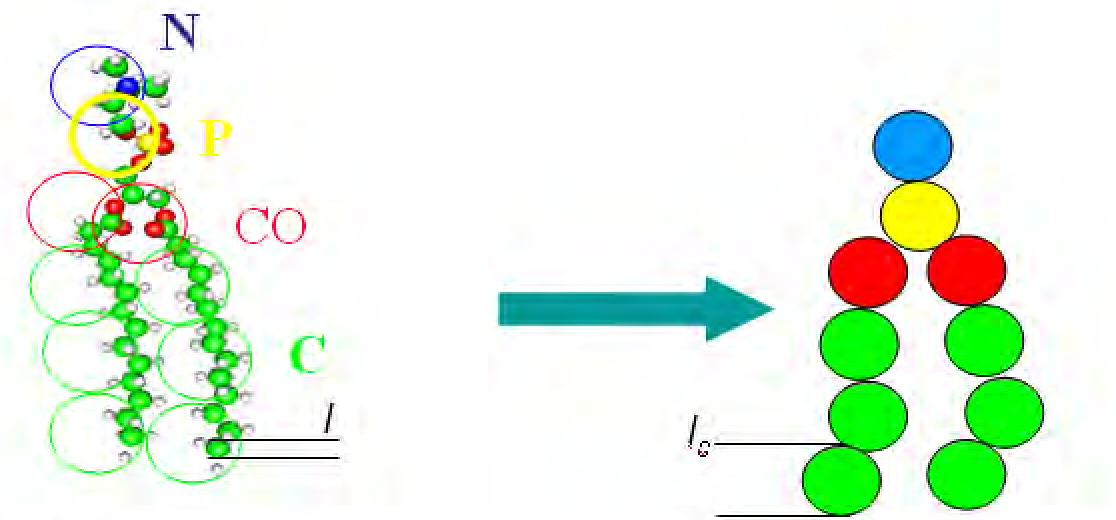
d. Applications:
  colloidal suspension
  Surfactant
  dilute polymer solutions
  biological membranes
  macromolecular movements

More efficient than MD (larger time step & scale)

A model of lipid

Maximum time-step

$$\Delta t_{\max} \sim l\sqrt{\frac{m}{k_B T}}$$



All-atom model
118 atoms

Coarse-grained model
10 sites

Hoogerbrugge, Koelman, *Europhys Lett* , 1992

Liu MB et al., ACME, 2015

2. DPD – Method development

2.1 Governing equations

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

Conservative force

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

Dissipative force

$$\mathbf{F}_{ij}^D = -\gamma w^D\left(r_{ij}\right)\left(\hat{\mathbf{r}}_{ij} \cdot \mathbf{v}_{ij}\right)\hat{\mathbf{r}}_{ij}$$

Random force

$$\mathbf{F}_{ij}^R = \sigma w^R\left(r_{ij}\right)\xi_{ij}\hat{\mathbf{r}}_{ij}$$

Fluctuation-Dissipation theorem

$$w^D(r) = \left[w^R(r)\right]^2 \quad , \quad \gamma = \frac{\sigma^2}{2k_B T},$$

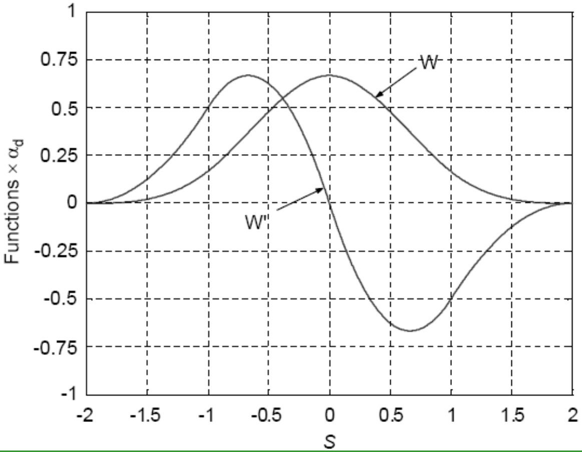
2. DPD – Method development

2.2 Constructing new DPD interaction

1. Conventional conservative weight function $W_c(r) = 1 - r$

Corresponding potential $U(r) = 0.5 - (r - 05r^2)$

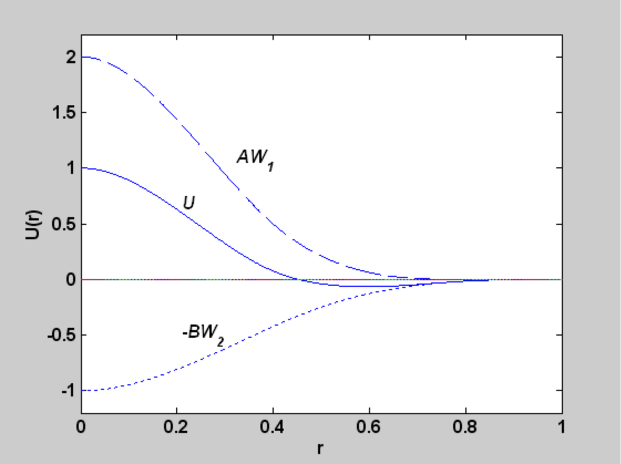
Purely repulsive, only for gas



2. New conservative interaction potential

***W*, SPH smoothing function**

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



- ***W*(*r*) : purely repulsive, -*W*(*r*): purely attractive**
- **U shape 🡐 A, B, r_{c1}, r_{c2}**

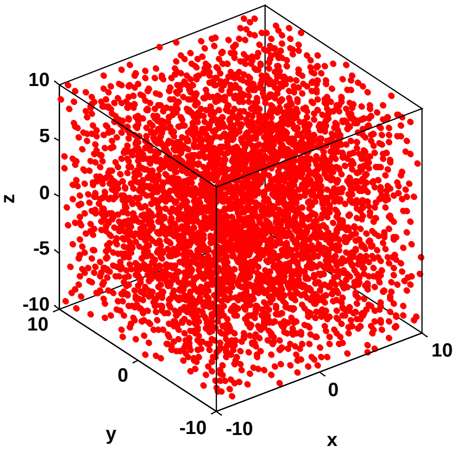
- **Fluid properties 🡐 U shape**
- **It is feasible to model liquid/gas co-existing systems like multiphase fluid transport.**

Liu M. B. et al., *Phys Fluids*, 2006

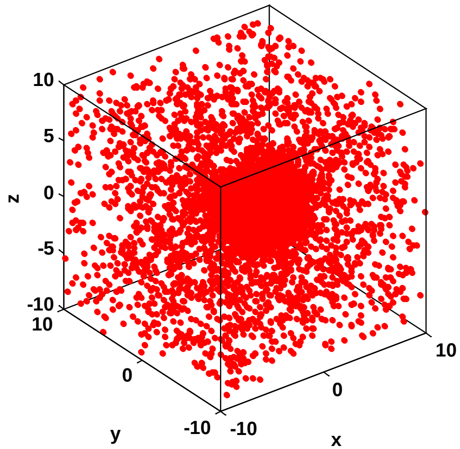
Liu MB et al., ACME, 2015

2. DPD – Method development

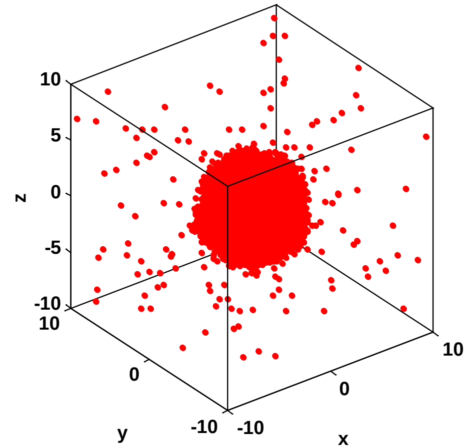
$$U(r) = 18.75[2W_1(r,0.8) - BW_2(r,1.0)]$$ → **Surface tension**



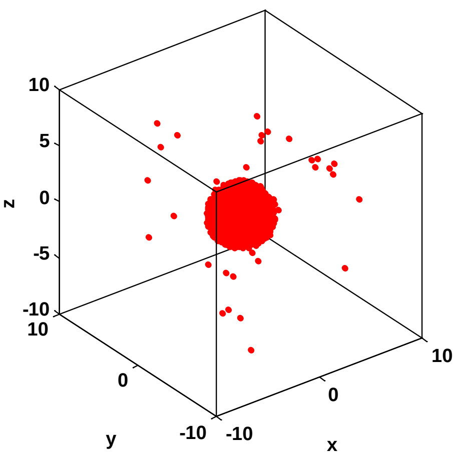
B = 0.0



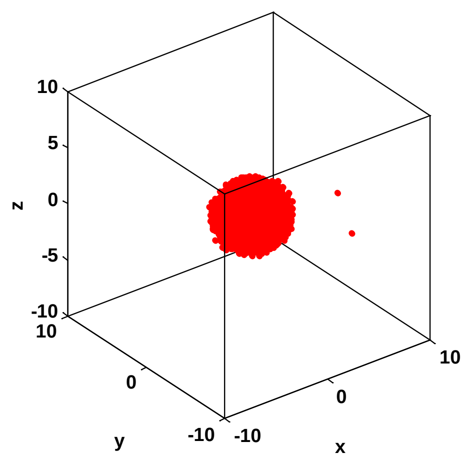
B = 0.5



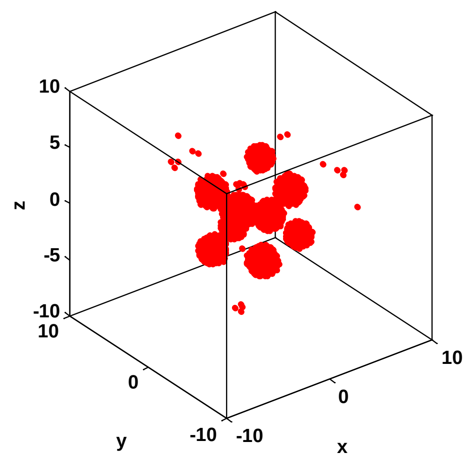
B = 0.9



B = 1.0



B = 1.05



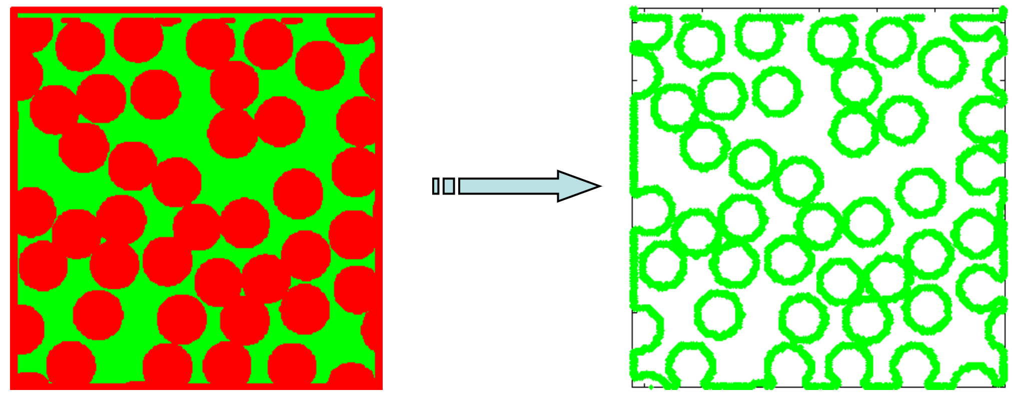
B = 1.20

Different interaction parameters determines different fluid properties.

2. DPD – Method development

2.3 Treating complex solid boundary

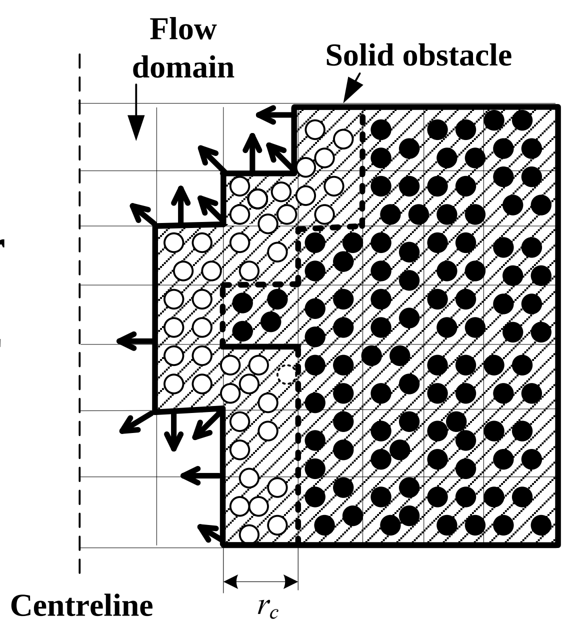
1.Solid matrix

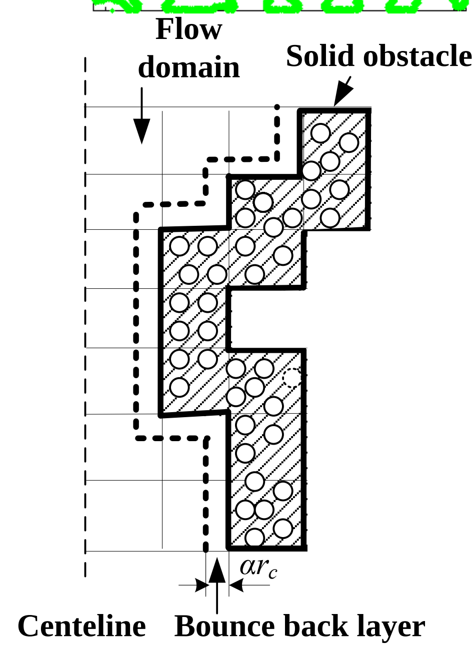


2.Solid boundary

a. fluid boundary layer

b. reflective/mirror BC



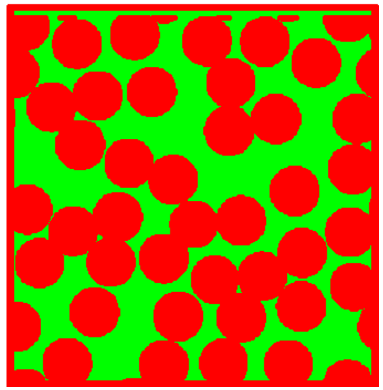


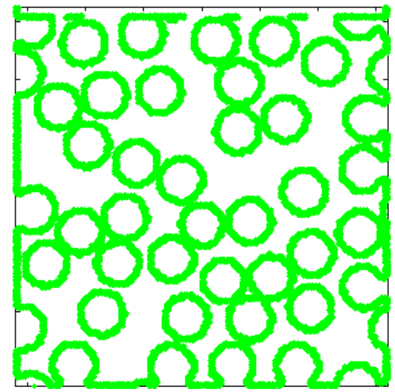
Liu MB et al., ACME, 2015

2. DPD – Method development

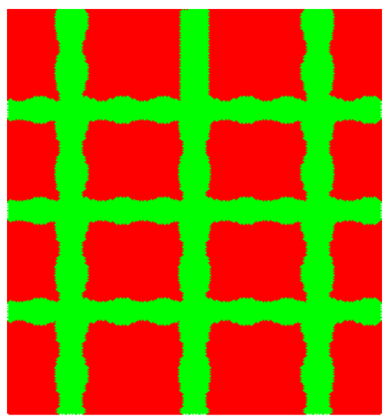
Flow geometry | **Simulation setup**

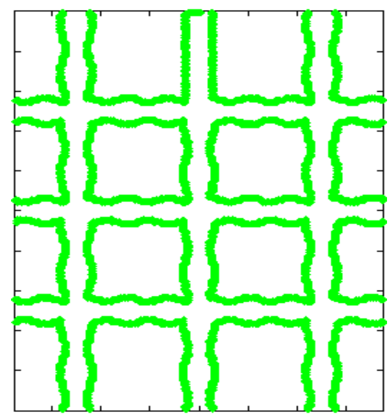
Porous media





Channel network





Examples

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

Liu MB et al., ACME, 2015

2. DPD – Method development

2.4 Modeling wetting phenomenon

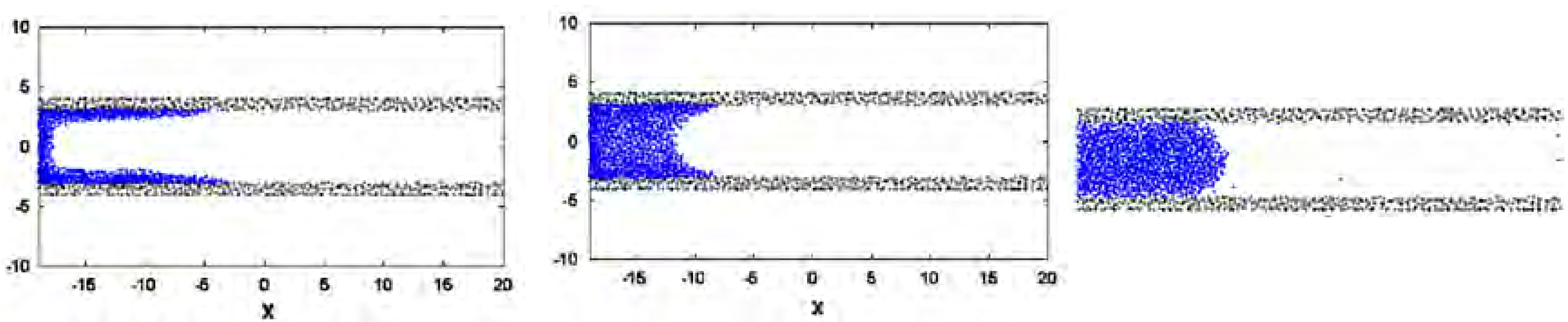
The particle-particle interactions between fluid-solid and fluid-fluid determine the contact line dynamics and wetting behavior

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

Fluid-Fluid $a_{f\text{-}f}$ → **Surface tension**

→ **Wetting behavior** a_{f-f} / a_{f-w}

Fluid-Wall $a_{f\text{-}w}$ → **Adhesion effects**



Different strength ratio leads to different wetting behaviors

2. DPD – Method development

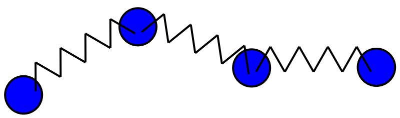
2.5 Modeling chained or net structure

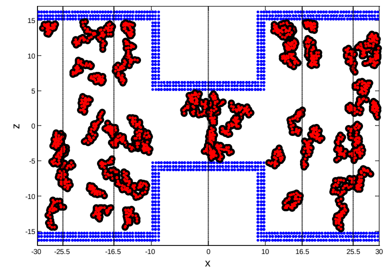
Bead-Chain Model

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

$$\mathbf{F}_{\mathbf{ij}}^{\mathbf{S}} = \frac{H\mathbf{r}_{\mathbf{ij}}}{1-\left(r_{ij}/r_{\max}\right)^2}$$





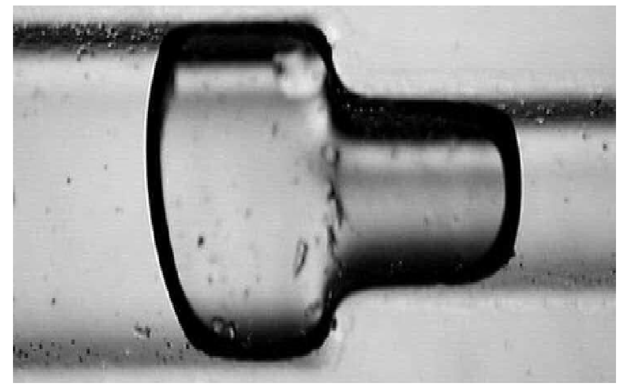
Other models like worm-like chain (WLC)

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

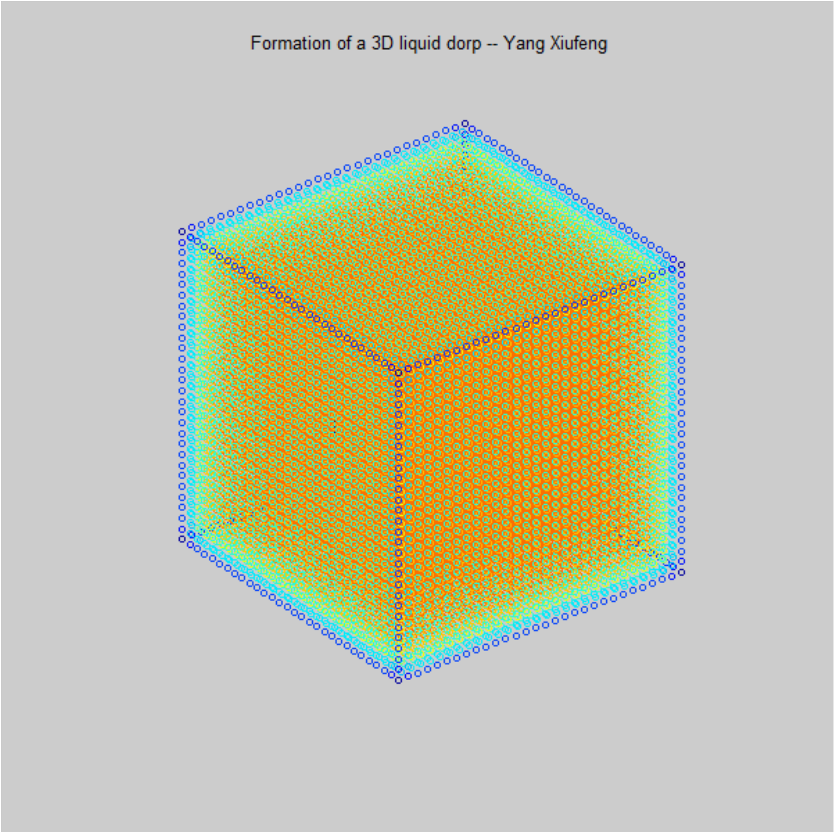


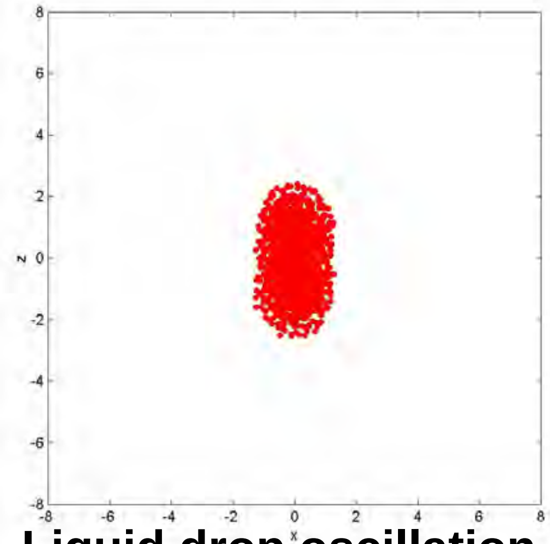
Liquid drop stuck in a micro channel due to non-wetting effects

water droplet on a caterpillar

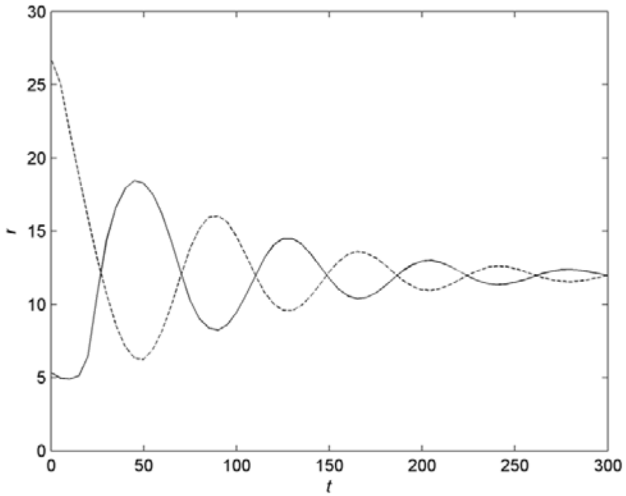
3. Micro drop dynamics with DPD

Formation of liquid drop





Liquid drop oscillation

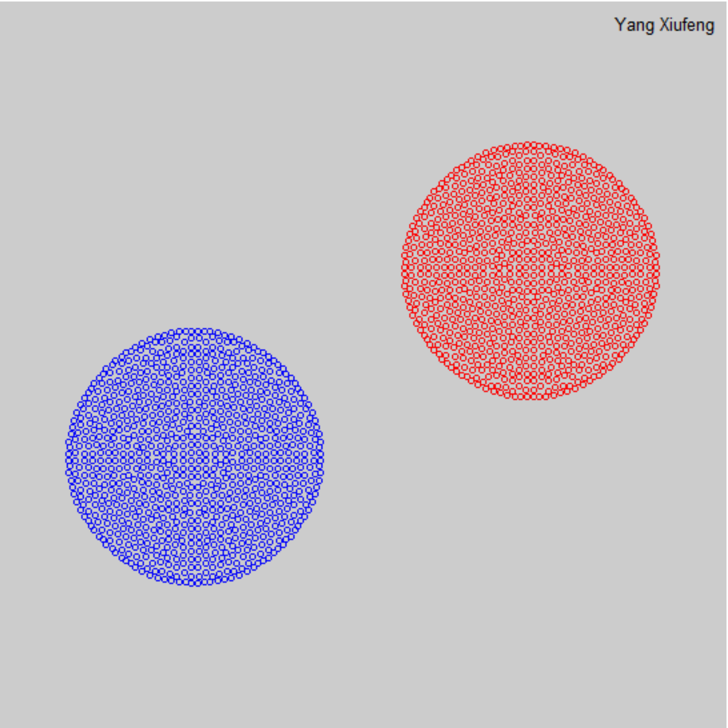


Evolution of axis

3. Micro drop dynamics with DPD

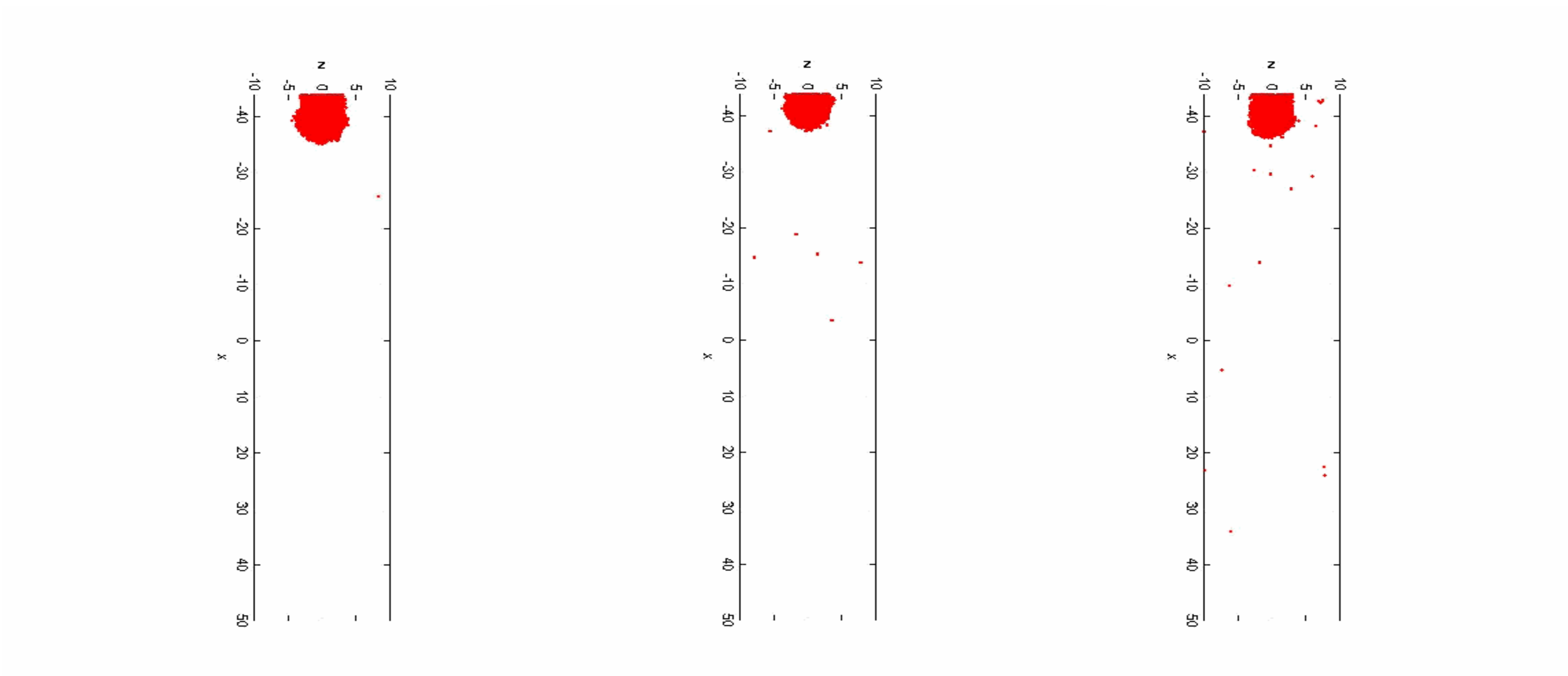
Head-on collision

Off-center collision



3. Micro drop dynamics with DPD

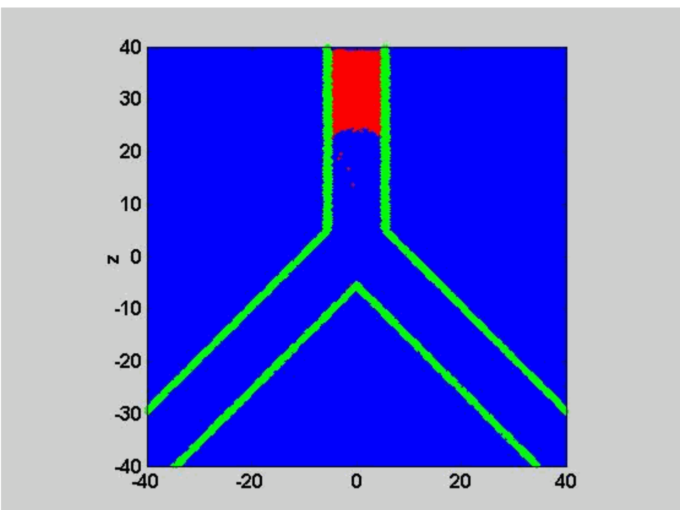
Dripping flow



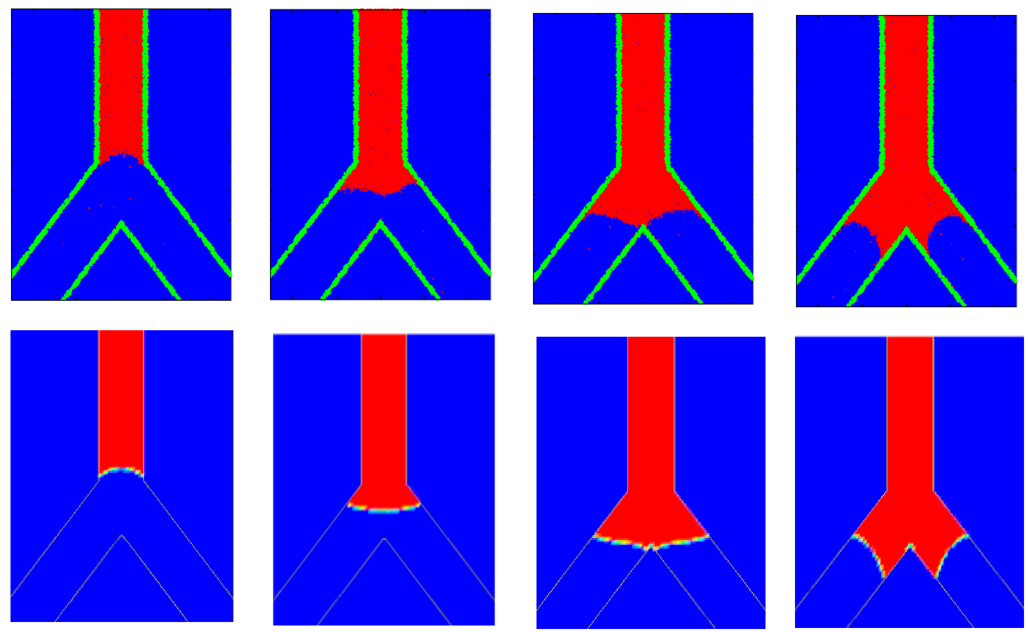
Continuous flow → dripping flow → liquid drops

Liu & Liu, WSPC, 2015

4.1 Two phase flow – Inverted Y channel



DPD VS VOF

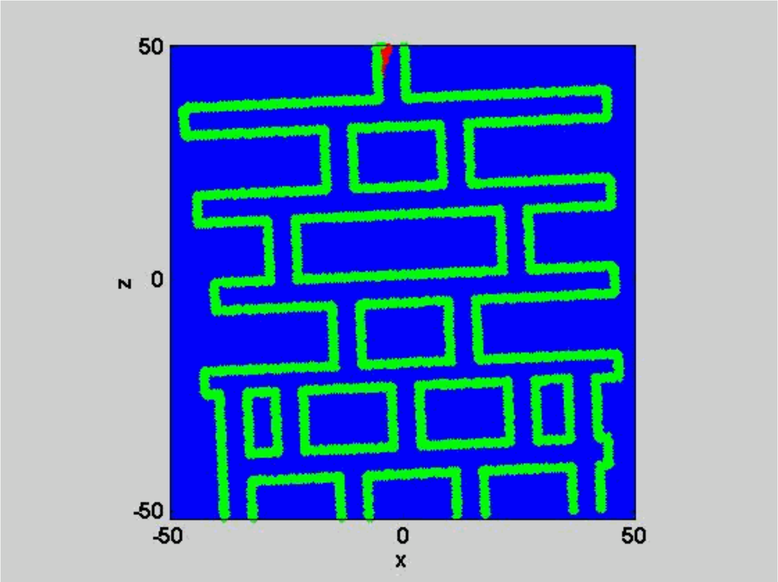


Liu M. B. et al., *J Comput Phys*, 2007

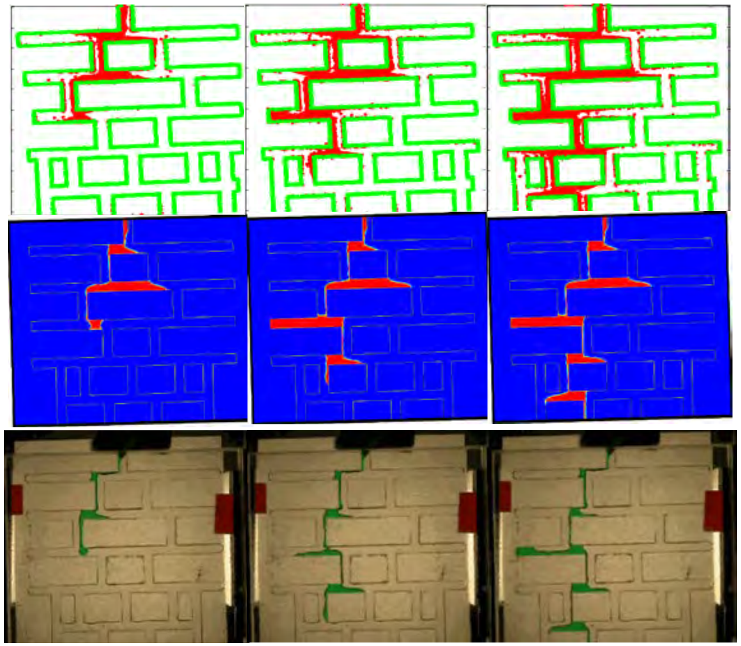
Liu & Liu, WSPC, 2015

4. Multiphase flows with DPD

4.2 Two phase flow – channel network



DPD VS VOF、Experiment

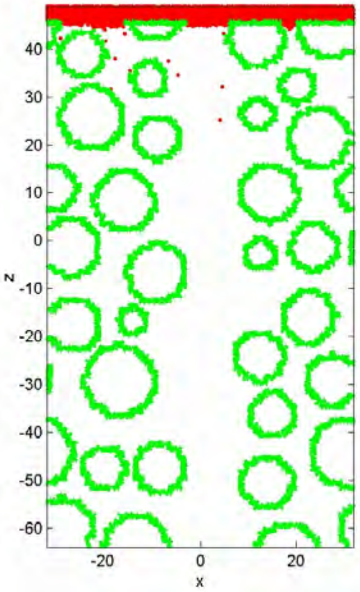


Liu M. B. et al., *Phys Fluids*, 2007

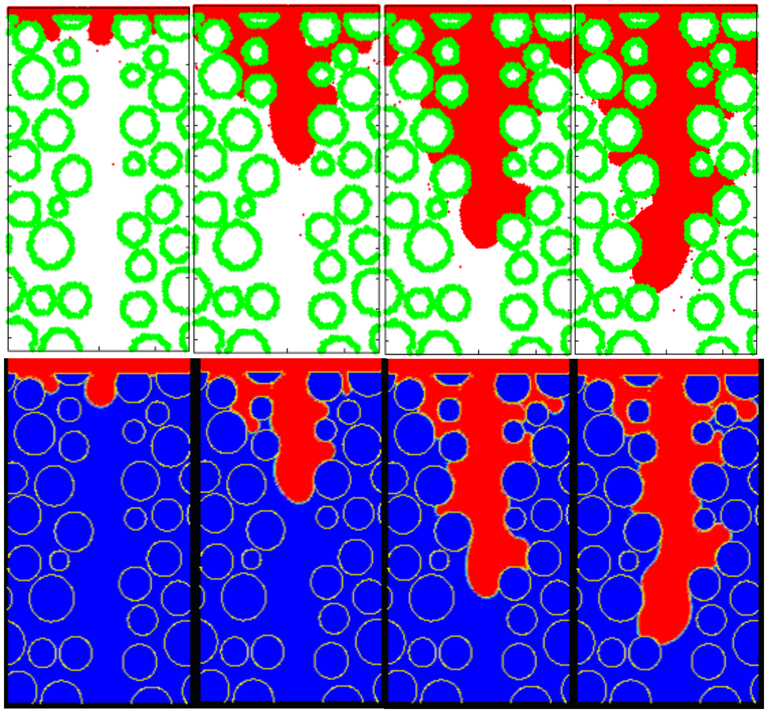
Liu & Liu, WSPC, 2015

4. Multiphase flows with DPD

4.3 Two phase flow – Porous media



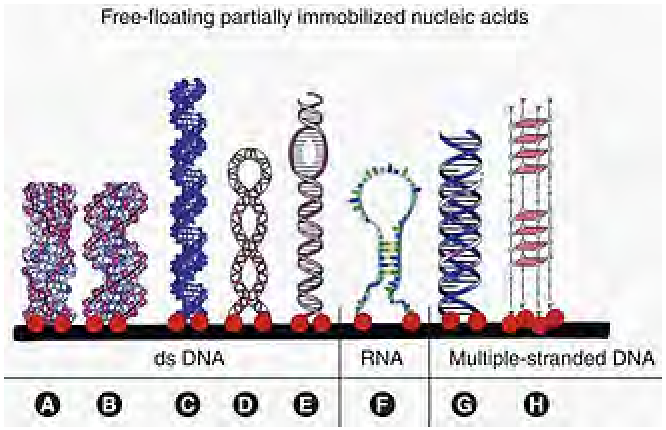
DPD VS VOF

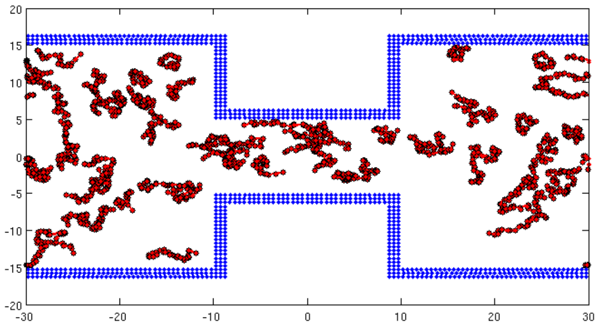


Liu M. B. et al., *Water Resour Res*, 2007

Liu & Liu, WSPC, 2015

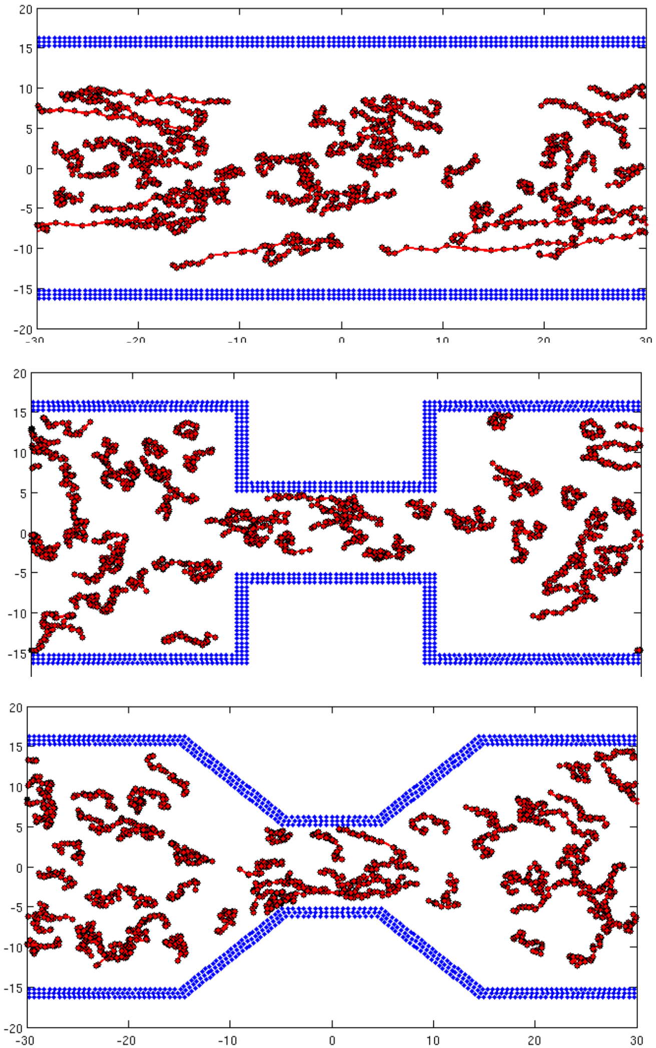
5. Complex fluids in micro channels

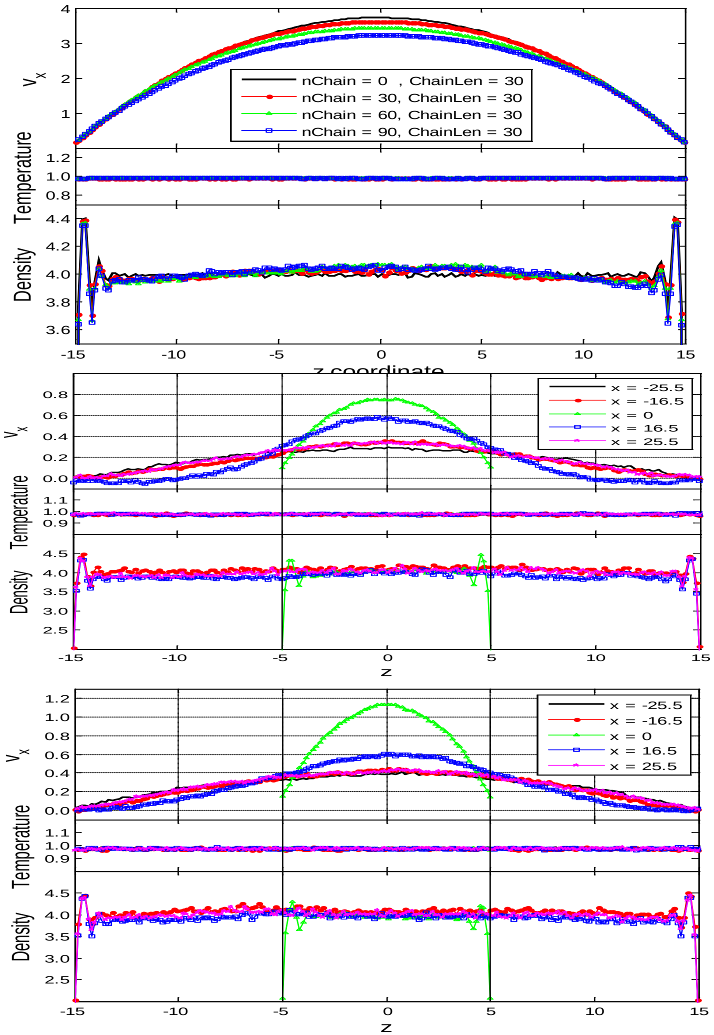




- Micro-devices enable processing, analyzing, and delivering biochemical materials in a wide range of biomedical and biological applications.
- Micro-channels are the main field to deliver and control injected materials. By designing optimal structures of micro-channels or micro-channel networks, it 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

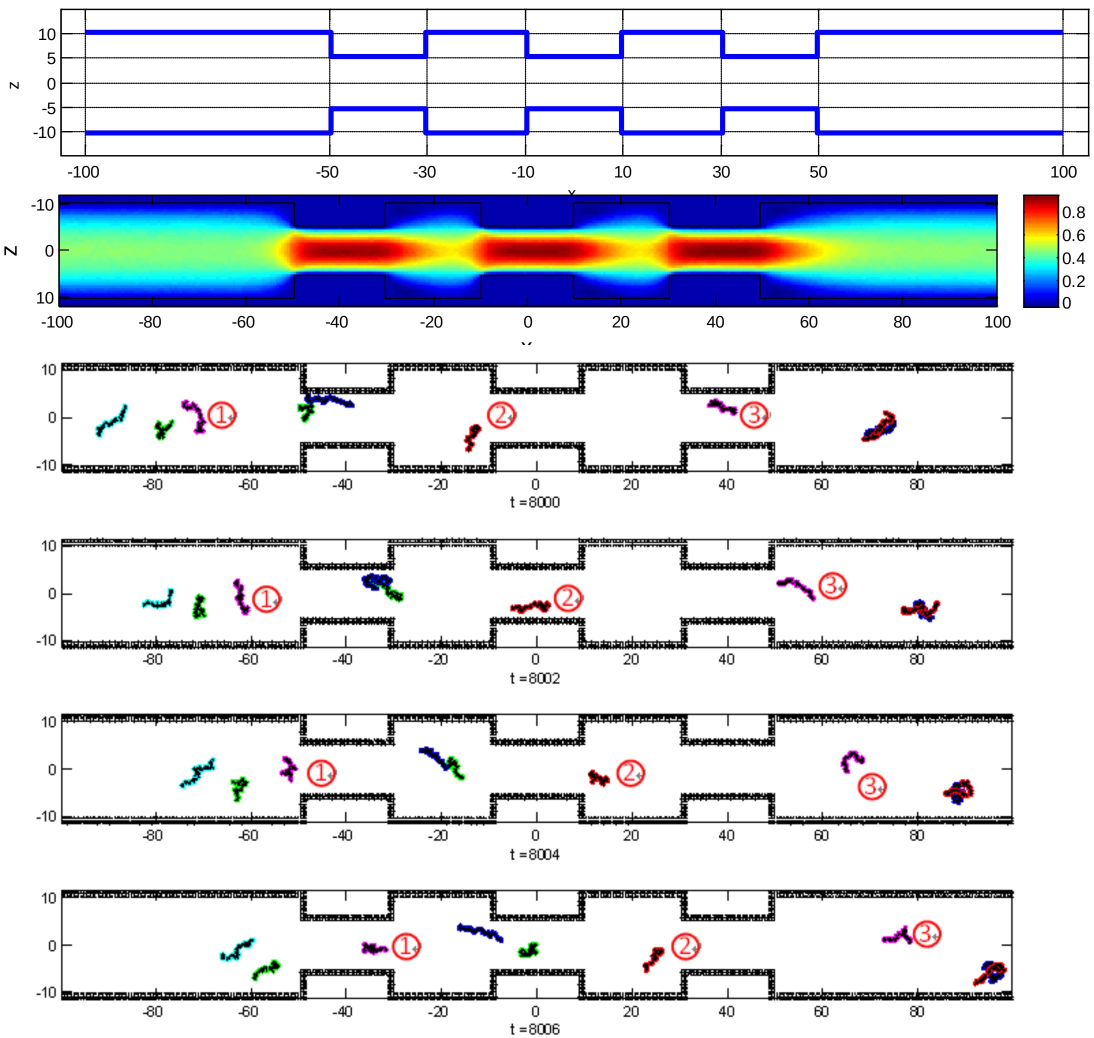
5. Complex fluids in micro channels

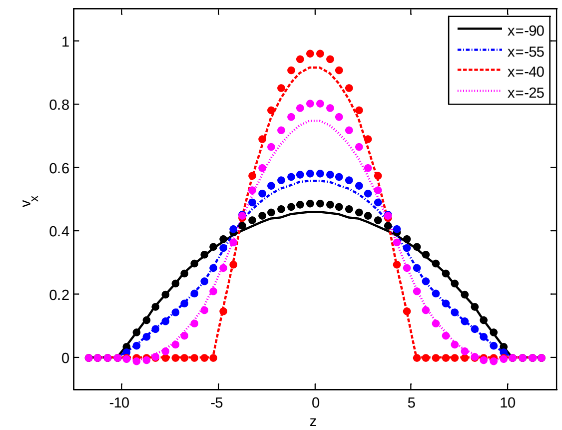


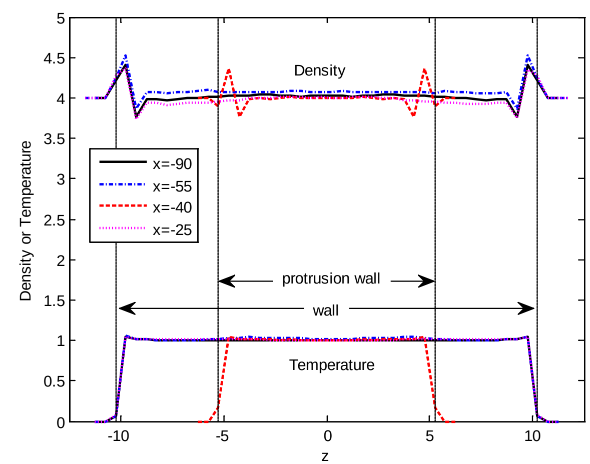


Zhou, Liu, Chang, Acta Polymerica Sinica 2012

5. Complex fluids in micro channels

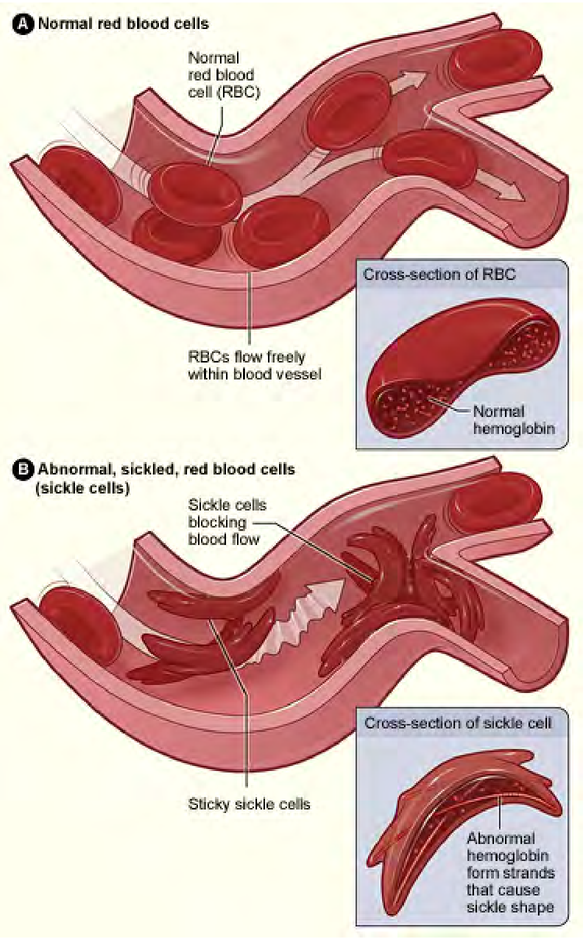






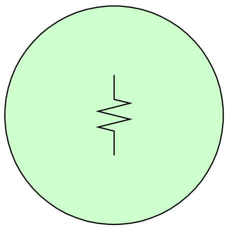
Zhou, Liu, Chang, IMMIJ, 2013

6. Modeling single cells with DPD

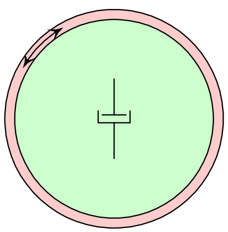


- The study of the movement and deformation of single cells (in blood vessels) is important for understanding mechanical properties of cells.
- The changes in mechanical properties of cells may be closely related to severe cell diseases.
- Modern physiology medicine have established the relationship of mechanical changes between healthy and pathological cells.
- Differences of mechanical properties could be used to distinguish between normal and diseased cells

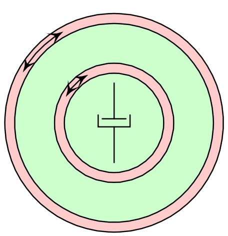
6. Modeling single cells with DPD



Solid model



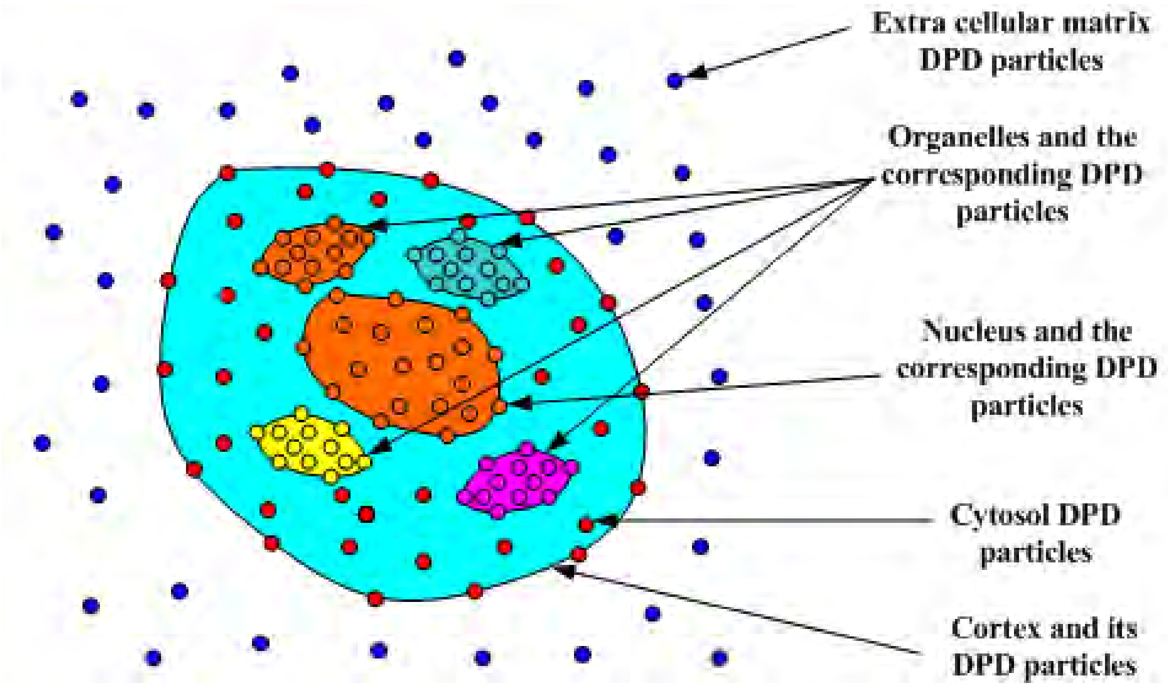
Liquid drop model



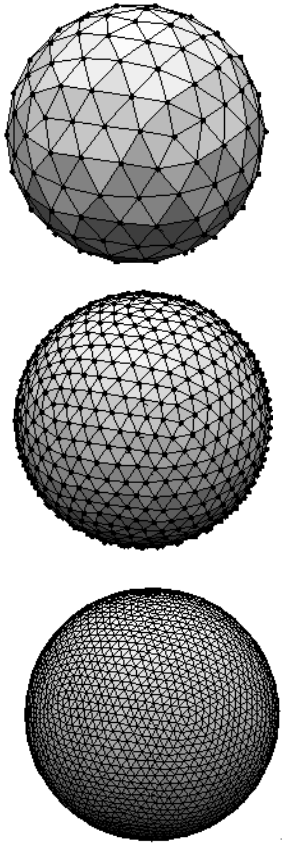
Compound drop model

- **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 assums the nucleus to be an encapsulated liquid drop.

6. Modeling single cells with DPD



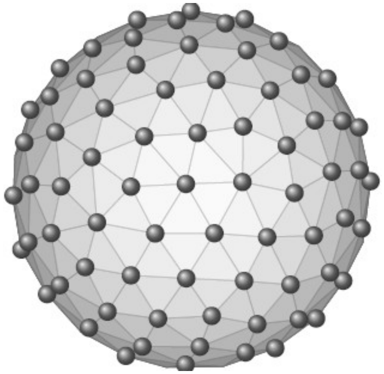
DPD modeling of a cell and its environment



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**



$$U(\{\mathbf{r}_i\}) = U_{\text{plane}} + U_{\text{bending}} + U_{\text{area}} + U_{\text{volume}}$$

Zhou, Liu, Chang, IJCM, 2016

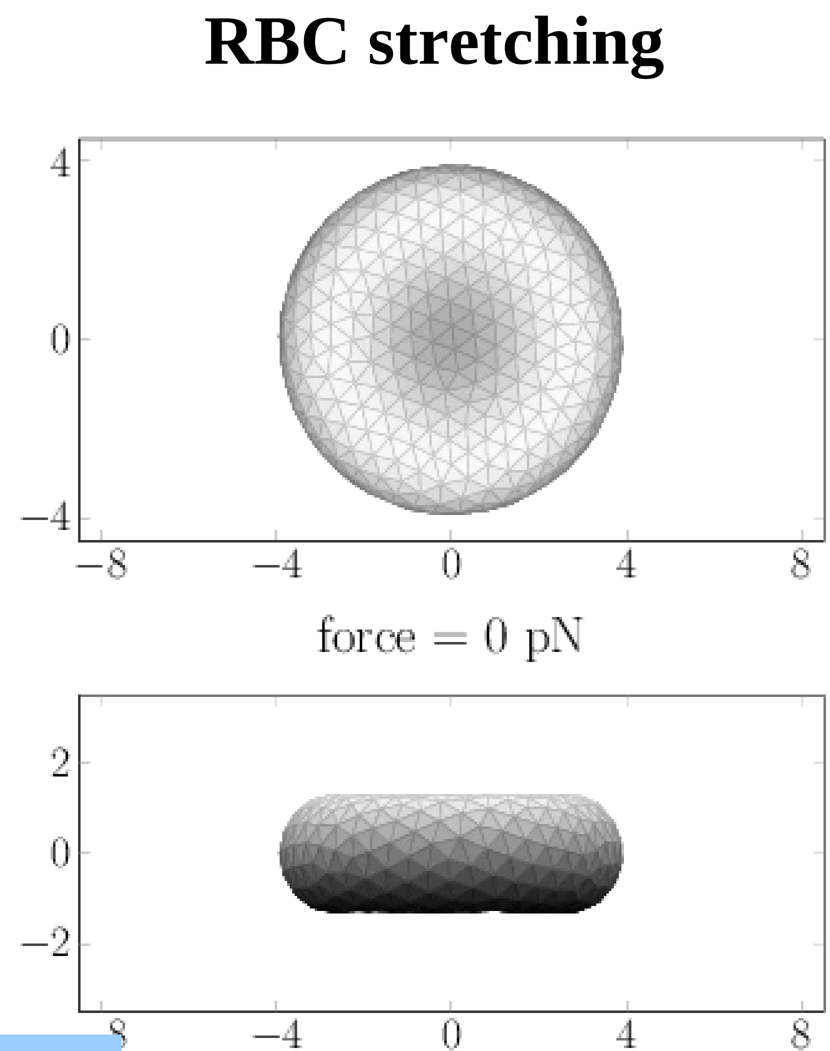
6. Modeling single cells with DPD

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)

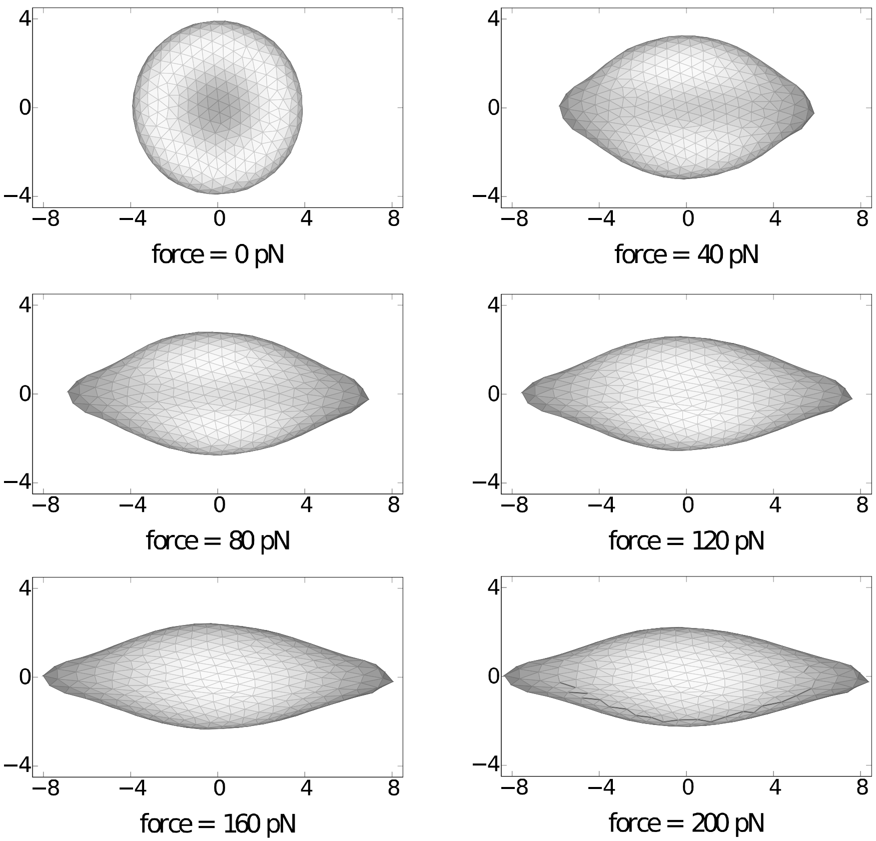


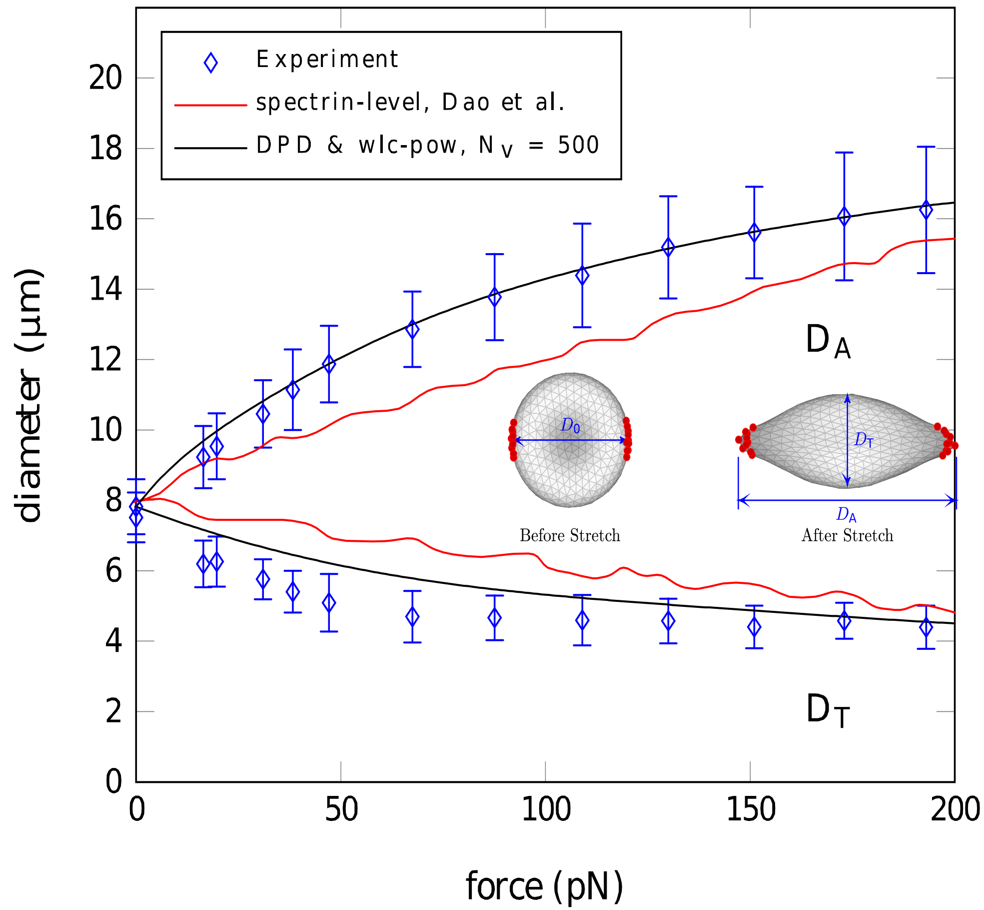
Zhou, Liu, Chang, IJCM, 2016

6. Modeling single cells with DPD

6.1 Biconcave cell (RBC)

RBC stretching

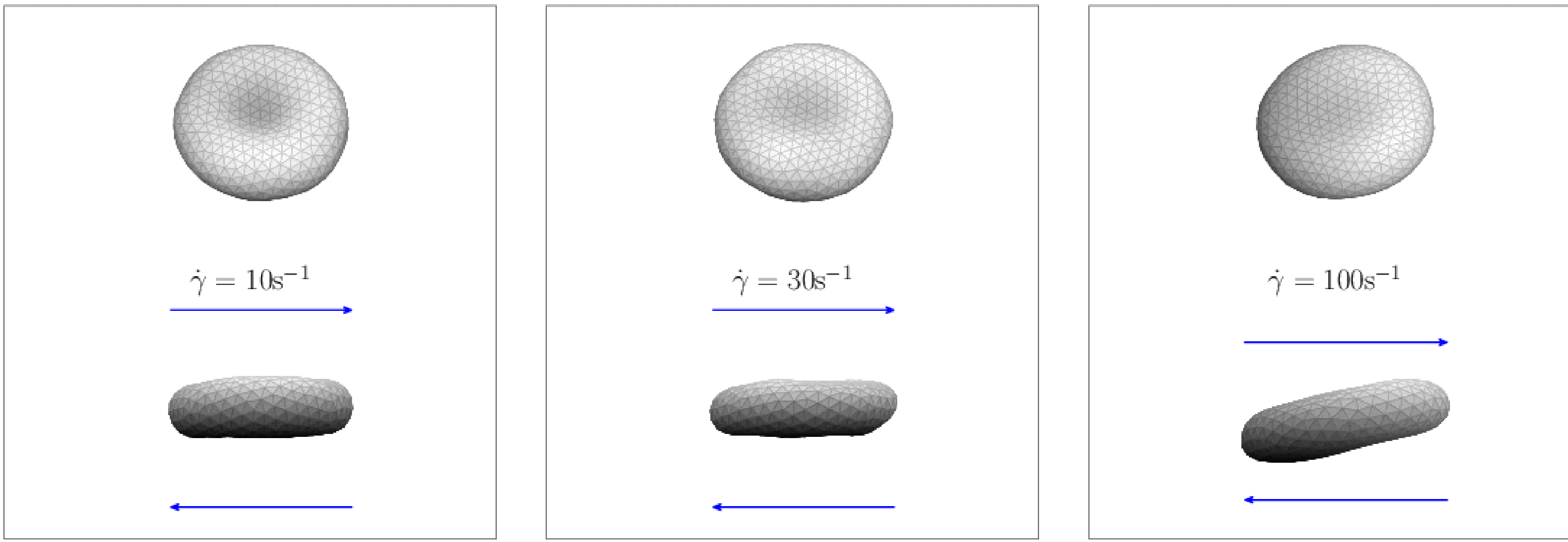




6. Modeling single cells with DPD

6.1 Biconcave cell (RBC)

RBCs in shear flows

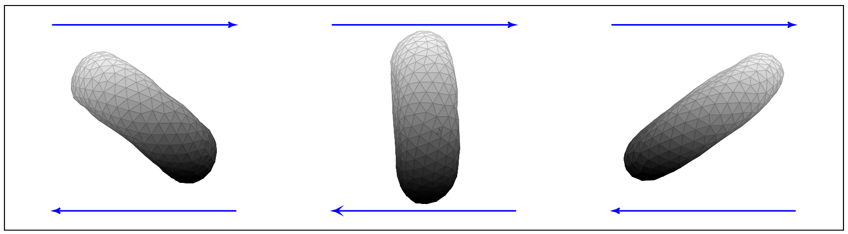


Tumbling **Intermediate** **Tank-treading**

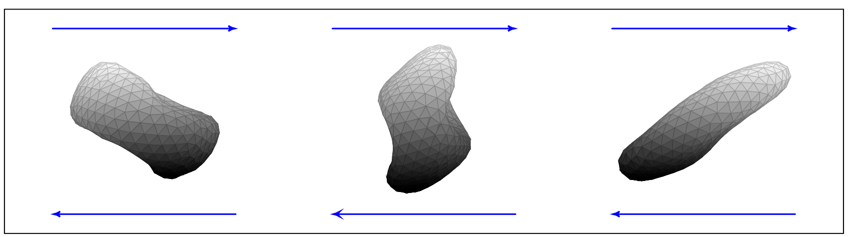
6. Modeling single cells with DPD

6.1 Biconcave cell (RBC)

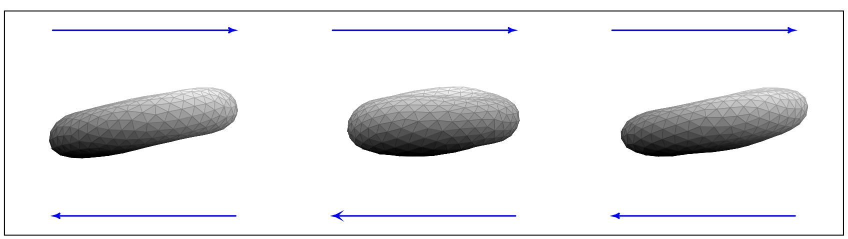
RBCs in shear flows



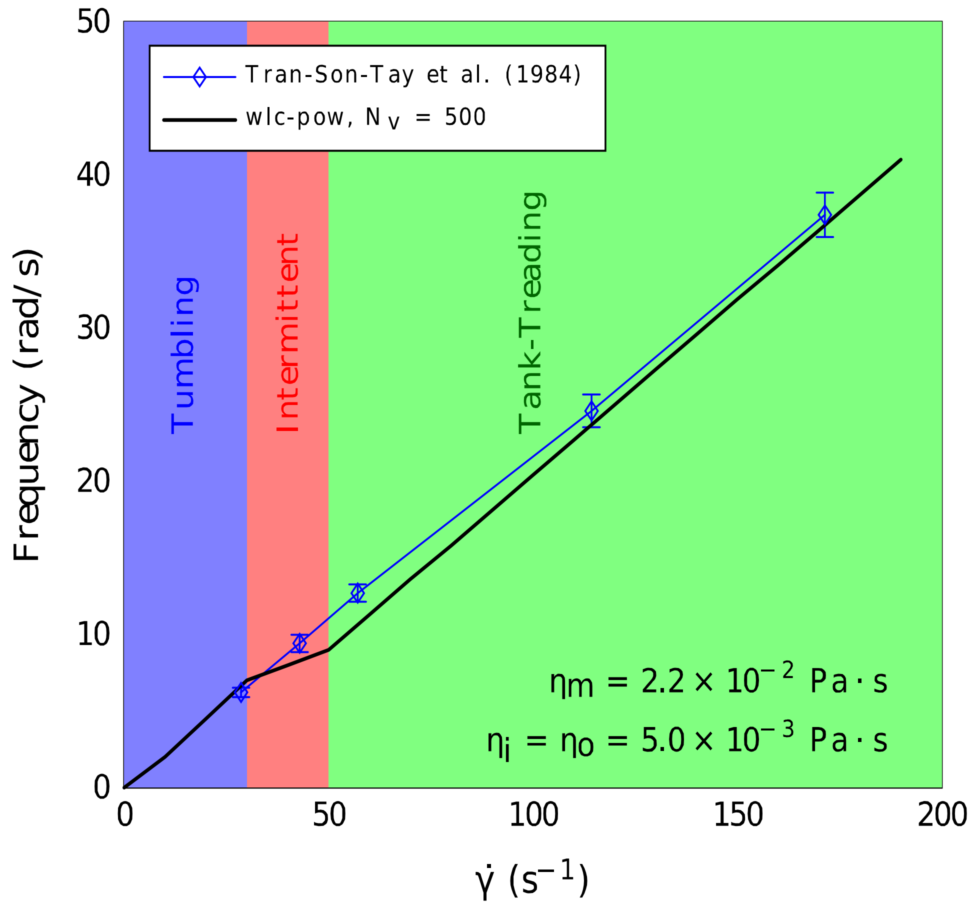
$\dot{\gamma} = 10\mathrm{s}^{-1}$



$\dot{\gamma} = 30\mathrm{s}^{-1}$



$\dot{\gamma} = 100\mathrm{s}^{-1}$

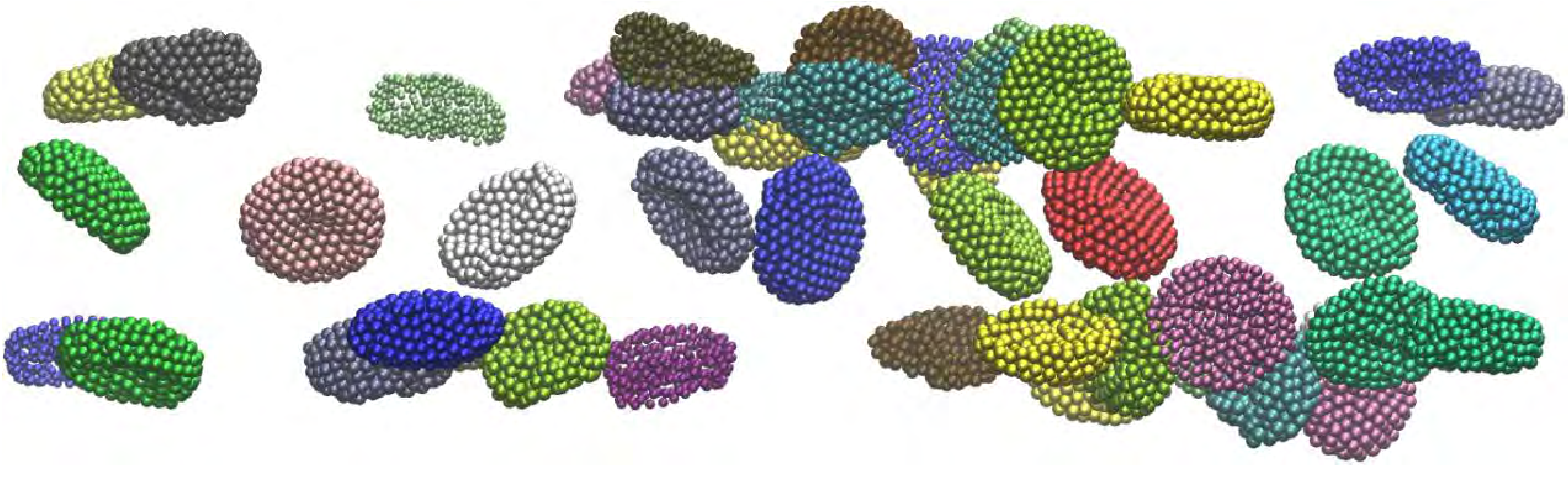


6. Modeling single cells with DPD

6.1 Biconcave cell (RBC)

Multi-RBCs in Poiseuille flow in a tube

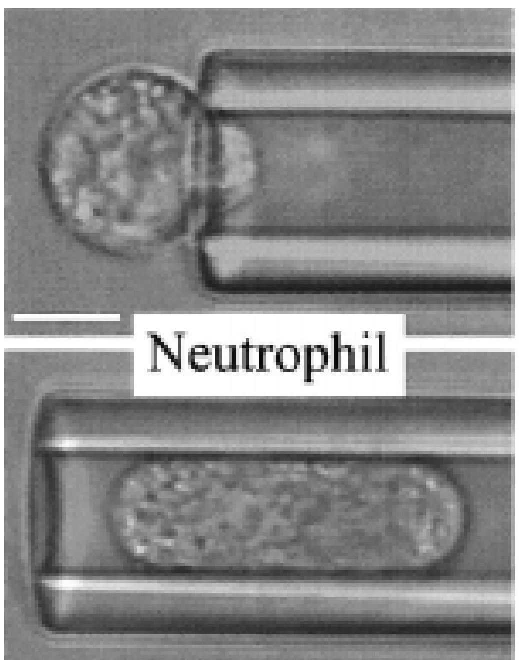
- Based on proper simulations of single RBCs with accurate mechanics, rheology and dynamics, more complicated situations can further be simulated. One of those situations is blood flow.

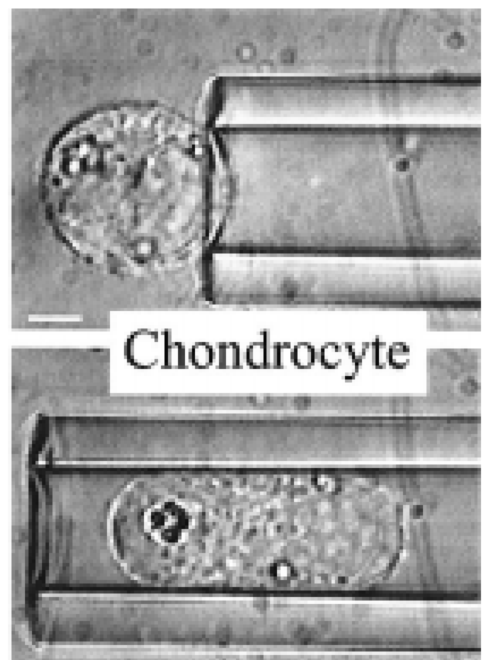


6.2 Spherical cells

Cell passing through channel

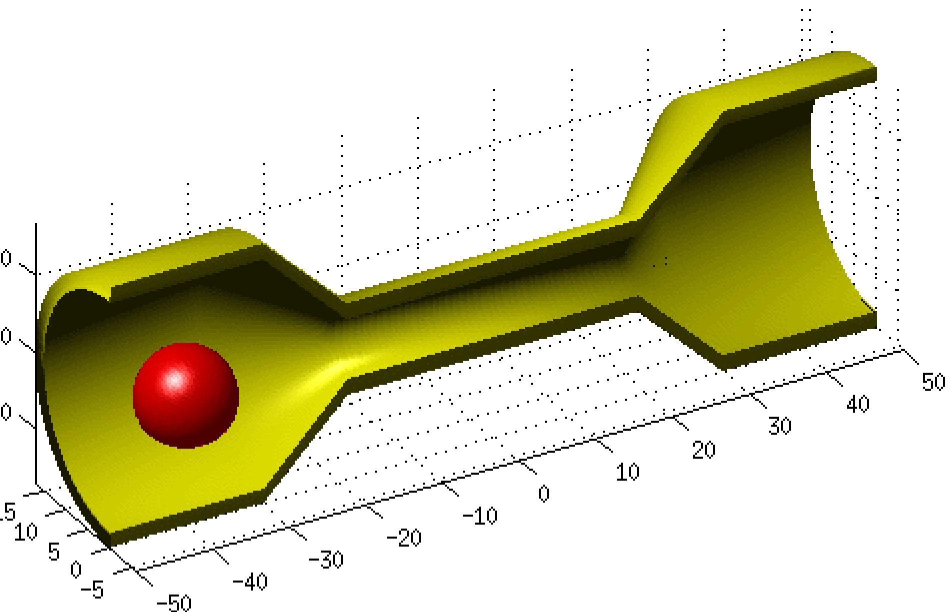
The deformation and dynamic response of a cell passing through a micro-channel can be used to investigate the mechanic, physical and biological features of a cell, and thus can be used to cell classification, separation, and disease diagnosis.

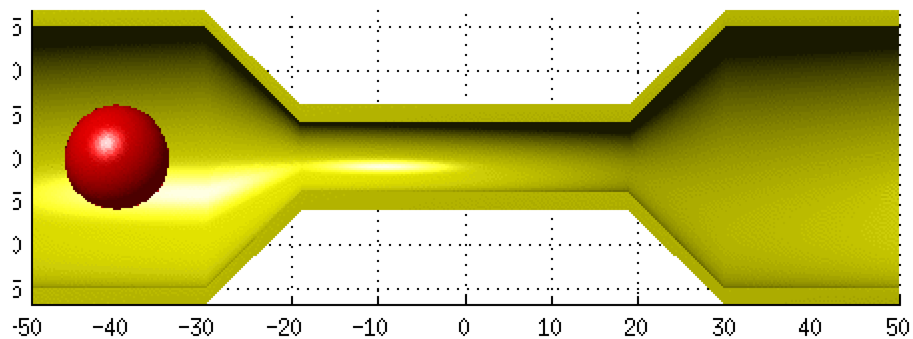




6. Modeling single cells with DPD

6.2 Spherical cells

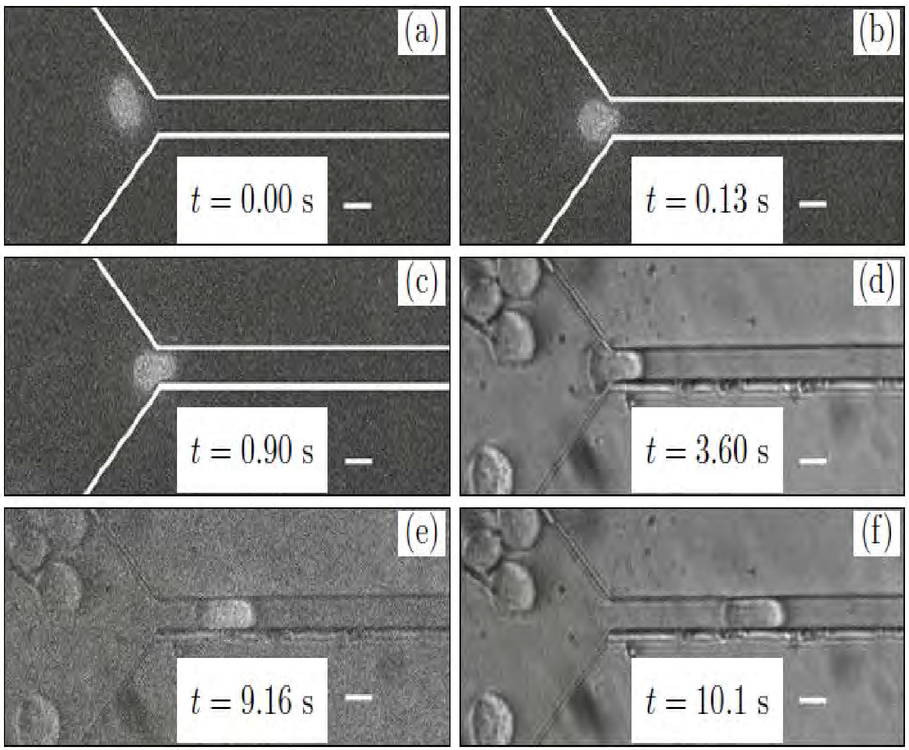


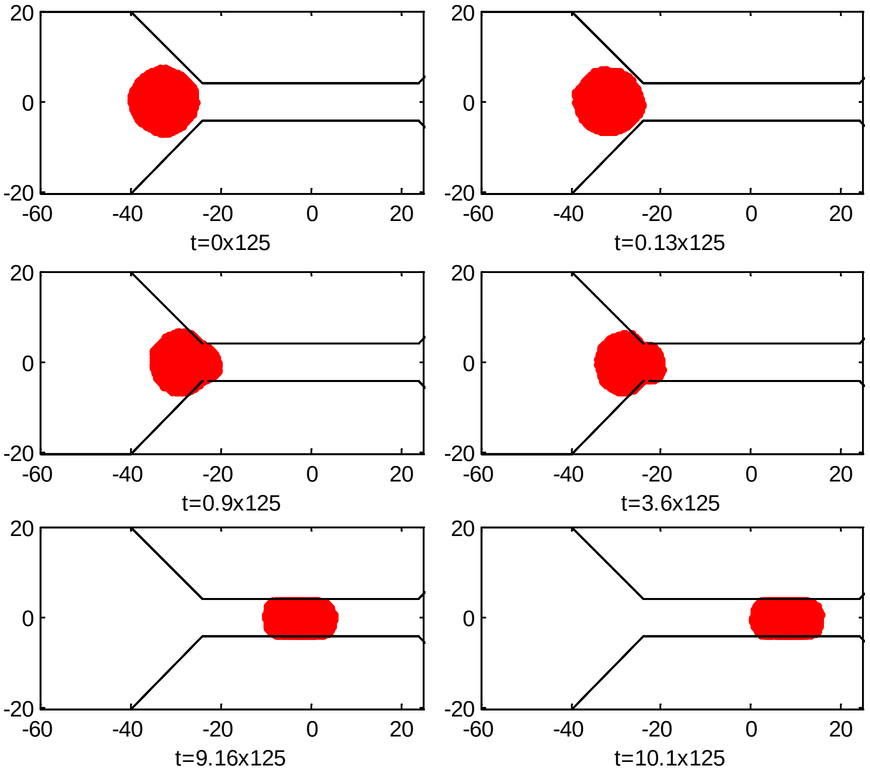


Entry process of benign breast epithelial cells (MCF-10A)

6. Modeling single cells with DPD

6.2 Spherical cells

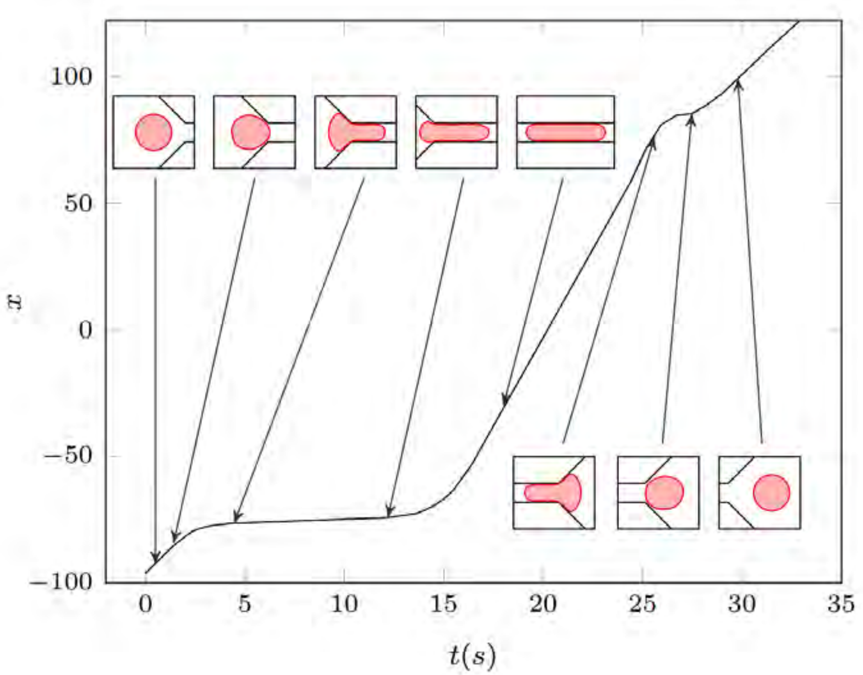




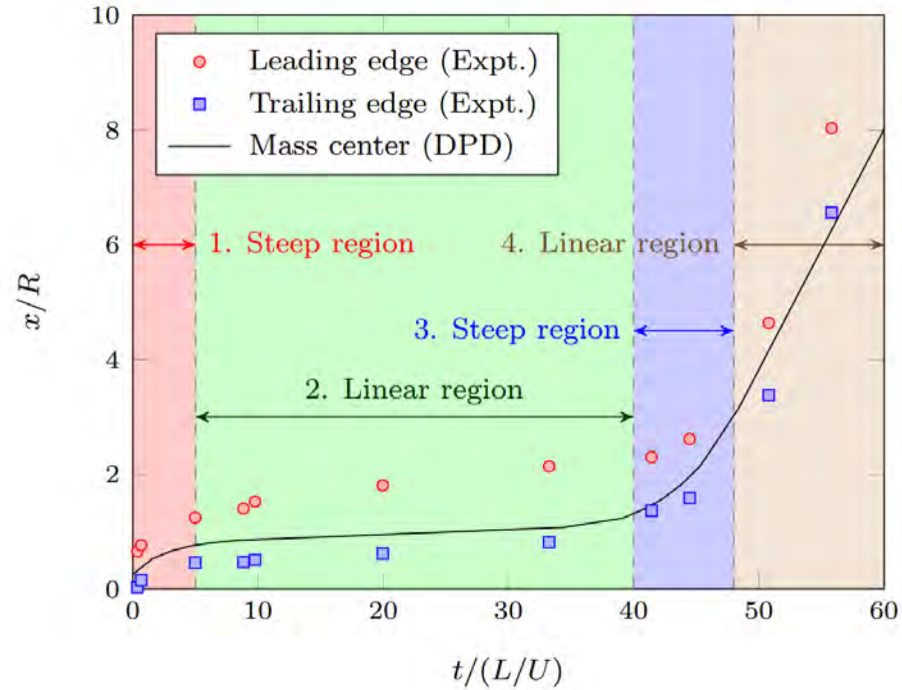
F.Y.Leong et al. Biomechanics and modeling in mechanobiology 10, 755766 (2011)

6. Modeling single cells with DPD

6.2 Spherical cells



Cell displacement and deformation pattern



Cell displacement vs experimental data

Approaching（reduce speed）→partially enter（v→0,long time duration）→fully enter（acceleration-roughly constant）→partially exit（accelerate suddenly → reduce speed）

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!