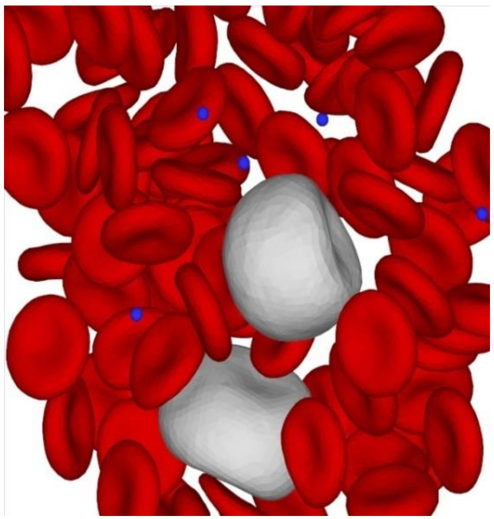
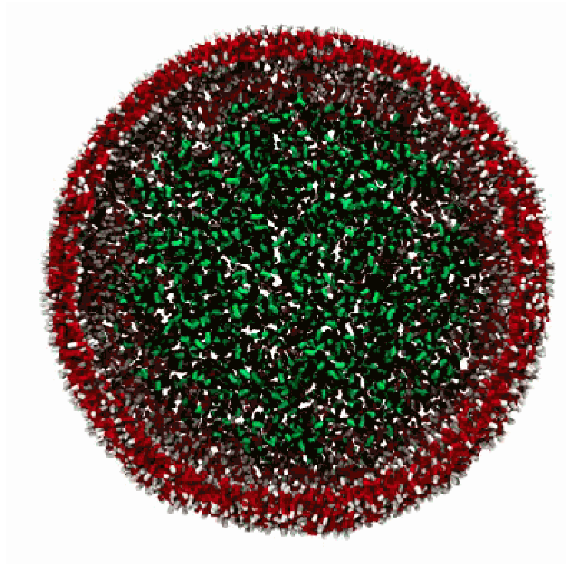
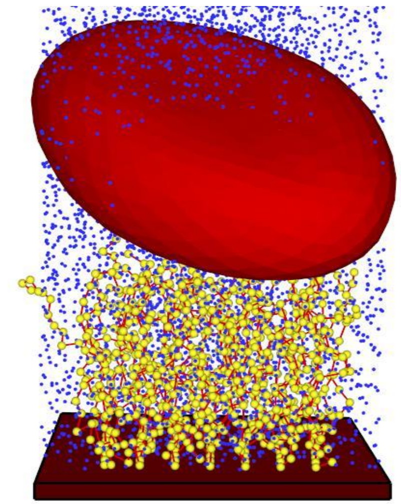
# Dissipative Particle Dynamics: Foundation, Evolution and Applications

## *Lecture 3:* New methods beyond traditional DPD

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& Pacific Northwest National Laboratory, CM4

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

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# Outline

## 1. Single Particle DPD

Particle size: mono-size → multi-size

## 2. Many-body DPD

Quadratic EOS → Higher-order EOS

## 3. Energy conserving DPD

Isothermal system → Non-isothermal system

## 4. Smoothed DPD

Bottom-up approach → Top-down approach

## 5. Other DPD models

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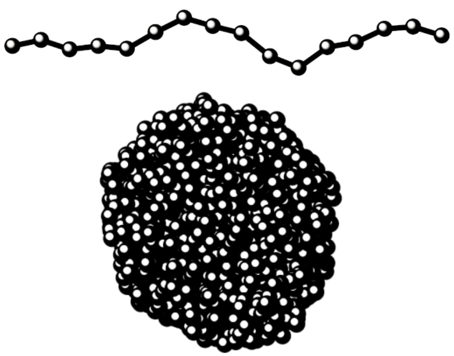
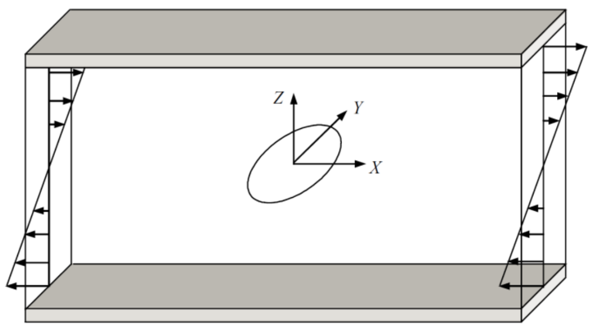
# Successful DPD applications using mono-size particles

## **Application 1:** Polymer drops in a shear flow

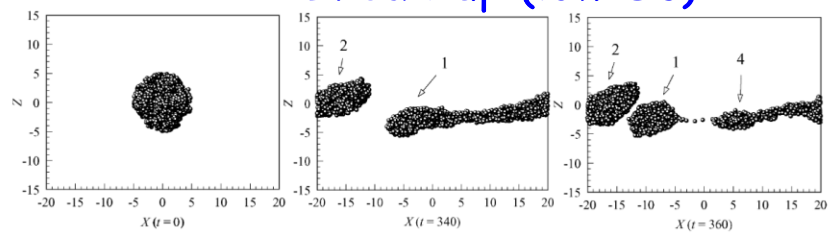
— Chen, Phan-Thien, Fan & Khoo, J. Non-Newtonian Fluid Mech., 2004.



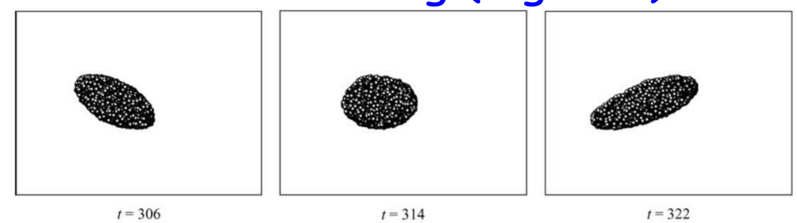
N = 2096




Break-up (low Sc)

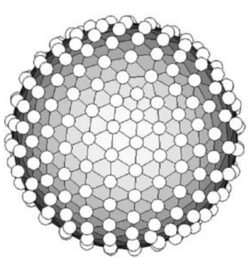



Tumbling (high Sc)

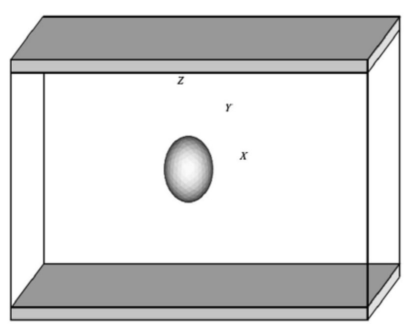


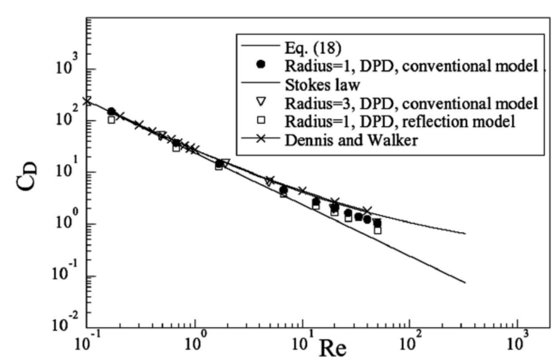

## **Application 2:** Flow around spheres

— Chen, Phan-Thien, Khoo & Fan, Phys. Fluids, 2006.



N = 452

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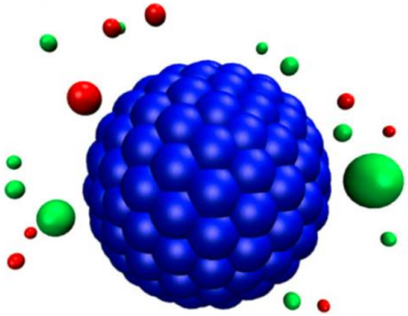
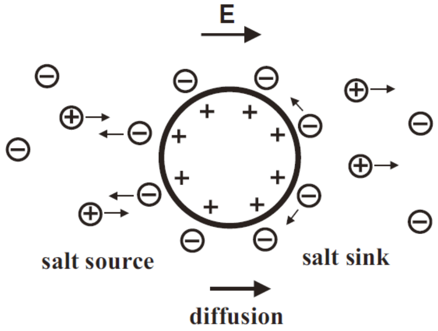
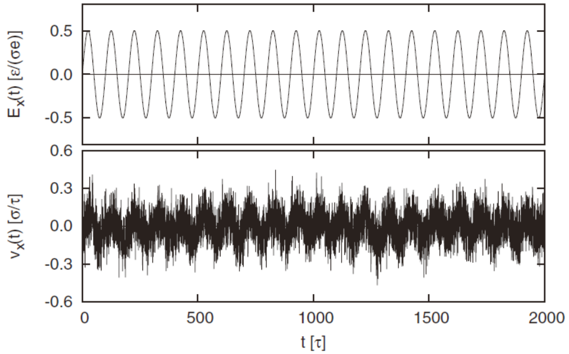
# Successful DPD applications using mono-size particles

## Application 3: Dynamic of colloids in electric fields

— Zhou, Schmitz, Dunweg & Schmid, J Chem. Phys., 2013.

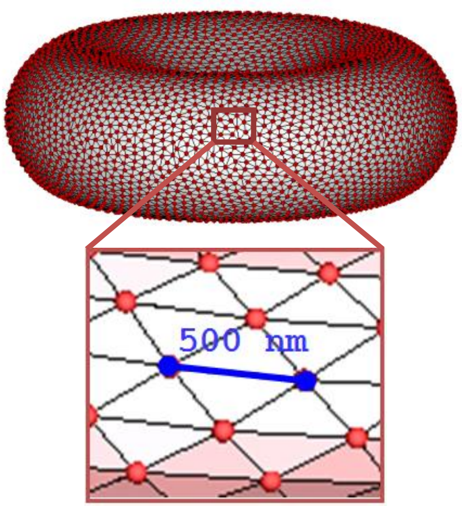


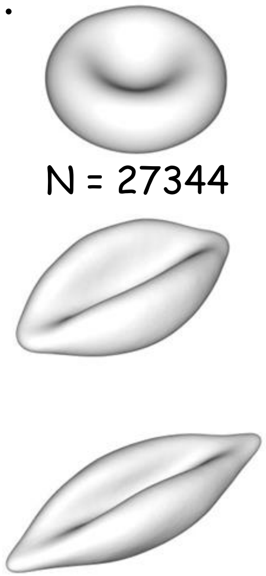


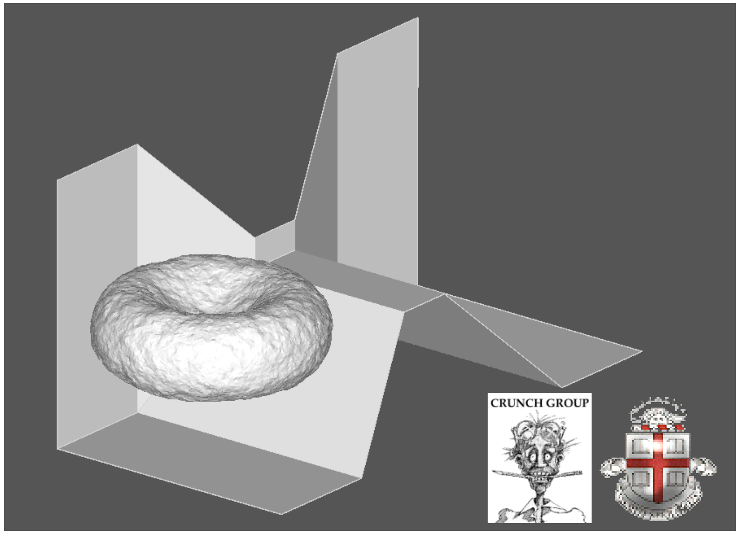




## Application 4: Accurate Modeling of Red Blood Cells

— Pivkin & Karniadakis, PRL, 2008.

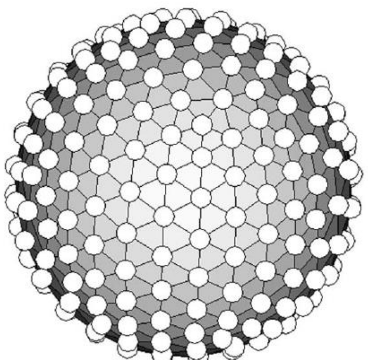


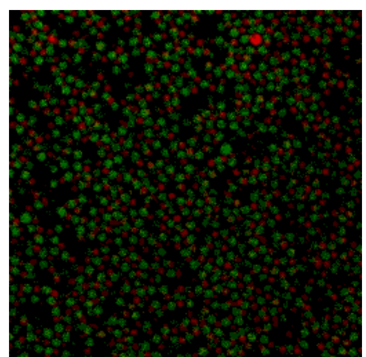
# Disadvantage of using mono-size particles

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



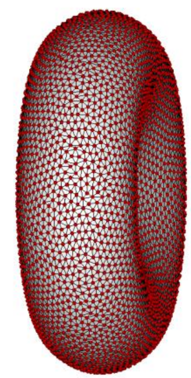
Chen, S., et al., Phys. Fluids, 2006.

N = 452

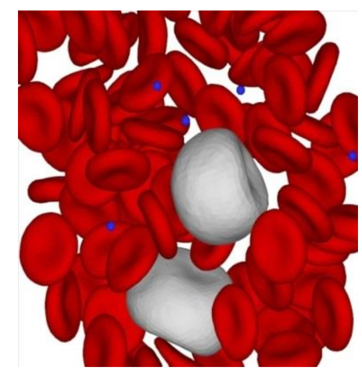


www.teunvissers.nl

Many colloids



N = 27344



Many RBCs

**Solution:** Multi-size particles.

— **Single Particle DPD model**

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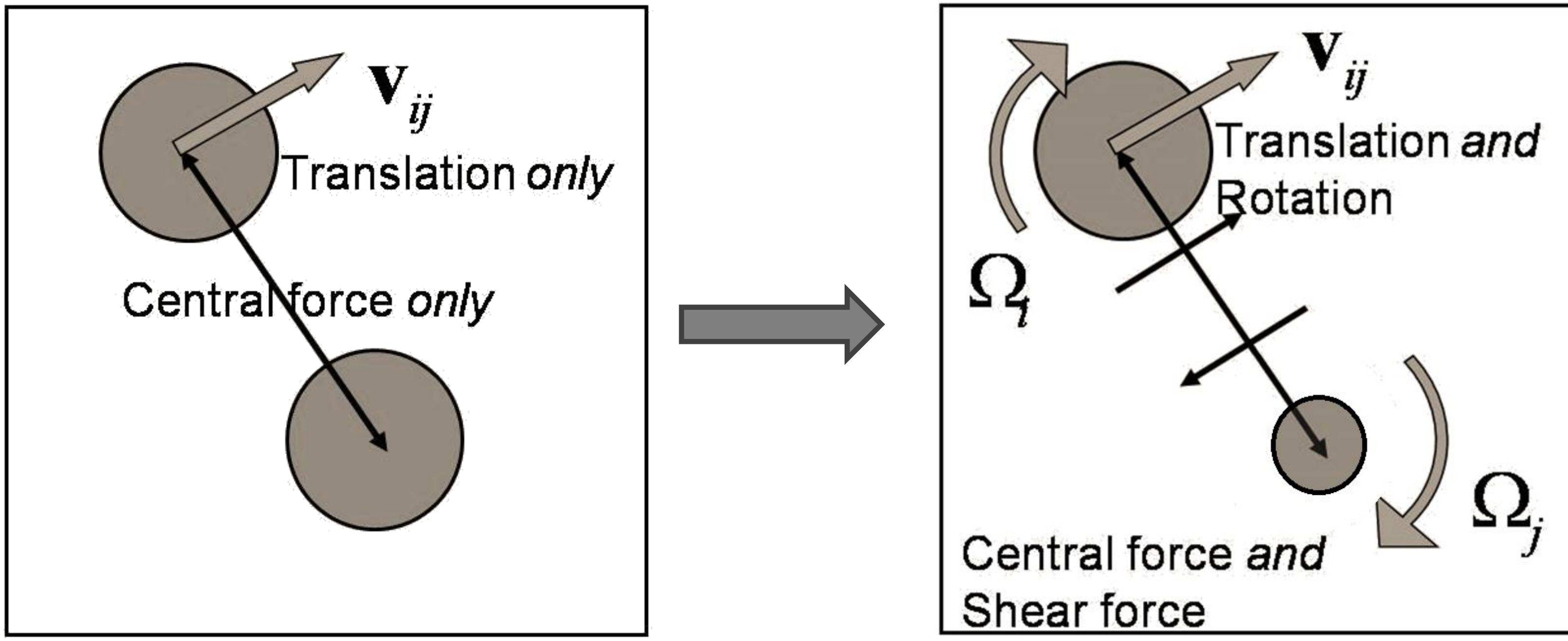
# Single Particle DPD model

## DPD Generalization:




Extra requirements:

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

— Pan, Pivkin & Karniadakis, Europhys. Lett., 2008.

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# Single Particle DPD model

## Equations of Motion:

$$\dot{\mathbf{r}}_i = \mathbf{v}_i$$

$$\dot{\mathbf{v}}_i = \frac{1}{m}\sum_{j \neq i} \mathbf{F}_{ij}$$

$$\dot{\mathbf{\Omega}}_i = \frac{1}{I}\sum_{j \neq i} \mathbf{T}_{ij}$$

$$\mathbf{F}_i = \sum_j \mathbf{F}_{ij}$$

$$\mathbf{T}_i = -\sum_j \lambda_{ij}\,\mathbf{r}_{ij} \times \mathbf{F}_{ij}$$

$$\mathbf{F}_{ij} = \mathbf{F}^C_{ij} + \mathbf{F}^T_{ij} + \mathbf{F}^R_{ij} + \widetilde{\mathbf{F}}_{ij}$$

$$\mathbf{F}^C_{ij} = -V'(r_{ij})\mathbf{e}_{ij}$$ Conservative force

$$\mathbf{F}^T_{ij} = -\gamma_{ij} m\, \mathbf{\Gamma}_{ij} \cdot \mathbf{v}_{ij}$$ Translational force

$$\mathbf{F}^R_{ij} = -\gamma_{ij} m\, \mathbf{\Gamma}_{ij} \cdot \left[ \mathbf{r}_{ij} \times (\lambda_{ij}\mathbf{\Omega}_i + \lambda_{ji}\mathbf{\Omega}_j) \right]$$ Rotational force

$$\widetilde{\mathbf{F}}_{ij} dt = (2k_B T \gamma_{ij} m)^{1/2} \left[ \widetilde{A}(r_{ij})\overline{d\mathbf{W}^S_{ij}} + \widetilde{B}(r_{ij})\frac{1}{d}\mathrm{tr}[d\mathbf{W}_{ij}]\mathbf{1} + \widetilde{C}(r_{ij})d\mathbf{W}^A_{ij} \right] \cdot \mathbf{e}_{ij}$$ Random force

$$\lambda_{ij} = \frac{R_i}{R_i + R_j}, \quad \text{and } \lambda_{ij} = 1/2 \quad \text{when } R_i = R_j$$

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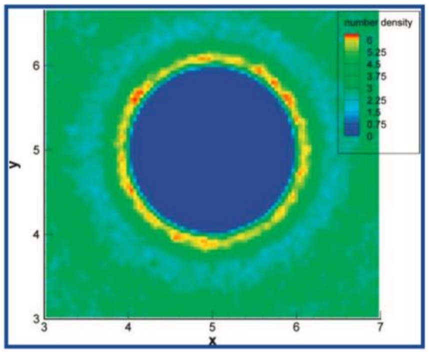
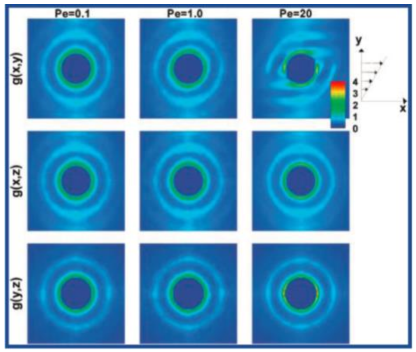
— Pan, Pivkin & Karniadakis, Europhys. Lett., 2008.

# Examples of Single Particle DPD

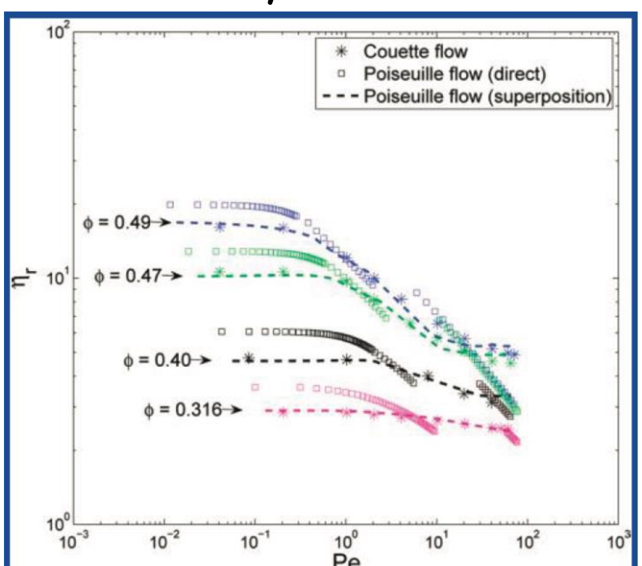
## Rheology in Colloidal Suspensions:

— Pan, Caswell & Karniadakis, Langmuir, 2010.



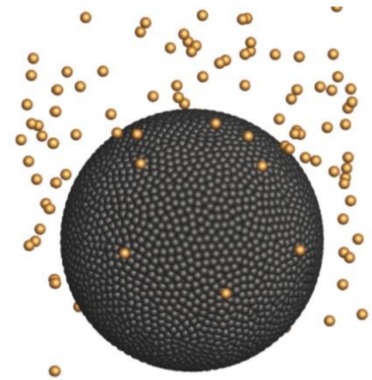

Relative viscosity vs ***Pe*** number:



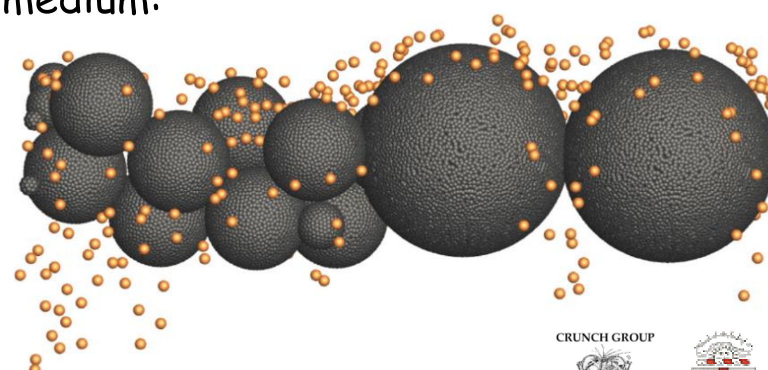

## Colloid transport in porous media:

— Pan and Tartakovsky, Adv. Water Resour., 2013.

Colloid transport surrounding a single collector:



Colloid transport in a polysized porous medium:



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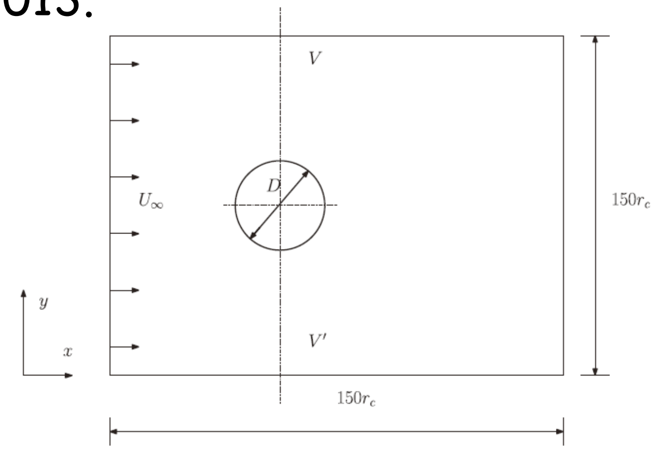
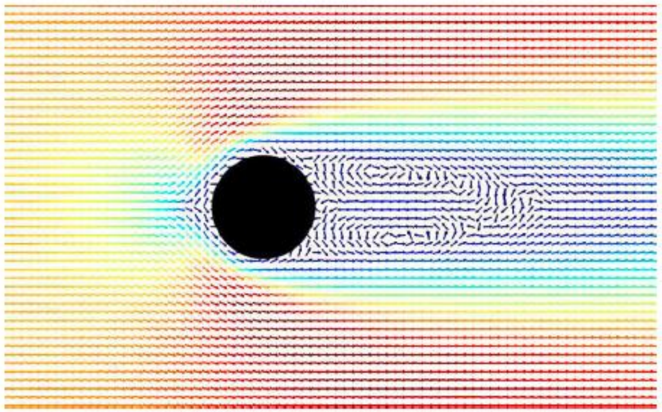
# Examples of Single Particle DPD

## Flow around a circular cylinder:

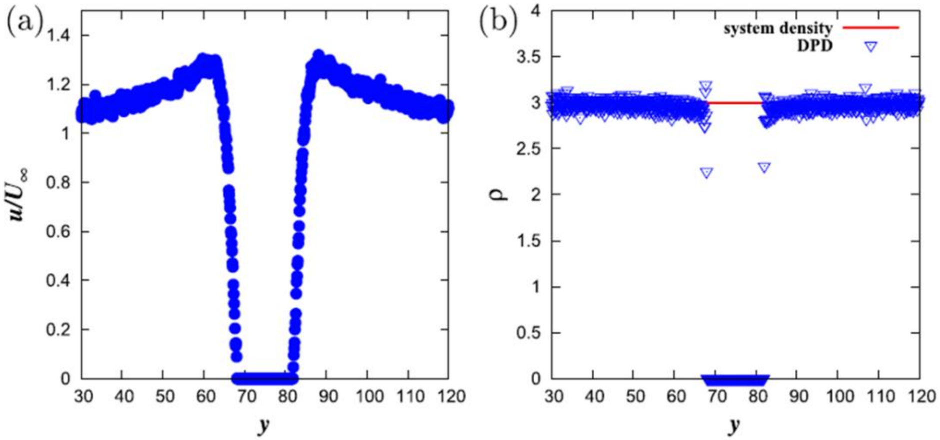
— Ranjith, et al., J. Comput. Phys., 2013.




Velocity vector:



Velocity and density profiles across the cylinder:

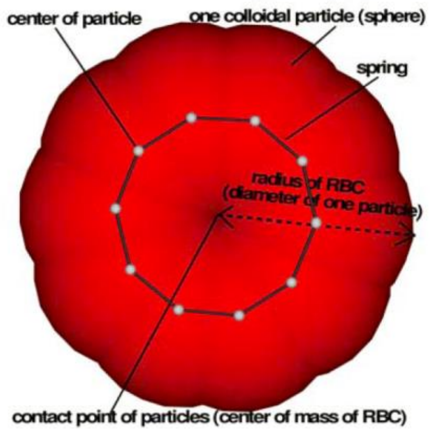



Comparison of drag coefficients:

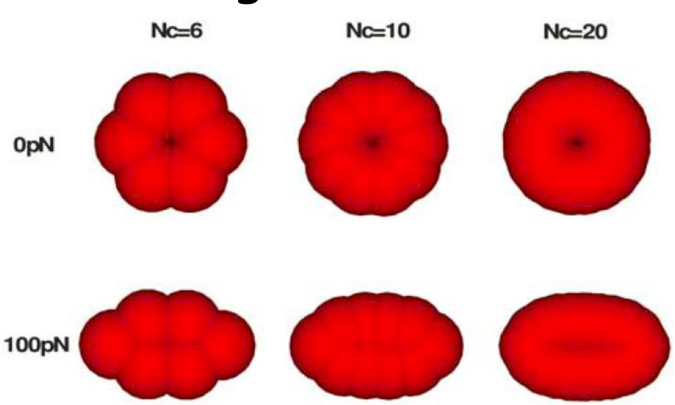
| Re | Experiment | DPD |
|---|---|---|
| 10 | 2.93 | 2.99 |
| 20 | 2.08 | 2.14 |
| 30 | 1.76 | 1.74 |
| 40 | 1.58 | 1.66 |

# Examples of Single Particle DPD

## Low-dimensional model for the red blood cell:

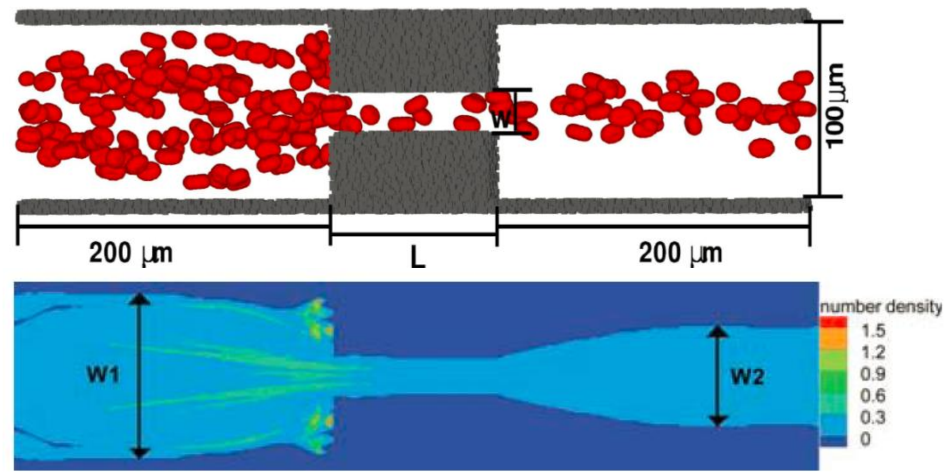



RBC shapes at various stretching forces:



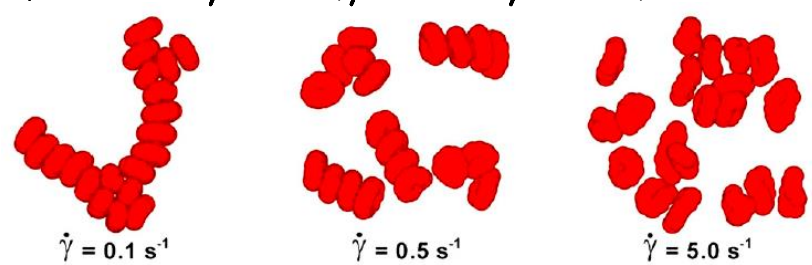

RBCs in a channel with a geometrical constriction:

— Pan, et al., Soft Matter, 2010.




Aggregation of RBCs under shear:

— Fedosov, et al., PNAS, 2011.



# Outline

1. Single Particle DPD
   Particle size: mono-size → multi-size
2. **Many-body DPD**
   Quadratic EOS → Higher-order EOS
3. Energy conserving DPD
   Isothermal system → Non-isothermal system
4. Smoothed DPD
   Bottom-up approach → Top-down approach
5. Other DPD models

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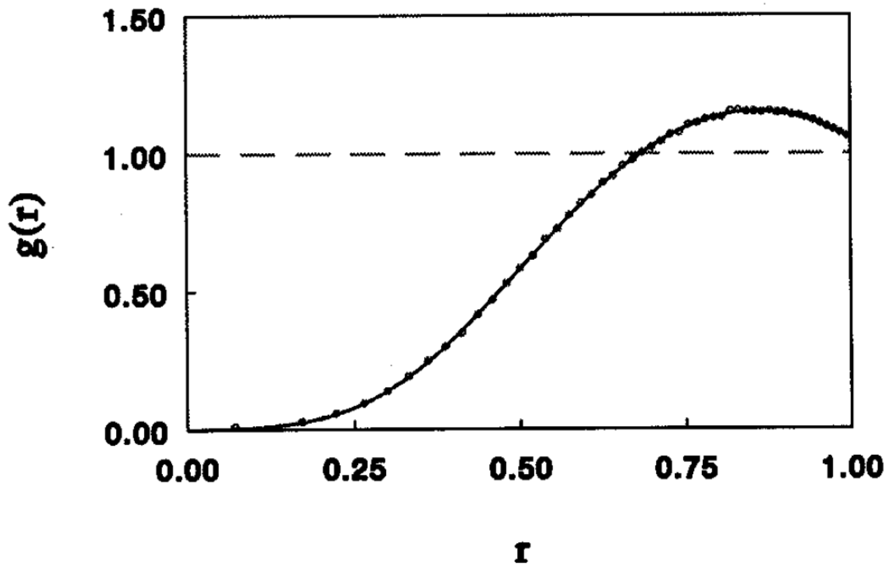
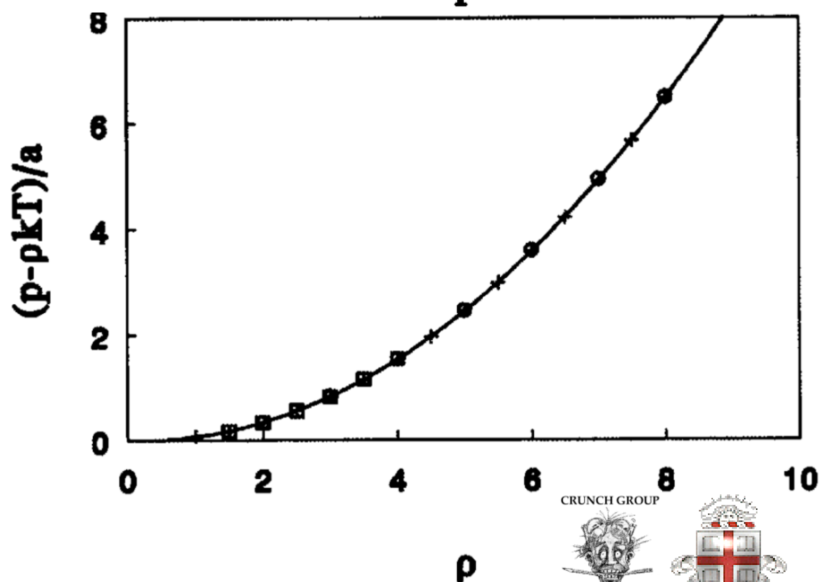
# Equation of State (EOS) of traditional DPD

$$
\begin{aligned}
P &= \rho k_B T + \frac{1}{3V}\left\langle \sum_i \mathbf{r}_i \cdot \mathbf{F}_i \right\rangle \\
&= \rho k_B T + \frac{1}{3V}\left\langle \sum_i \sum_{j>i} \mathbf{r}_{ij} \cdot \mathbf{F}_{ij}^C \right\rangle \\
&= \rho k_B T + \frac{2\pi}{3}\rho^2 \int_0^1 r F^C(r) g(r) r^2 dr
\end{aligned}
$$

$$F^C(r) = a(1-r)$$

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

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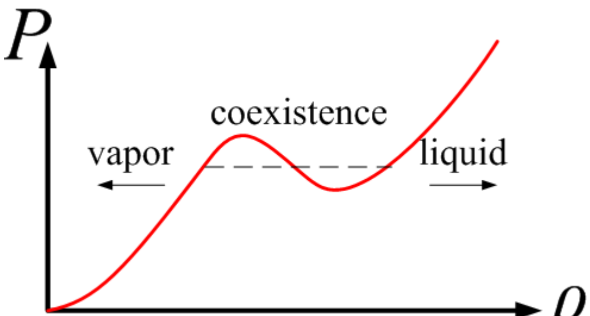
— Groot & Warren, J. Chem. Phys., 1997.

# Making conservative force density dependent

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



van der Waal's equation

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

EOS with high order terms:

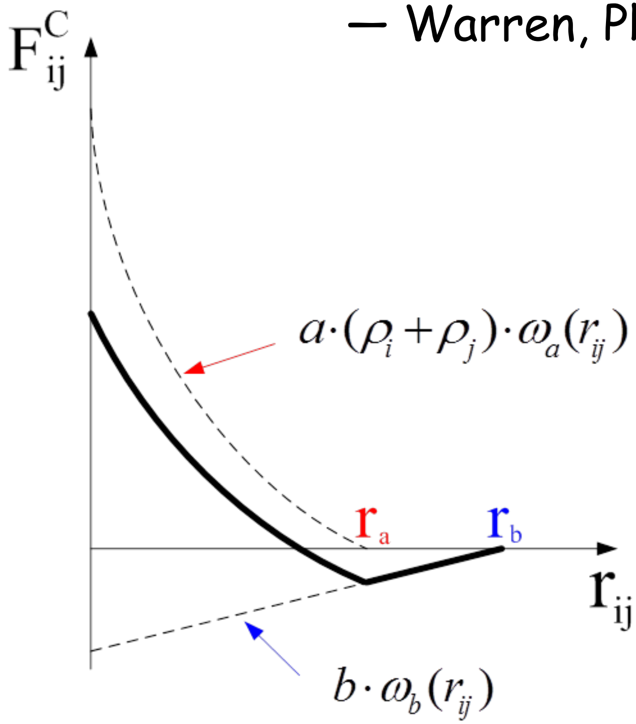
| | Traditional DPD | Many-body DPD |
|---|---|---|
| Force | $\mathbf{F}_{ij}^{C} = a \cdot \omega_C(r_{ij})\mathbf{e}_{ij}$ | $\mathbf{F}_{ij}^{C} = \frac{1}{2}\left(a(\rho_i) + a(\rho_j)\right) \cdot \omega_C(r_{ij})\mathbf{e}_{ij}$ |
| EOS | $P = \rho k_B T + \lambda a \rho^2$ | $P = \rho k_B T + \lambda a(\rho)\rho^2$ |

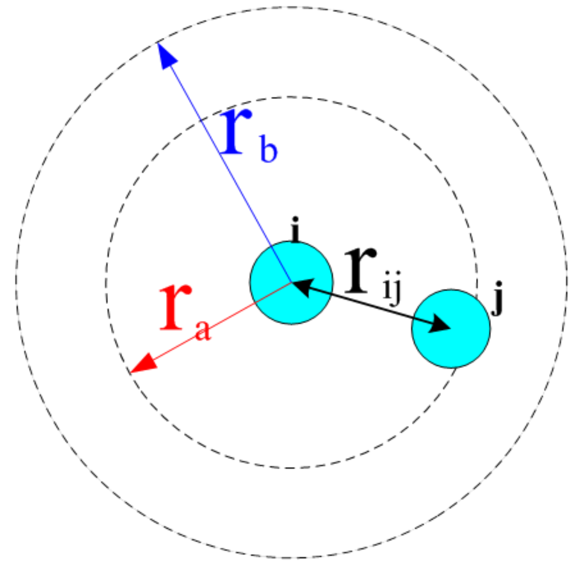
— Warren, Phys. Rev. E, 2003.

# Making conservative force density dependent

A common choice: $F_{ij}^{C} = a\cdot(\rho_i+\rho_j)\cdot\omega_a(r_{ij})\mathbf{e}_{ij} + b\cdot\omega_b(r_{ij})\mathbf{e}_{ij}$

— Warren, Phys. Rev. E, 2003.




Other approach: $F^{C} = \nabla\left(k_B T\ln\left(1-b\cdot\rho\right)+a\cdot\rho\right)+\kappa\nabla\nabla^2\rho$

— Tiwari & Abraham, Phys. Rev. E, 2006.

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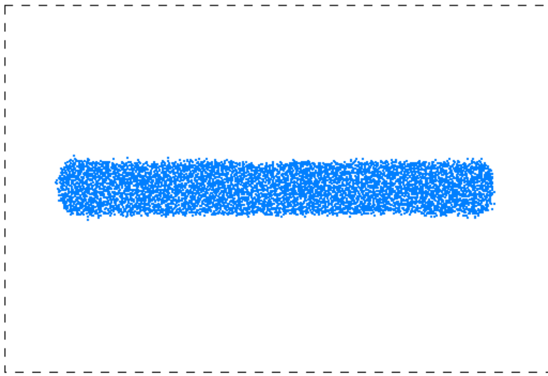
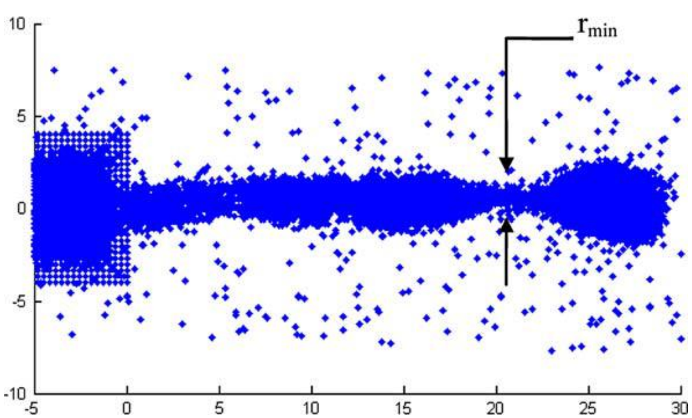
# Examples of Many-body DPD

## Free oscillation of a droplet:

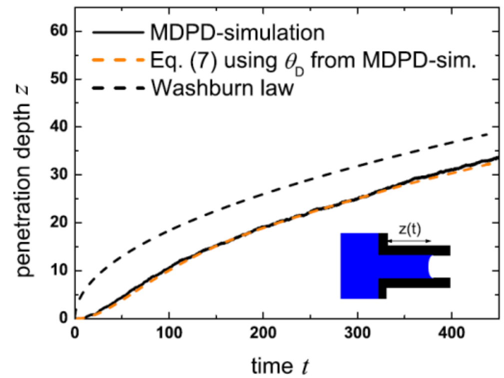


## Nano-Jet:

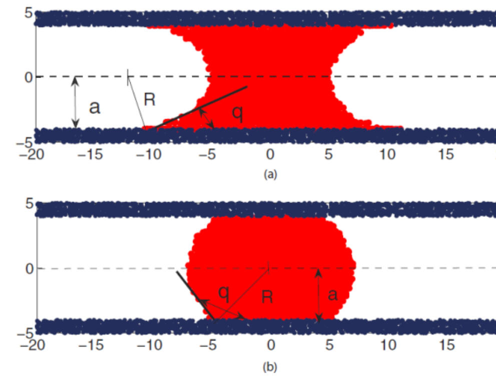
— Tiwari, et al. Microfluid Nanofluid, 2008.



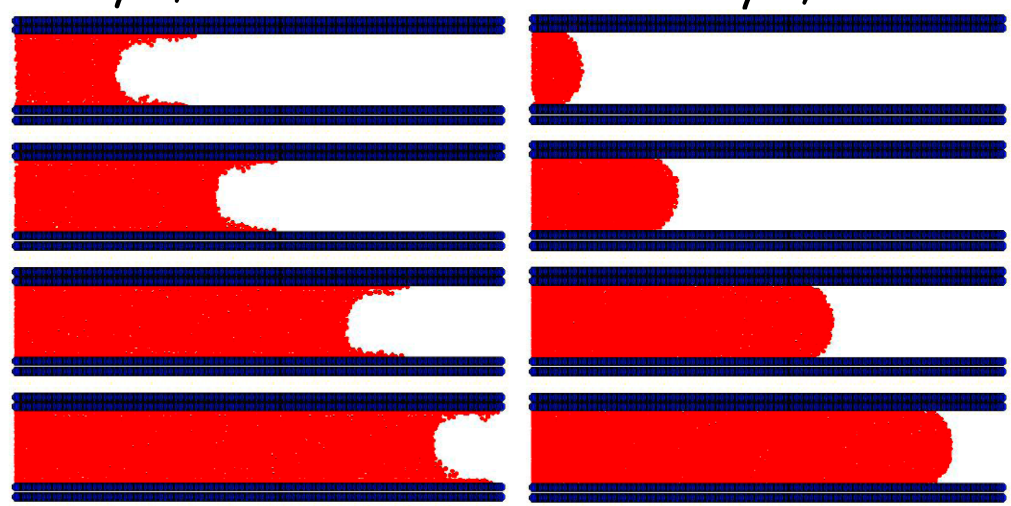

## Droplets wetting microchannels:




— Cupelli, et al. New J. Phys., 2008.




— Arienti, et al., J Chem. Phys., 2011.



— Pan, W.X., Ph.D Thesis, Brown University. 2010.

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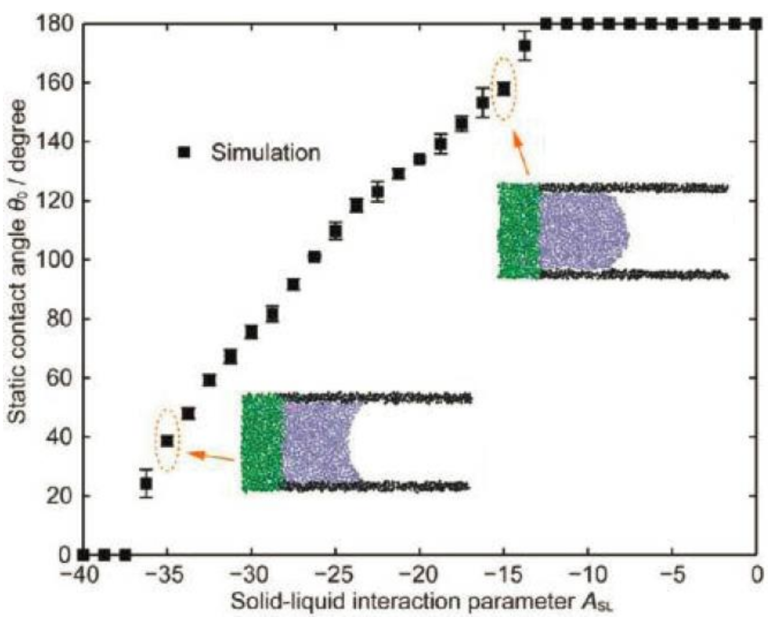
# Examples of Many-body DPD

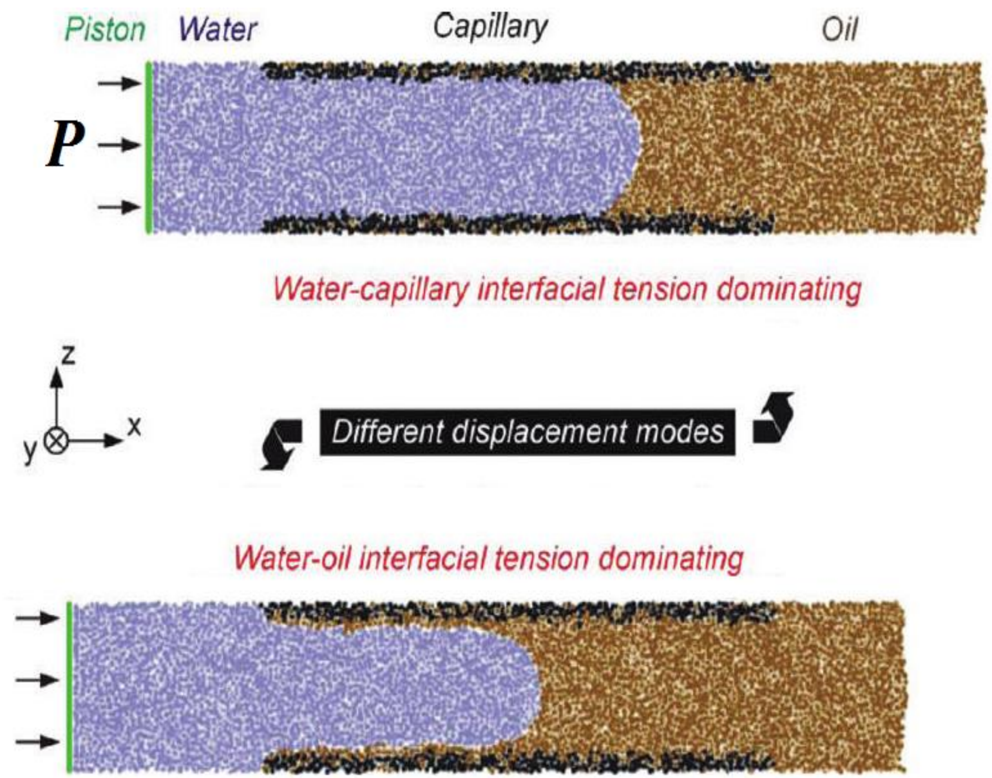
## Forced Water-Oil movement in capillary:

— Chen, Zhuang, Li, Dong & Lu, Langmuir, 2012.

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:

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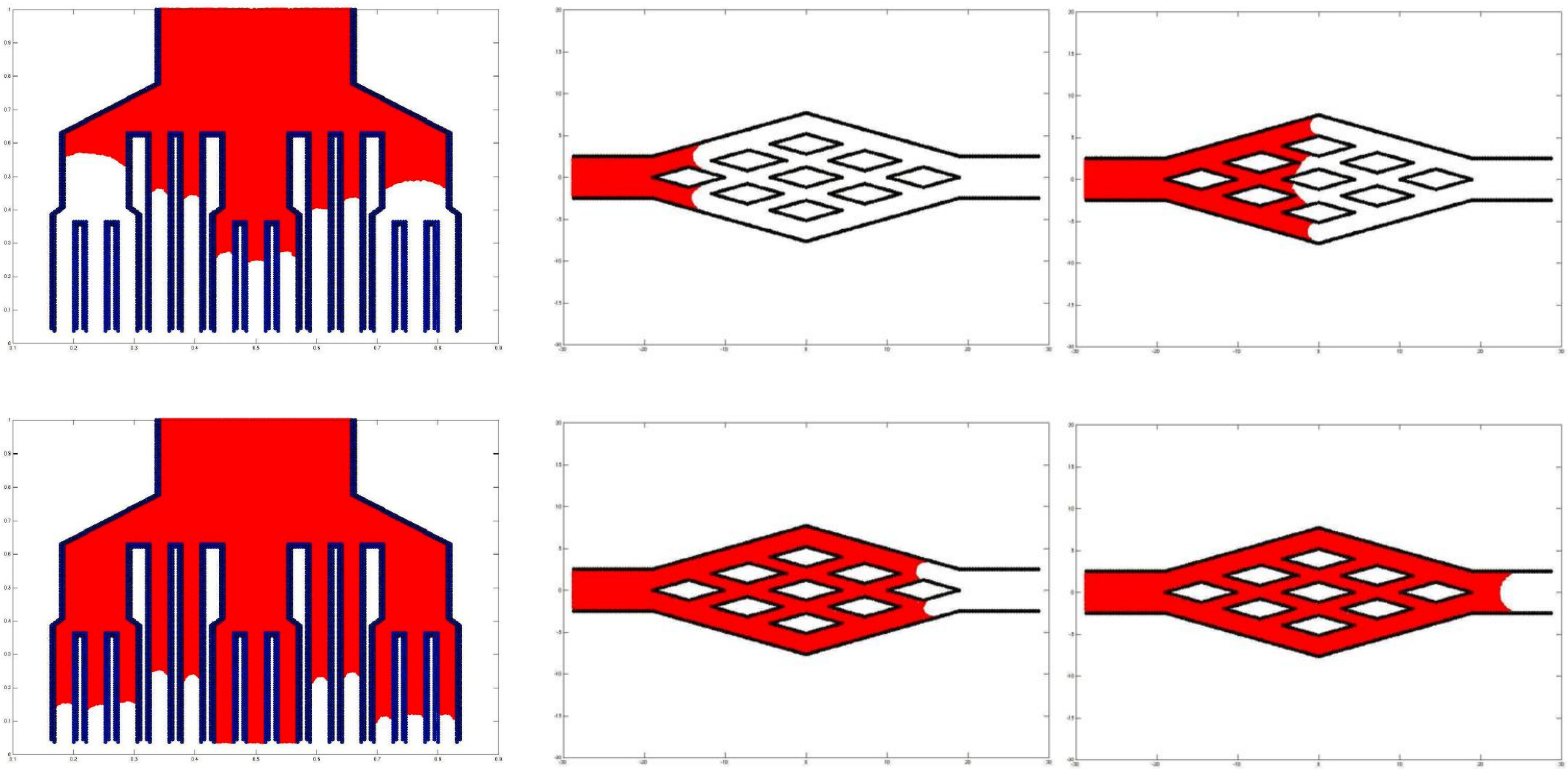
# Examples of Many-body DPD

## Flow with wetting in microchannel network:

– Pan, W.X., Ph.D Thesis, Brown University. 2010.



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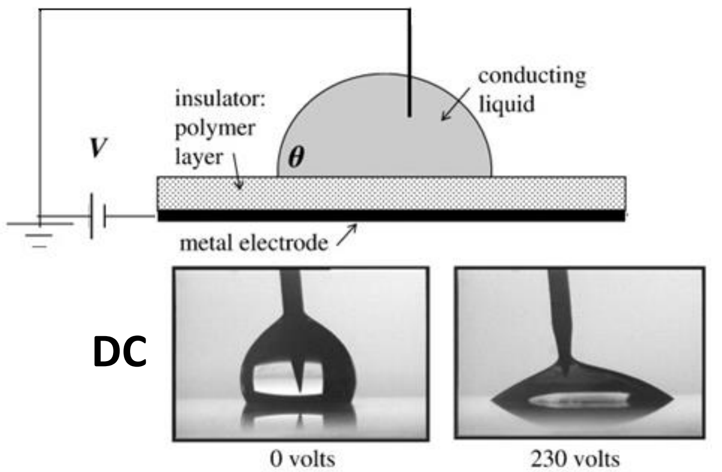
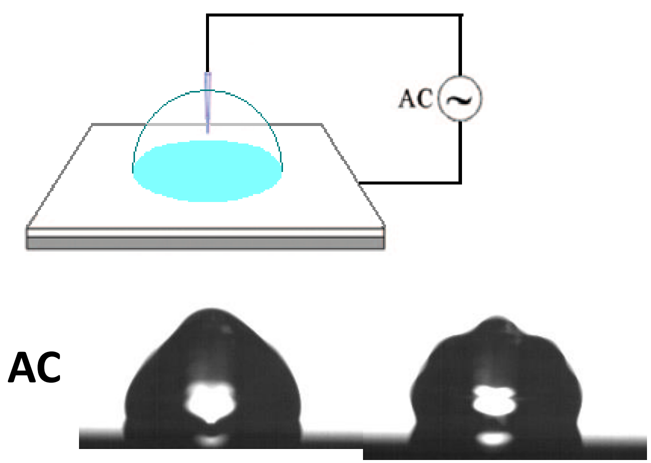
# Examples of Many-body DPD

## Electrowetting of a droplet:

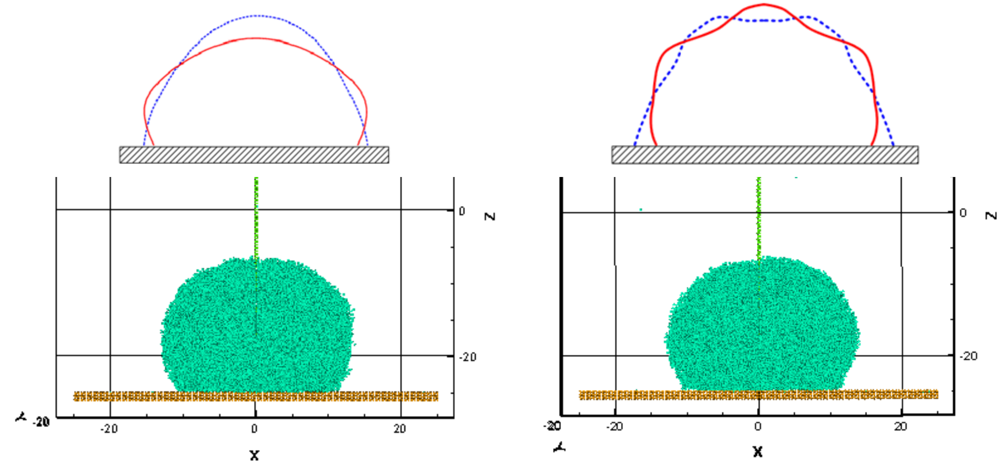


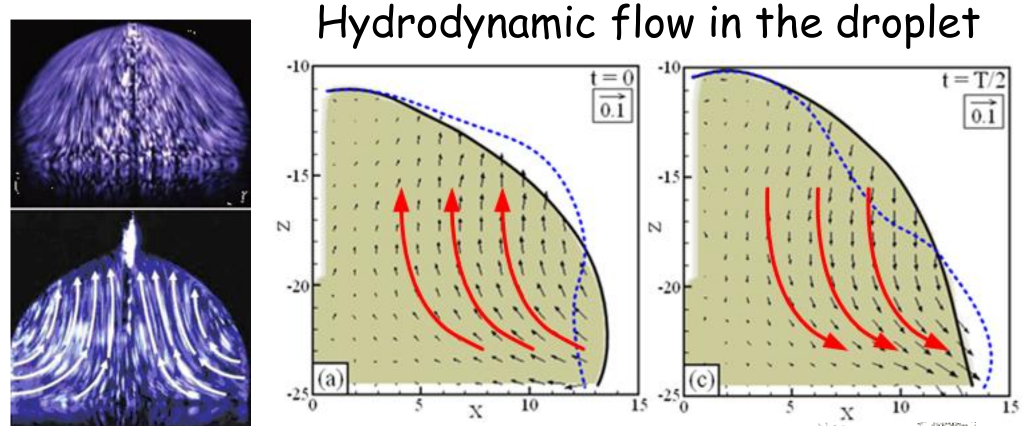

— Hong et al. J. Micromech. Microeng. 2012.

Low frequency mode

High frequency mode




Hydrodynamic flow in the droplet




— Ko, et al., Langmuir, 2008.

— Li, et al., J Adhes. Sci. Technol., 2012.

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# Energy is not conserved in traditional DPD

Equations of DPD:

$$\mathbf{F}_{ij}^{C} = a\omega_C(r_{ij})\mathbf{e}_{ij}$$

$$\mathbf{F}_{ij}^{D} = -\gamma\omega_D(r_{ij})(\mathbf{e}_{ij}\cdot\mathbf{v}_{ij})\mathbf{e}_{ij}$$

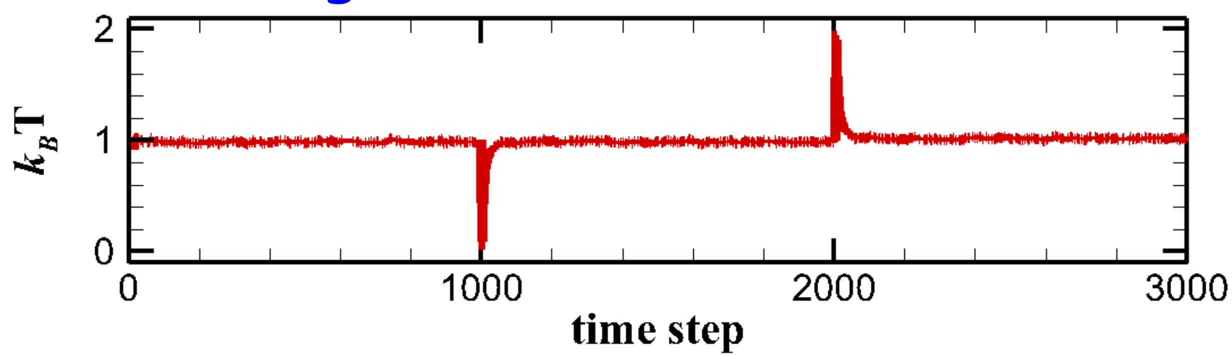
$$\mathbf{F}_{ij}^{R} = \sigma\omega_R(r_{ij})\zeta_{ij}dt^{-1/2}\mathbf{e}_{ij}$$

$$\omega_C(r) = 1 - r/r_c$$

$$[w_R]^2 = w_D = (1 - r/r_c)^2$$

$$\sigma^2 = 2\gamma k_B T$$

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.

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# Energy-conserving DPD Model for non-isothermal fluid systems

## Include the energy equation:

$$\mathbf{F}_{ij}^C = \alpha \omega^C(r_{ij})\mathbf{e}_{ij}$$

$$\mathbf{F}_{ij}^D = -\gamma \omega^D(r_{ij})(\mathbf{e}_{ij}\cdot\mathbf{v}_{ij})\mathbf{e}_{ij}$$

$$\mathbf{F}_{ij}^R = \sigma \omega^R(r_{ij})\zeta_{ij} dt^{-1/2}\mathbf{e}_{ij}$$

$$\omega^C(r) = 1 - r / r_c$$

$$[w_R]^2 = w_D = \left(1 - \frac{r}{r_c}\right)^S$$

$$\sigma_{ij}^{\ 2} = \frac{4\gamma_{ij} k_B T_i \cdot T_j}{T_i + T_j}$$

— Ripoll & Español, Int. J. Mod. Phys. C, 1998.

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

$$q_{ij}^{cond} = \sum_{j\neq i} k_{ij} w_{CT}(r_{ij})\left(\frac{1}{T_i} - \frac{1}{T_j}\right)$$

Heat conduction

$$q_{ij}^{visc} = \frac{1}{2C_v}\sum_{j\neq i}\left(w_D(r_{ij})\left[\gamma_{ij}\left(\mathbf{e}_{ij}\cdot\mathbf{v}_{ij}\right)^2 - \frac{\left(\sigma_{ij}\right)^2}{m}\right] - \sigma_{ij} w_R(r_{ij})\left(\mathbf{e}_{ij}\cdot\mathbf{v}_{ij}\right)\zeta_{ij}\right)$$

Viscous heating

$$q_{ij}^{R} = \sum_{j\neq i} \alpha_{ij} w_{RT}(r_{ij}) dt^{-1/2}\zeta_{ij}^{e}$$

Fluctuating term

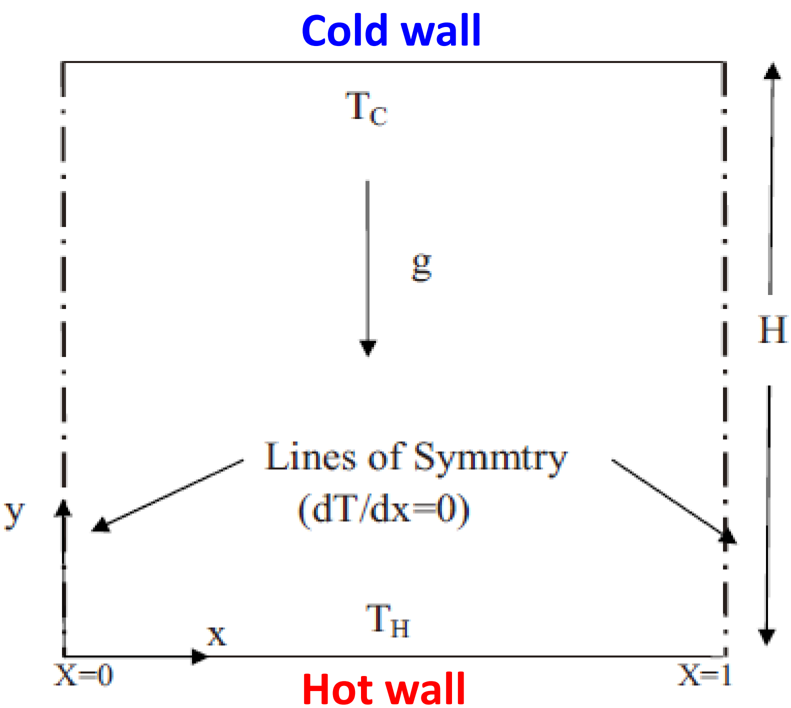
$$w_{CT}(r_{ij}) = \left[w_{RT}(r_{ij})\right]^2 = \left(1 - \frac{r_{ij}}{r_{cut}}\right)^{S_T}$$

$$\alpha_{ij} = \sqrt{2k_B k_{ij}}, \qquad k_{ij} = C_v^2 \kappa (T_i + T_j)^2 / 4k_B$$

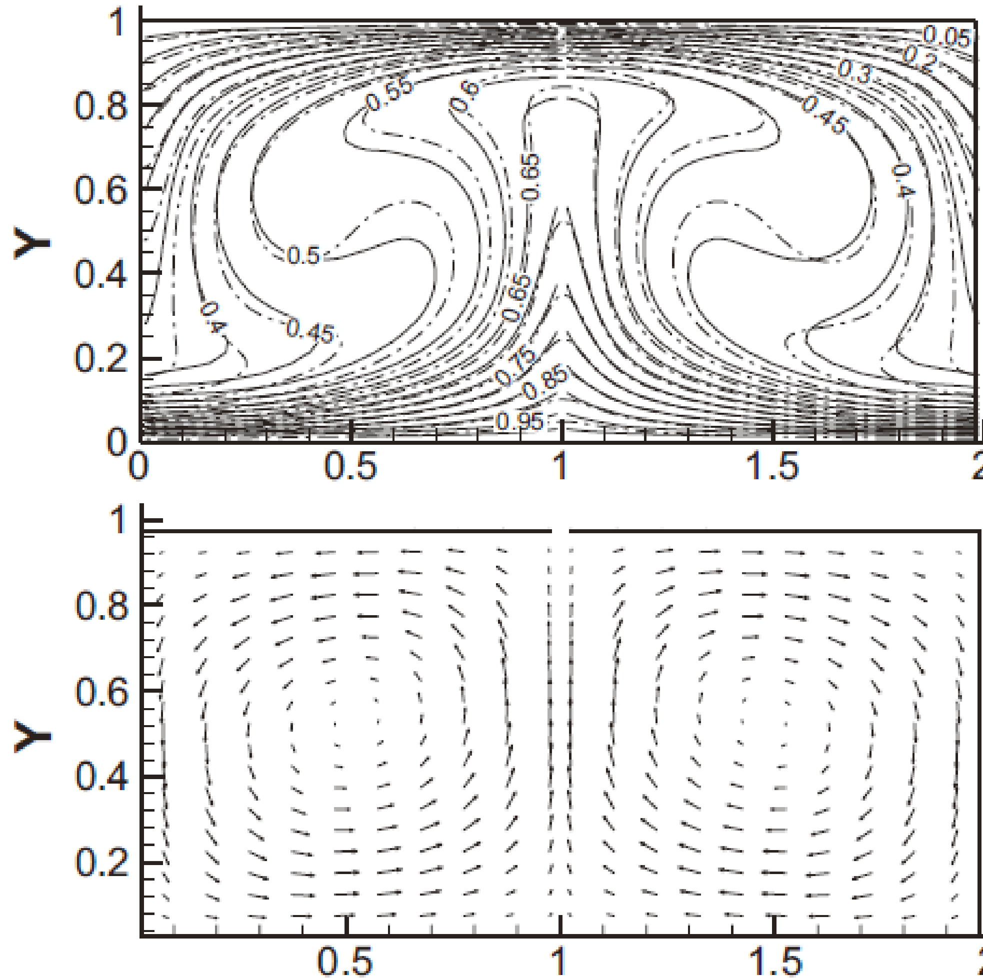
# Examples of Energy-conserving DPD

Natural convection heat transfer simulation:

— Abu-Nada, E., Phys. Rev. E, 2010.



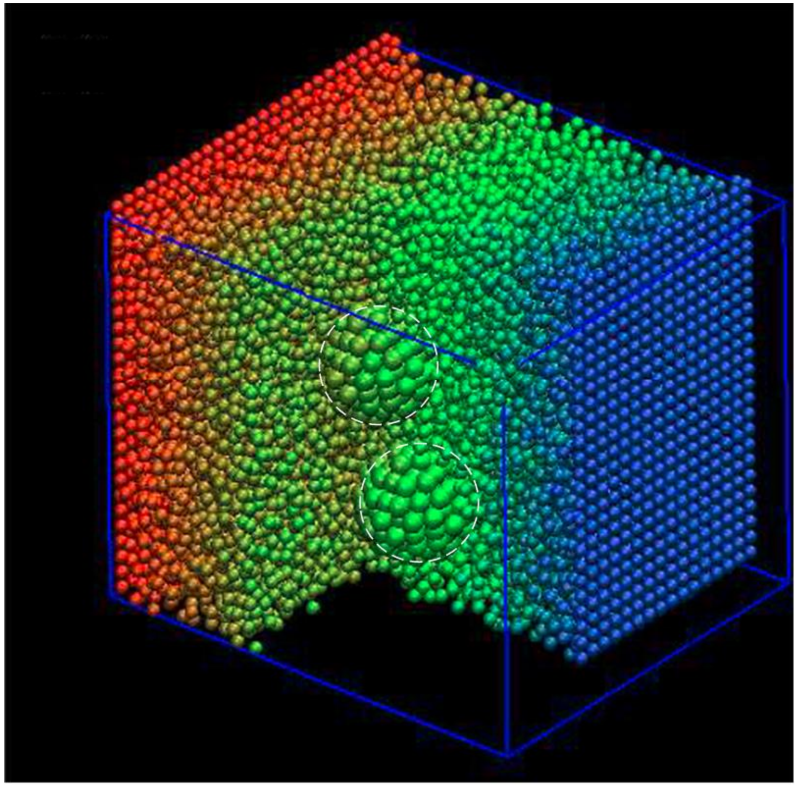

Temperature isotherms and velocity field (sold lines: eDPD, dashed dotted lines: finite volume solutions):



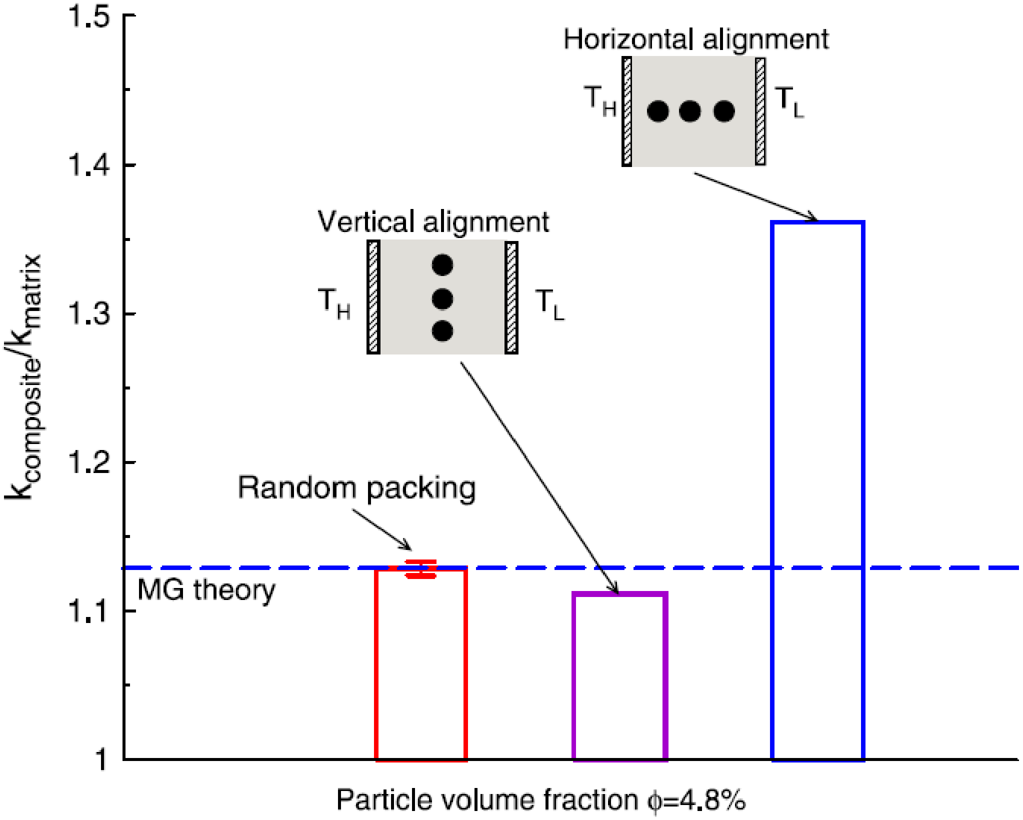
# Examples of Energy-conserving DPD

## Heat conduction in nanocomposite:

— Qiao and He, Molecular Simulation, 2007.



Thermal conductivity enhancement by nanoparticles:

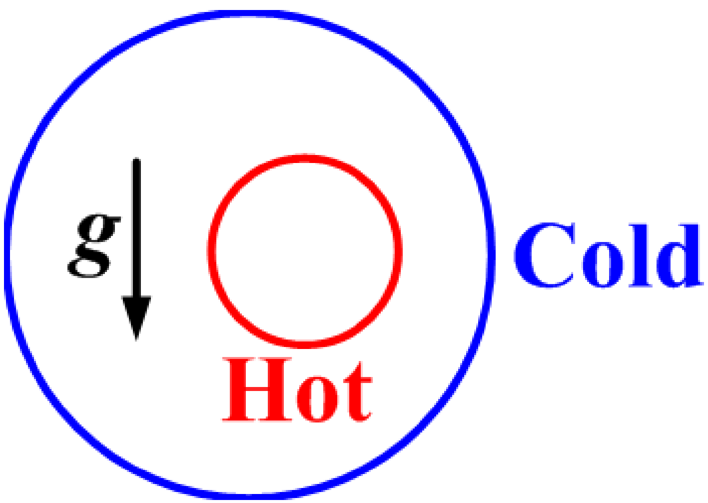


# Examples of Energy-conserving DPD

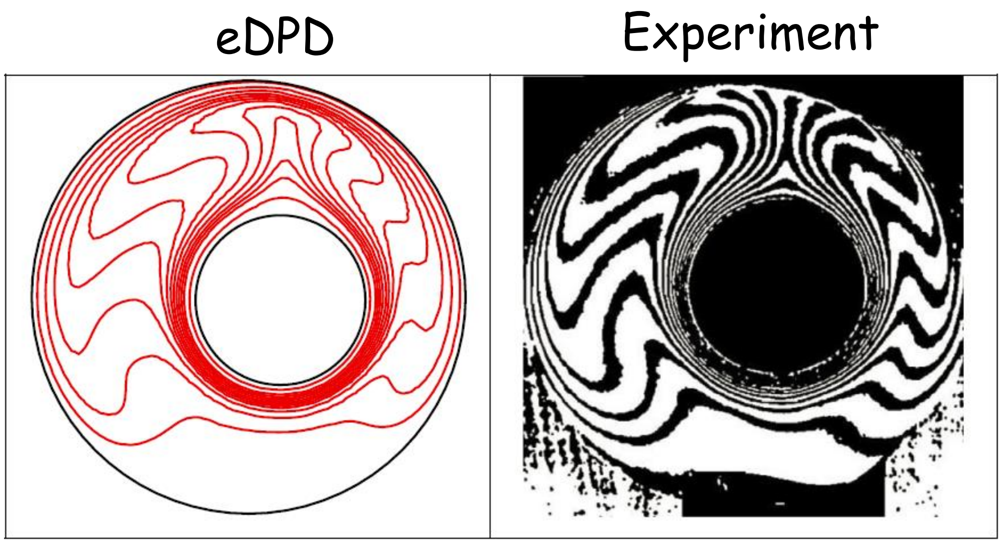
## Natural convection in eccentric annulus:

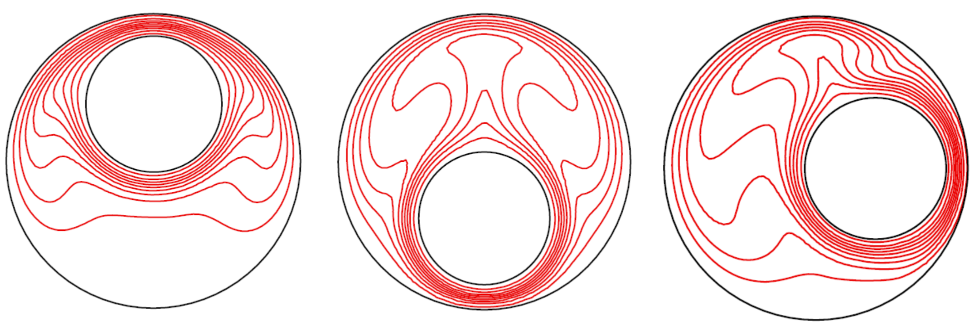
— Cao, et al., Int. J. Heat Mass Transfer, 2013.

Physical model:




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



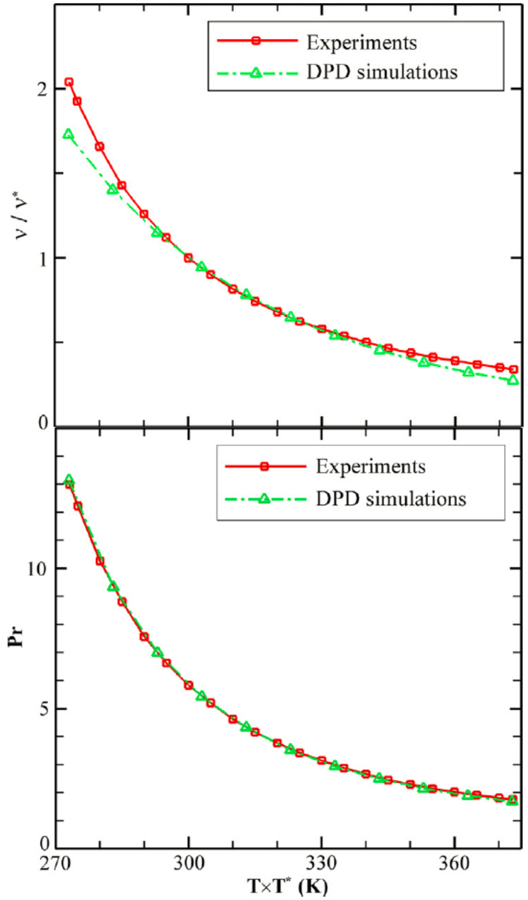



# Examples of Energy-conserving DPD

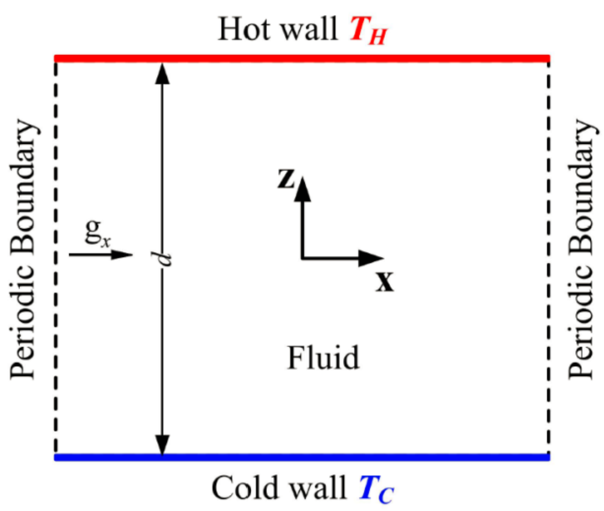
## Flow between Cold-Hot walls:

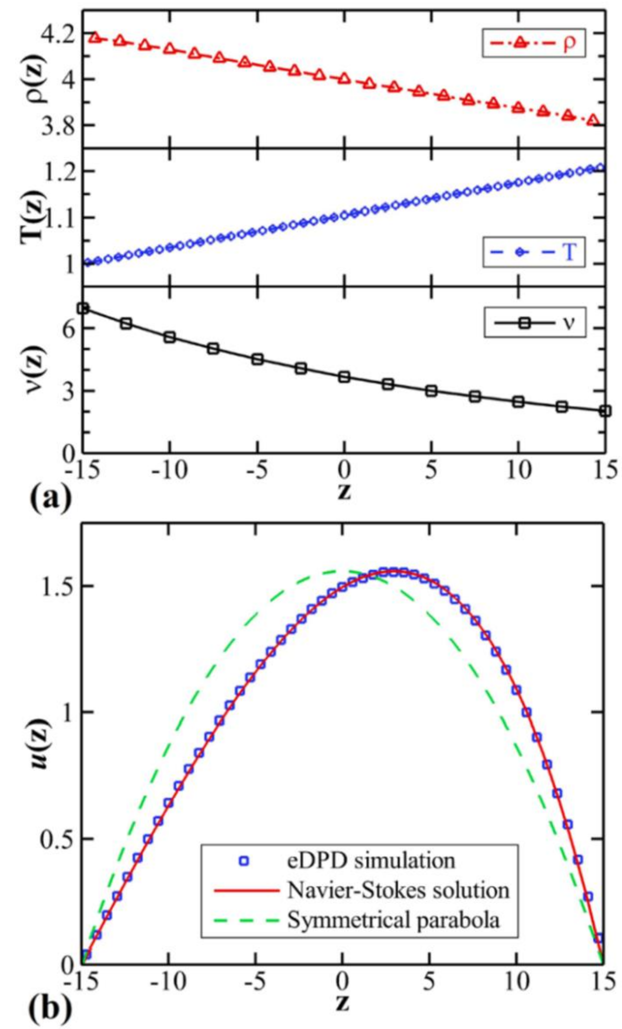
— Li, Tang, Lei, Caswell & Karniadakis, J. Comput. Phys., 2014.

Temperature-dependent properties:




Coupling of flow and heat conduction:



# Examples of Energy-conserving DPD

## An easy way to compute the thermal conductivity:

— Li, Tang, Lei, Caswell & Karniadakis, J. Comput. Phys., 2014.

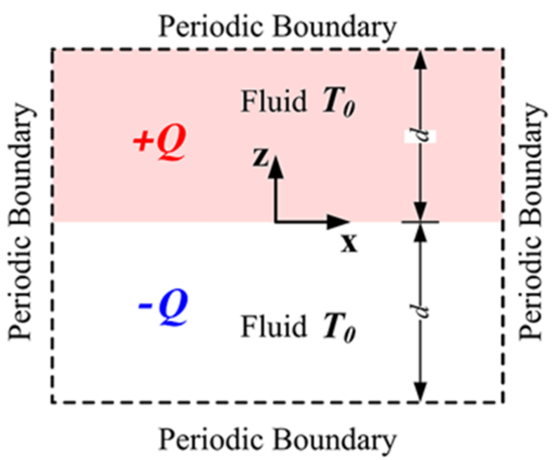
The heat conduction of a fluid is governed by

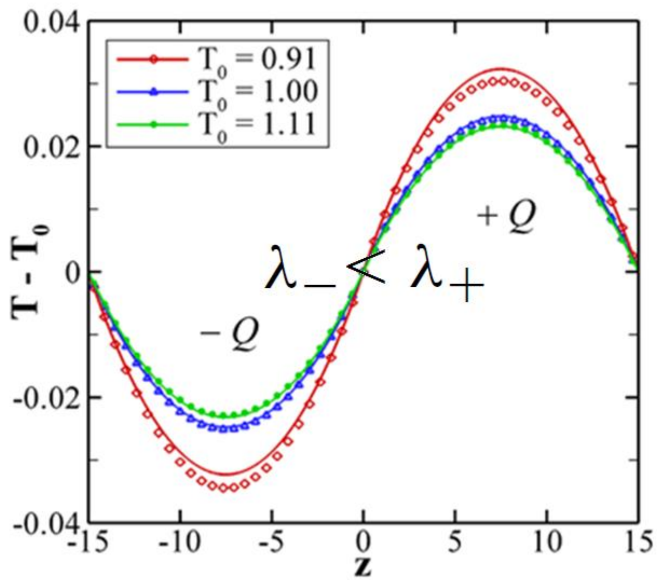
$$\rho C_v \frac{\partial T}{\partial t} = \eta \nabla^2 T + \rho q \quad \text{For steady state} \quad \boxed{\lambda \nabla^2 T = -Q} \longleftrightarrow \boxed{\upsilon \nabla^2 \mathbf{V} = -g}$$

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

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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# Outline

## 1. Single Particle DPD

Particle size: mono-size → multi-size

## 2. Many-body DPD

Quadratic EOS → Higher-order EOS

## 3. Energy conserving DPD

Isothermal system → Non-isothermal system

## 4. Smoothed DPD

Bottom-up approach → Top-down approach

## 5. Other DPD models

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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.

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

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# DPD and Smoothed DPD

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

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# 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 $\boldsymbol{\eta}$, $\boldsymbol{\zeta}$ and the thermal conductivity $\boldsymbol{\kappa}$. They are input parameters.

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

$$d\mathbf{r}_i = \mathbf{v}_i dt$$

$$m\,d\mathbf{v}_i = \underbrace{\sum_j \left[\frac{P_i}{d_i^2} + \frac{P_j}{d_j^2}\right]F_{ij}\mathbf{r}_{ij}dt}_{F^C} \underbrace{- \sum_j (1-d_{ij})a_{ij}\mathbf{v}_{ij}dt - \sum_j (1-d_{ij})\left(\frac{a_{ij}}{3} + b_{ij}\right)\mathbf{e}_{ij}\mathbf{e}_{ij}\cdot\mathbf{v}_{ij}dt}_{F^D} \underbrace{+ m\,d\tilde{\mathbf{v}}_i}_{F^R}$$

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

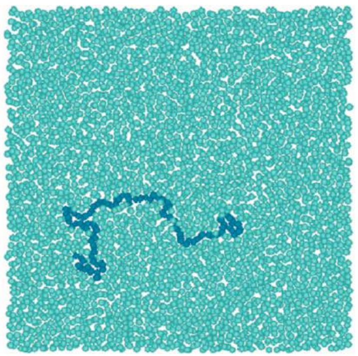
$$-2\kappa\sum_j \frac{F_{ij}}{d_i d_j}T_{ij}dt - 2\kappa\frac{k_B}{C_i}\sum_j{}' \frac{F_{ij}}{d_i d_j}T_j dt + T_i d\tilde{S}_i\,.$$

— Español and Revenga, Phys. Rev. E, 2003.

# Examples of Smoothed DPD

## Polymer chain in suspension:

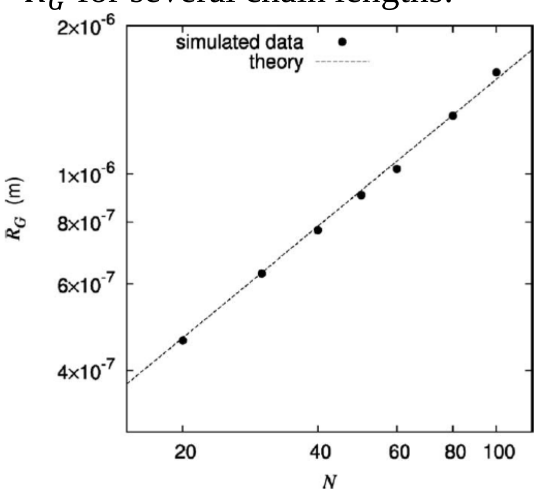
— Litvinov, Ellero, Hu & Adams, Phys. Rev. E, 2008.



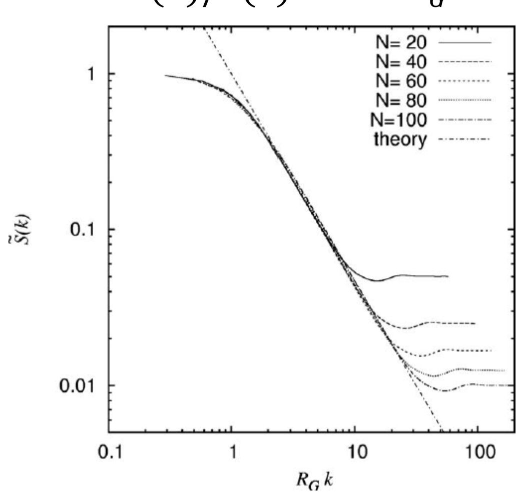
**Solvent:**
Newtonian fluid

**Polymer chain:**
Finitely Extendable Nonlinear Elastic (FENE) springs

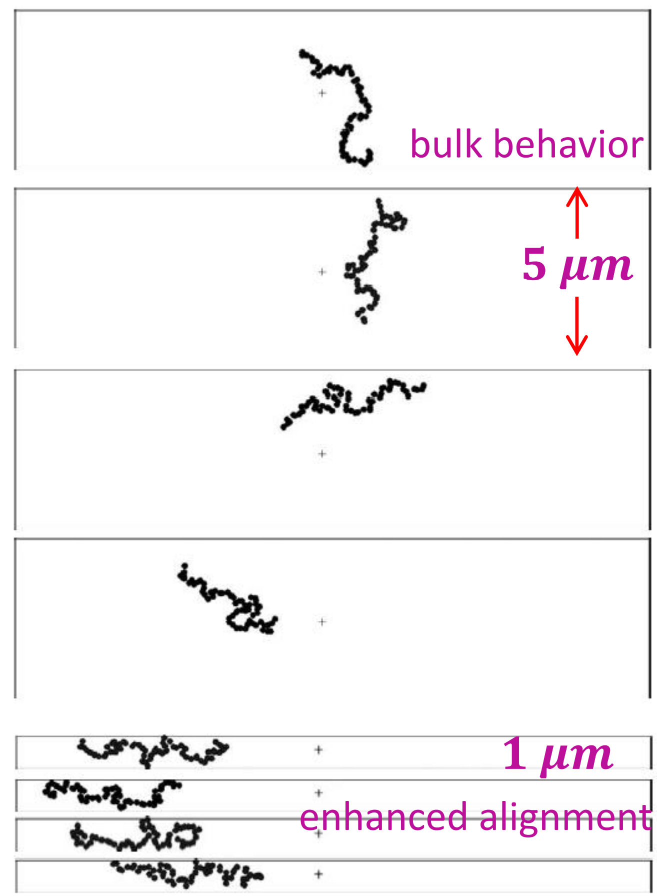
Scaling of the radius of gyration $R_G$ for several chain lengths:




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




Polymer conformations under confinement:



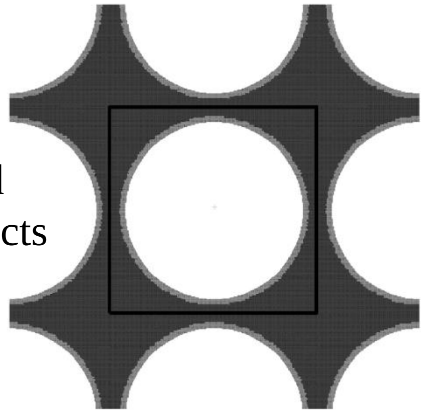
# Examples of Smoothed DPD

## Flow through porous media:

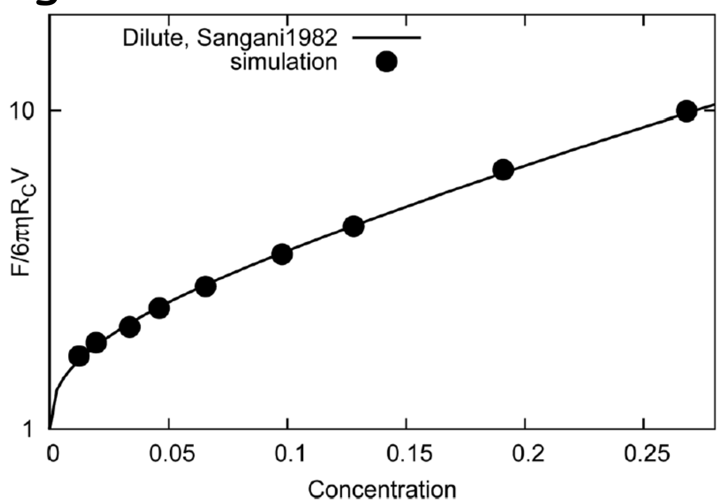
— Bian, Litvinov, Qian, Ellero & Adams, Phys. Fluids, 2012.

Model:

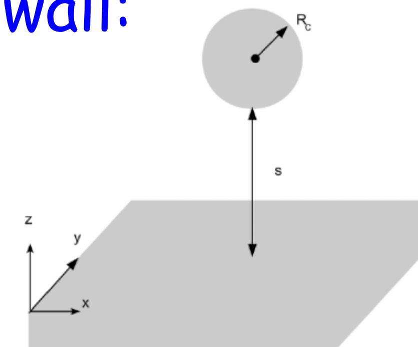
Periodic array of fixed circular/spherical objects



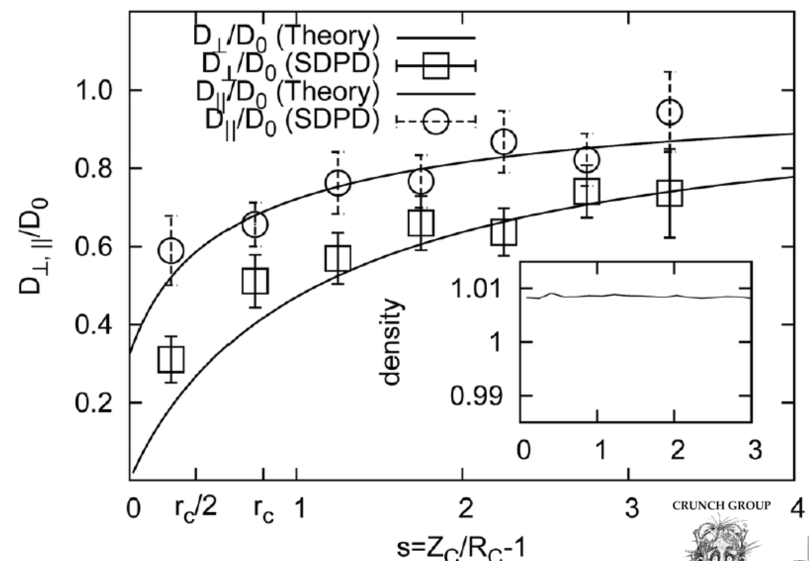
Three-dimensional dimensionless drag coefficient:




## A colloidal particle near a rigid wall:




Diffusion coefficients perpendicular and parallel to the wall:

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# Outline

1. **Single Particle DPD**

   Particle size: mono-size ⟶ multi-size

2. **Many-body DPD**

   Quadratic EOS ⟶ Higher-order EOS

3. **Energy conserving DPD**

   Isothermal system ⟶ Non-isothermal system

4. **Smoothed DPD**

   Bottom-up approach ⟶ Top-down approach

5. **Other DPD models**

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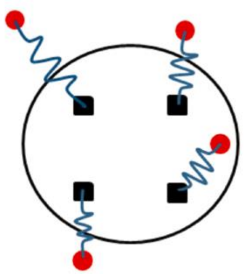
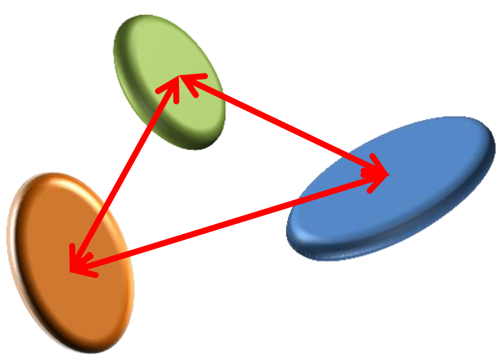
# Other DPD models

1. Low-mass DPD model for an approximation of incompressible fluids.
    - Phan-Thien, N., Mai-Duy, N., Pan, D. and Khoo, B. C., Exponential-time differencing schemes for low-mass DPD systems. Computer Physics Communications, 2014. **185**(1): 229-235.

2. Spring model for colloids in suspension.
    - Phan-Thien, N., Mai-Duy, N. and Khoo, B.C., A spring model for suspended particles in dissipative particle dynamics. Journal of Rheology, 2014. **58**(4): 839-867.



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



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- Bian, X., S. Litvinov, R. Qian, M. Ellero and N.A. Adams, *Multiscale modeling of particle in suspension with smoothed dissipative particle dynamics.* Physics of Fluids, 2012. **24:** 012002.
- Li, Z., Y.H. Tang, H. Lei, B. Caswell, and G.E. Karniadakis, *Energy-conserving dissipative particle dynamics with temperature-dependent properties.* Journal of Computational Physics, 2014. **265**: 113-127.


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