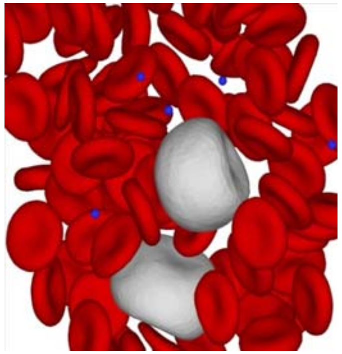
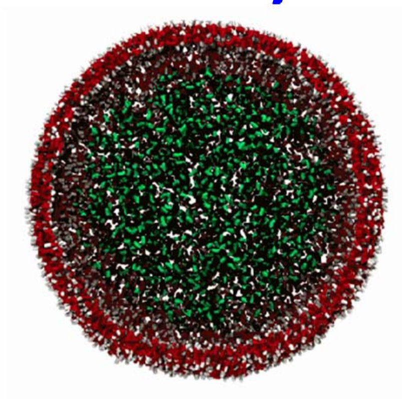
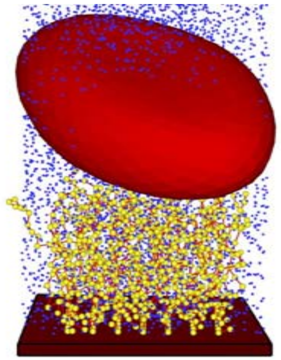
APMA 2811T
Dissipative Particle Dynamics

Instructor: **Professor George Karniadakis**
Location: **170 Hope Street, Room 118**
Time: **Thursday 12:00pm - 2:00pm**

Today's topic:

Dissipative Particle Dynamics:
Foundation, Evolution and Applications

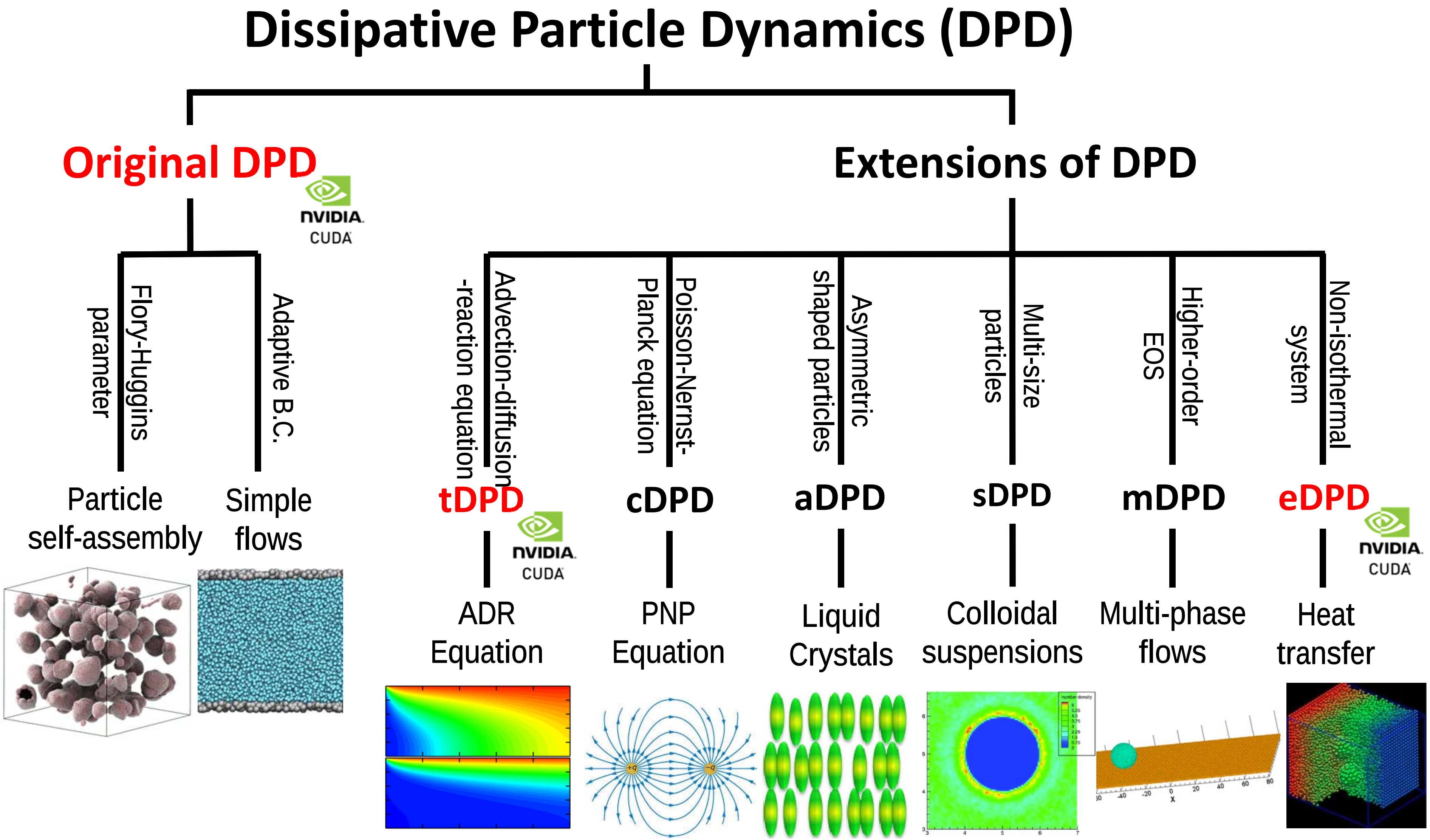
Lecture 3: New Methods beyond traditional DPD

By **Zhen Li**
Division of Applied Mathematics, Brown University

Sep. 22, 2016

State-of-the-art



Extensions of DPD: complete the DPD framework

Flow field (DPD) + **Temperature field** (eDPD) + **Concentration field** (tDPD) + **Electric field** (cDPD)

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**

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

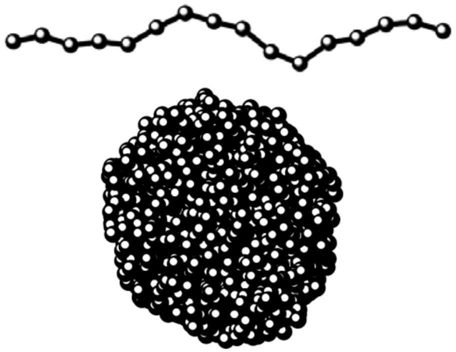
5. Other DPD models

CRUNCH GROUP

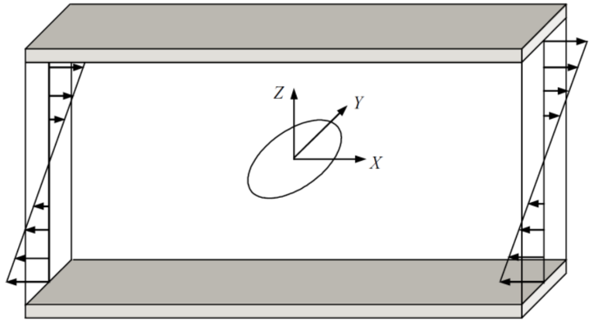
Successful DPD applications using mono-size particles

Application 1: Polymer drops in a shear flow

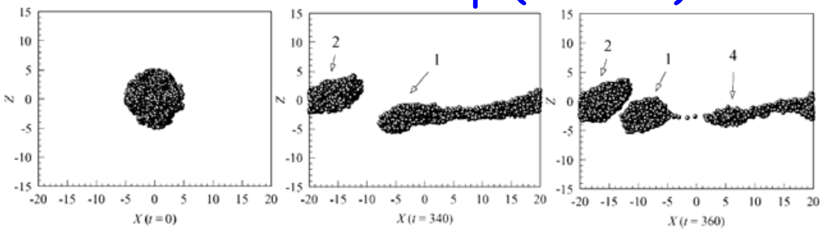
— Chen, Phan-Thien, Fan & Khoo, J. Non-Newtonian Fluid Mech., 2004.



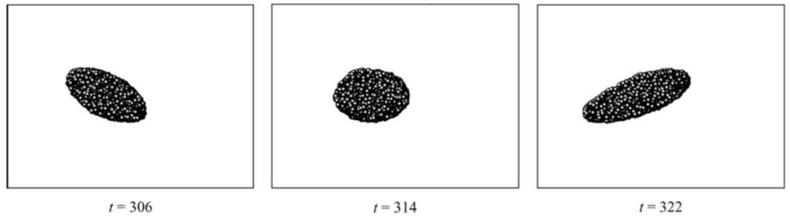
N = 2096



Break-up (low Sc)

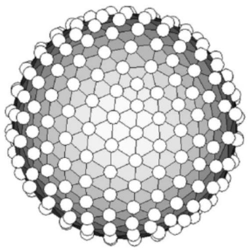


Tumbling (high Sc)

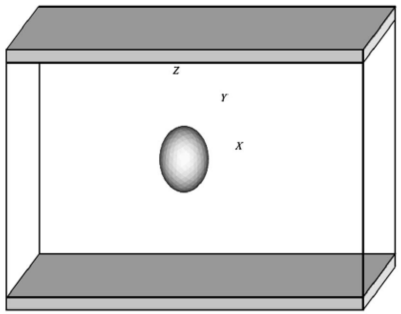


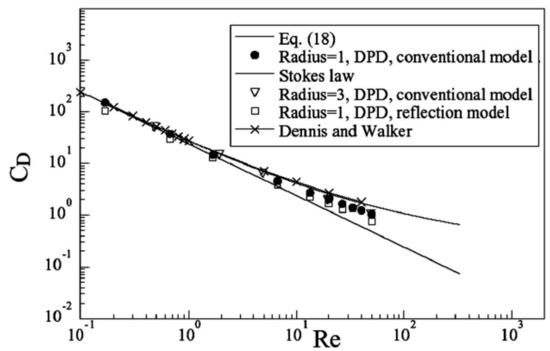
Application 2: Flow around spheres

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



N = 452



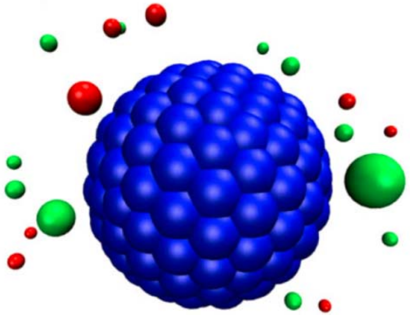


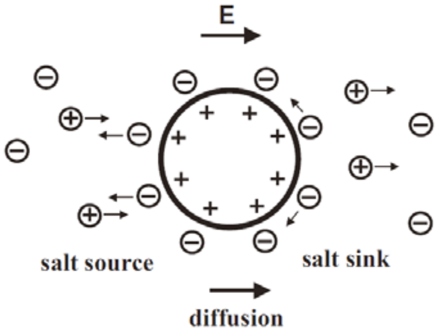
CRUNCH GROUP

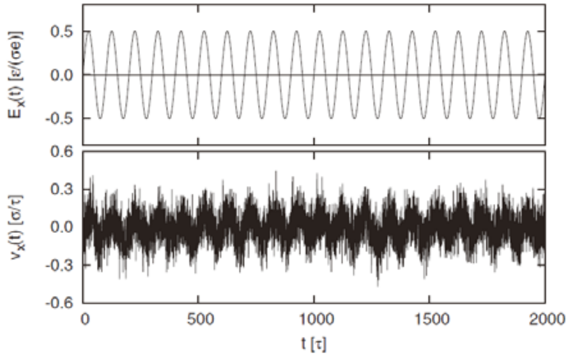
Successful DPD applications using mono-size particles

Application 3: Dynamic of colloids in electric fields

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

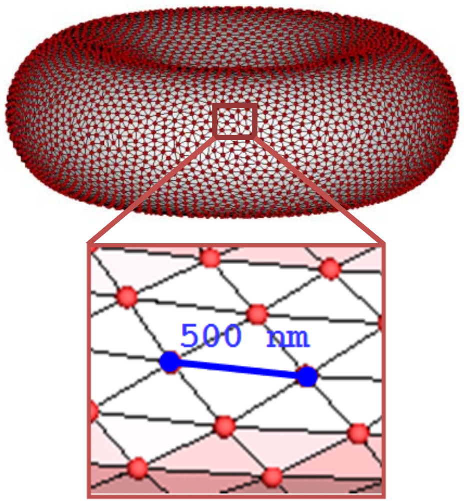


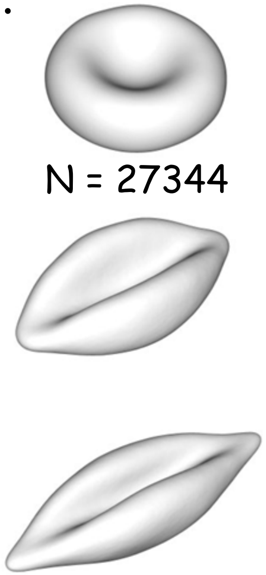


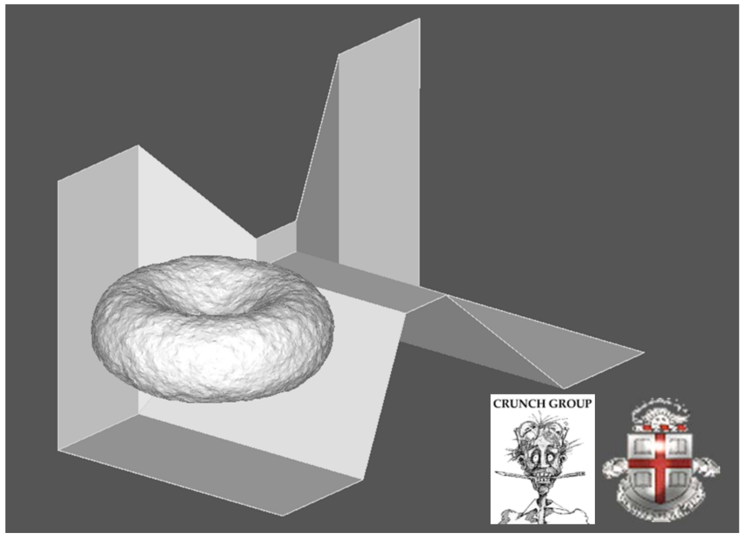


Application 4: Accurate Modeling of Red Blood Cells

— Pivkin & Karniadakis, PRL, 2008.

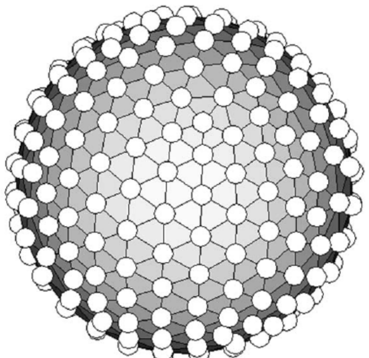






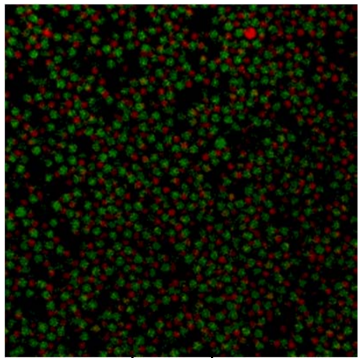
Disadvantage of using mono-size particles

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



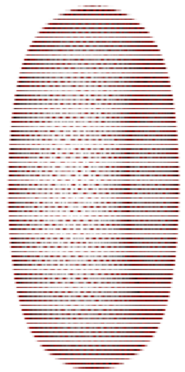
Chen, S., et al., Phys. Fluids, 2006.

N = 452

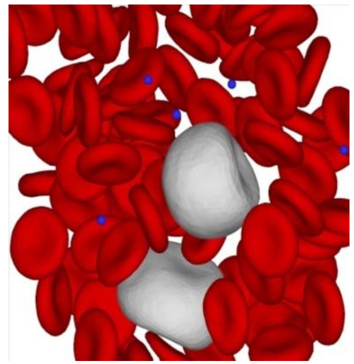


www.teunvissers.nl

Many colloids



N = 27344



Many RBCs

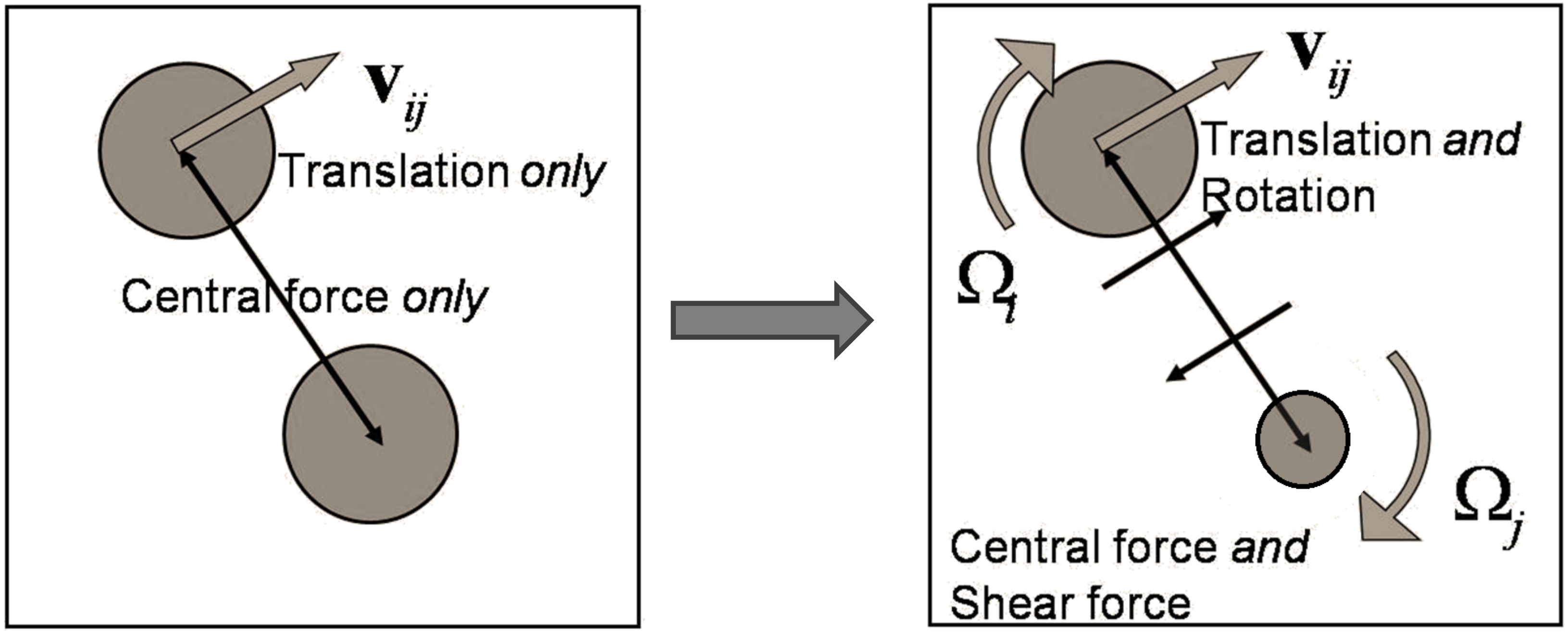
Solution: Multi-size particles.

— **Single Particle DPD model**

CRUNCH GROUP

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.

CRUNCH GROUP

Single Particle DPD model

Equations of Motion:

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

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

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

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

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

$$\mathbf{F}_{ij} = \mathbf{F}_{ij}^C + \mathbf{F}_{ij}^T + \mathbf{F}_{ij}^R + \widetilde{\mathbf{F}}_{ij}$$

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

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

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

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

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

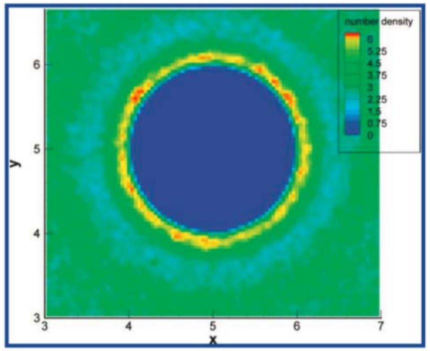
CRUNCH GROUP

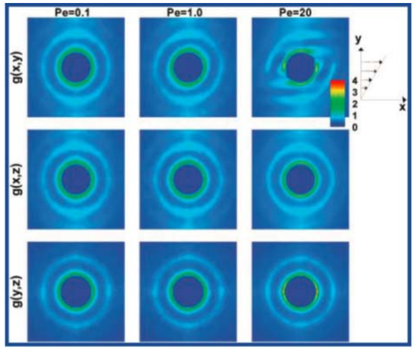
— Pan, Pivkin & Karniadakis, Europhys. Lett., 2008.

Examples of Single Particle DPD

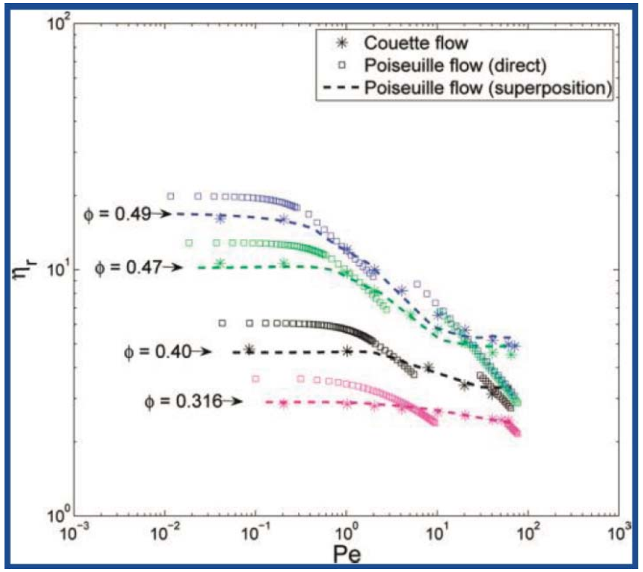
Rheology in Colloidal Suspensions:

— Pan, Caswell & Karniadakis, Langmuir, 2010.





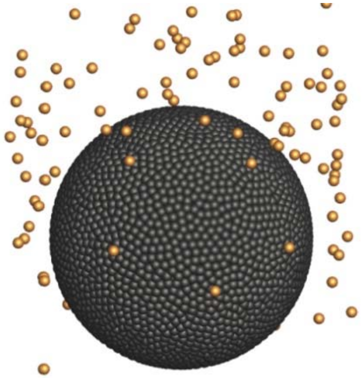
Relative viscosity vs *Pe* number:



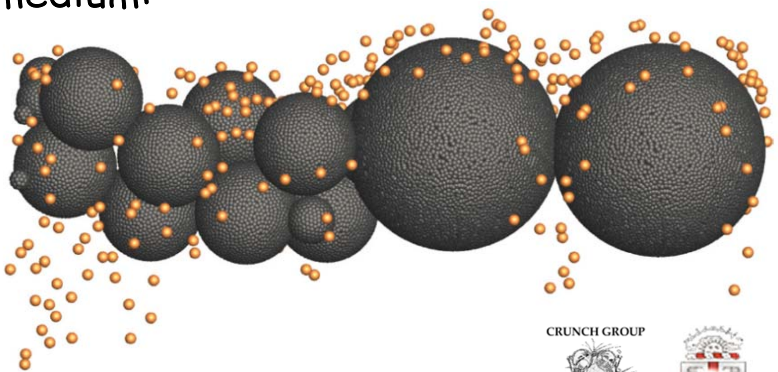
Colloid transport in porous media:

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

Colloid transport surrounding a single collector:



Colloid transport in a polysized porous medium:

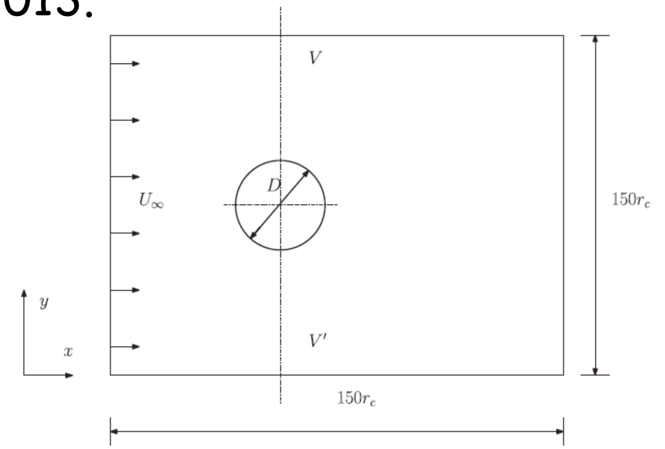


CRUNCH GROUP

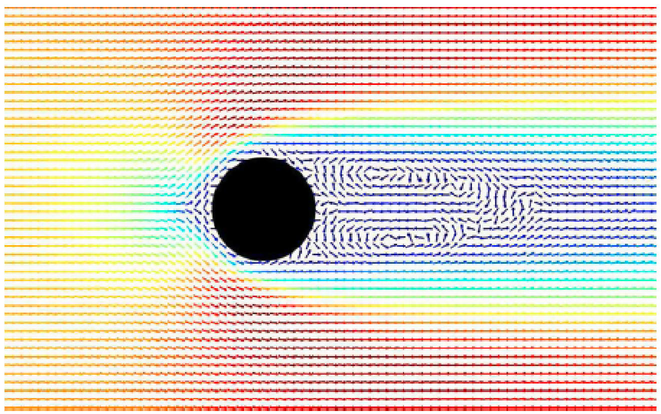
Examples of Single Particle DPD

Flow around a circular cylinder:

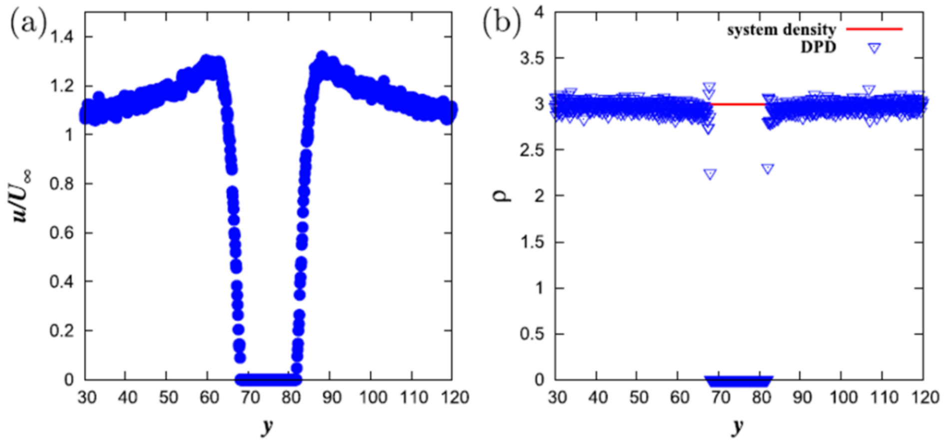
— Ranjith, et al., J. Comput. Phys., 2013.



Velocity vector:



Velocity and density profiles across the cylinder:

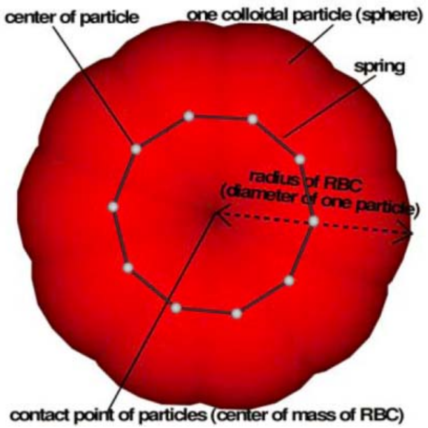


Comparison of drag coefficients:

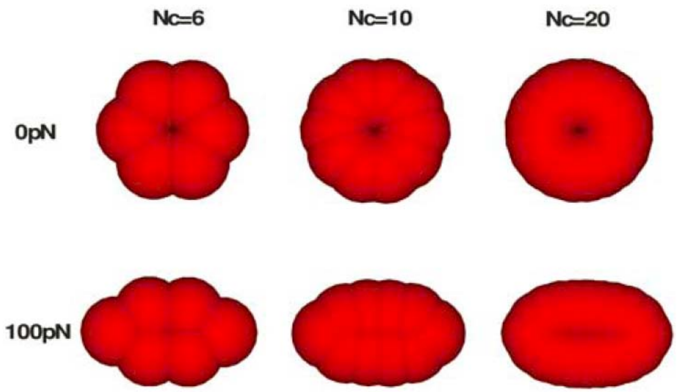
Re	Experiment	DPD
10	2.93	2.99
20	2.08	2.14
30	1.76	1.74
40	1.58	1.66

Examples of Single Particle DPD

Low-dimensional model for the red blood cell:

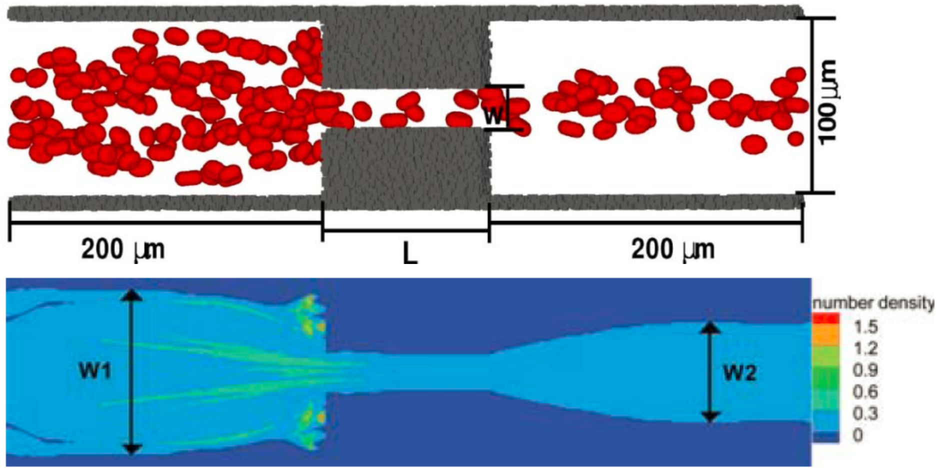


RBC shapes at various stretching forces:



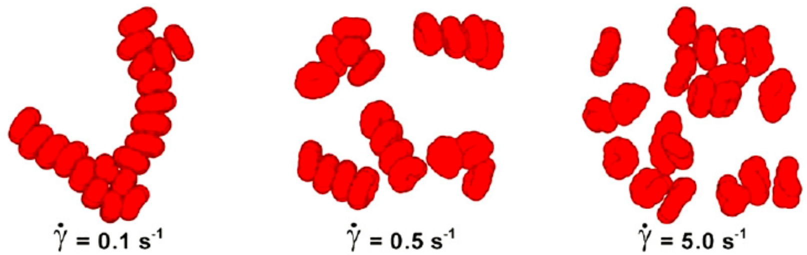
RBCs in a channel with a geometrical constriction:

— 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

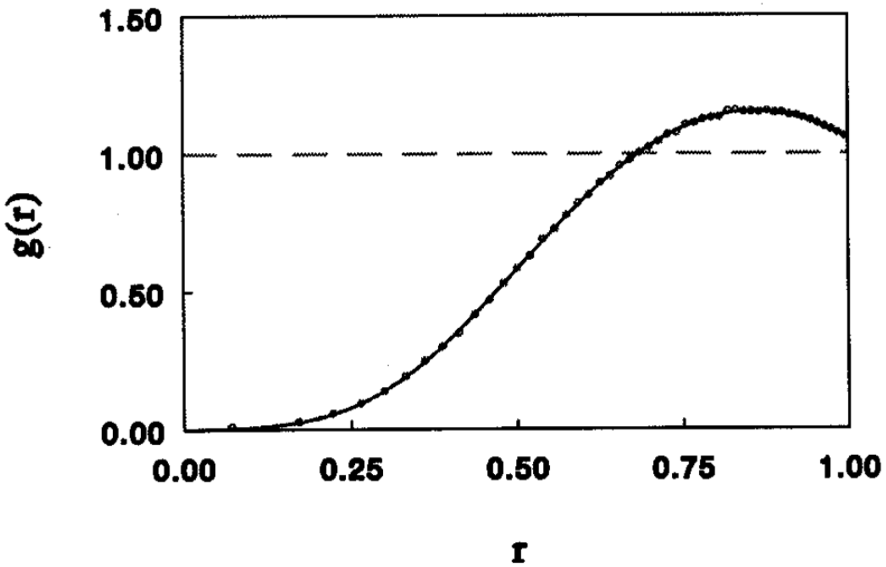
CRUNCH GROUP

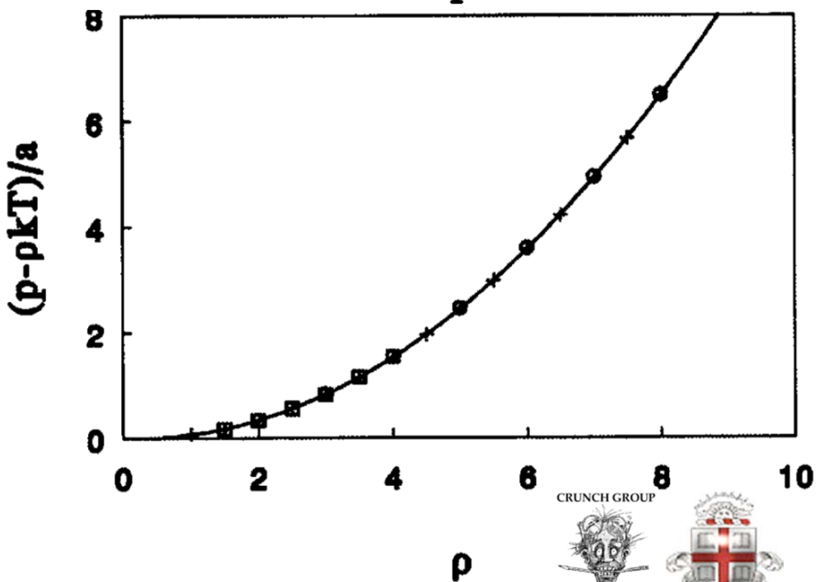
Equation of State (EOS) of traditional DPD

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

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

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



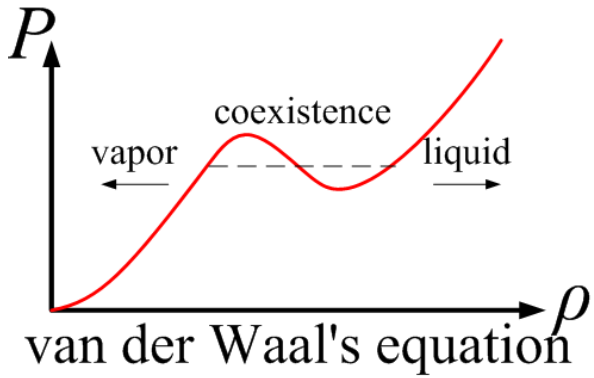


CRUNCH GROUP

— 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.



EOS needs high order terms of ρ to model liquid-vapor coexistence.

EOS with high order terms:

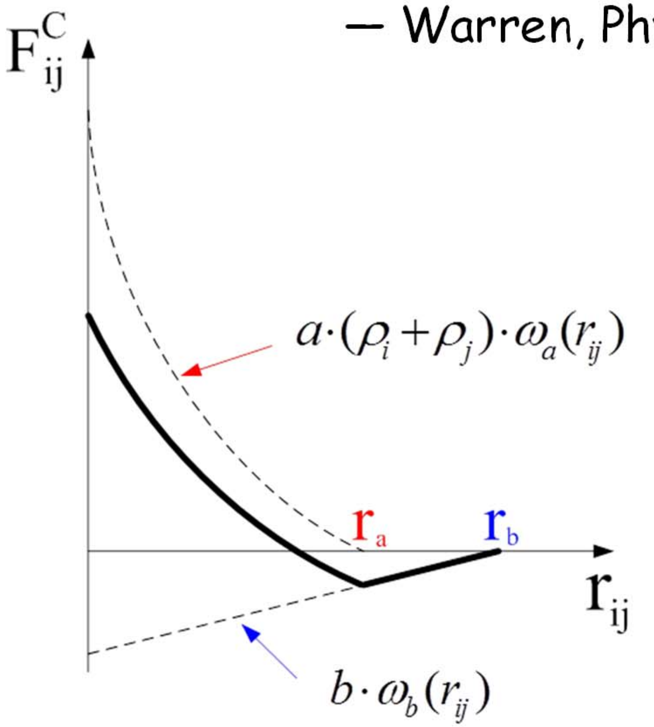
	Traditional DPD	Many-body DPD
Force	$\mathbf{F}_{ij}^{C} = a \cdot \omega_C(r_{ij})\mathbf{e}_{ij}$	$\mathbf{F}_{ij}^{C} = \frac{1}{2}\left(a(\rho_i) + a(\rho_j)\right) \cdot \omega_C(r_{ij})\mathbf{e}_{ij}$
EOS	$P = \rho k_B T + \lambda a \rho^2$	$P = \rho k_B T + \lambda a(\rho)\rho^2$

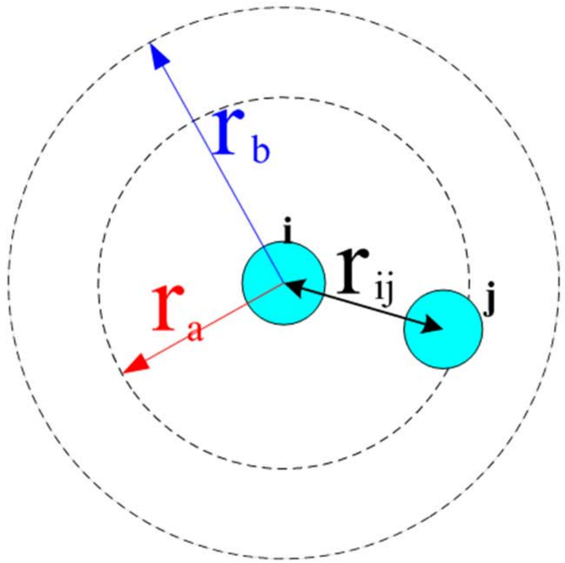
— Warren, Phys. Rev. E, 2003.

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.



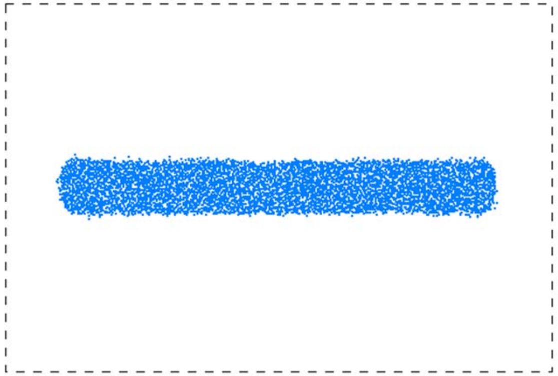


Other approach: $F^{C} = \nabla\left(k_B T \ln\left(1 - b \cdot \rho\right) + a \cdot \rho\right) + \kappa \nabla \nabla^2 \rho$

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

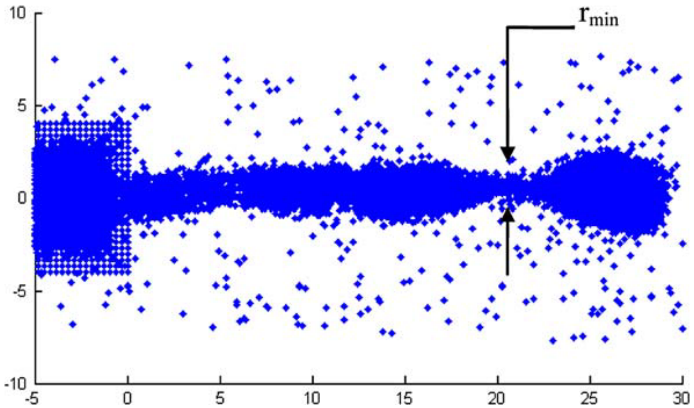
Examples of Many-body DPD

Free oscillation of a droplet:

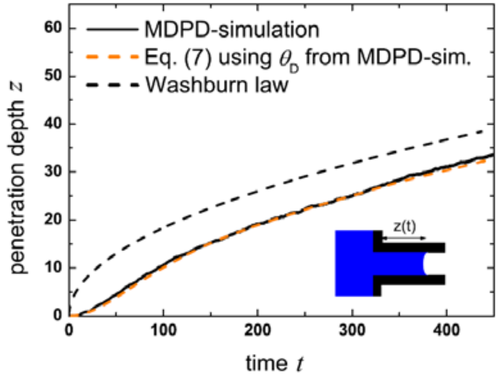


Nano-Jet:

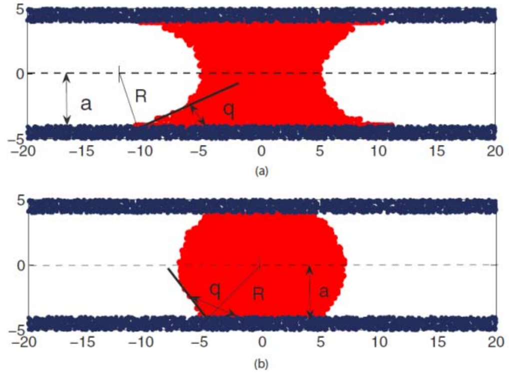
— Tiwari, et al. Microfluid Nanofluid, 2008.



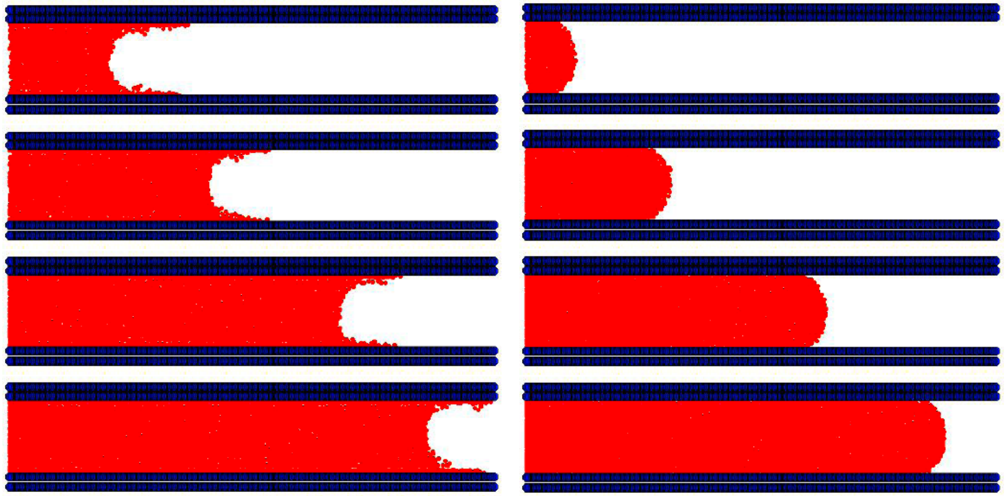
Droplets wetting microchannels:



— Cupelli, et al. New J. Phys., 2008.



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



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

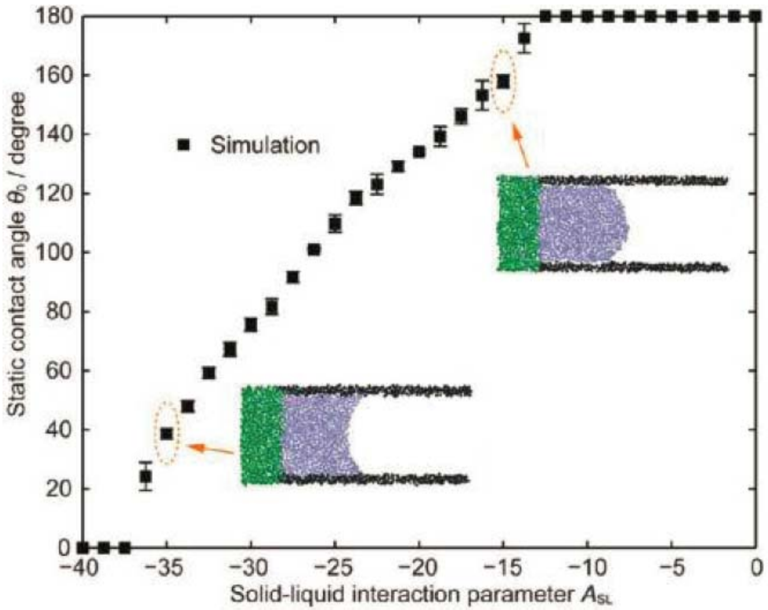
CRUNCH GROUP

Examples of Many-body DPD

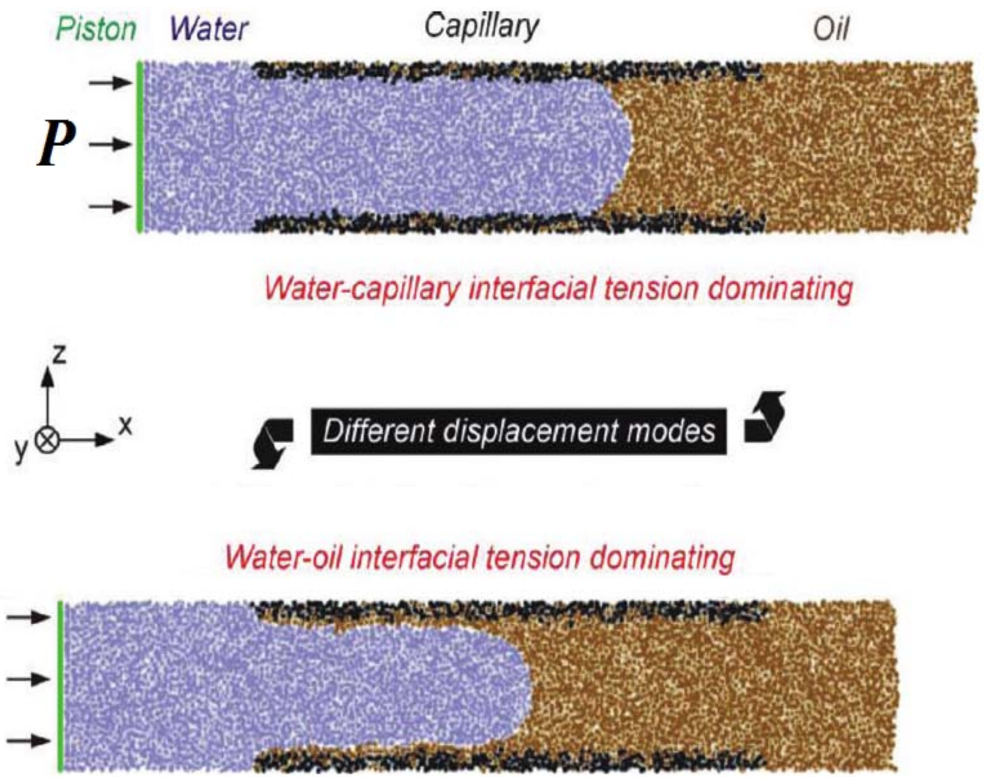
Forced Water-Oil movement in capillary:

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

Calibration of the solid-liquid interaction parameter A_{SL} related to the static contact angle θ_0 :



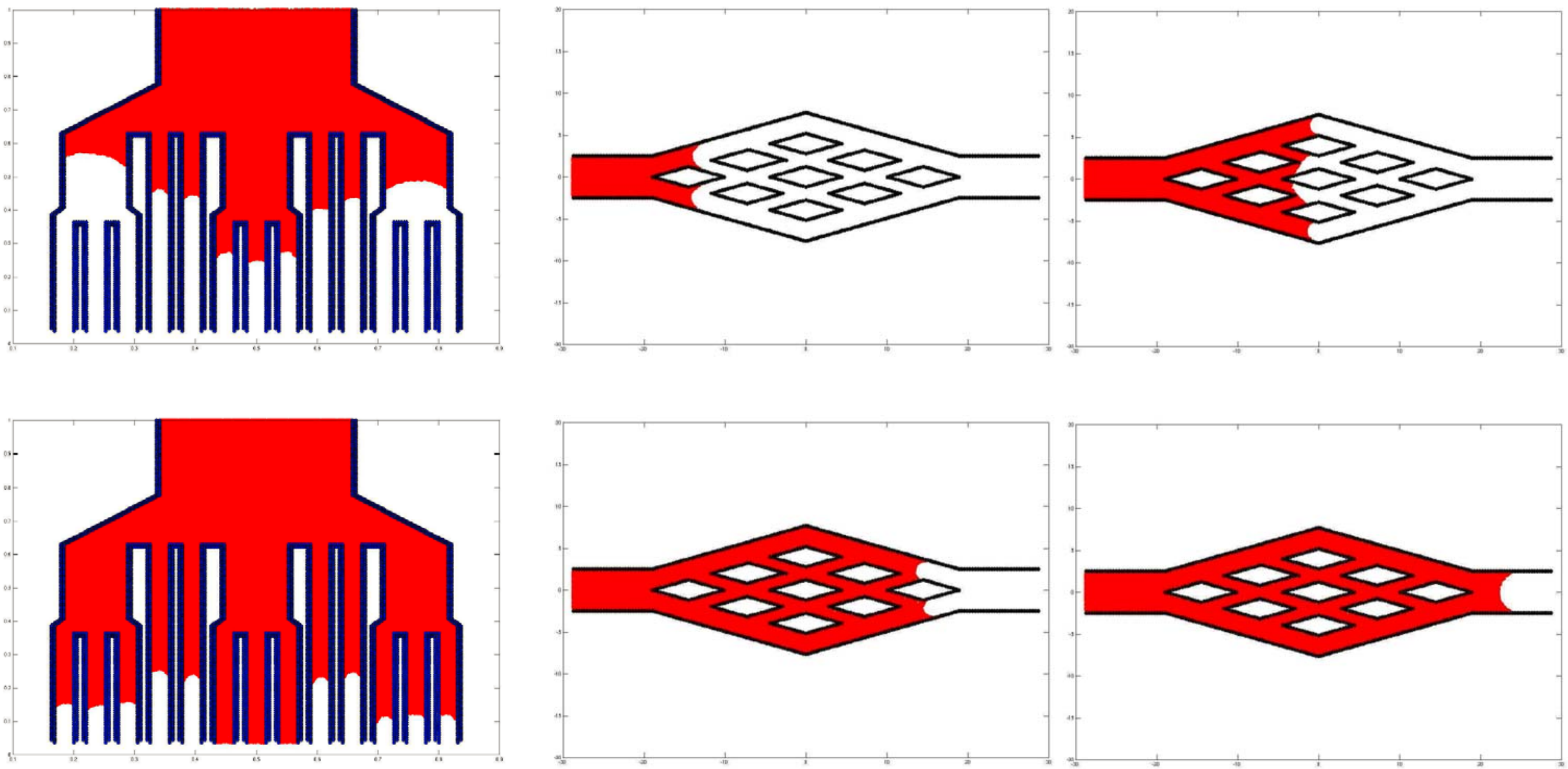
Two different modes of the water-oil displacement:



Examples of Many-body DPD

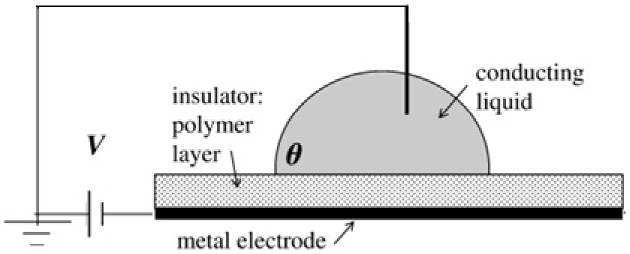
Flow with wetting in microchannel network:

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

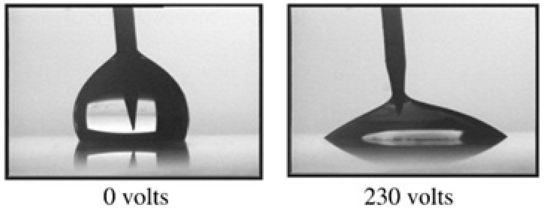


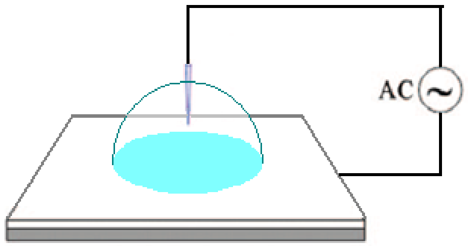
Examples of Many-body DPD

Electrowetting of a droplet:

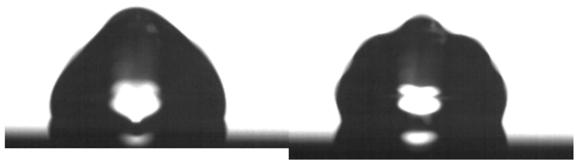


DC





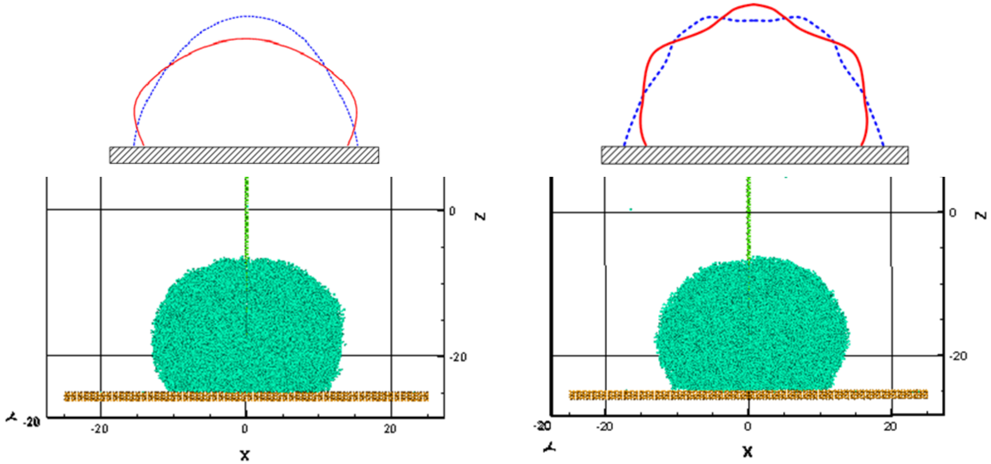
AC



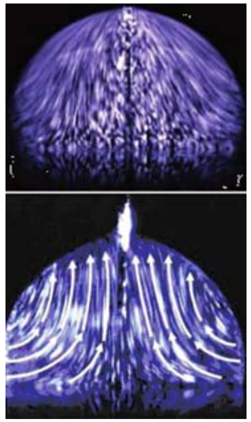
— Hong et al. J. Micromech. Microeng. 2012.

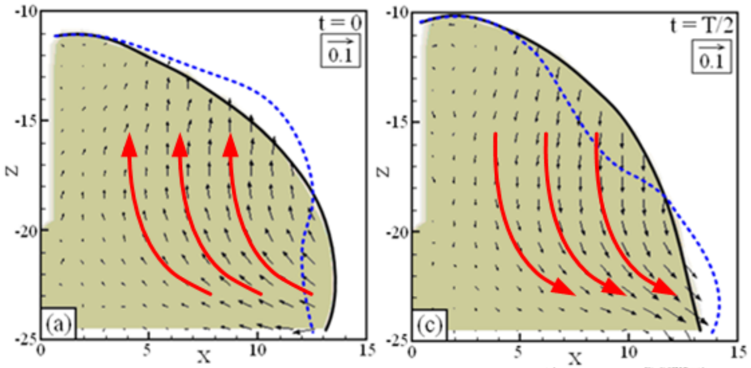
Low frequency mode

High frequency mode



Hydrodynamic flow in the droplet





— Ko, et al., Langmuir, 2008.

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

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

CRUNCH GROUP

Energy is not conserved in traditional DPD

Equations of DPD:

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

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

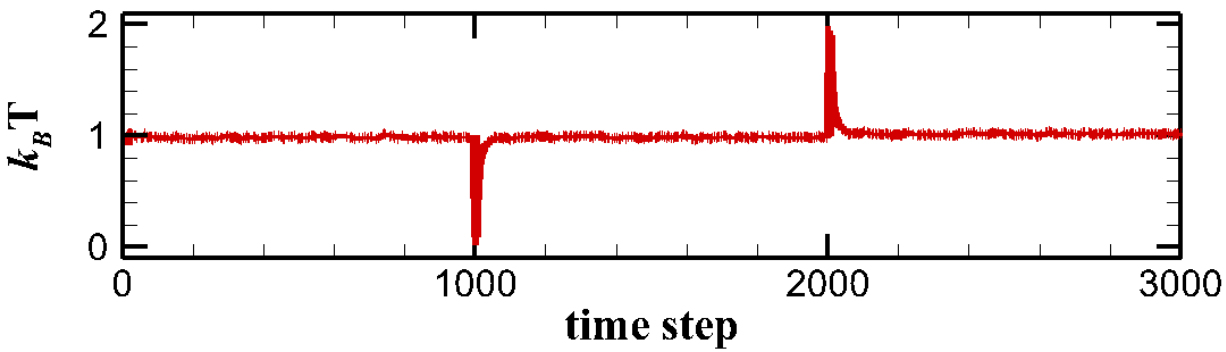
$$\mathbf{F}_{ij}^{R} = \sigma\omega_R(r_{ij})\zeta_{ij}dt^{-1/2}\mathbf{e}_{ij}$$

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

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

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

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.

CRUNCH GROUP

Energy-conserving DPD Model for non-isothermal fluid systems

Include the energy equation:

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

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

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

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

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

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

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

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

Heat conduction

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

Viscous heating

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

Fluctuating term

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

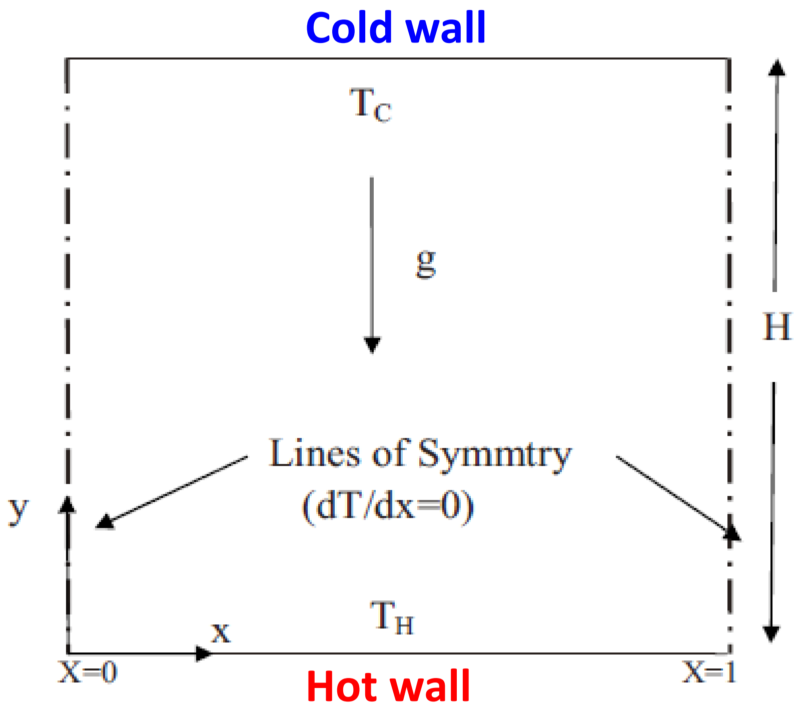
$$\alpha_{ij} = \sqrt{2k_B k_{ij}}, \qquad k_{ij} = C_v^2 \kappa (T_i + T_j)^2 / 4k_B$$

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

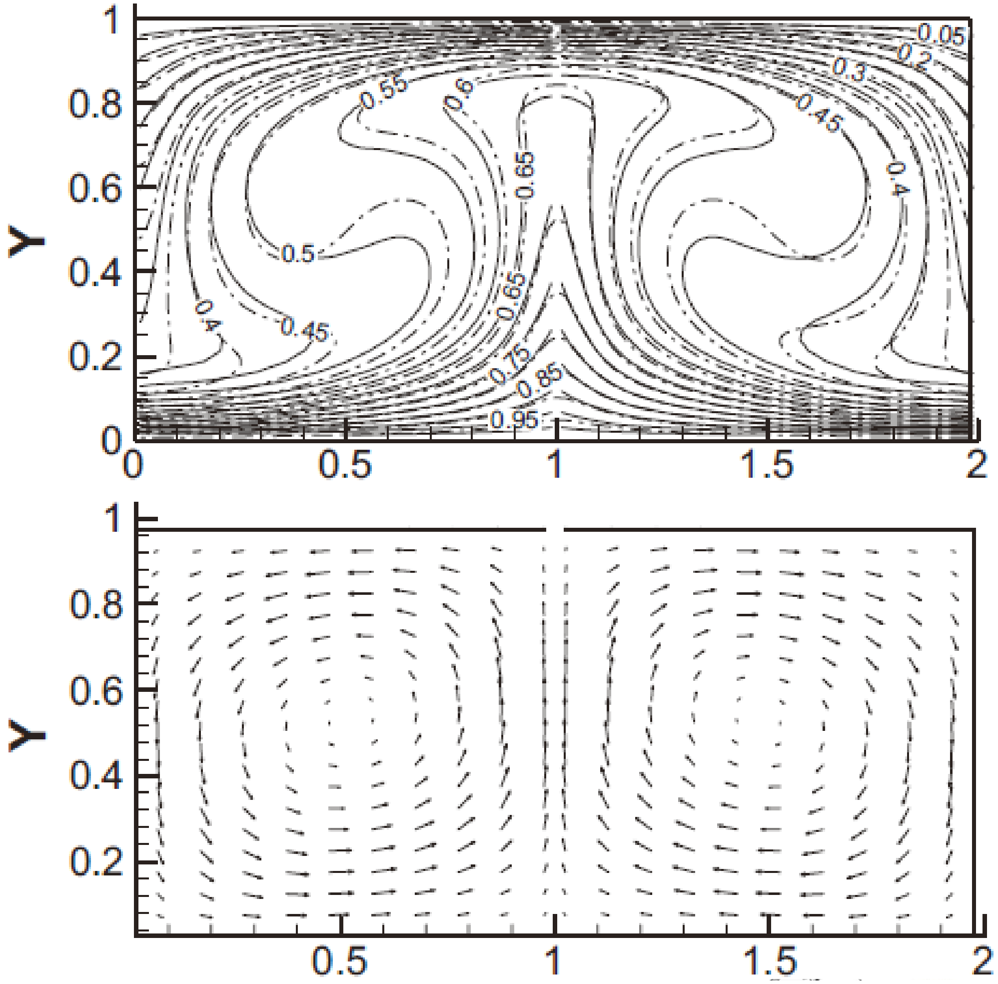
Examples of Energy-conserving DPD

Natural convection heat transfer simulation:

— Abu-Nada, E., Phys. Rev. E, 2010.



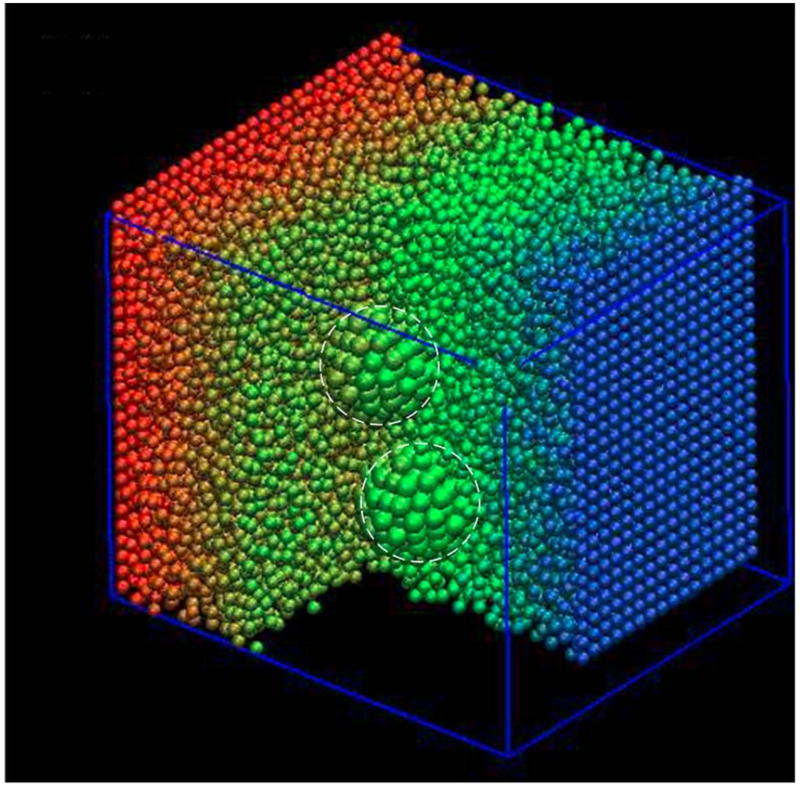
Temperature isotherms and velocity field (sold lines: eDPD, dashed dotted lines: finite volume solutions):



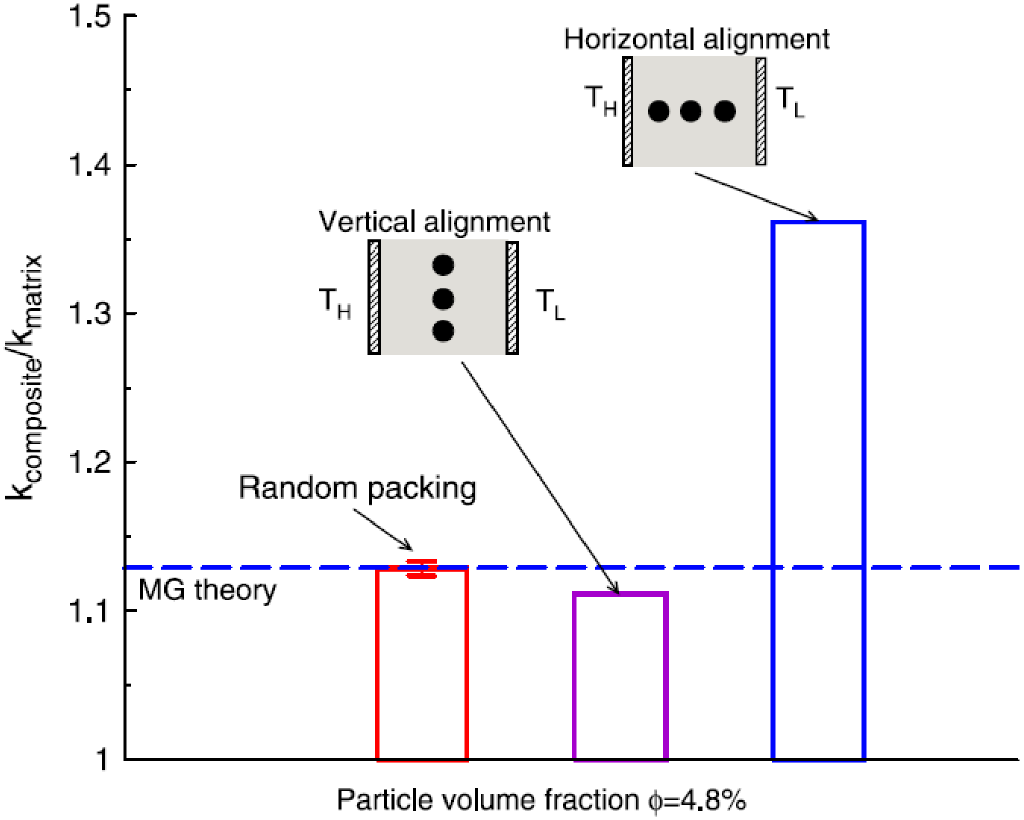
Examples of Energy-conserving DPD

Heat conduction in nanocomposite:

– Qiao and He, Molecular Simulation, 2007.



Thermal conductivity enhancement by nanoparticles:

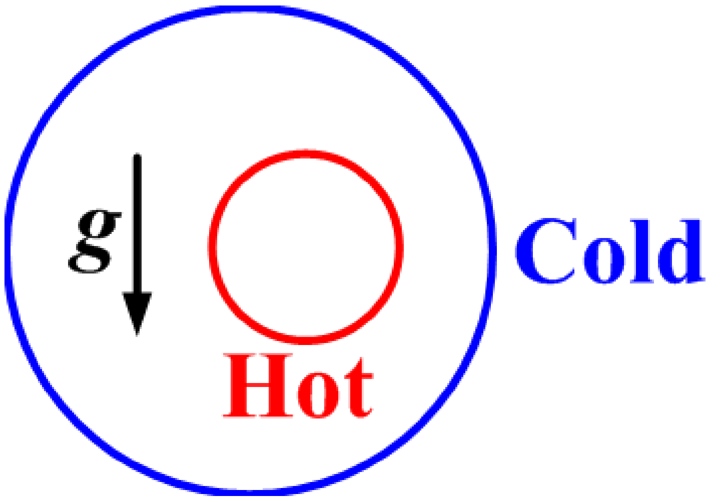


Examples of Energy-conserving DPD

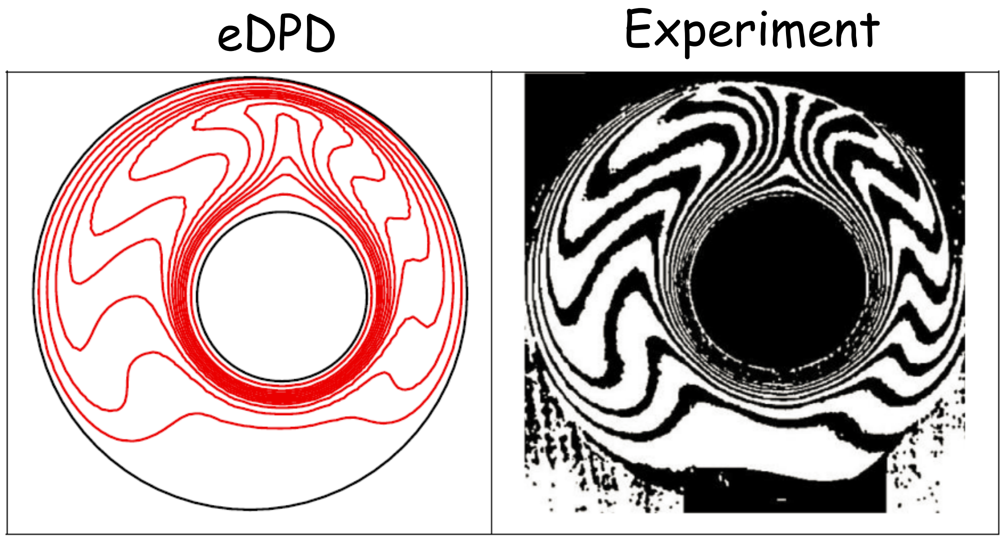
Natural convection in eccentric annulus:

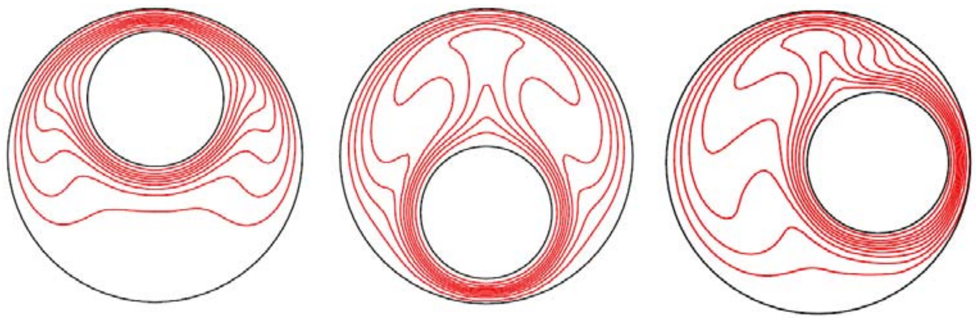
— Cao, et al., Int. J. Heat Mass Transfer, 2013.

Physical model:



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



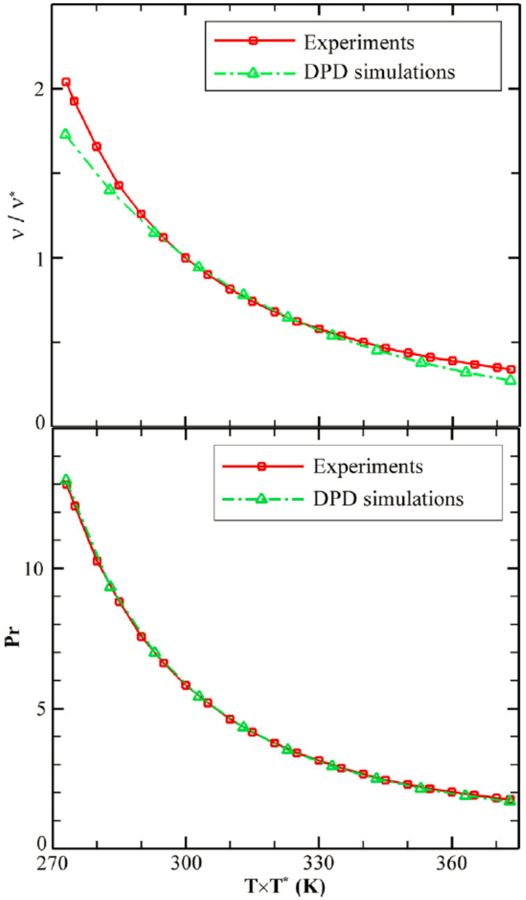


Examples of Energy-conserving DPD

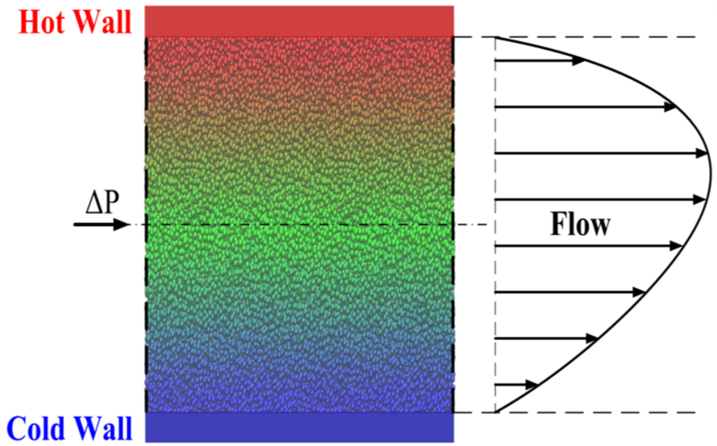
Flow between Cold-Hot walls:

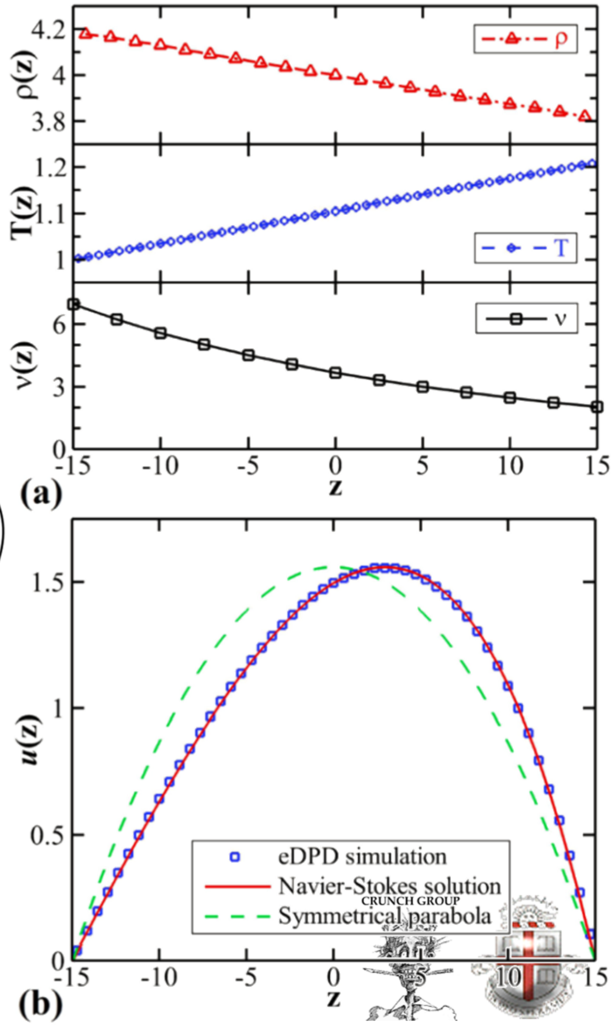
— Li, Tang, Lei, Caswell & Karniadakis, J. Comput. Phys., 2014.

Temperature-dependent properties:



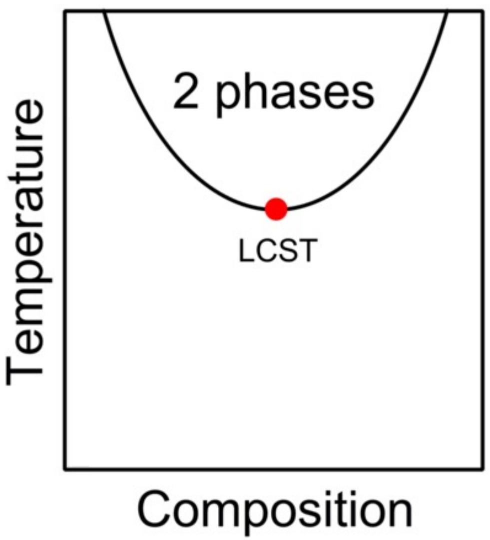
Coupling of flow and heat conduction:





Application of eDPD
Thermoresponsive polymers

Polymers have a drastic and discontinuous change of their **solubility** in given solvents with **temperature**.



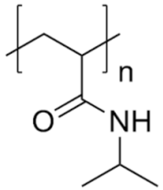
LCST:
Lower
Critical
Solution
Temperature

~ 90% are LCST-type

LCST-type polymer:

This demo is obtained from YouTube.

A quick example for introduction of smart materials:

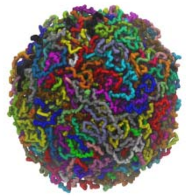


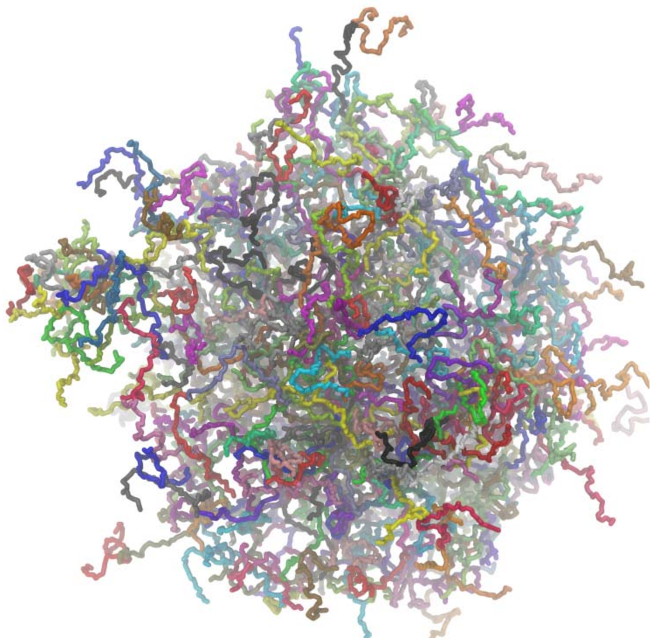
PNIPAM

$T_C = 32^o C$

Drug delivery

$\mathbf{T > T_c}$

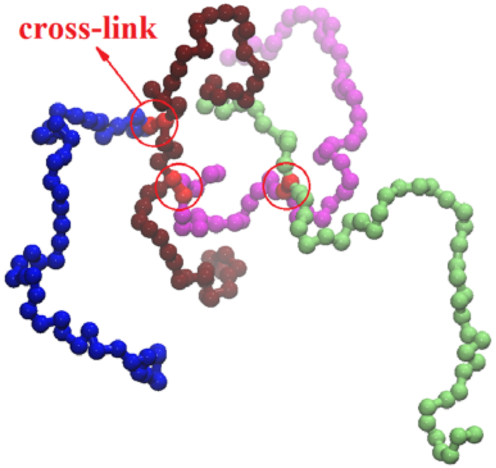


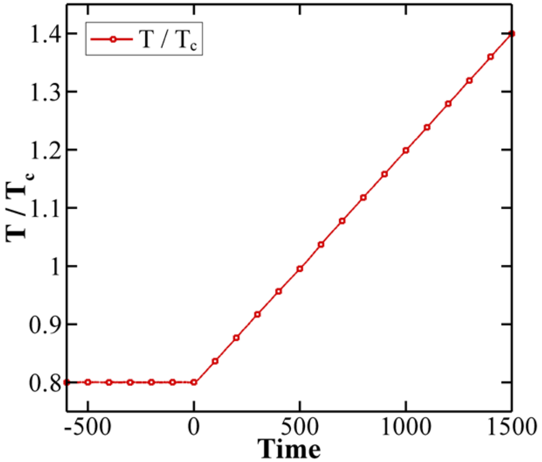


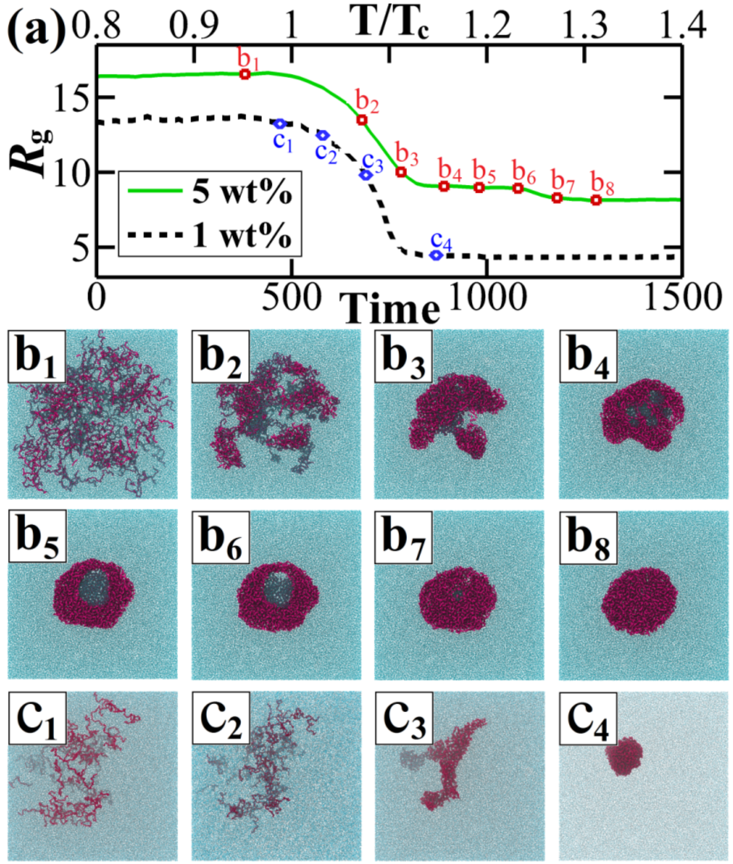
$\mathbf{T < T_c}$

Thermally induced phase transition:

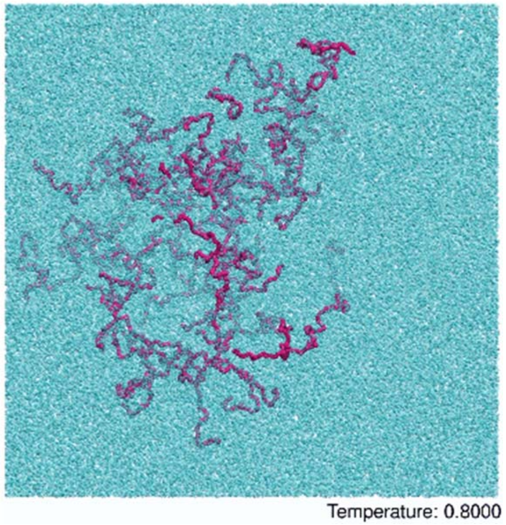
— Li, Tang, Li & Karniadakis, Chem. Comm., 2015.



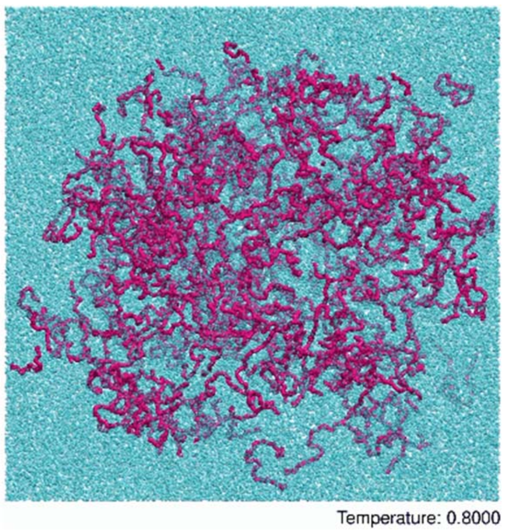




Phase transition dynamics:

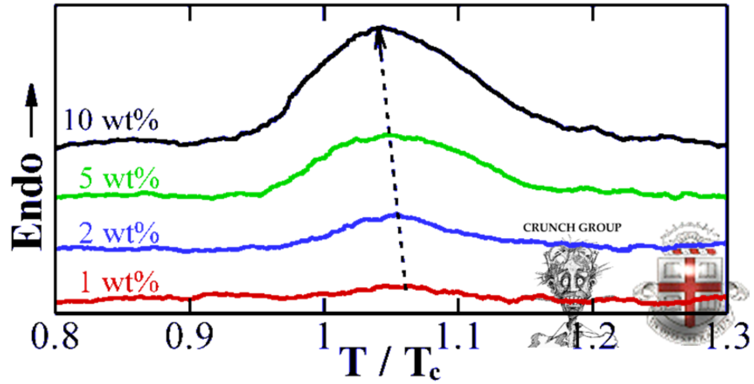


1 wt%



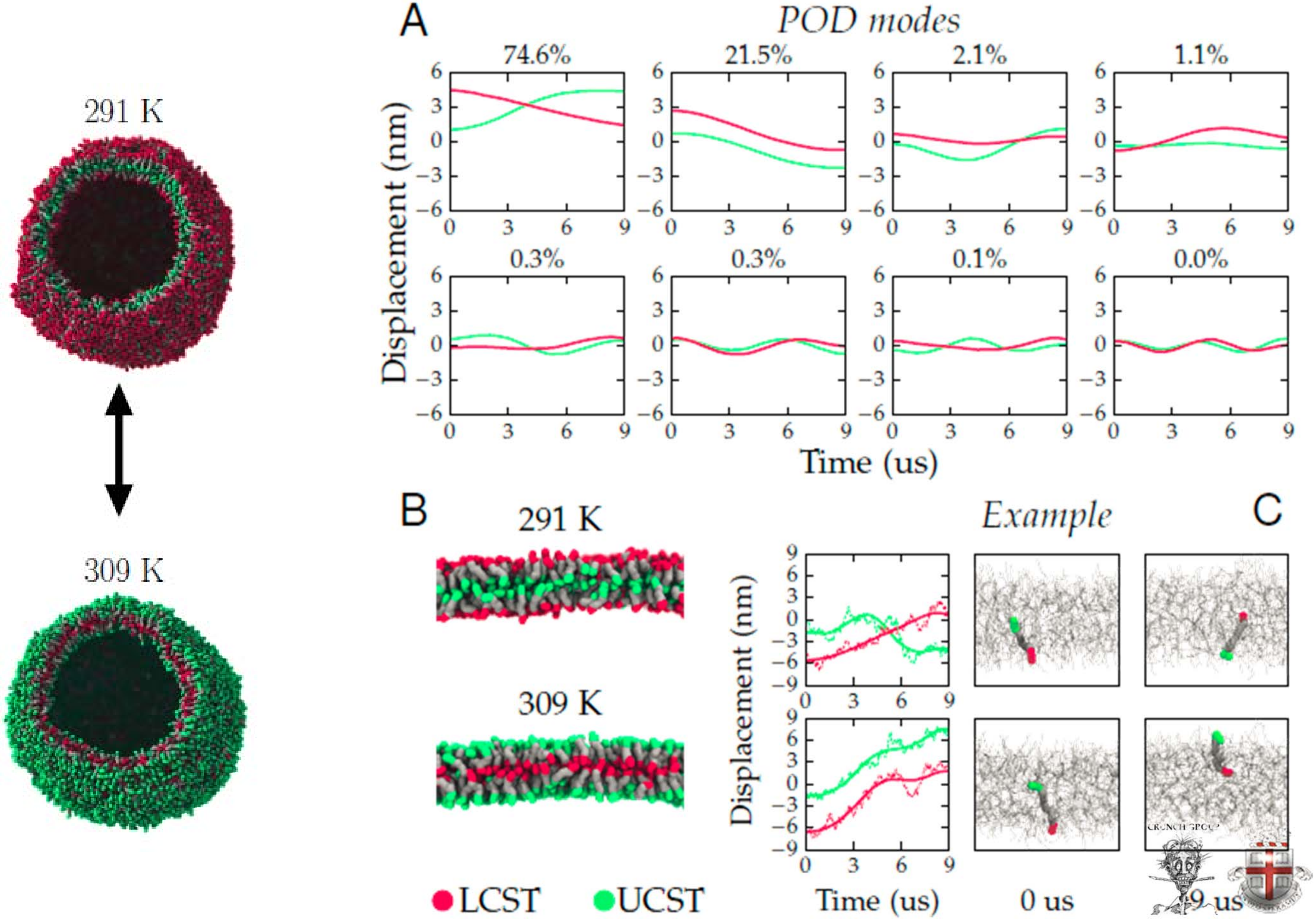
5 wt%

Energy changes:



Thermoresponsive vesicles, as drug delivery vehicle

— Tang, Li, Li, Deng & Karniadakis, Macromolecules, 2016.



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**

CRUNCH GROUP

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.

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

CRUNCH GROUP

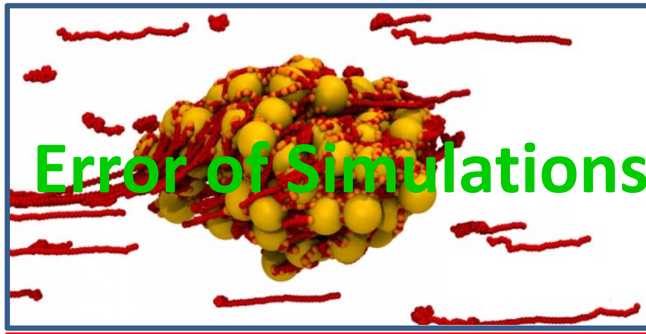
DPD and Smoothed DPD

	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. 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. 2. Need to map DPD units to physical units based on output properties.	Must know the constitutive equation and properties of the system.

Top-down v.s. Bottom-up

- Material can be modeled as a continuous mass that fills the entire region of space it occupies.
- No underlying inhomogeneous microstructure, that is, matter can be divided infinitely without change of material properties.
- It ignores the fact that matter is made of atoms.
- Only valid on length scales much greater than that of inter-atomic distances.

Continuum assumption: (PDEs, Top-Down)



Error of Simulations = Modeling Error + Discretization Error

Atomistic description: (F=ma, Bottom-Up)

- Born-Oppenheimer (BO) approximation (do not consider quantum effects)
- Material is made of discrete atoms.
- More fundamental description of the world, does not distinguish different subjects (physics, chemistry, biology, material science, et. al.)

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:

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

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

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

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

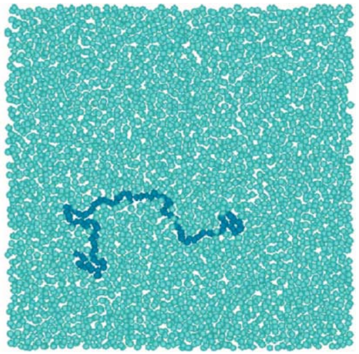
— Español and Revenga, Phys. Rev. E, 2003.

CRUNCH GROUP

Examples of Smoothed DPD

Polymer chain in suspension:

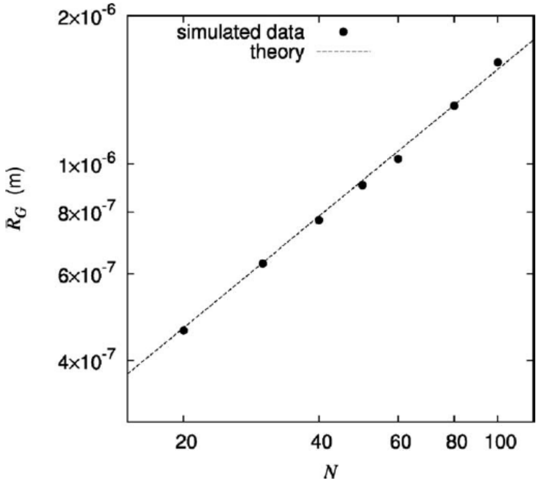
— Litvinov, Ellero, Hu & Adams, Phys. Rev. E, 2008.



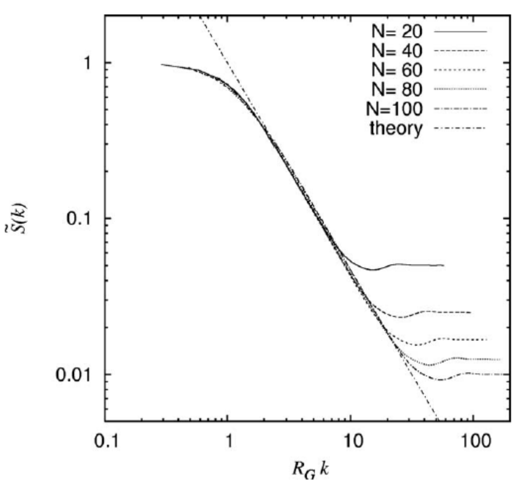
Solvent:
Newtonian fluid

Polymer chain:
Finitely Extendable Nonlinear Elastic (FENE) springs

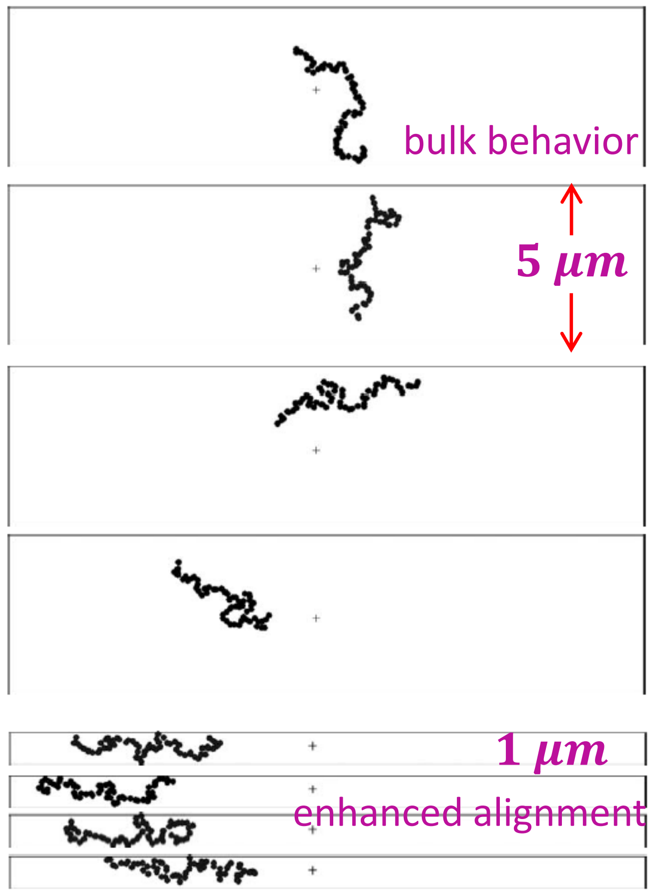
Scaling of the radius of gyration R_G for several chain lengths:



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



Polymer conformations under confinement:

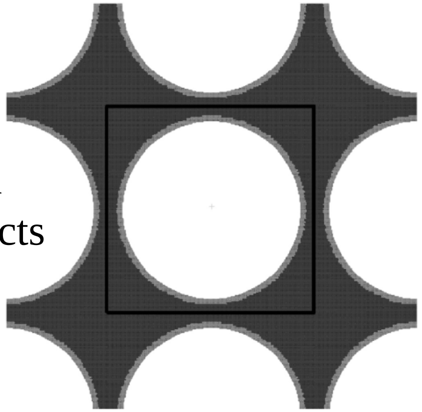


Examples of Smoothed DPD

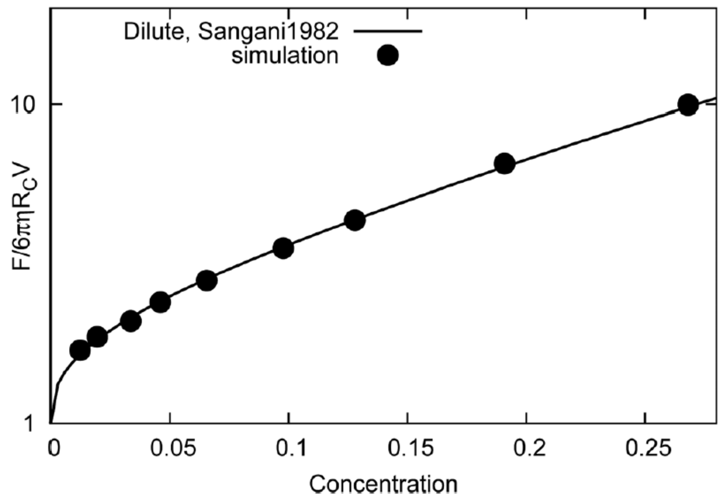
Flow through porous media:

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

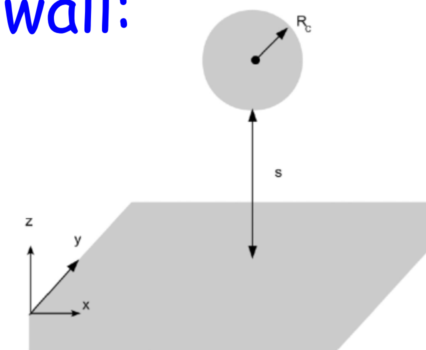
Model:
Periodic array of fixed circular/spherical objects



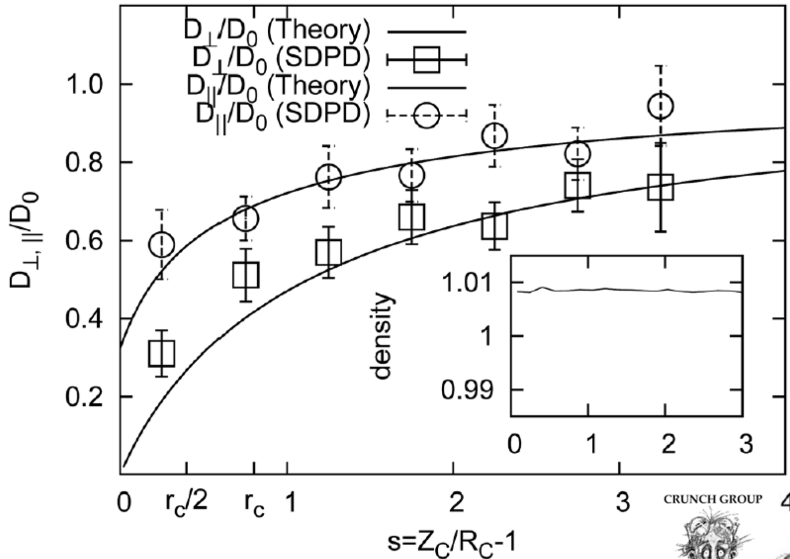
Three-dimensional dimensionless drag coefficient:



A colloidal particle near a rigid wall:



Diffusion coefficients perpendicular and parallel to the wall:



CRUNCH GROUP

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

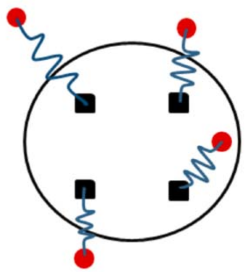
5. **Other DPD models**

CRUNCH GROUP

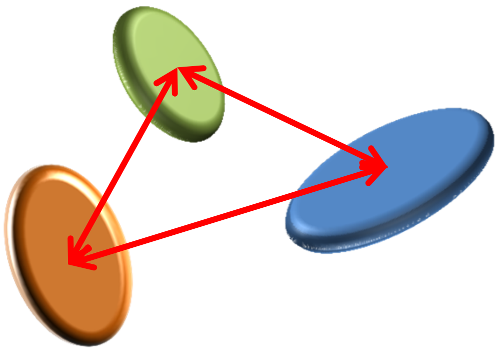
Other DPD models

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.

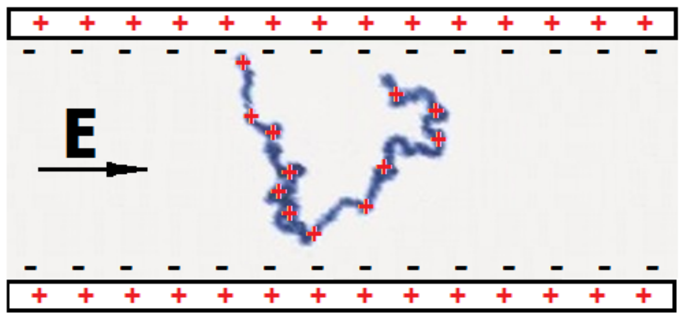
2. Spring model for colloids in suspension.
    - Phan-Thien, N., Mai-Duy, N. and Khoo, B.C., A spring model for suspended particles in dissipative particle dynamics. Journal of Rheology, 2014. **58**(4): 839-867.



3. Anisotropic DPD particles, and charged DPD particles



aDPD



cDPD

CRUNCH GROUP

References

- Hoogerbrugge, P.J. and J.M.V.A. Koelman, *Simulating Microscopic Hydrodynamic Phenomena with Dissipative Particle Dynamics.* Europhysics Letters, 1992. **19**: 155-160.
- Espanol, P. and P. Warren, *Statistical mechanics of dissipative particle dynamics.* Europhysics Letters, 1995. **30**: 191-196.
- Groot, R.D. and P.B. Warren, *Dissipative particle dynamics: Bridging the gap between atomistic and mesoscopic simulation*. Journal of Chemical Physics, 1997. **107**: 4423-4435.
- Marsh, C.A., G. Backx, and M.H. Ernst, *Static and dynamic properties of dissipative particle dynamics*. Physical Review E, 1997. **56**: 1676-1691.
- Espanol, P., *Dissipative particle dynamics with energy conservation*. Europhysics Letters, 1997. **40**: 631-636.
- Espanol, P., *Fluid particle model*. Physical Review E, 1998. **57**: 2930-2948.
- Lowe, C.P., *An alternative approach to dissipative particle dynamics*. Europhysics Letters, 1999. **47**: 145-151.
- Español, P. and M. Revenga, *Smoothed dissipative particle dynamics*. Physical Review E, 2003. **67**: 026705.
- Soddemann, T., B. Dunweg, and K. Kremer, *Dissipative particle dynamics: A useful thermostat for equilibrium and nonequilibrium molecular dynamics simulations*. Physical Review E, 2003. **68**: 046702.
- Warren, P.B., *Vapor-liquid coexistence in many-body dissipative particle dynamics*. Physical Review E, 2003. **68**: 066702.
- Pan, W.X., I.V. Pivkin, and G.E. Karniadakis, *Single-particle hydrodynamics in DPD: A new formulation.* Europhysics Letters, 2008. **84**: 10012.
- Pivkin, I.V. and G.E. Karniadakis, *Accurate Coarse-Grained Modeling of Red Blood Cells.* Physical Review Letters, 2008. **101**: 118105.
- Pan, W.X., B. Caswell, and G.E. Karniadakis, *A low-dimensional model for the red blood cell.* Soft Matter, 2010. **6**: 4366-4376.
- Arienti, M., W.X. Pan, X.Y. Li and G.E. Karniadakis, *Many-body dissipative particle dynamics simulation of liquid/vapor and liquid/solid interactions.* Journal of Chemical Physics, 2011. **134**: 204114.
- 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.

CRUNCH GROUP