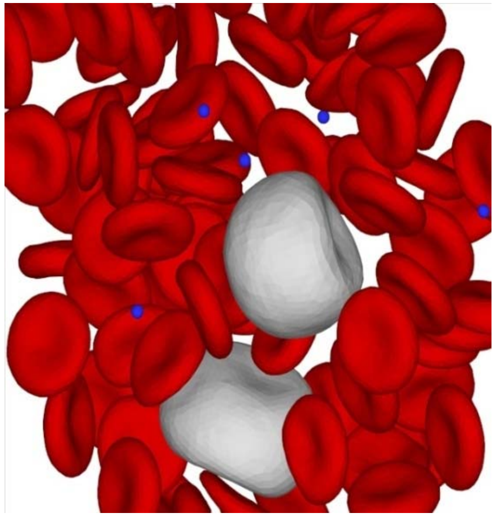
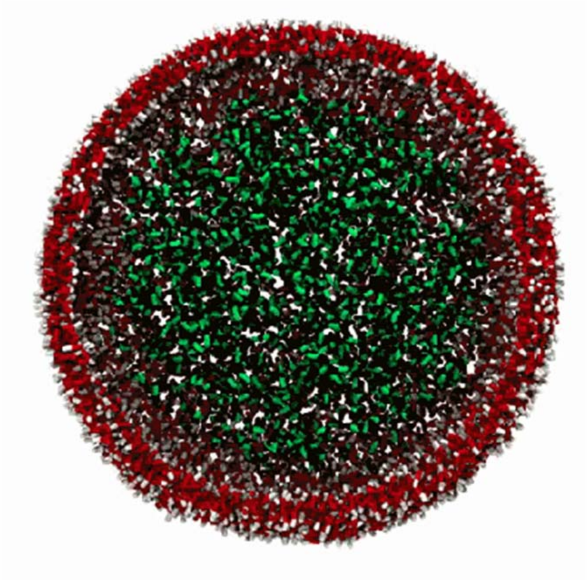
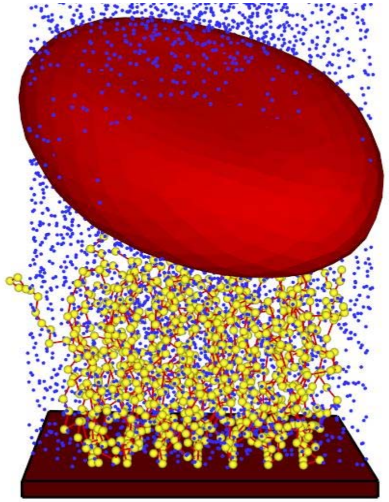
Dissipative Particle Dynamics: Foundation, Evolution and Applications

Lecture 4: DPD in soft matter and polymeric applications







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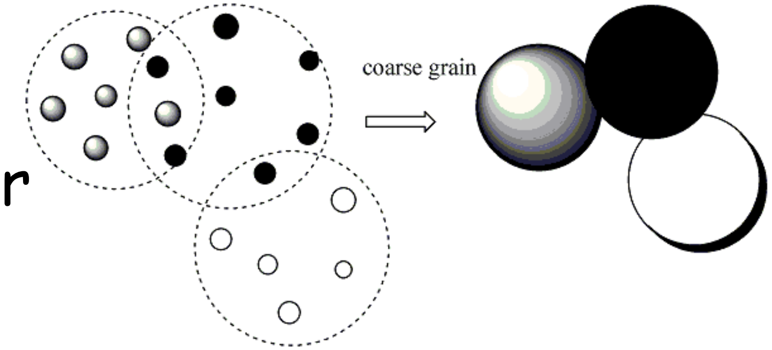
The CRUNCH group: www.cfm.brown.edu/crunch

Outline

- Dissipative Particle Dynamics (DPD)
- Applications:
  - Fluid Flow
    - Boundary conditions
    - Triple-Decker: MD – DPD - NS
  - Blood Flow
  - Amphiphilic Self-assembly
- Future of DPD

Dissipative Particle Dynamics (DPD)



- Stochastic simulation approach for simple and complex fluids.

- Mesoscale approach to simulate soft matter.

- Conserve momentum locally & preserve hydrodynamics.

- Access to longer time and length scales than are possible using conventional MD simulations.

Simulations with DPD

- Applying appropriate boundary conditions, so we can simulate problems of interest.

- A choice for the inter-particle forces, so we can model materials of interest.

- DPD has been applied to model a diverse range of systems:
  - Fluid flow (pipes, porous media)
  - Complex fluids (Colloidal suspension, blood)
  - Self-assembly (polymers, lipids, surfactants, nanoparticles)
  - Phase phenomena (polymer melts, dynamic wetting)

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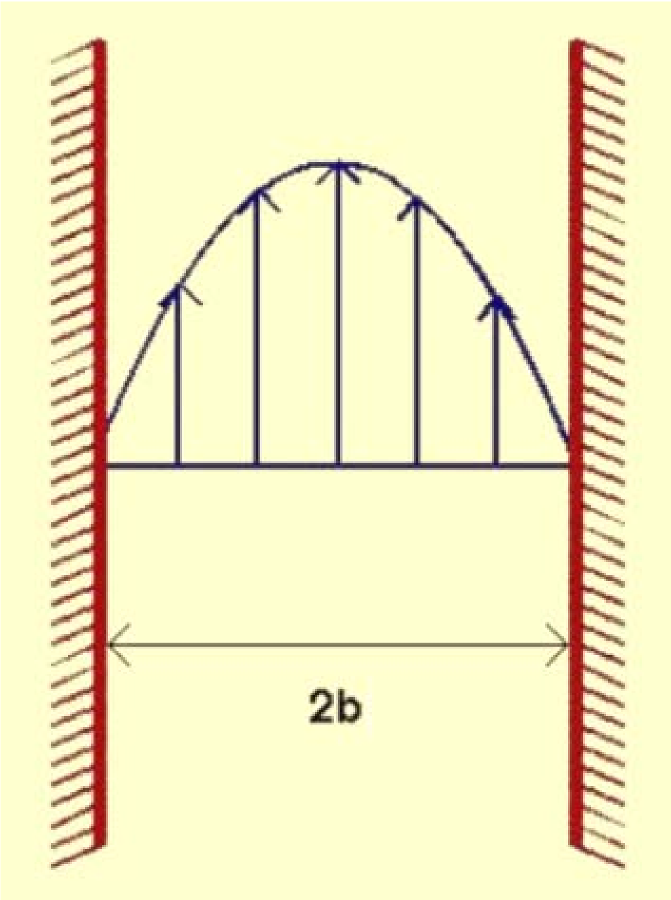
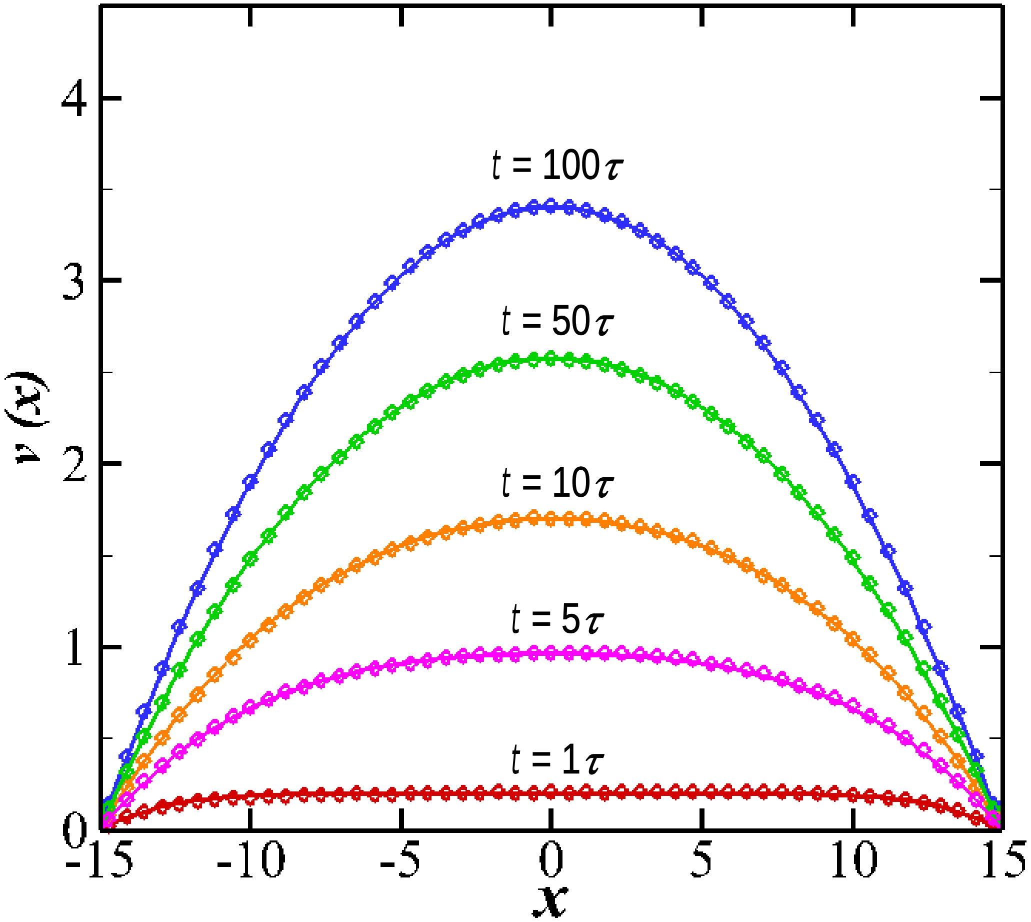
Fluid flow





The development of velocity profiles in Poiseuille flow

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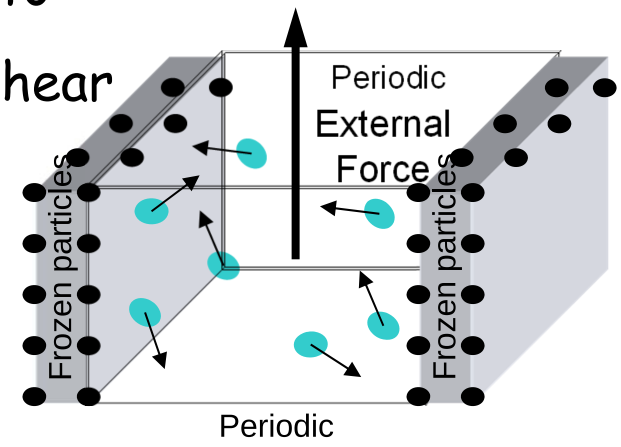
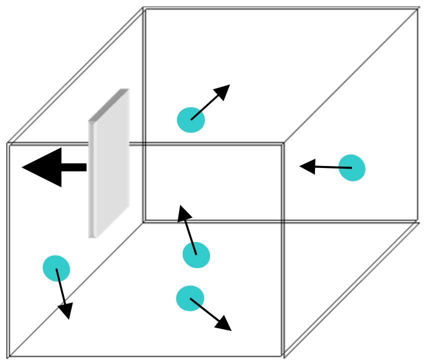
Boundary Conditions in DPD

- Lees-Edwards boundary conditions can be used to simulate an infinite but periodic system under shear



- Revenga et al. (1998) created a solid boundary by freezing the particles on the boundary of solid object; no repulsion between the particles was used.

- Willemsen et al. (2000) used layers of ghost particles to generate no-slip boundary conditions.



- Pivkin & Karniadakis (2005) proposed new wall-fluid interaction forces.

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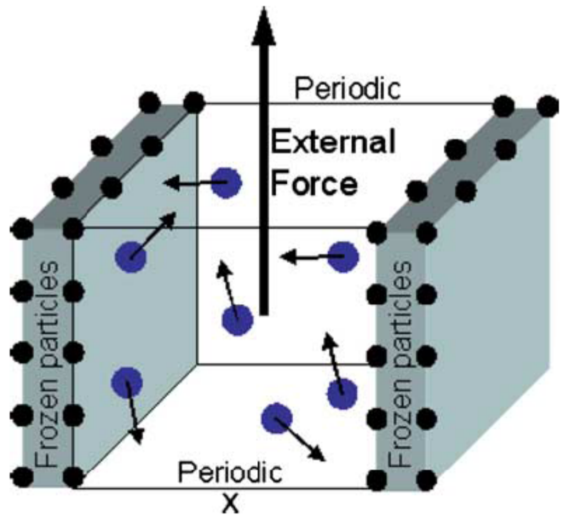
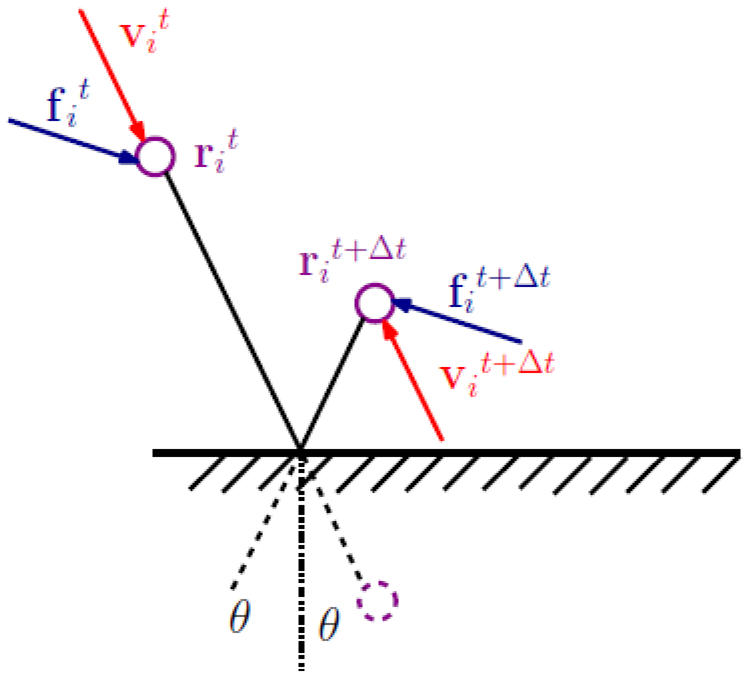
Boundary conditions in DPD

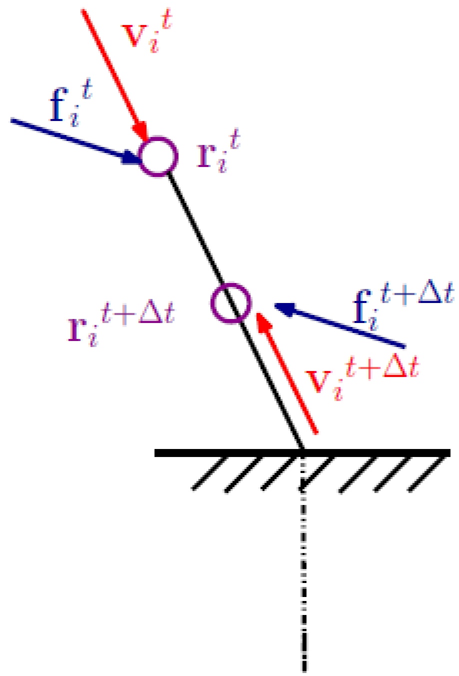
Frozen wall boundary condition

- Fluid in between parallel walls
- Walls are simulated by freezing DPD particles
- Flow induced by external body force





Bounce forward reflection



Bounce back reflection

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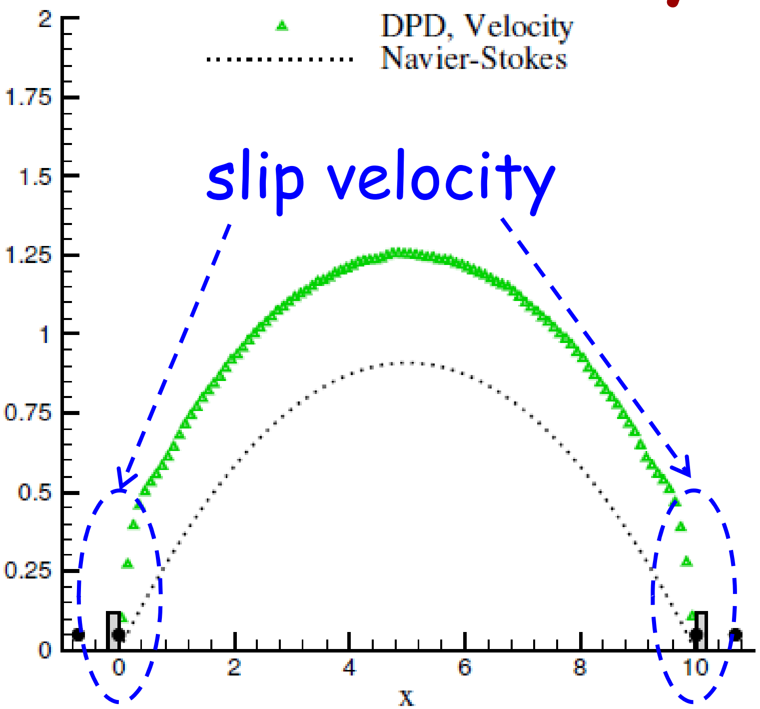
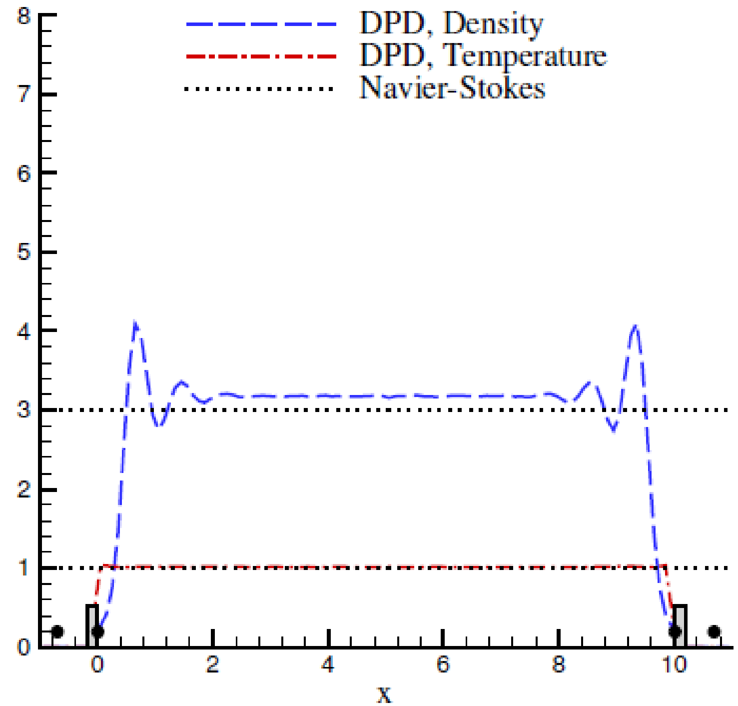
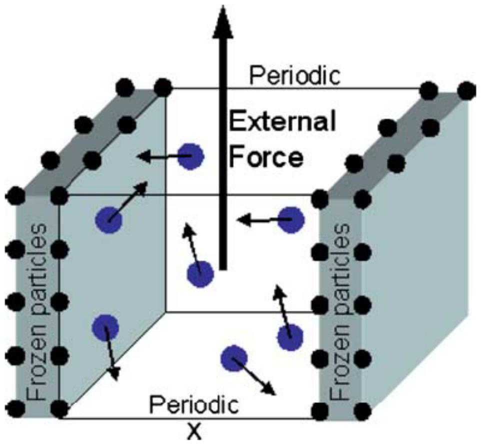
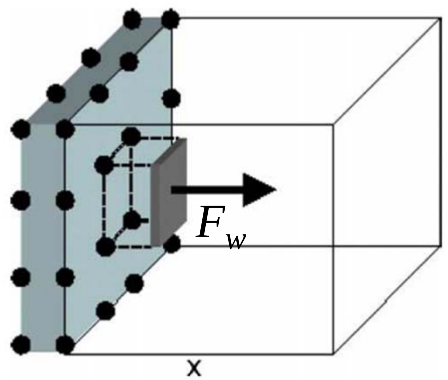
Boundary conditions in DPD





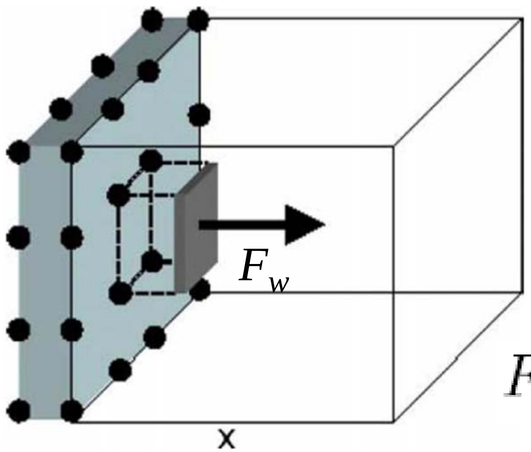
No-slip boundary condition

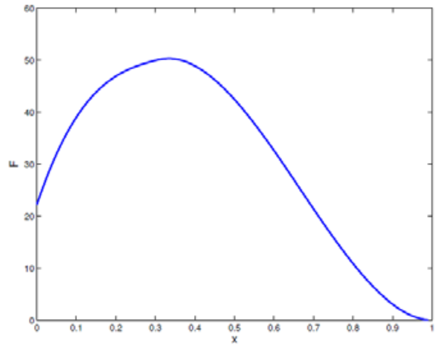




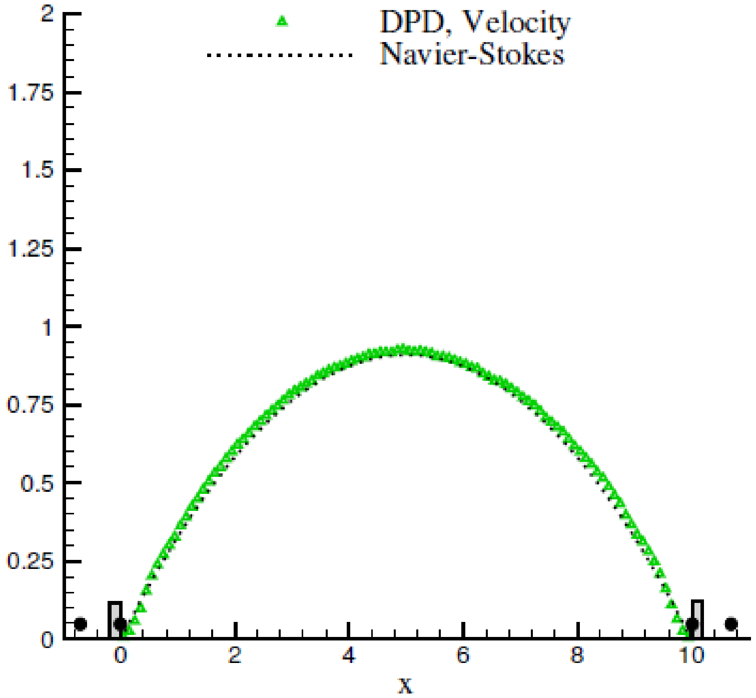
Pivkin & Karniadakis. J. Comput. Phys., 2005.

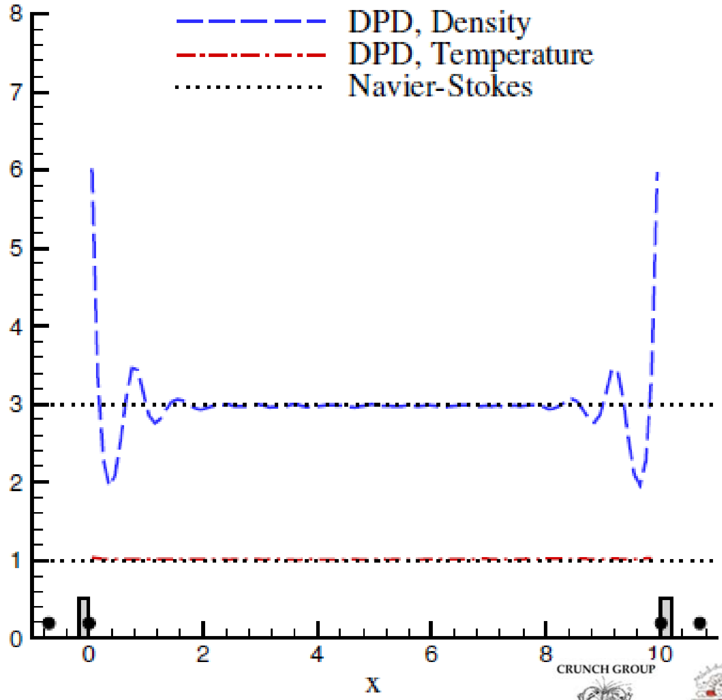
Poiseuille flow results





$$F_w = a_e(0.0303n_w^2 + 0.5617n_w - 0.8536)$$

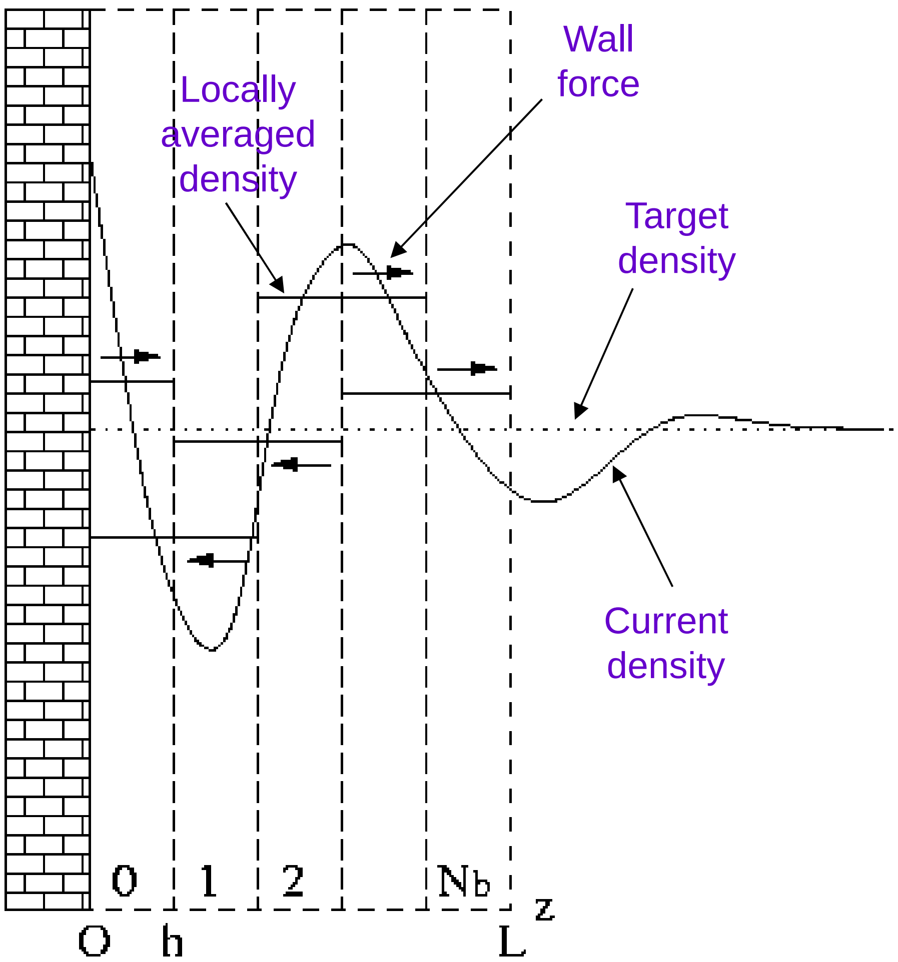


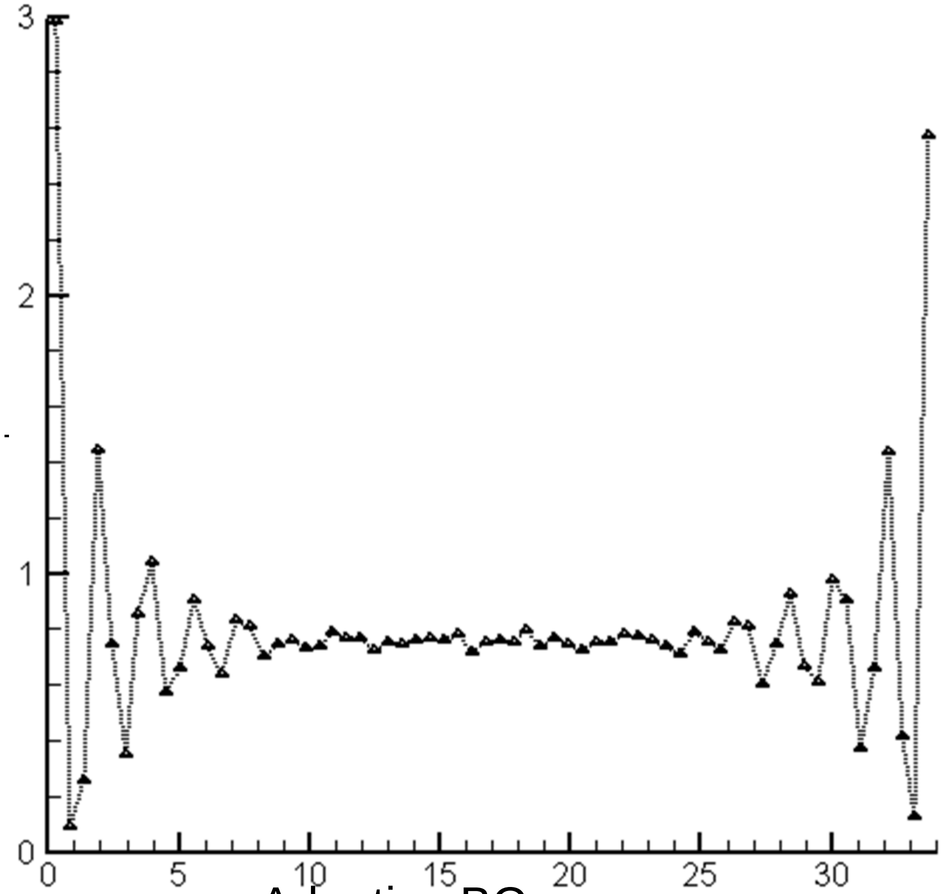


<u>**Pivkin & Karniadakis. J. Comput. Phys., 2005.**</u>

Boundary conditions in DPD

Adaptive boundary condition





Iteratively adjust the wall repulsion force in each bin based on the averaged density values.

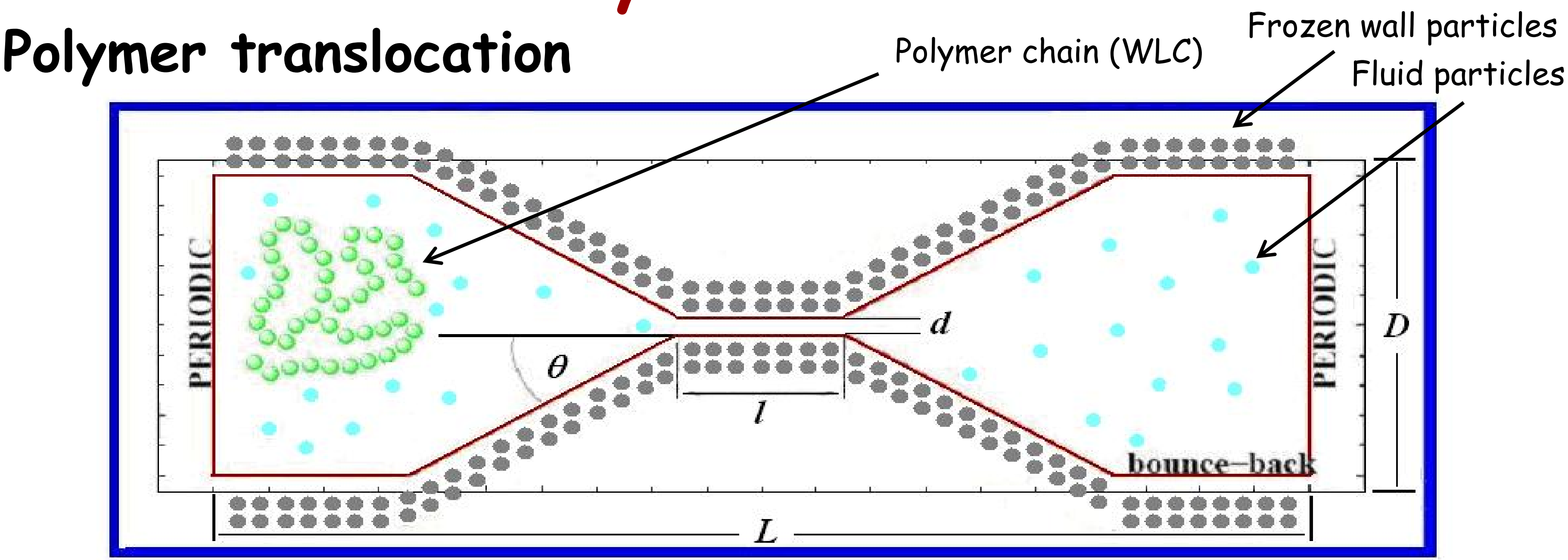
Adaptive BC:

- layers of particles
- bounce back reflection
- adaptive wall force

Pivkin & Karniadakis, PRL, 2006

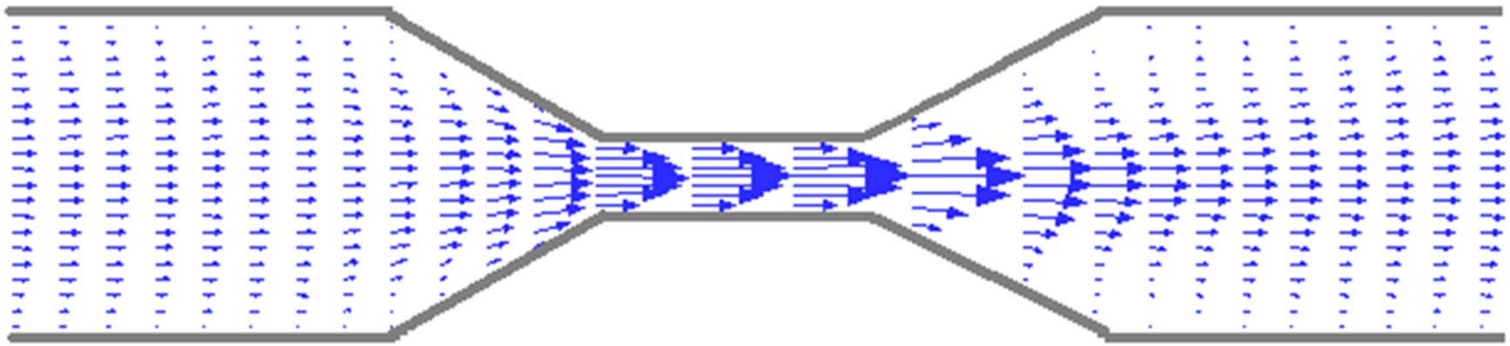
Boundary conditions in DPD

Polymer translocation



Schematic representation of simulation model

No-slip B.C. + Adaptive B.C.



velocity vector field

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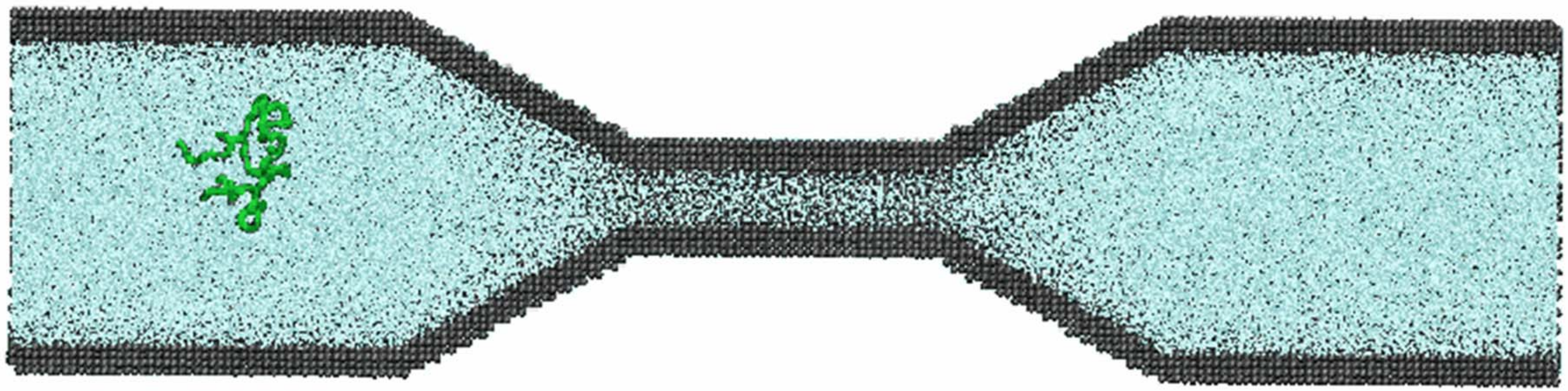
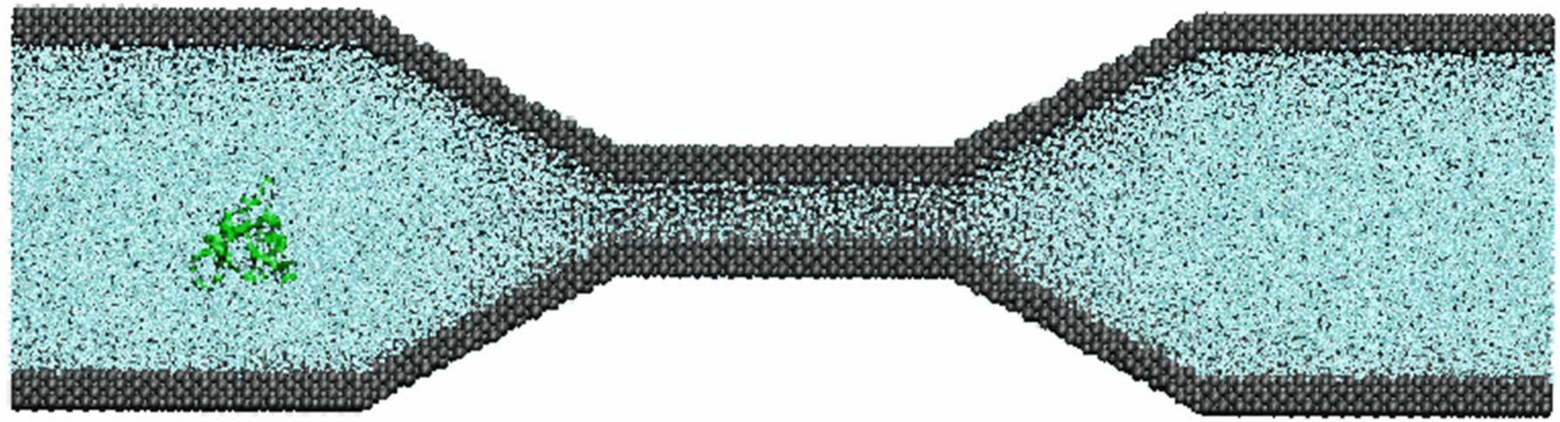
Boundary conditions in DPD

Polymer translocation



Translocation of polymer in single-file conformations



Translocation of polymer in double-folded conformations

<u>**Guo, Li, Liu & Liang, J. Chem. Phys., 2011**</u>

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Macro-Meso-Micro Coupling

NS + DPD + MD

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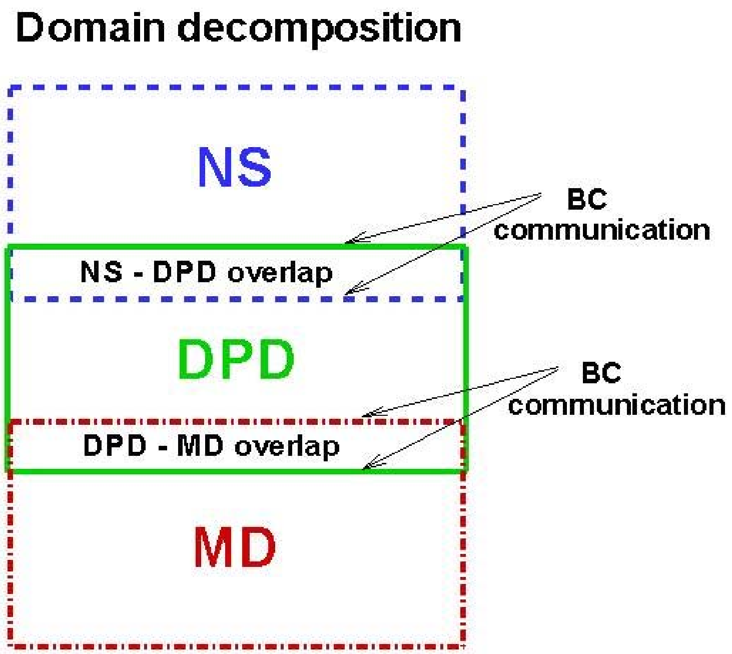
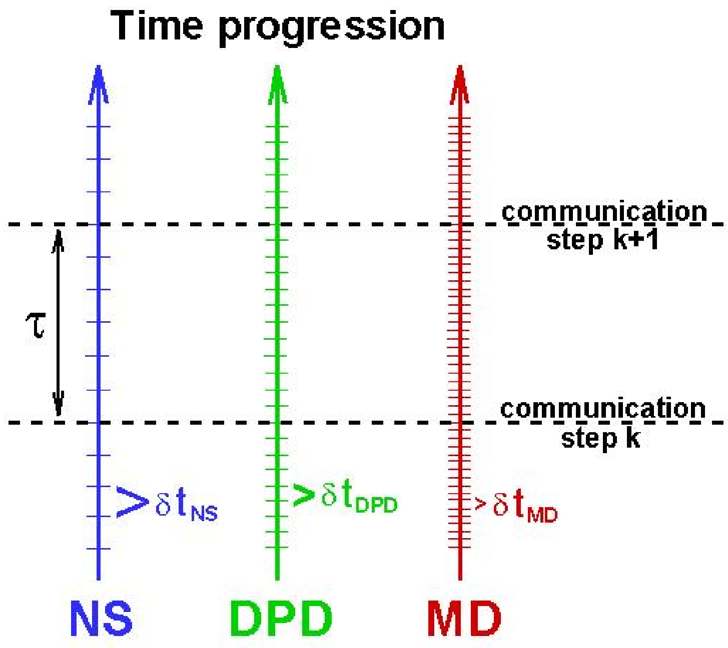
Triple-Decker Algorithm





- Atomistic – Mesoscopic - Continuum Coupling
- Efficient time and space decoupling
- Subdomains are integrated independently and are coupled through the boundary conditions every time τ

<u>**Fedosov & Karniadakis, J. Comput. Phys., 2009**</u>

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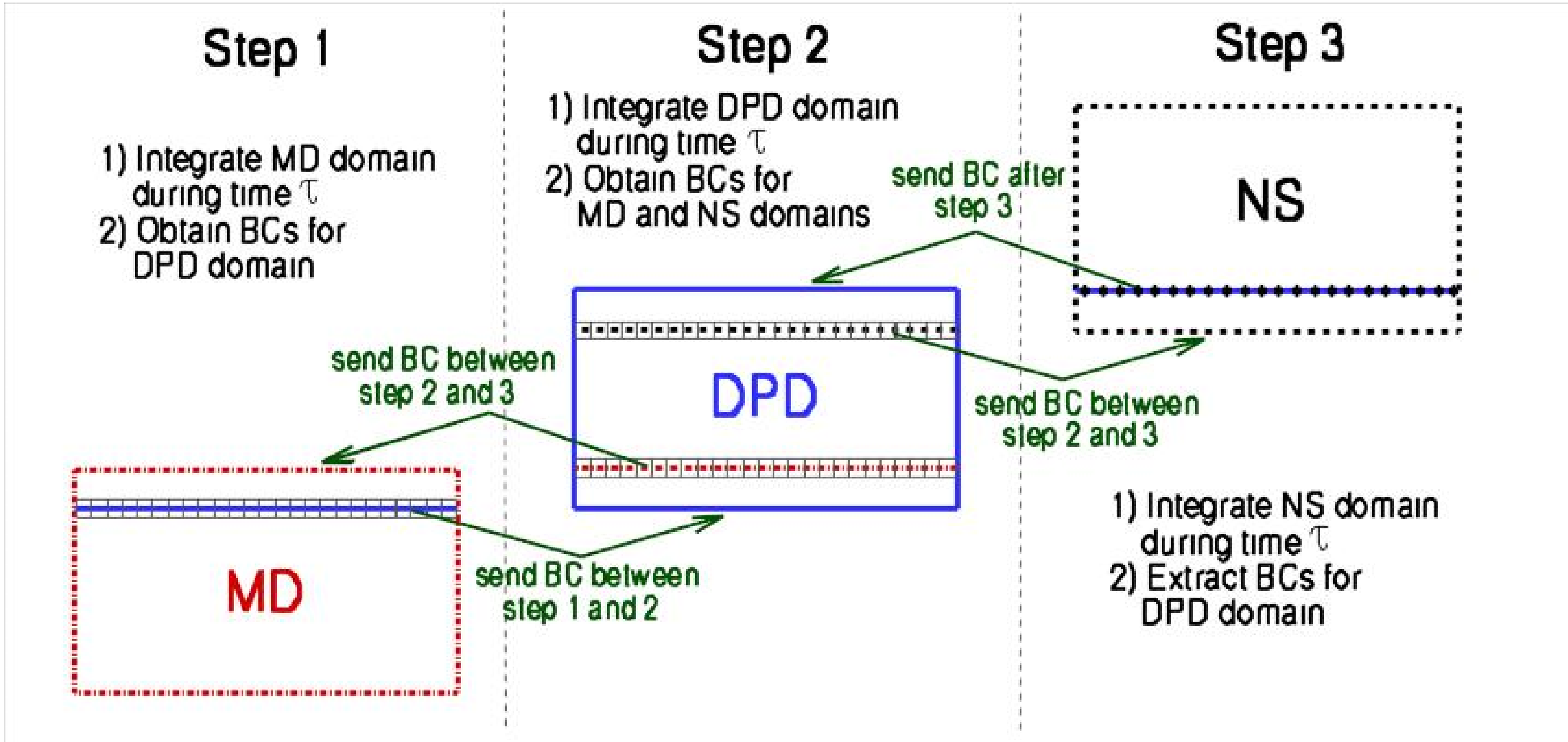
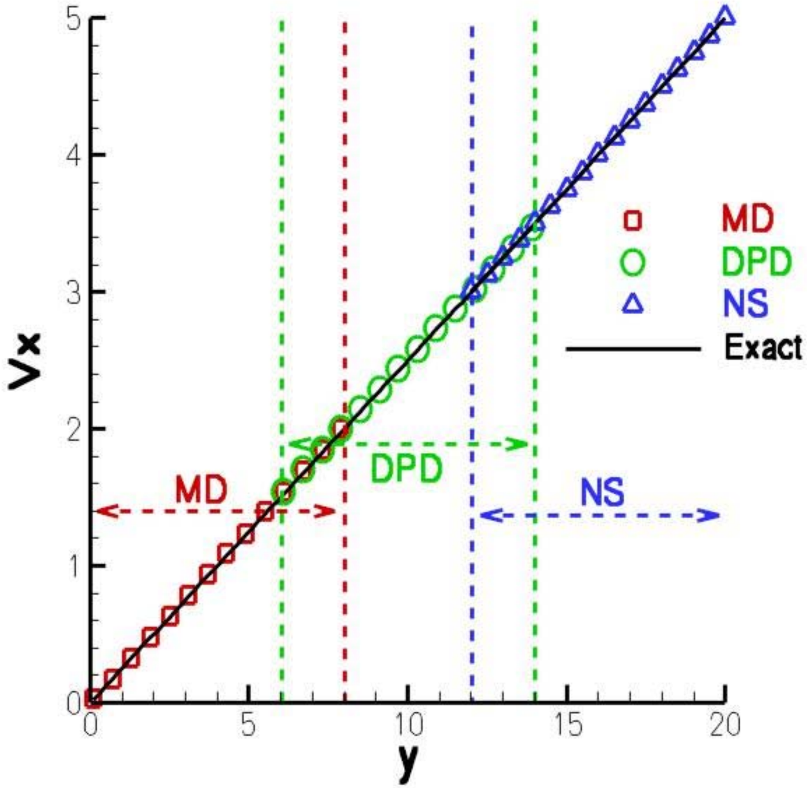
Triple-Decker Algorithm



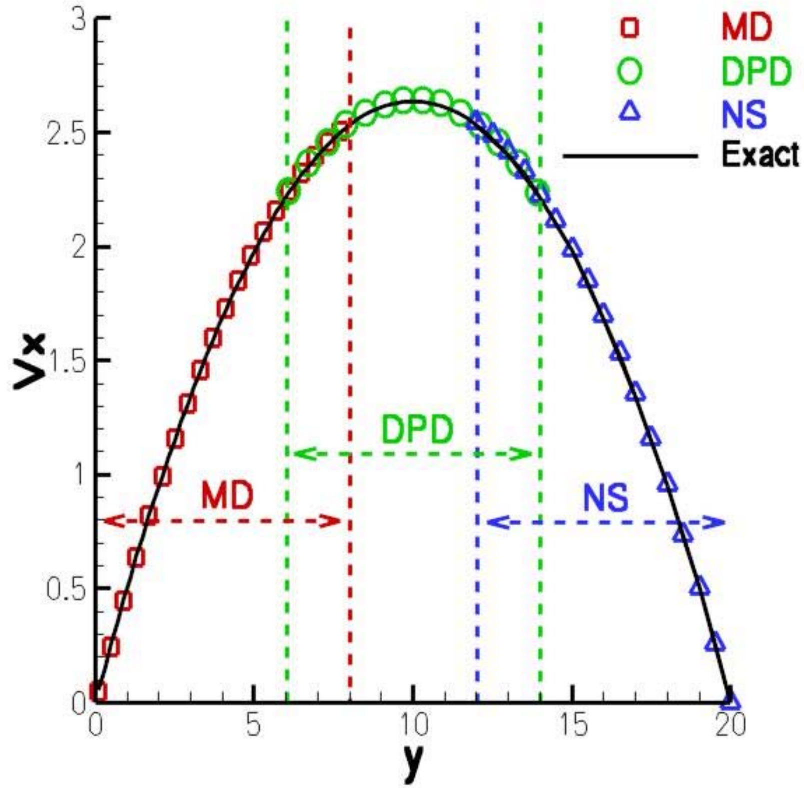
Fedosov & Karniadakis, J. Comput. Phys., 2009

Algorithm validation: 1D flows

Couette flow



Poiseuille flow



Fedosov & Karniadakis, J. Comput. Phys., 2009

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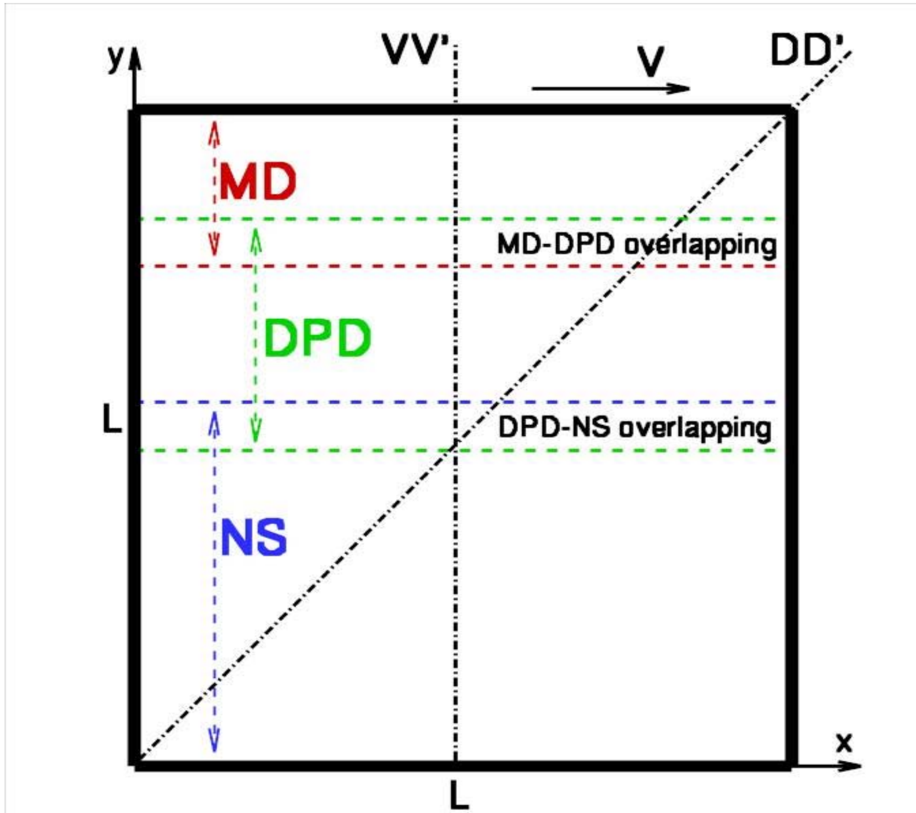
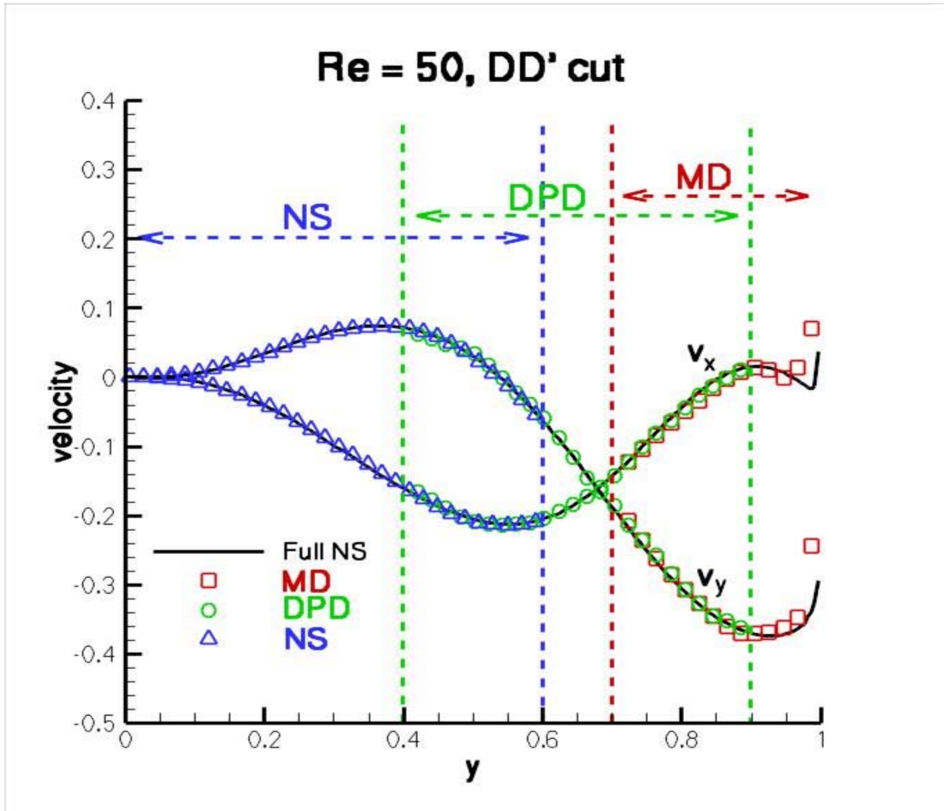
Square cavity flow

Square cavity, upper wall is moving to the right





Fedosov & Karniadakis, J. Comput. Phys., 2009

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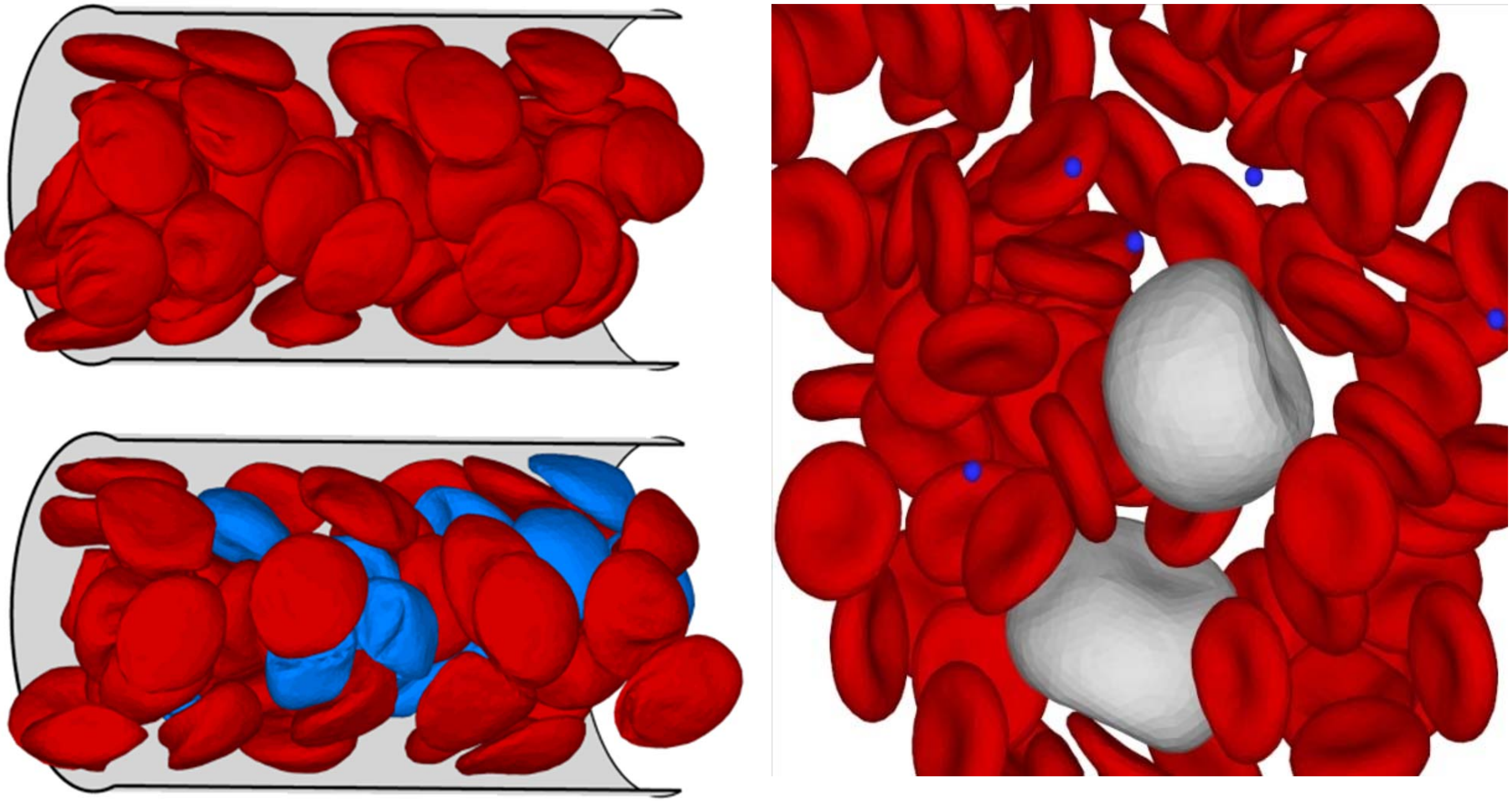
Blood flow



Modeling human blood flow in health and disease

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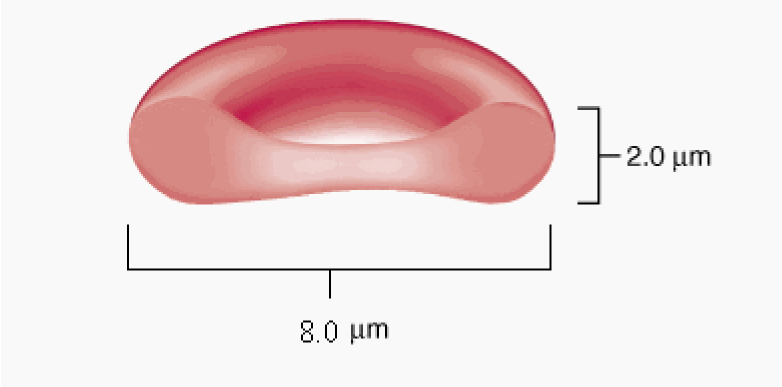
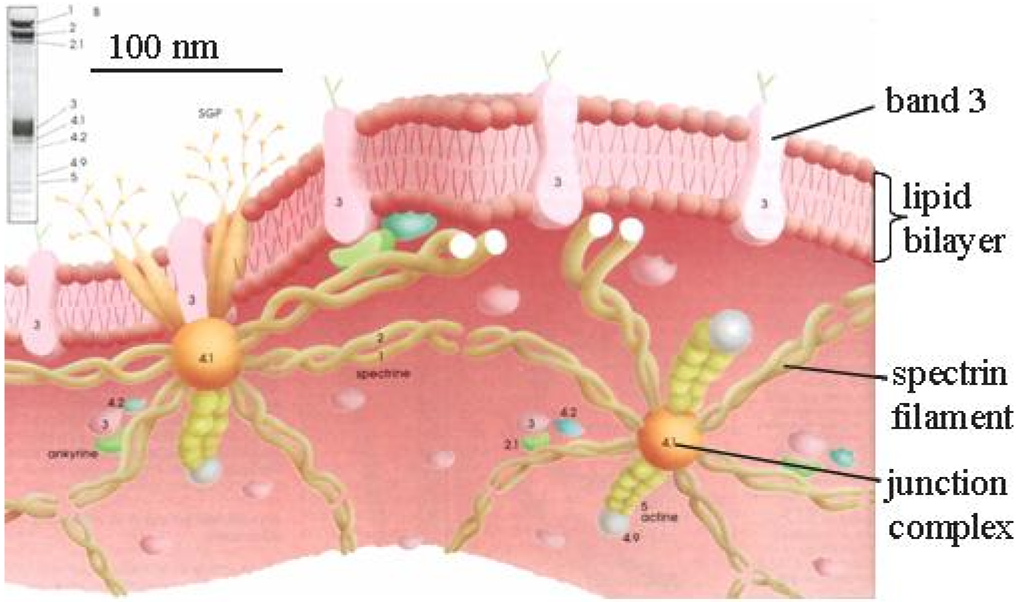
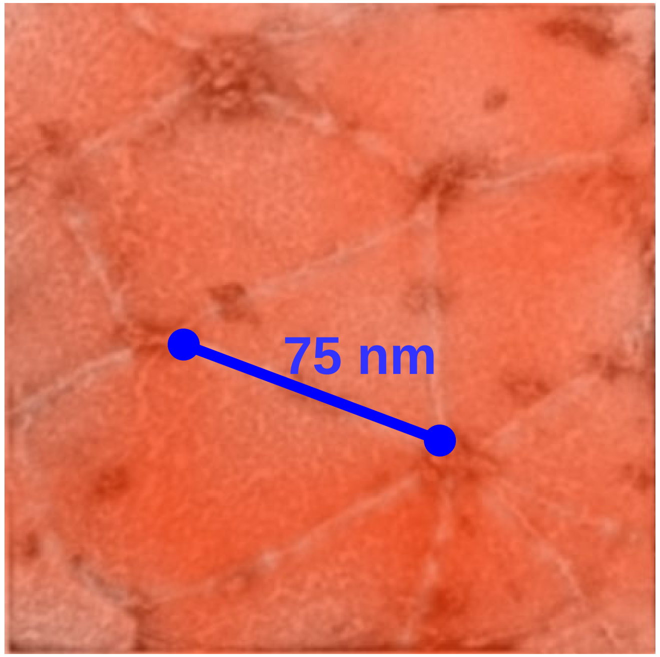
Red Blood Cells



50-100 *nm* spectrin length between junctions

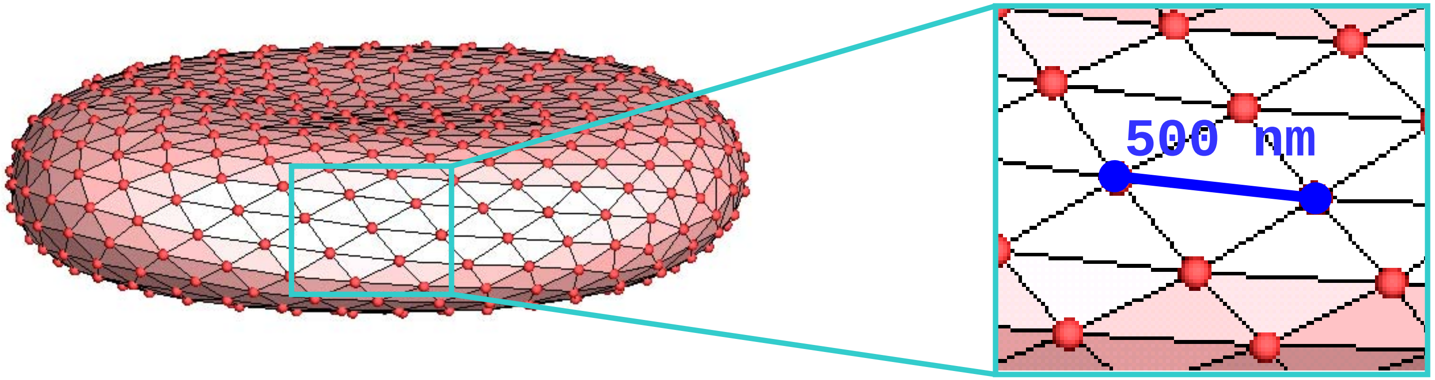
27000 – 40000 of junctions per RBC





General Spectrin-level and Multiscale RBC Models

- RBCs are immersed into the DPD fluid
- The RBC particles interact with fluid particles through DPD forces
- Temperature is controlled using DPD thermostat



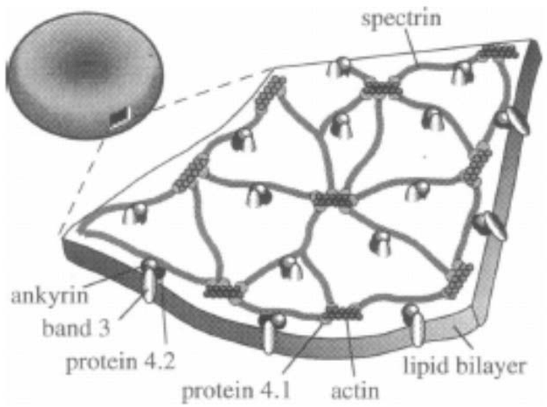
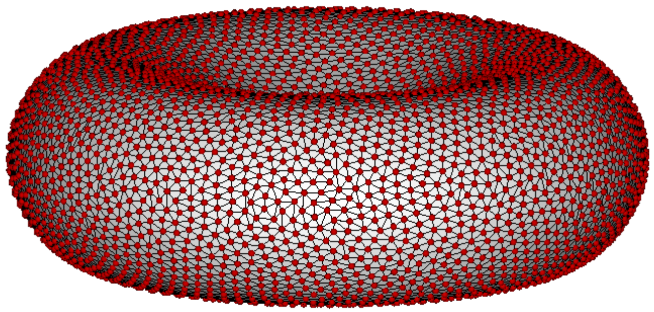


FIGURE 1 Arrangement of the major components of the RBC membrane skeleton.



1. Pivkin & Karniadakis, PRL, 2008;
2. Fedosov, Caswell & Karniadakis, Biophys. J, 2010.

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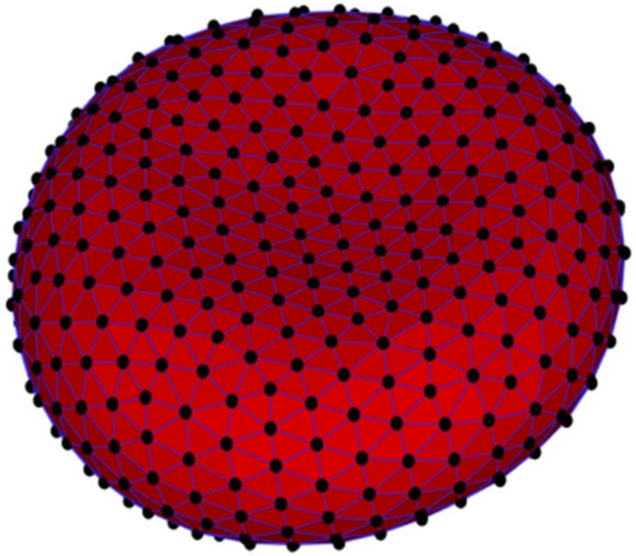
Multiscale RBC model

Triangular mesh:

- each vertex – a DPD particle



- each edge – a viscoelastic spring

$$U_{POW-WLC}(x) = \boxed{\frac{k_p}{(n-1)x^{n-1}}} + \boxed{\frac{k_B T L_m}{4p} \times \frac{3(x/L_m)^2 - 2(x/L_m)^3}{1 - x/L_m}} + U_{visc}$$

- bending resistance of lipid bilayer

$$U_{BEND}(\theta_{\alpha\beta}) = k_b \left[1 - \cos(\theta_{\alpha\beta} - \theta_0)\right]$$

- shear resistance of cytoskeleton

Fedosov, Caswell and Karniadakis. Biophys. J., 2010

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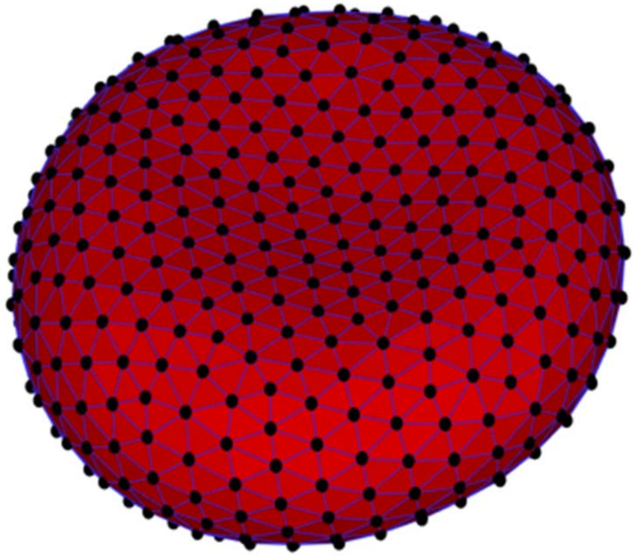
Multiscale RBC model

Triangular mesh:



- constant surface area

$$U_{AREA}(A) = \frac{k_A (A - A_0^{tot})^2}{2A_0^{tot}} + $$

$$+ \sum_{j \in 1 \ldots N_f} \frac{k_d (A_j - A_0)^2}{2A_0}$$

- constant volume

$$U_{VOLUME}(V) = \frac{k_V (V - V_0^{tot})^2}{2V_0^{tot}}$$

Fedosov, Caswell and Karniadakis. Biophys. J., 2010.

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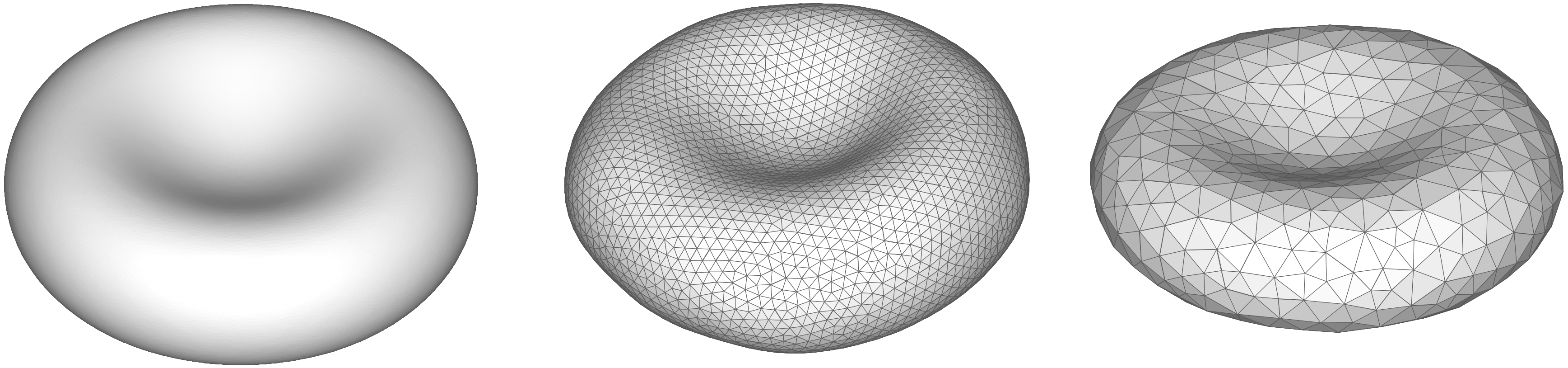
Spectrin-level/Coarse RBC Representation



N = 27344 $\qquad$ N = 3000 $\qquad$ N = 500

The membrane macroscopic elastic properties are found analytically for all representations: from spectrin-level to coarse-level.

Pivkin & Karniadakis, PRL, 2008

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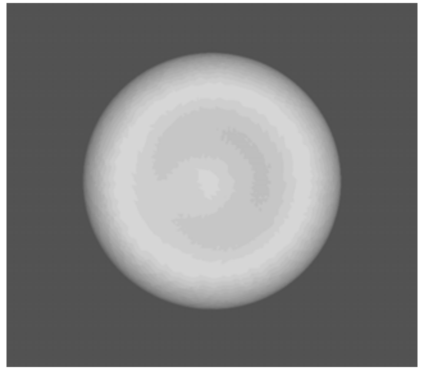
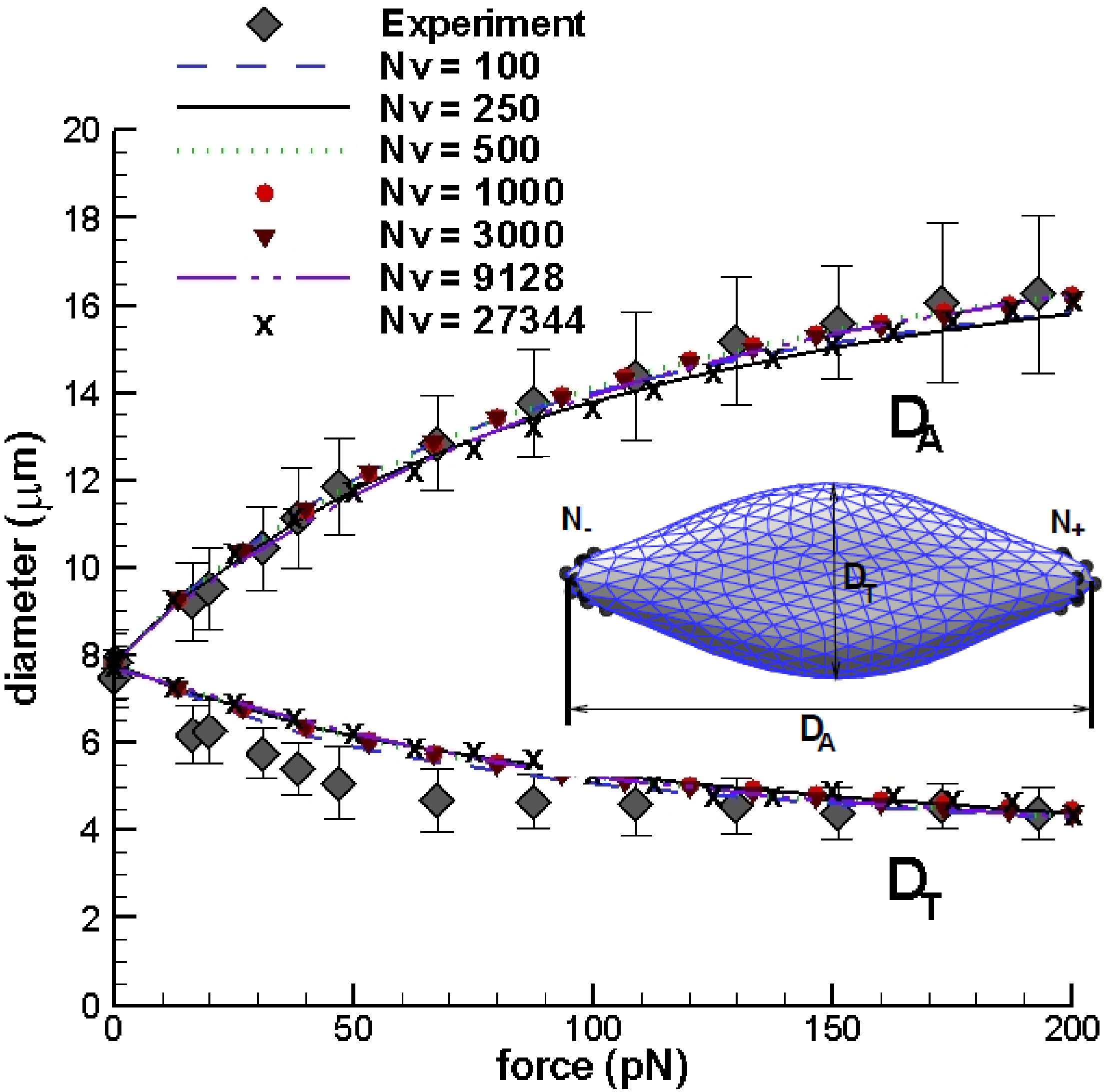
MS-RBC mechanics: healthy





$$\mu_0 = 6.3 \times 10^{-6} \, \frac{N}{m}$$

$$Y = 18.9 \times 10^{-6} \, \frac{N}{m}$$

$$k_c = 2.4 \times 10^{-19} J$$

Experiment - Suresh et al., *Acta Biomaterialia*, 1:15-30, 2005

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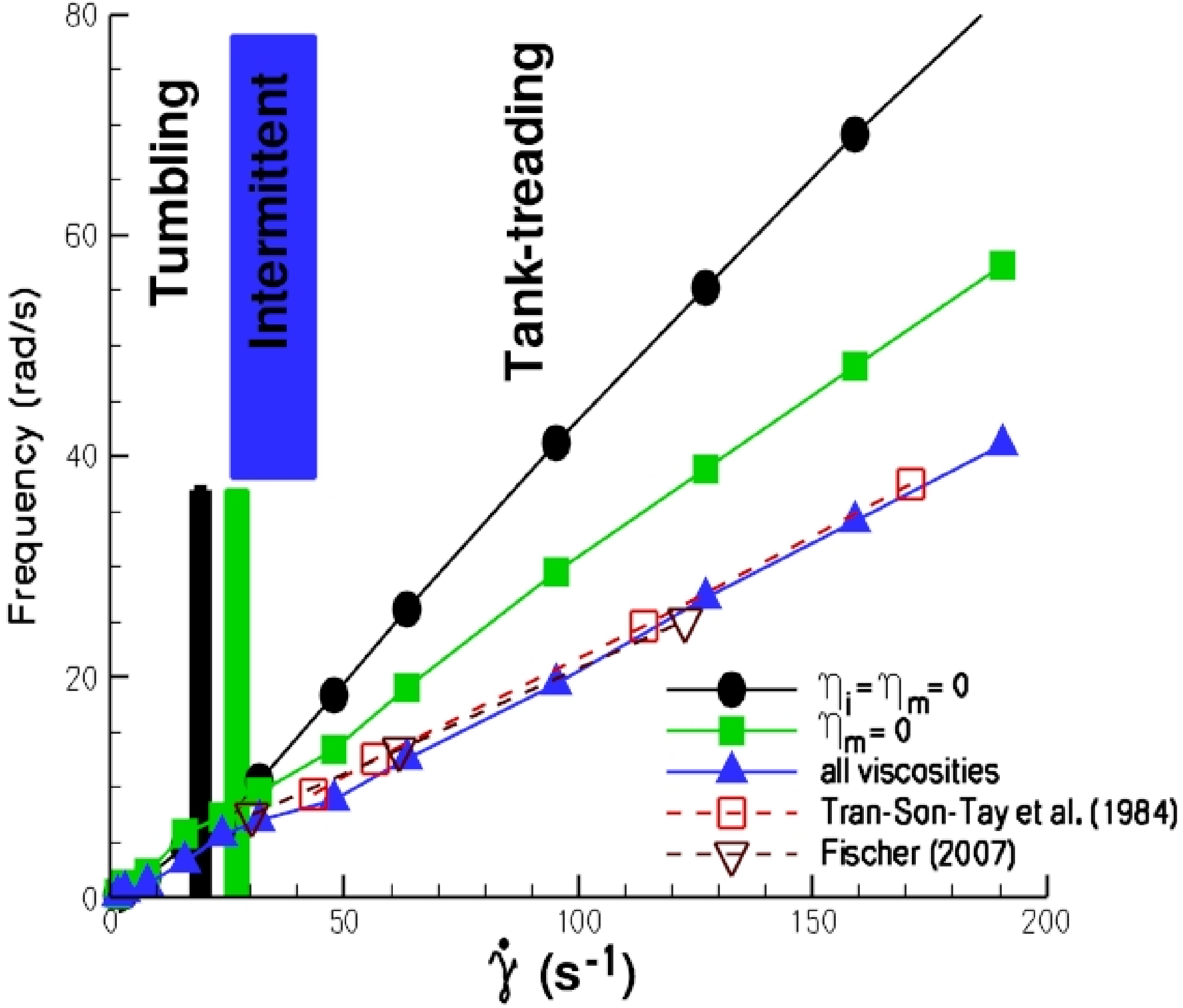
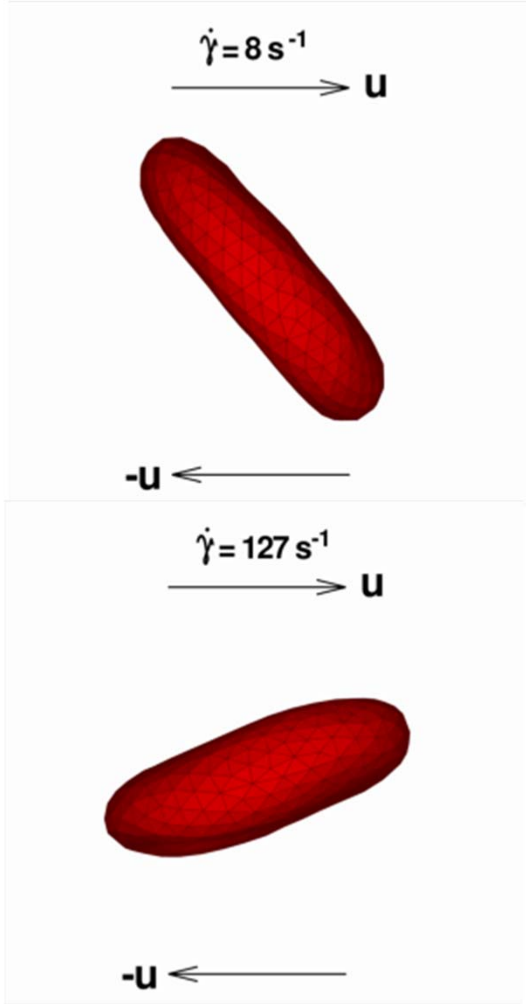
RBC dynamics in shear flow





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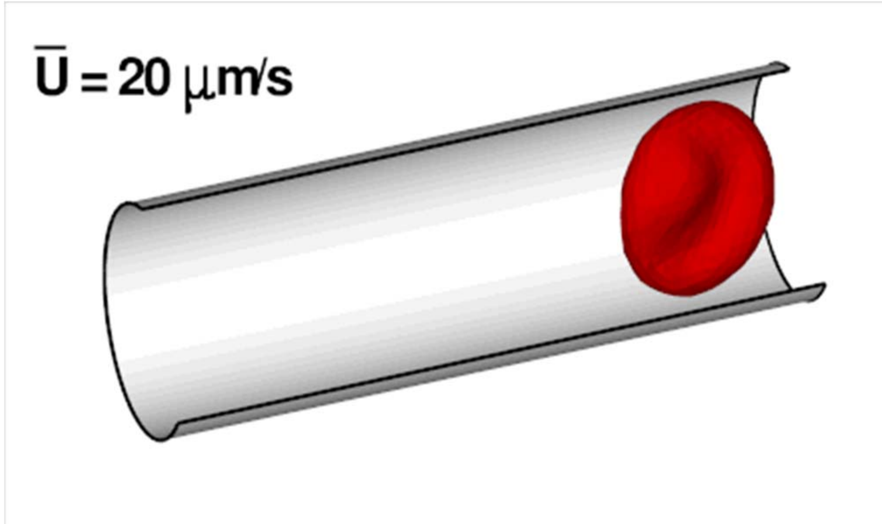
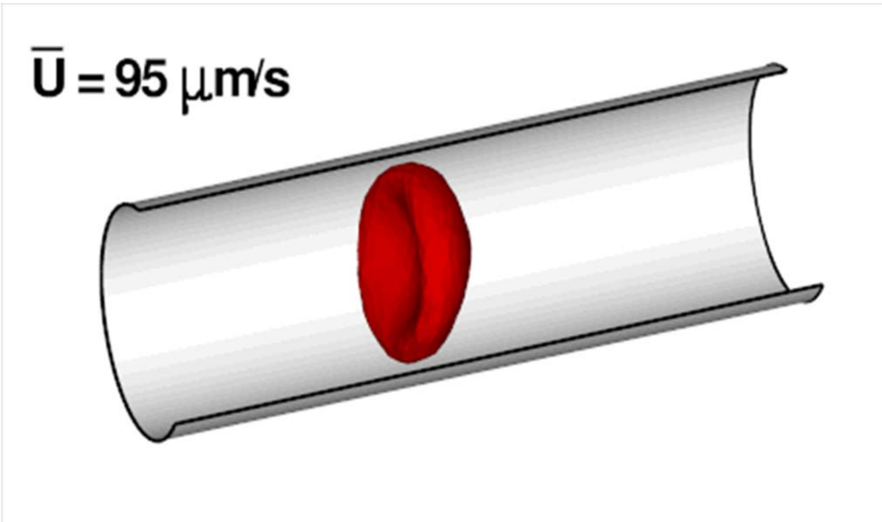
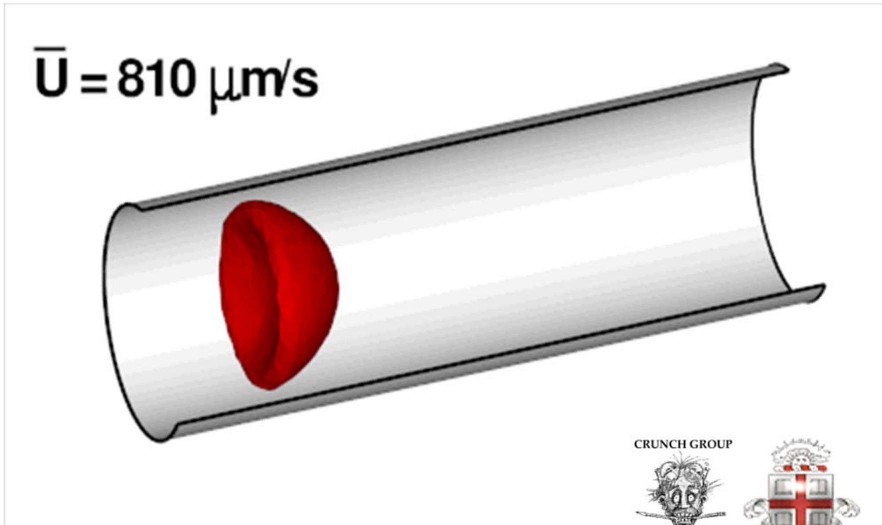
RBC dynamics in Poiseuille flow

D = 9 μm - tube diameter

C = 0.05 – RBC volume fraction







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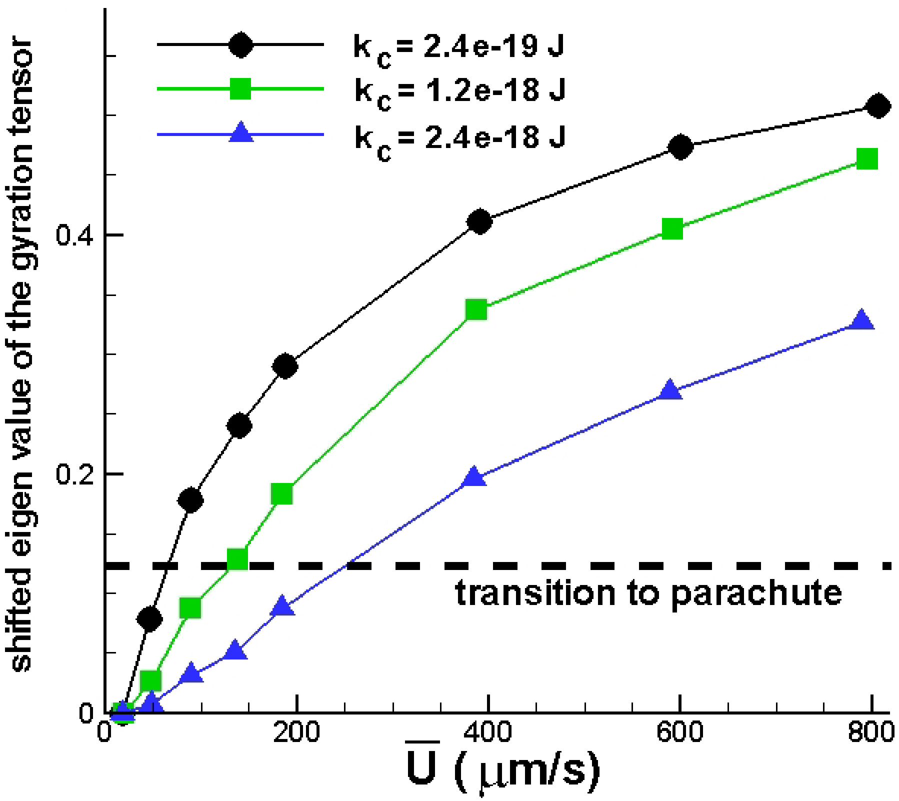
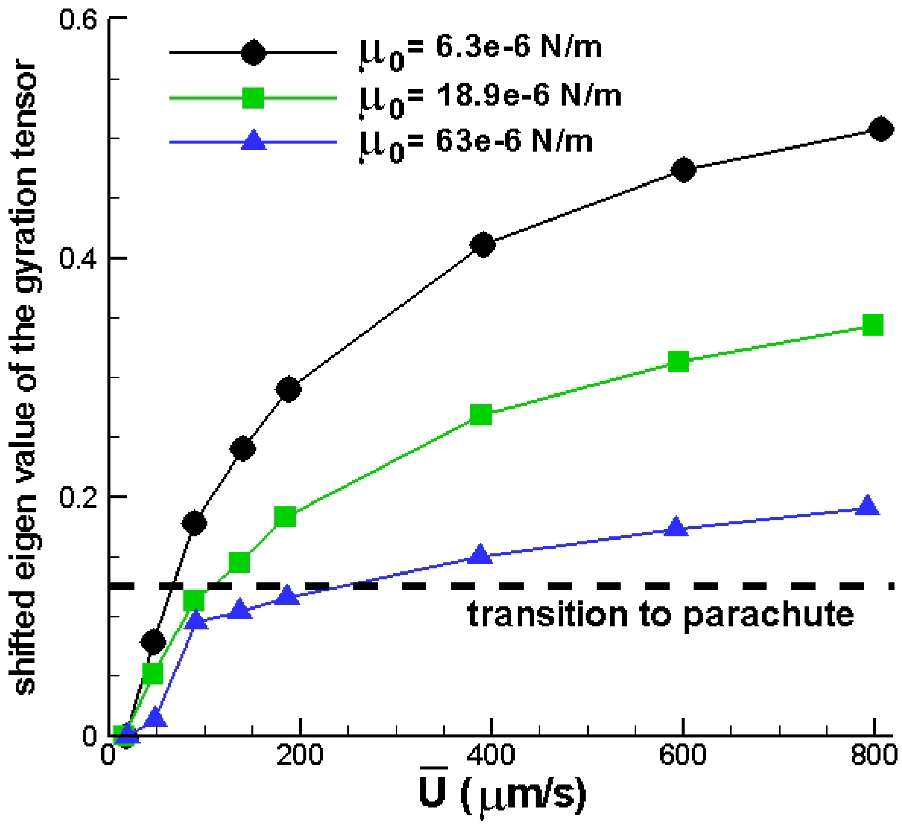
RBC dynamics in Poiseuille flow

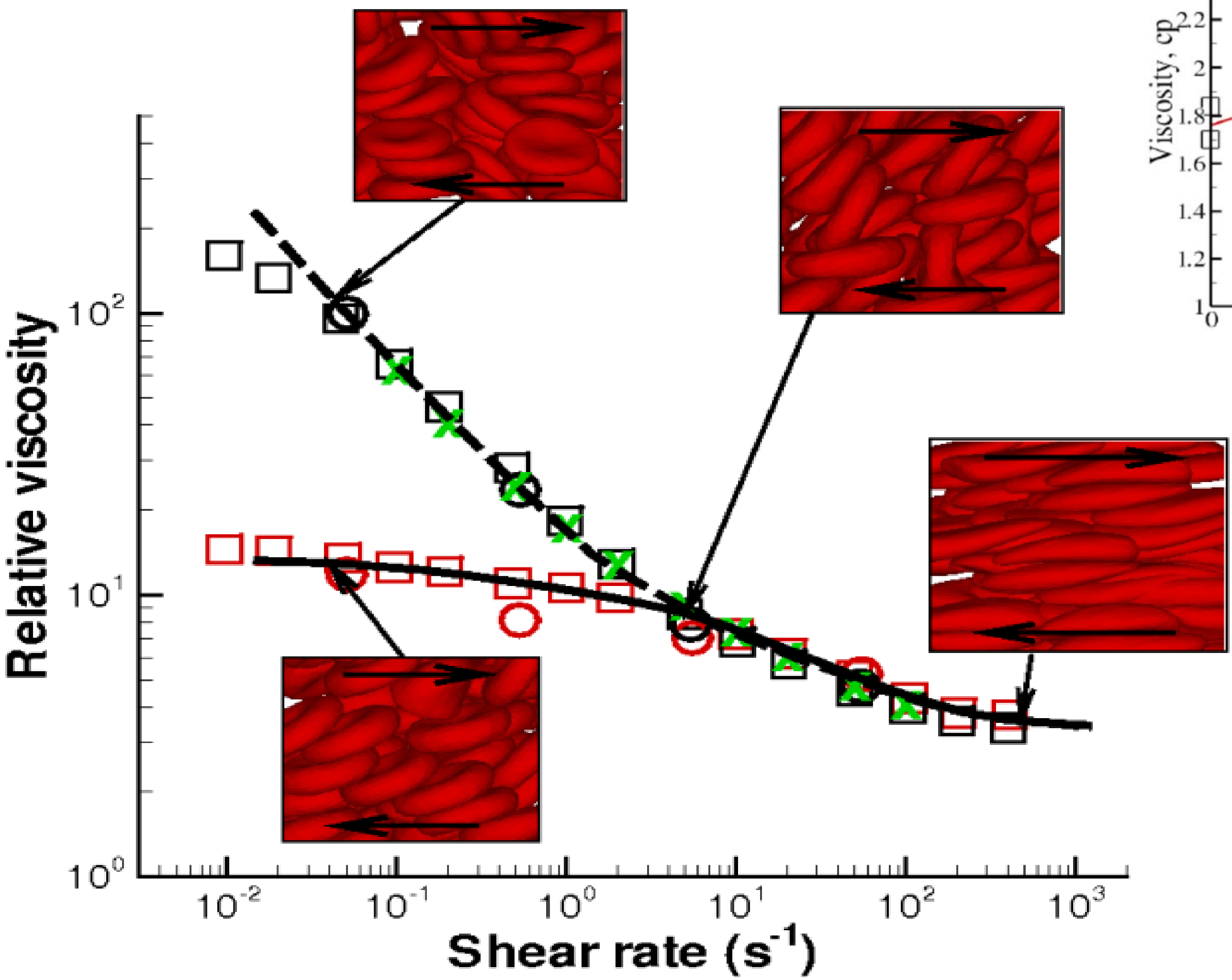
$$\overline{U} = \frac{\int v(r)dA}{A} \qquad G_{mn} = \frac{1}{N}\sum_i (r_m^i - r_m^{CM})(r_n^i - r_n^{CM})$$ - gyration tensor

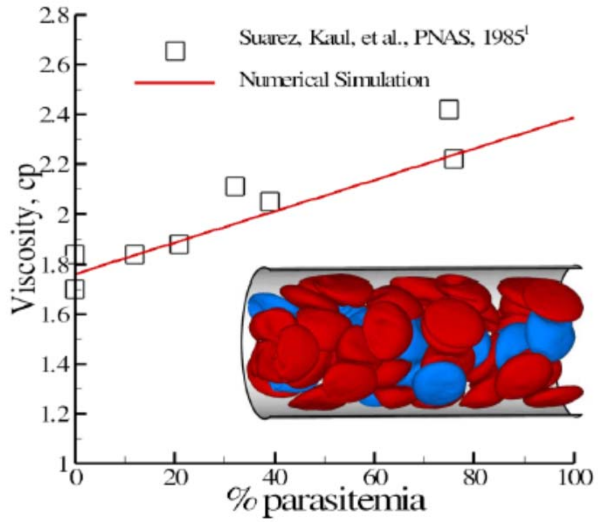




Prediction of Human Blood Viscosity *In Silico*

Healthy Blood



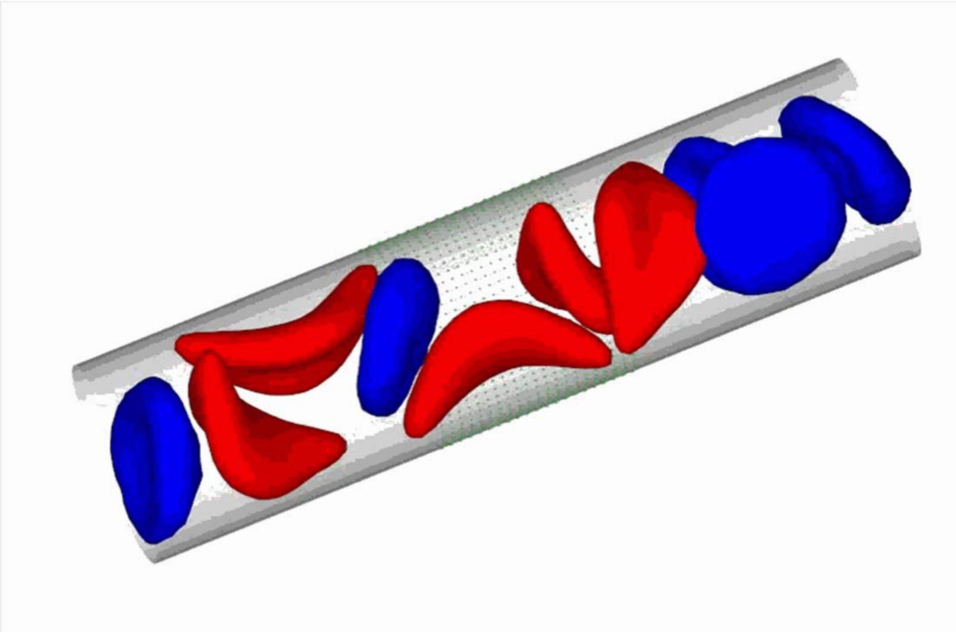


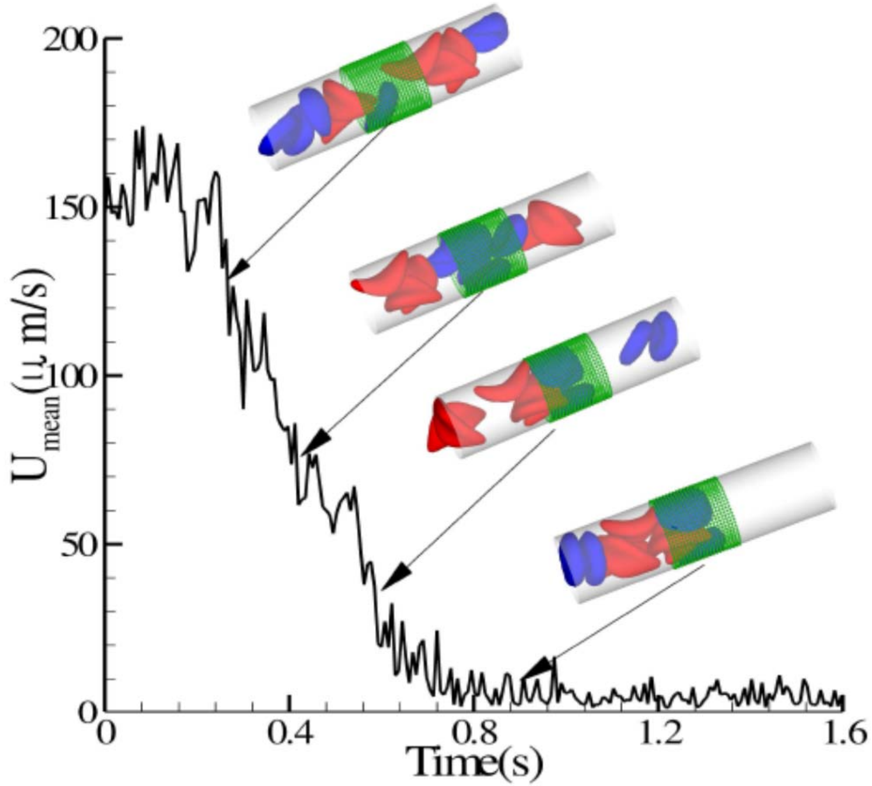
Malaria-infected Blood

<u>Fedosov, Pan, Caswell, Gompper & Karniadakis, PNAS, 2011</u>

Vaso-occlusion in sickle cell disease

Pipe flow (SS2 + SS4)





Deformable SS2 cells adherent to post capillary

Trap rigid SS4 cells (mostly Irreversible sickle cells)

Blood occlusion in post capillary

Lei & Karniadakis, PNAS, 2013

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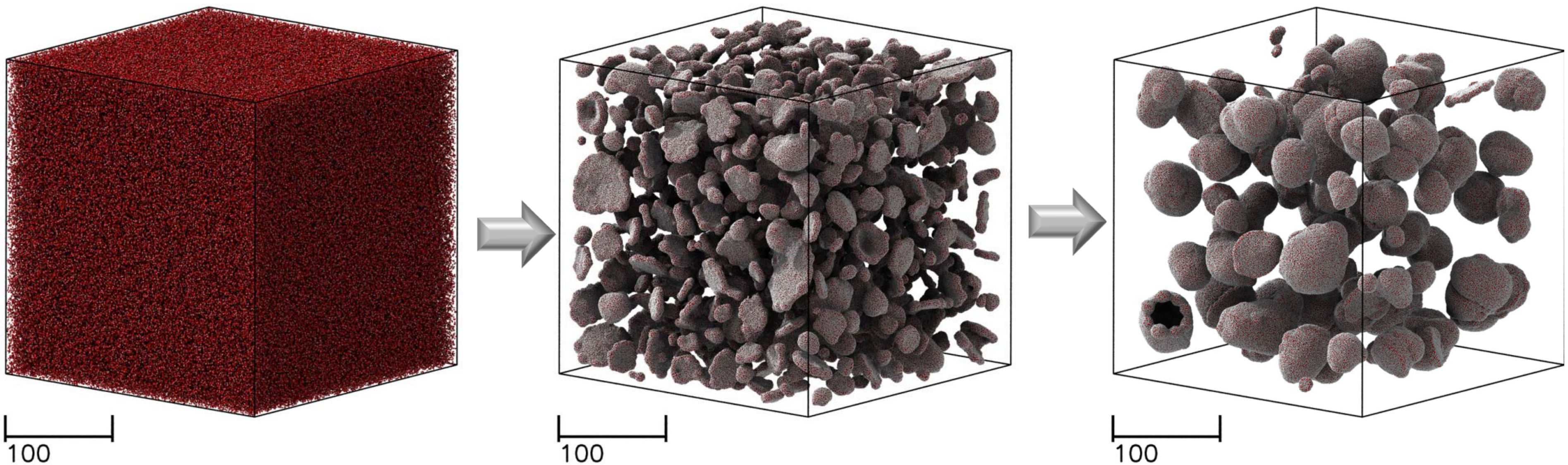
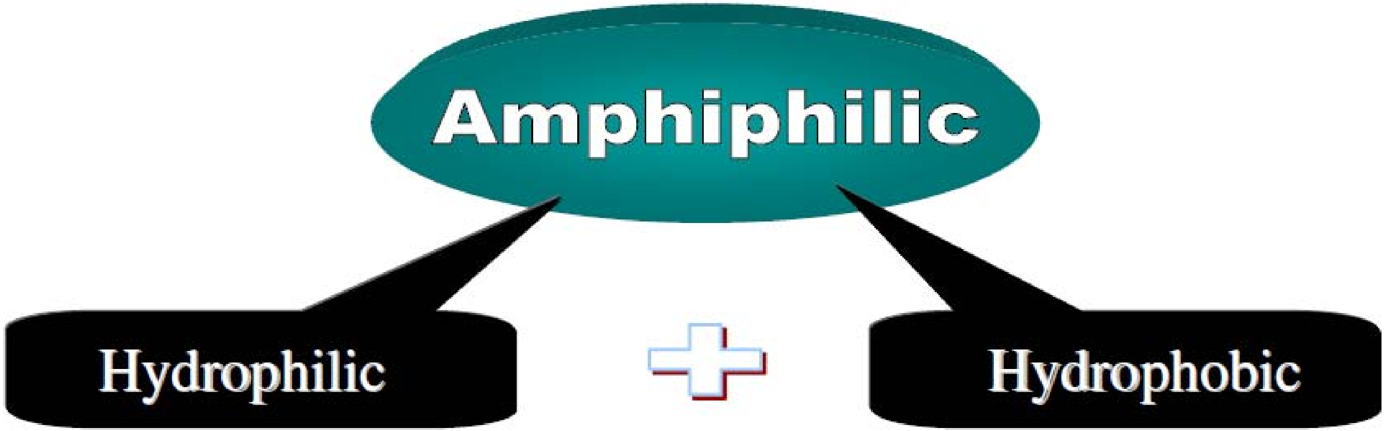
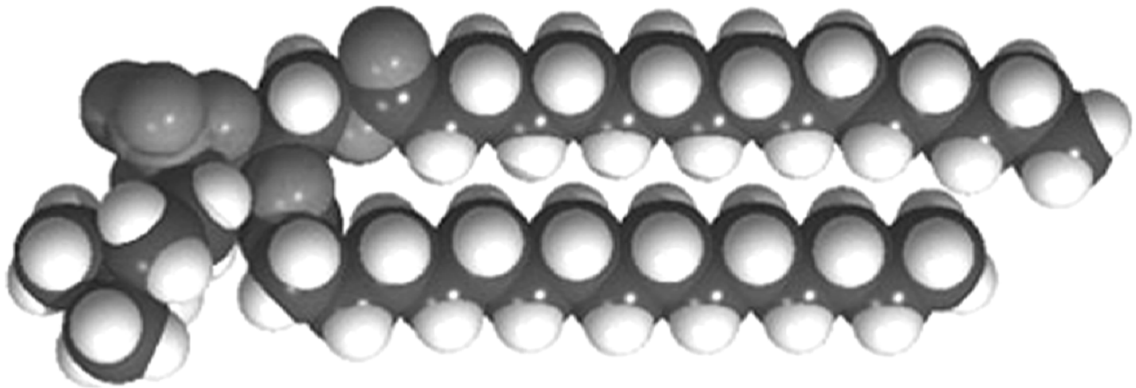
Amphiphilic self-assembly



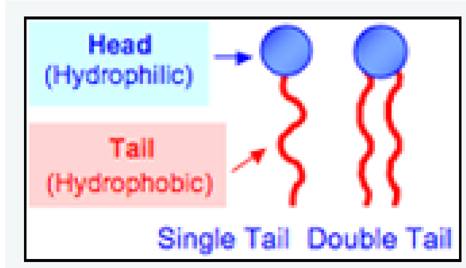
Self-assembled vesicles from 128M particle simulations

Amphiphilic self-assembly

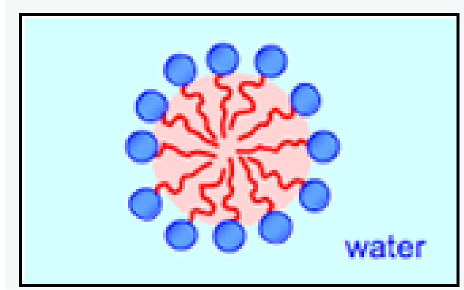




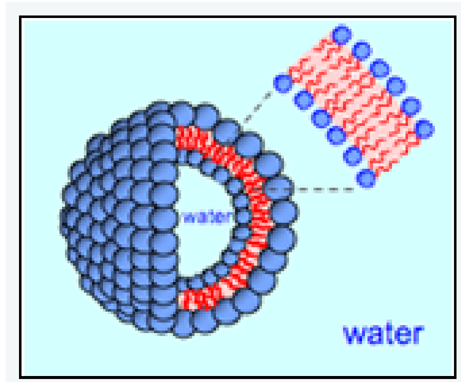
hydrophilic head *hydrophobic tail*



Amphiphilic molecule



Micelle



Vesicle

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Amphiphilic self-assembly

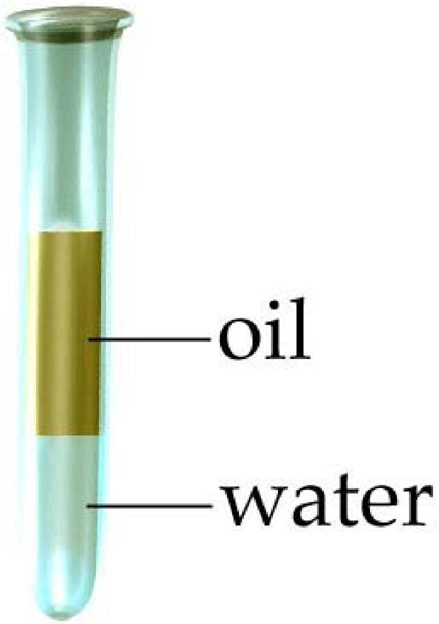
DPD repulsion parameter

$$\boxed{a_{ij} = a_{ii} + \Delta a}$$

Hydrophilic and hydrophobic molecules need differences in the repulsion parameters otherwise they would mix

How do we define 'not mixing' and separation ?

Phase separation: mean-field theory



$\chi N < 10.5$ homogeneous or disordered system

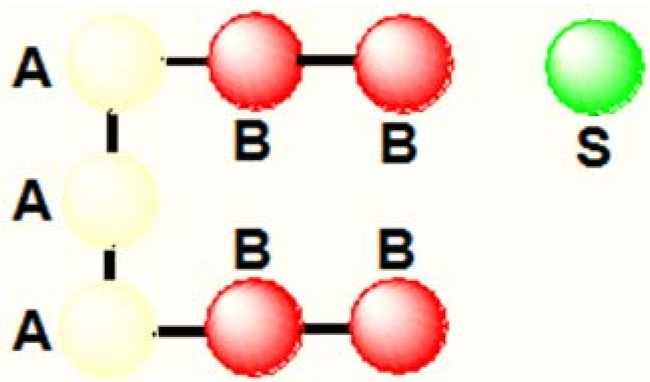
$\chi N \cong 10.5$ weak segregation demixing

$\chi N >> 10.5$ strong segregation demixing

$$\boxed{\frac{\chi N k_B T}{\Delta a} = 0.306 N}$$ [Groot & Warren (1997)]

Amphiphilic self-assembly

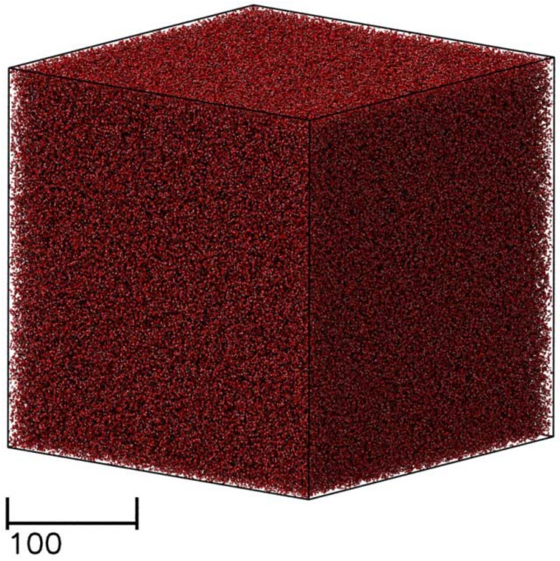
DPD model



A: hydrophilic

B: hydrophobic

S: solvent



Particle density: $\rho = 5$; Polymer length: $N = 7$

DPD parameters

Two alike particles

(A-A, B-B, S-S, A-S)

$$a_{ii} = 75 \frac{k_B T}{\rho r_c^4}$$

$$a_{ii} = 15$$

Two unlike particles

(A-B, B-S)

$$a_{ij} = a_{ii} + \Delta a$$

$$\frac{\chi N k_B T}{\Delta a} = 0.306N$$

$\chi N \sim 32.1$

strong segregation regime

$$a_{ij} = 120$$

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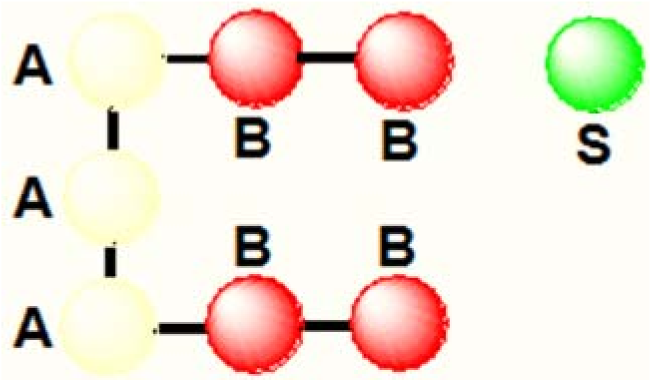
Amphiphilic self-assembly



A: hydrophilic

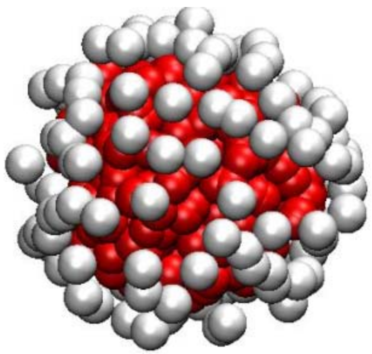
B: hydrophobic

S: solvent

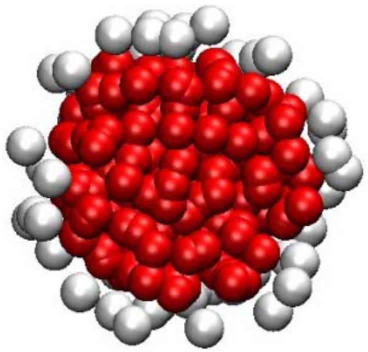
Repulsive parameters:

$$a_{ij} = \begin{array}{c} \\ A \\ B \\ S \end{array} \begin{array}{c} \begin{matrix} A & B & S \end{matrix} \\ \begin{pmatrix} 15 & 120 & 15 \\ 120 & 15 & 120 \\ 15 & 120 & 15 \end{pmatrix} \end{array}$$

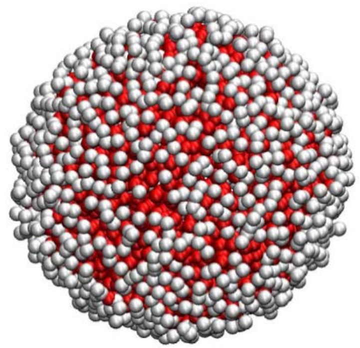
Self-assembled microstructures:



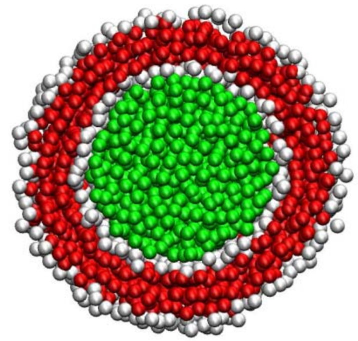
spherical micelle



slice



vesicle



slice

<u>**Li, Tang, Liang & Karniadakis, Chem Commun, 2014**</u>

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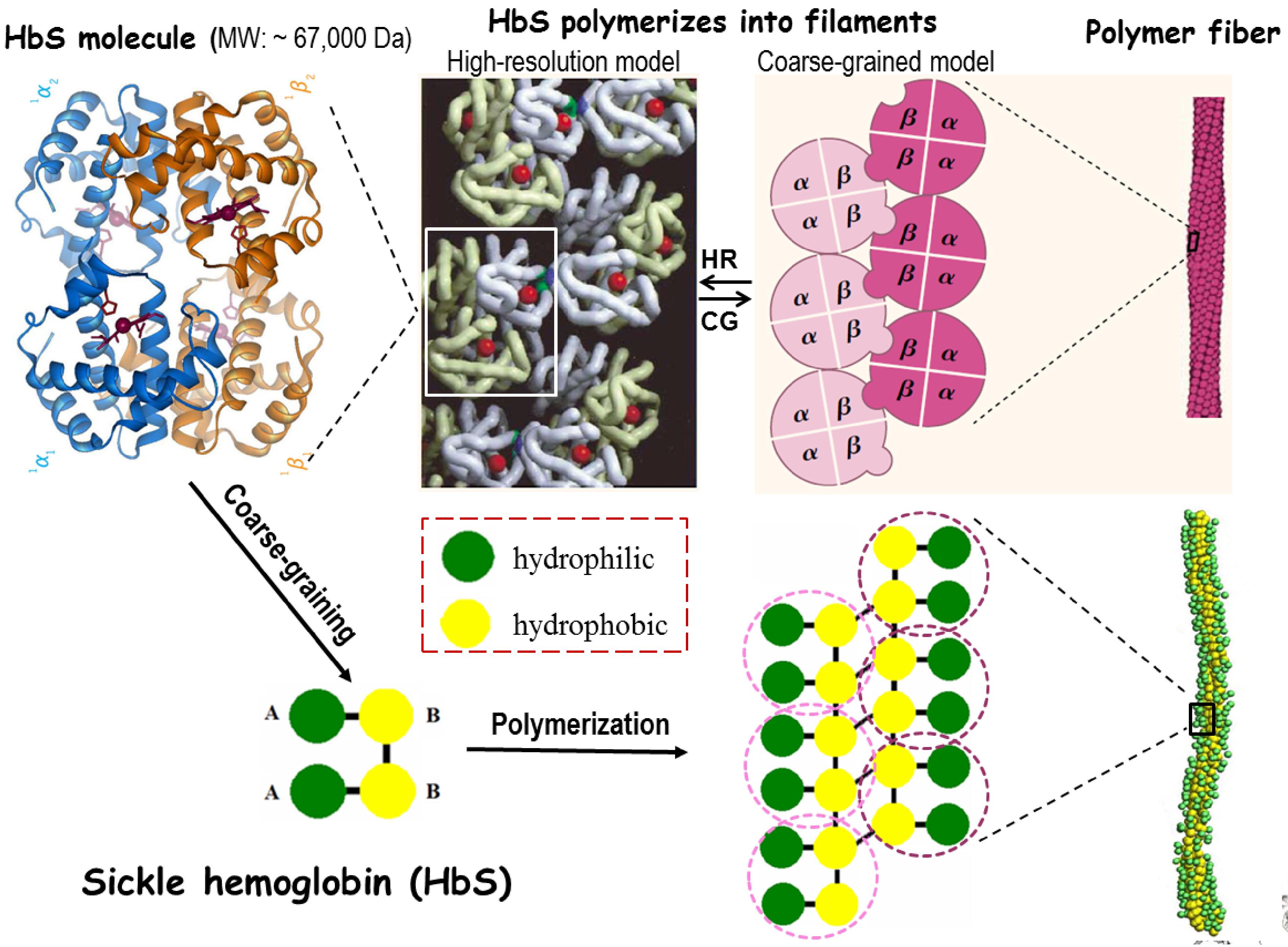
Chirality controls molecular self-assembly



Chirality controls molecular self-assembly

DPD interactions:

$$V_{\text{tot}} = V_{\text{bonded}} + V_{\text{nonbonded}} = \left(V_{\text{str}} + V_{\text{bend}} + V_{\text{tors}}\right) + \left(V_{\text{vdw}} + V_{\text{es}} + \cdots\right)$$

Bonded interactions:

Hookean spring interaction:

$$V_{\text{str}} = k_{\text{str}}\left(r - r_0\right)^2$$

(a)

Bond-bending interaction:

$$V_{\text{bend}} = k_{\text{bend}}\left(\theta - \theta_0\right)^2$$

(b1)

Control chain rigidity

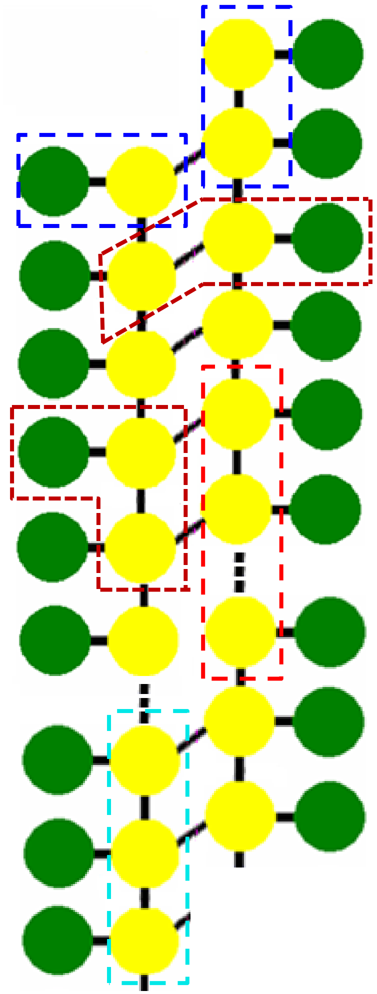
(b2)

Bending FENE interaction:

$$F_{\text{FENE}} = k_{\text{BEND}}\left[\frac{\theta - \theta_0}{1 - (\theta - \theta_0)/\Delta\theta_{\max}}\right]$$

(c)

Describe chain chirality

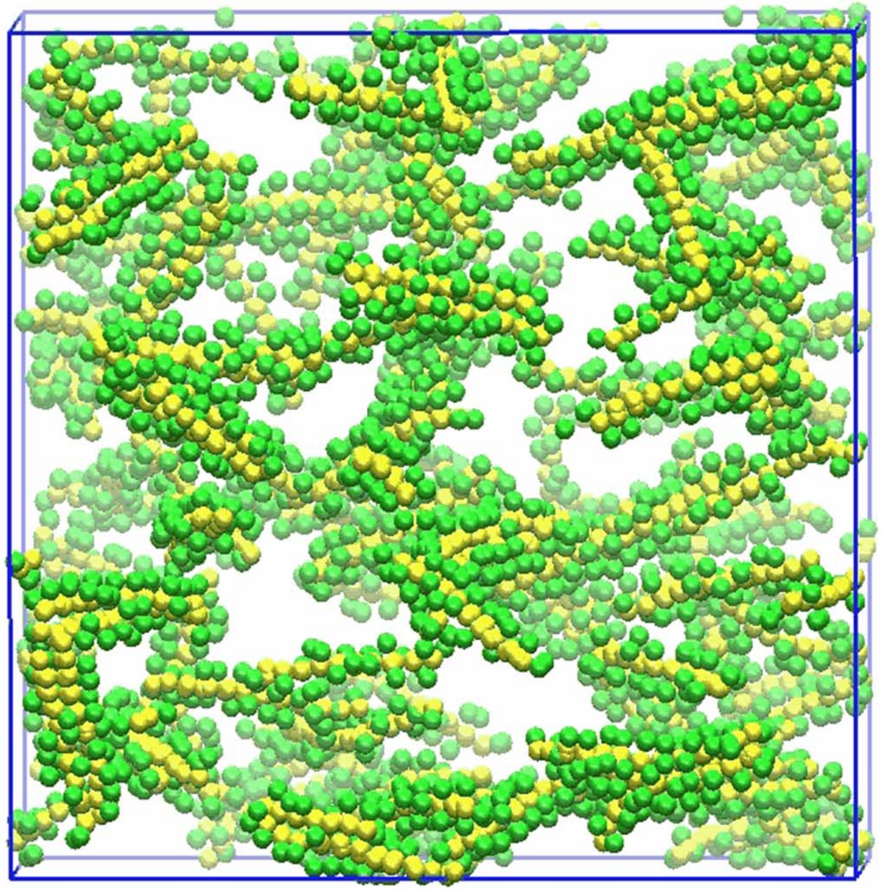


Non-bonded interactions:

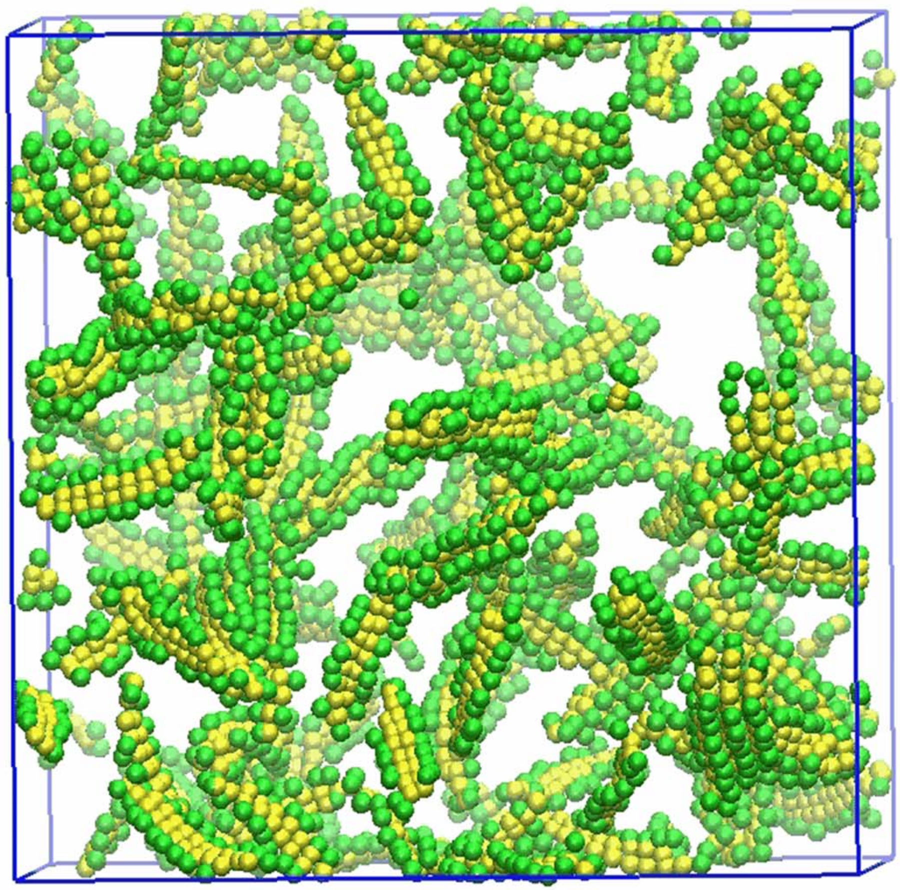
Pairwise DPD conservative interaction:

$$V_{\text{non-bonded}} = -\frac{a_{ij}}{2}\left(1 - r_{ij}/r_c\right)^2$$

Chirality controls molecular self-assembly



Elongated step-like fiber



Elongated sheet-like membrane

<u>Li, Caswell & Karniadakis, Biophys. J., 2012</u>

Summary

Dissipative Particle Dynamics is a powerful tool to

- treat boundary conditions in microchannel flows
- simulate the dynamic and rheological properties of simple and complex fluids
- understand the dynamic behavior of polymer and DNA chains
- model blood flow in health and disease

The future of DPD

- Multiscale modeling: MD – DPD – SDPD - SPH
- Complex fluids and complex geometries
- Parameterization development for simulating real fluids
- Structural models

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