JÜLICH FORSCHUNGSZENTRUM

Vesicles and Red Blood Cells in Microcapillary Flows

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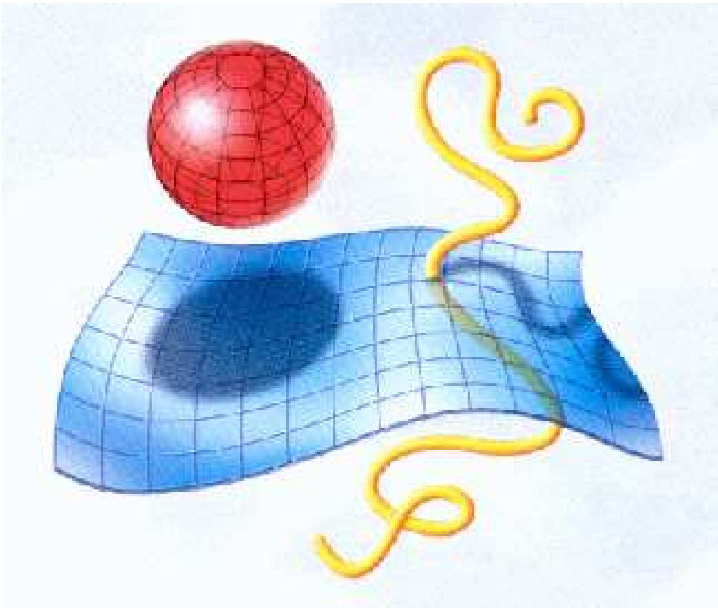
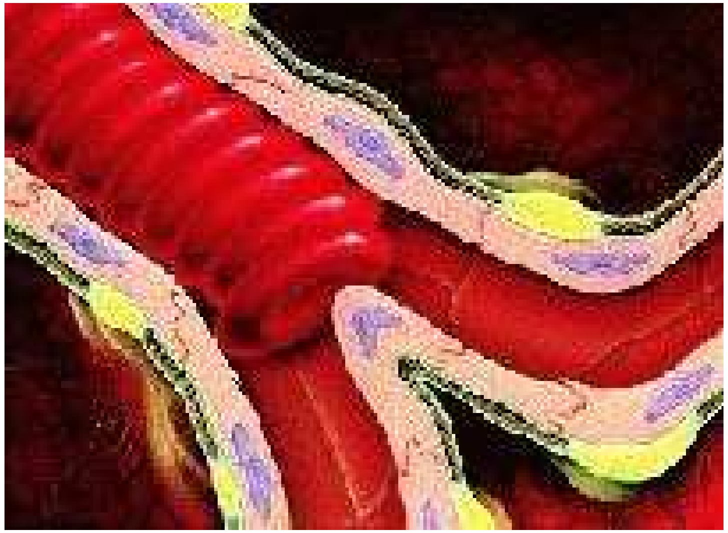
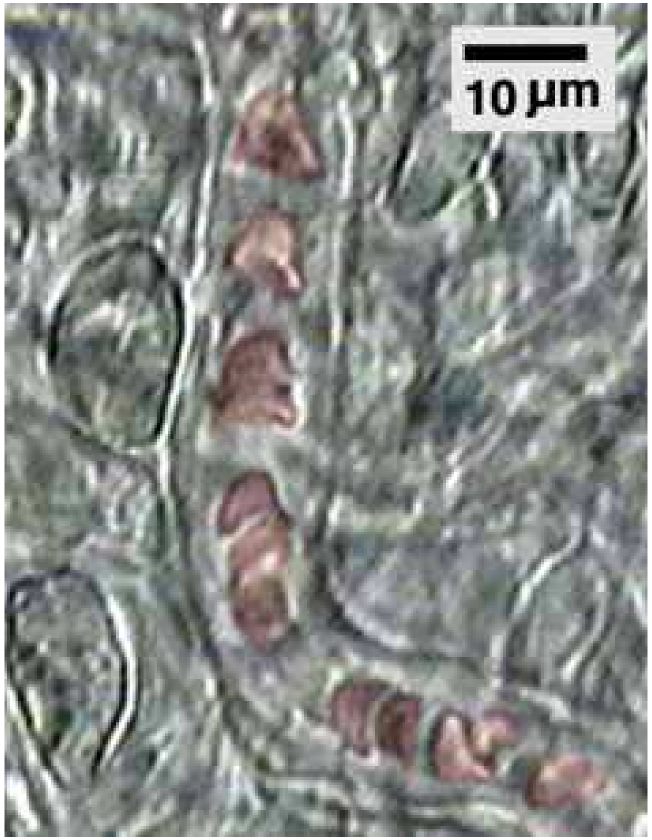


Soft Matter Hydrodynamics

Cells and vesicles in flow:

- Red blood cells in microvessels:



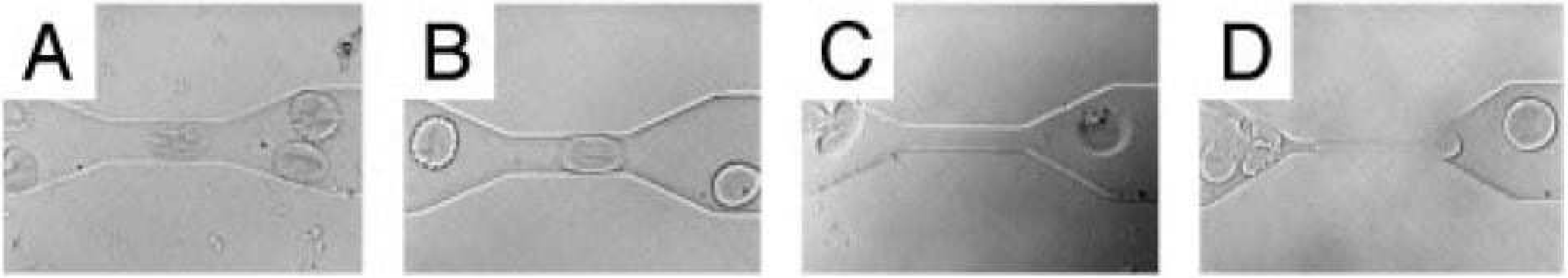


Diseases such as diabetes reduce deformability of red blood cells!

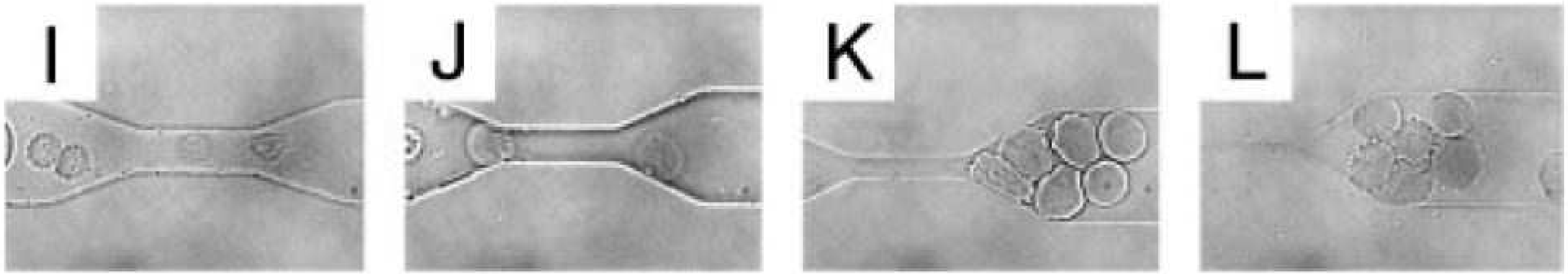
Soft Matter Hydrodynamics

Example: Flow behavior of malaria-infected red blood cells in microchannels

Just after infection:



Late stage:



Diameter: 8 μm 6 μm 4 μm 2 μm

J.P. Shelby et al., Proc. Natl. Acad. Sci. **100** (2003)

Mesoscale Flow Simulations

Complex fluids: length- and time-scale gap between

- atomistic scale of solvent
- mesoscopic scale of dispersed particles (colloids, polymers, membranes)

$\longrightarrow$ **Mesoscale Simulation Techniques**

Basic idea:

- drastically simplify dynamics on molecular scale
- respect conservation laws for mass, momentum, energy

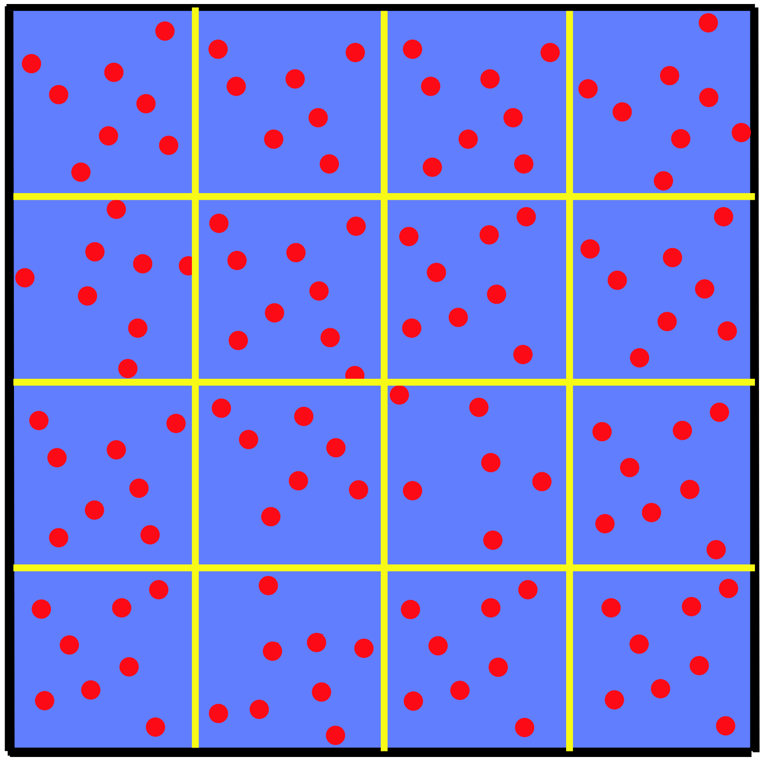
Examples:

- Lattice Boltzmann Method (LBM)
- Dissipative Particle Dynamics (DPD)
- Multi-Particle-Collision Dynamics (MPC)

Alternative approach: Hydrodynamic interactions via Oseen tensor

Mesoscale Hydrodynamics Simulations

Multi-Particle-Collision Dynamics (MPC)



- coarse grained fluid
- point particles
- off-lattice method
- collisions inside “cells”
- thermal fluctuations

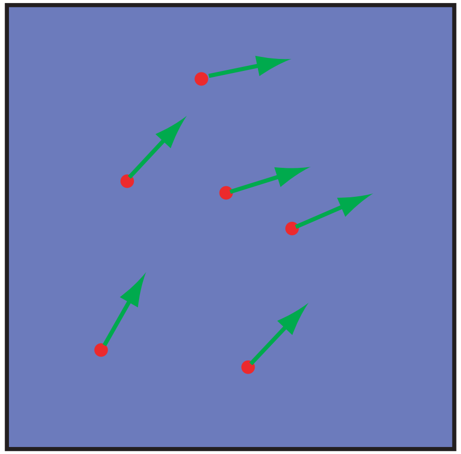
A. Malevanets and R. Kapral, J. Chem. Phys. **110** (1999)

A. Malevanets and R. Kapral, J. Chem. Phys. **112** (2000)

Multi-Particle Collision Dynamics (MPC)

Flow dynamics: Two step process

Streaming



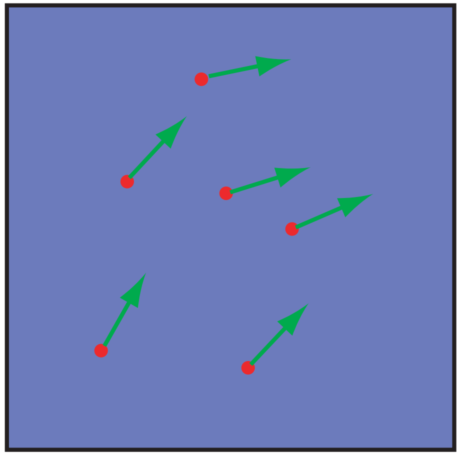
- ballistic motion

  $$\mathbf{r}_i(t+h) = \mathbf{r}_i(t) + \mathbf{v}_i(t)h$$

Multi-Particle Collision Dynamics (MPC)

Flow dynamics: Two step process

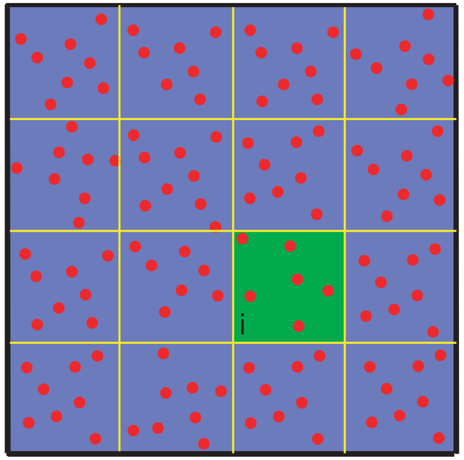
Streaming

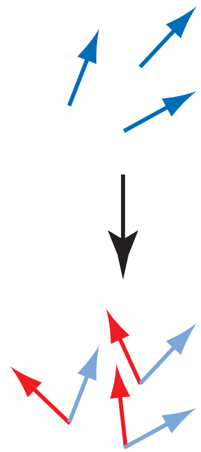


- ballistic motion

$$\mathbf{r}_i(t+h) = \mathbf{r}_i(t) + \mathbf{v}_i(t)h$$

Collision





- mean velocity per cell

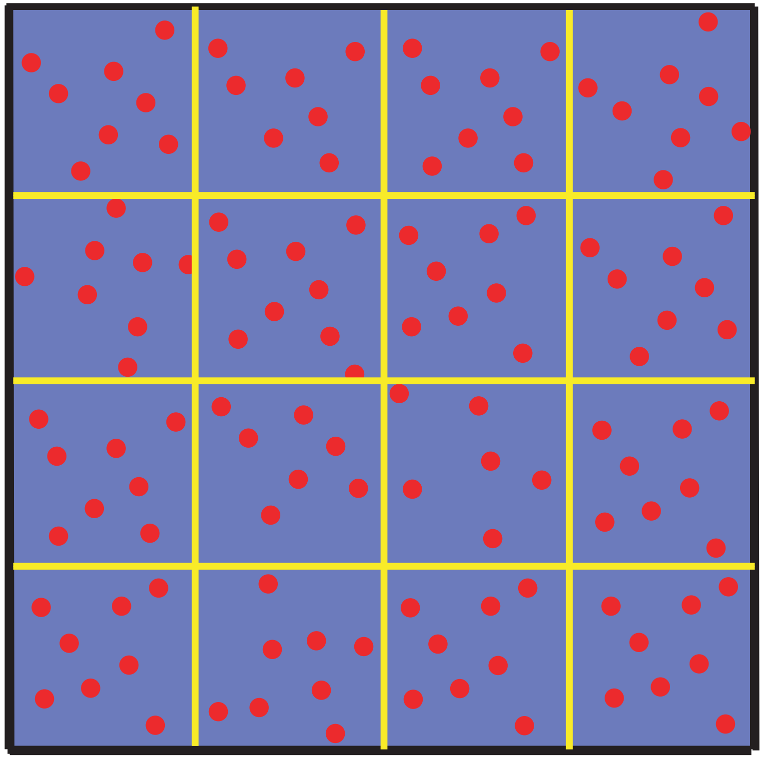
$$\bar{\mathbf{v}}_i(t) = \frac{1}{n_i}\sum_{j\in C_i}^{n_i} \mathbf{v}_j(t)$$

- rotation of relative velocity by angle α

$$\mathbf{v}_i' = \bar{\mathbf{v}}_i + \mathbf{D}(\alpha)(\mathbf{v}_i - \bar{\mathbf{v}}_i)$$

Mesoscale Flow Simulations: MPC

- Lattice of collision cells: breakdown of Galilean invariance
- Restore Galilean invariance exactly: random shifts of cell lattice



T. Ihle and D.M. Kroll, Phys. Rev. E **63** (2001)

Mesoscale Flow Simulations: MPC

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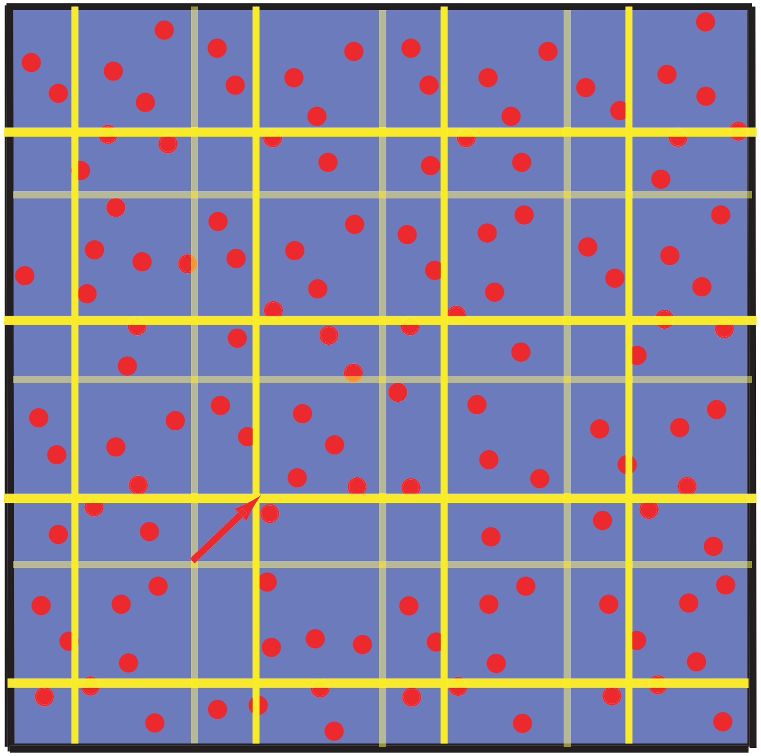


T. Ihle and D.M. Kroll, Phys. Rev. E **63** (2001)

Low-Reynolds-Number Hydrodynamics

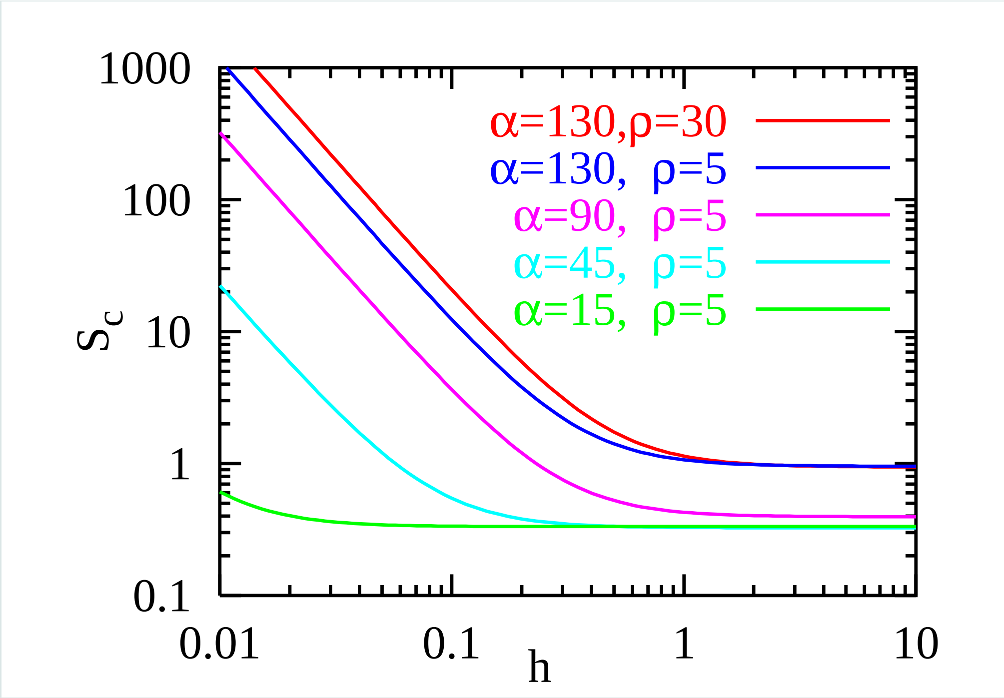
- Reynolds number $Re = v_{\rm max} L/\nu \sim$ inertia forces / friction forces

  For soft matter systems with characteristic length scales of μm:

  $Re \simeq 10^{-3}$

- Schmidt number $Sc = \nu/D \sim$ momentum transp. / mass transp.

  Gases: $Sc \simeq 1$, liquids: $Sc \simeq 10^3$



M. Ripoll, K. Mussawisade, R.G. Winkler and G. Gompper, Europhys. Lett. **68** (2004)

Other MPC Methods

- Anderson thermostat (MPC-AT-a):

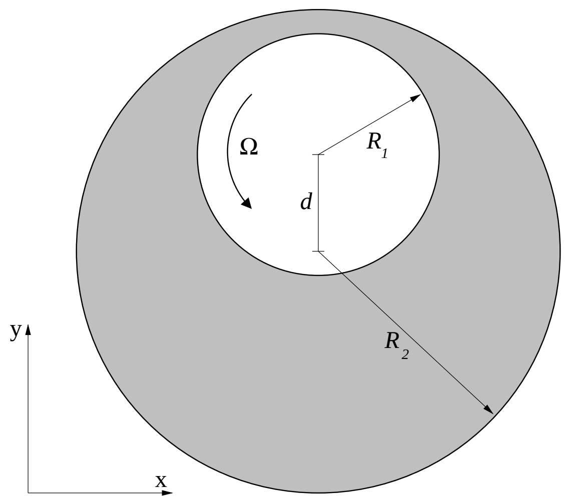
  Choose new relative velocities from Maxwell-Boltzmann distribution

- Angular-momentum conservation (MPC-AT+a):

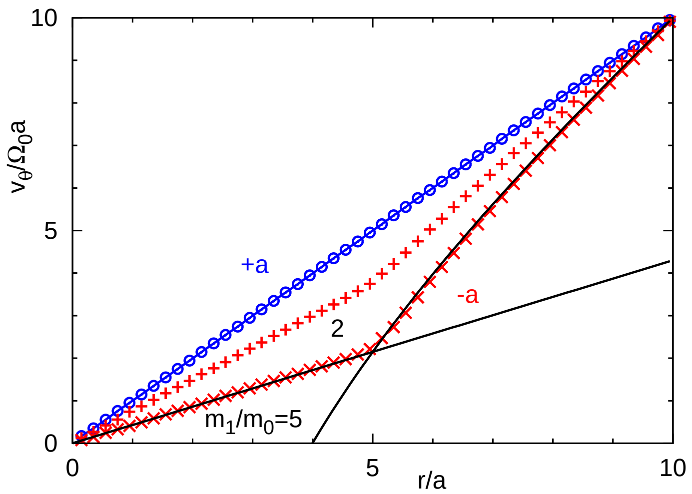
  Modify collision rule to conserve angular momentum

- Importance of angular-momentum conservation:

  Rotating fluid drop with different viscosity in circular Couette flow



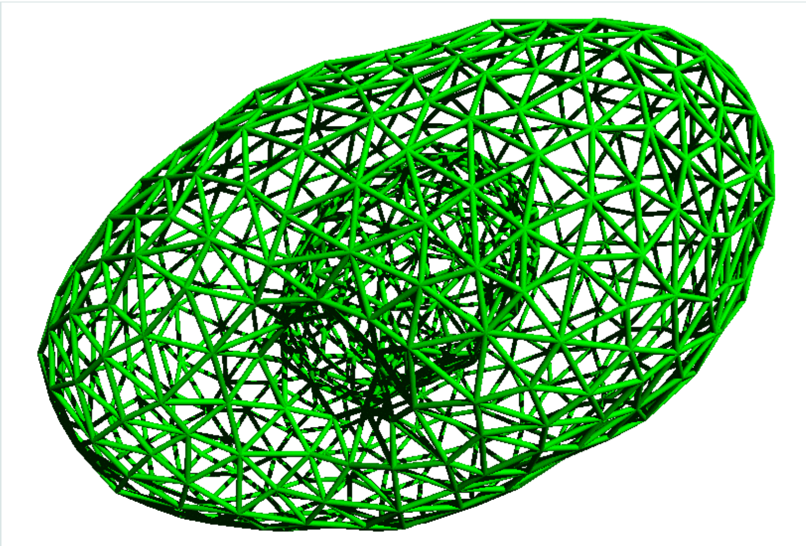
Angular velocity profile:



H. Noguchi, N. Kikuchi, G. Gompper, Europhys. Lett. **78** (2007); I.O. Götze, H. Noguchi, G. Gompper, Phys. Rev. E **76** (2007)

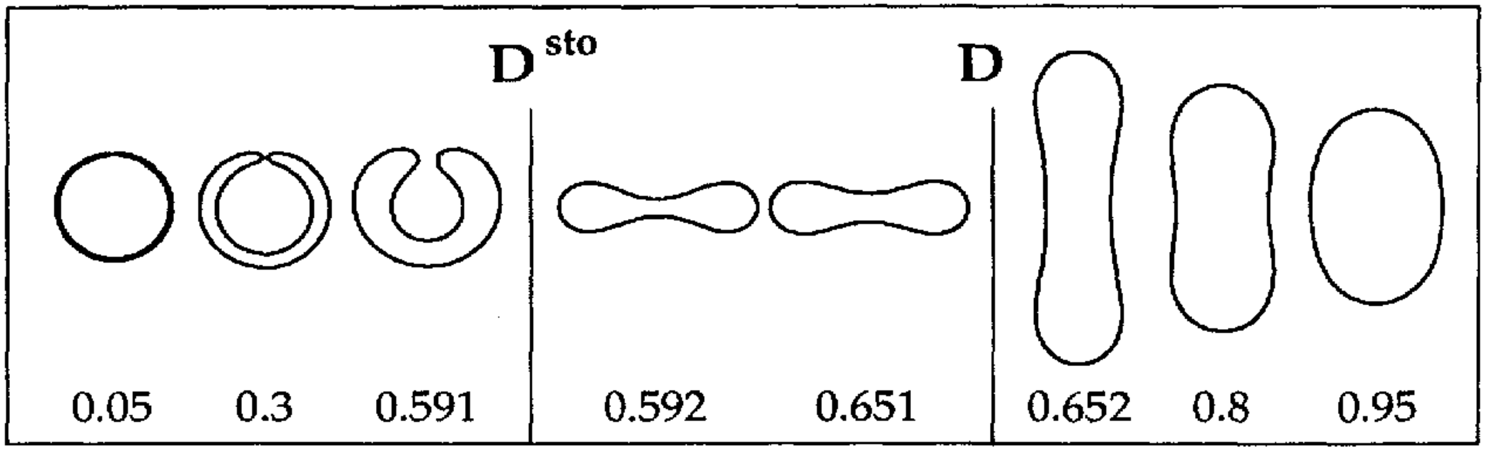
Membranes

Hydrodynamics of Membranes and Vesicles



Equilibrium Vesicle Shapes

Minimize curvature energy for fixed area $A = 4\pi R_0^2$ and reduced volume $V^* = V/V_0$, where $V_0 = 4\pi R_0^3/3$:

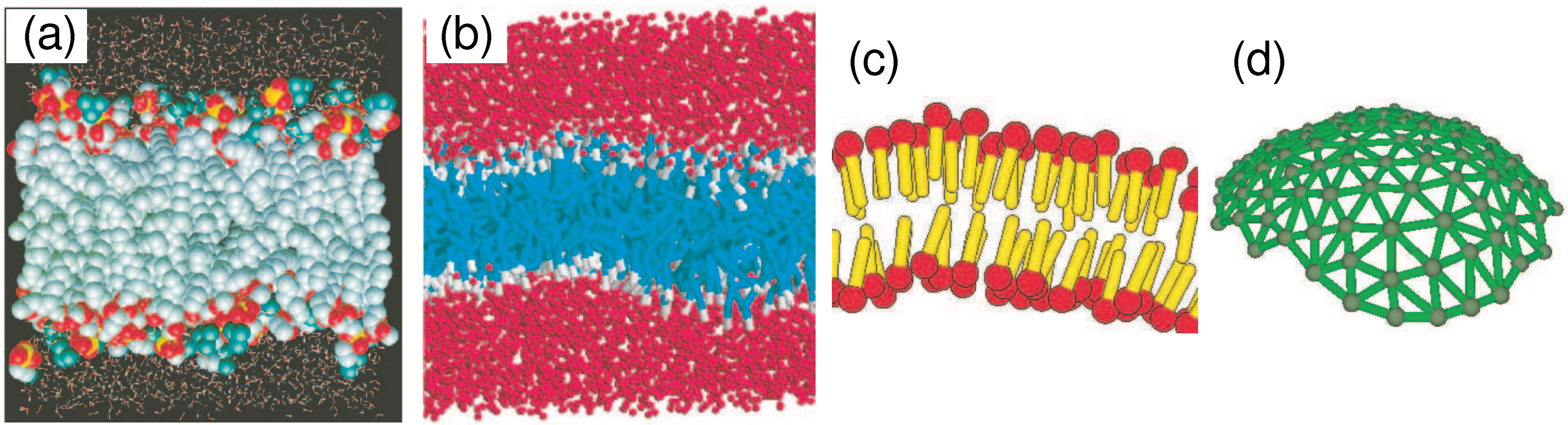


stomatocyte discoctyte prolate

U. Seifert, K. Berndl, and R. Lipowsky, Phys. Rev. A **44** (1991)

Simulations of Membranes

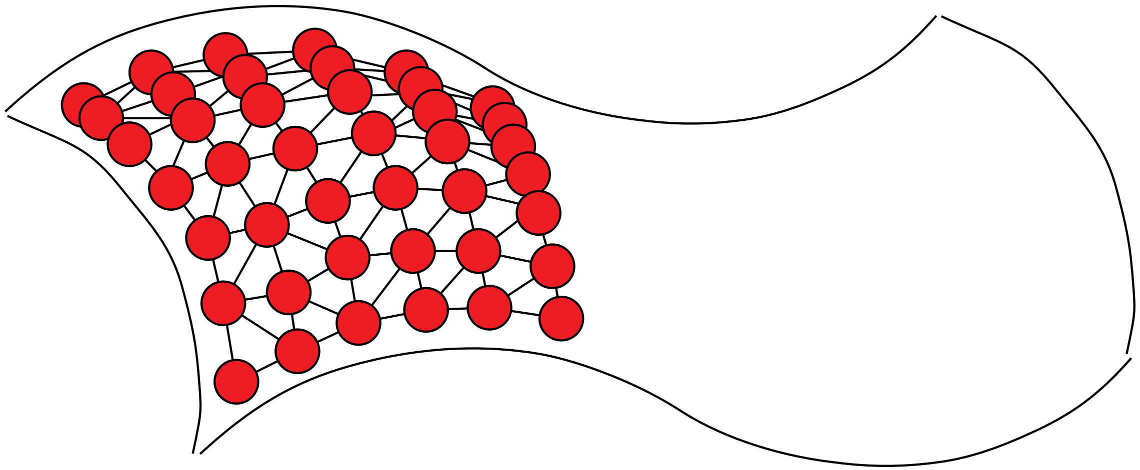
Modelling of membranes on different length scales:



atomistic coarse-grained solvent-free triangulated

Simulations of Membranes

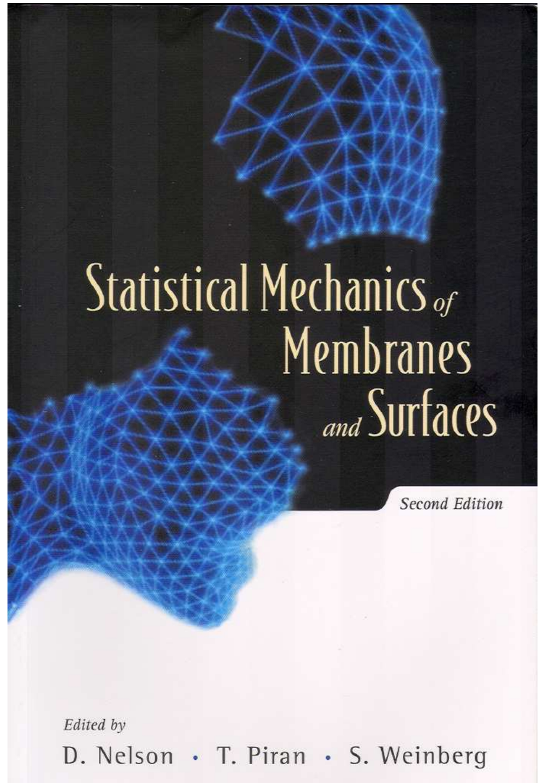
Dynamically triangulated surfaces



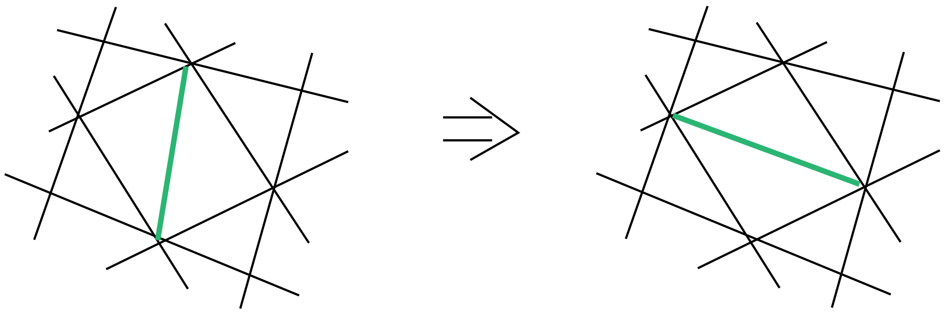
Hard-core diameter σ

Tether length L: $\sigma < L < \sqrt{3}\,\sigma$

--> self-avoidance



Dynamic triangulation:



G. Gompper & D.M. Kroll (2004)

Membrane Hydrodynamics

Interaction between membrane and fluid:

- Streaming step:

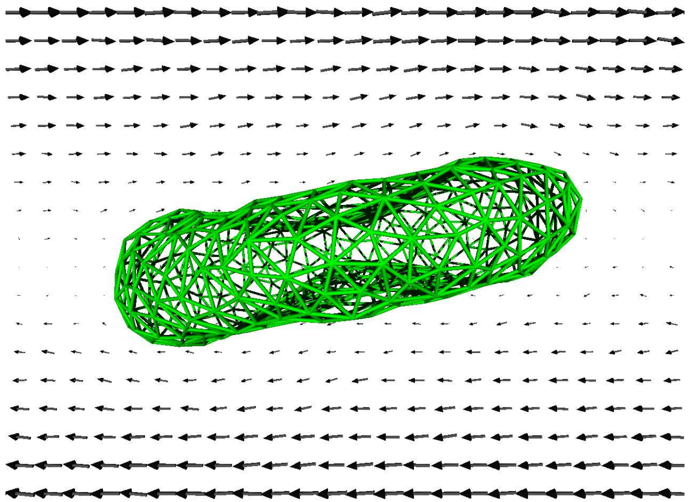
  bounce-back scattering of solvent particles on triangles

- Collision step:

  membrane vertices are included in MPC collisions

implies impenetrable membrane

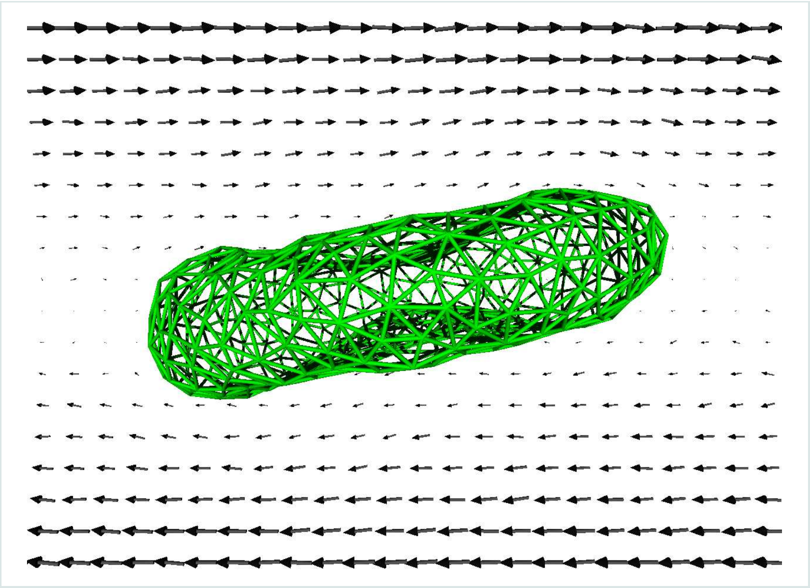
with no-slip boundary conditions.



H. Noguchi and G. Gompper, Phys. Rev. Lett. **93** (2004); Phys. Rev. E **72** (2005)

Membrane Hydrodynamics

Vesicle Dynamics in Shear Flow



Vesicles in Shear Flow

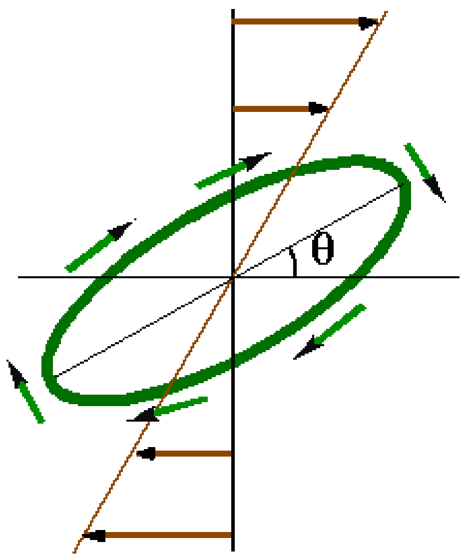
Parameter: shear rate $\dot{\gamma}$

Variables:

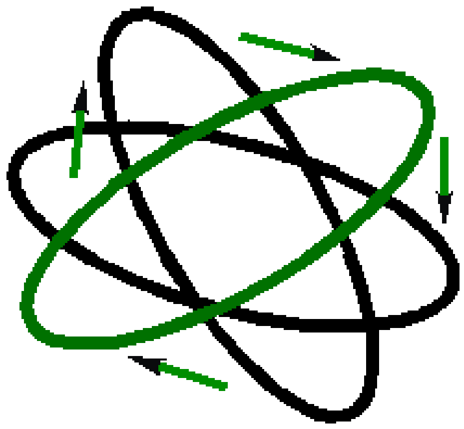
- Reduced volume V^*
- Shape
- Membrane viscosity η_{mb}
- Internal viscosity η_{in}

Behavior in shear flow:

- Tank-treading
- Tumbling
- Swinging (vacillating-breathing, trembling)
- Shape transformations

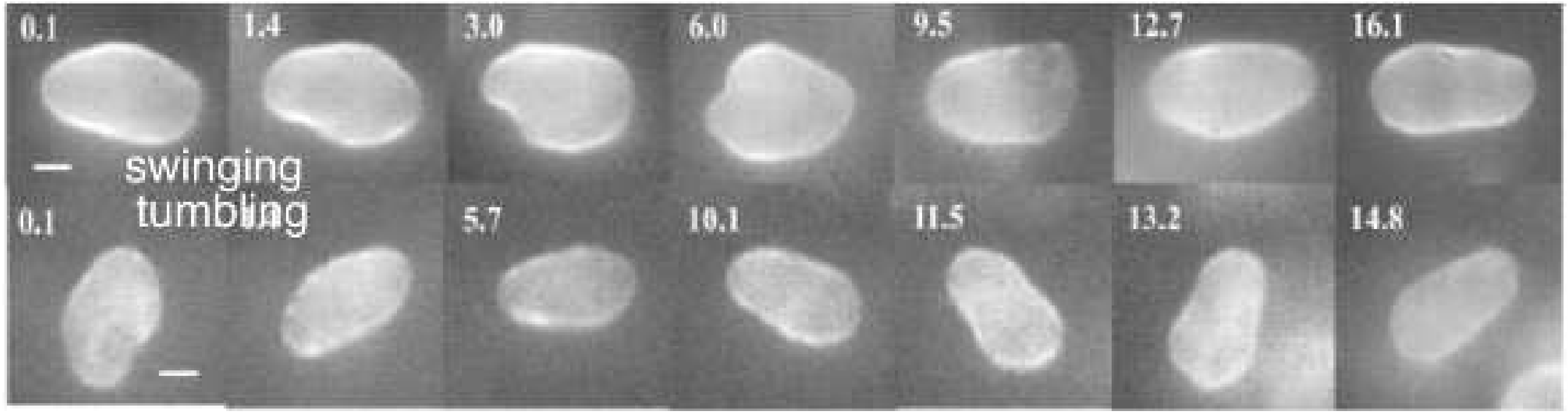


low viscosity



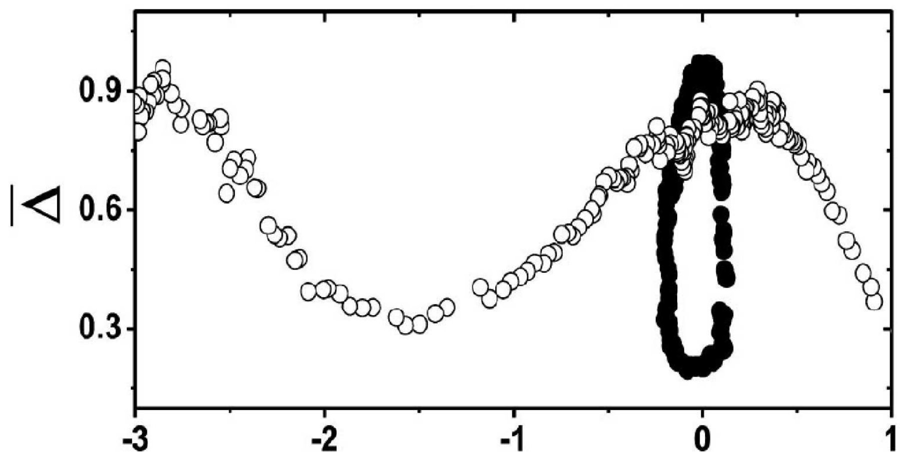
high viscosity

Swinging, Vacillating-breathing, Trembling



$\dot{\gamma} = 1.8 s^{-1}$

$\dot{\gamma} = 1.7 s^{-1}$



inclination angle θ

Transition fom tumbling to swinging with increasing shear rate $\dot{\gamma}$

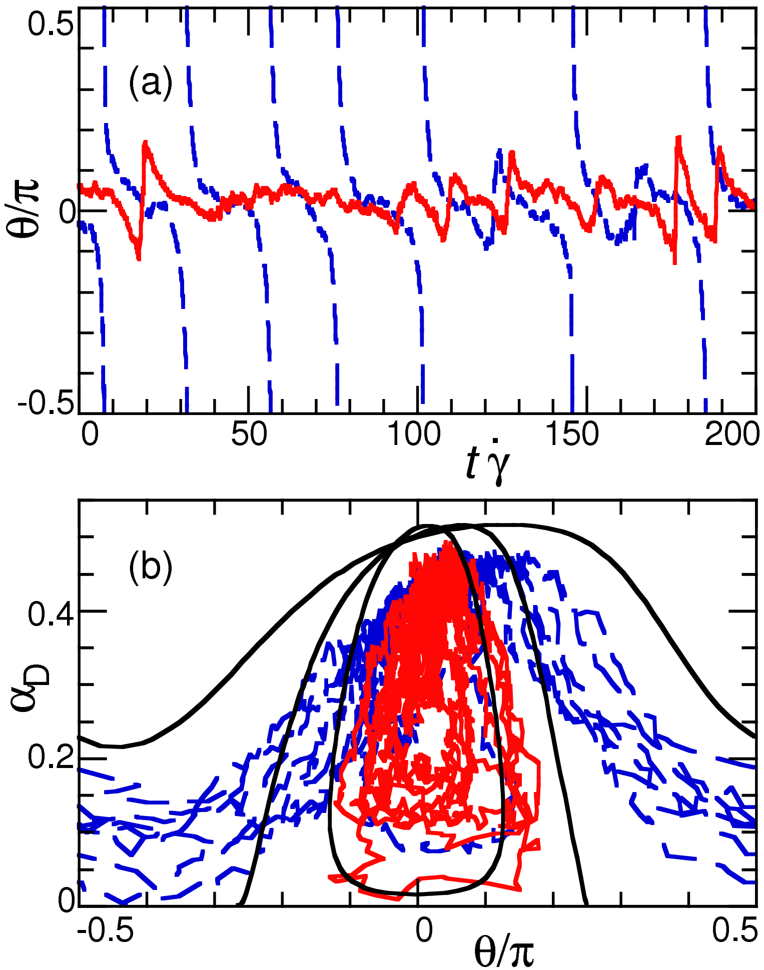
V. Kantsler and V. Steinberg,

Phys. Rev. Lett. **96** (2006)

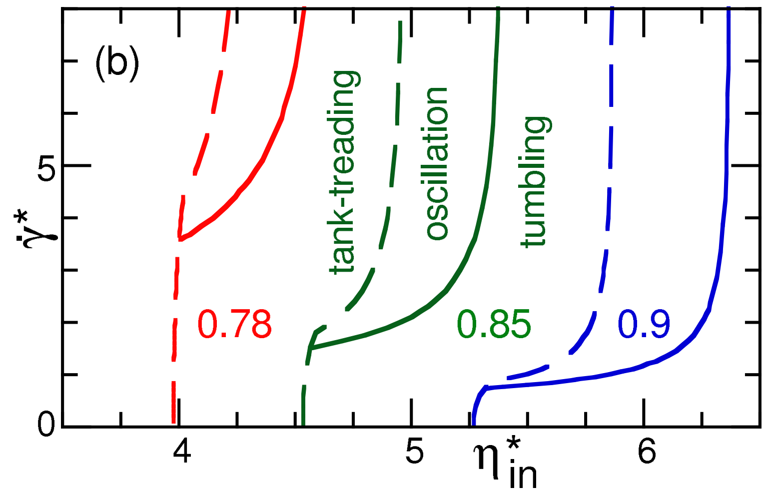
Theory: C. Misbah, Phys. Rev. Lett. **96** (2006); H. Noguchi and G. Gompper, Phys. Rev. Lett. **98** (2007); P.M. Vlahovska and R.S. Garcia, Phys. Rev. E **78** (2007); V.V. Lebedev et al., Phys. Rev. Lett. **99** (2007) ...

Swinging of Fluid Vesicles: Theory

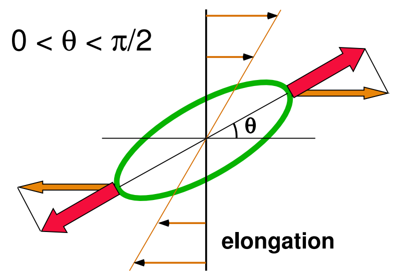
Shape dynamics:

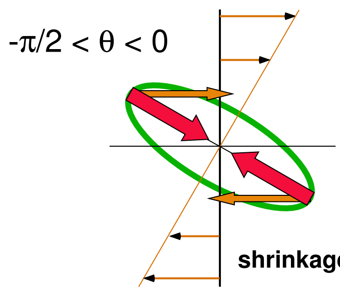


Phase diagram:



Mechanism:





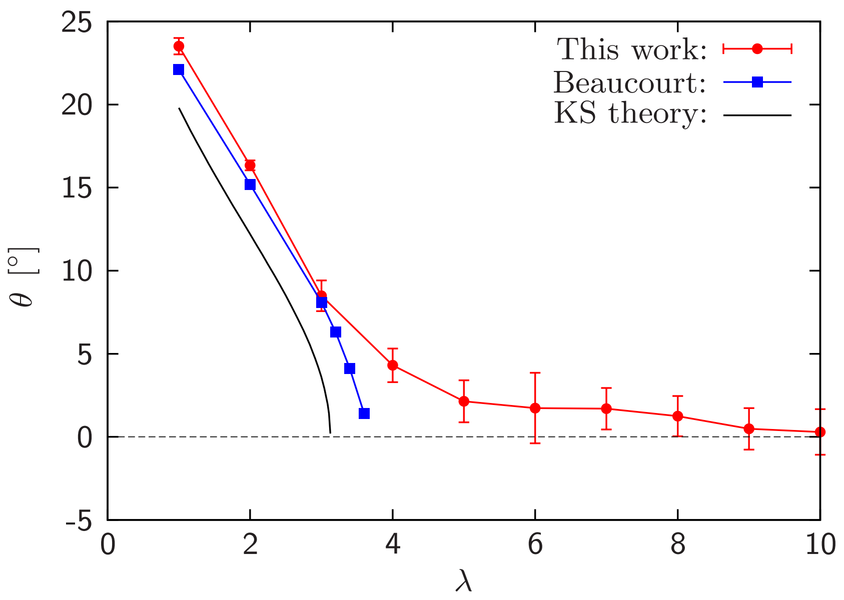
→ tumbling

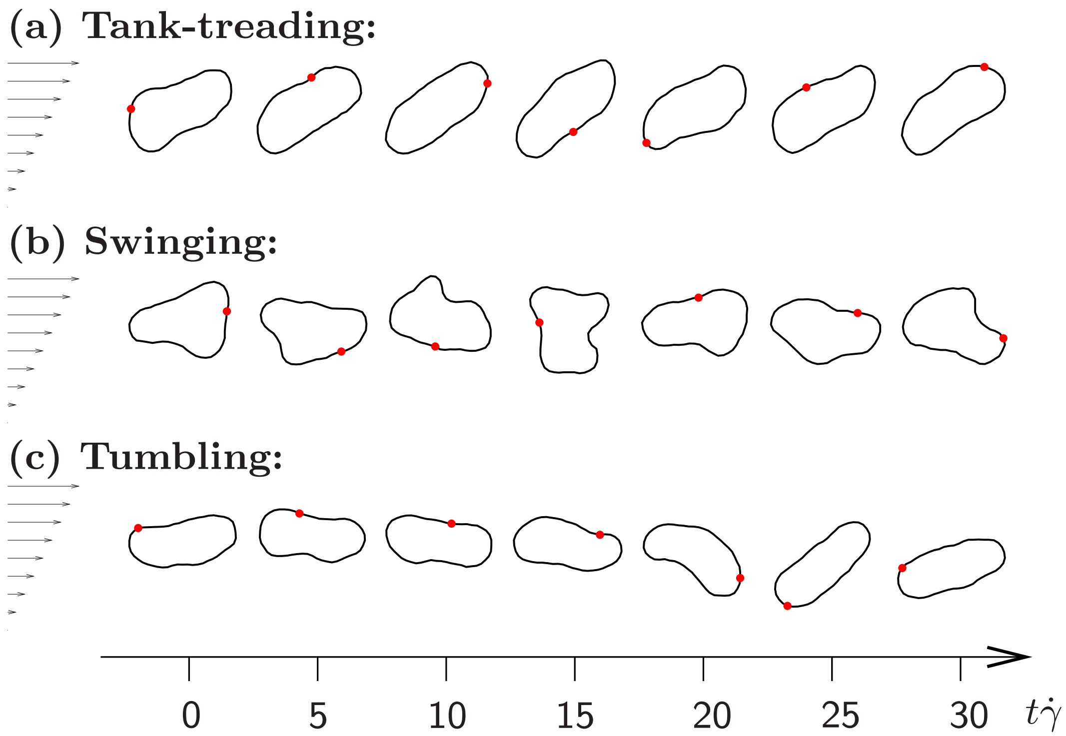
→ tank-treading

H. Noguchi and G. Gompper, Phys. Rev. Lett. **98** (2007)

Vesicles with Viscosity Contrast in Bulk

- Two-dimensional vesicles in shear flow
- Employ MPC-AT+a (with angular momentum conservation)
- Change viscosity contrast λ by varying mass of fluid particles

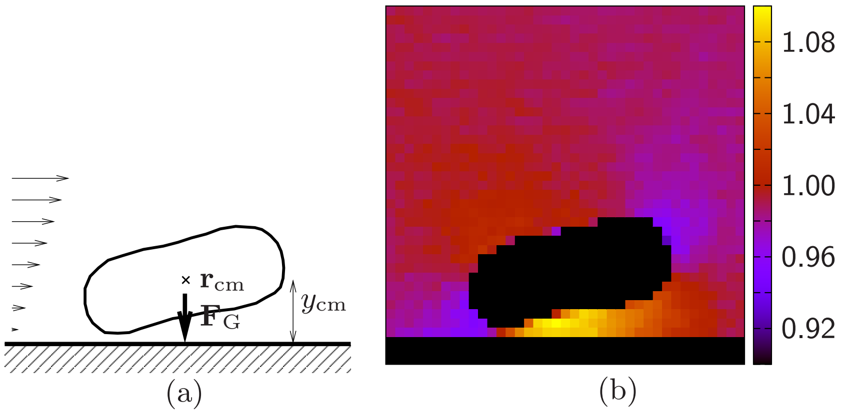




S. Messlinger, B. Schmidt, H. Noguchi and G. Gompper, Phys. Rev. E **80** (2009)

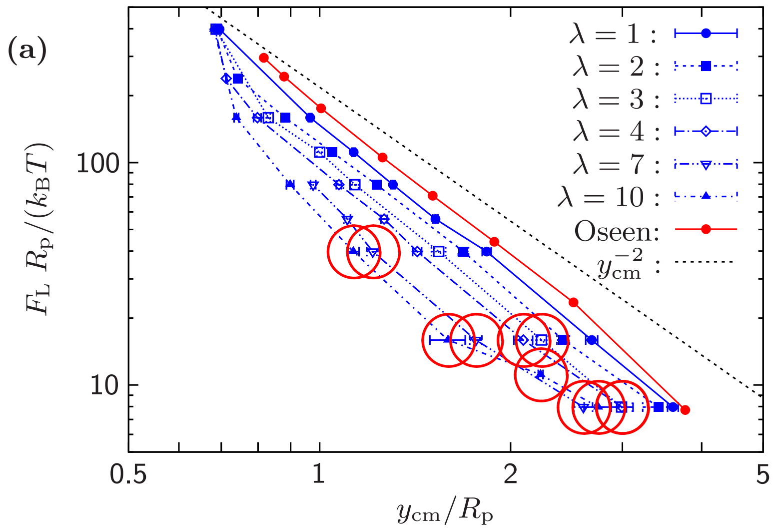
Vesicles with Viscosity Contrast near Wall

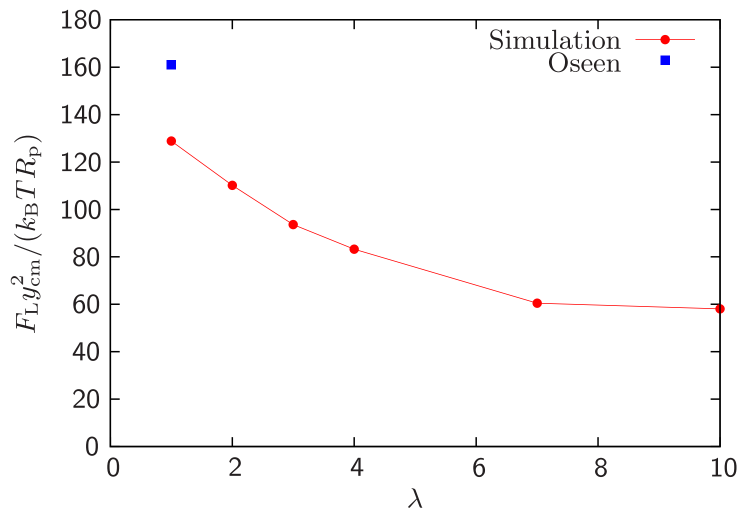
Vesicle in gravitational field near wall:



Lift force F_L balanced by gravitational force F_G

Lift force depends on viscosity contrast $\lambda = \eta_{in}/\eta_{out}$

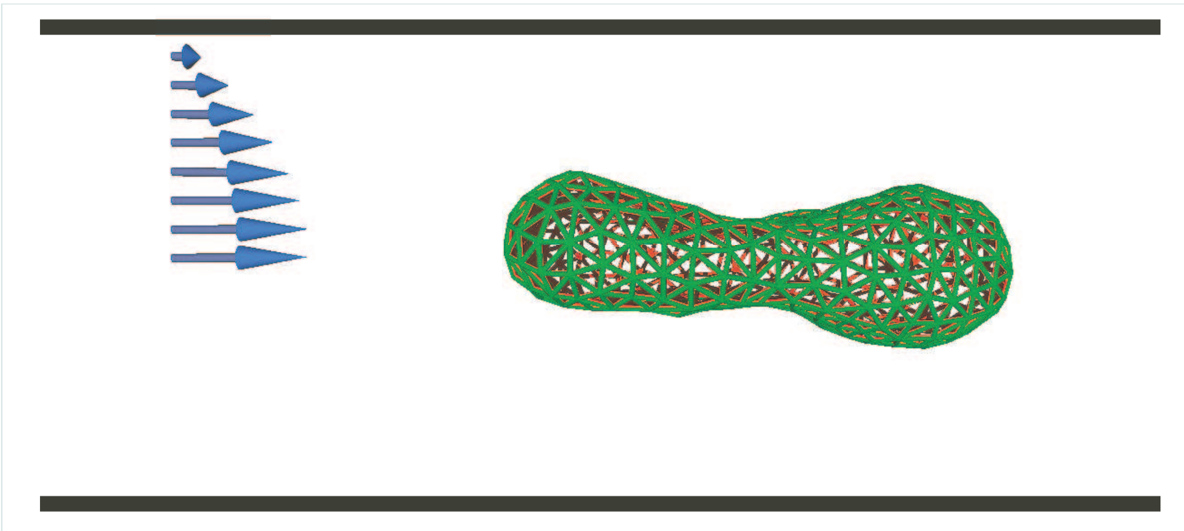




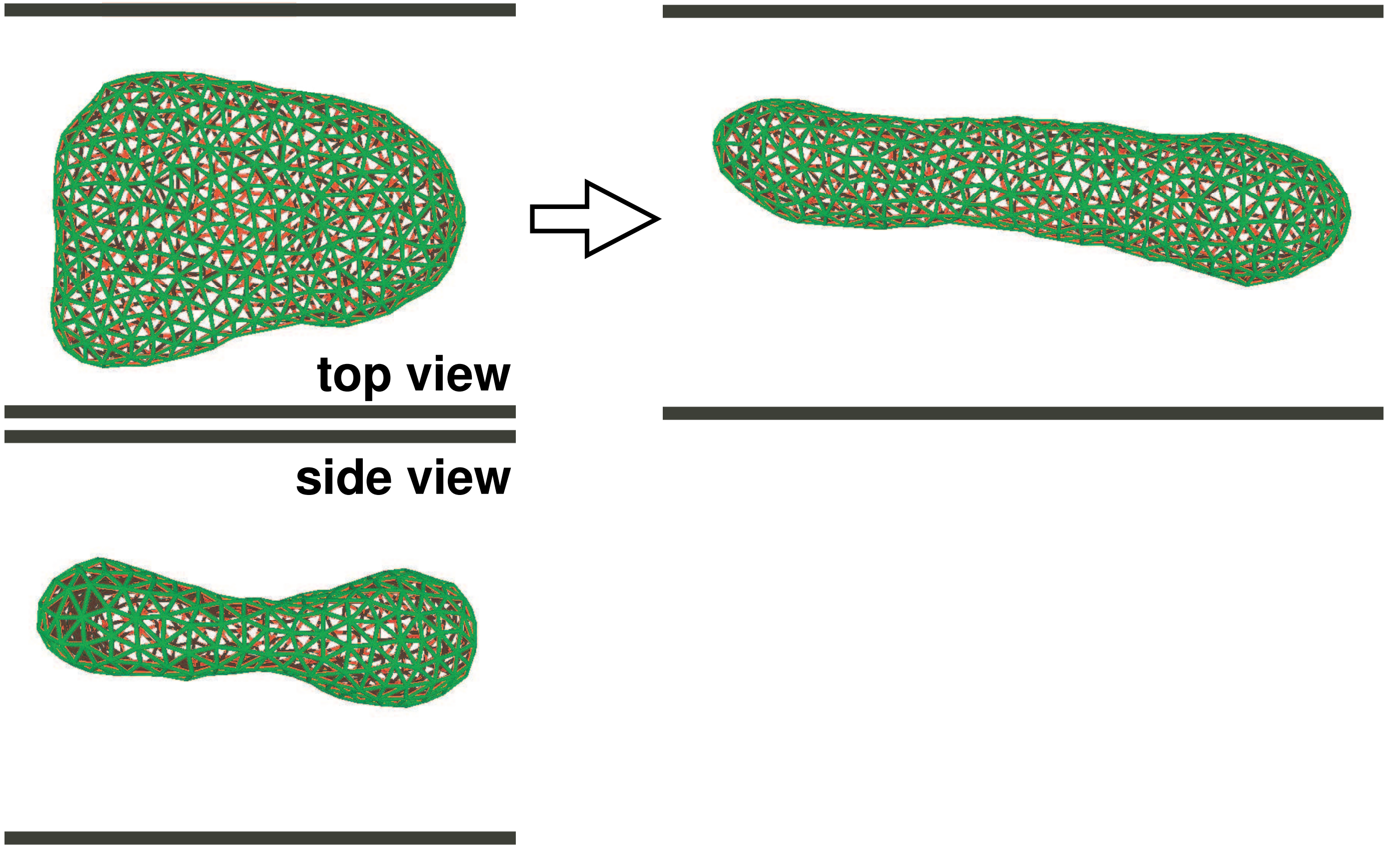
S. Messlinger, B. Schmidt, H. Noguchi and G. Gompper, Phys. Rev. E **80** (2009)

Membrane Hydrodynamics

Vesicle and Cells in Capillary Flow



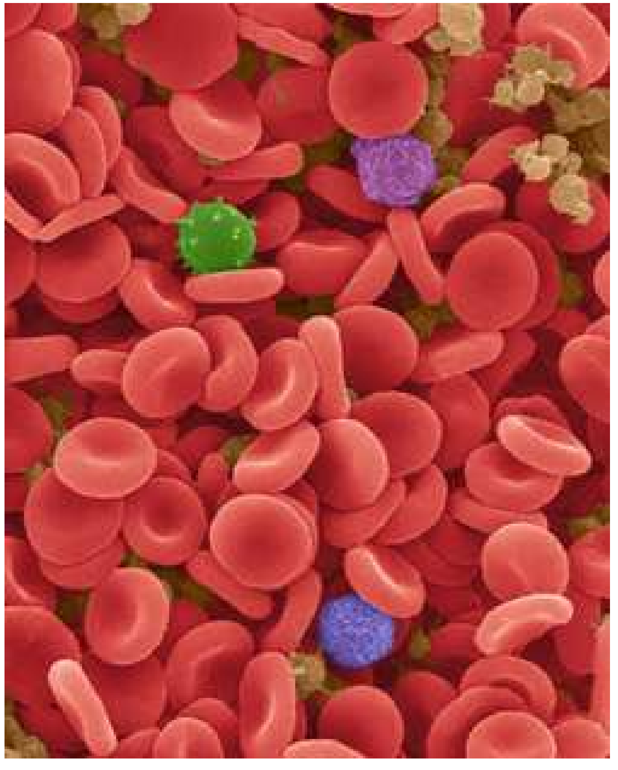
Capillary Flow: Fluid Vesicles

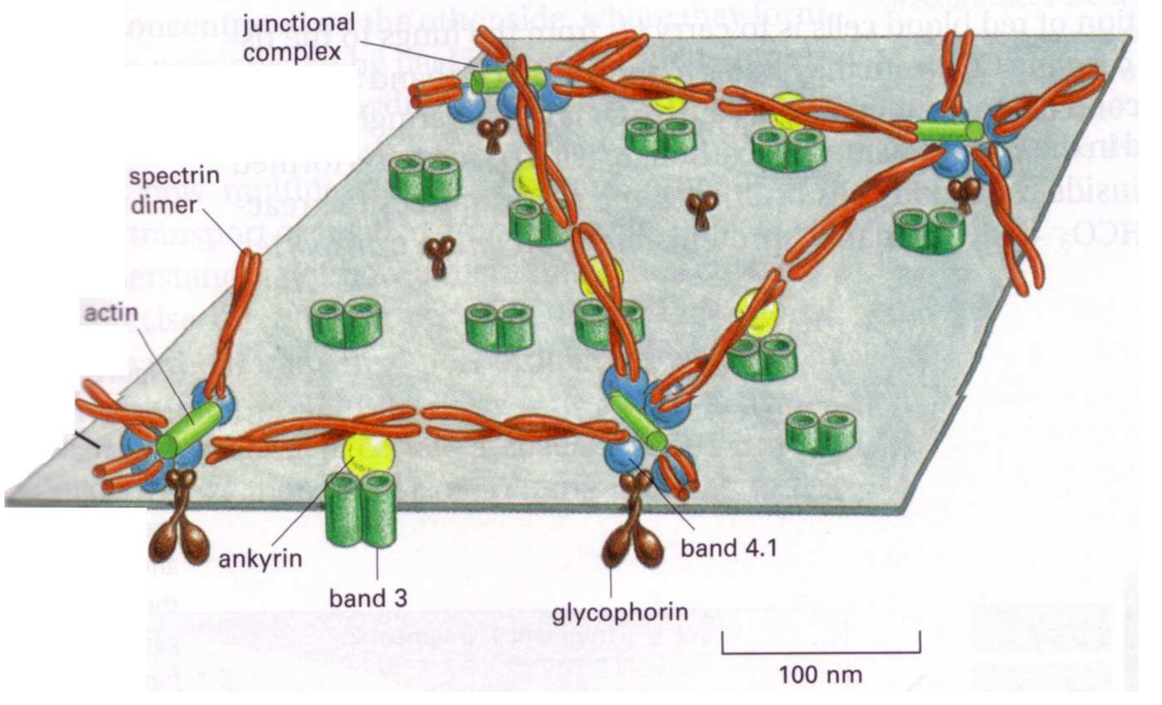


- small flow velocities: vesicle axis perpendicular to capillary axis $\longrightarrow$ no axial symmetry!
- discocyte-to-prolate transition with increasing flow

H. Noguchi and G. Gompper, Proc. Natl. Acad. Sci. USA **102** (2005)

Capillary Flow: Red Blood Cells



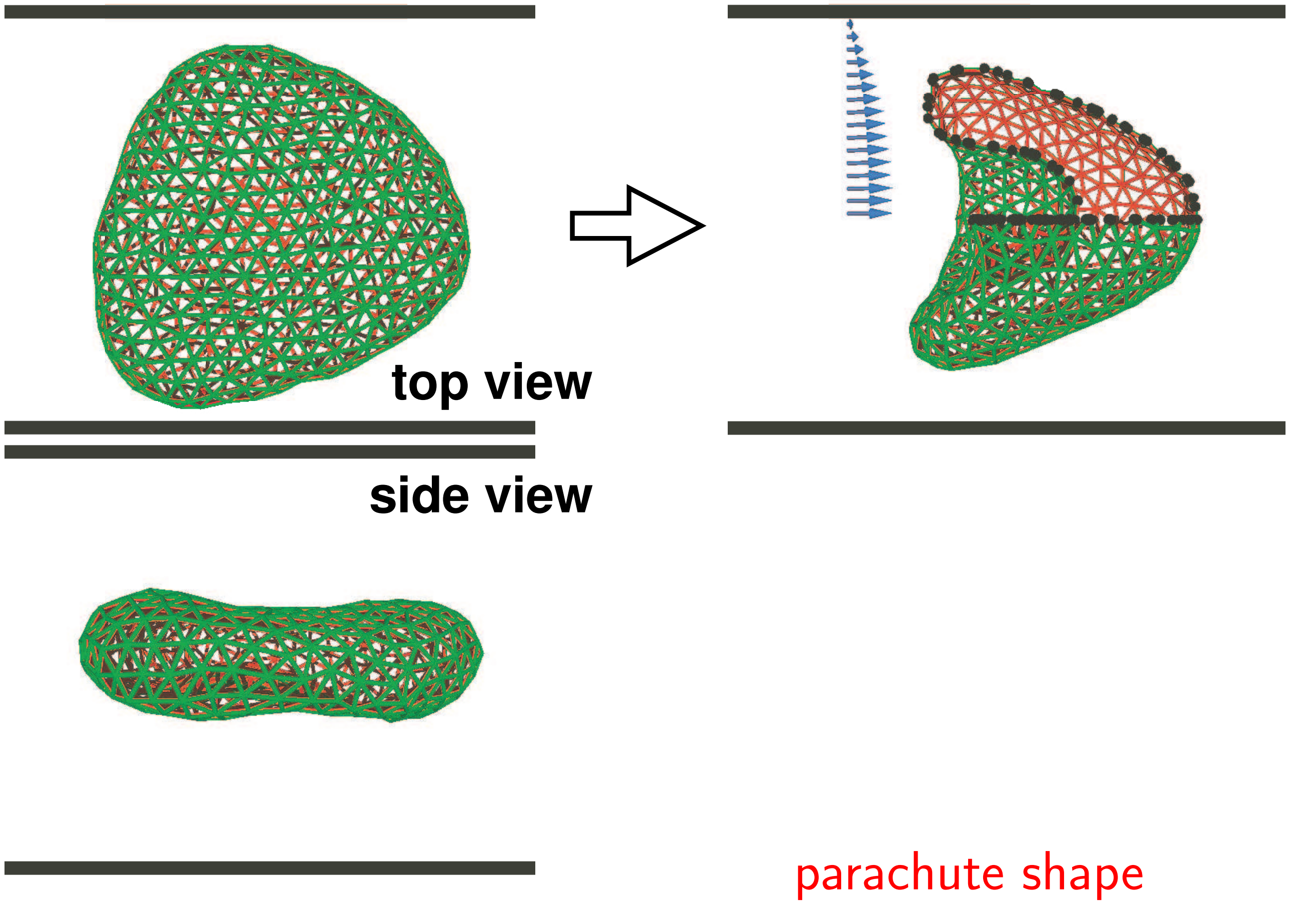


- Spectrin network induces shear elasticity μ of composite membrane
- Elastic parameters: $\kappa/k_BT = 50$, $\mu R_0^2/k_BT = 5000$

Capillary Flow: Elastic Vesicles

Elastic vesicle:

- curvature and shear elasticity $(\kappa = 20\, k_BT,\ \mu = 110\, k_BT/R_0^2)$
- model for red blood cells



Capillary Flow: Elastic Vesicles

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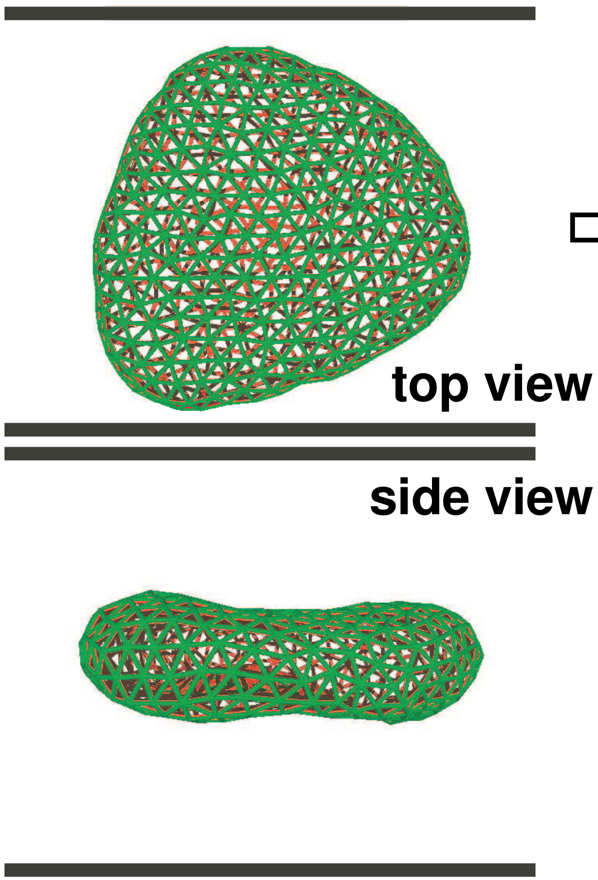
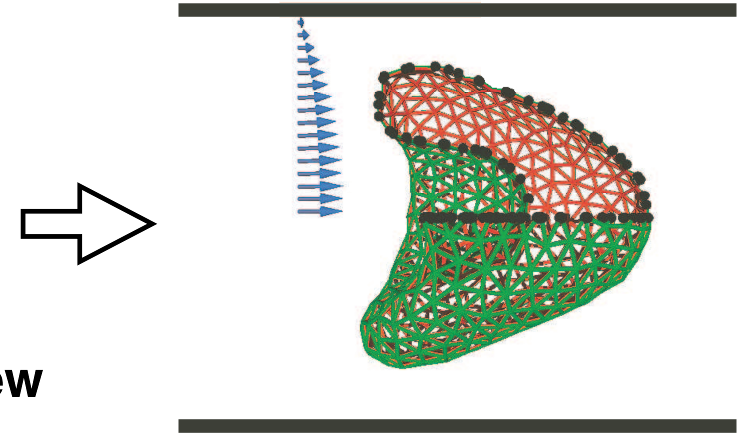
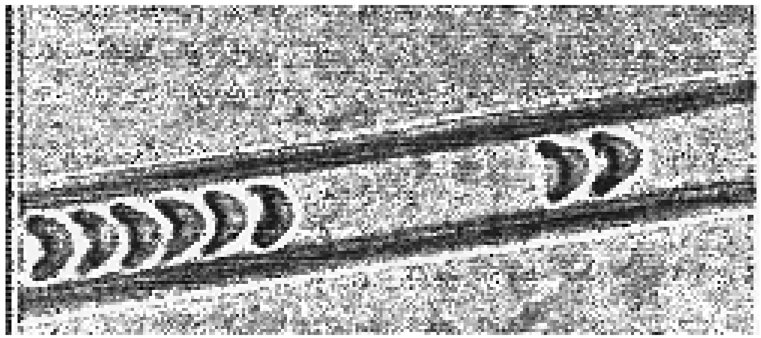




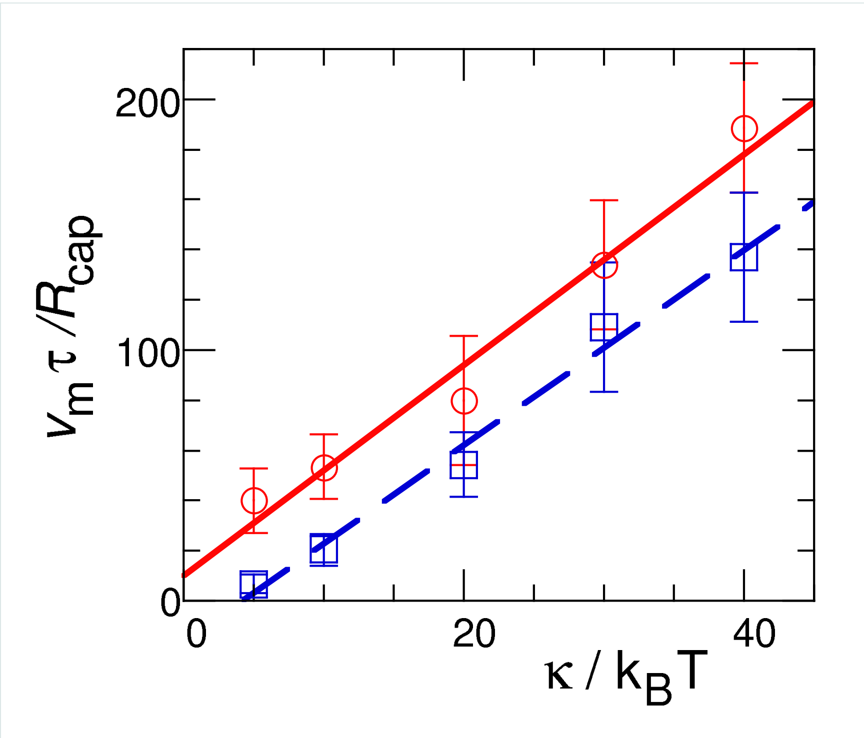


Tsukada et al., Microvasc. Res. **61** (2001)

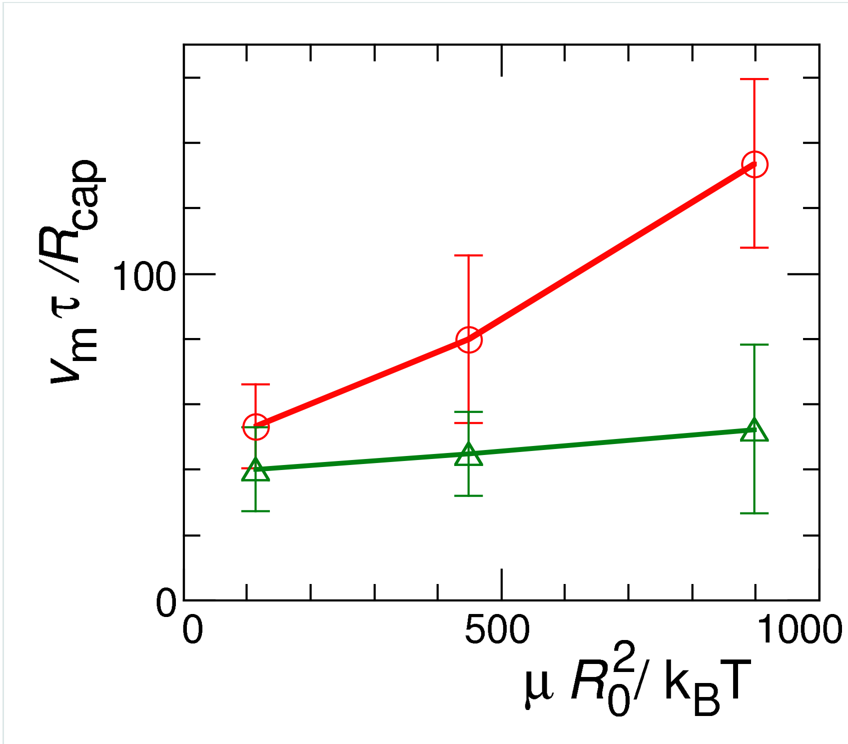
Capillary Flow: Red Blood Cells

Shear elasticity suppresses prolate shapes (large deformations)

Flow velocity at discocyte-to-parachute transition



bending rigidity



shear modulus

Implies for RBCs: $v_{trans} \simeq 0.2mm/s$ for $R_{cap} = 4.6\mu m$

RBC Clustering & Alignment in Flow

Physiological conditions: Hematocrit (volume fraction of RBCs) $H = 0.45$

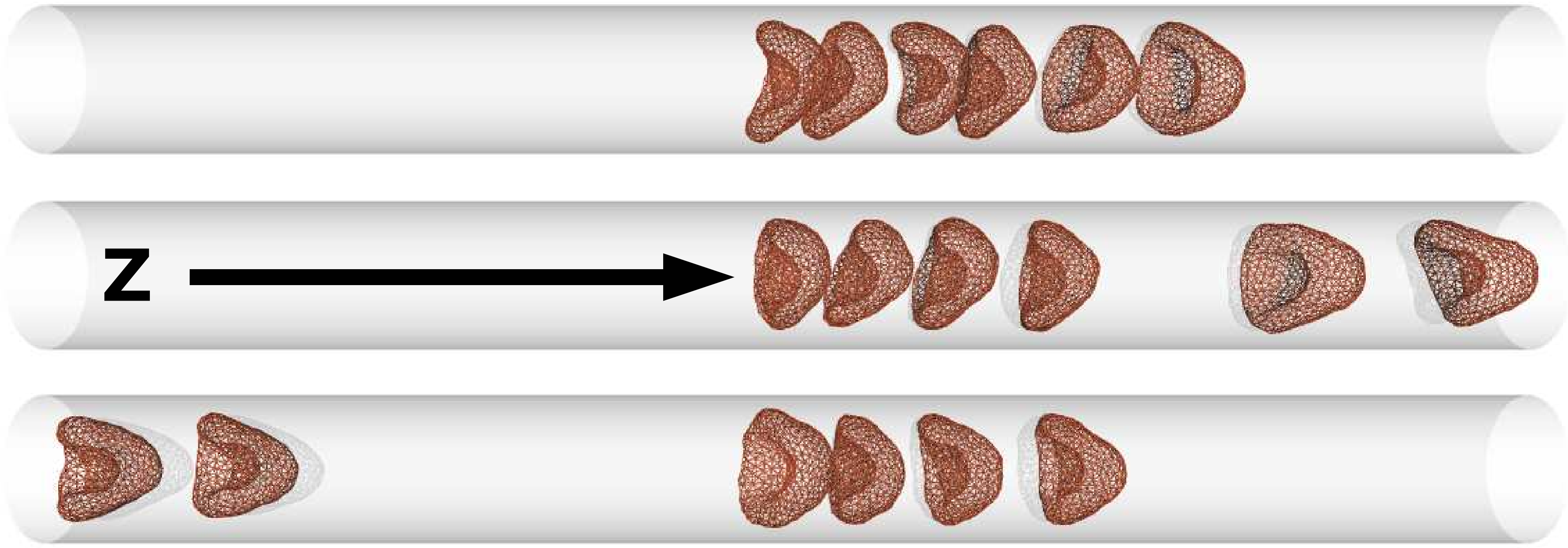
Lower in narrow capillaries $H_T = 0.1 ... 0.2$

Therefore: Hydrodynamic interactions between RBCs very important

Note: No direct attractive interactions considered!

RBC Clustering & Alignment in Flow

Low hematocrit H_T:

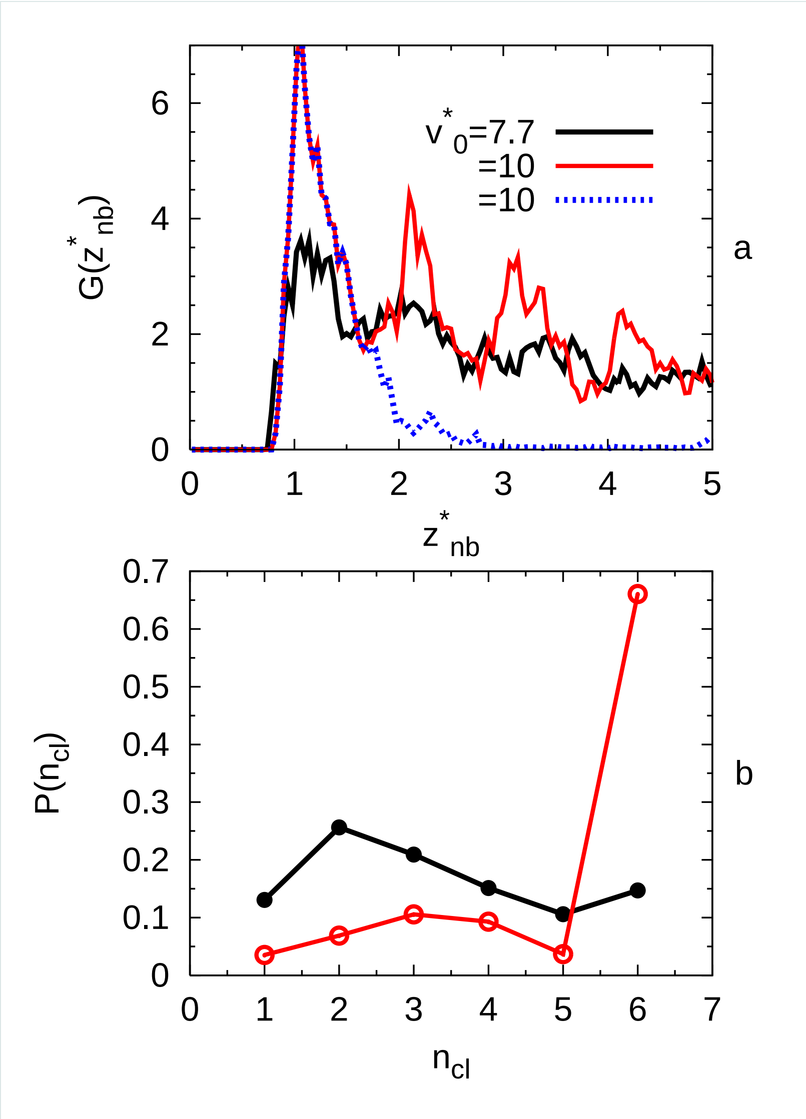


- Single vesicles more deformed $\longrightarrow$ move faster
- Effective hydrodynamic attraction stabilizes clusters

J.L. McWhirter, H. Noguchi, G. Gompper, Proc. Natl. Acad. Sci. **106** (2009)

RBC Clustering & Alignment in Flow

Low hematocrit H_T:



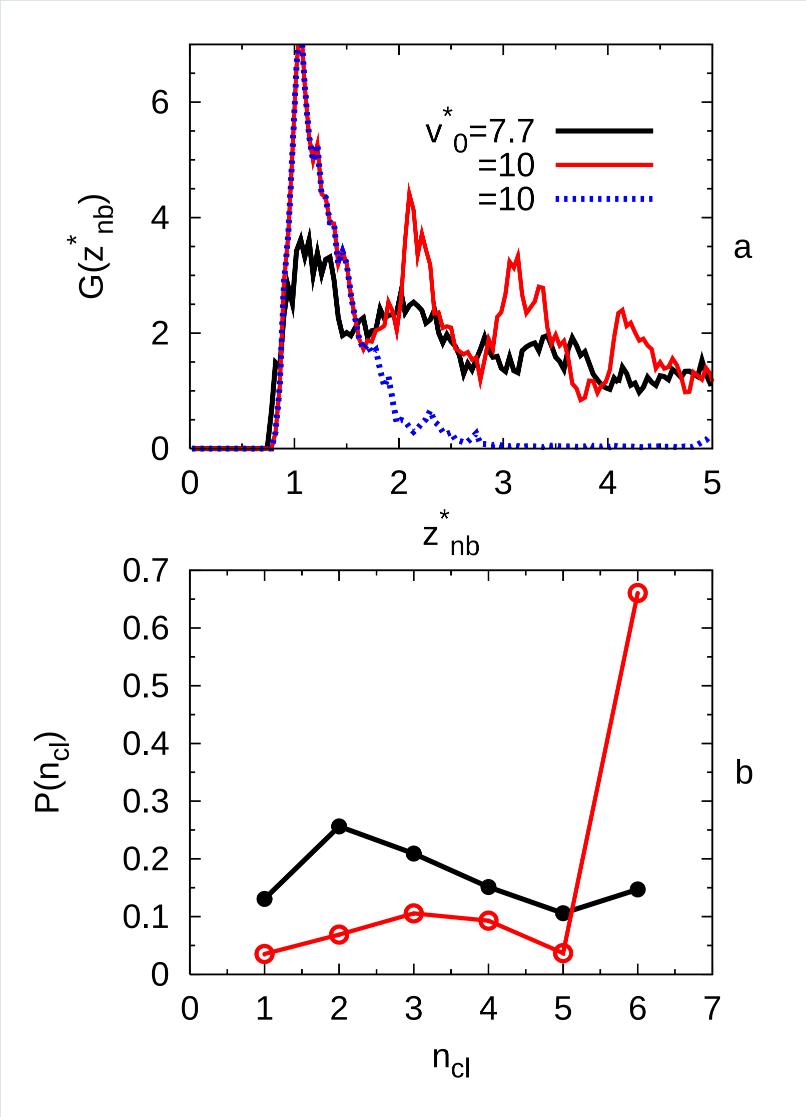
Positional correlation function

Probability for cluster size n_{cl}

Clustering tendency increases with increasing flow velocity

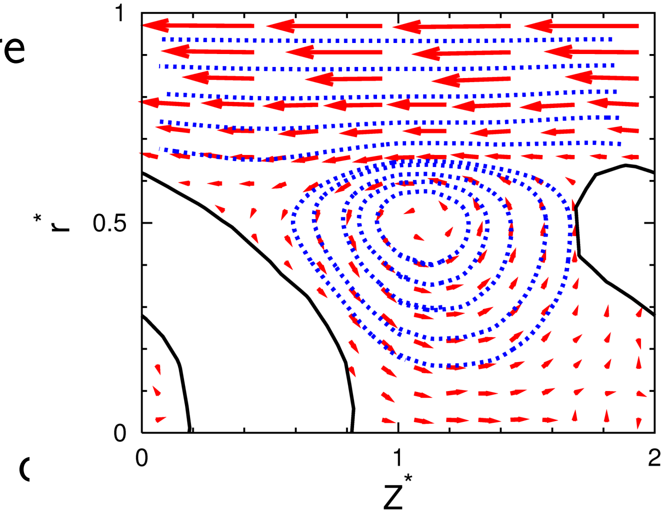
RBC Clustering & Alignment in Flow

Low hematocrit H_T:



Positional corre

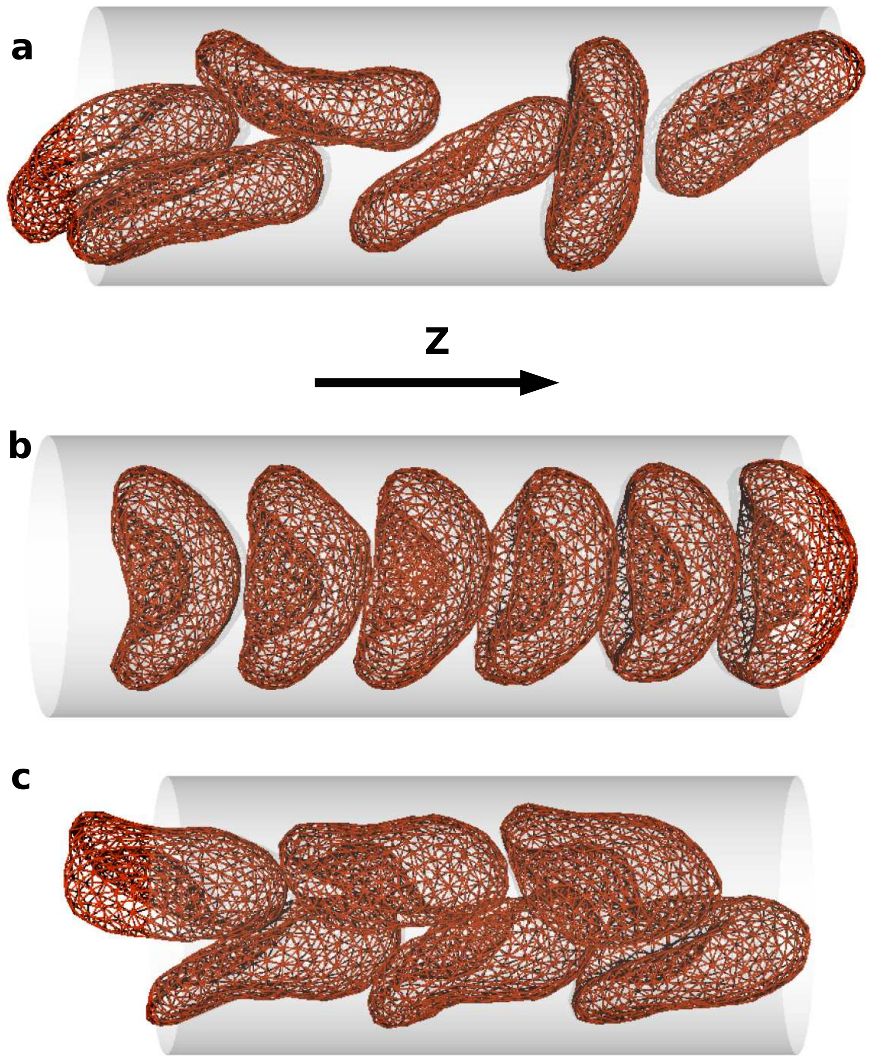
Probability for c



Clustering tendency increases with increasing flow velocity

RBC Clustering & Alignment in Flow

High hematocrit H_T:



disordered discocyte

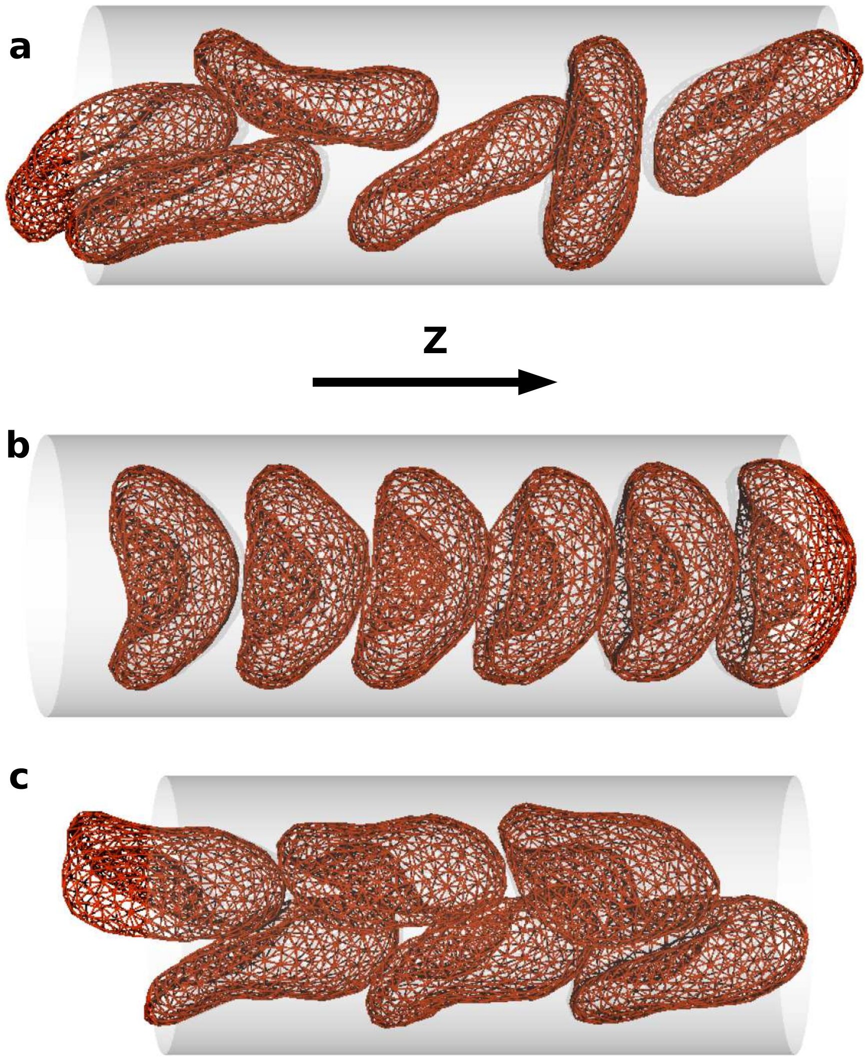
aligned parachute

zig-zag slipper

J.L. McWhirter, H. Noguchi, G. Gompper, Proc. Natl. Acad. Sci. **106** (2009)

RBC Clustering & Alignment in Flow

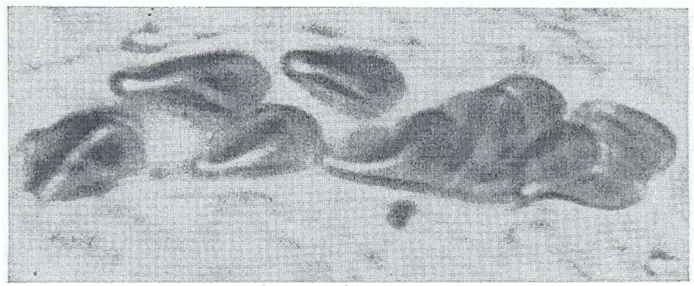
High hematocrit H_T:



disordered discocyte

aligned parachute

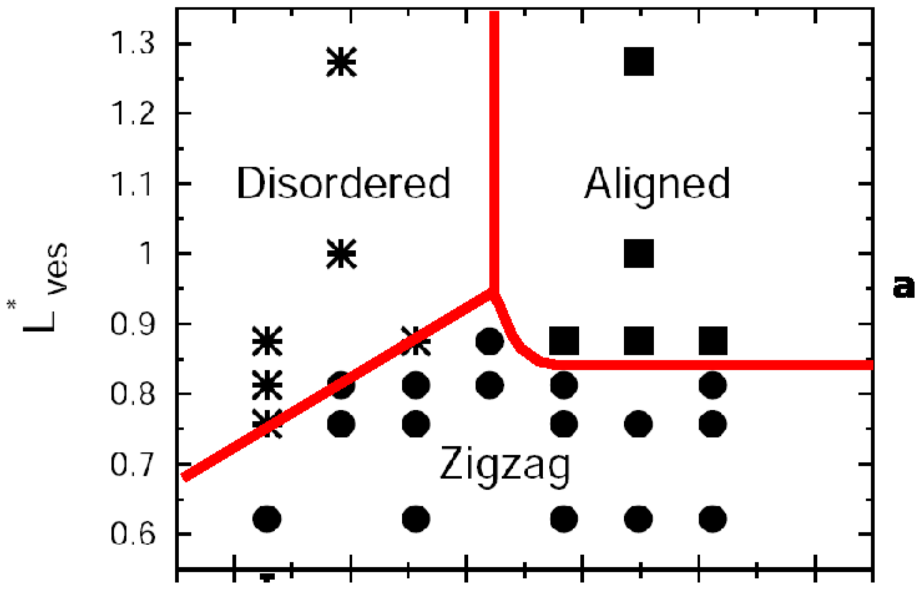
zig-zag



Skalak, Science (1969)

Clustering & Alignment in Flow

Phase diagram:



flow velocity v_0^*

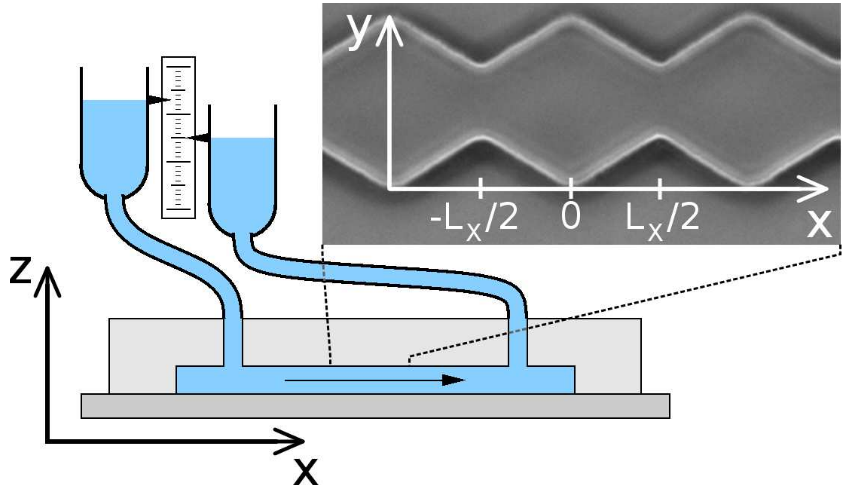
Hematocrit $H_T = 0.28/L^*_{ves}$

Transition to zig-zag phase despite higher flow resistance than aligned-parachute phase!

Vesicles in Structured Channels

Vesicle motion through zig-zag shaped channel ($L_x = 100\mu m$):

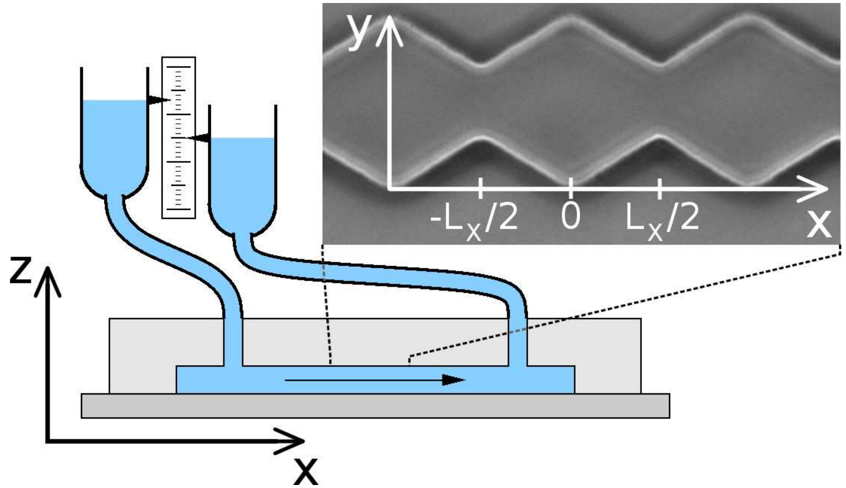
time-dependent flow

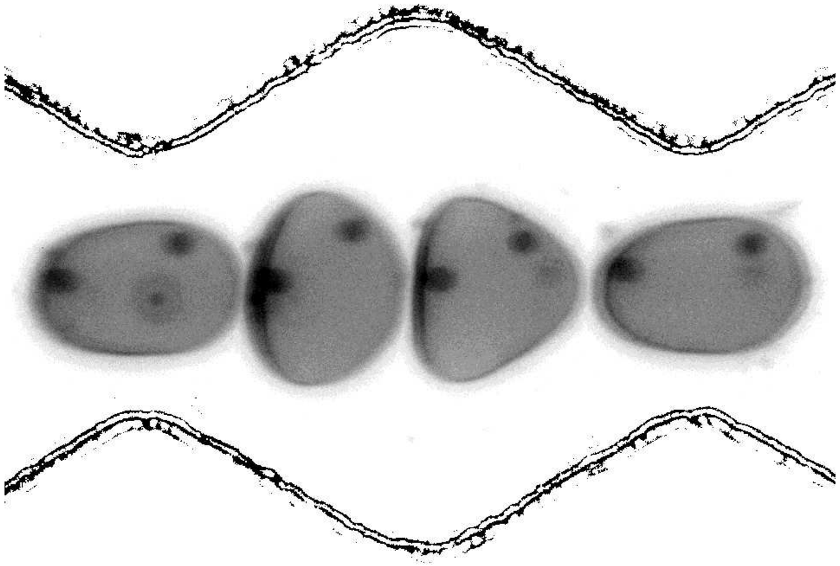


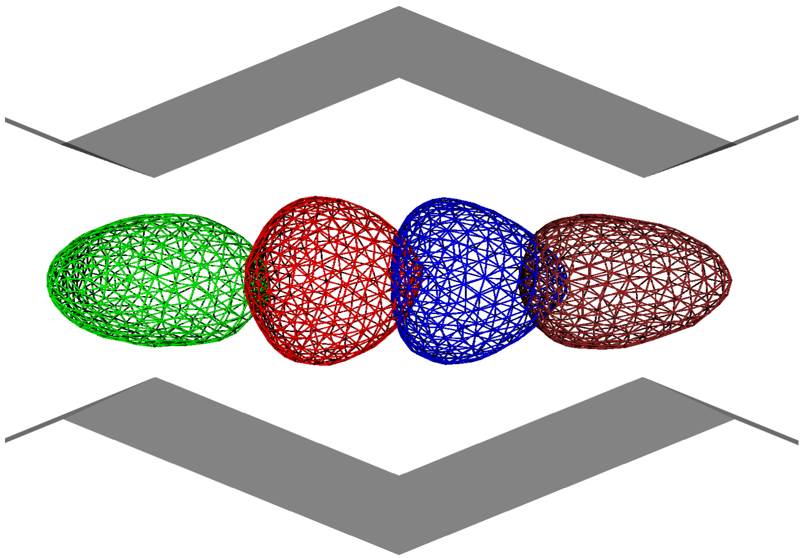
Vesicles in Structured Channels

Vesicle motion through zig-zag shaped channel ($L_x = 100\mu m$):

time-dependent flow







H. Noguchi, G. Gompper, L. Schmid, A. Wixforth, and T. Franke, EPL **89** (2010)

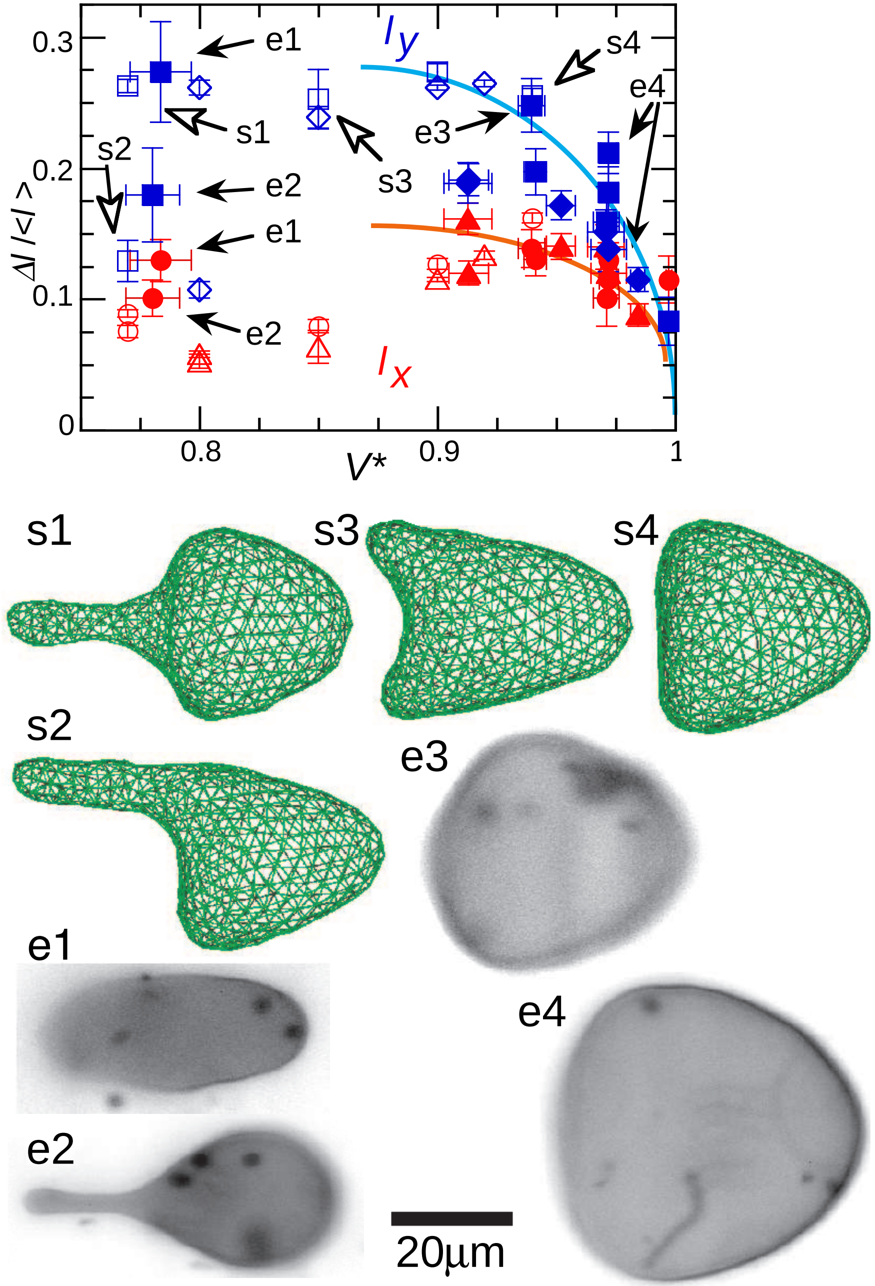
Vesicles in Structured Channels

Large reduced volume V^*:

- Fast flows: Symmetric shape oscillations
- Slow flows: Orientational oscillations

Smaller reduced volume V^*:

- Symmetric double tail
- Asymmetric single tail



Summary

- Mesoscale simulation techniques are powerful tool to bridge the length- and time-scale gap in complex fluids
- Multi-particle-collision dynamics well suited for hydrodynamics of embedded particles: colloids, polymers, vesicles, RBCs
- Vesicles in shear flow: tank-treading, tumbling, swinging, lift force
- Red blood cells in capillary flow: shear elasticity implies parachute shapes, hydrodynamic clustering and alignment
- Vesicles in structured channels: single- and double-tailed shapes

Review: G. Gompper, T. Ihle, D.M. Kroll, R.G. Winkler, Adv. Polym. Sci. **221**, 1 (2009)