Mesoscale simulation of blood flow in microcapillaries

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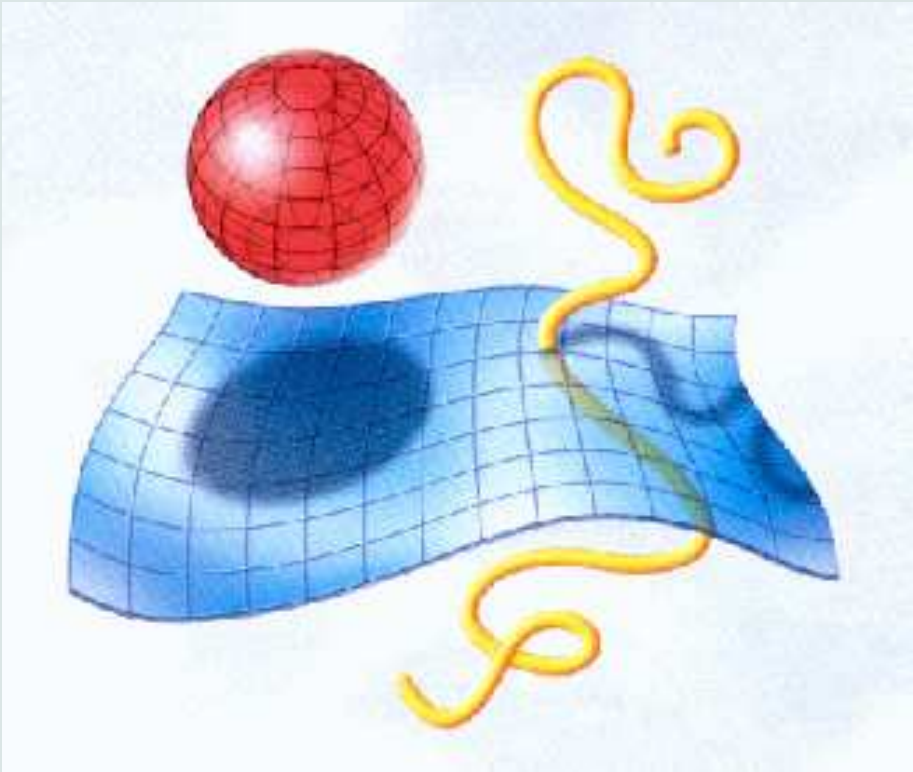


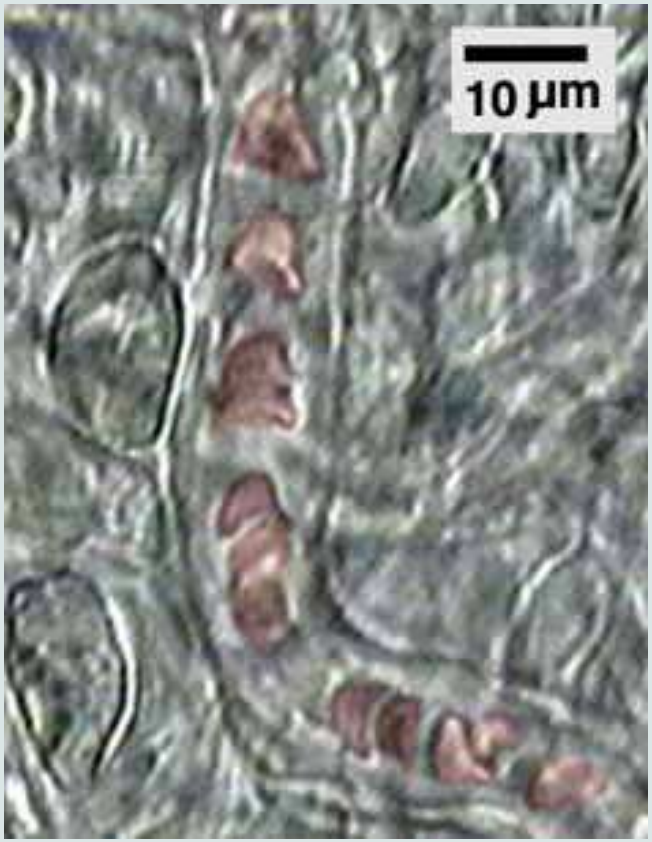
Work done during the last year in the Soft Matter Theory group in Jülich. Involved people include

- Hiroshi Noguchi (now in Tokyo)
- J. Liam McWhirter (now in Helsinki)
- Julia Fornleitner
- Dmitry Fedosov
- Matti Peltomäki
- Prof. Gerhard Gompper

Soft Matter Hydrodynamics

Cells and vesicles in flow:

- Red blood cells in microvessels:



Diseases such as diabetes reduce deformability of red blood cells!

Mesoscale 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:

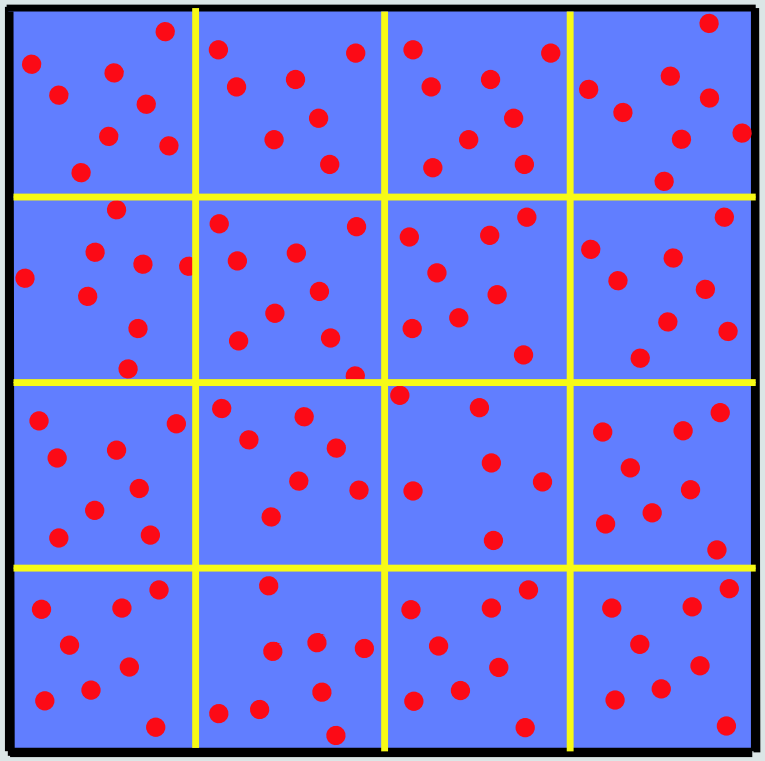
- drastically simplify dynamics on molecular scale
- respect conservation laws for mass, momentum, energy

Examples:

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

Mesoscale Simulations: MPC

Multi-Particle-Collision Dynamics (MPC)



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

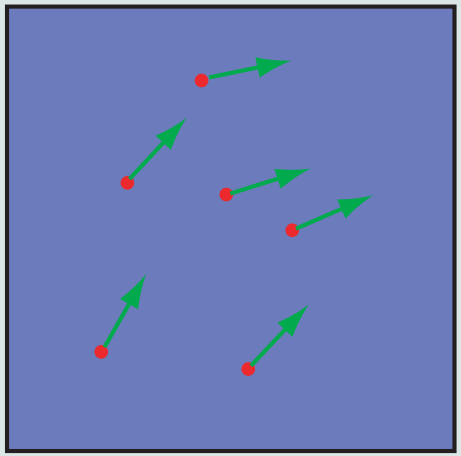
A. Malevanets and R. Kapral, J. Chem. Phys. **110** (1999)

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

Mesoscale Simulations: MPC

Flow dynamics: Two step process

Streaming



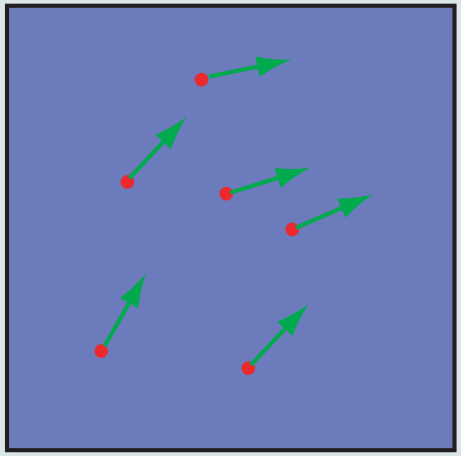
- ballistic motion

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

Mesoscale Simulations: MPC

Flow dynamics: Two step process

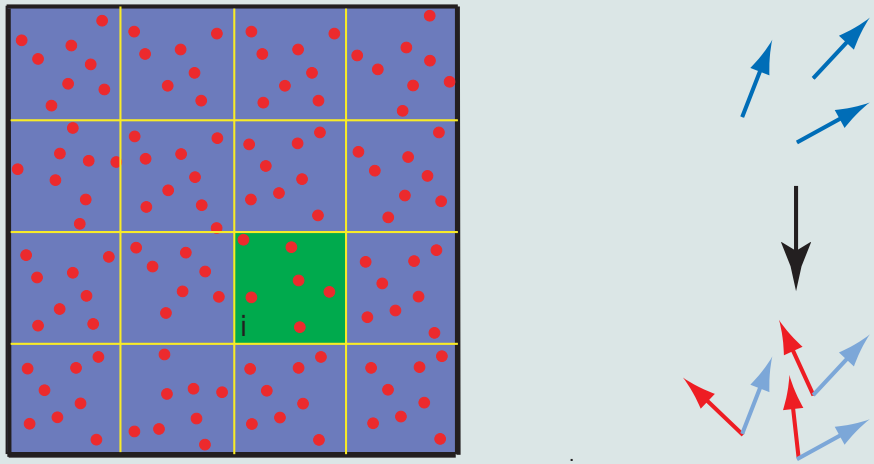
Streaming



- ballistic motion

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

Collision



- mean velocity per cell

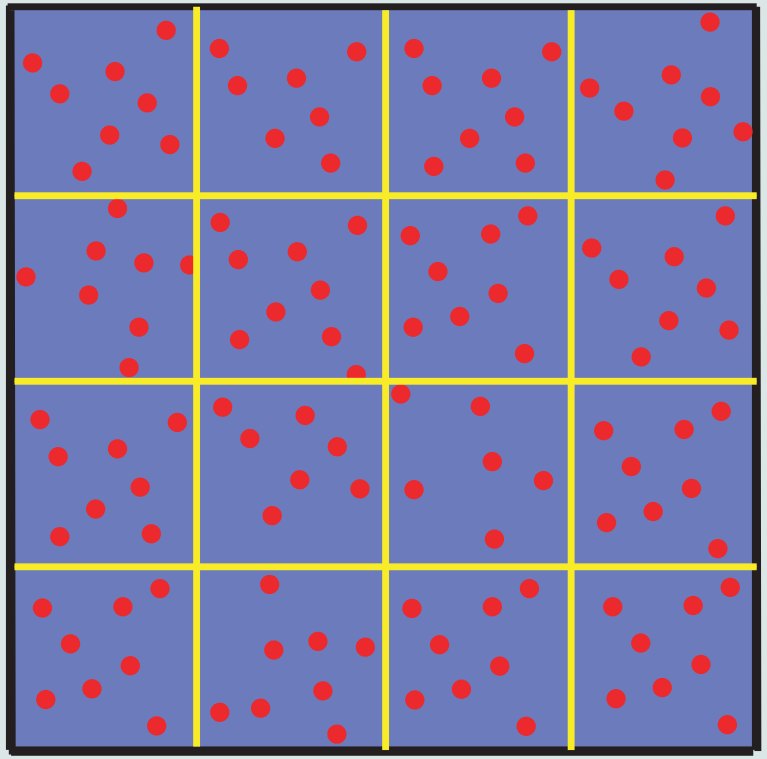
$$\bar{\mathbf{v}}_i(t) = \frac{1}{n_i}\sum_{j\in C_i}^{n_i} \mathbf{v}_j(t)$$

- 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 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 Simulations: MPC

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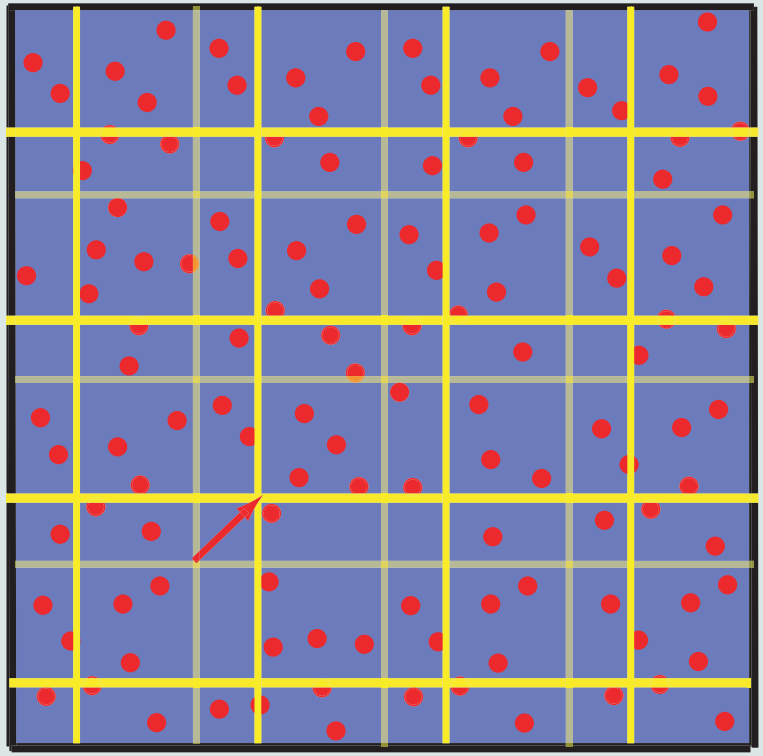


T. Ihle and D.M. Kroll, Phys. Rev. E **63** (2001)

Mesoscale Simulations: Reynolds and Schmidt Numbers

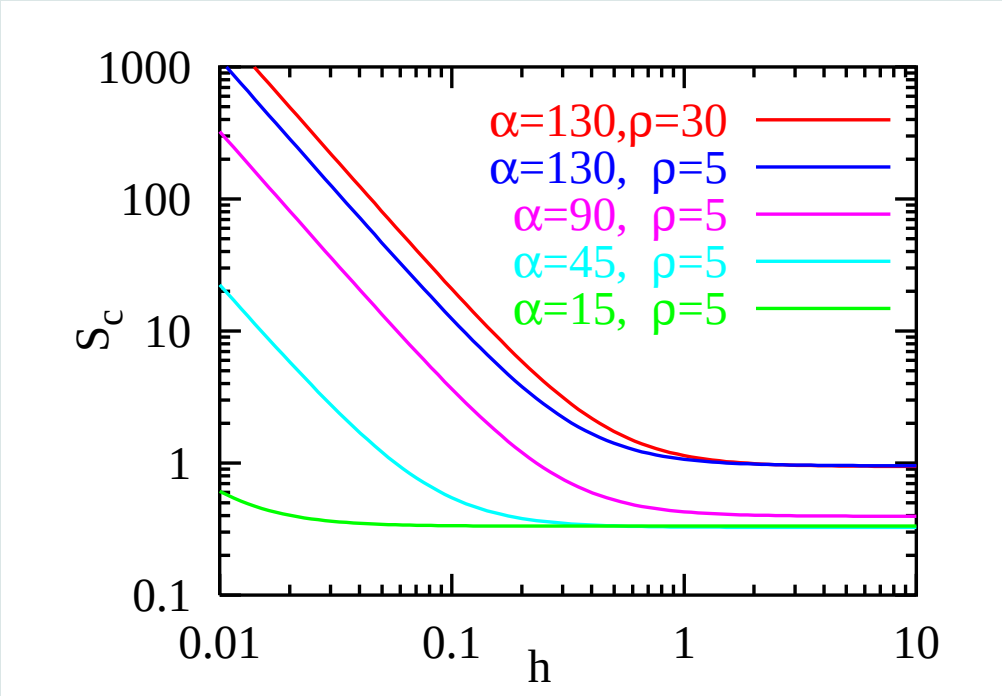
- Reynolds number $Re = v_{\max} L/\nu \sim$ inertia forces / friction forces

  For soft matter systems with characteristic length scales of μm:

  $Re \simeq 10^{-3}$

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

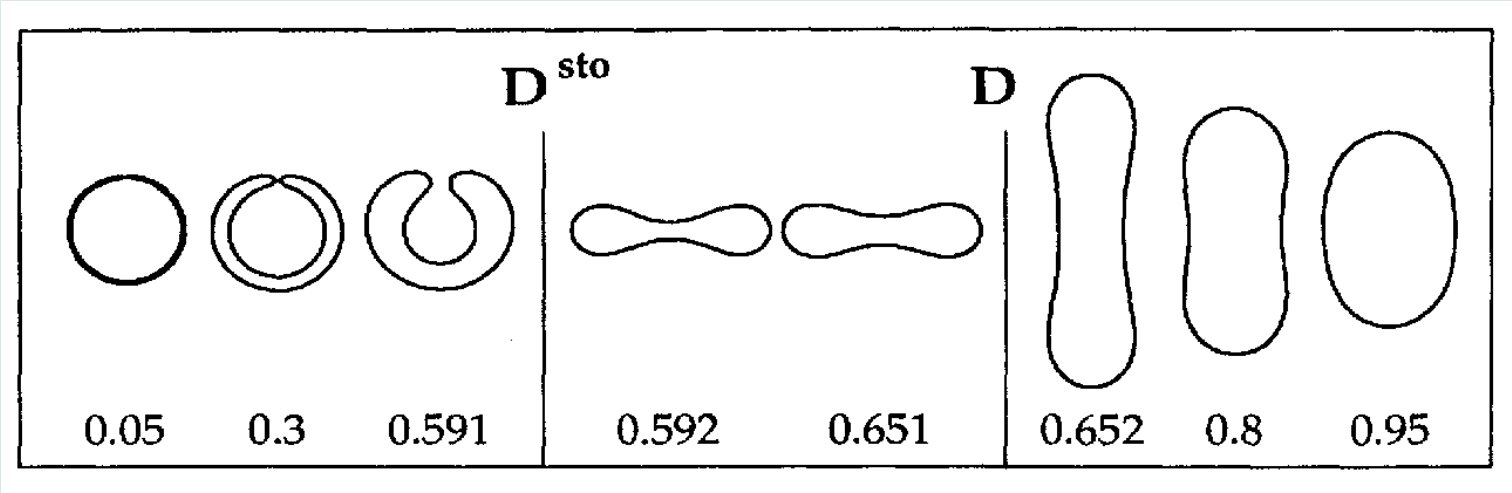
  Gases: $Sc \simeq 1$, liquids: $Sc \simeq 10^3$



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

Membranes and Vesicles: Equilibrium Shapes

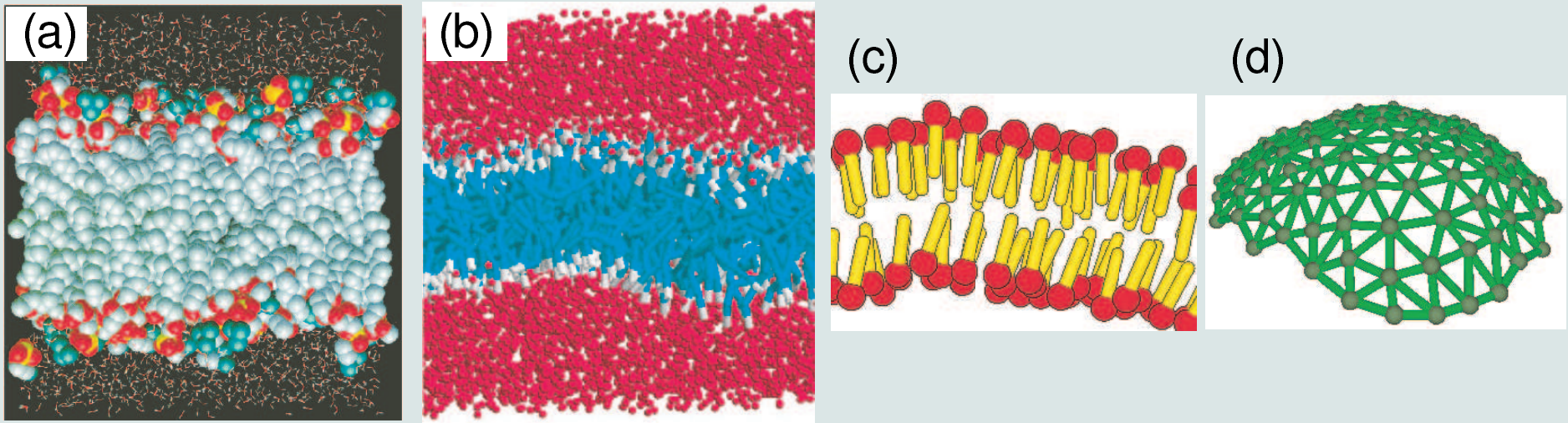
Minimize curvature energy for fixed area $A = 4\pi R_0^2$ and reduced volume $V^* = V/V_0$, where $V_0 = 4\pi R_0^3/3$:



stomatocyte discocyte prolate

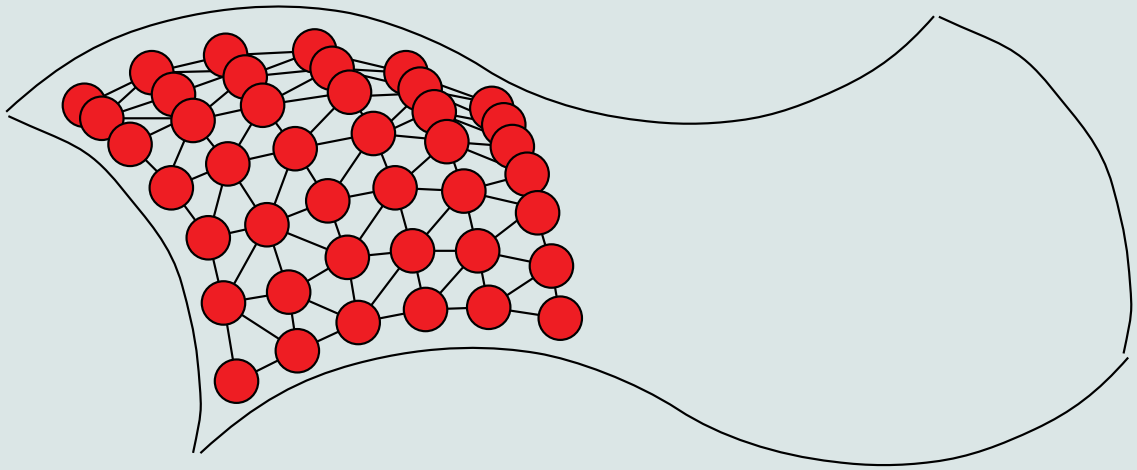
U. Seifert, K. Berndl, and R. Lipowsky, Phys. Rev. A **44** (1991)

Membranes and Vesicles: Different Length Scales



atomistic | coarse-grained | solvent-free | triangulated

Membranes and Vesicles: Triangulated Surfaces



- Closed 2D surface in 3D.
- N vertices (membrane particles)
- $3(N-2)$ edges
- $2(N-2)$ faces

Two- and many-body potentials:

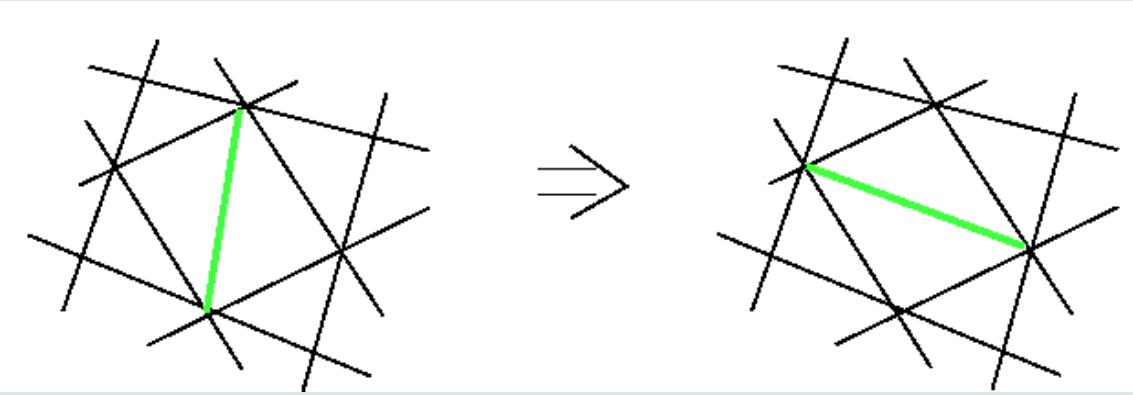
- Bending rigidity κ
- Pairwise soft repulsion
- Pairwise soft attraction (in the presence of an edge)
- Surface area constraint
- Volume constraint

G. Gompper, D.M.Kroll, J. Phys. Cond. Matt **9** (1997);

G. Gompper, D.M. Kroll, in *Statistical Mechanics of Membranes and Surfaces* (World Scientific, 2004)

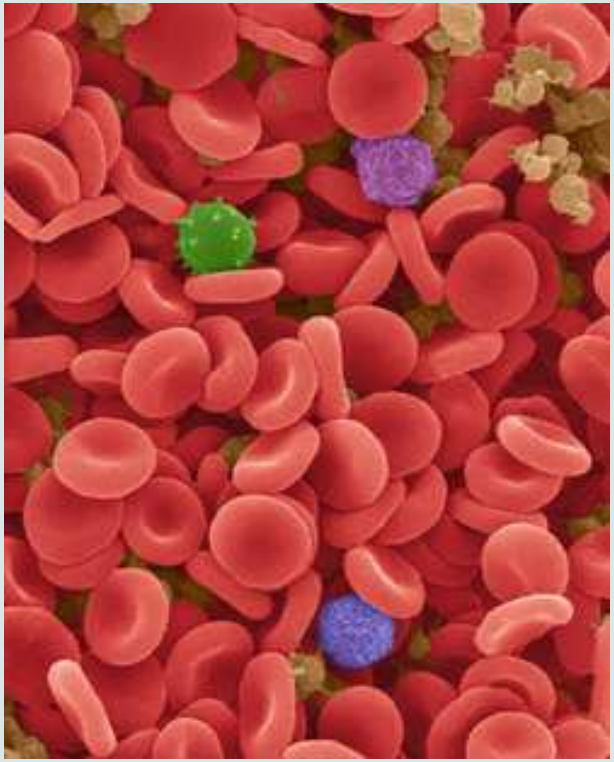
Membranes and Vesicles: Fluid Vesicles

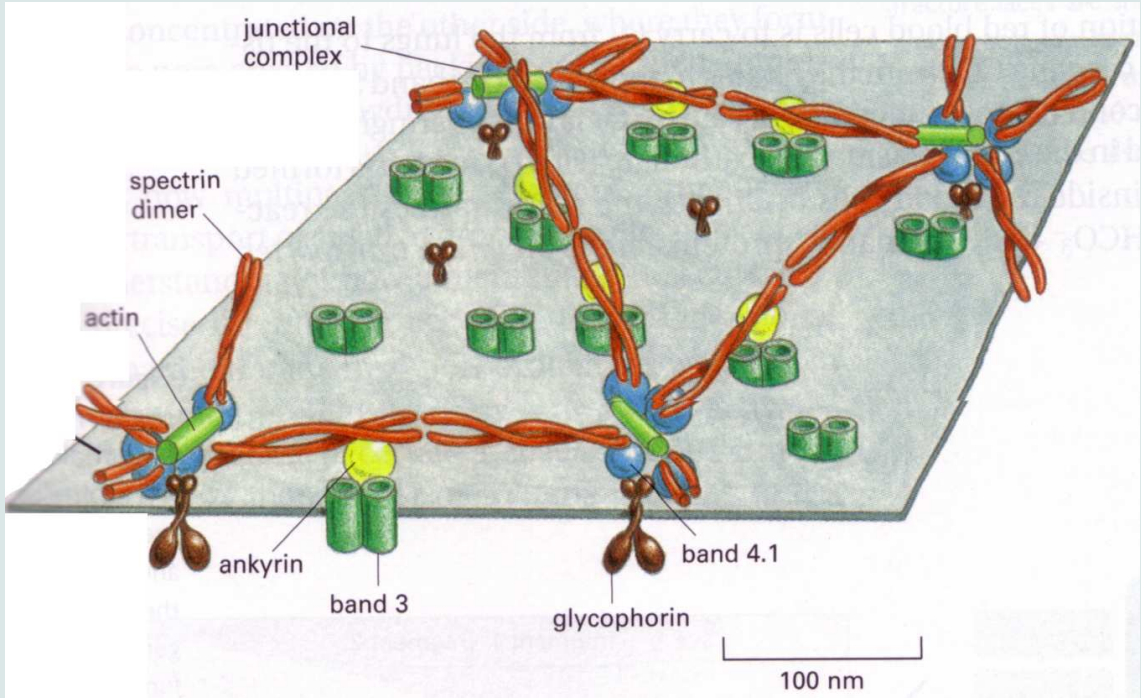
In fluid vesicles, the triangulation is dynamic:



The membrane viscosity can be controlled through the bond-flip rate.

Membranes and Vesicles: Red Blood Cells





- Spectrin network (no bond flips) induces shear elasticity μ of composite membrane
- For real RBCs: elastic parameters: $\kappa/k_BT = 50$, $\mu R_0^2/k_BT = 5000$

Membranes and Vesicles: Coupling to the Fluid

Interaction between membrane and fluid:

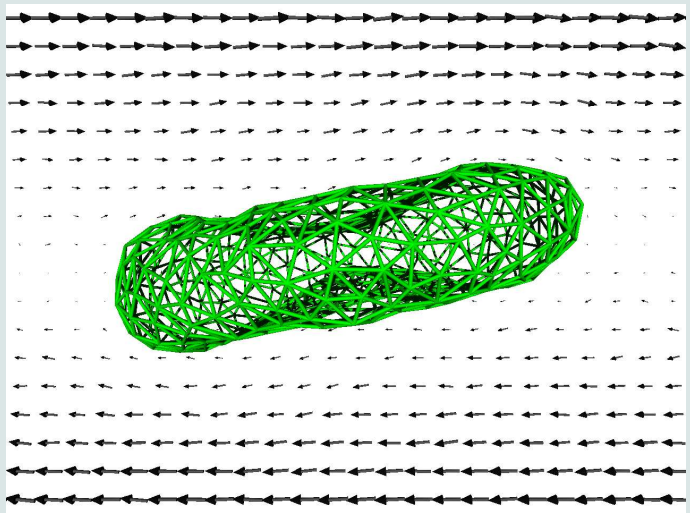
- Streaming step:

  bounce-back scattering of solvent particles on triangles

- Collision step:

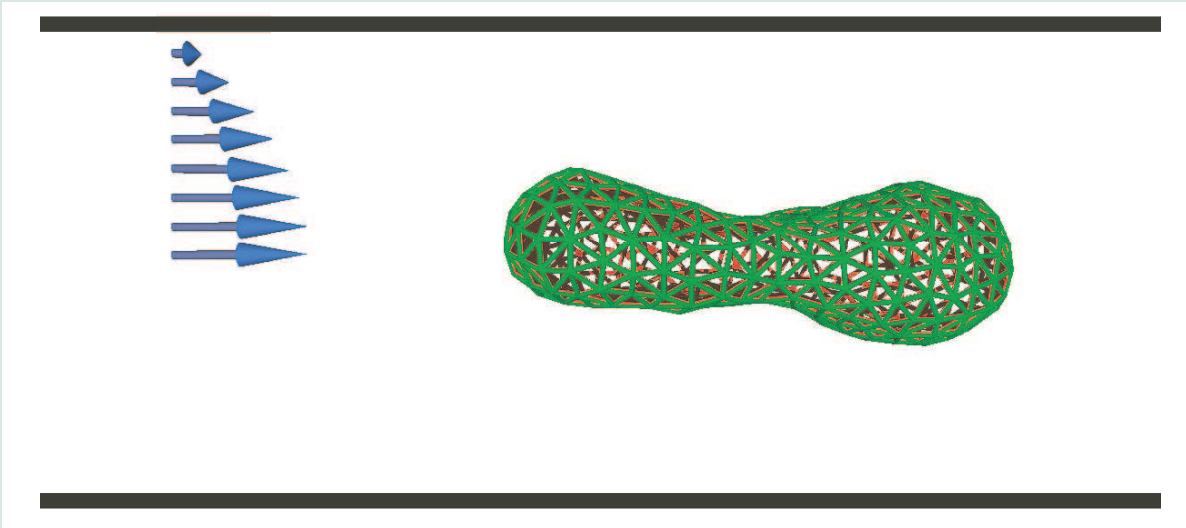
  membrane vertices are included in MPC collisions

implies impenetrable membrane with no-slip boundary conditions.

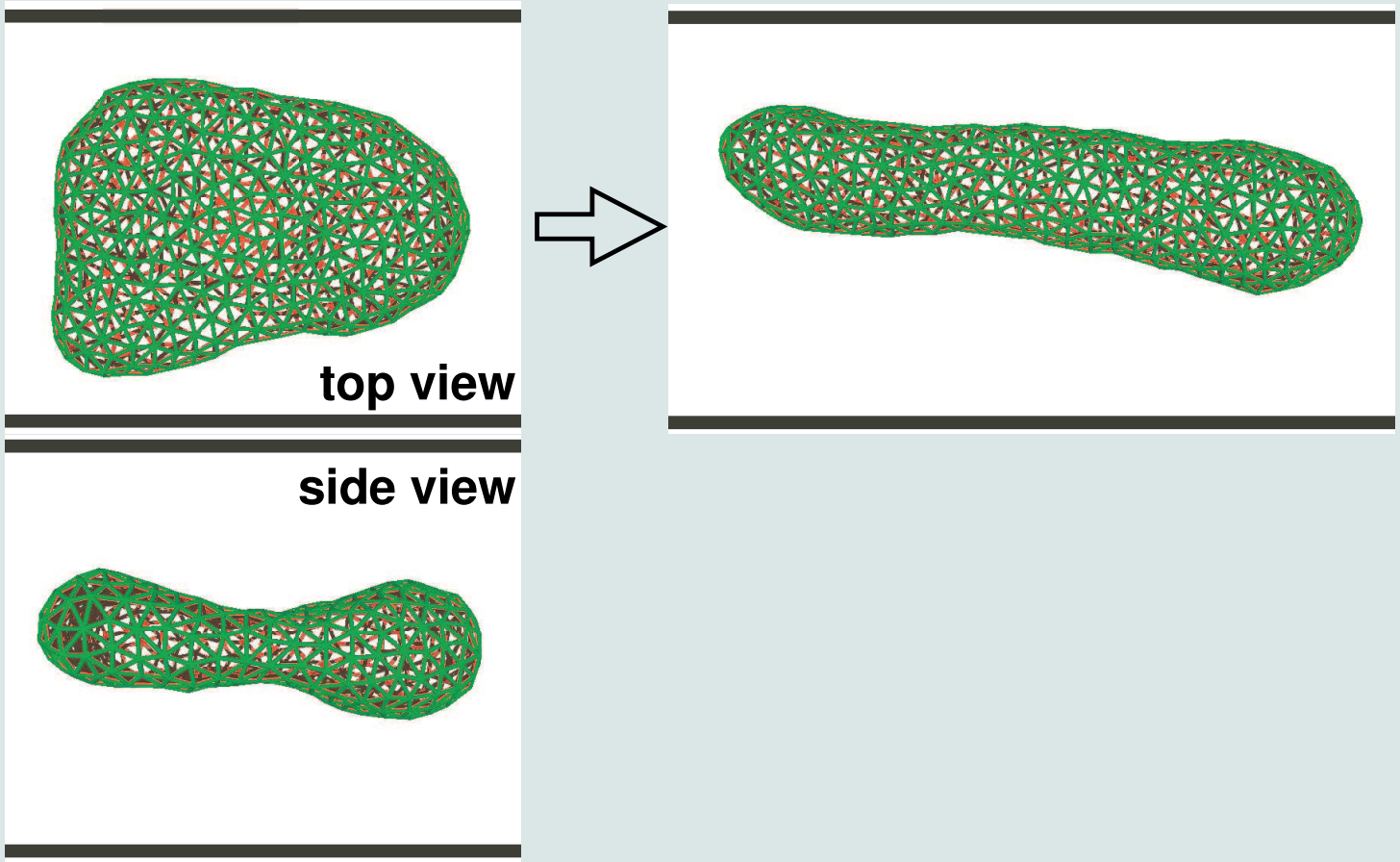


H. Noguchi and G. Gompper, Phys. Rev. Lett. **93** (2004); Phys. Rev. E **72** (2005)

Capillary Flow: Results for one vesicle



Capillary Flow: One Fluid Vesicle



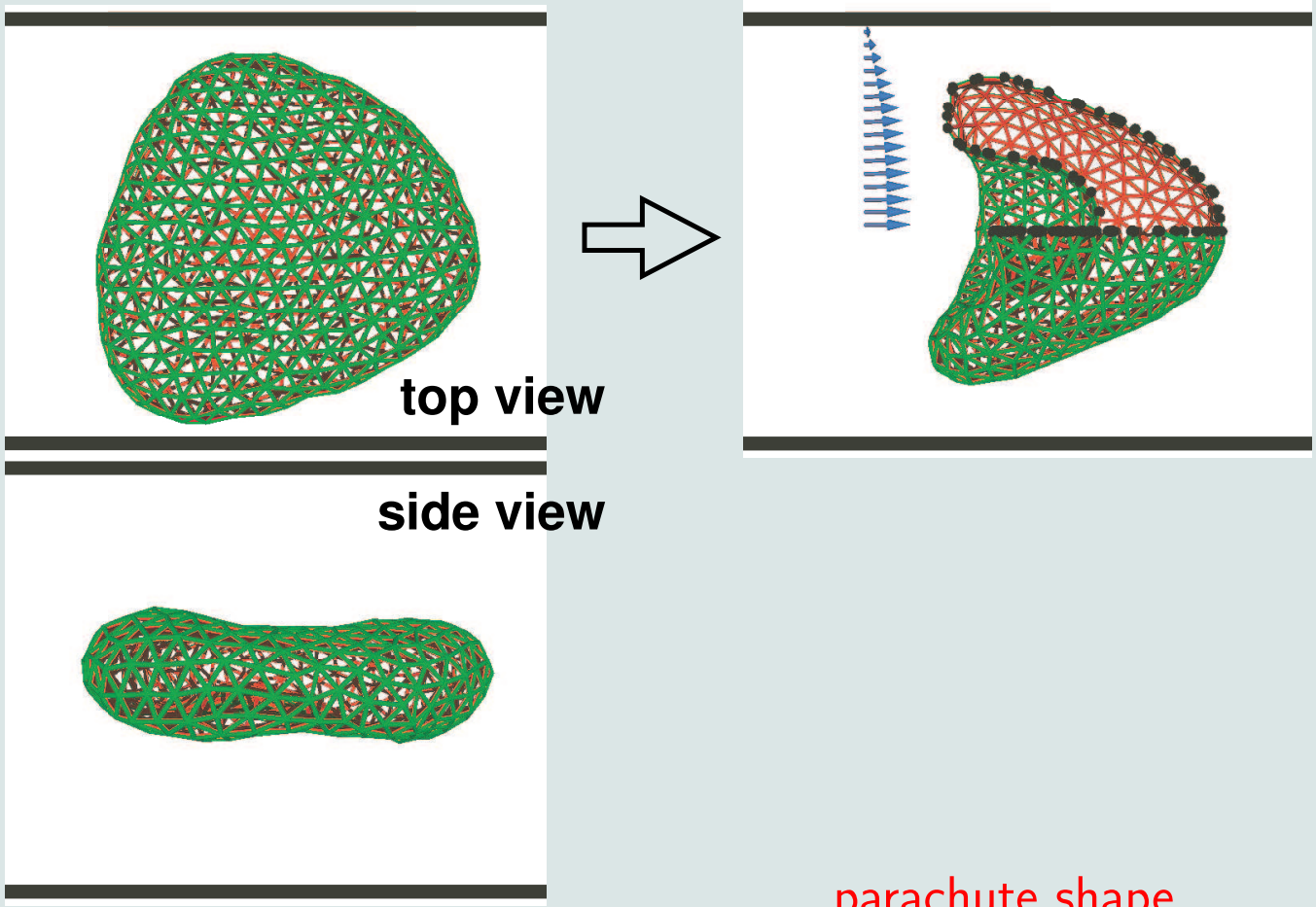
- small flow velocities: vesicle axis perpendicular to capillary axis $\longrightarrow$ no axial symmetry!
- discocyte-to-prolate transition with increasing flow

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

Capillary Flow: One Elastic Vesicle

Elastic vesicle:

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



parachute shape

Capillary Flow: One Elastic Vesicle

Elastic vesicle:

- curvature and shear elasticity
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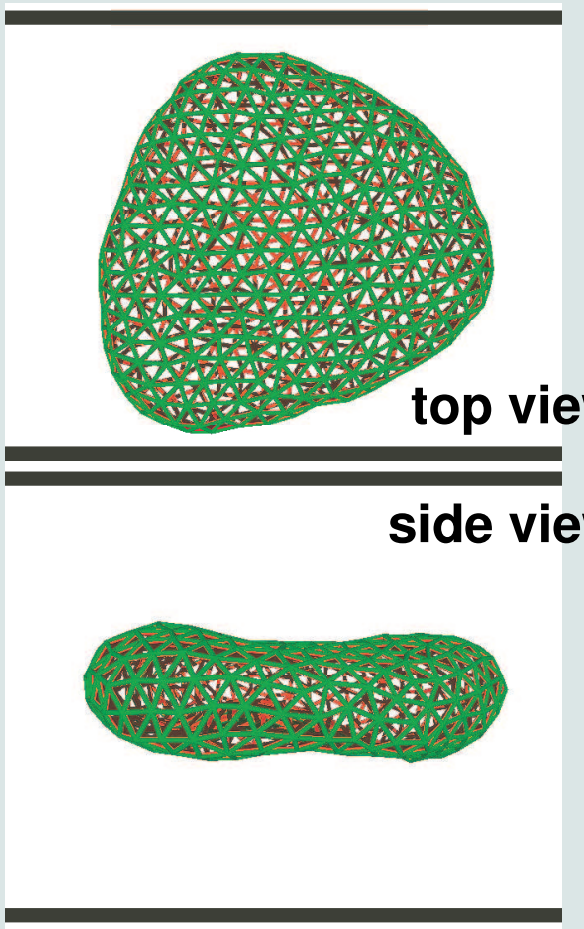
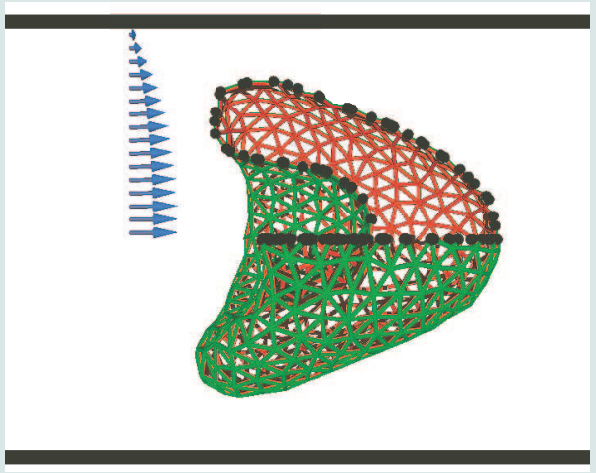
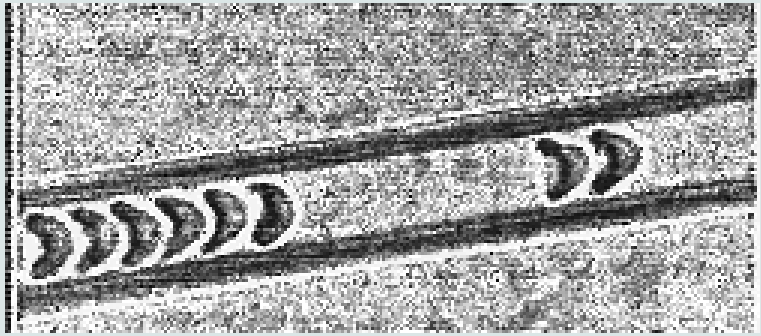


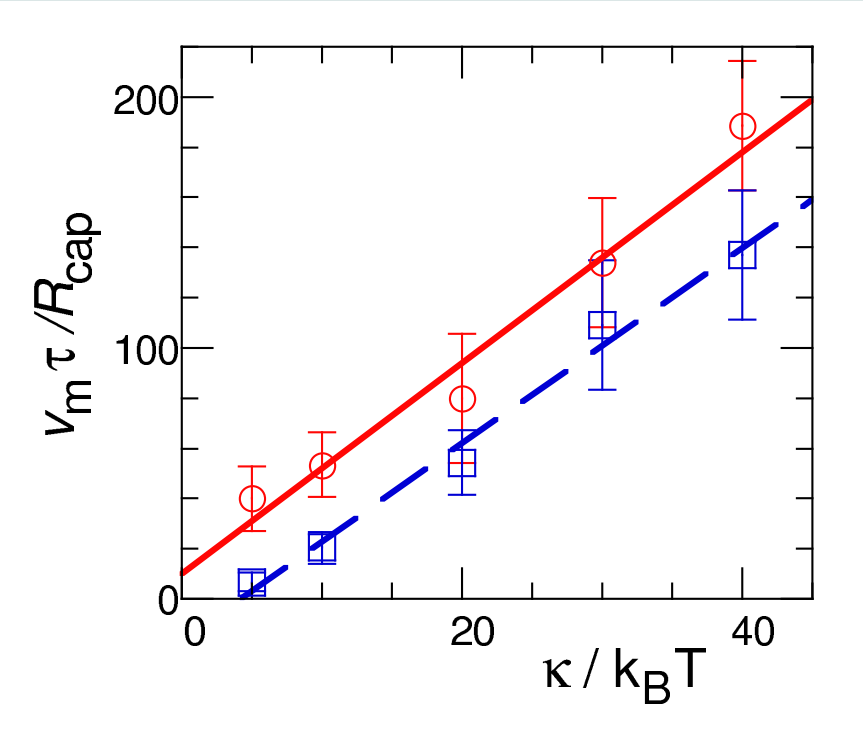




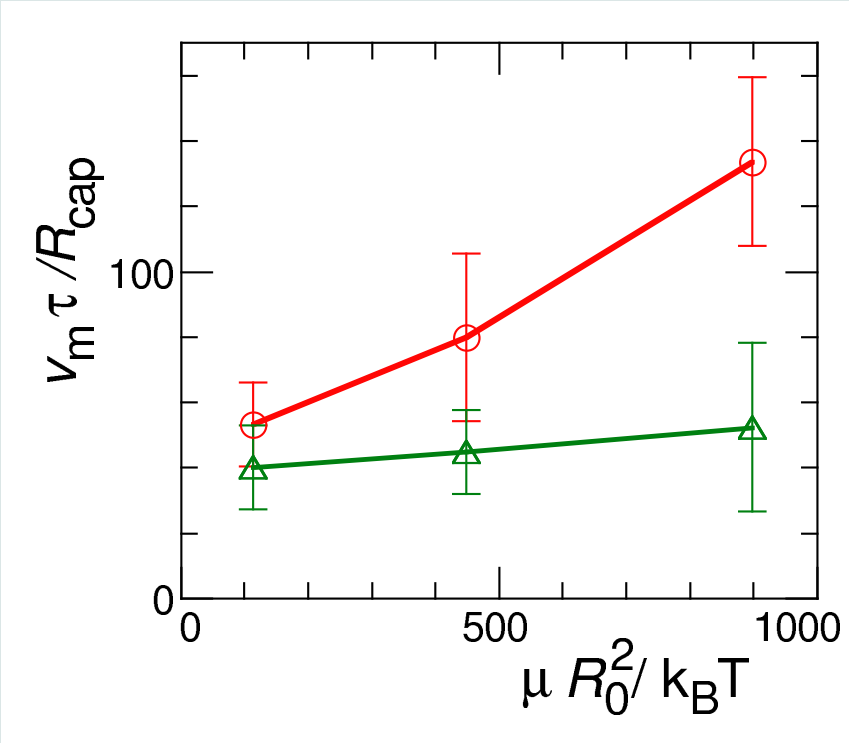
Tsukada et al., Microvasc. Res. **61** (2001)

Capillary Flow: One Elastic Vesicle

The discocyte–to–parachute transition takes place as a function of flow velocity $v_m\tau/R_{\rm cap}$



bending rigidity ($\mu = 110\,k_BT/R_0^2$)

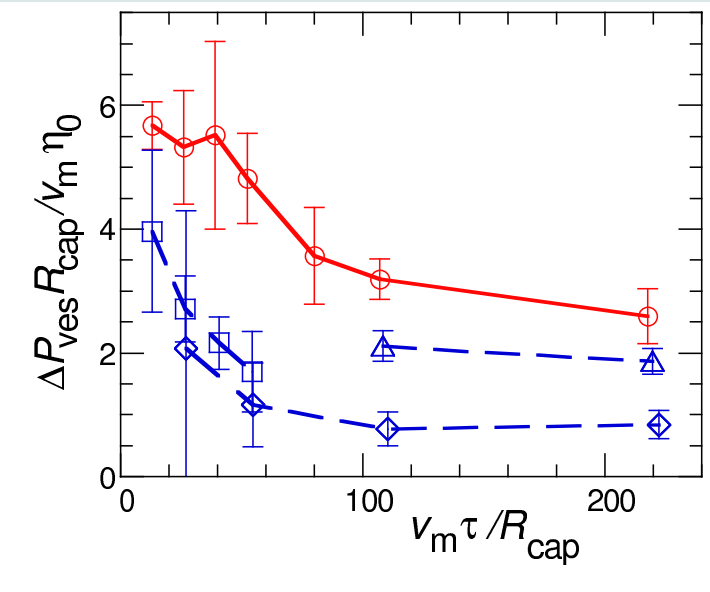


shear modulus ($\kappa = 20\,k_BT$)

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

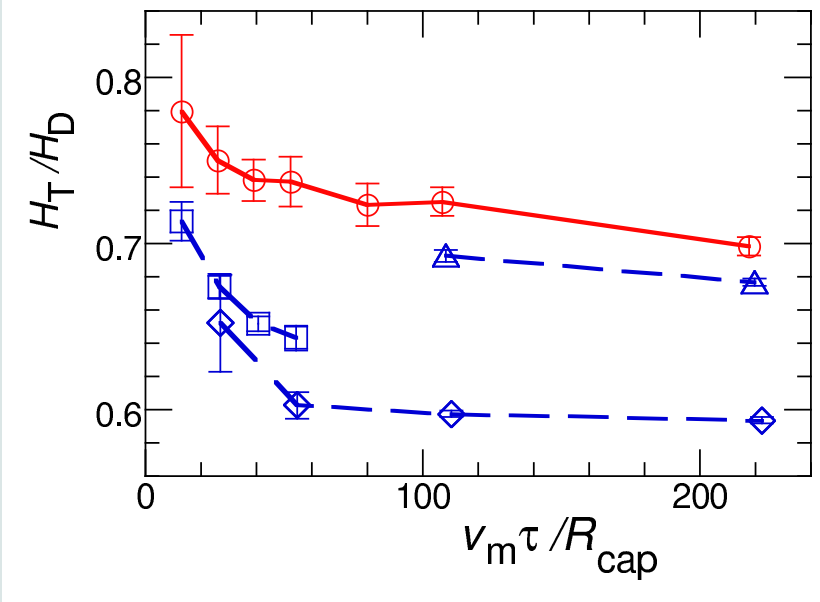
Capillary Flow: One Elastic Vesicle

Pressure drop due to vesicle



$$\Delta P = \frac{8\eta_0 (v_o - v_m) L_z}{R_{\rm cap}^2}$$

Hematocrit ratio $H_T/H_D = v_m/v_{ves}$



elastic vesicle

fluid vesicle:

□ discocyte

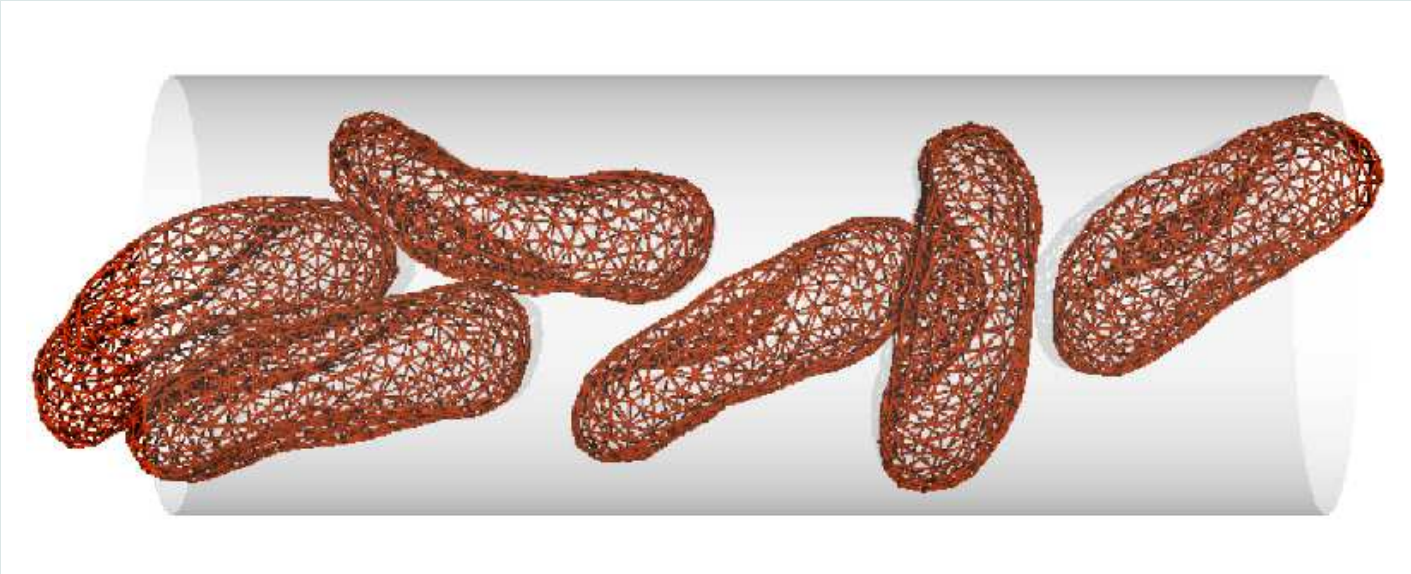
△ parachute

◇ prolate

vesicle velocity larger than fluid velocity (Fåhraeus effect)

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

Capillary Flow: Results for several vesicle



Capillary Flow: Clustering & Alignment

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

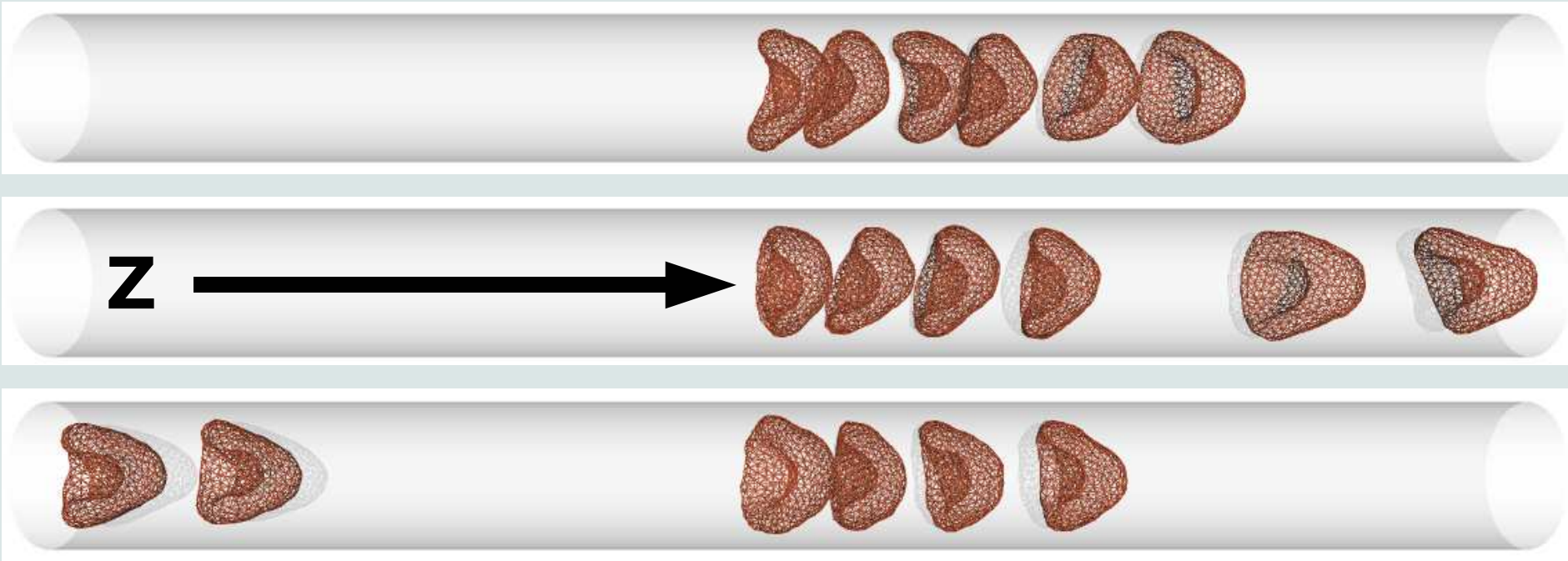
Lower in narrow capillaries $H_T = 0.1...0.2$

Therefore: Hydrodynamic interactions between RBCs very important

Note: No direct attractive interactions considered!

Capillary Flow: Clustering & Alignment

Low hematocrit H_T:

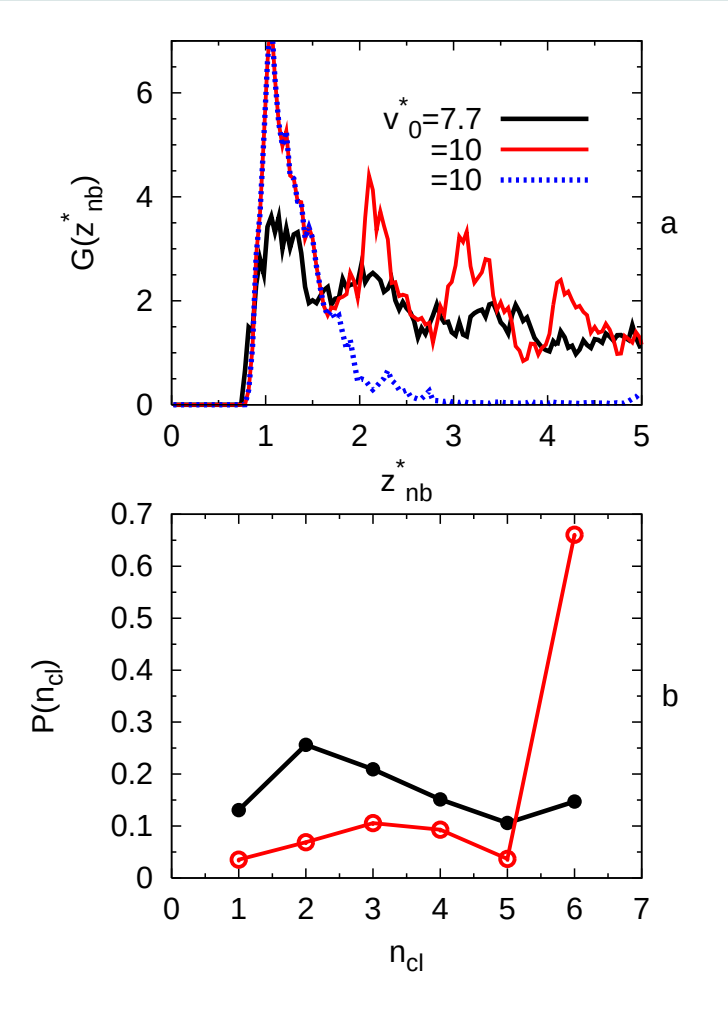


- Single vesicles more deformed $\rightarrow$ move faster
- Effective hydrodynamic attraction stabilizes clusters

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

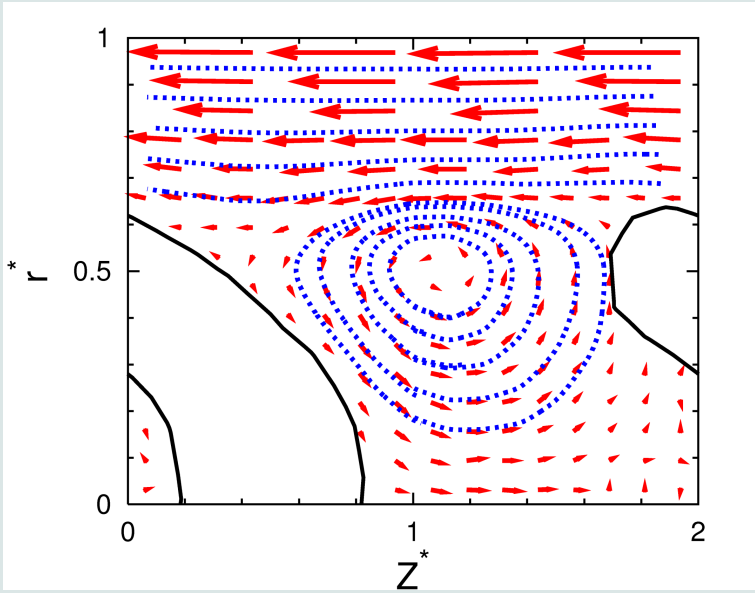
Capillary Flow: Clustering & Alignment

Low hematocrit H_T:



Positional correlation function

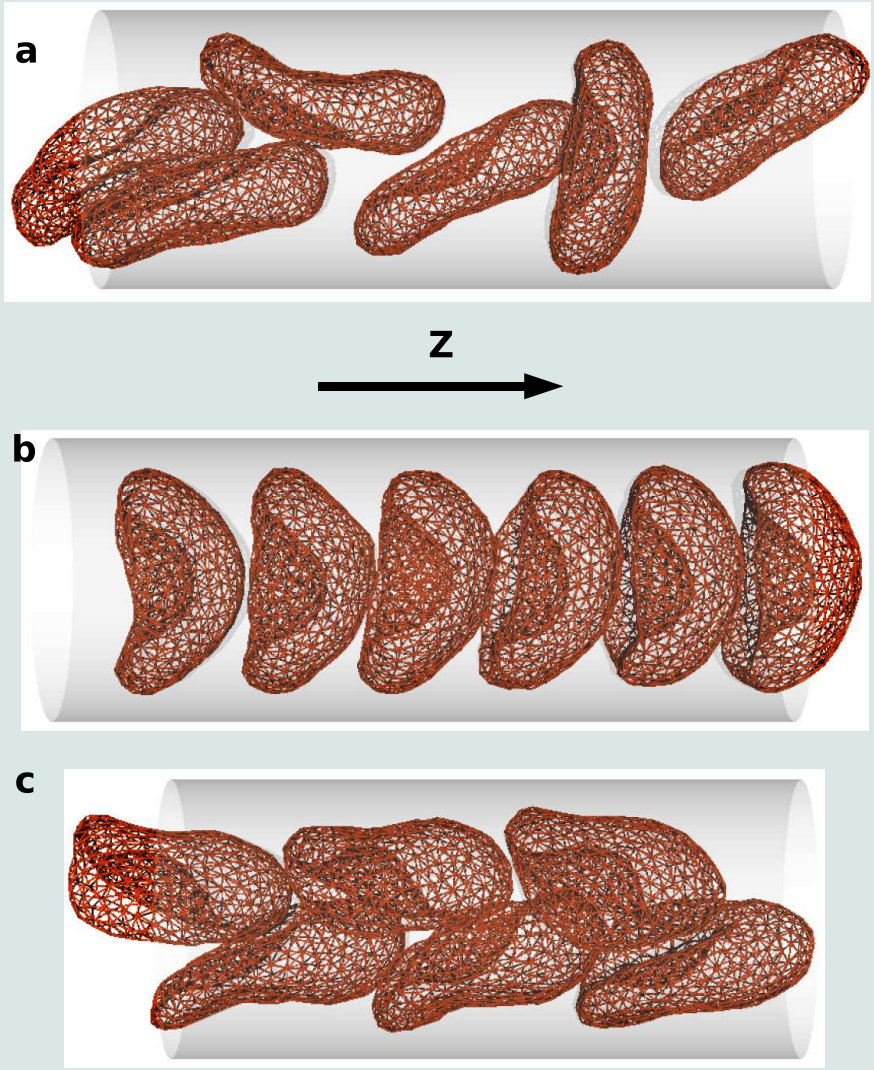
Probability for cluster size n_{cl}



Clustering tendency increases with increasing flow velocity

Capillary Flow: Clustering & Alignment

High hematocrit H_T:



disordered discocyte

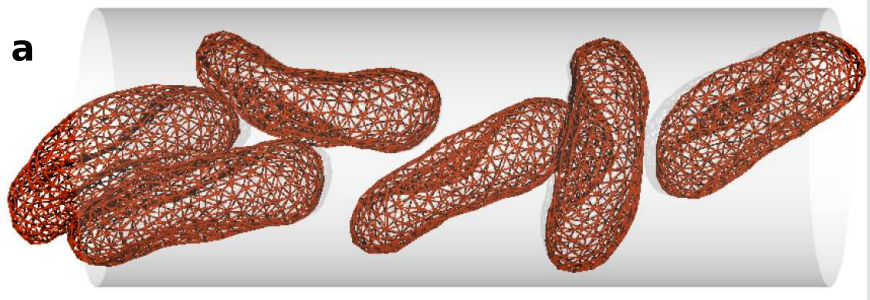
aligned parachute

zig-zag slipper

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

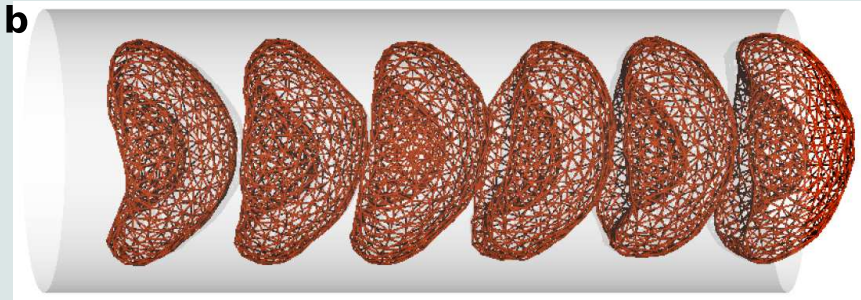
Capillary Flow: Clustering & Alignment

High hematocrit H_T:

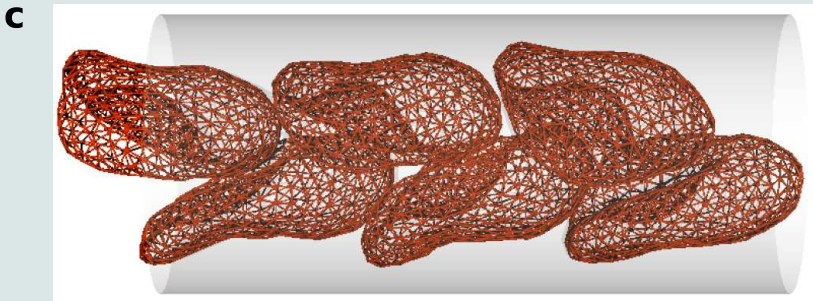


disordered discocyte

z



aligned parachute

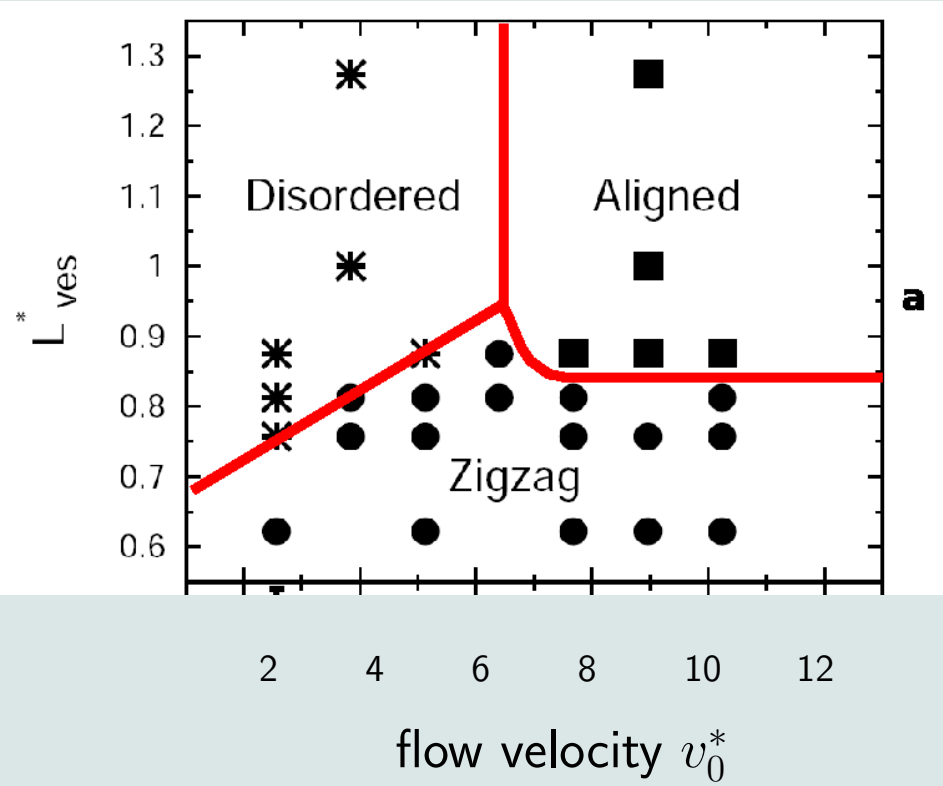


zig-zag slipper

Skalak, Science, 1969

Capillary Flow: Clustering & Alignment

Phase diagram:



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

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

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
- Red blood cells in capillary flow: shear elasticity implies parachute shapes, hydrodynamic clustering and alignment

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