CENTRE NATIONAL
DE LA RECHERCHE
SCIENTIFIQUE

Laboratoire de Spectrométrie Physique

Modelling vesicle dynamics in extended geometries and in microfluidic devices

Modélisation de vésicules en géométrie étendue et dans des systèmes micro-fluidiques

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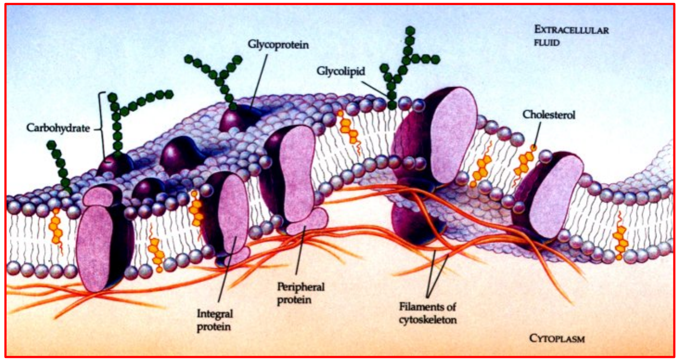
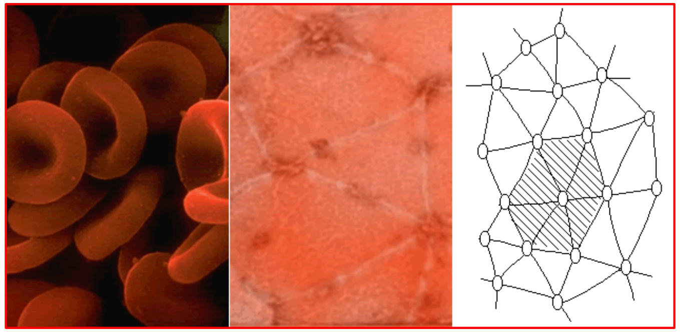
Contents

- Vesicle model
- Simple shear flow
- Unbounded Poiseuille flow
- Confined geometries and micro-fluidic devices
- Two interacting vesicles
- Conclusions

Vesicle model

What is a vesicle?





Hydrophilic phosphate head (polar)

Two hydrophobic fatty acid tails (non polar)

Phospholipid molecule

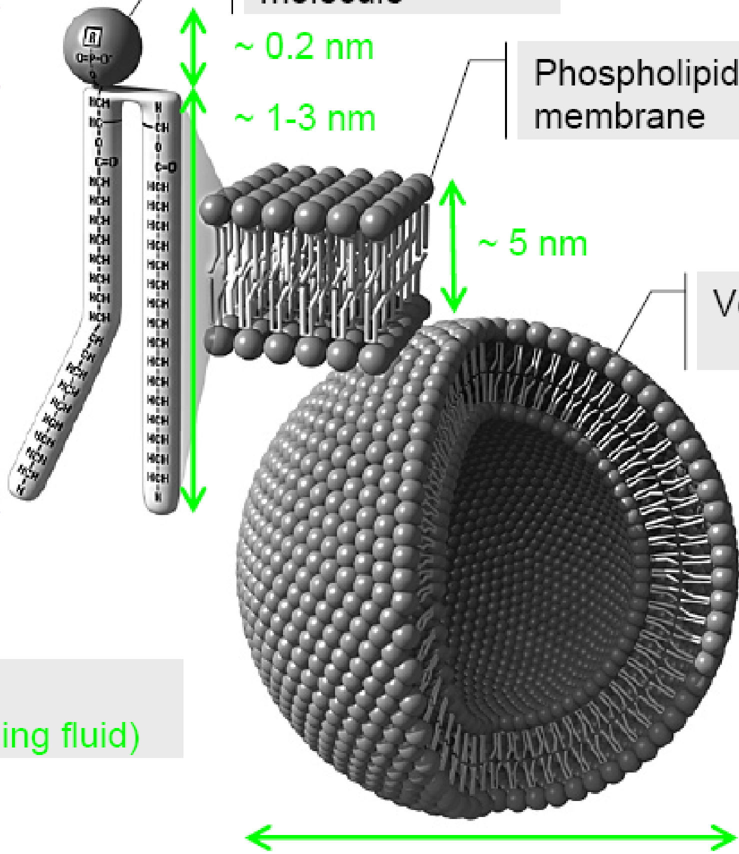
~ 0.2 nm

~ 1-3 nm

Phospholipid bilayer membrane

~ 5 nm

Vesicle



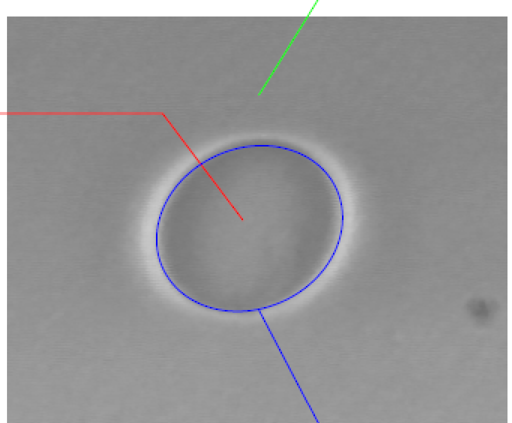
~ 10 μm

$\sim 10^{10}$ Molecules

(Nasa Astrobiology Institute)

External fluid (the suspending fluid)

Internal fluid (the encapsulated fluid)



Phospholipid membrane (fluid membrane)

A phase-contrast micrograph (V. Vitkova)

Vesicle properties

- A conserved volume V (area S in 2D)
- A conserved area S (perimeter L in 2D)
- The vesicle membrane energy:

Membrane rigidity
$\kappa \sim 10^{-19} J$

Local membrane curvature

$$E = \frac{\kappa}{2}\int_{\partial\Omega} H^2 dS + \int_{\partial\Omega} \zeta dS.$$

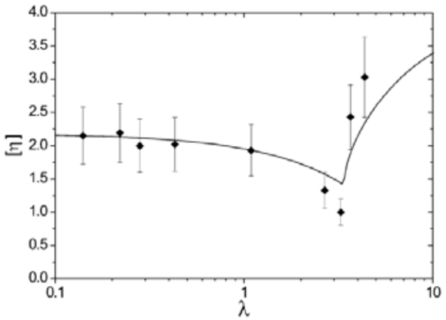
The Helfrich curvature energy

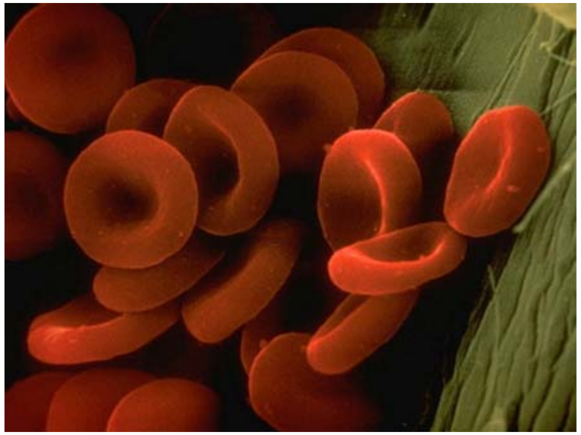
Lagrange multiplier
(area conservation constraint)

Membrane force

$$\mathbf{f} = -\frac{\delta E}{\delta \mathbf{r}}$$

Biomedical engineering applications

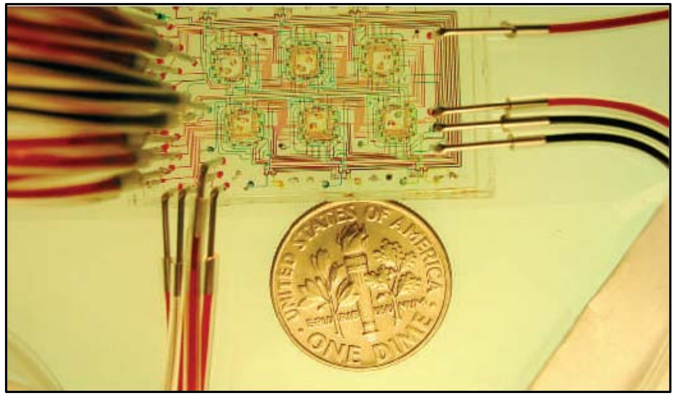




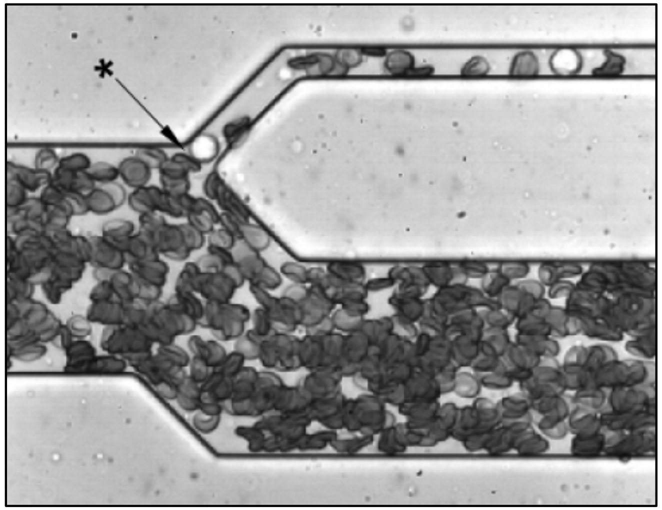
Blood rheology

A lab

A lab-on-chip



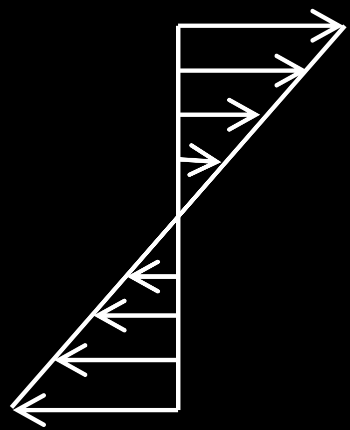
(S. R. Quake, Stanford University)



Microfluidic device to sort out WBCs
from a whole blood sample
(L. L. Munn, MGH)

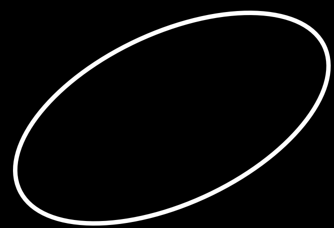
Medical diagnostic
on a drop of
blood using
a lab-on-chip (CNRS)

Vesicle dynamics under <u>shear flow</u>



Shear flow

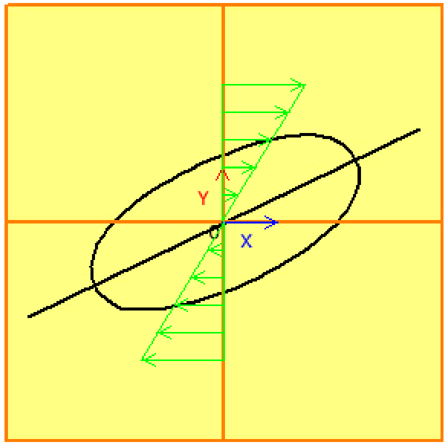
+



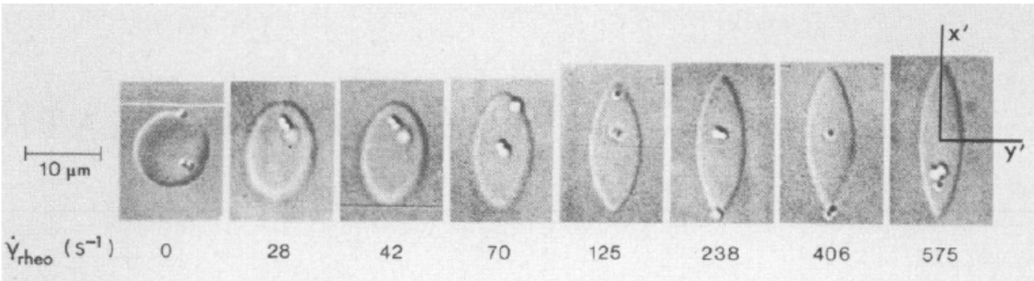
Vesicle

Dynamical regimes under shear flow

Tank-treading



T. M. Fischer *el al* Science (1978)



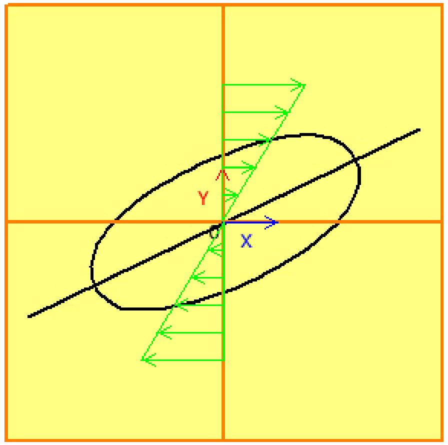
λ_C

1 → ∞

$$\lambda = \frac{\eta_{int}}{\eta_{ext}}$$

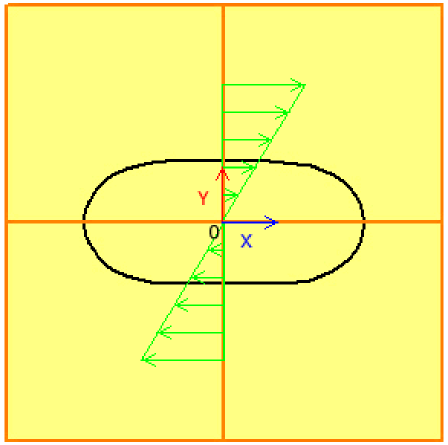
Dynamical regimes under shear flow

Tank-treading



T. M. Fischer *el al* Science (1978)

Tumbling



S. R. Keller & R. Skalak JFM (1982)

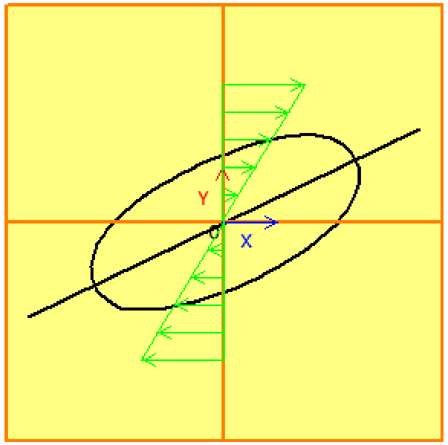
λ_C

1 ⟶ ∞

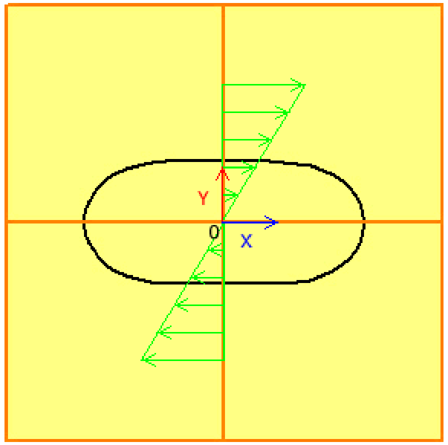
$$\lambda = \frac{\eta_{int}}{\eta_{ext}}$$

Dynamical regimes under shear flow

Tank-treading



Tumbling



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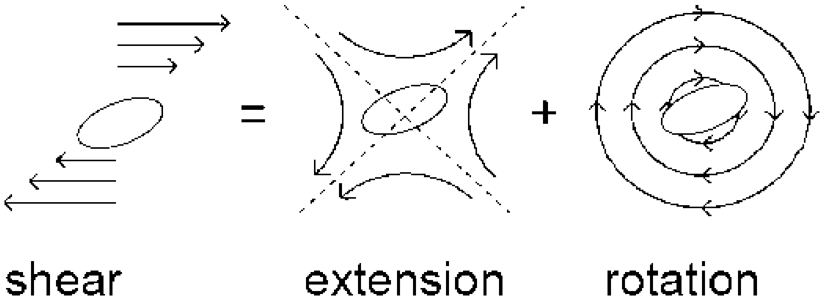


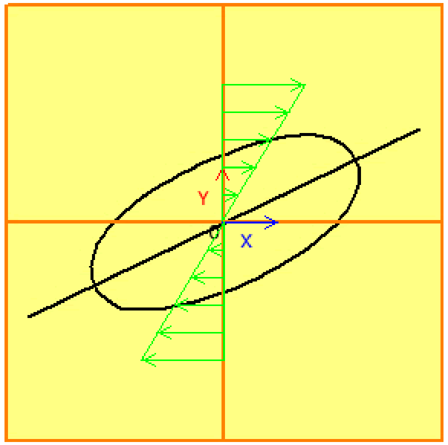
λ_C

1 ⟶ ∞

$$\lambda = \frac{\eta_{int}}{\eta_{ext}}$$

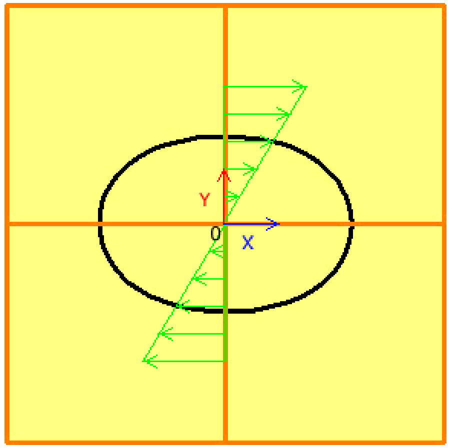
Dynamical regimes under shear flow

Tank-treading



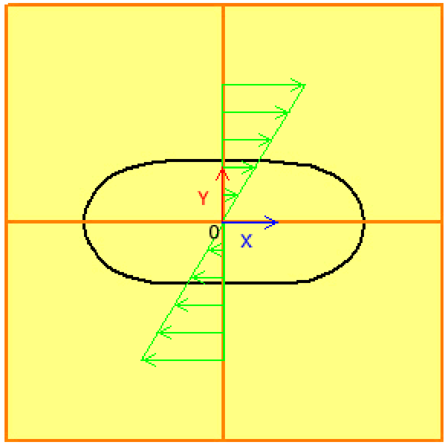
T. M. Fischer *el al* Science (1978)

Vacillating-breathing



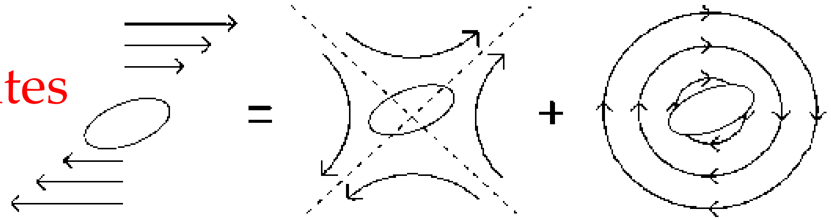
C. Misbah PRL (2006)

Tumbling



S. R. Keller & R. Skalak JFM (1982)

At higher shear rates



shear extension rotation

λ_C

1 ⟶ ∞

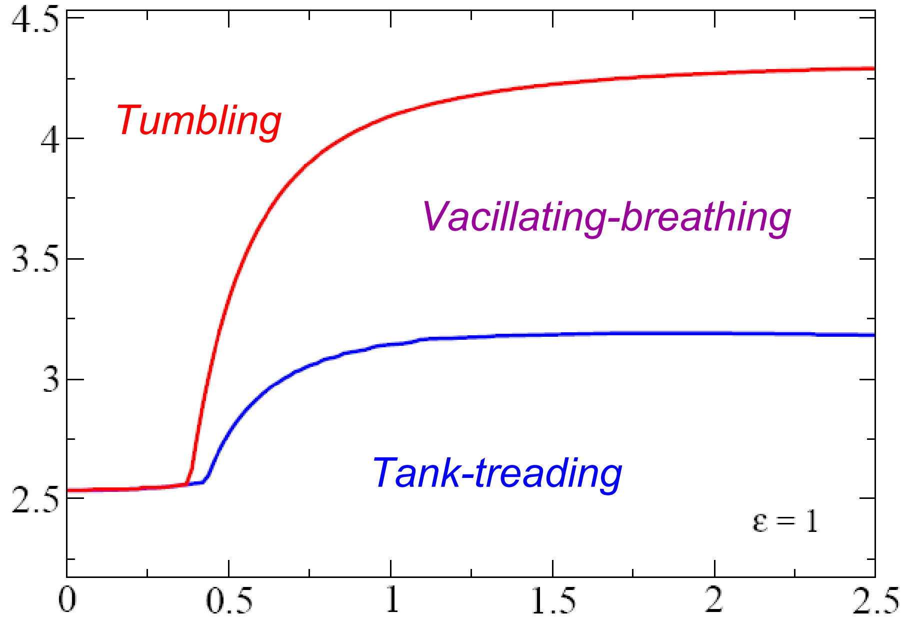
$$\lambda = \frac{\eta_{int}}{\eta_{ext}}$$

Three main key parameters

- The viscosity contrast: $\lambda = \frac{\eta_{int}}{\eta_{ext}}$
- The excess area: $A = (4\pi + \Delta)\, R_0^2$
- The capillary number: $Ca = \frac{\tau_{shape}}{\tau_{flow}} = \frac{\eta_{ext} R_0^3}{\kappa} \dot{\gamma}$

Phase-diagram

$$\lambda = \frac{\eta_{\rm int}}{\eta_{\rm ext}}$$



$$Ca = \frac{\eta_{\rm ext}\dot{\gamma}R_0^3}{\kappa}$$

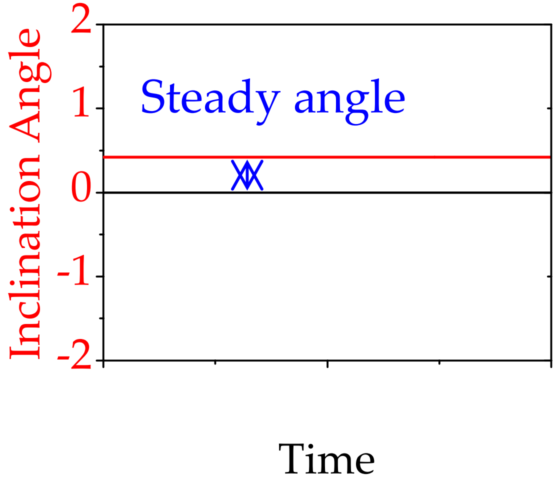
Theory

G. Danker *et al* PRE (2007)
V. V. Lebedev *et al* PRL (2007)
H. Noguchi & Gompper PRL (2007)

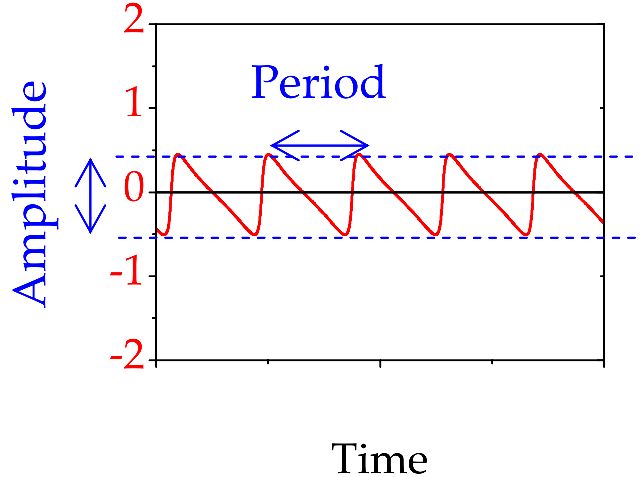
Experiment

J. Deschamps et al PRL (2009)

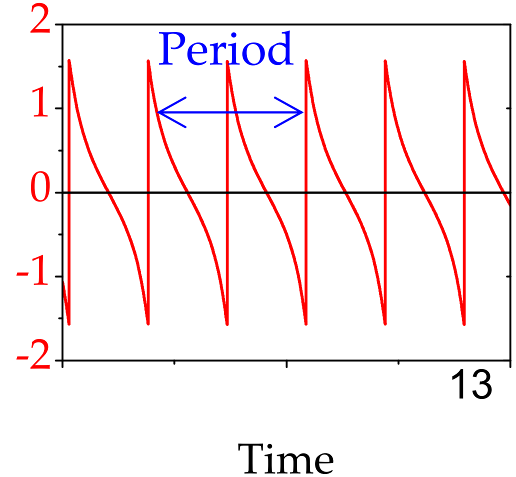
Tank-treading



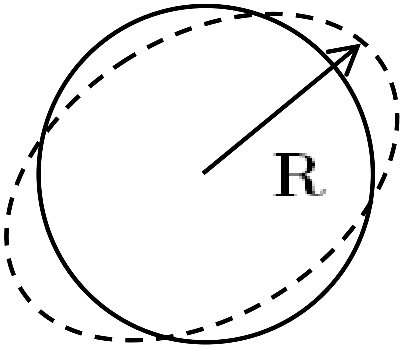
Vacillating-breathing



Tumbling



Small deformation theory



Vesicle shape deviation from a sphere

$$\mathbf{R}(\theta,\phi) = R_0\left[1+\epsilon f(\theta,\phi)\right]\mathbf{e}_\mathrm{r}$$

C. Misbah PRL (2006)

$$\epsilon = \sqrt{\Delta}$$

Spherical harmonics

$$f(\theta,\phi) = \sum_{m=-2}^{2} F_{2,m} Y_2^m = F_{2,-2}Y_2^{-2} + F_{2,0}Y_2^0 + F_{2,2}Y_2^2$$

Amplitude → Dynamics

Shear flow

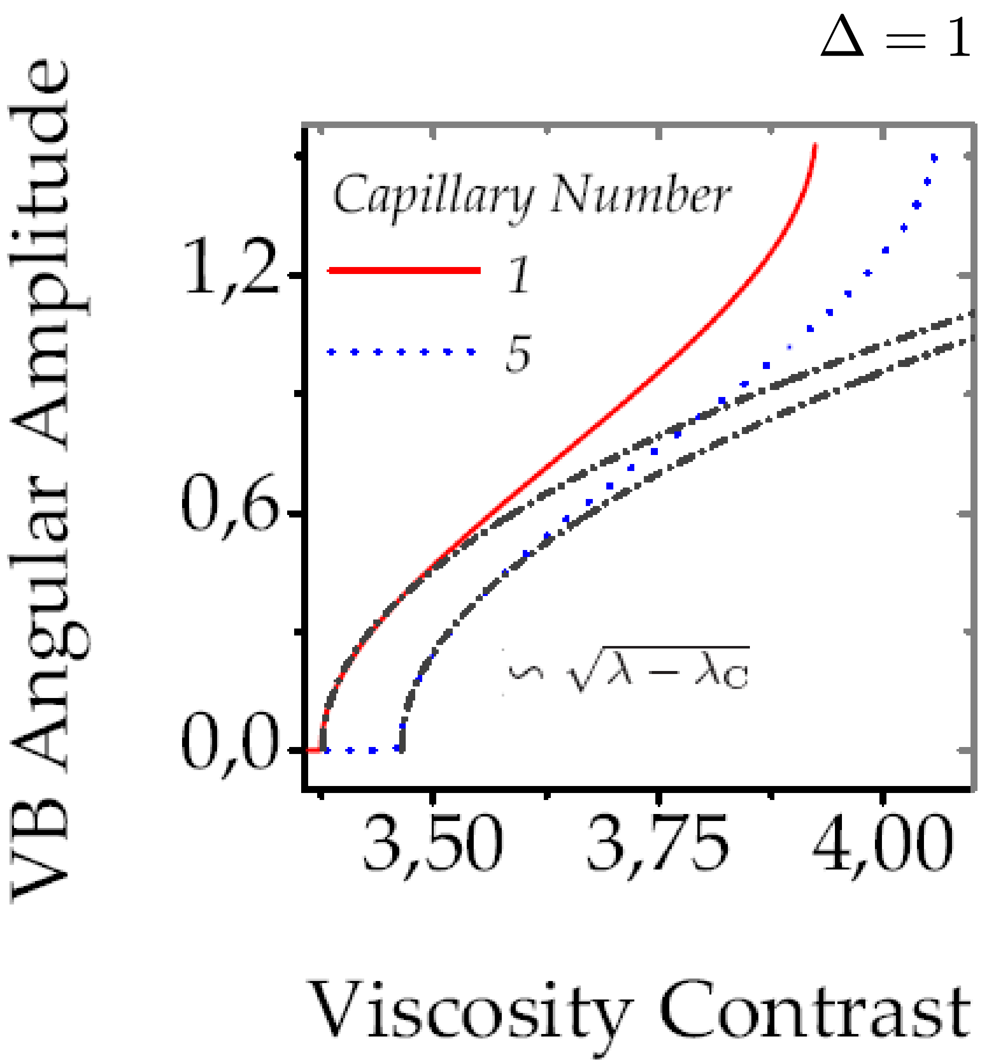
$$-i\epsilon\partial_t F_{22} = F_{22} - h + 2h\Delta^{-1}(|F_{22}|^2 - F_{22}^2) + \text{Higher order terms}$$

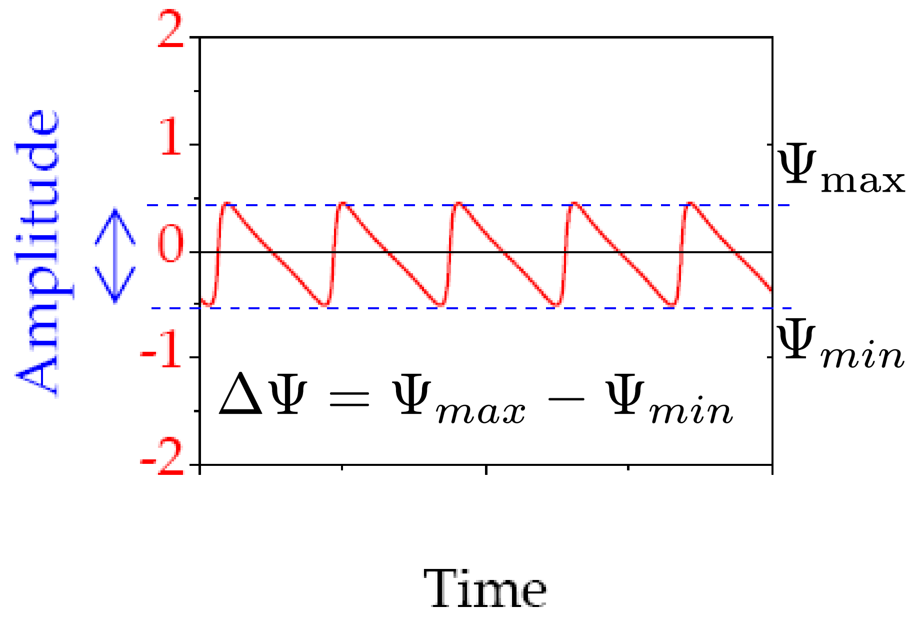
$$h = f(\lambda)$$

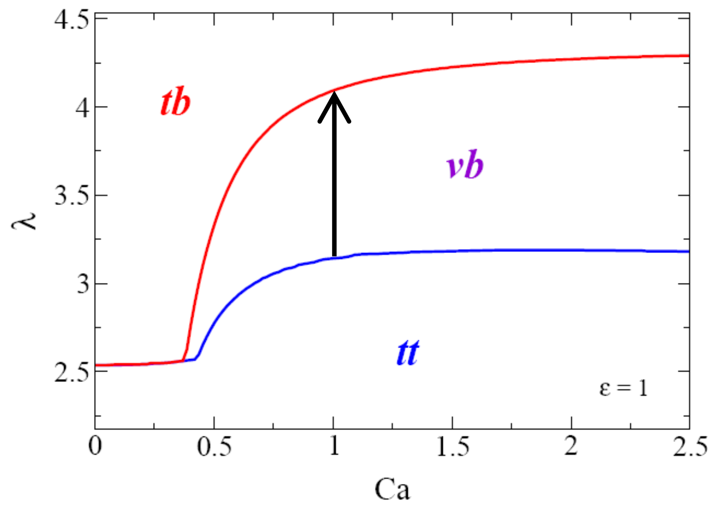
Dynamical equation

G. Danker *et al* PRE (2007)

Vacillathing-breathing (Amplitude)

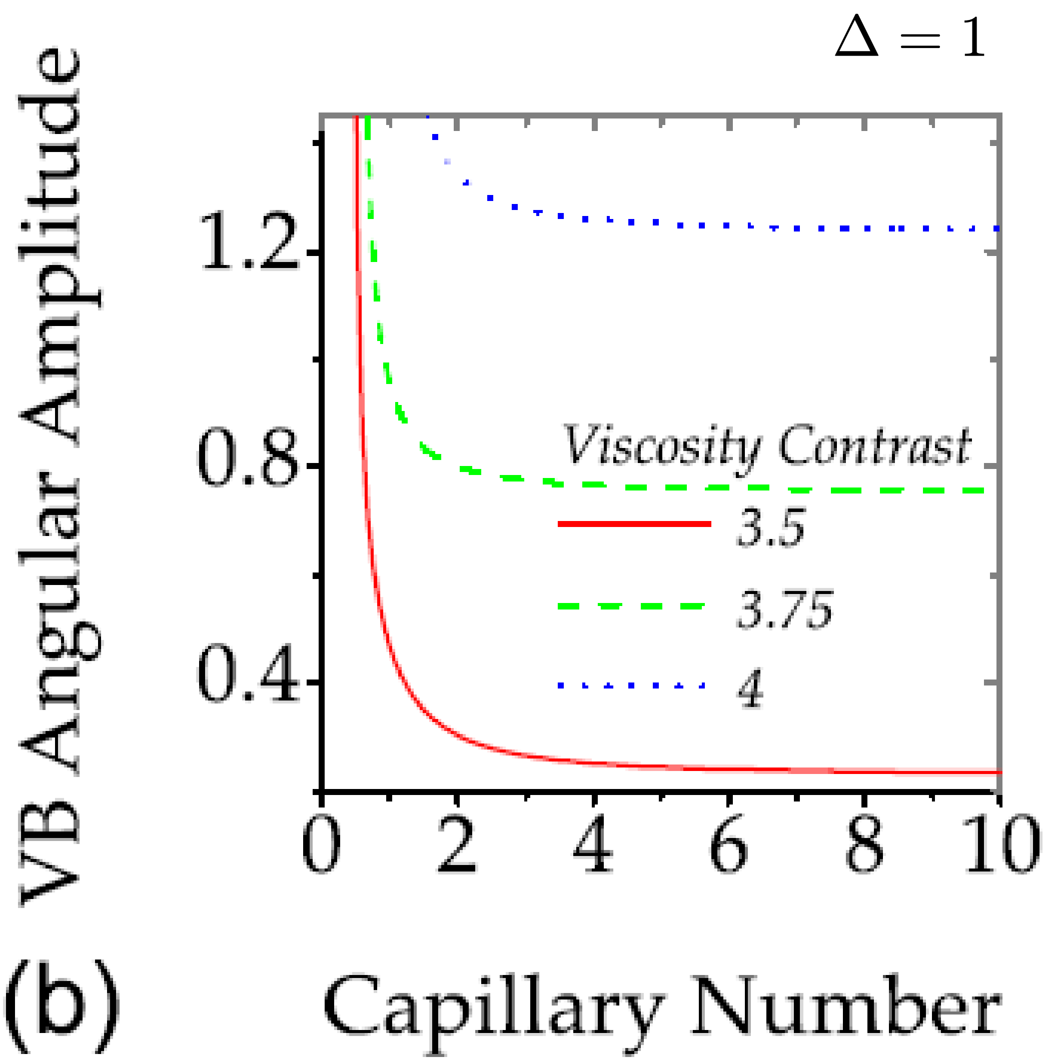


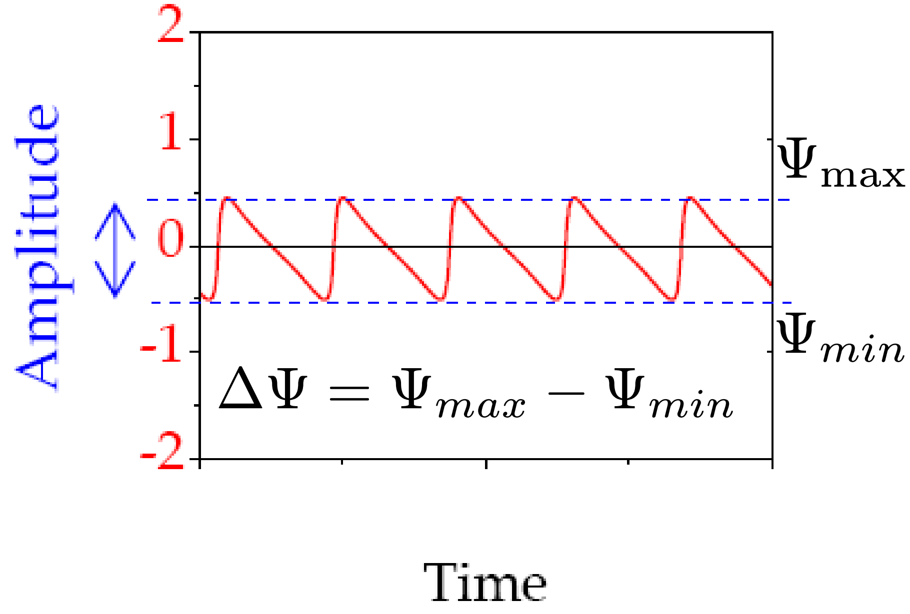


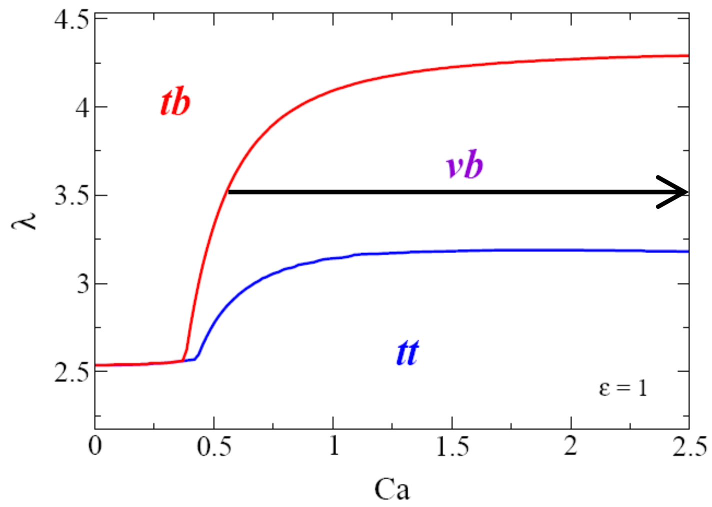


$$-\pi/4 < \Psi_{min} < \Psi_{max} < +\pi/4$$

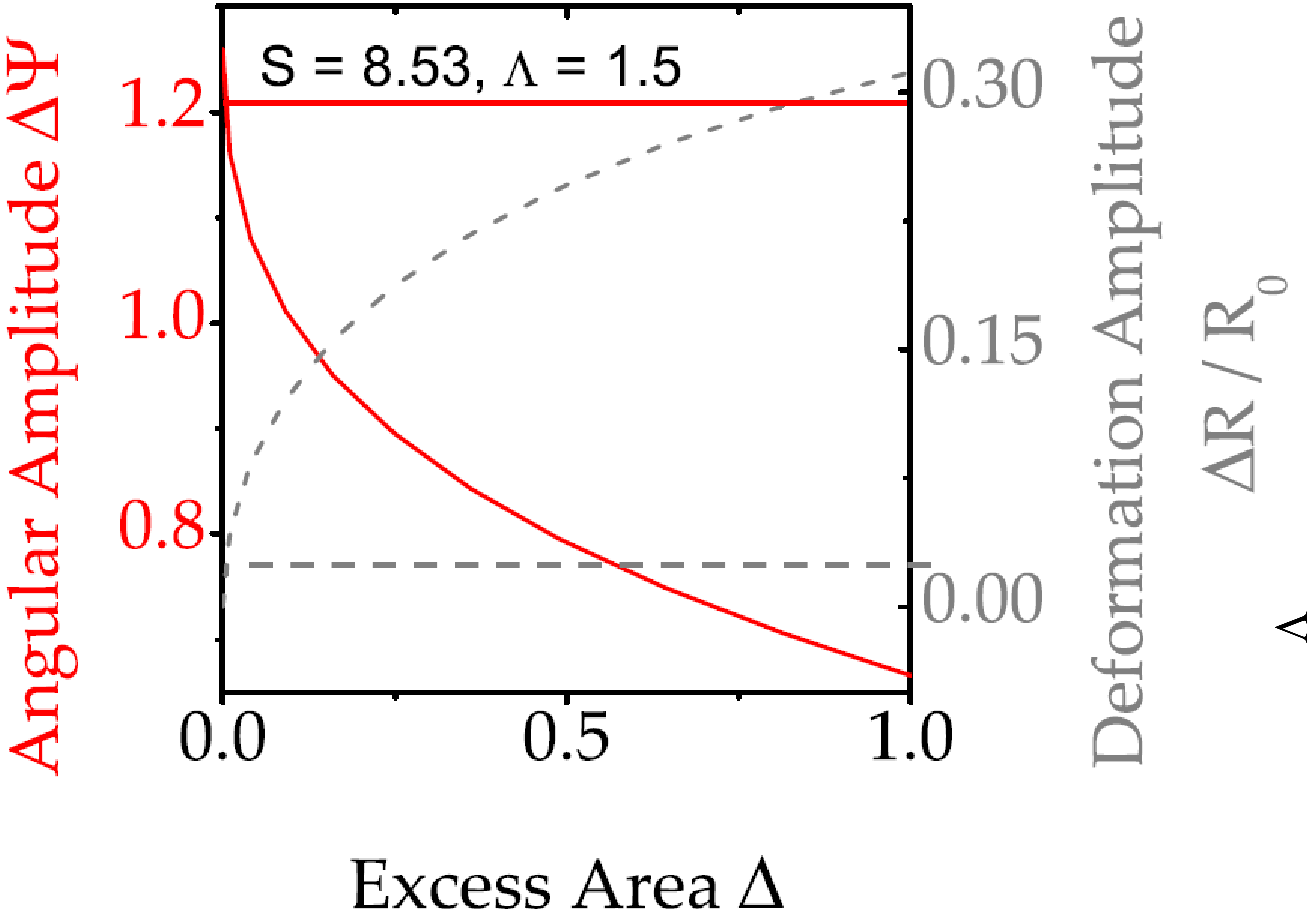
Vacillathing-breathing (Amplitude)

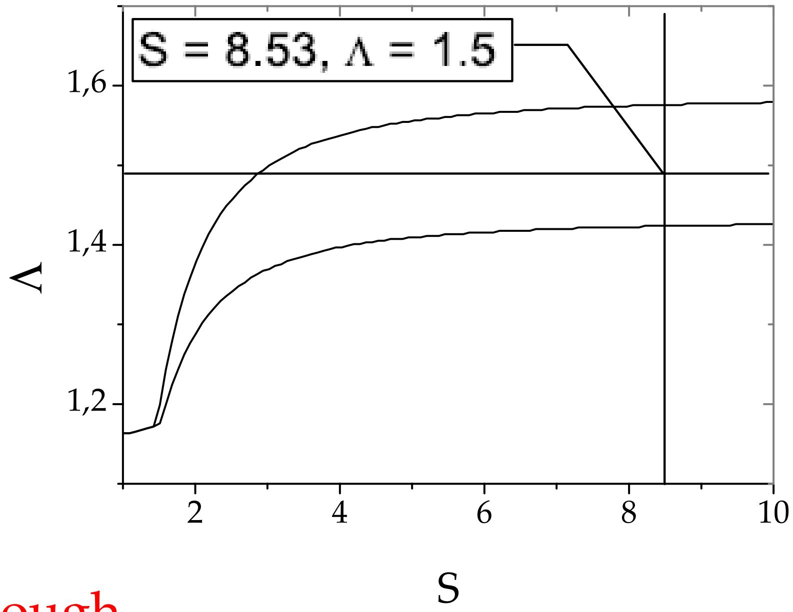






3 main key dimensionless parameters





Not enough

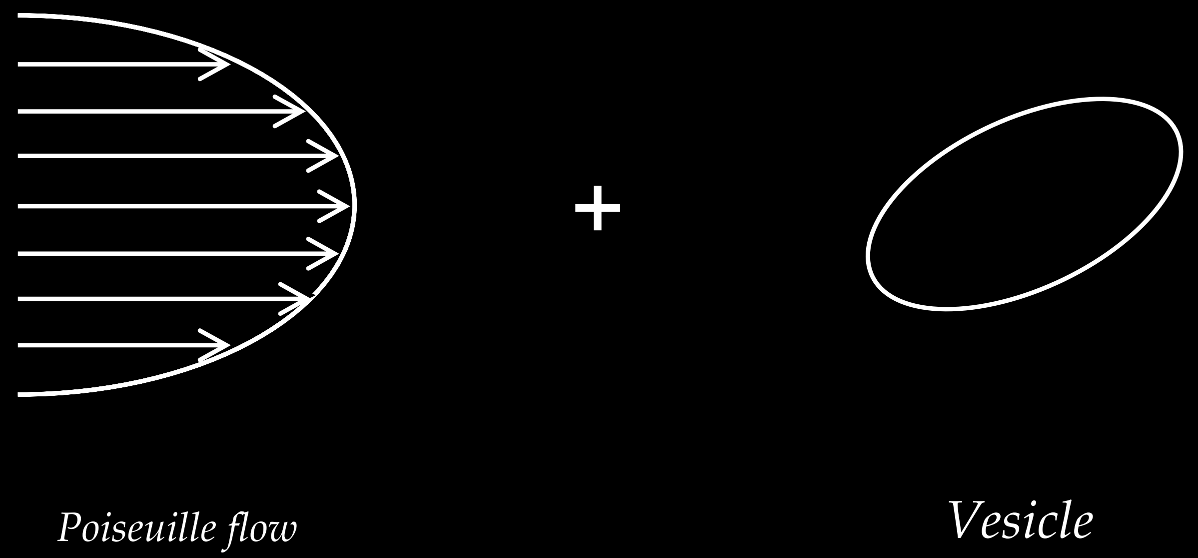
(Δ,λ,Ca) ~~(S,Λ)~~

$$S = f(Ca, \Delta)$$

$$\Lambda = f(\lambda, \Delta)$$

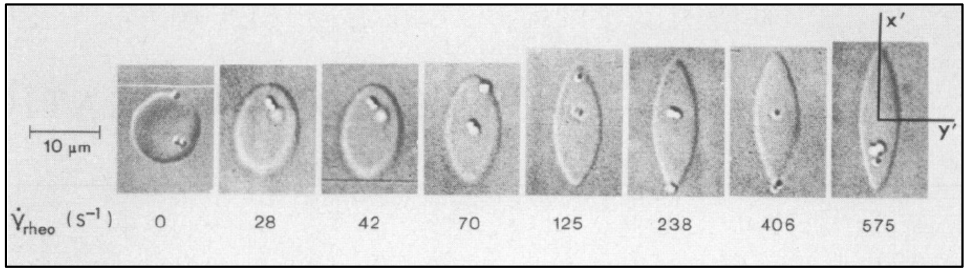
V. V. Lebedev *et al* PRL (2007)

Lateral migration and deformation of a vesicle in unbounded Poiseuille flow



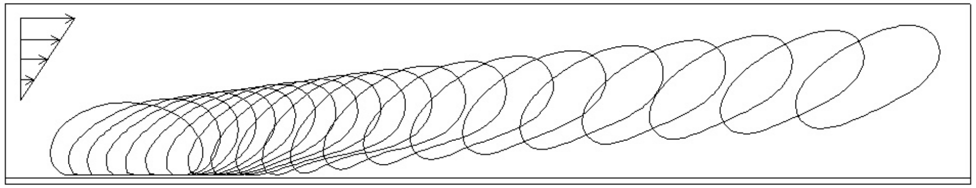
Motivations (Blood rheology)

Deformation of a RBC under shear flow



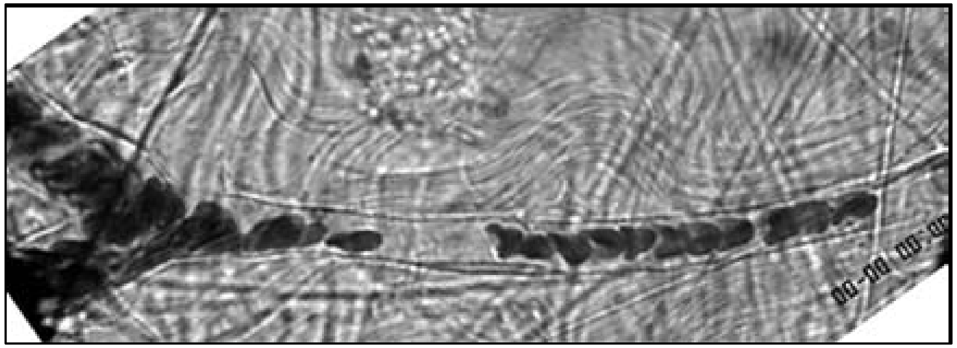
T. M. Fischer *el al* Science (1978)

Wall-induced lift force



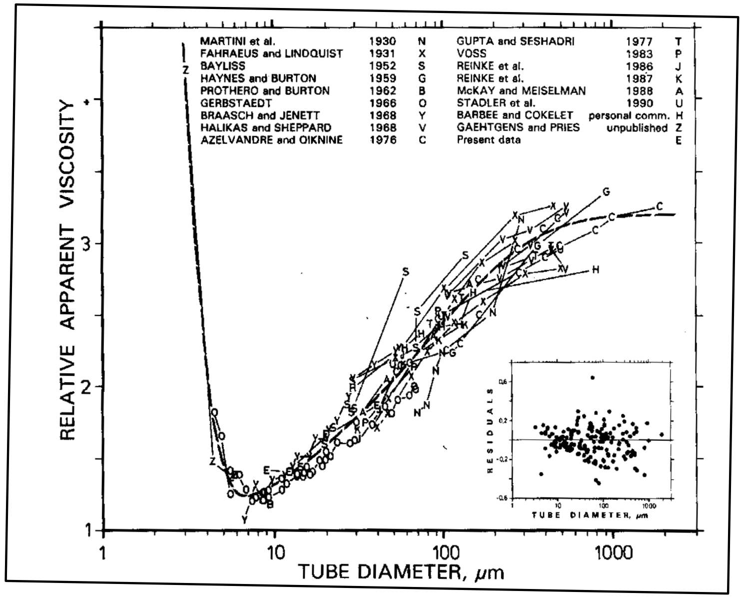
I. Cantat and C. Misbah PRL (1999)
M. Abkarian *et al* PRL (2002)

Lateral migration of RBCs



T. W. Secomb *et al* ABE (2007)

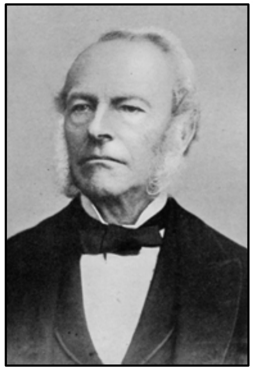
Fahraeus-Lindqvist effect



R. Fahraeus and T. Lindqvist, Am. J. Physiol. (1931)

The boundary integral method (BIM)

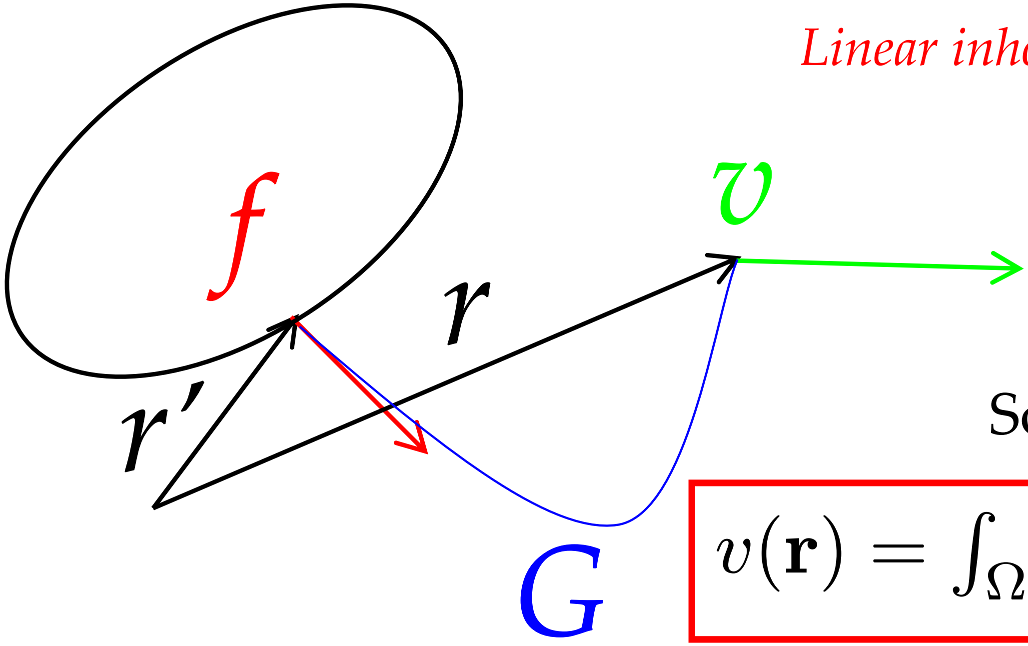
G. G. Stokes
(1819-1903)



Stokes equations

$$\eta \nabla^2 v(\mathbf{r}) - \nabla p(\mathbf{r}) = -f(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}')$$
$$\nabla . v(\mathbf{r}) = 0$$

Linear inhomogeneous partial differential equations



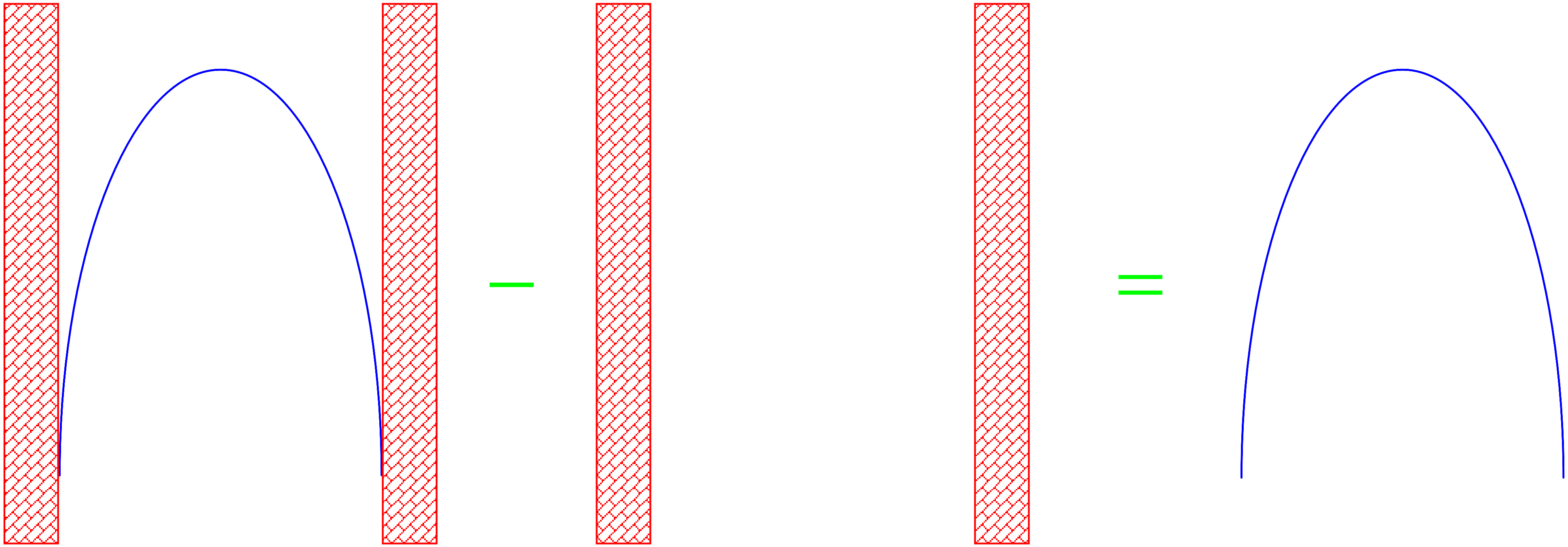
Solution (Integral equation)

$$v(\mathbf{r}) = \int_\Omega \mathbf{G}(\mathbf{r},\mathbf{r}')f(\mathbf{r}')ds(\mathbf{r}') + \mathbf{v}_{\mathrm{Pois}}(\mathbf{r})$$

Solution in terms of the Green's function

C. Pozrikidis (1992)
M. Kraus *et al* PRL (1996)
I. Cantat and C. Misbah PRL (1999)

What is an unbounded Poiseuille flow?



The Poiseuille flow
in a
confined geometry

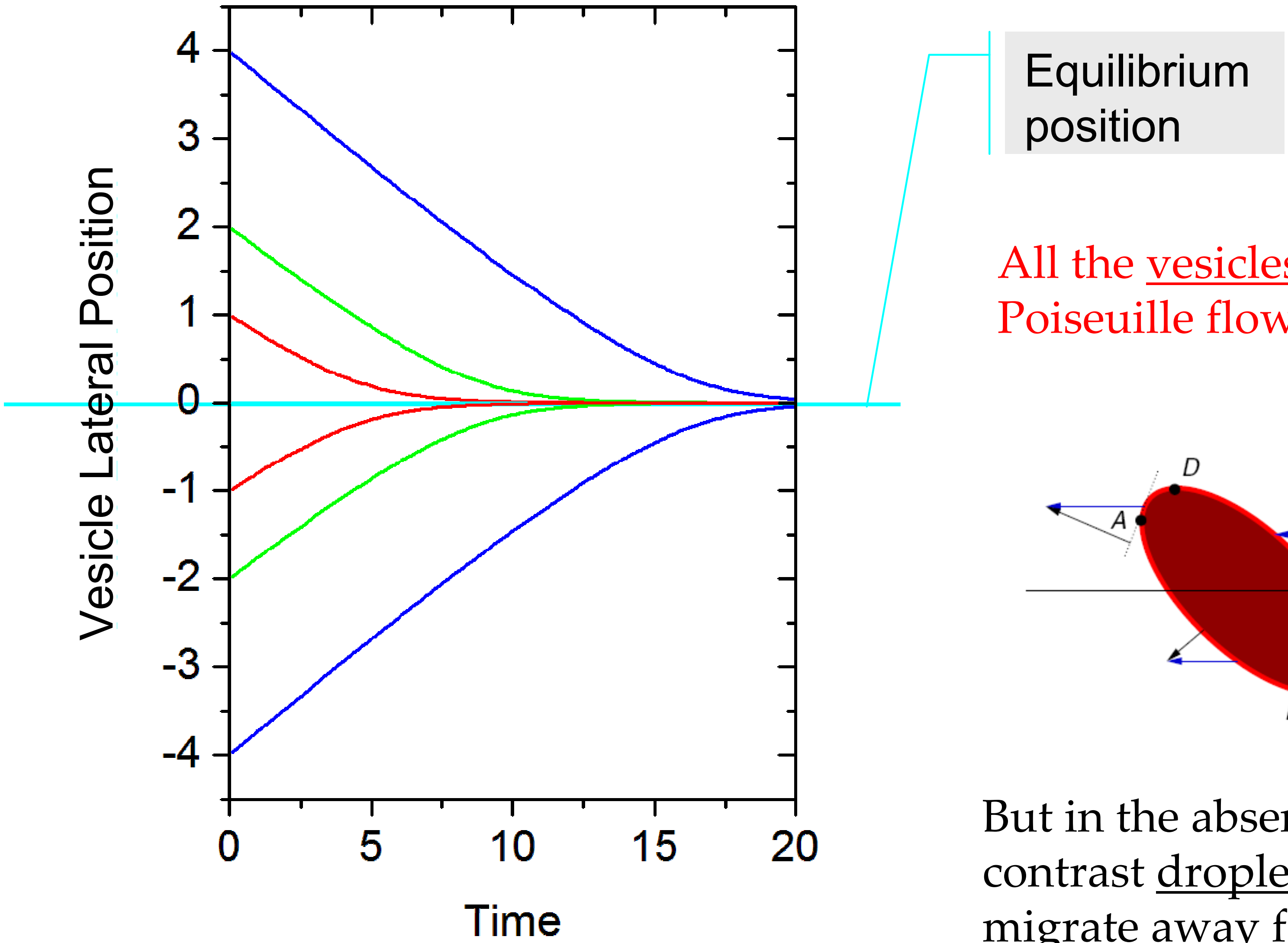
The bounded walls

The Unbounded
Poiseuille flow

$$v_x = cy^2$$

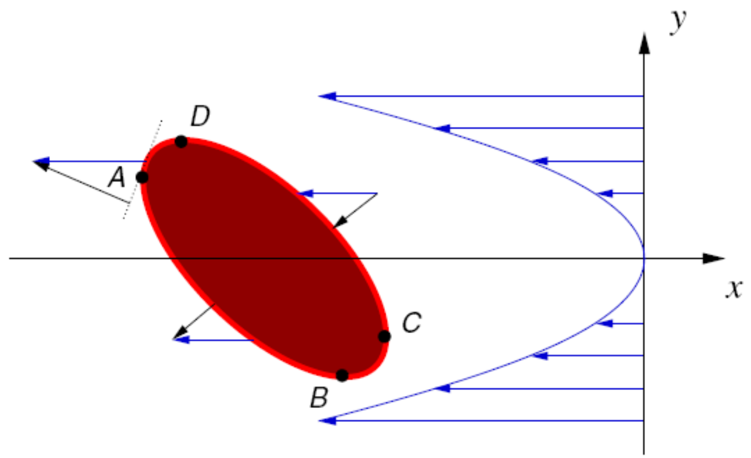
To avoid any wall induced lift force

The lateral migration



The aspect ratio $R_0/w \ll 1$

All the vesicles migrate to the Poiseuille flow centre-line

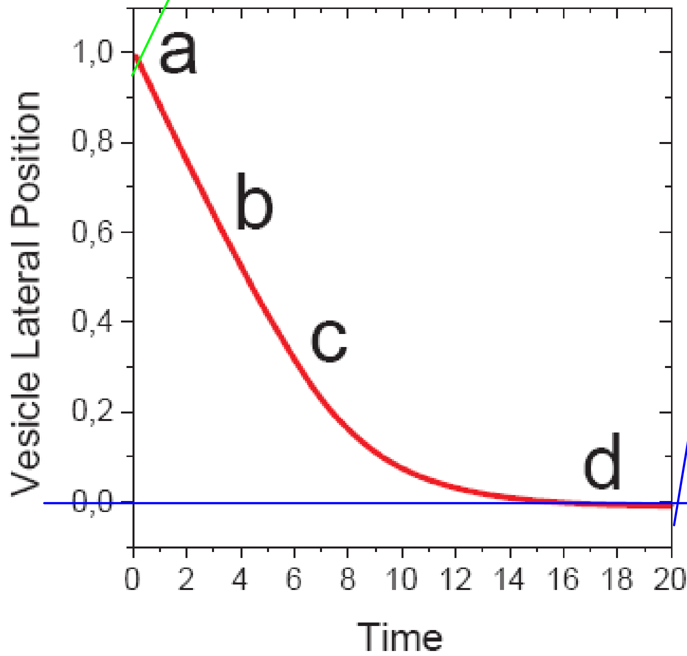


But in the absence of the viscosity contrast droplets are known to migrate away from the centre-line (L. G. Leal 1980)

B. Kaoui *et al* PRE (2008)

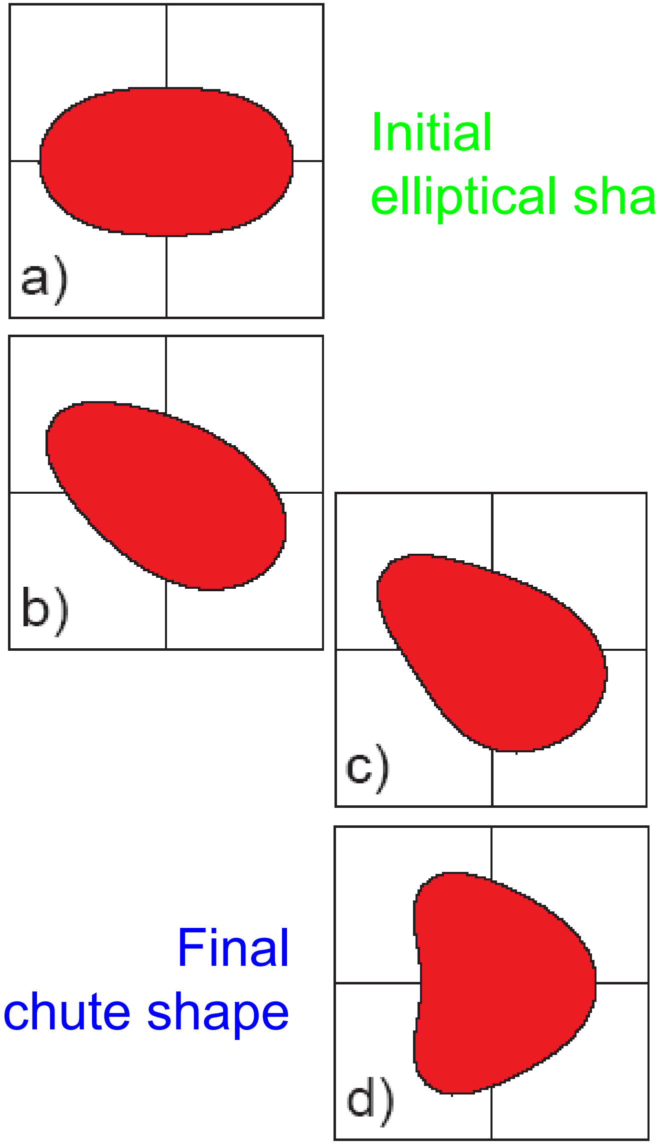
Vesicle shape deformation

Initial position



Final equilibrium position

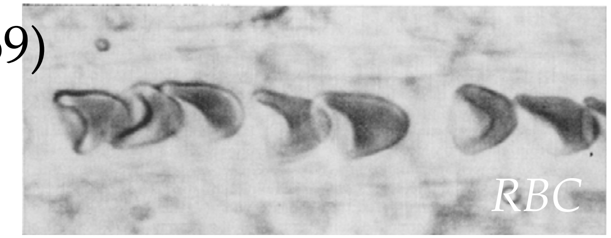
Vesicle shapes as a function of the distance from the Poiseuille flow centre-line.



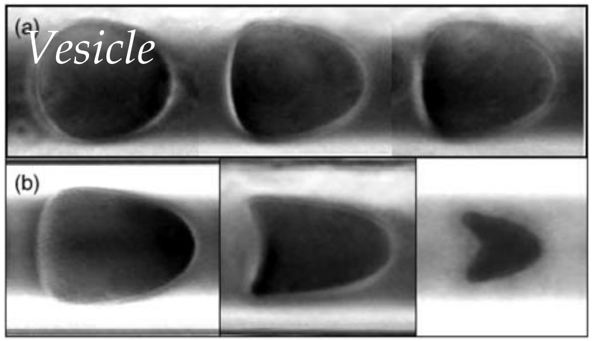
Initial elliptical shape

Final parachute shape

R. Skalak *et al* Science (1969)



Parachute shapes obtained in <u>capillary flows</u>



V. Vitkova *et al* EPL (2004)

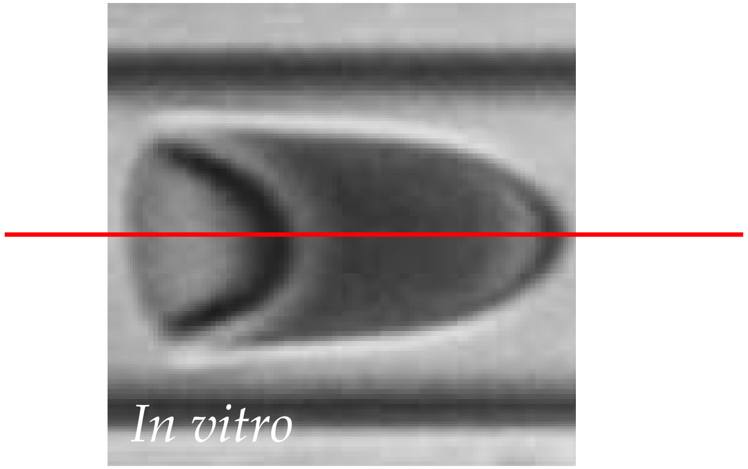
- axisymmetric shape
- obtained without presence of <u>any bounded walls</u>

Why RBCs move ASYMMETRIC even in a SYMMETRIC flow?

Asymmetric shapes 1

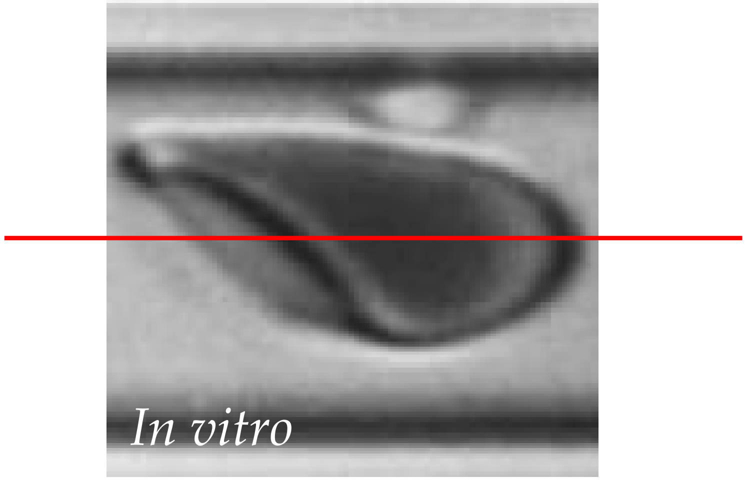
Collaboration with G. Biros

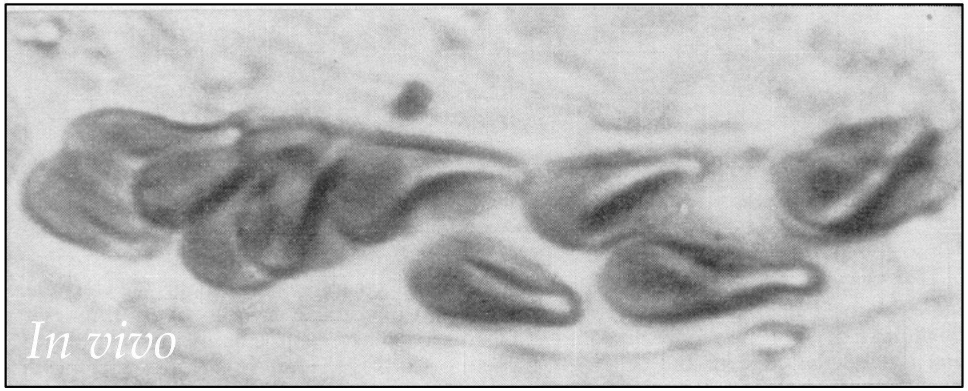
Parachute-like shape
(Axisymmetric shape)



T. W. Secomb *et al* ABE (2007)

Slipper-like shape
(Non-axisymmetric shape)





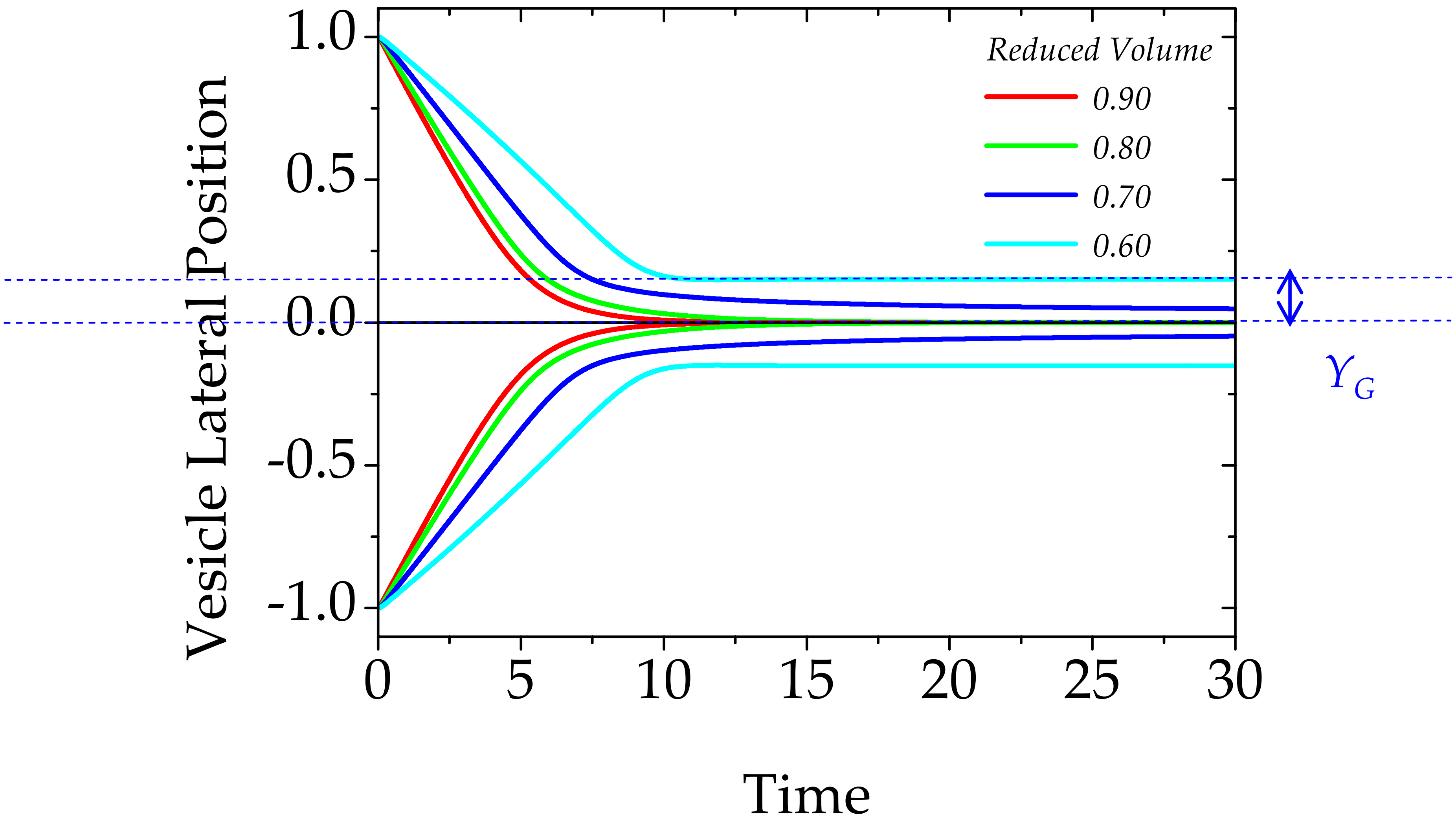
R. Skalak *et al* Science (1969)

Why RBCs move ASYMMETRIC even in a SYMMETRIC flow?

T. W. Secomb and R. Skalak MR (1982)

Librucation theory:
Confinement + Shear elasticity

Asymmetric shapes (Lateral migration)



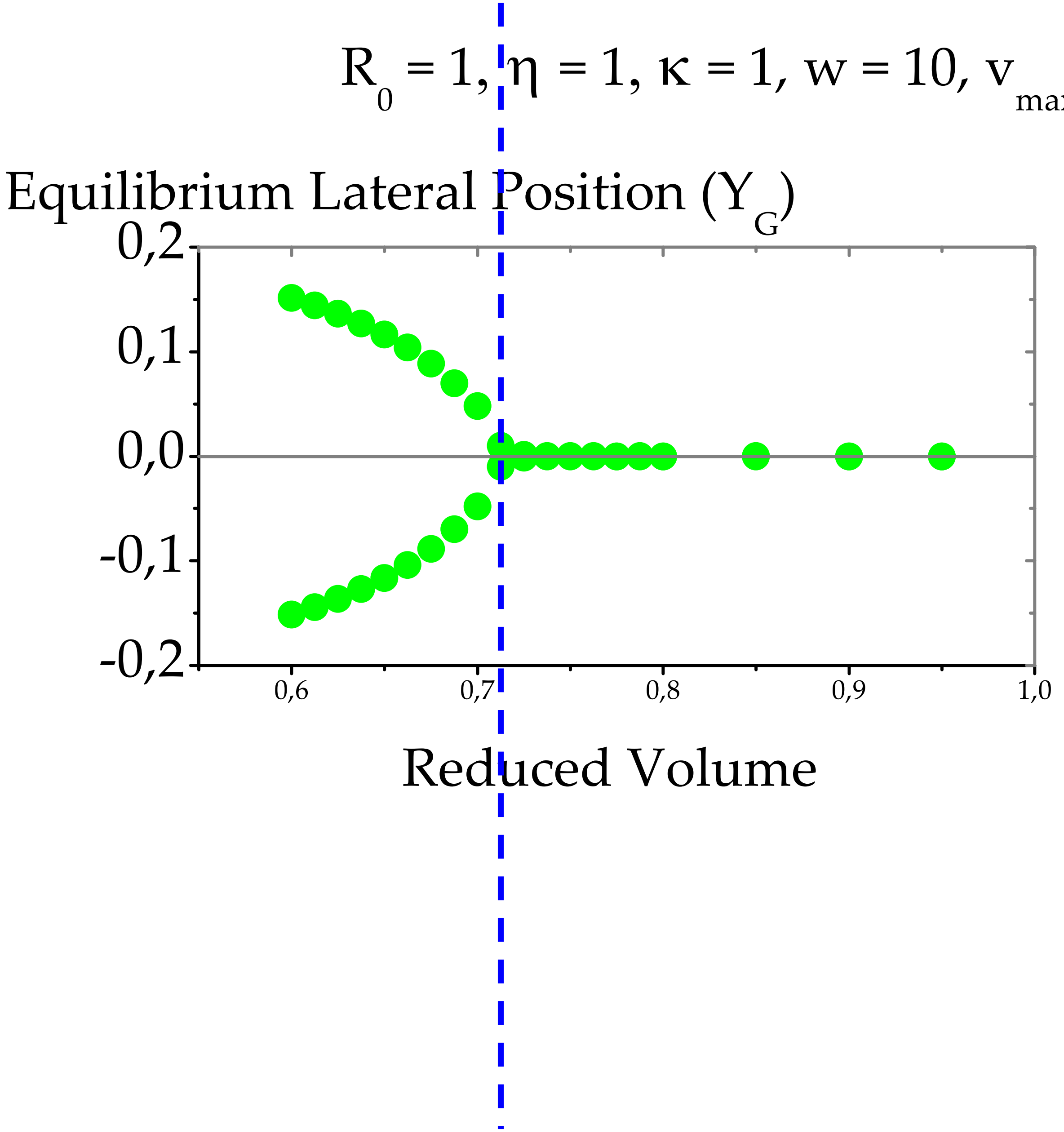
Reduced volume (2D) : $\nu = \frac{A}{A_c} = \frac{4\pi S}{L^2}$

Asymmetric shapes (Bifurcation)

$R_0 = 1, \eta = 1, \kappa = 1, w = 10, v_{max} = 800$

$Y_G \neq 0$

Non centered



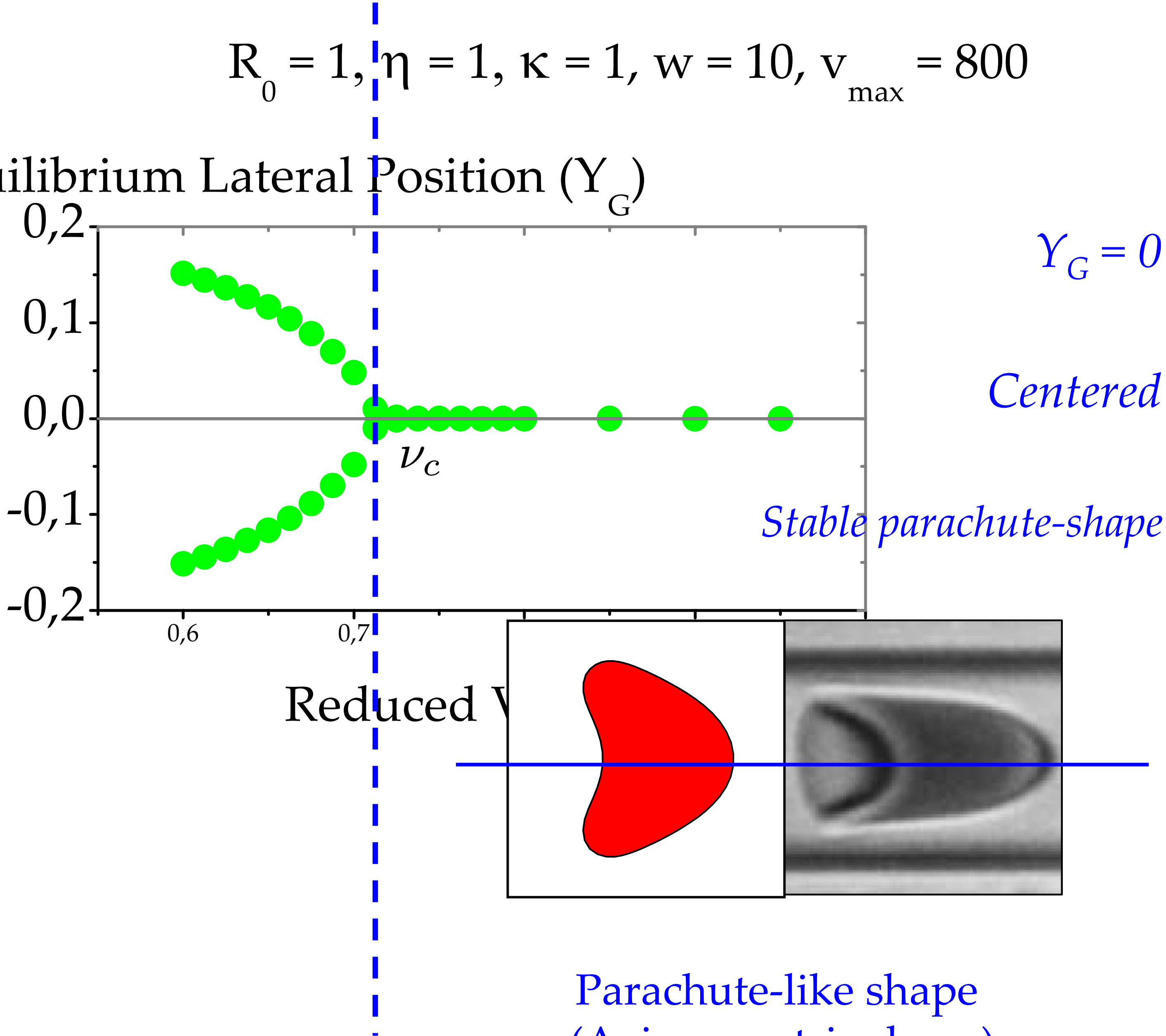
$Y_G = 0$

Centered

Asymmetric shapes (Bifurcation)

$Y_G \neq 0$

Non centered

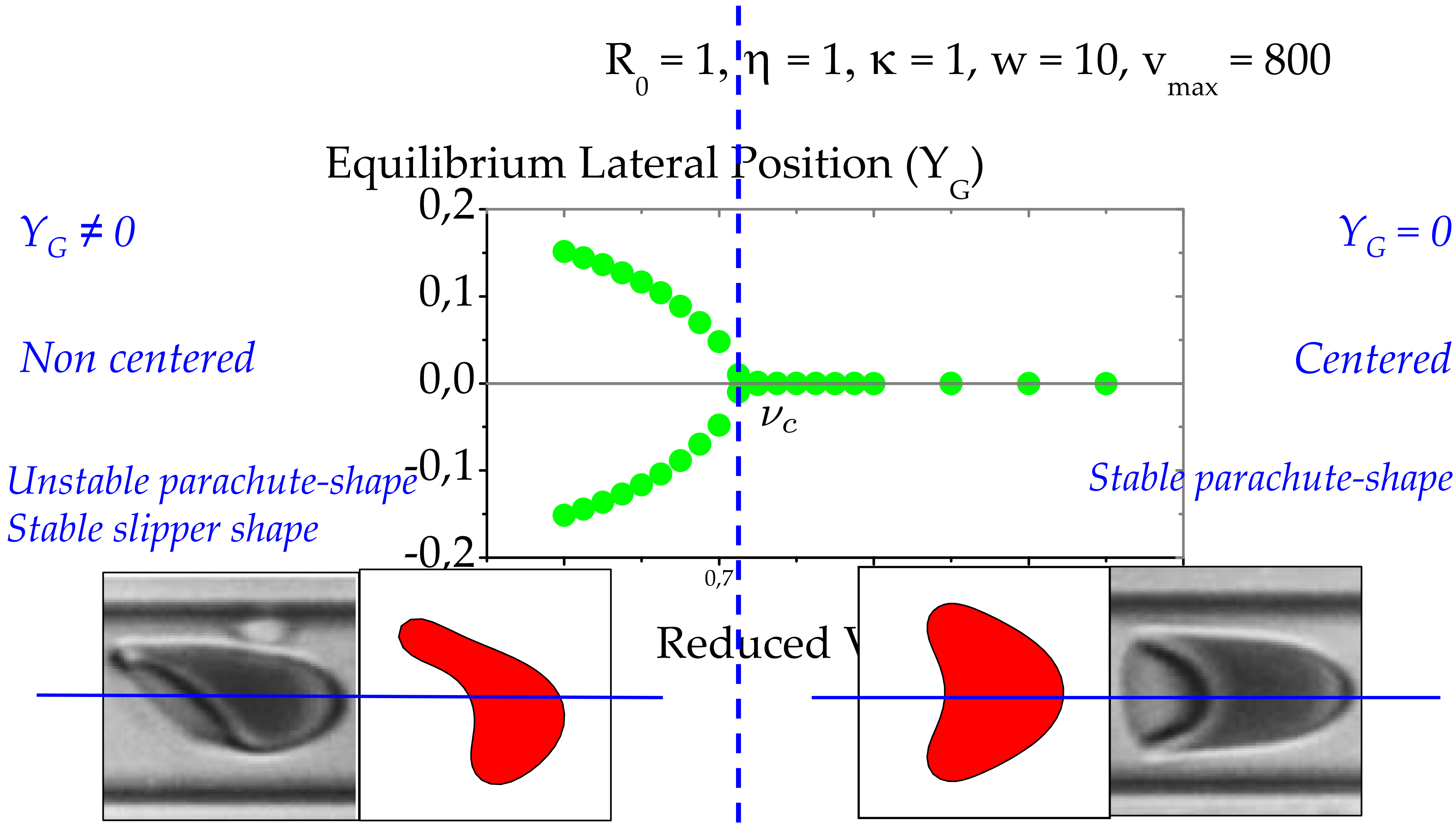


$Y_G = 0$

Centered

Parachute-like shape
(Axisymmetric shape)

Asymmetric shapes (Bifurcation)



Slipper-like shape
(Non-axisymmetric shape)

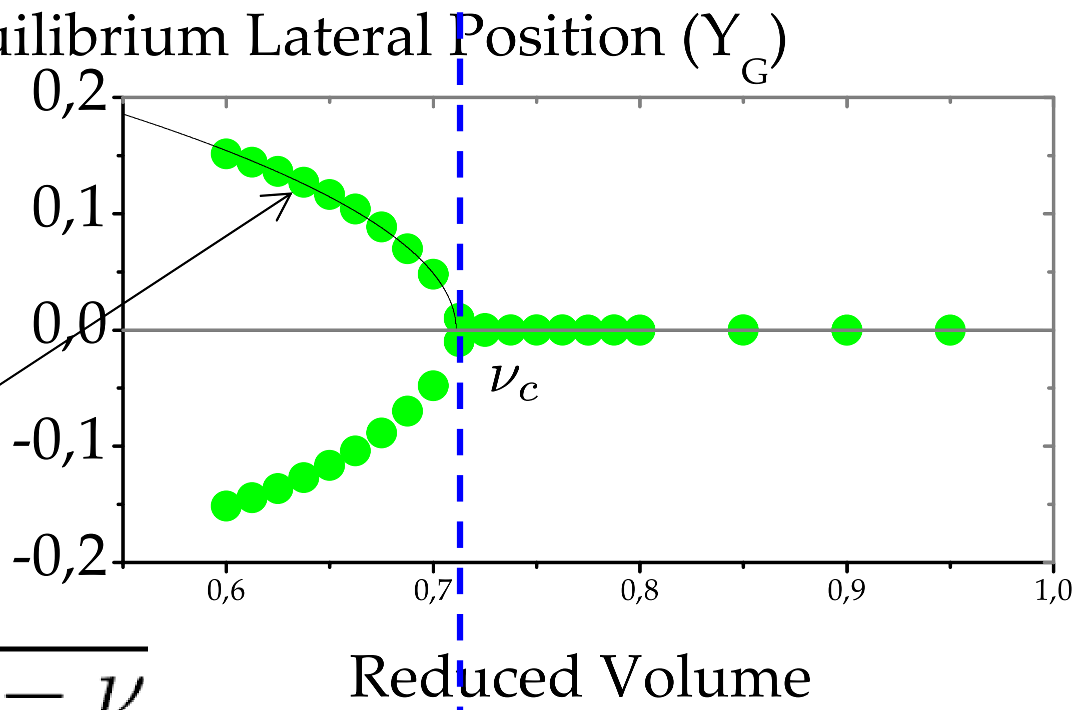
Parachute-like shape
(Axisymmetric shape)

Asymmetric shapes (Bifurcation)

$R_0 = 1, \eta = 1, \kappa = 1, w = 10, v_{max} = 800$

$Y_G \neq 0$

Non centered



$Y_G = 0$

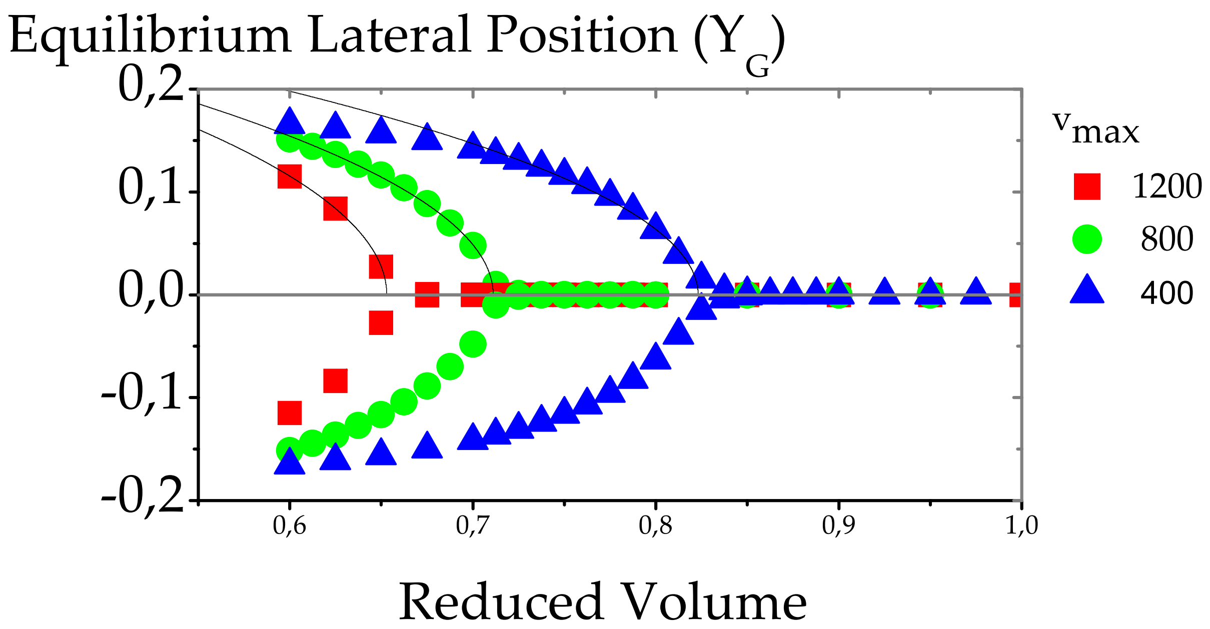
Centered

$$Y_G = \pm\sqrt{\nu_c - \nu}$$

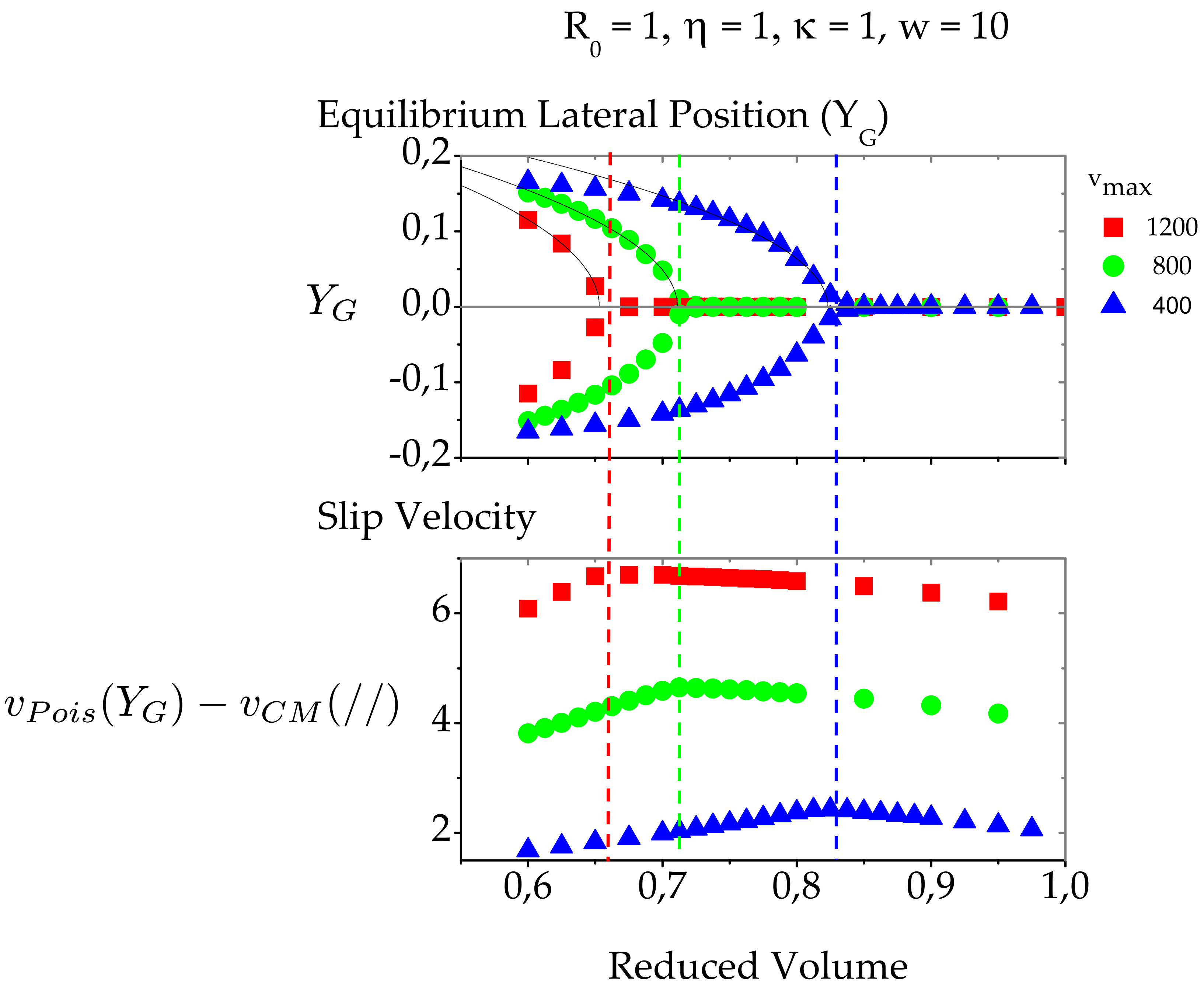
Supercritical bifurcation

Asymmetric shapes (Bifurcation)

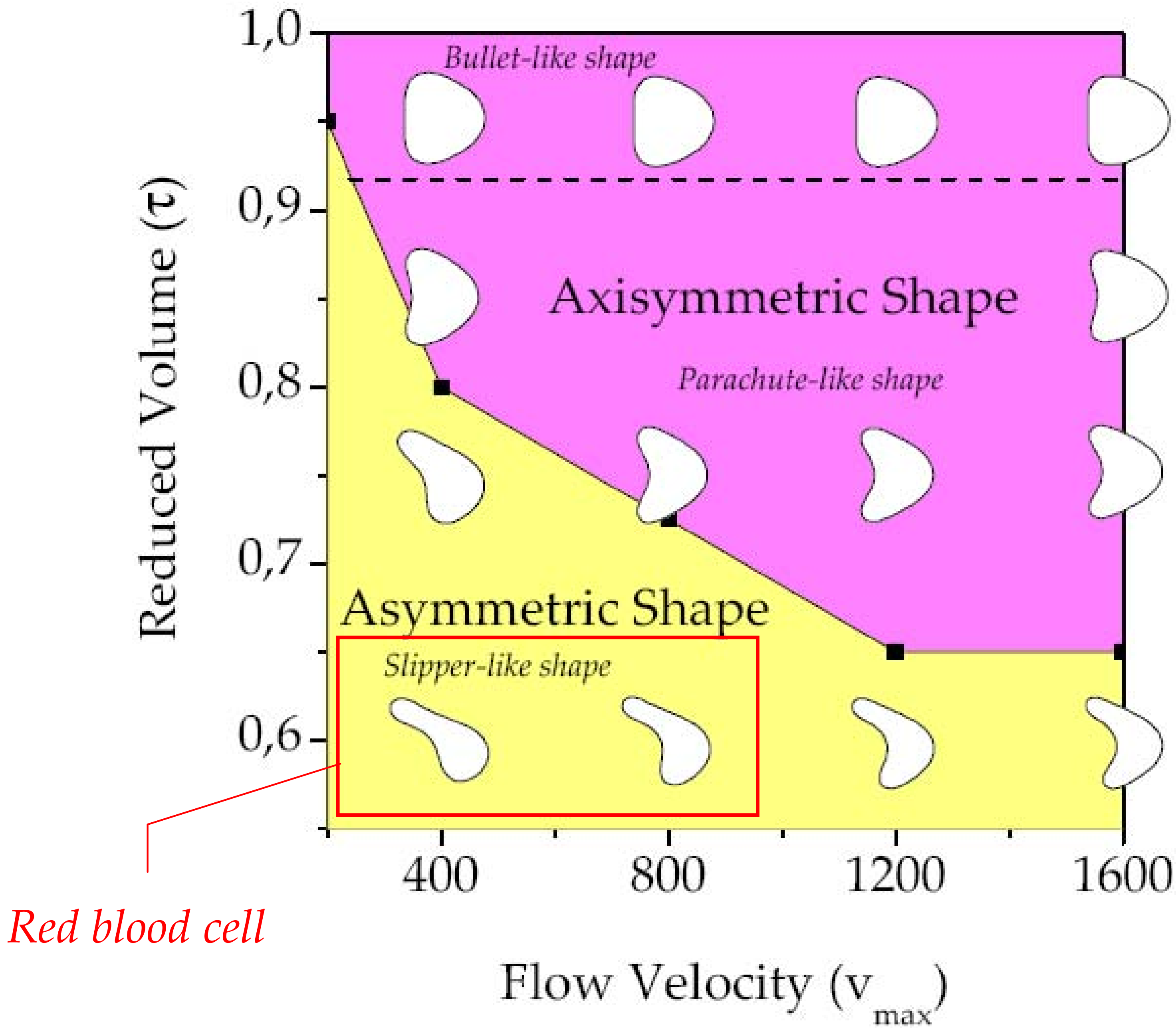
$R_0 = 1, \eta = 1, \kappa = 1, w = 10$



Asymmetric shapes (Slip velocity)



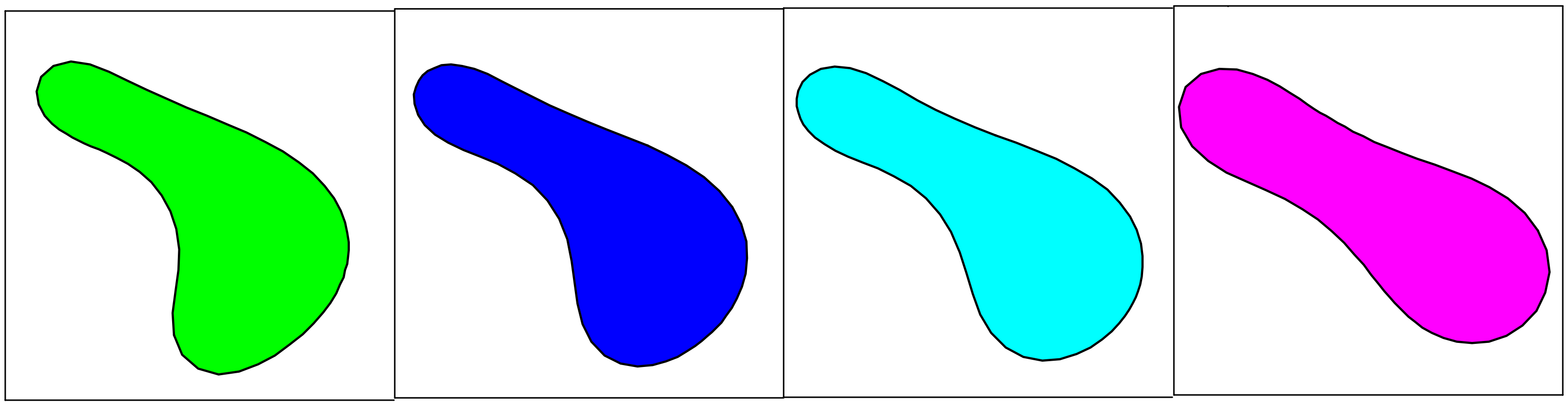
Asymmetric shapes (Phase-diagram)



Asymmetric shapes (Effect of rigidity)

Increasing membrane rigidity →

$\nu = 0.6$

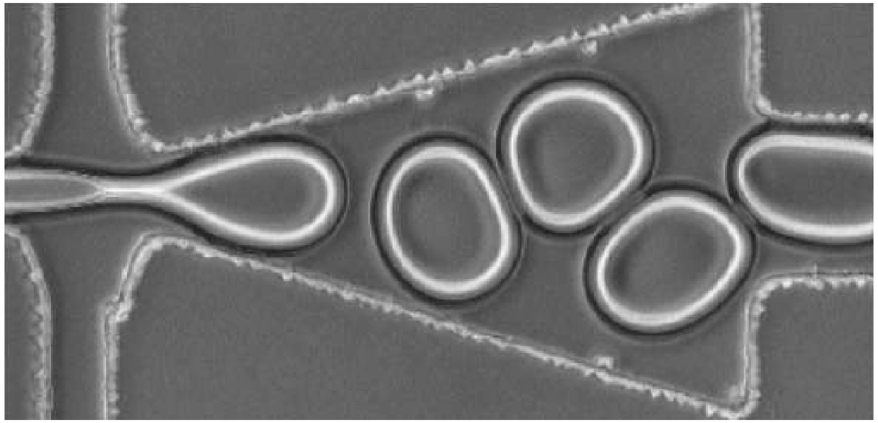


$\kappa = 1$ $\kappa = 1.5$ $\kappa = 2$ $\kappa = 5$

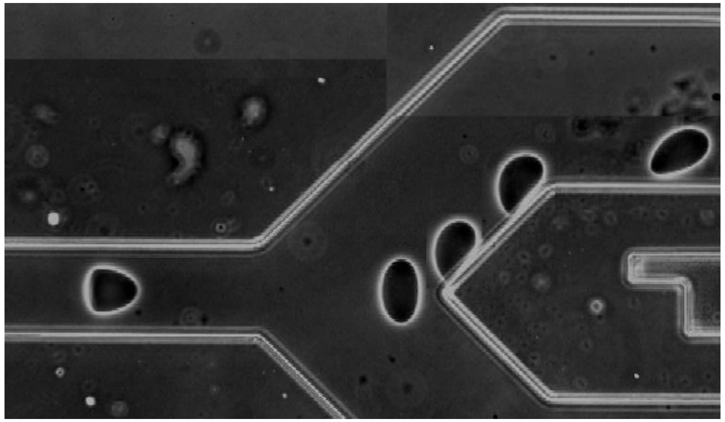
Vesicle dynamics in confined geometries and in micro-fluidic devices

The main goal

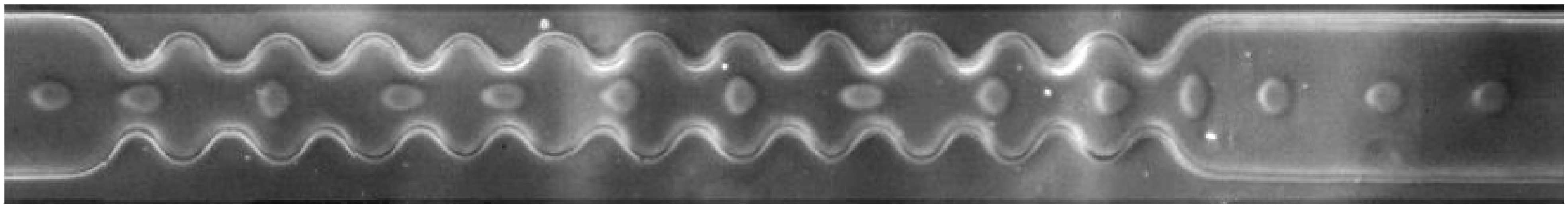
- Simulation of vesicles (deformable particles) flowing in micro-fluidic devices (complex geometries)



A microfluidic device used to produce monodisperse vesicles (V. Vitkova).



A Y-junction used to study the lateral migration of vesicles in micro-channels (G. Coupier).



A microfluidic device used to measure the mechanical properties of vesicles (H. A. Stone).

Fluid flow: *Lattice-Boltzmann 1* Collaboration with J. Harting

- The main central quantity:

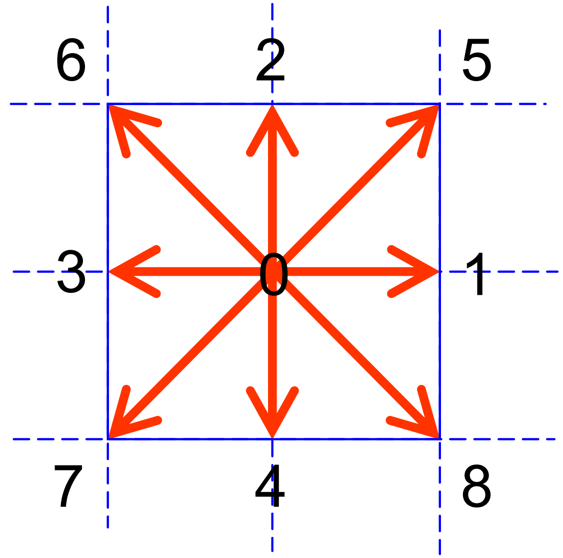
$$f_i(\mathbf{r}, t)$$

- In the LBMs not only the positions are <u>discretized</u> but also <u>velocities</u>:

Two-dimensional space

D2Q9 lattice

9 possible discrete velocity vectors



- The evolution in time of $f_i(\mathbf{r}, t)$:

The collision operator

$$f_i^{\mathrm{new}}(\mathbf{r} + \mathbf{c}_i \Delta t, t + \Delta t) - f_i^{\mathrm{old}}(\mathbf{r}, t) = \Delta t \left(\Omega_i + F_i \right)$$

Free streaming

An external applied force

Fluid flow: *Lattice-Boltzmann 2*

- The Bhatnagar-Gross-Krook (BGK) approximation:

$$\nu = \frac{2\tau - 1}{6}$$

The kinematic viscosity

$$\Omega_{\mathrm{i}} = -\frac{1}{\tau}\left(f_{\mathrm{i}}^{\mathrm{old}}(\mathbf{r},t) - f_{\mathrm{i}}^{\mathrm{eq}}(\mathbf{r},t)\right)$$

$$f_i^{eq}(\mathbf{r},t) = w_i\rho(\mathbf{r},t)\left[c_1 + c_2(\mathbf{c}_i \cdot \mathbf{u}) + c_2(\mathbf{c}_i \cdot \mathbf{u})^2 + c_4(\mathbf{u}\cdot\mathbf{u})\right]$$

The equilibrium distribution

- Fluid flow:

$$\mathbf{u}(\mathbf{r},t) = \frac{1}{\rho(\mathbf{r},t)}\sum_{\mathrm{i}=0}^{8} f_{\mathrm{i}}(\mathbf{r},t)\mathbf{c}_{\mathrm{i}}$$

Velocity

$$\rho(\mathbf{r},t) = \sum_{\mathrm{i}=0}^{8} f_{\mathrm{i}}(\mathbf{r},t)$$

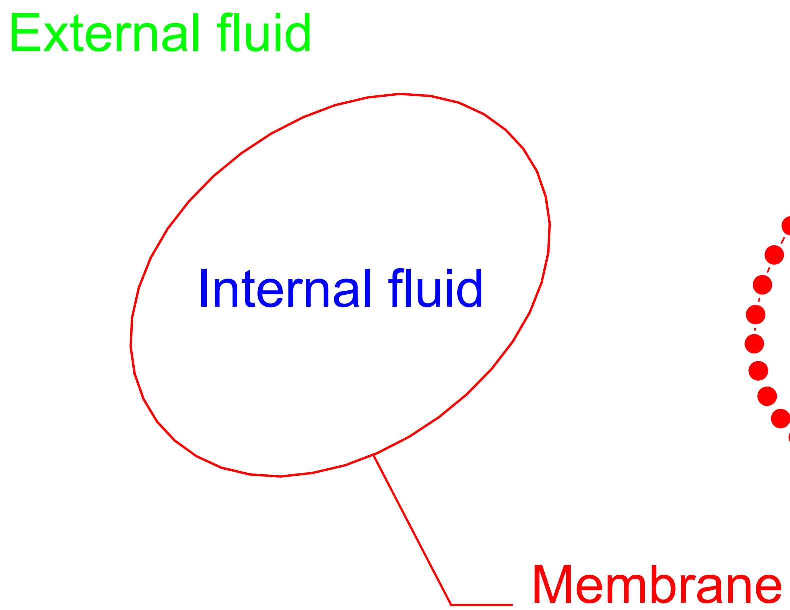
Density

$$p(\mathbf{r},t) = \rho(\mathbf{r},t)c_{\mathrm{S}}^2$$

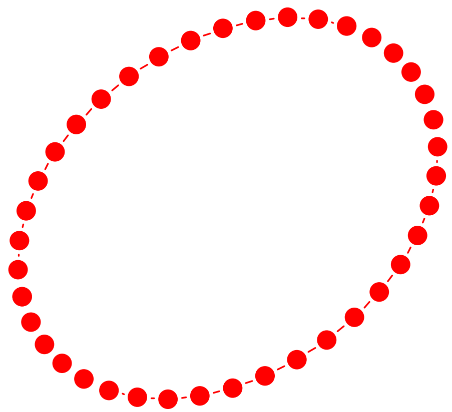
Pressure

Fluid-vesicle coupling 1

Immersed boundary method

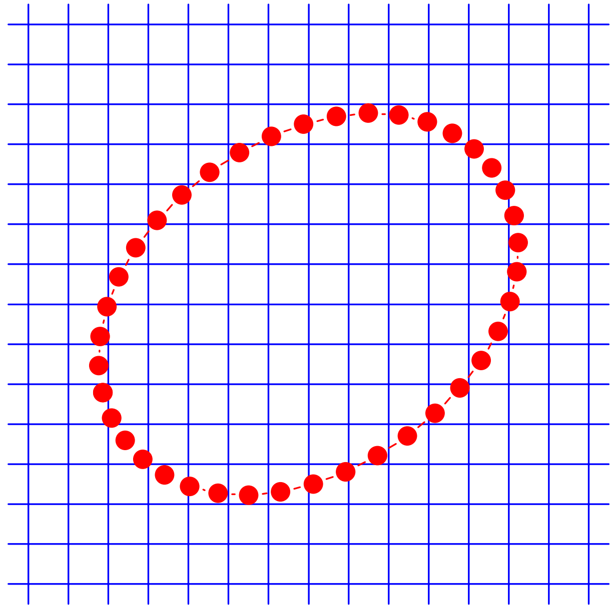


Moving Lagrangian mesh
(vesicle)



Neighboring nodes are inter-connected by an elastic spring

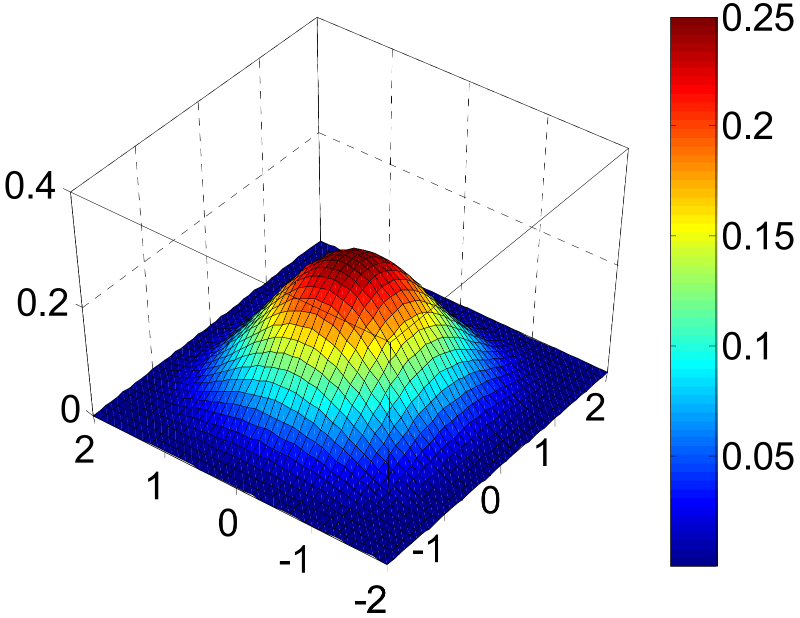
Fixed Eulerian mesh
(fluid)



Fluid flow computed using the lattice-Boltzmann method

C. S. Peskin. J. Comp. Phys. (1977)

Fluid-vesicle coupling 2

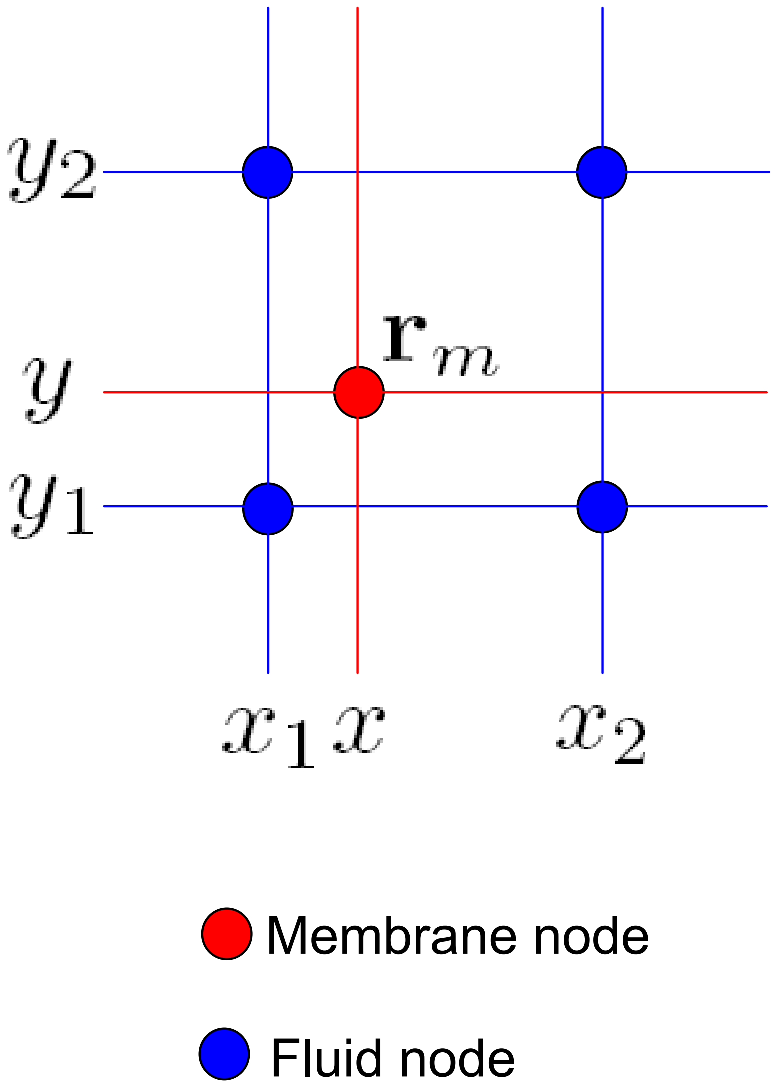


$$\Delta(\mathbf{x}) = \begin{cases} \frac{1}{16 l_s^2}\left(1+\cos\frac{\pi x}{2 l_s}\right)\left(1+\cos\frac{\pi y}{2 l_s}\right) & \text{for} \quad |x| \leqslant 2 l_s \quad \text{and} \quad |y| \leqslant 2 l_s, \\ 0 & \text{otherwise,} \end{cases}$$

<u>a discrete Dirac delta function</u>

C. S. Peskin, Acta Numerica 11, 479 (2002)

Fluid-vesicle coupling 3



Fluid flow → Membrane dynamics

$$\mathbf{v}(\mathbf{r}_m) = \sum_f \Delta(\mathbf{r}_f - \mathbf{r}_m)\mathbf{u}(\mathbf{r}_f)$$

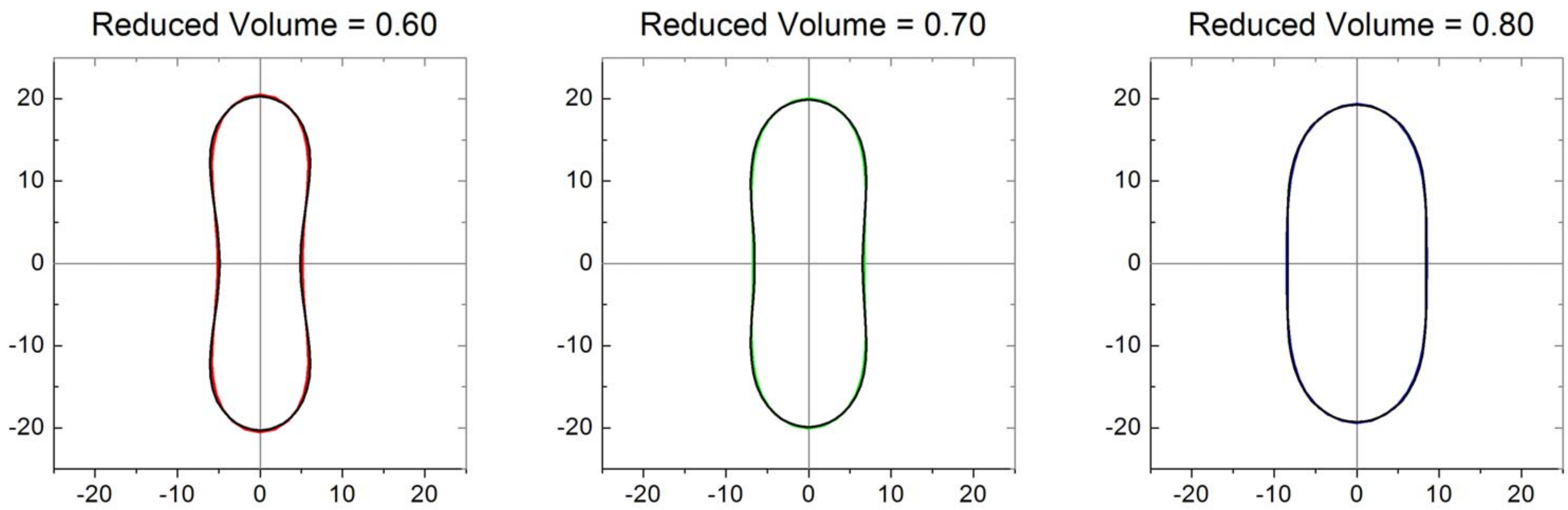
Advection (Euler scheme):

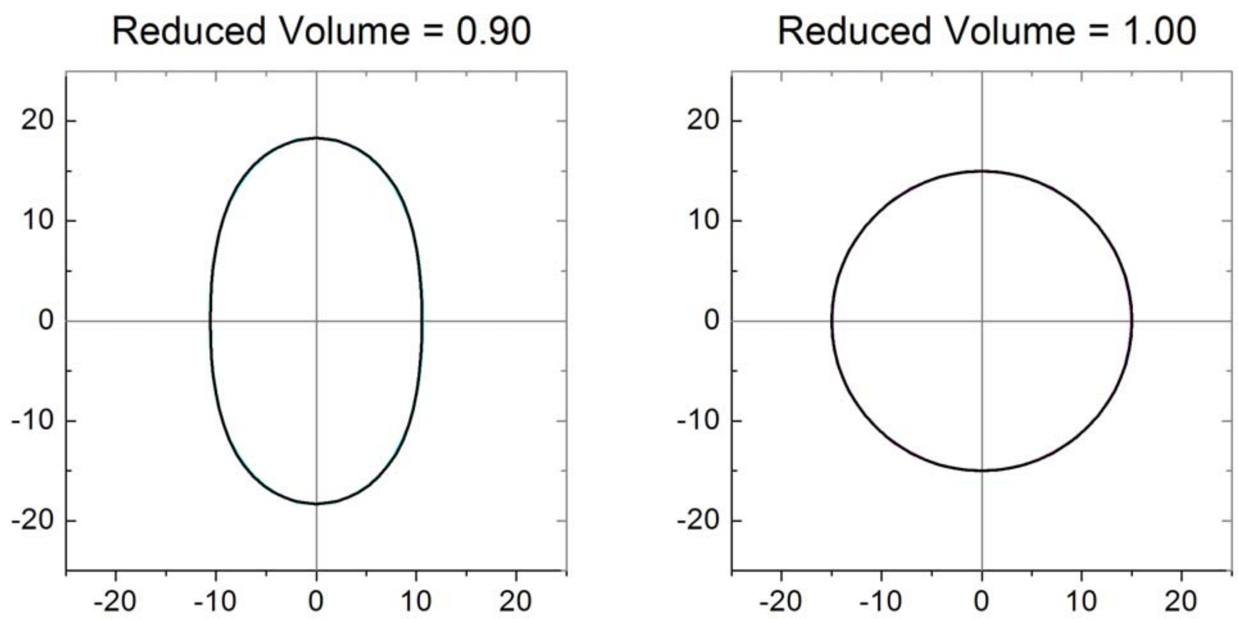
$$\mathbf{r}(t+dt) = \mathbf{v}(\mathbf{r},t)dt + \mathbf{r}(t)$$

Membrane dynamics → Fluid flow

$$\mathbf{F}(\mathbf{r_f}) = \sum_m \mathbf{f}(\mathbf{r_m})\delta(\mathbf{r_f} - \mathbf{r_m})$$

Computed equilibrium shapes

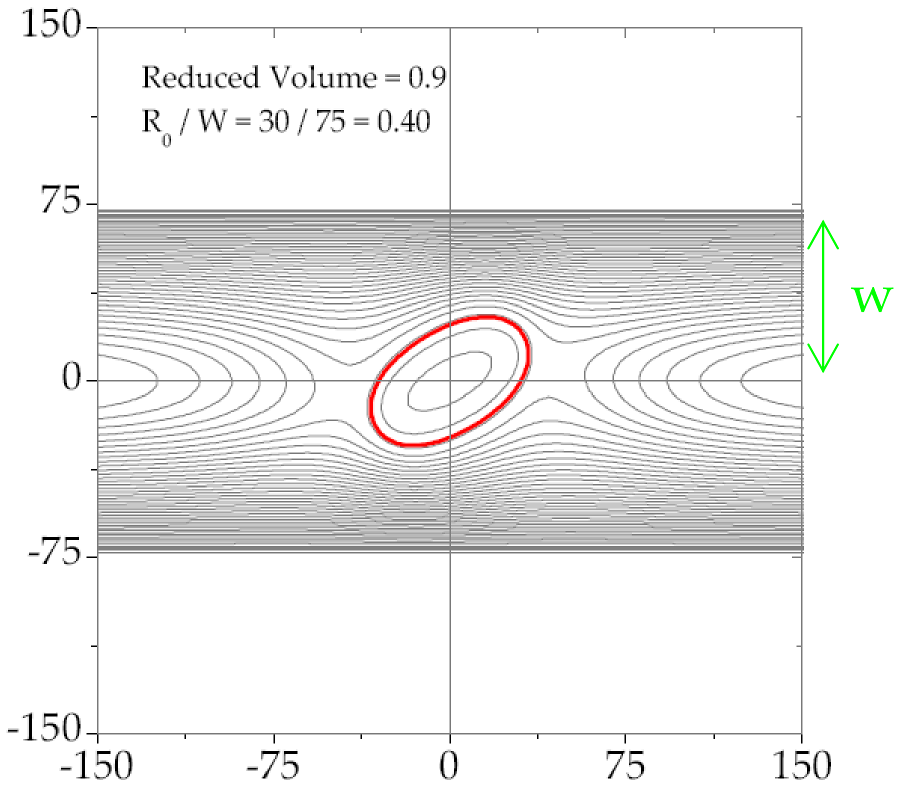


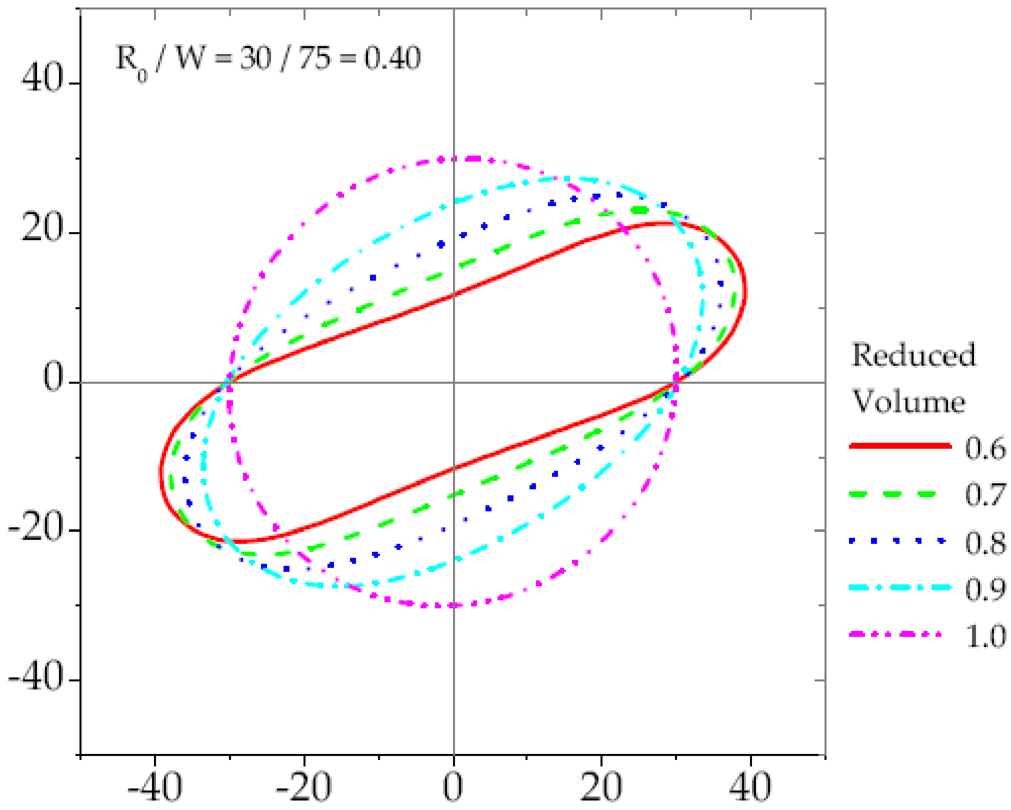


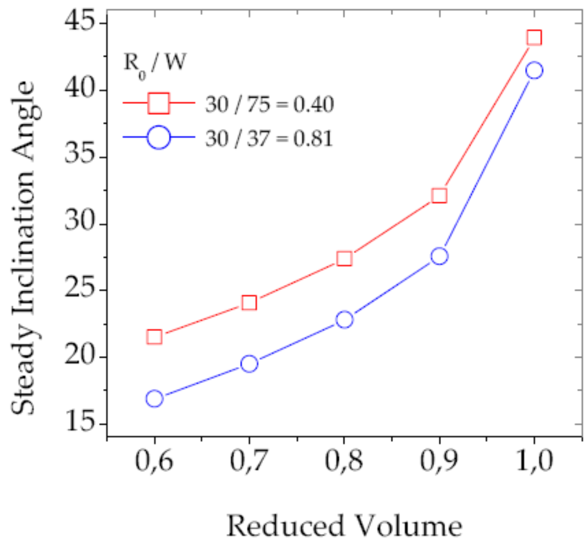
Solid black lines are the equilibrium shapes computed by the <u>boundray integral method</u>.

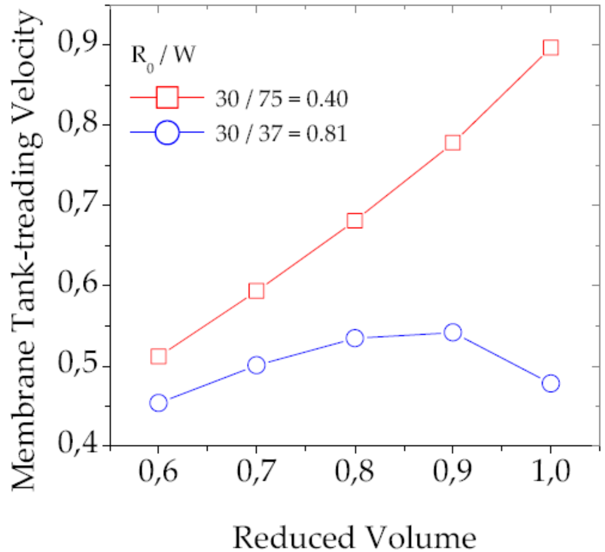
The same equilibrium shapes are obtained by the two Methods!

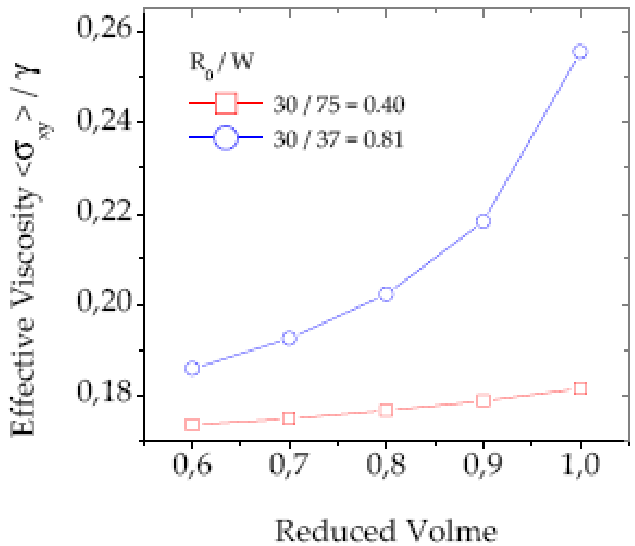
Tank-treading under shear flow





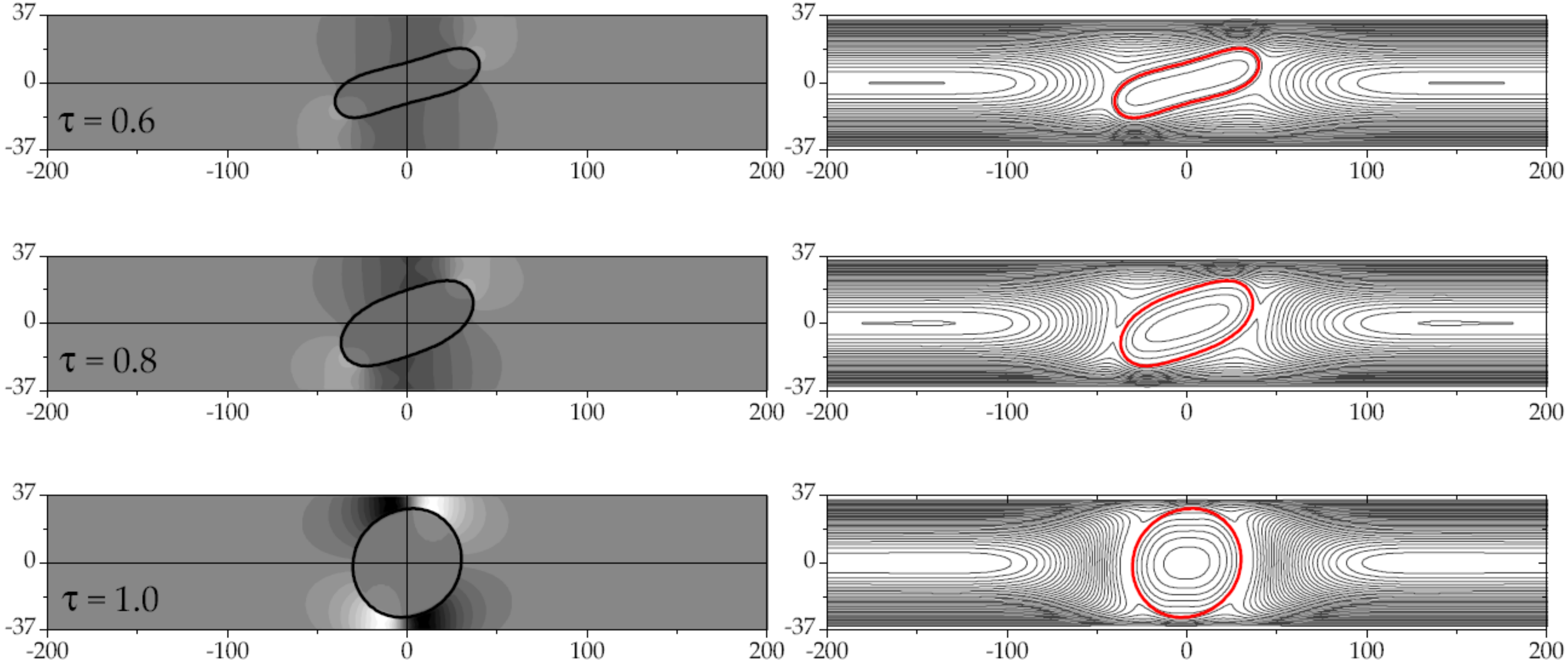


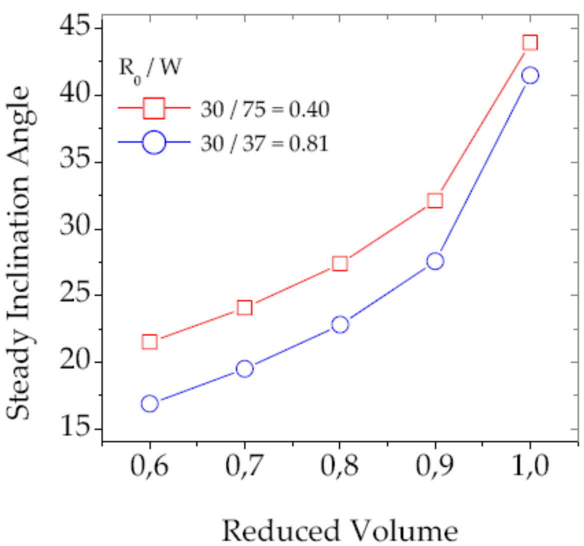


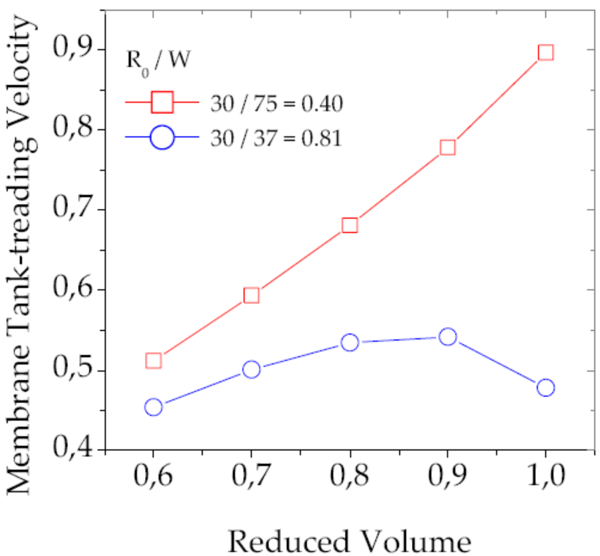


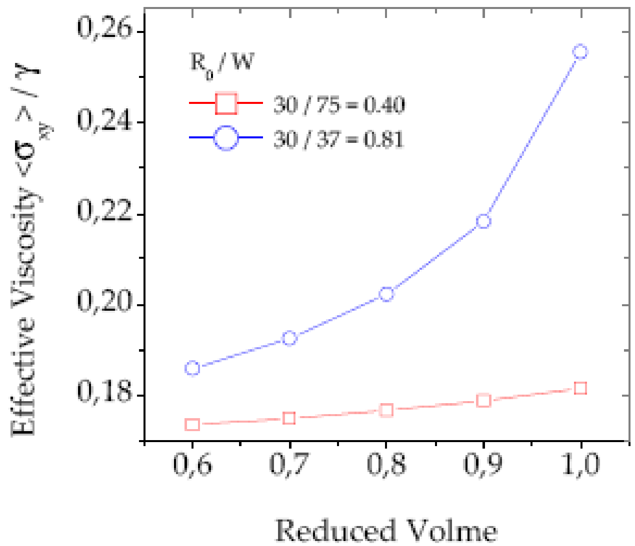
Tank-treading under shear flow

$$R_0/w = 30/37 = 0.81$$

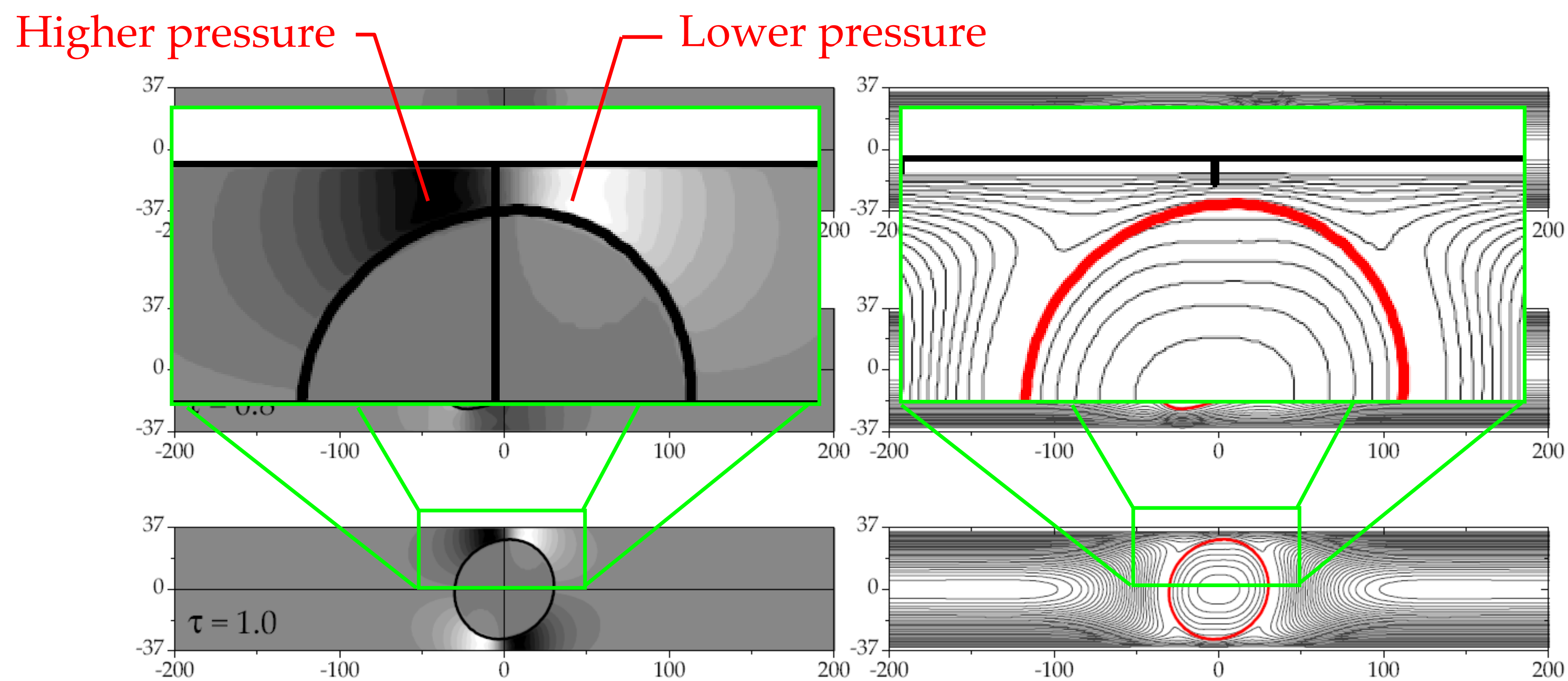


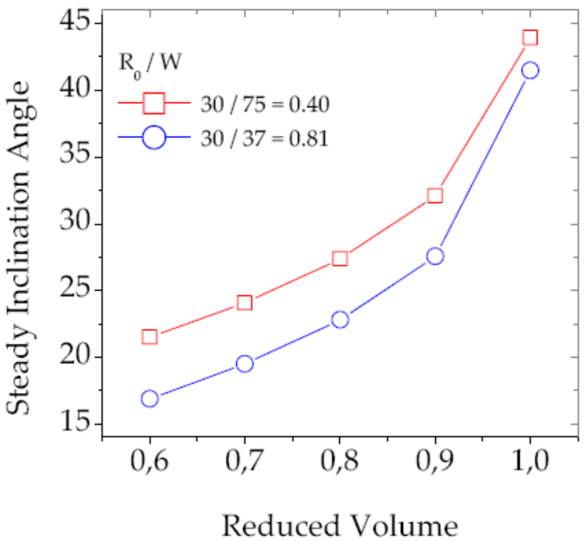


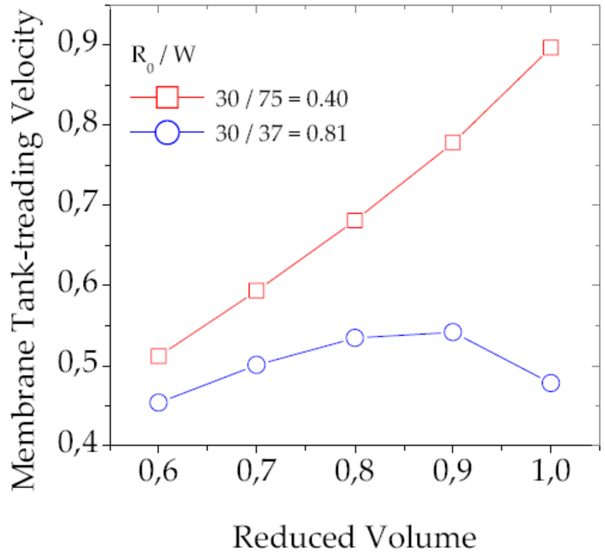


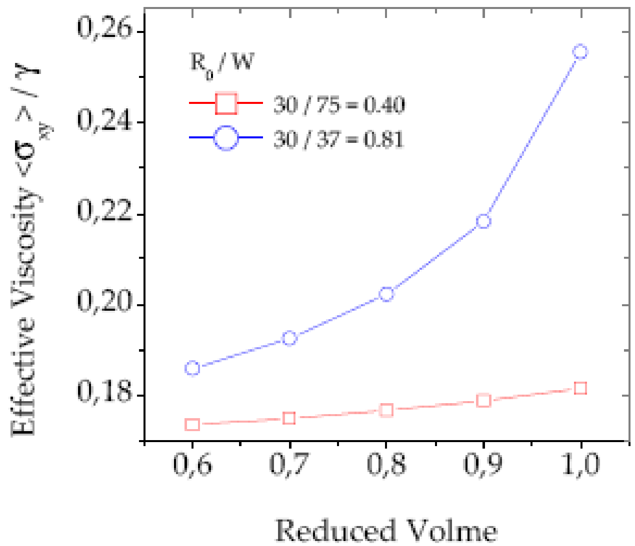


Tank-treading under shear flow

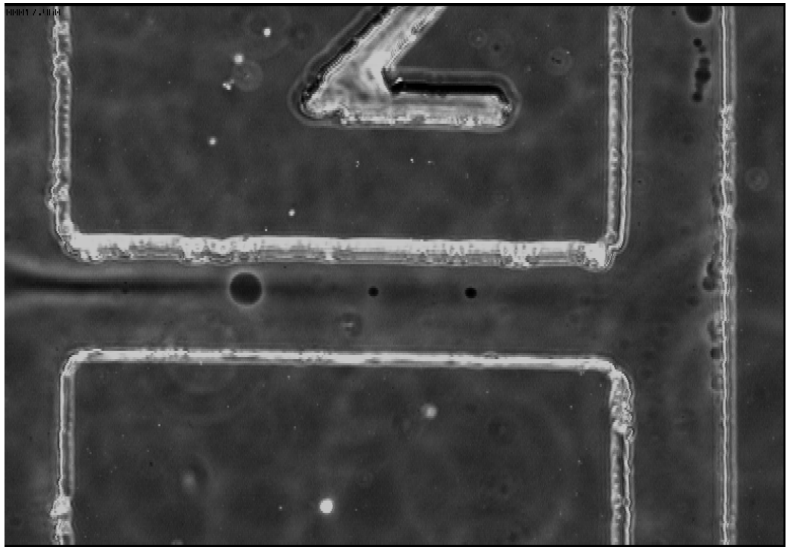




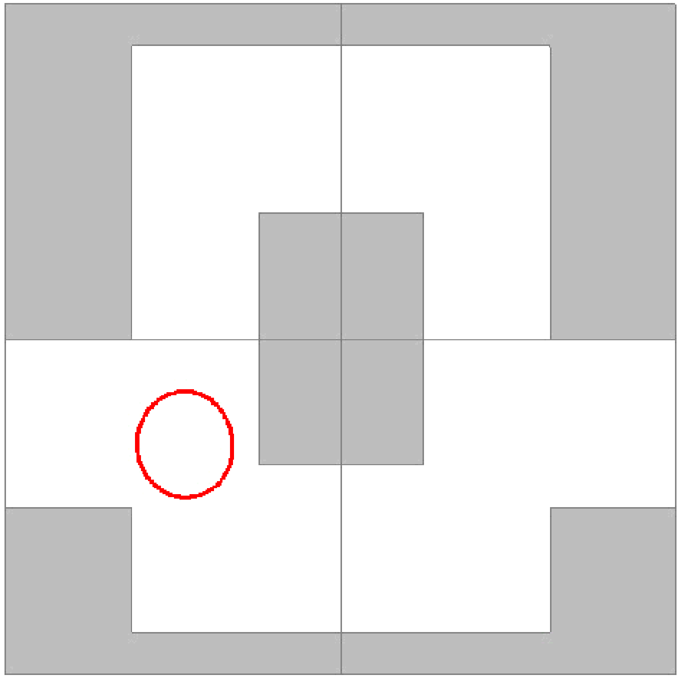


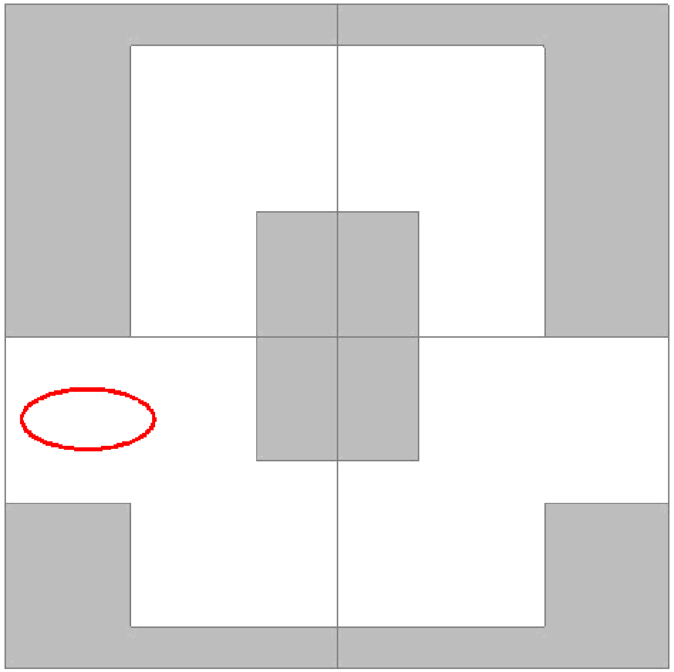


Double-T junction

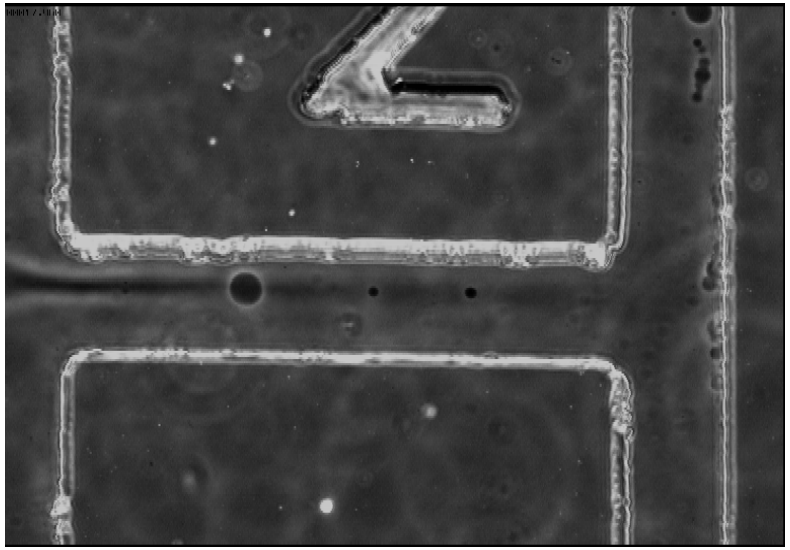


Experiment (T. Podgorski & G. Coupier)

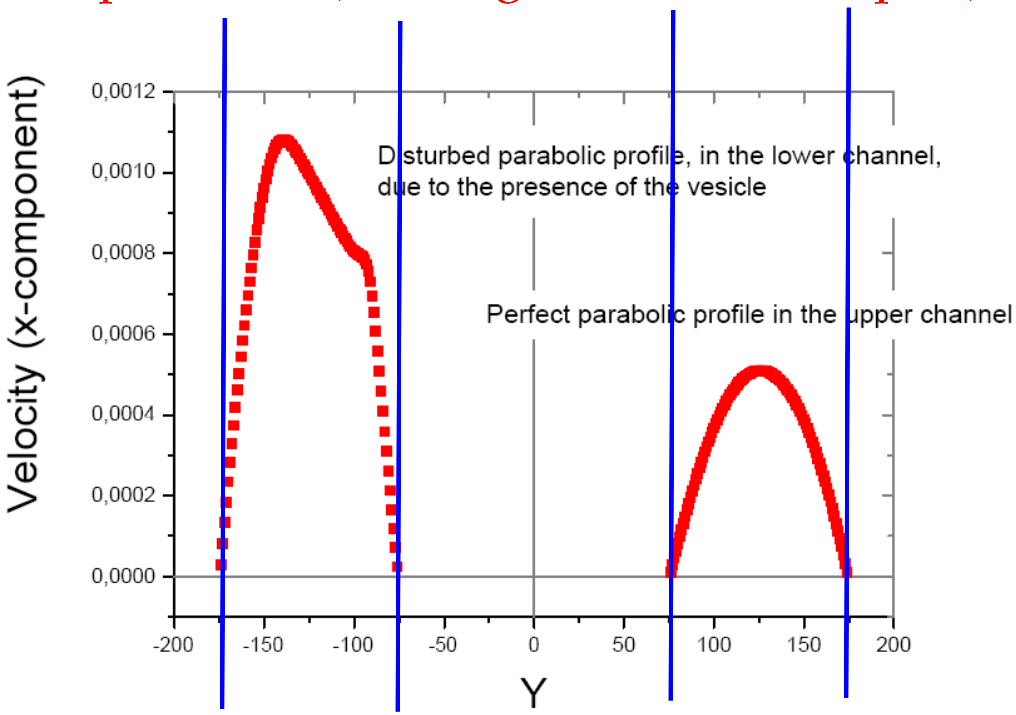


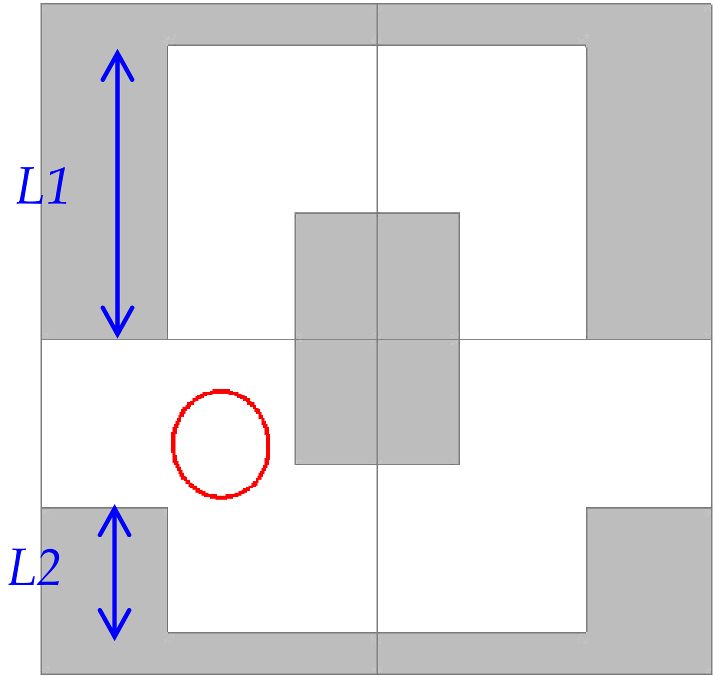


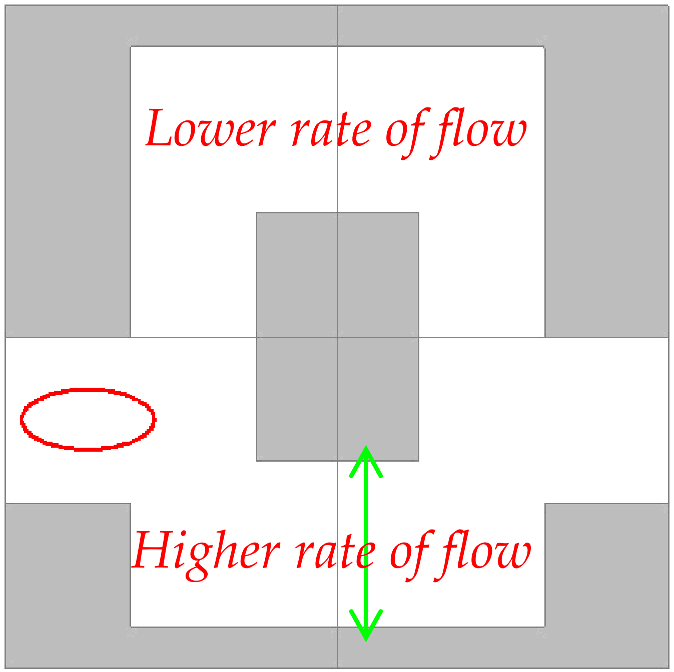
Double-T junction



Experiment (T. Podgorski & G. Coupier)

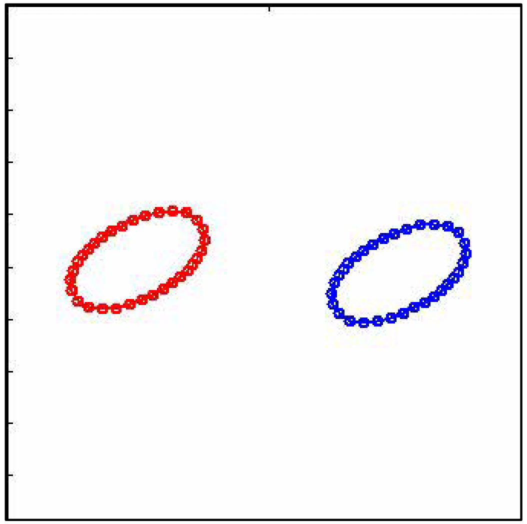






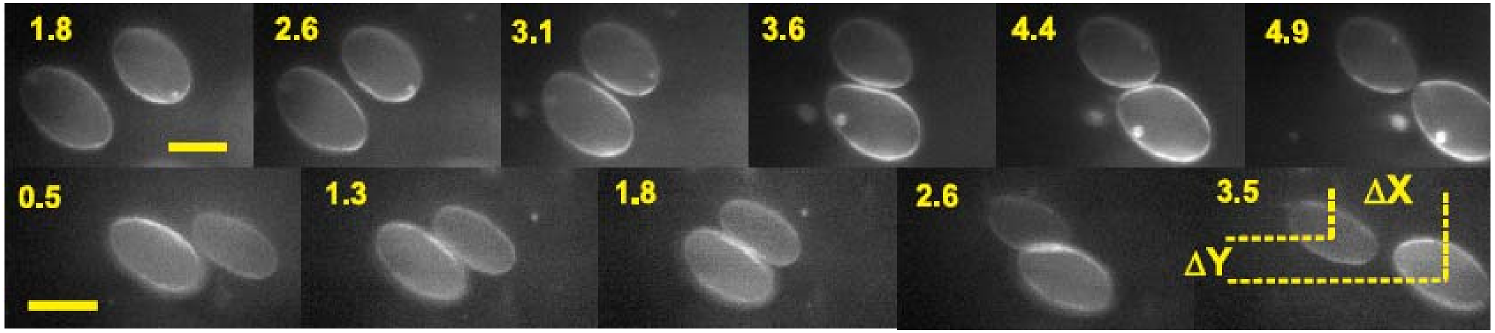
Two interacting vesicles under shear flow

Two interacting vesicles (Reduced volume)

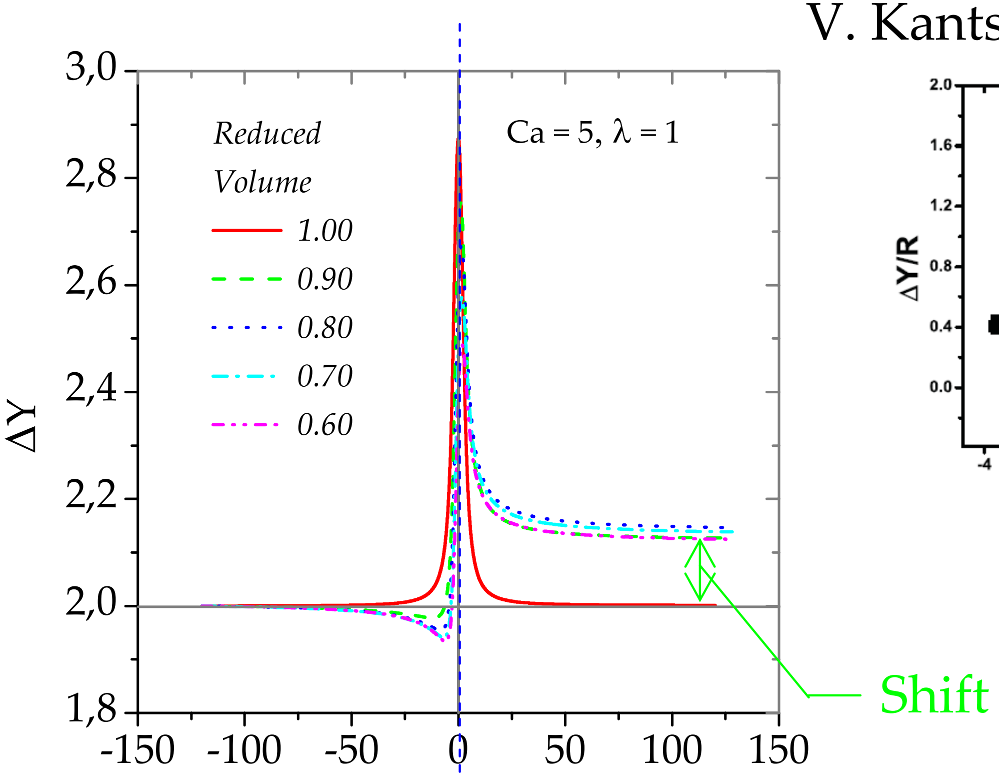


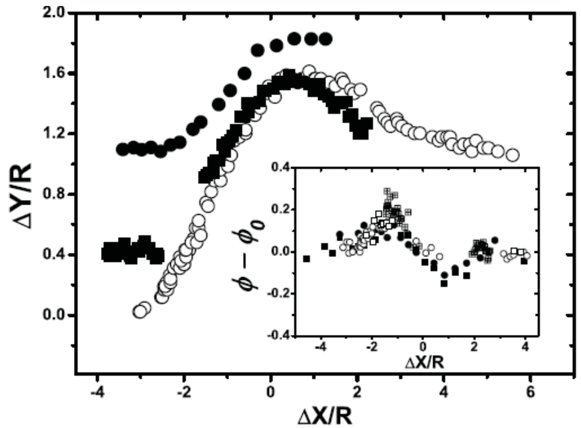
BIM Simulation

Experiment



V. Kantsler *et al* EPL (2008)





Experiment

Two vesicles with different reduced volumes

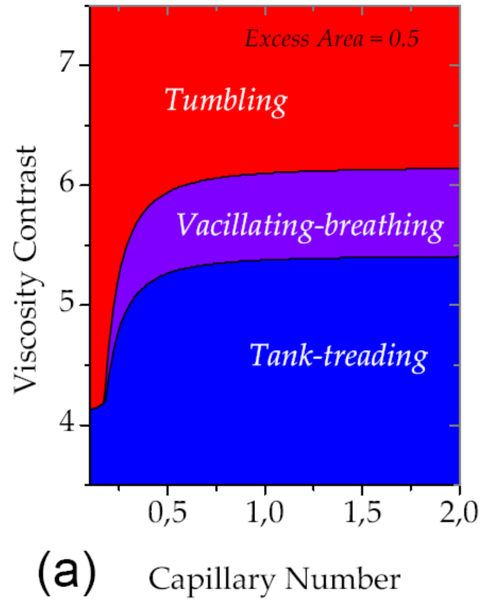
Before the collision

ΔX

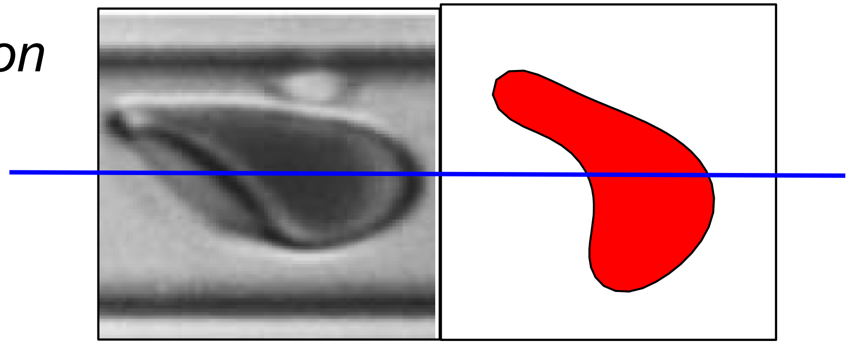
After the collision

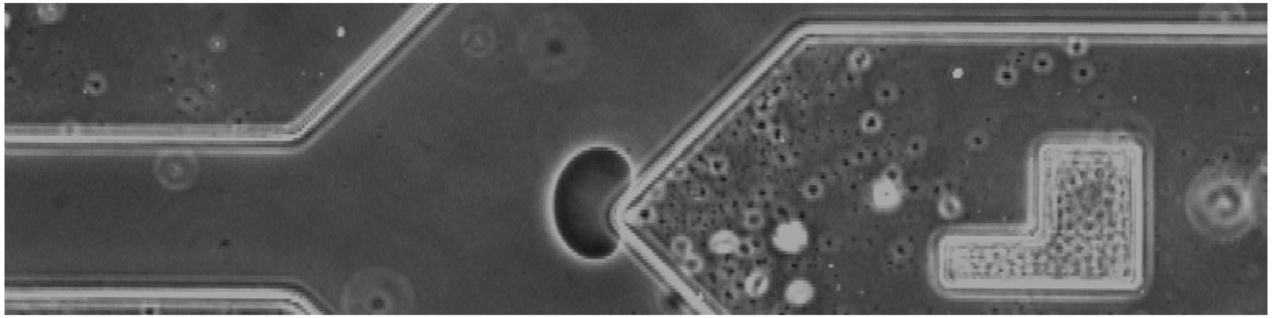
Conclusions

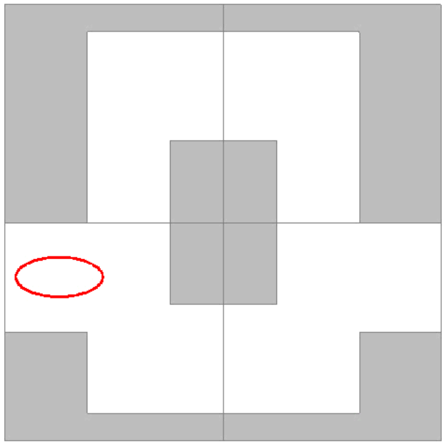
Dynamics under shear flow



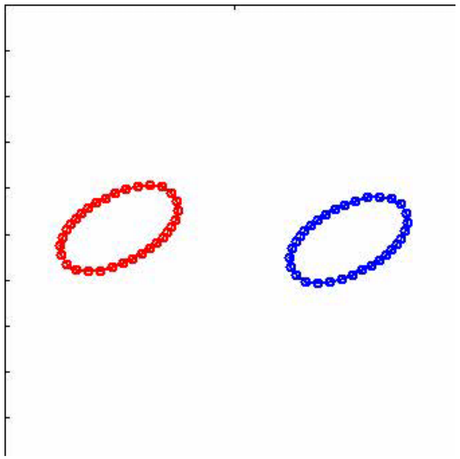
Lateral migration (Slipper)







T-junction



Interaction