Immersed Boundary Methods for Interfacial Flows

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Outline of my talk

Three different Immersed Boundary (IB) Method applications

1. Moving contact lines with surfactant, CiCP, vol 8, pp. 735-757, (2010)
2. Two-dimensional dry foam and von Neumann law, JCP, vol 229, pp. 5194-5207, (2010)
3. Dynamics of inextensible vesicles, JCP, vol 229, pp. 4840-4853, (2010)

Joint work with

- Charlie Peskin (Courant Institute, New York University)
- Huaxiong Huang (York University)
- Yongsam Kim (Chung-Ang University, Korea)
- Zhilin Li (North Carolina State University)
- Yu-Hau Tseng, Chung-Yin Huang, Yi-Min Huang (NCTU)

Moving contact lines with surfactant

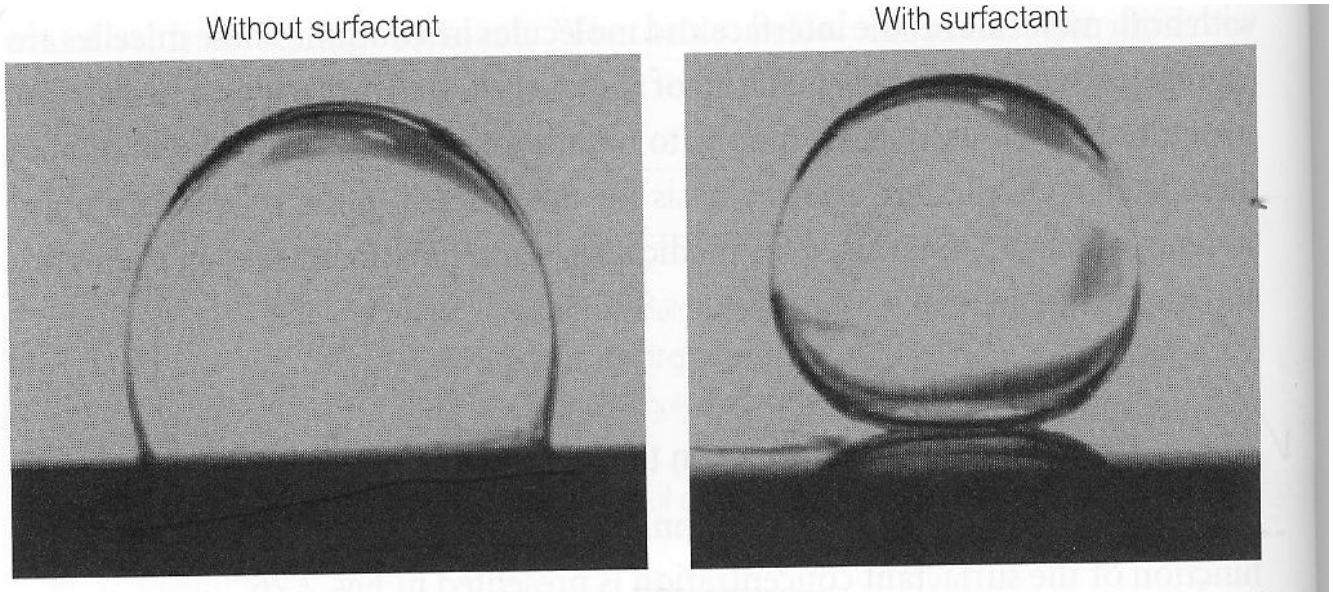
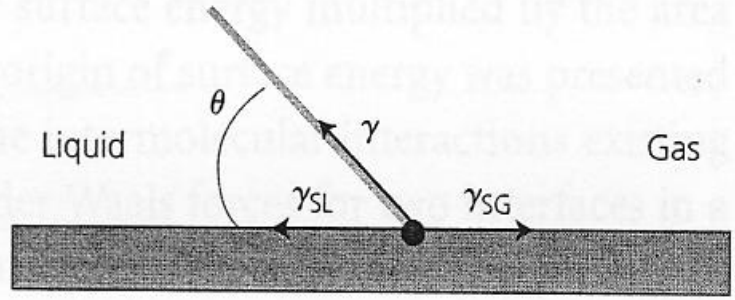


Figure 2.27 The effect of detergence in a water-tetradecane system. On increasing the concentration of surfactant (SPAN 80), the system goes from a partial wetting regime to a total wetting regime of tetradecane on the substrate. The water droplet thus tends to detach itself from the substrate.

Two issues: moving contact lines and surfactant

Equilibrium contact angle: static case

Figure 2.21 Diagram showing a solid–liquid–gas contact line, for which Young's relation is applied.



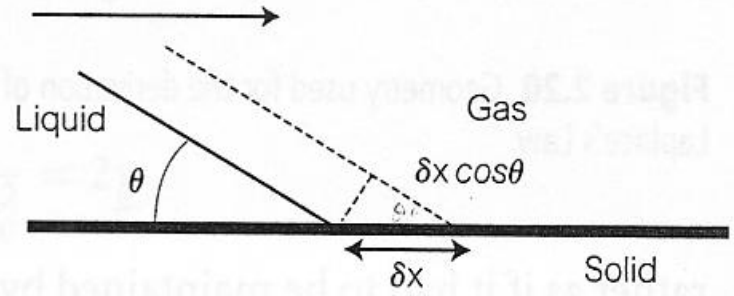


Figure 2.22 Solid–liquid–gas contact line, subjected to an infintessimal displacement δx.

- Surface energy: γ_{SG} (solid/gas), γ_{LS} (liquid/solid), and γ (liquid/gas)
- Equilibrium contact angle: $\gamma_{SG} = \gamma_{SL} + \gamma cos\theta$

Moving contact line paradox: slip vs. no-slip

- Huh & Scriven, J. Colloid Interf. Sci. 35, 85-101 (1971), a planar fluid interface moving steadily over a flat solid surface, 2D Stokes flow with no-slip boundary condition at the solid surface, it leads to non-integrable stress
- Dussan & Davis, JFM 65, 71-95 (1974), if the contact line moves and no sip boundary condition is enforced, then the tangential force exerted by the fluid on the solid surface is infinite

Some remedies

- Slip boundary condition, Dussan V. 1976
- Generalized Navier boundary condition, Qian, Wang & Sheng, 2006, phase-field formulation, is verified by MD simulation
- Effective boundary condition, Ren & E, 2007, Navier slip BC at solid wall away from contact line, effective BC at the contact line results from the deviation of the contact angle from its static value
- Many others

Some selected numerical works

- Front-tracking method: Huang, Liang & Wetton 2004
- Volume of fluid: Renardy, Renardy & Li, 2001; Sikalo et. al. 2005;
- Level set method: Spelt 2005
- Phase field method: Qian, Wang & Sheng, 2006; Zhou et. al. 2010
- Sharp interface method: Liu, Krishnan, Marella & Udaykumar 2005
- Immersed interface method: Li, Lai, He & Zhao, 2010
- Others

Surfactant (Surface active agent)

- Molecules prefer to reside at interfaces rather than staying immersed in the liquid
- Surfactant are usually organic compounds that are amphiphilic, containing both hydrophilic (likes water) heads and hydrophobic (avoids water) tails
- Soap(anionic), CTAB(cationic), non-ionic, detergent
- Surfactant are wetting agents that lower the surface tension of a liquid, allowing easier spreading, and lower the interfacial tension between two liquid. Tap water surface tension $\sigma = 40$ dynes/cm
- Soap bubbles, emulsions, soap boat
- Insoluble surfactant
- Journal of Surfactants and Detergents

Immersed boundary formulation

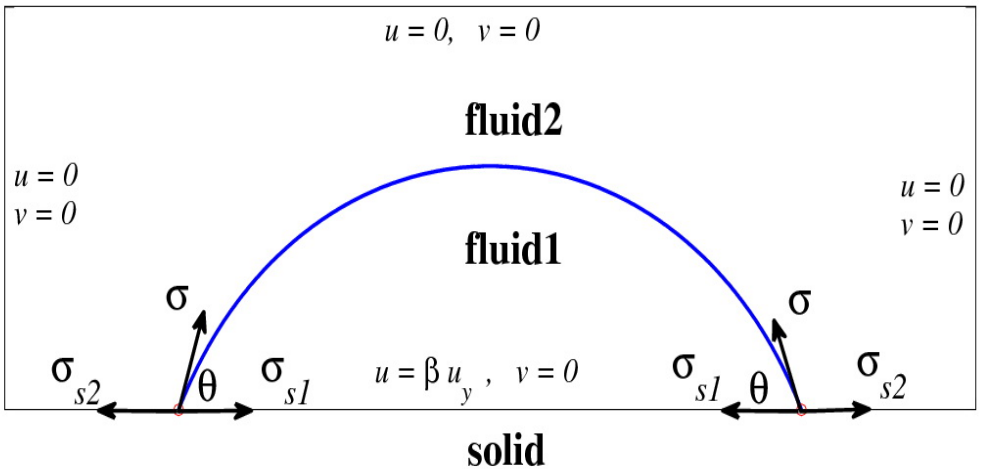


Figure: The diagram of contact lines and the problem set up. Assumption: Insoluble surfactant, same fluid viscosity, no gravity. The fluid domain $\Omega = [a, b] \times [c, d]$, where the fluid/soild surface is at $y = c$. The fluid/fluid interface $\Sigma(t) = \{\mathbf{X}(s, t) | s \in [0, L_b]\}$, where s is the Lagrangian parameter, so $s = 0$ and $s = L_b$ represent the right and left contact lines, respectively.

IB formulation for interfacial flows with surfactant, Lai, Tseng & Huang, JCP 227, 7279-7293, (2008)

$$
\begin{aligned}
\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p &= \frac{1}{Re}\nabla^2\mathbf{u} + \frac{1}{ReCa}\mathbf{f}, \quad \text{in } \Omega \\
\nabla\cdot\mathbf{u} &= 0, \quad \text{in } \Omega \\
\mathbf{f}(\mathbf{x},t) &= \int_\Sigma \mathbf{F}(s,t)\,\delta(\mathbf{x}-\mathbf{X}(s,t))\,ds, \quad \text{in } \Omega \\
\frac{\partial \mathbf{X}(s,t)}{\partial t} = \mathbf{U}(s,t) &= \int_\Omega \mathbf{u}(\mathbf{x},t)\,\delta(\mathbf{x}-\mathbf{X}(s,t))d\mathbf{x}, \quad \text{on } \Sigma
\end{aligned}
$$

$$
\mathbf{F}(s,t) = \frac{\partial}{\partial s}(\sigma(s,t)\boldsymbol{\tau}(s,t)), \qquad \boldsymbol{\tau}(s,t) = \frac{\frac{\partial \mathbf{X}}{\partial s}}{\left|\frac{\partial \mathbf{X}}{\partial s}\right|} \quad \text{on } \Sigma
$$

$$
\begin{aligned}
\frac{D\Gamma}{Dt} + (\nabla_s\cdot\boldsymbol{U})\,\Gamma &= \frac{1}{Pe_s}\,\nabla_s^2\,\Gamma, \quad \text{on } \Sigma \\
\sigma(\Gamma) &= \sigma_c(1+\ln(1-\eta\,\Gamma))
\end{aligned}
$$

$\mathbf{u}(\mathbf{x},t)$: fluid velocity; $p(\mathbf{x}$,t): fluid pressure, $\Gamma(s,t)$: surfactant concentration

Slip boundary condition and contact line condition

- Navier slip boundary condition $u = \beta \frac{\partial u}{\partial y}, v = 0$ at solid wall, β is the slip length
- Unbalanced Young's forces at contact lines $s = 0$ and $s = L_b$:

$$F_{cl} = \sigma_{s2} - \sigma_{s1} - \sigma \cos\theta = \sigma_{cl}(\cos\theta_e - \cos\theta),$$

where θ_e is the equilibrium contact angle

Effective boundary condition at the contact line, Ren & E 2007

At the contact lines

$$\beta_{cl} u_{cl} = \sigma_{cl}(\cos\theta_e - \cos\theta),$$

where β_{cl} is the effective friction coefficient

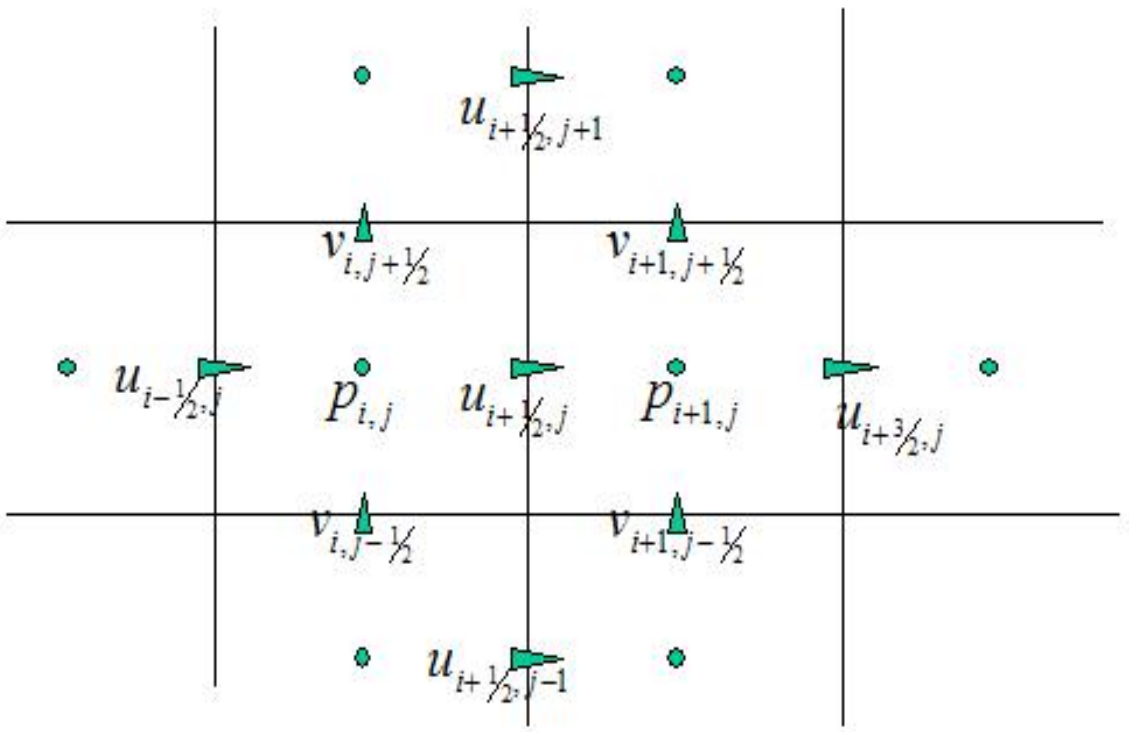
Surface gradient, divergence, and Laplacian

$$
\begin{aligned}
\nabla_s \Gamma &= \frac{\partial \Gamma}{\partial \boldsymbol{\tau}} \boldsymbol{\tau} = \left(\frac{\partial \Gamma}{\partial s} \boldsymbol{\tau} \right) / |\boldsymbol{X}_s| \\
\nabla_s \cdot \boldsymbol{U} &= \frac{\partial \boldsymbol{U}}{\partial \boldsymbol{\tau}} \cdot \boldsymbol{\tau} = \left(\frac{\partial \boldsymbol{U}}{\partial s} \cdot \boldsymbol{\tau} \right) / |\boldsymbol{X}_s|, \\
\nabla_s^2 \Gamma &= \nabla_s \cdot \nabla_s \Gamma = \frac{\partial}{\partial s} \left(\frac{\partial \Gamma}{\partial s} / |\boldsymbol{X}_s| \right) / |\boldsymbol{X}_s|.
\end{aligned}
$$

Numerical scheme

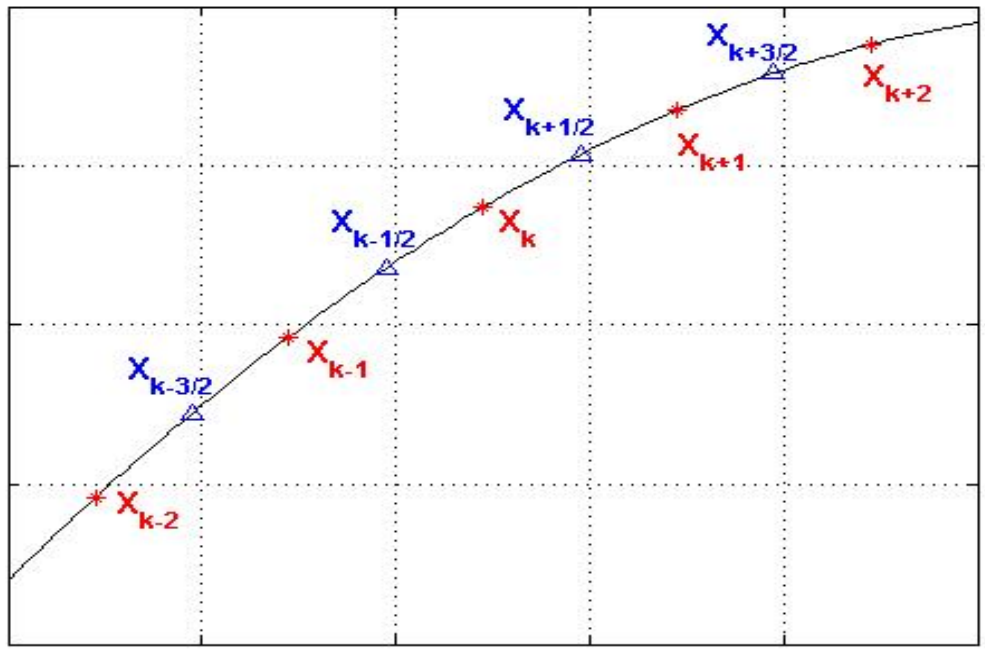
Fluid variables

- Staggered marker-and-cell (MAC) mesh introduced by Harlow & Welsh, 1965



Lagrangian variables

- The Lagrangian markers are denoted by $\mathbf{X}_k = \mathbf{X}(s_k) = (X_k, Y_k)$, where $s_k = k\Delta s, k = 0, 1, \ldots M$. $k = 0$ and $k = M$ represent the right and left contact lines, respectively.
- The surfactant concentration Γ_k, surface tension σ_k are defined at the "half-integer" points given by $s_{k+1/2} = (k + 1/2)\Delta s$.



- For any function defined on the interface $\phi(s)$,

$$D_s\phi(s) = \frac{\phi(s + \Delta s/2) - \phi(s - \Delta s/2)}{\Delta s}.$$

  Interface stretching factor $|D_s \boldsymbol{X}_k|$, and the unit tangent vector $\boldsymbol{\tau}_k$ are also defined at the "half-integer" points.

- Let Δt be the time step size, and n be the superscript time step index. At the beginning of each time step n, the variables $\mathbf{u}^n = \mathbf{u}(\mathbf{x}, n\Delta t)$, $\mathbf{X}_k^n = \mathbf{X}(s_k, n\Delta t)$, $\Gamma_k^n = \Gamma(s_{k+1/2}, n\Delta t)$, and $p^{n-1/2} = p(\mathbf{x}, (n - 1/2)\Delta t)$ are all given.

Time integration

- Step 1: Compute the surface tension and unit tangent on the interface as

$$\begin{aligned} \sigma_k^n &= \sigma_c(1+\ln(1-\eta\Gamma_k^n) \\ \boldsymbol{\tau}_k^n &= \frac{D_s \boldsymbol{X}_k^n}{|D_s \boldsymbol{X}_k^n|} \end{aligned}$$

both of which hold for $s_{k+1/2} = (k+1/2)\Delta s$. Then we define the interface force as

$$\boldsymbol{F}_k^n = D_s(\sigma_k^n \boldsymbol{\tau}_k^n),$$

at point $\mathbf{X}_k, k = 1, 2 \ldots M-1$.
The unbalanced Young's force at the contact lines ($k = 0$ and $k = M$) can be computed by

$$\begin{aligned} \boldsymbol{F}_0^n &= (\sigma_{s2} - \sigma_{s1} - \sigma_0^n \cos\theta_0^n)\, \boldsymbol{e}_1, \\ \boldsymbol{F}_M^n &= -(\sigma_{s2} - \sigma_{s1} - \sigma_M^n \cos\theta_M^n)\, \boldsymbol{e}_1, \end{aligned}$$

where $\boldsymbol{e}_1 = (1, 0)$ and $\cos\theta_k^n = -\boldsymbol{\tau}_k^n \cdot \boldsymbol{e}_1$.

- Step 2: Distribute the force from the markers to the fluid by

$$\boldsymbol{f}^n(\boldsymbol{x}) = \sum_{k=1}^{M-1} \boldsymbol{F}_k^n \, \delta_h(\boldsymbol{x} - \boldsymbol{X}_k^n) \, \Delta s + \sum_{k=0,M} \boldsymbol{F}_k^n \, \delta_h(\boldsymbol{x} - \boldsymbol{X}_k^n),$$

  where the smooth version of Dirac delta function in is used.

- Step 3: Solve the Navier-Stokes equations. Second-order accurate projection method (Brown, Cortez & Minion 2001), Adams-Bashforth for convection and Crank-Nicholson for diffusion terms.

$$
\begin{aligned}
(\boldsymbol{u}\cdot\nabla_h)\mathbf{u}^{n+1/2} &= \frac{3}{2}(\boldsymbol{u}^n\cdot\nabla_h)\mathbf{u}^n - \frac{1}{2}(\boldsymbol{u}^{n-1}\cdot\nabla_h)\mathbf{u}^{n-1} \\
\frac{\mathbf{u}^*-\mathbf{u}^n}{\Delta t} &+ (\boldsymbol{u}\cdot\nabla_h)\mathbf{u}^{n+1/2} = -\nabla_h p^{n-1/2} \\
&\quad + \frac{1}{2Re}\nabla_h^2(\mathbf{u}^*+\mathbf{u}^n) + \frac{\mathbf{f}^n}{Re\,Ca} \\
\boldsymbol{u}^* = 0 \quad \text{on } \partial\Omega, &\qquad u^* = \beta\,\frac{\partial u^*}{\partial y}, v^* = 0 \quad \text{on } y = c, \\
\nabla_h^2\phi^{n+1} &= \frac{\nabla_h\cdot\boldsymbol{u}^*}{\Delta t}, \qquad \frac{\partial\phi^{n+1}}{\partial\mathbf{n}}|_{\partial\Omega} = 0, \\
\boldsymbol{u}^{n+1} &= \boldsymbol{u}^* - \Delta t\,\nabla_h\phi^{n+1}, \\
p^{n+1/2} &= p^{n-1/2} + \phi^{n+1} - \frac{\nabla_h\cdot\boldsymbol{u}^*}{2\,Re}.
\end{aligned}
$$

- Step 4: Update the interface positions.

$$\begin{aligned}
\boldsymbol{U}_k^{n+1} &= \sum_{\boldsymbol{x}} \boldsymbol{u}^{n+1}\delta_h(\boldsymbol{x}-\boldsymbol{X}_k^n)h^2, k=0,1,\dots M \\
\boldsymbol{X}_k^{n+1} &= \boldsymbol{X}_k^n + \Delta t \boldsymbol{U}_k^{n+1}, k=1,2\dots M-1 \\
X_k^{n+1} &= X_k^n + \Delta t\, U_k^{n+1}, \quad k=0,M, \qquad Y_0^{n+1} = Y_M^{n+1} = c
\end{aligned}$$

- Step 5: Update the surfactant distribution.
  Let

$$\frac{\partial \Gamma}{\partial t}\left|\frac{\partial \mathbf{X}}{\partial s}\right| + (\nabla_s \cdot \boldsymbol{U})\left|\frac{\partial \mathbf{X}}{\partial s}\right|\Gamma = \frac{1}{Pe_s}\frac{\partial}{\partial s}\left(\frac{\partial \Gamma}{\partial s}\Big/\left|\frac{\partial \mathbf{X}}{\partial s}\right|\right).$$

  and then

$$\frac{\partial \Gamma}{\partial t}\left|\frac{\partial \mathbf{X}}{\partial s}\right| + \frac{\partial}{\partial t}\left|\frac{\partial \mathbf{X}}{\partial s}\right|\Gamma = \frac{1}{Pe_s}\frac{\partial}{\partial s}\left(\frac{\partial \Gamma}{\partial s}\Big/\left|\frac{\partial \mathbf{X}}{\partial s}\right|\right).$$

Use Crank-Nicholson scheme in a symmetric way as

$$\begin{aligned}
& \frac{\Gamma_k^{n+1}-\Gamma_k^n}{\Delta t}\,\frac{\left|D_s\boldsymbol{X}_k^{n+1}\right|+\left|D_s\boldsymbol{X}_k^n\right|}{2}+\frac{\left|D_s\boldsymbol{X}_k^{n+1}\right|-\left|D_s\boldsymbol{X}_k^n\right|}{\Delta t}\,\frac{\Gamma_k^{n+1}+\Gamma_k^n}{2} \\
= & \frac{1}{2\,Pe_s}\,\frac{1}{\Delta s}\left(\frac{(\Gamma_{k+1}^n-\Gamma_k^n)/\Delta s}{(\left|D_s\boldsymbol{X}_{k+1}^n\right|+\left|D_s\boldsymbol{X}_k^n\right|)/2}-\frac{(\Gamma_k^n-\Gamma_{k-1}^n)/\Delta s}{(\left|D_s\boldsymbol{X}_k^n\right|+\left|D_s\boldsymbol{X}_{k-1}^n\right|)/2}\right) \\
+ & \frac{1}{2\,Pe_s}\,\frac{1}{\Delta s}\left(\frac{(\Gamma_{k+1}^{n+1}-\Gamma_k^{n+1})/\Delta s}{(\left|D_s\boldsymbol{X}_{k+1}^{n+1}\right|+\left|D_s\boldsymbol{X}_k^{n+1}\right|)/2}-\frac{(\Gamma_k^{n+1}-\Gamma_{k-1}^{n+1})/\Delta s}{(\left|D_s\boldsymbol{X}_k^{n+1}\right|+\left|D_s\boldsymbol{X}_{k-1}^{n+1}\right|)/2}\right)
\end{aligned}$$

Easy to check (with no flux BC at the contact lines):

$$\sum_k \Gamma_k^{n+1}\,\left|D_s\boldsymbol{X}_k^{n+1}\right|\,\Delta s=\sum_k \Gamma_k^n\,\left|D_s\boldsymbol{X}_k^n\right|\,\Delta s.$$

Implicit scheme and total mass conserved!

An equi-distributed technique for Lagrangian markers

Goal: To make the Lagrangian markers to be equidistributed in arc-length along the interface without changing the shape of the interface (Hou, Lowengrub & Shelley, JCP 114, 312-338, (1994))
Idea: To introduce an artificial tangential velocity such that the marker $\mathbf{X}(s,t)$ satisfies $|\boldsymbol{X}_s|_s = 0$.

$$\frac{\partial \mathbf{X}(s,t)}{\partial t} = \mathbf{U}(s,t) + U^A(s,t)\,\boldsymbol{\tau} = \int_\Omega \mathbf{u}(\mathbf{x},t)\,\delta(\mathbf{x}-\mathbf{X}(s,t))d\mathbf{x} + U^A(s,t)\,\boldsymbol{\tau}$$

Let $L_s = \left|\frac{\partial \boldsymbol{X}}{\partial s}\right| = |\boldsymbol{X}_s|$. Then $|\boldsymbol{X}_s|_s = L_{s,s} = 0$ implies that L_s is independent of s and is dependent on t.

$$L_s(t) = \frac{1}{L_b}\int_0^{L_b} L_{s'}(s',t)\,ds'$$

$$L_{s,t}(t) = \frac{1}{L_b}\int_0^{L_b} L_{s',t}(s',t)\,ds'$$

$$L_{s,t} = \frac{\partial}{\partial t}|\boldsymbol{X}_s| = \frac{\partial \boldsymbol{U}}{\partial s} \cdot \boldsymbol{\tau} + \frac{\partial U^A}{\partial s}$$

Proof:

$$\begin{aligned}
\frac{\partial}{\partial t}|\boldsymbol{X}_s| &= \frac{\boldsymbol{X}_s \cdot \boldsymbol{X}_{s,t}}{|\boldsymbol{X}_s|} \\
&= \frac{\boldsymbol{X}_s \cdot (\boldsymbol{U} + U^A \boldsymbol{\tau})_s}{|\boldsymbol{X}_s|} \\
&= \frac{1}{|\boldsymbol{X}_s|}\left(\boldsymbol{X}_s \cdot (\frac{\partial \boldsymbol{U}}{\partial s} + \frac{\partial U^A}{\partial s}\boldsymbol{\tau} + U^A \frac{\partial \boldsymbol{\tau}}{\partial s})\right) \\
&= \frac{\partial \boldsymbol{U}}{\partial s} \cdot \boldsymbol{\tau} + \frac{\partial U^A}{\partial s} \\
&= (\nabla_s \cdot \boldsymbol{U})\,|\boldsymbol{X}_s| + \frac{\partial U^A}{\partial s}
\end{aligned}$$

$$\left(\boldsymbol{\tau} = \frac{\boldsymbol{X}_s}{|\boldsymbol{X}_s|}, \quad \frac{\partial \boldsymbol{\tau}}{\partial s} = \kappa \boldsymbol{n}|\boldsymbol{X}_s|, \quad \nabla_s \cdot \boldsymbol{U} = \frac{\partial \boldsymbol{U}}{\partial \boldsymbol{\tau}} \cdot \boldsymbol{\tau}\right)$$

Thus, we have

$$\begin{aligned}\frac{\partial \boldsymbol{U}}{\partial s}\cdot\boldsymbol{\tau}+\frac{\partial U^A}{\partial s}(s,t) &= \frac{1}{L_b}\int_0^{L_b}\frac{\partial \boldsymbol{U}}{\partial s'}\cdot\boldsymbol{\tau}'+\frac{\partial U^A}{\partial s'}\,ds' \\ &= \frac{1}{L_b}\int_0^{L_b}\frac{\partial \boldsymbol{U}}{\partial s'}\cdot\boldsymbol{\tau}'ds'\end{aligned}$$

Integrating with respect to s, we obtain

$$U^A(s,t)-U^A(0,t)=-\int_0^s\frac{\partial \boldsymbol{U}}{\partial s'}\cdot\boldsymbol{\tau}'ds'+\frac{s}{L_b}\int_0^{L_b}\frac{\partial \boldsymbol{U}}{\partial s'}\cdot\boldsymbol{\tau}'ds'$$

Since $U^A(0,t)=0$ (no artificial velocity at the contact line), we obtain the artificial tangential velocity as

$$U^A(s,t)=\frac{s}{L_b}\int_0^{L_b}\frac{\partial \boldsymbol{U}}{\partial s'}\cdot\boldsymbol{\tau}'ds'-\int_0^s\frac{\partial \boldsymbol{U}}{\partial s'}\cdot\boldsymbol{\tau}'ds'$$

Note: The above formula is without the calculation of the curvature! Similar derivation has been found from Ceniceros' work (Phys. Fluids, 15, 245-256 (2003)) in terms of tangential velocity, normal velocity and curvature.

How about the new surfactant evolution equation?

From the surfactant equation

$$\frac{D\Gamma}{Dt} + (\nabla_s \cdot \boldsymbol{U})\,\Gamma = \frac{1}{Pe_s}\,\frac{\partial}{\partial s}\left(\frac{\partial \Gamma}{\partial s} \Big/ \left|\frac{\partial \mathbf{X}}{\partial s}\right|\right) \Big/ \left|\frac{\partial \mathbf{X}}{\partial s}\right|.$$

Using the identity

$$\frac{D\Gamma}{Dt} = \frac{\partial \Gamma}{\partial t} - (U^A \boldsymbol{\tau}) \cdot \nabla \Gamma = \frac{\partial \Gamma}{\partial t} - (U^A \boldsymbol{\tau}) \cdot \nabla_s \Gamma = \frac{\partial \Gamma}{\partial t} - U^A \frac{\partial \Gamma}{\partial \boldsymbol{\tau}}$$

and multiplying $|\boldsymbol{X}_s|$ on both sides, we have

$$\frac{\partial \Gamma}{\partial t}\,|\boldsymbol{X}_s| - U^A \frac{\partial \Gamma}{\partial s} + (\nabla_s \cdot \boldsymbol{U})\,\Gamma\,|\boldsymbol{X}_s| = \frac{1}{Pe_s}\,\frac{\partial}{\partial s}\left(\frac{\partial \Gamma}{\partial s} \Big/ \left|\frac{\partial \mathbf{X}}{\partial s}\right|\right).$$

$$(\nabla_s \cdot \boldsymbol{U})\,|\boldsymbol{X}_s| = \frac{\partial}{\partial t}|\boldsymbol{X}_s| - \frac{\partial U^A}{\partial s}$$

$$\frac{\partial \Gamma}{\partial t}\,|\boldsymbol{X}_s| - \frac{\partial}{\partial s}(U^A\,\Gamma) + \Gamma\,\frac{\partial}{\partial t}|\boldsymbol{X}_s| = \frac{1}{Pe_s}\,\frac{\partial}{\partial s}\left(\frac{\partial \Gamma}{\partial s} \Big/ \left|\frac{\partial \mathbf{X}}{\partial s}\right|\right).$$

A modified numerical scheme

- Step 1,2 and 3 are same as before
- Step 4 should be modified as follows. Find the artificial velocity U_k^A. Then

$$\boldsymbol{X}_k^{n+1} = \boldsymbol{X}_k^n + \Delta t \boldsymbol{U}_k^{n+1} + \Delta t U_k^A \boldsymbol{\tau}_k^n.$$

  No artificial velocity is needed at the contact lines.
- Solve the modified surfactant equation. Extra term can be discretized as

$$\frac{\partial}{\partial s}(U^A \Gamma) = \frac{1}{\Delta s}\left(U_{k+1}^A \frac{\Gamma_{k+1} + \Gamma_k}{2} - U_k^A \frac{\Gamma_k + \Gamma_{k-1}}{2}\right)$$

- The total mass is still conserved!

Extension to 3D axis-symmetric case

Lai, Huang & Huang, IJNAM, vol 8, 105-107 (2011). Interface forces, and surface divergence are different from 2D! Total surfactant mass is still conserved.

Numerical Results

Numerical parameters

- $\Omega = [-1, 1] \times [0, 1]$
- A half circular drop with radius 0.5 on the substrate with $\Gamma(s, 0) = 1$
- $\sigma_c = 1$, $\eta = 0$ (clean interface), $\eta = 0.3$ (contaminated interface)
- $Re = 10$, $Ca = 0.1$, $Pe_s = 20$
- Slip length $\beta = h/4$, h is the mesh width
- No artificial velocity is imposed at the contact lines

Grid Information

- Uniform Cartesian grid: $h = \Delta x = \Delta y = 1/128$
- Lagrangian grid: $\Delta s \approx h$
- Time step: $\Delta t = h/10$

Convergence test

h	$\|u - u_{ref}\|_2$	rate	$\|v - v_{ref}\|_2$	rate	$\|\Gamma - \Gamma_{ref}\|_2$	rate
1/16	5.8079e-03	-	3.3148e-03	-	3.1818e-02	-
1/32	2.9639e-03	0.97	1.9179e-03	0.79	1.7977e-02	0.82
1/64	1.4773e-03	1.00	1.0805e-03	0.82	9.8698e-03	0.86
1/128	5.9179e-04	1.32	4.6628e-04	1.21	4.2087e-03	1.23

Table: The mesh refinement analysis of the velocity (u, v), and surfactant concentration Γ. $\sigma_{s1} = 0.5, \sigma_{s2} = 1, \sigma_c = 1$, $\theta_e = \pi/3$, $T = 6.25$.

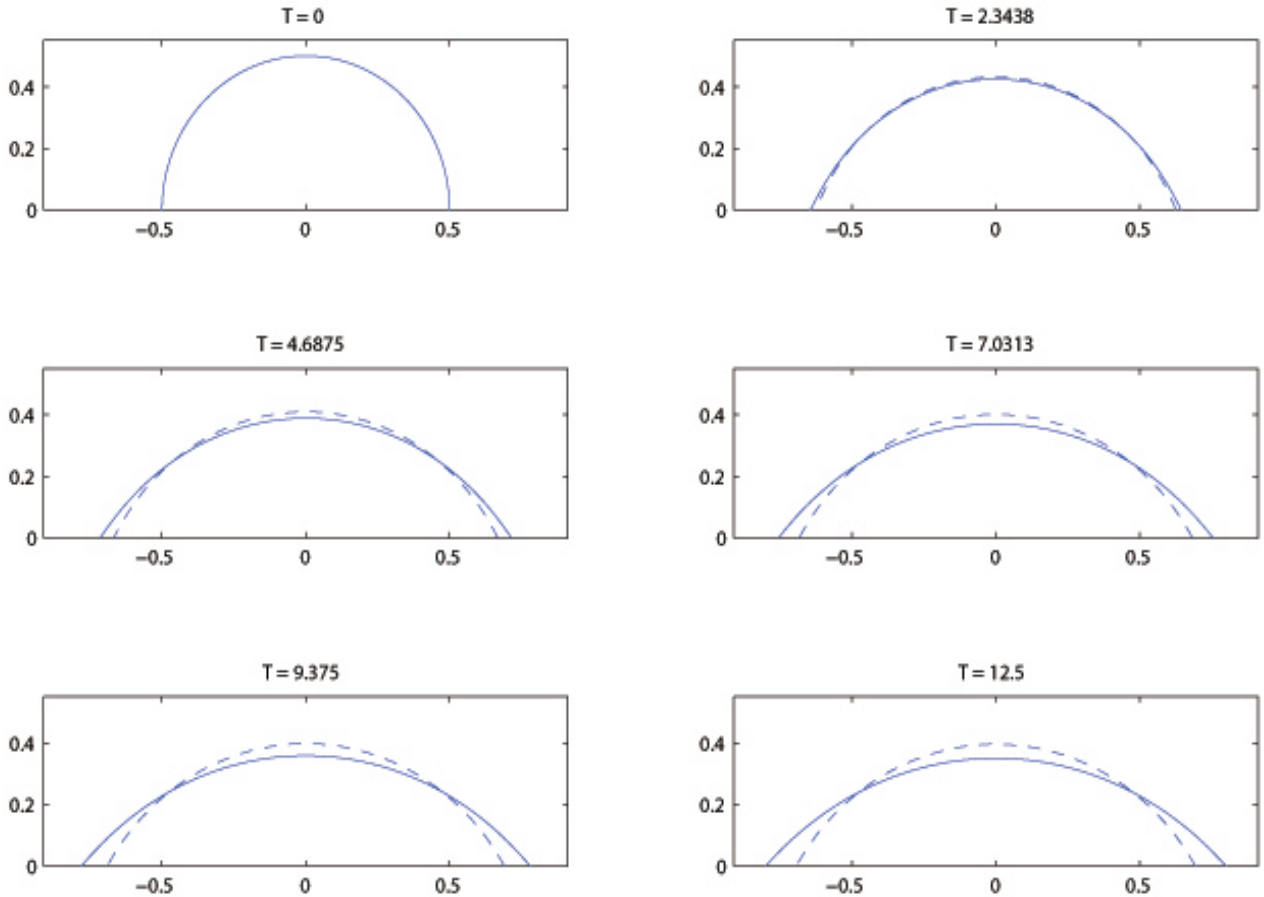
h	$\|\boldsymbol{X} - \boldsymbol{X}_{ref}\|_\infty$	rate	$\|\cos(\theta) - \cos(\theta_{ref})\|$	rate	$\|A - A_{ref}\|/A_r$
1/16	4.76e-02	-	1.03e-01	-	1.15e-01
1/32	2.42e-02	0.98	6.39e-02	0.69	5.67e-02
1/64	1.14e-02	1.08	3.69e-02	0.79	2.75e-02
1/128	4.17e-03	1.45	2.17e-02	0.77	1.31e-02

Table: The mesh refinement analysis of interface positions, the contact angles, and the area of drop.

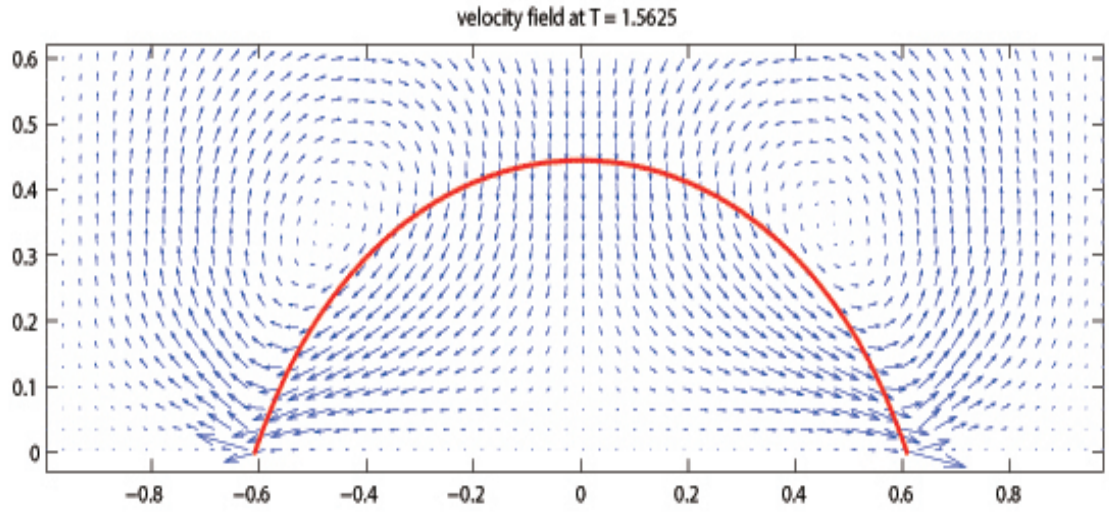
Hydrophilic case

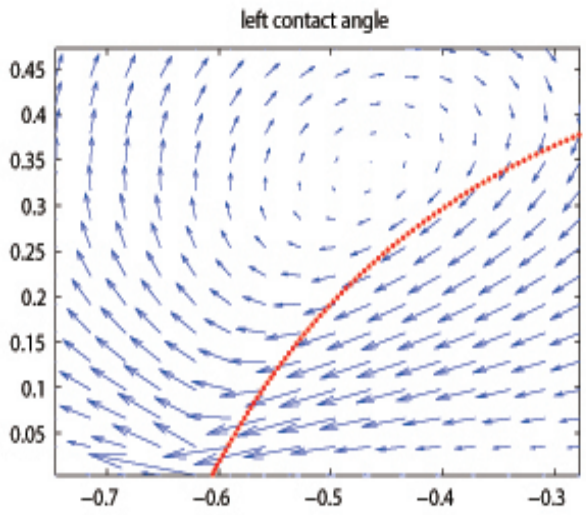
$\sigma_{s1} = 0.5, \sigma_{s2} = 1, \sigma_c = 1$, so the equilibrium contact angle $\theta_e = \pi/3$ (without surfactant)

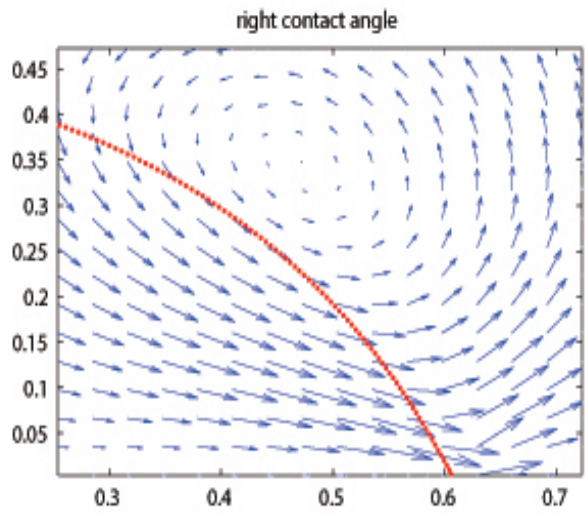
With surfactant (solid line); without surfactant (dashed line)



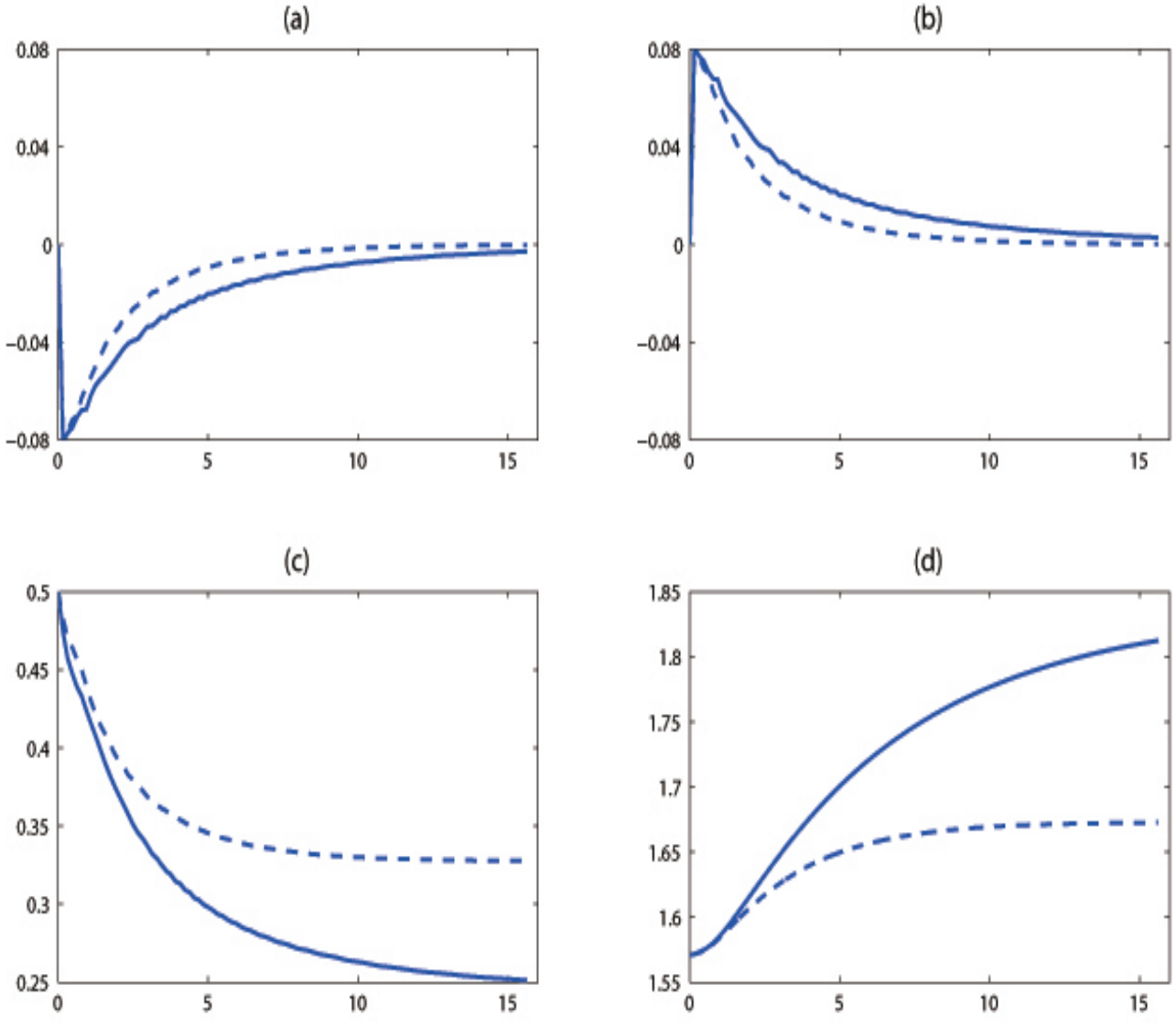
Velocity field near contact lines (with surfactant)





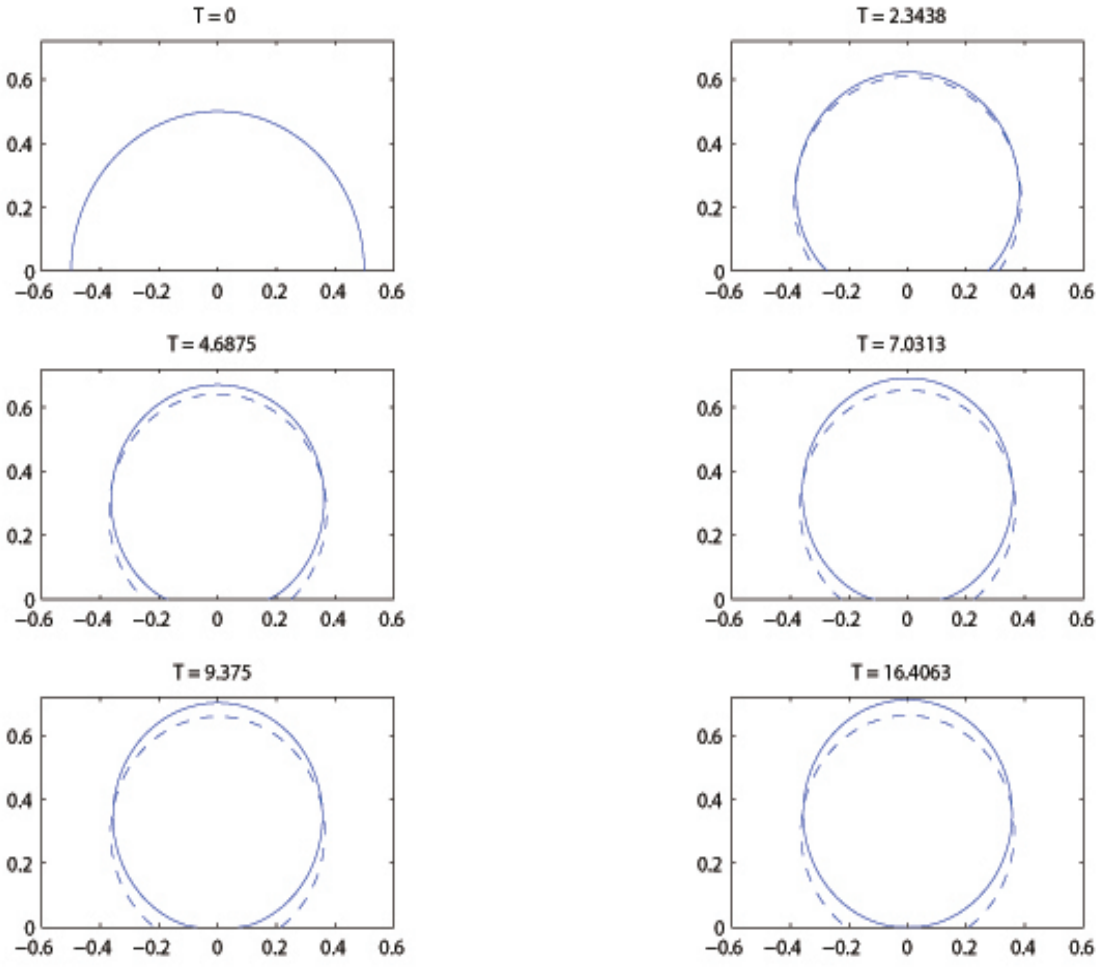


(a) left contact line speed; (b) right contact line speed; (c) contact angles in units of π; (d) total length of the drop.

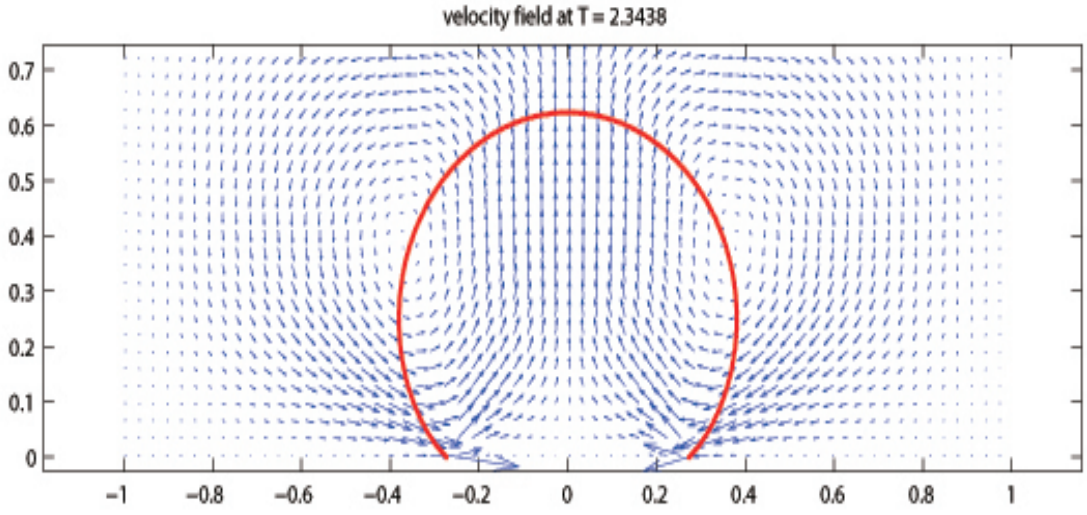


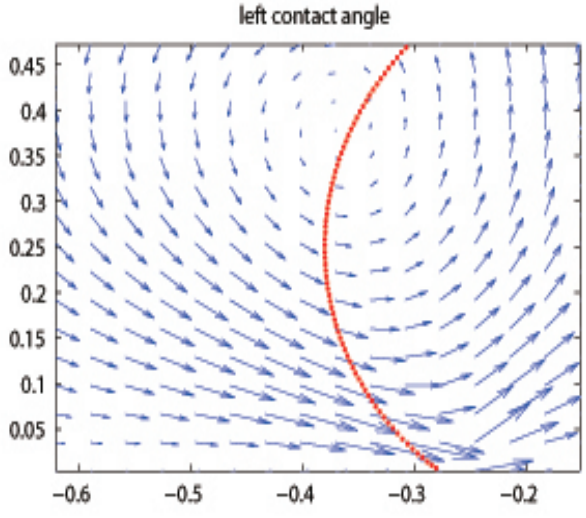
Hydrophobic case

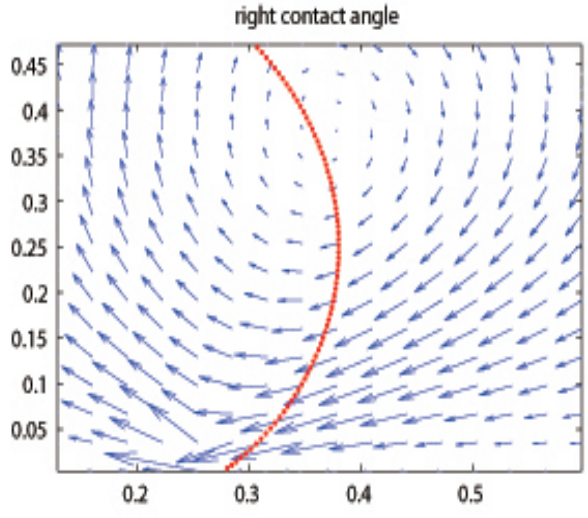
$\sigma_{s1} = 1, \sigma_{s2} = 0.1557, \sigma_c = 1$, so the equilibrium contact angle $\theta_e = 0.82\pi$ (without surfactant)



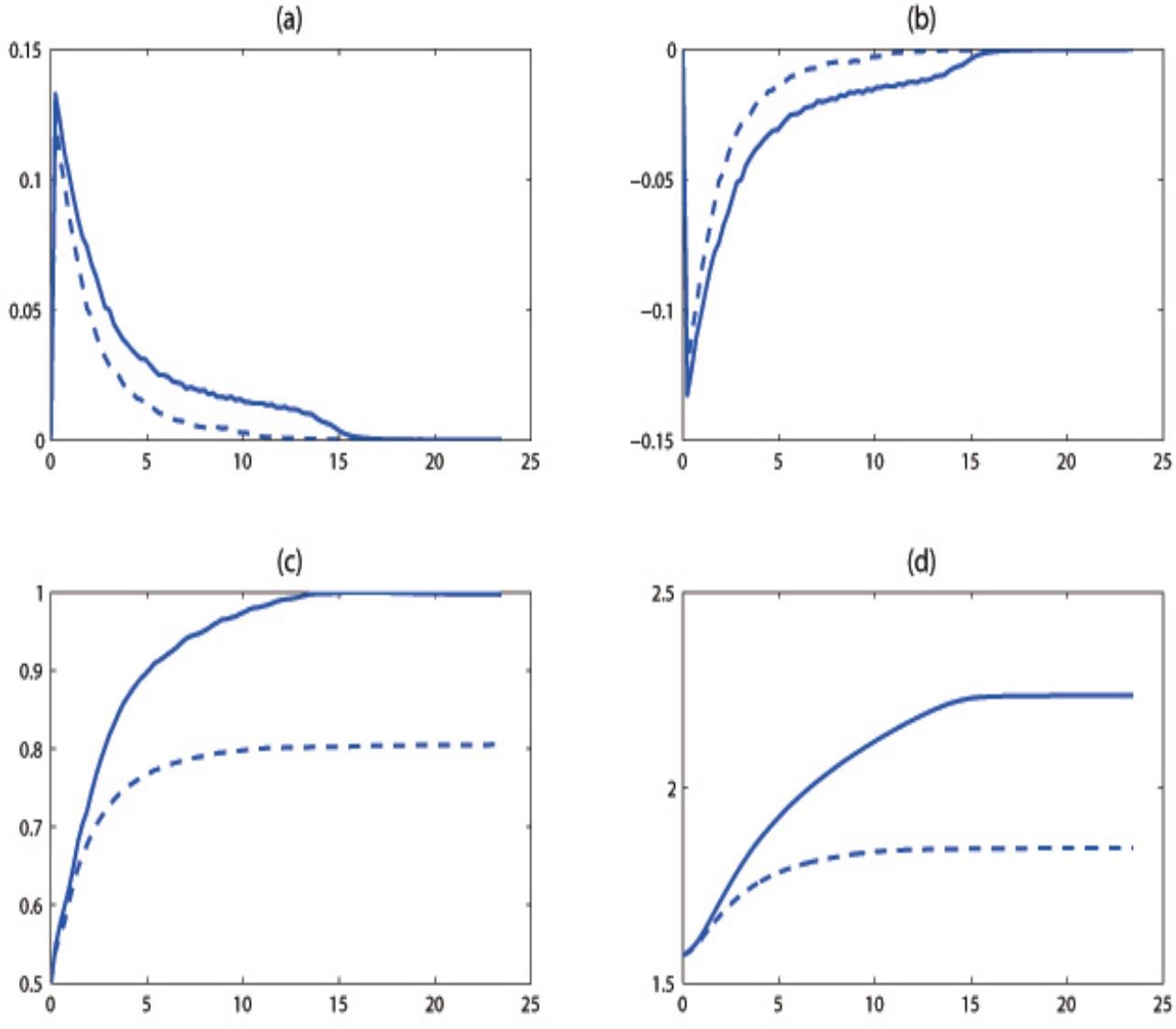
Velocity field near contact lines (with surfactant)







(a) left contact line speed; (b) right contact line speed; (c) contact angles in units of π; (d) total length of the drop.

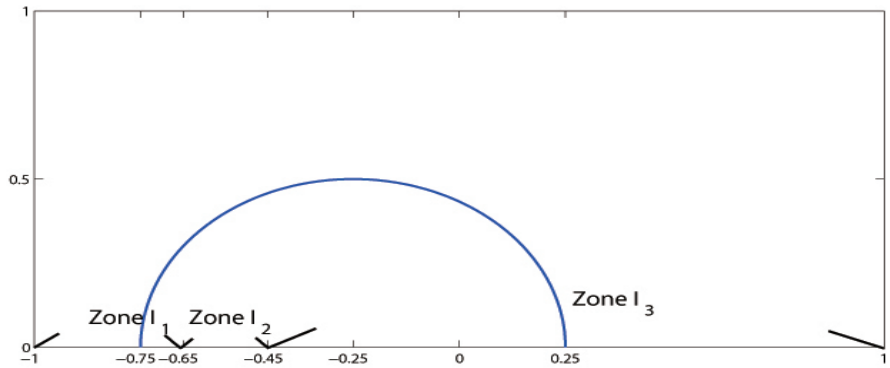


Hydrophilic-hydrophobic case

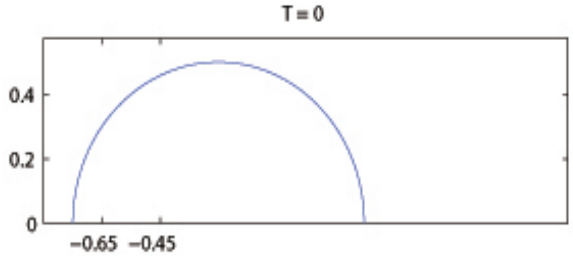
$\sigma_{s1} = 1, \sigma_c = 1$

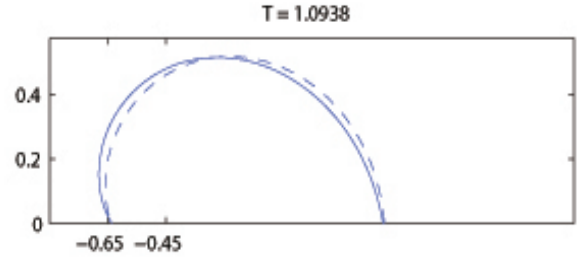
$$\sigma_{s2}(x) = \begin{cases} 0.191, & \text{Hydrophobic} \quad x \in I_1 = [-1, -0.65] \\ 5.59\,(x + 0.65) + 0.191, & x \in I_2 = (-0.65, -0.45) \\ 1.309, & \text{Hydrophilic} \quad x \in I_3 = [-0.45, 1]. \end{cases}$$

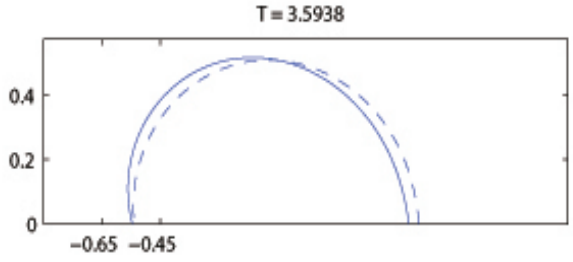
$$\Gamma(\alpha) = -\frac{8}{5\pi^3}\alpha^3 + \frac{12}{5\pi^2}\alpha^2 + 0.5, \quad \alpha \in (0, \pi).$$

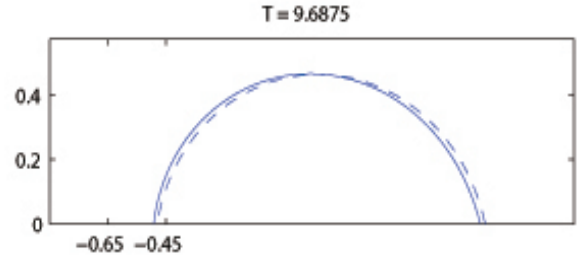


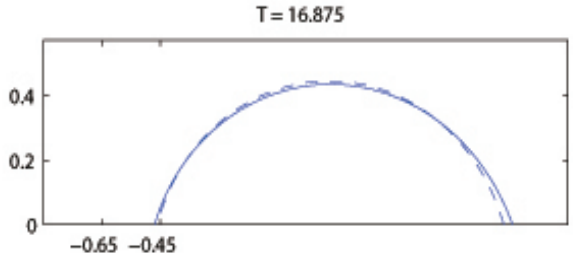
Drop behavior

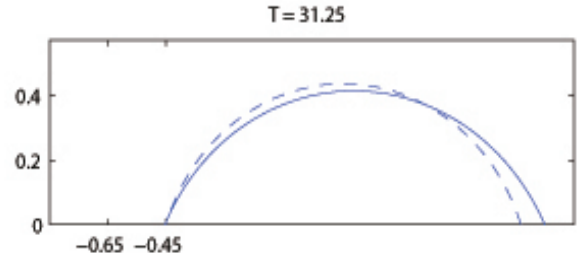




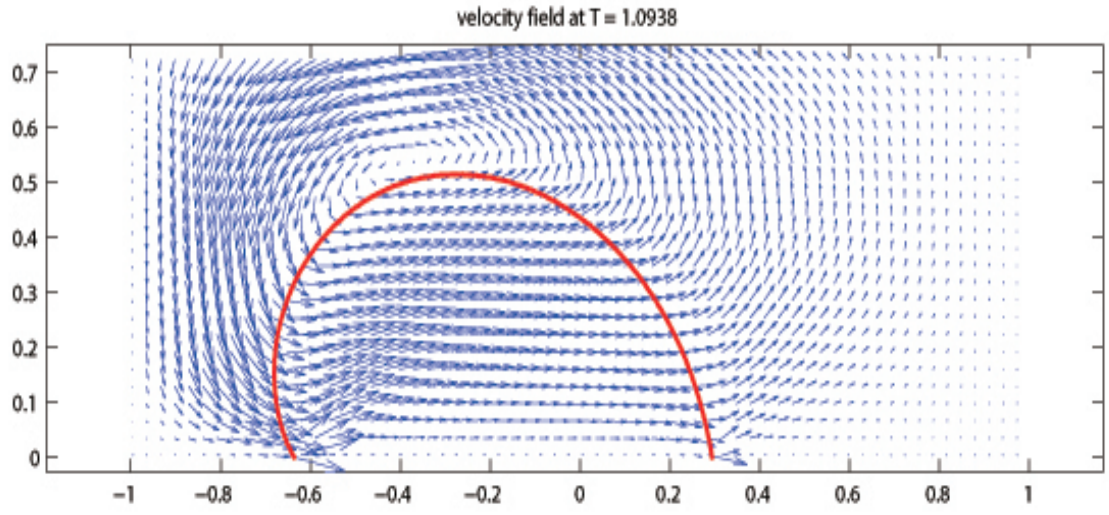


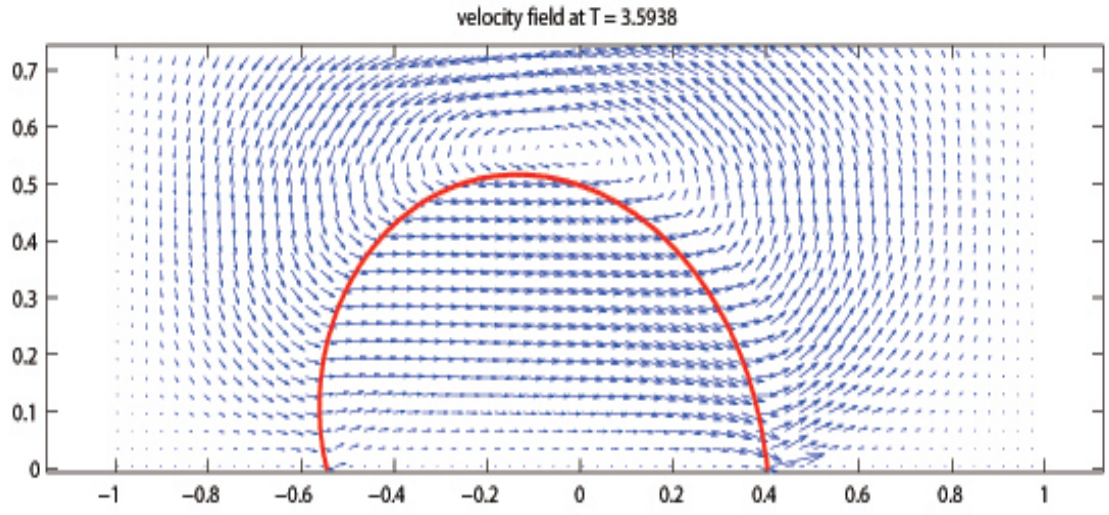




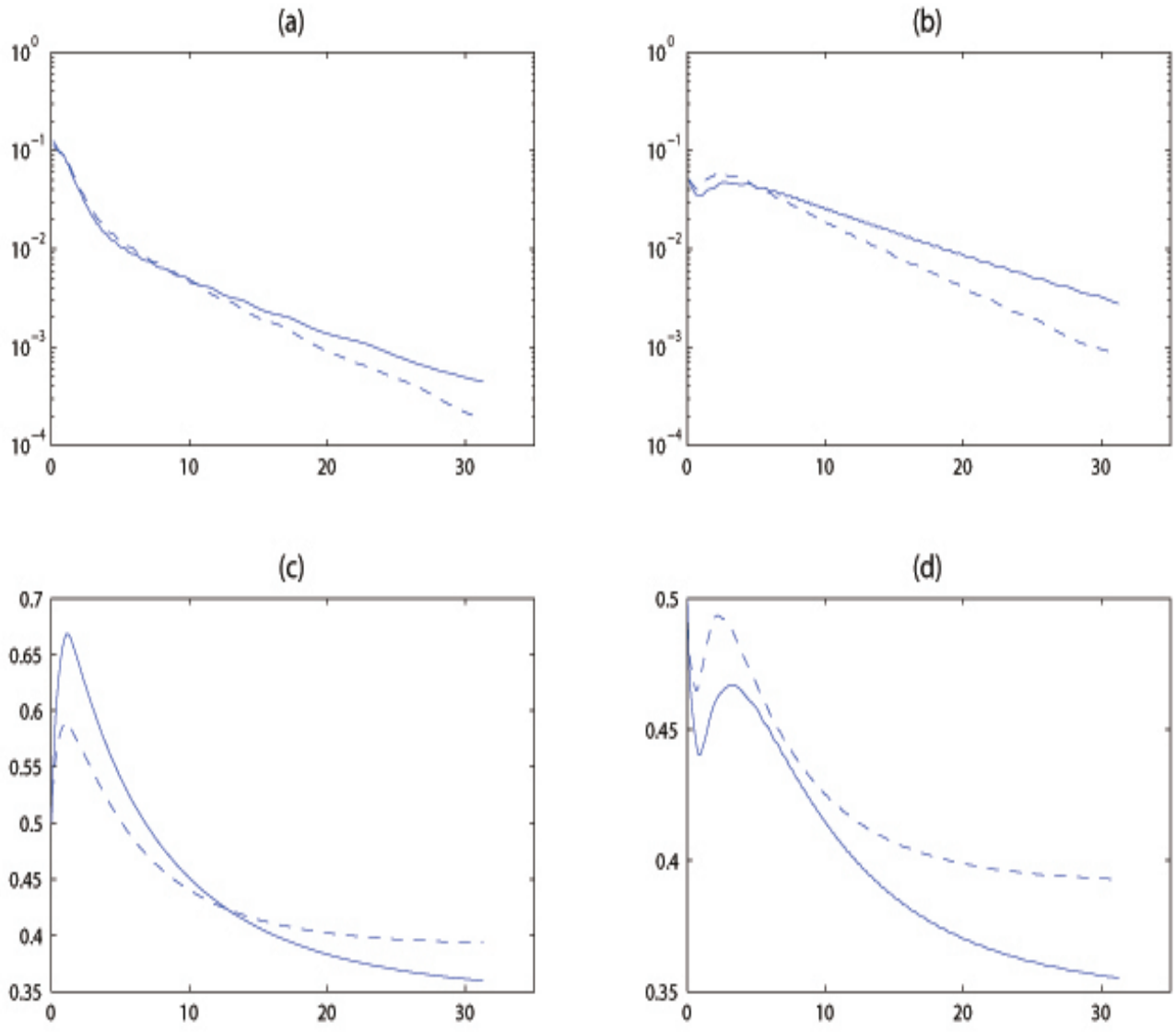


Velocity field near contact lines (with surfactant)



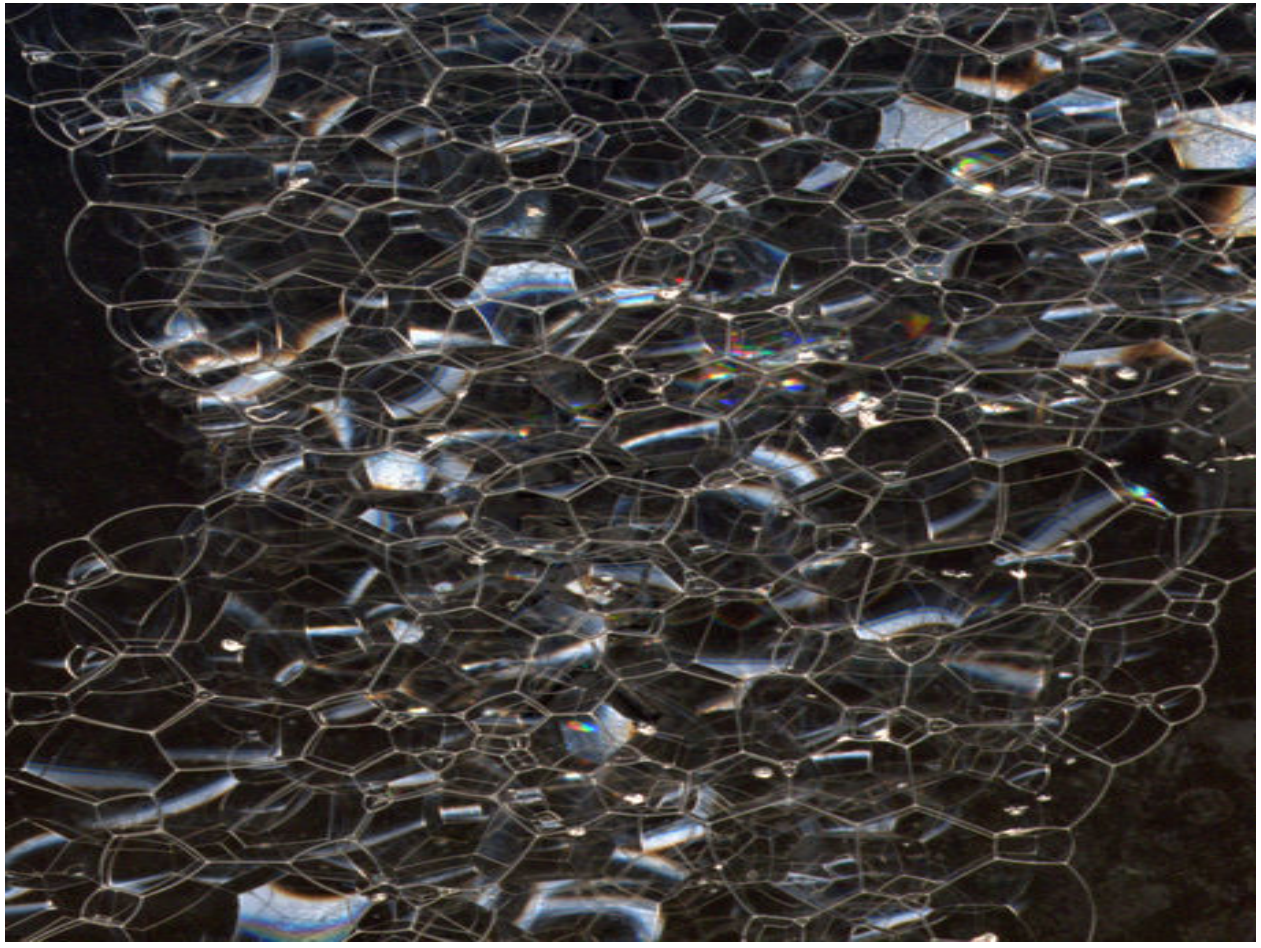


(a) left contact line speed; (b) right contact line speed; (c) left contact angles in units of π; (d) right contact angles in units of π;



2D dry foam and von Neumann law

Foam: soap bubble growth



Why FOAM?

- A gas-liquid mixture
- The physics of foam is poorly understood
- The head on a pint of bear
- Foundations Of Applied Mathematics
- Foam Optics And Mechanics (International Space Station), exploring the critical point of foams

Some references

- The Physics of Foams, D. Weaire & S. Hutzler, Oxford Univ. Press, 1999
- The Mathematics of Foam, C. Breward Ph.D thesis, 1999

Two type of foams

Wet foam: liquid fraction is about $10\% - 20\%$, spherical shape
Dry foam: liquid fraction is less than 10%, polyhedral shape

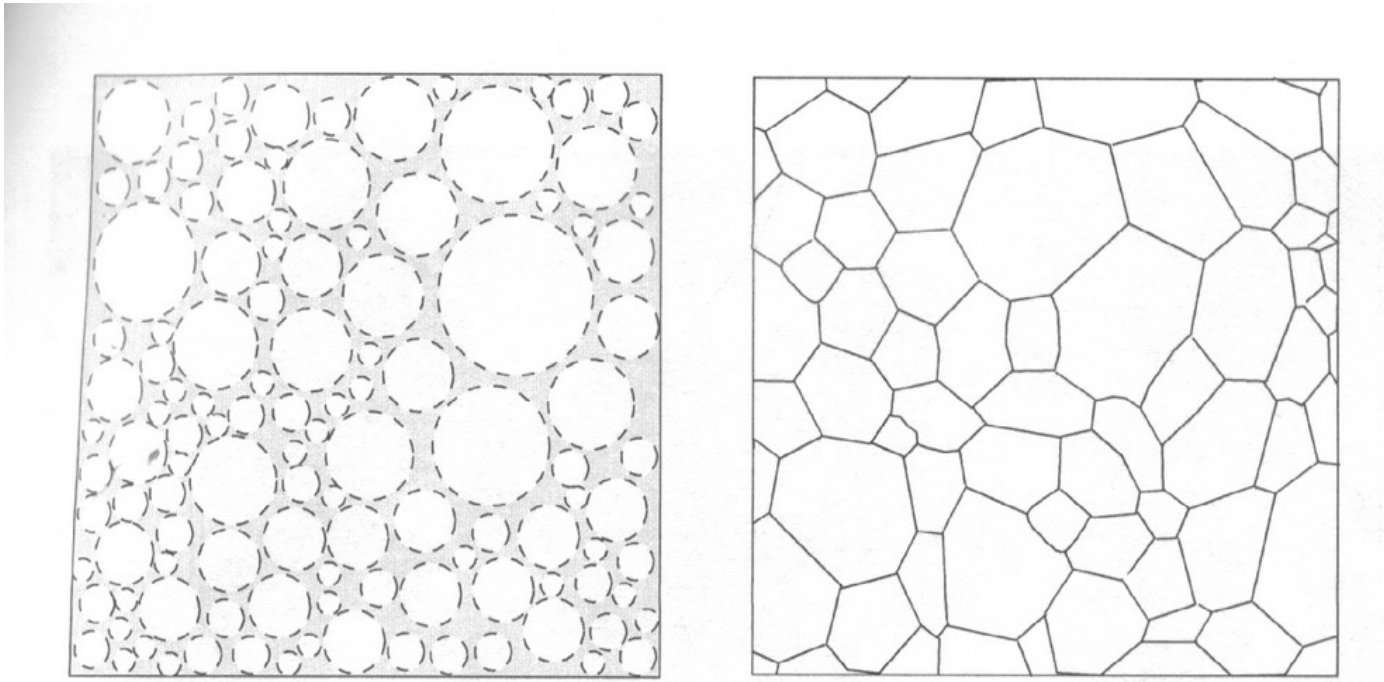


Figure 1.1: Schematic of (a) a wet foam and (b) a dry foam.

von Neumann law for 2D dry foam

The area change for an individual 2D cell (soap bubble or idealized grain) with n sides is proportional to $n - 6$.

Figure: John von Neumann (December 28, 1903 - February 8, 1957)

Some references

- J. von Neumann, Metal interfaces, American Society for Metals, Cleveland 1952, pp 108-110. Soap bubble with circular arcs
- W. W. Mullins 1956, idealized grain boundaries with arbitrary shape
- H. Stone et. al. 2001, a statistical version for 3D foams
- R. D. MacPherson & D. J. Srolovitz, 3D von Neumann Law, Nature 2007

Law of Plateau

- For a dry foam, the cell boundaries can intersect only three at a time, and must do so at 120 degree.
- The 120 rule is required by the equilibrium of three equal surface tension force vectors acting at the triple junction.

Figure: Joseph Antoine Ferdinand Plateau (October 14, 1801 - September 15, 1883)

Derivation of von Neumann law

Fick's Law:

$$\begin{aligned} \frac{dV}{dt} &= -M \cdot dS \cdot (p_1 - p_2) \qquad \text{3D, } dS\text{: film area} \\ \frac{dA}{dt} &= -M \cdot dl \cdot (p_1 - p_2) \qquad \text{2D, } dl\text{: film arc-length} \\ &= -M \cdot dl \cdot \gamma \cdot \kappa \end{aligned}$$

where p_1 and p_2 are inside and outside pressure, respectively.

$$\begin{aligned} \frac{dA_n}{dt} &= -M\,\gamma \int \kappa\, dl \qquad \text{by Law of Plateau} \\ &= -M\,\gamma(2\pi - \frac{n\pi}{3}) = -2\pi\, M\,\gamma\,(1 - n/6) \end{aligned}$$

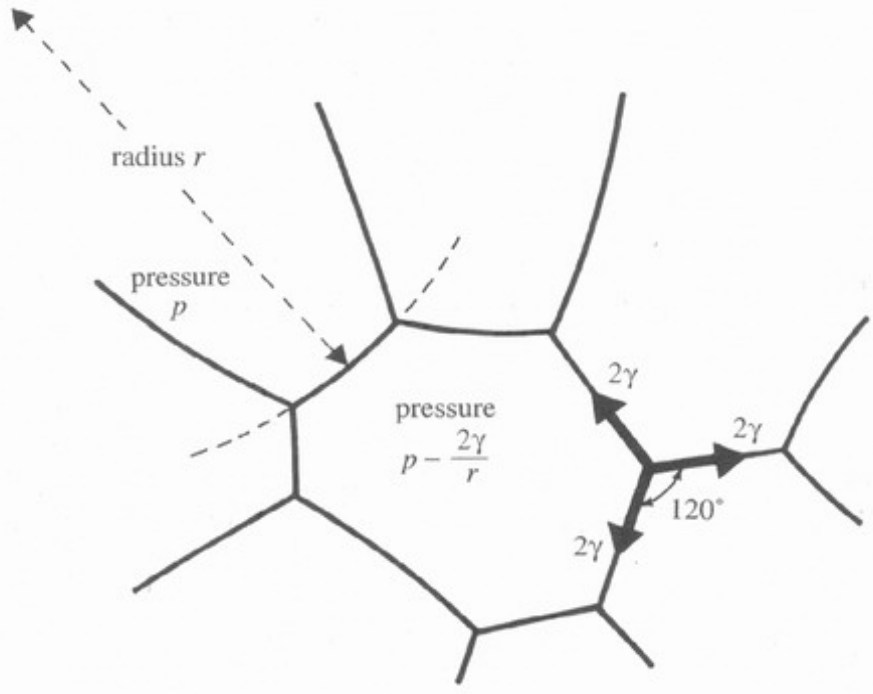


Fig. 2.3 A two-dimensional dry foam consists of circular arcs, whose curvature is consistent with the pressure difference between cells.

Foam coarsening

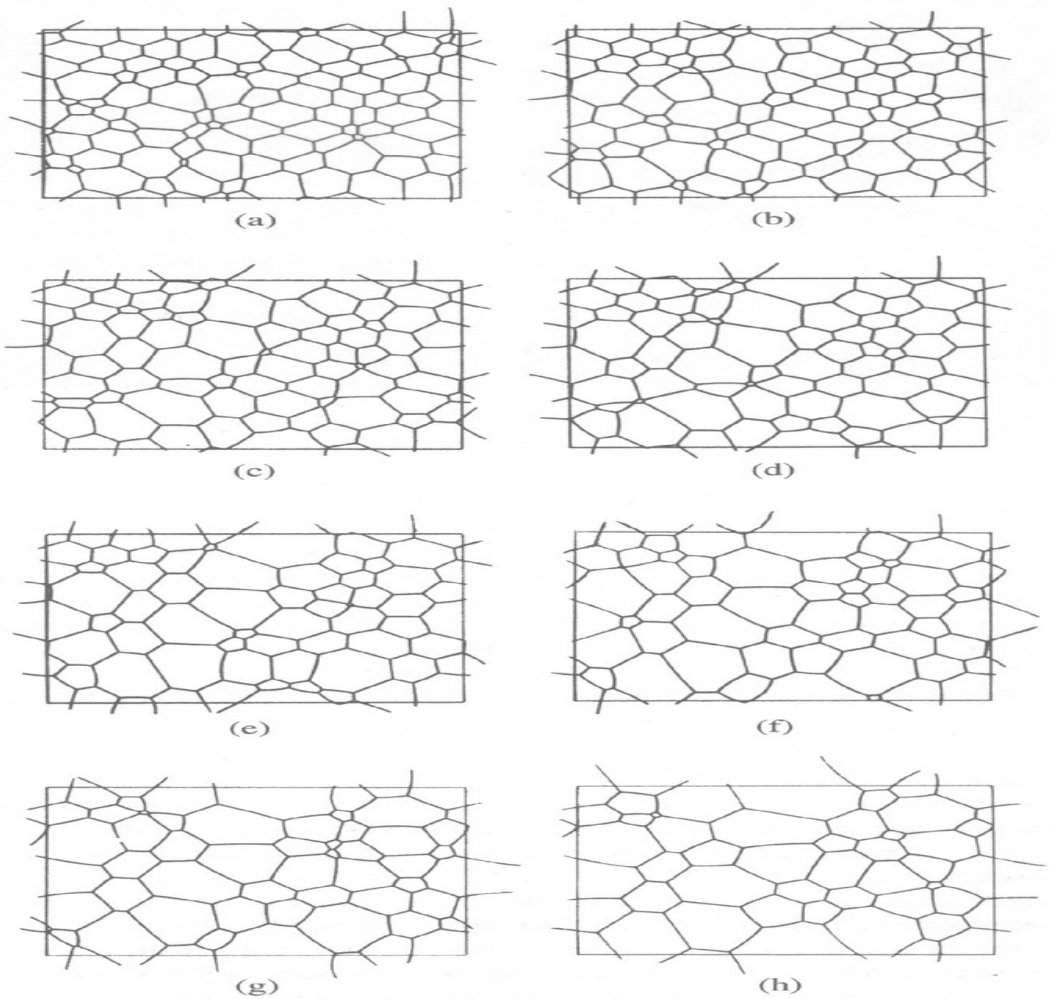


Fig. 7.1 Sequence of simulated soap cell structures (using the model of Section 6.1) at roughly equal time intervals.

Some selected numerical works

Without hydrodynamics

- T. Herdtle & H. Aref, JFM (1992), 2D dry foam
- A. M. Kraynik & D. A. Reinelt, (1999), foam microrheology
- K. A. Brakke, Surface Evolver

With hydrodynamics - Boundary Integral Method

- X. Li, H. Zhou & C. Pozrikidis, JFM (1995), 2D shearing motion of foams
- I. B. Bazhlekov, P. D. Anderson & H. E. H. Meijer, Phys. Fluids (2004), 3D shearing motion of foams

2D dry foam simulation by IB method

Basic assumptions:

- 2D dry foam
- The foam system comprises one single fluid (gas) only
- Cell boundary has zero thickness and is immersed in the fluid
- Cell boundary is permeable so the boundary is slip in the normal direction

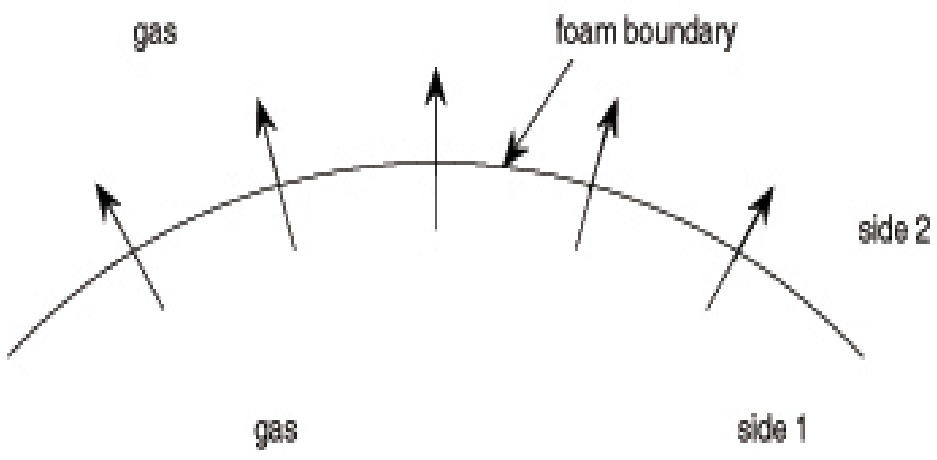


Figure: A foam boundary with permeability.

Equations of motion

$$\rho(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u}) = -\nabla p + \mu \nabla^2 \mathbf{u} + \mathbf{f},$$

$$\nabla \cdot \mathbf{u} = 0,$$

$$\mathbf{f}(\mathbf{x}, t) = \int \mathbf{F}(s, t) \delta(\mathbf{x} - \mathbf{X}(s, t)) ds,$$

$$\mathbf{F}(s, t) = \frac{\partial}{\partial s}(\gamma \boldsymbol{\tau}) = \gamma \frac{\partial \boldsymbol{\tau}}{\partial s}$$

$$\begin{aligned} \frac{\partial \mathbf{X}}{\partial t}(s, t) &= \mathbf{U}(s, t) + M \mathbf{F} / \left| \frac{\partial \mathbf{X}}{\partial s} \right|, \\ &= \int \mathbf{u}(\mathbf{x}, t) \delta(\mathbf{x} - \mathbf{X}(s, t)) d\mathbf{x} + M \mathbf{F} / \left| \frac{\partial \mathbf{X}}{\partial s} \right|, \end{aligned}$$

$$\boldsymbol{\tau}(s, t) = \frac{\partial \mathbf{X}}{\partial s} / \left| \frac{\partial \mathbf{X}}{\partial s} \right|$$

M: permeability $\qquad$ γ: surface tension

Foam boundary equation

Consider a patch of the foam boundary of length $|\frac{\partial \mathbf{X}}{\partial s}|ds$. The flux through this patch is

$$M\,(p_1 - p_2)\left|\frac{\partial \mathbf{X}}{\partial s}\right| ds = (\mathbf{U}(s,t) - \frac{\partial \mathbf{X}}{\partial t}(s,t)) \cdot \mathbf{n} \left|\frac{\partial \mathbf{X}}{\partial s}\right| ds,$$

$$M(p_1 - p_2) = (\mathbf{U}(s,t) - \frac{\partial \mathbf{X}}{\partial t}(s,t)) \cdot \mathbf{n}.$$

Since the pressure jump $p_1 - p_2 = \gamma\kappa$ (Laplace-Young condition) can be related to the normal component of the boundary force $\mathbf{F}(s,t)$ as

$$(p_1 - p_2)\left|\frac{\partial \mathbf{X}}{\partial s}\right| + \mathbf{F} \cdot \mathbf{n} = 0.$$

$$\left(\frac{\partial \mathbf{X}}{\partial t}(s,t) - \mathbf{U}(s,t)\right) \cdot \mathbf{n} = M\,\mathbf{F} \cdot \mathbf{n} / \left|\frac{\partial \mathbf{X}}{\partial s}\right|.$$

$$\left(\frac{\partial \mathbf{X}(s,t)}{\partial t} - \mathbf{U}(s,t)\right) \cdot \boldsymbol{\tau} = 0.$$

Time integration: $\boldsymbol{X}_k^n, \boldsymbol{u}^n$ are given

Step 1: Compute the boundary force $\mathbf{F}(s,t) = \gamma \frac{\partial \boldsymbol{\tau}}{\partial s}$

$$\mathbf{F}_k^n = \frac{\gamma}{\Delta s}\left(\frac{\mathbf{X}_{k+1}^n - \mathbf{X}_k^n}{|\mathbf{X}_{k+1}^n - \mathbf{X}_k^n|} - \frac{\mathbf{X}_k^n - \mathbf{X}_{k-1}^n}{|\mathbf{X}_k^n - \mathbf{X}_{k-1}^n|}\right)$$

Step 2: Distribute the boundary force into the fluids

$$\mathbf{f}^n(\mathbf{x}) = \sum_k \mathbf{F}_k^n \delta_h(\mathbf{x} - \mathbf{X}_k^n)\Delta s,$$

$$\delta_h(\mathbf{x}) = h^{-2}\phi(\frac{x_1}{h})\phi(\frac{x_2}{h}),$$

$$\phi(r) = \begin{cases} \frac{3-2|r|+\sqrt{1+4|r|-4r^2}}{8} & , \quad \text{if} \quad |r| \leq 1 \\ \frac{5-2|r|-\sqrt{-7+12|r|-4r^2}}{8} & , \quad \text{if} \quad 1 \leq |r| \leq 2 \\ 0 & , \quad \text{if} \quad 2 \leq |r|. \end{cases}$$

Step 3: Solve the Navier-Stokes equations

$$\rho\Big(\frac{\mathbf{u}^{n+1}-\mathbf{u}^n}{\Delta t}+\frac{1}{2}\sum_{i=1,2}\left(u_i D_i^0\mathbf{u}+D_i^0(u_i\mathbf{u})\right)^n\Big)+\mathbf{D}^0 p^{n+1}=\mu\,\Delta_h\mathbf{u}^{n+1}+\mathbf{f}^n,$$

$$\mathbf{D}^0\cdot\mathbf{u}^{n+1}=0$$

Step 4: Move the foam boundary

$$\frac{\mathbf{X}_k^{n+1}-\mathbf{X}_k^n}{\Delta t}=\sum_{\mathbf{x}}\mathbf{u}^{n+1}(\mathbf{x})\delta_h(\mathbf{x}-\mathbf{X}_k^n)h^2+\frac{M\,\mathbf{F}_k^n\,\Delta s}{(|\mathbf{X}_{k+1}^n-\mathbf{X}_k^n|+|\mathbf{X}_k^n-\mathbf{X}_{k-1}^n|)/2},$$

Some implementation details

- No permeability at the junctions. That is, the junctions move at the local fluid velocity.
- The maintenance of foam boundary point resolution.

Numerical results

Problem setup

- $[0,1] \times [0,1]$ fluid domain
- Fluid density $\rho = 1$, viscosity $\mu = 0.001$, surface tension $\gamma = 2$
- No slip boundary condition on the computational domain
- The mesh width $h = \Delta x = \Delta y = 1/256$, and the time step $\Delta t = 2.5 \times 10^{-6}$
- Choose different permeability constant $M = 0, \quad 0.025, \quad 0.05$ to make comparisons

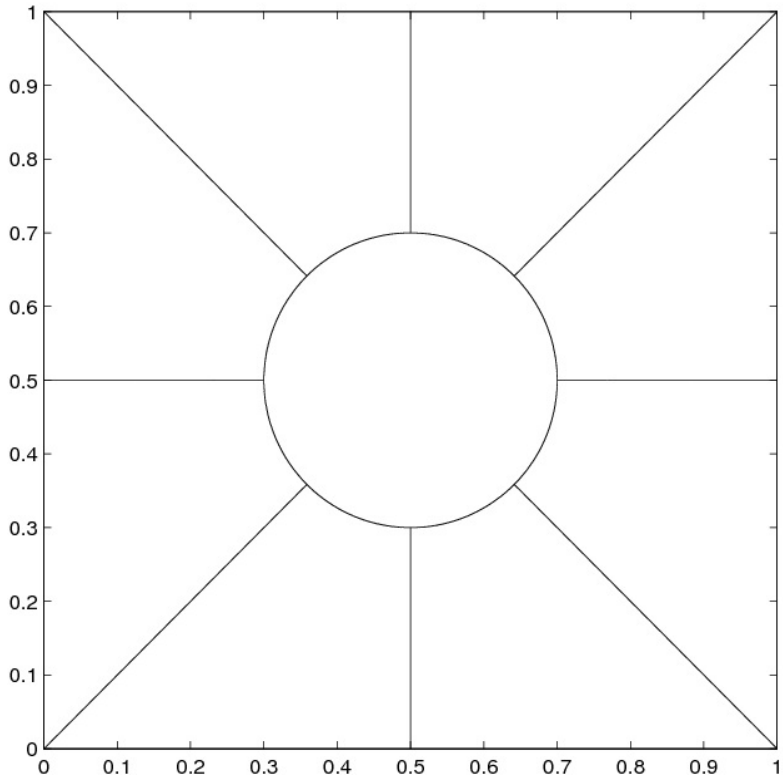


Figure: Initially, a single n-edged circular cell with radius 0.2 and n straight lines connect to the domain boundary.

Check of von Neumann law

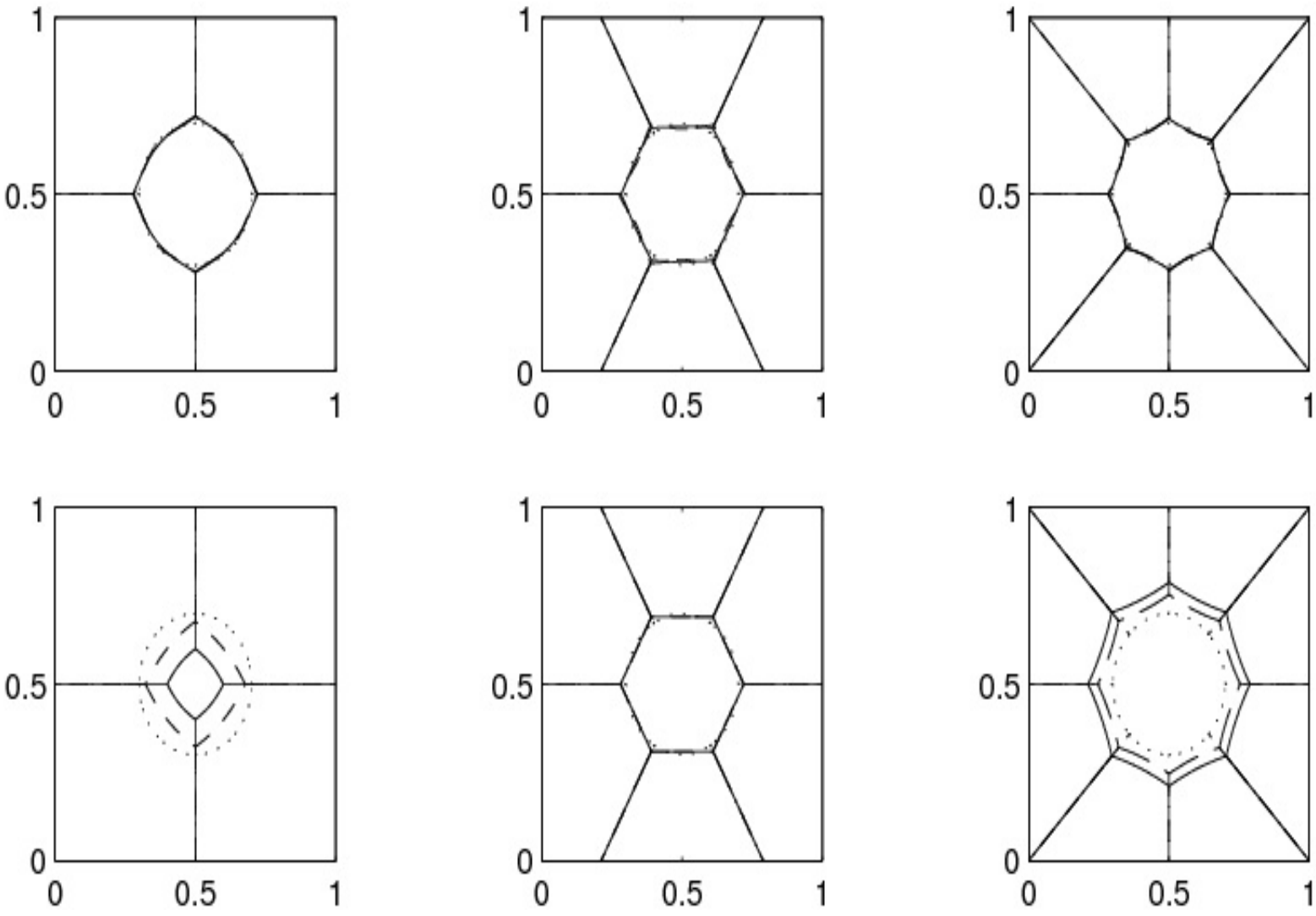


Figure: Motion of the foam boundaries. The permeability is $M = 0$ in the upper panels and $M = 0.05$ in the lower panels.

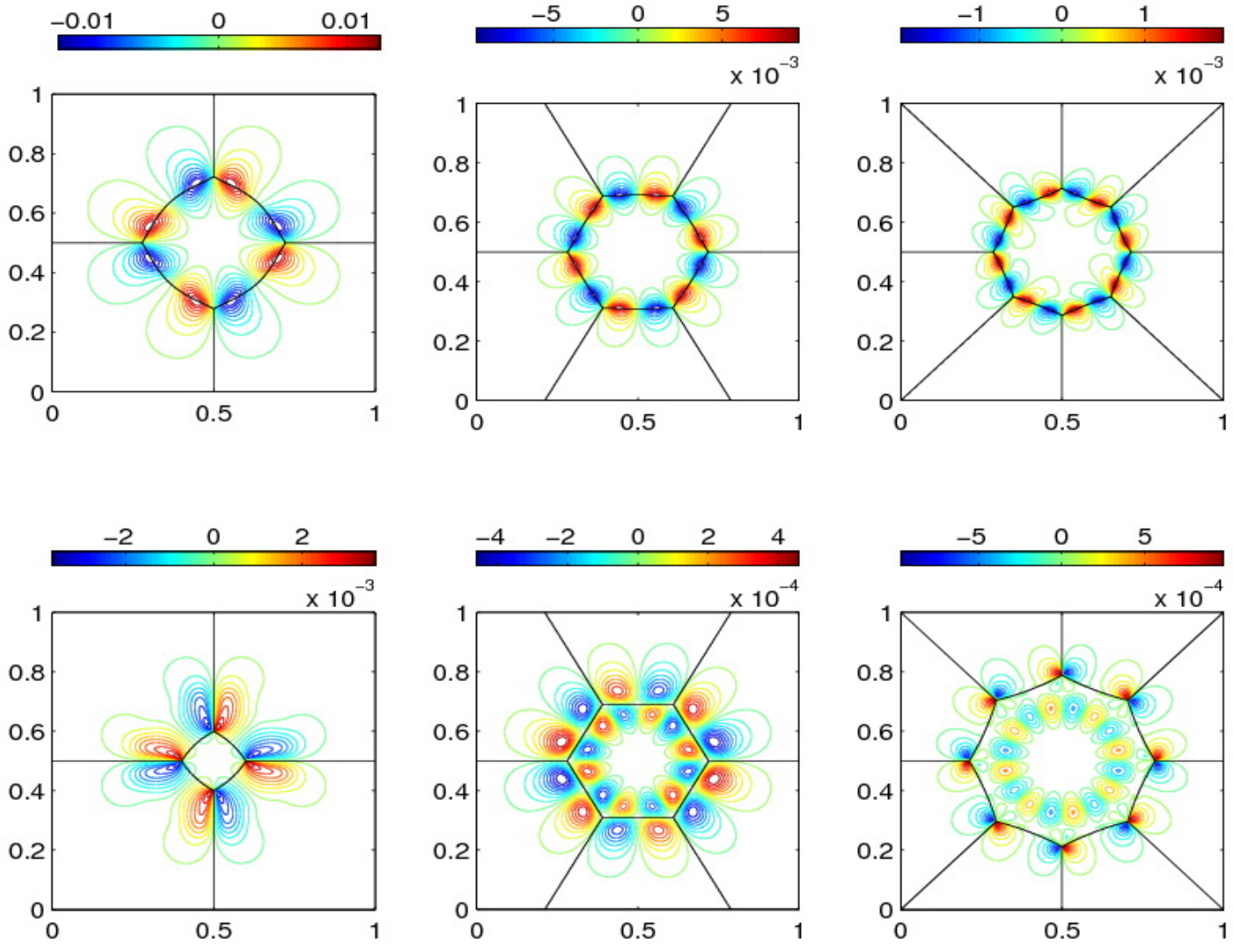


Figure: Streamlines of the velocity fields at time $t = 0.5$.

Check of area rate

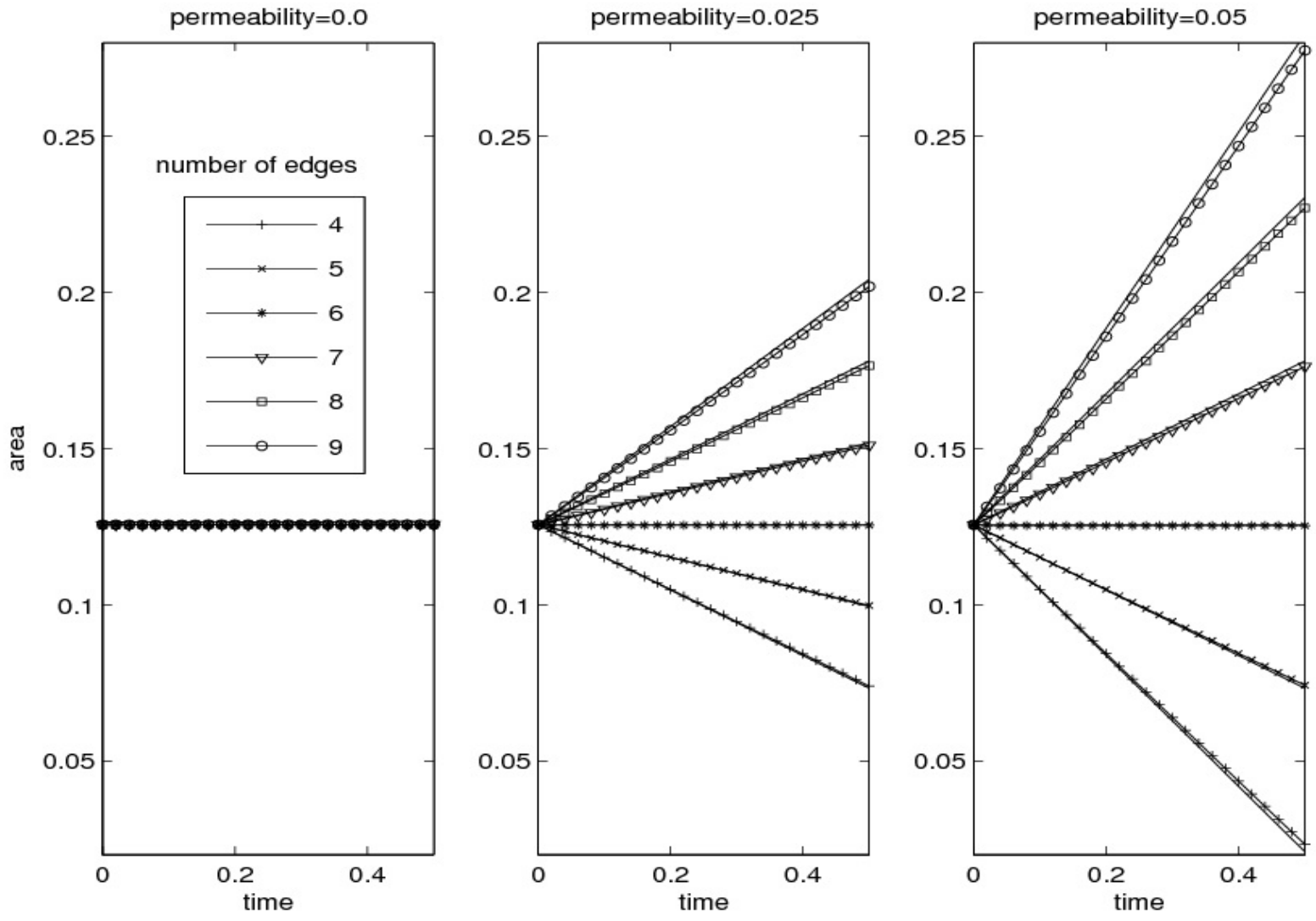


Figure: Area vs. Time for different n.

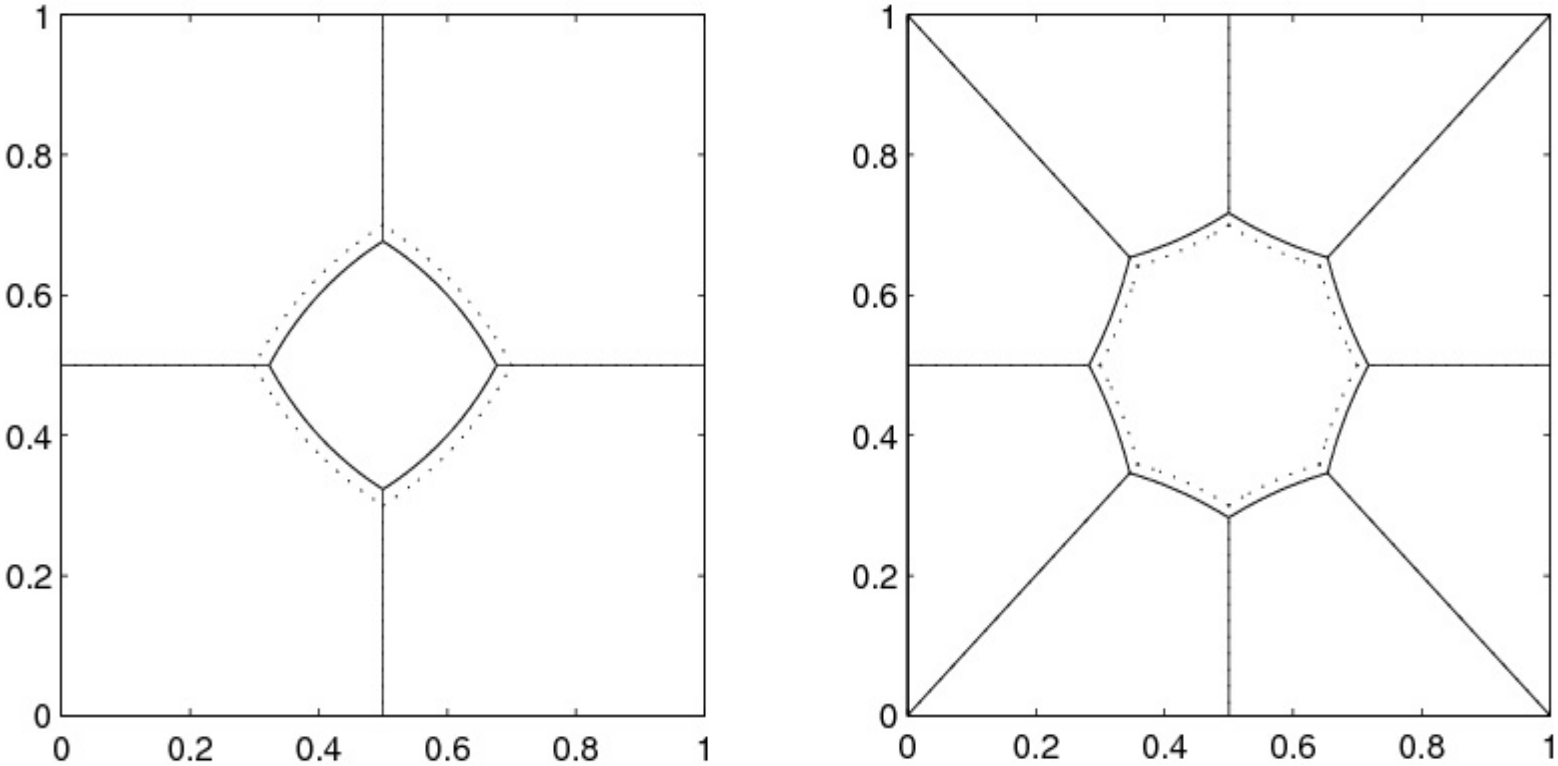


Figure: Foam boundary of 4-edged (left) and 8-edged (right) inner cells. The times are $t = 0$ (dotted line) and $t = 0.1$ (solid line).

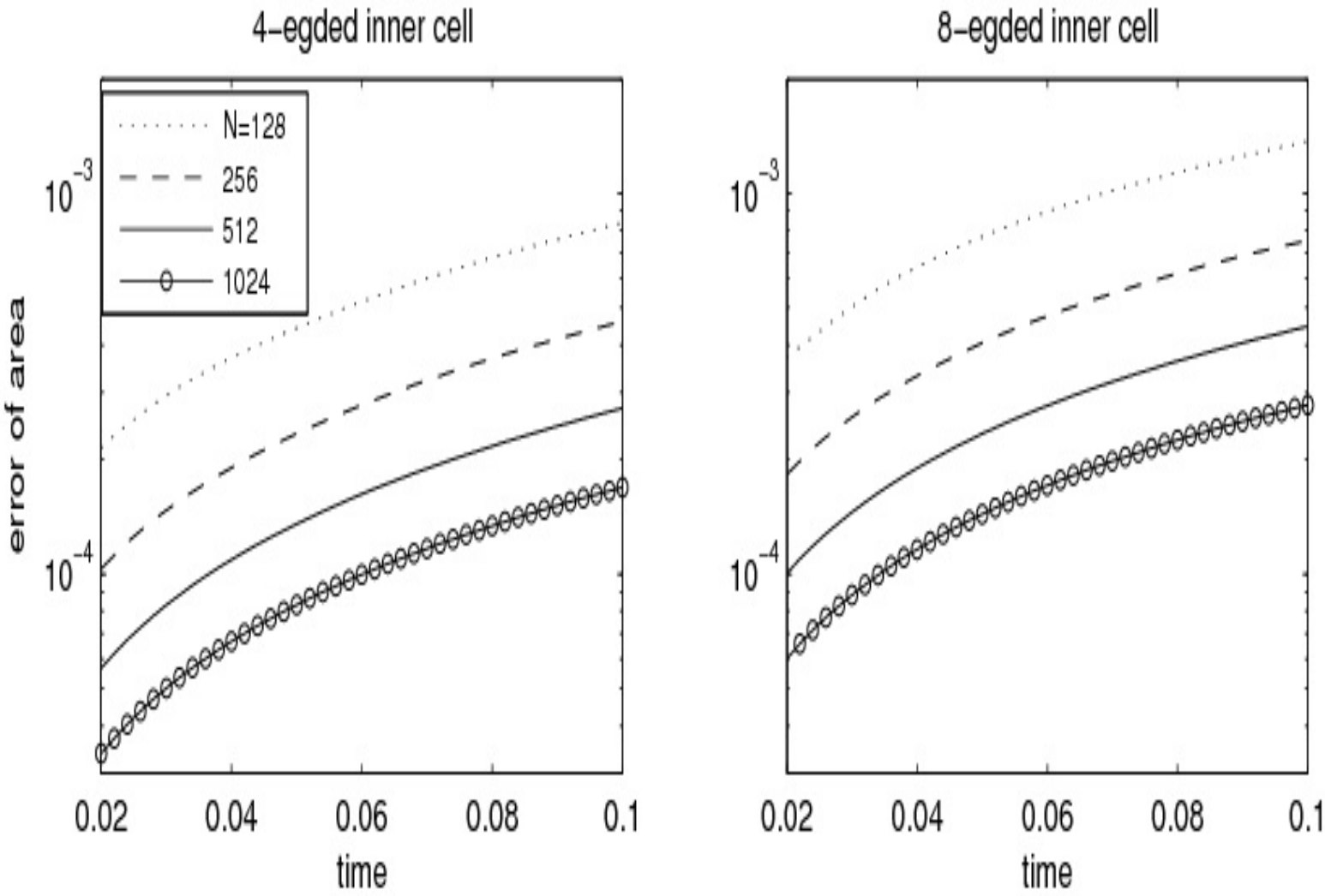


Figure: The errors of area in comparison to that predicted by the von Neumann relation are plotted as functions of time on a logarithmic vertical scale for each of the cases N=128, 256, 512, and 1024.

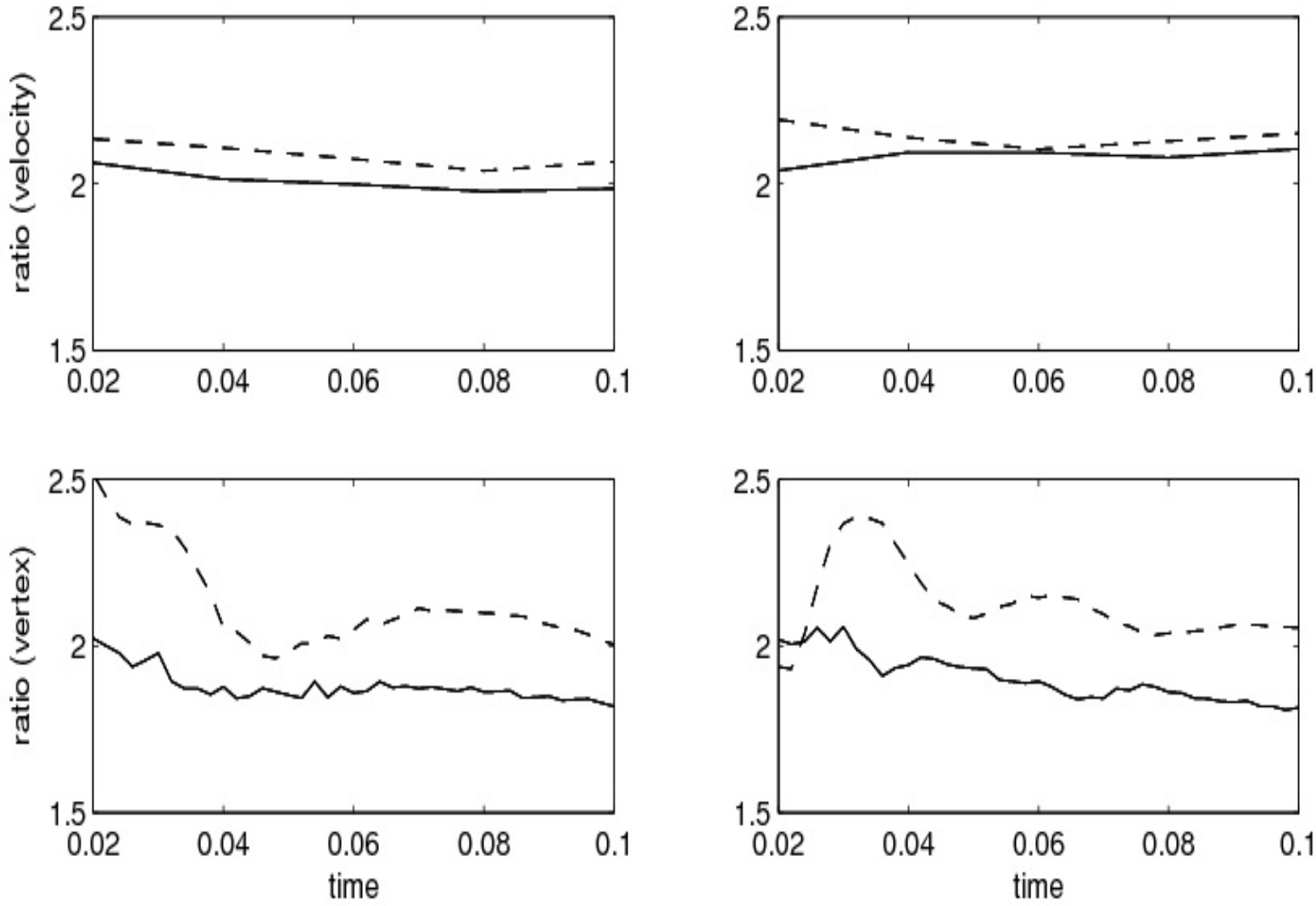
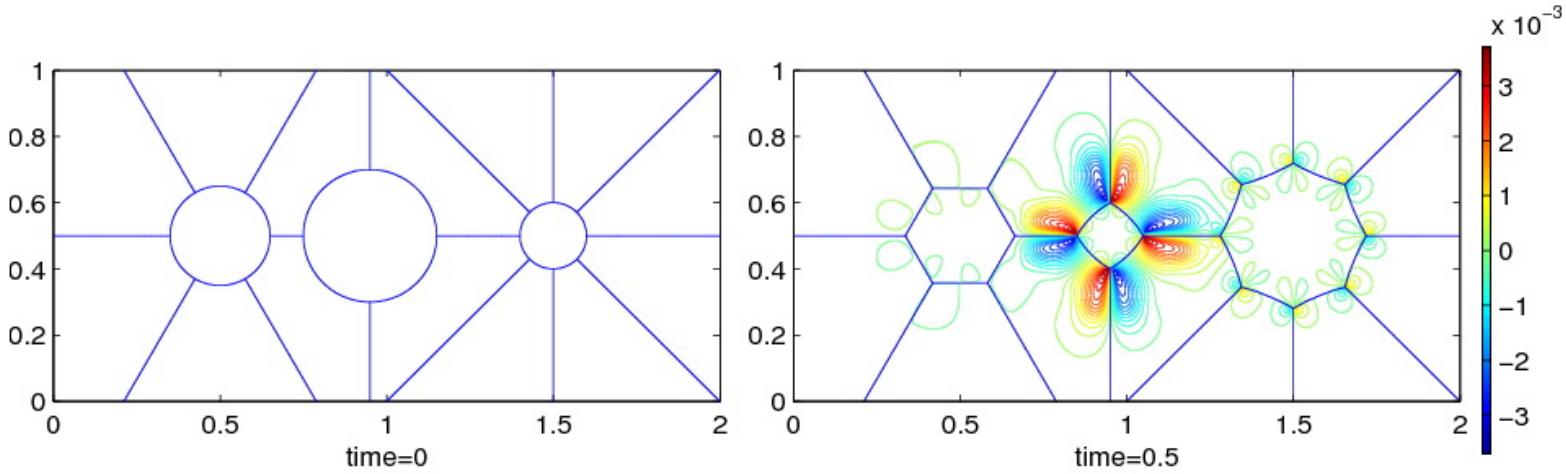
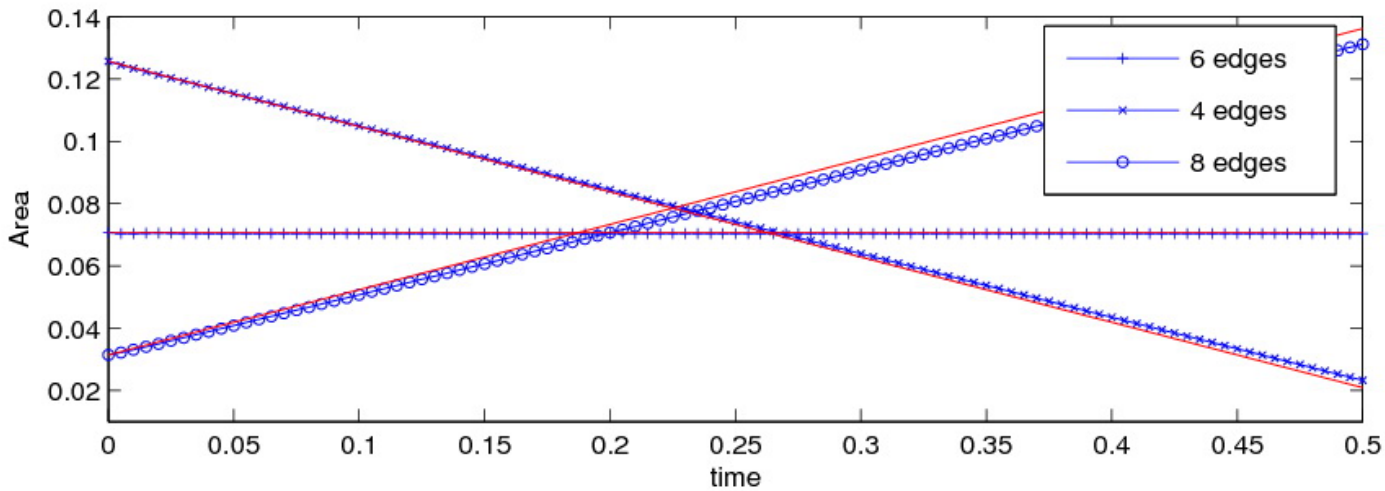


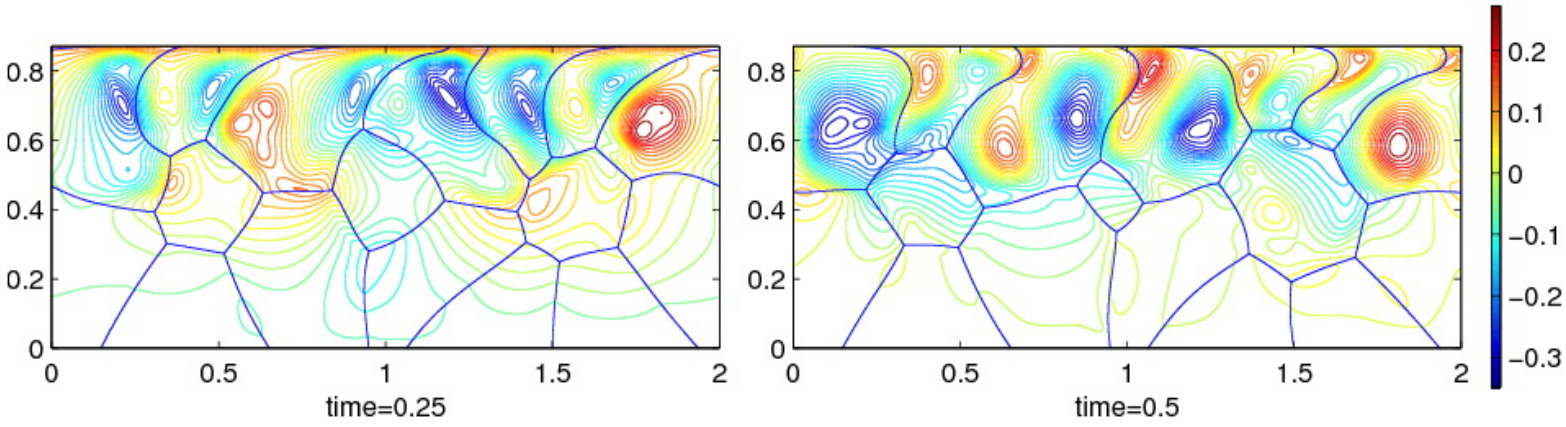
Figure: Convergence ratios of the computed velocity field $\mathbf{u}(\mathbf{x}, t)$ of the fluid (top) and the position (x_N^i, y_N^i) of vertices (bottom).

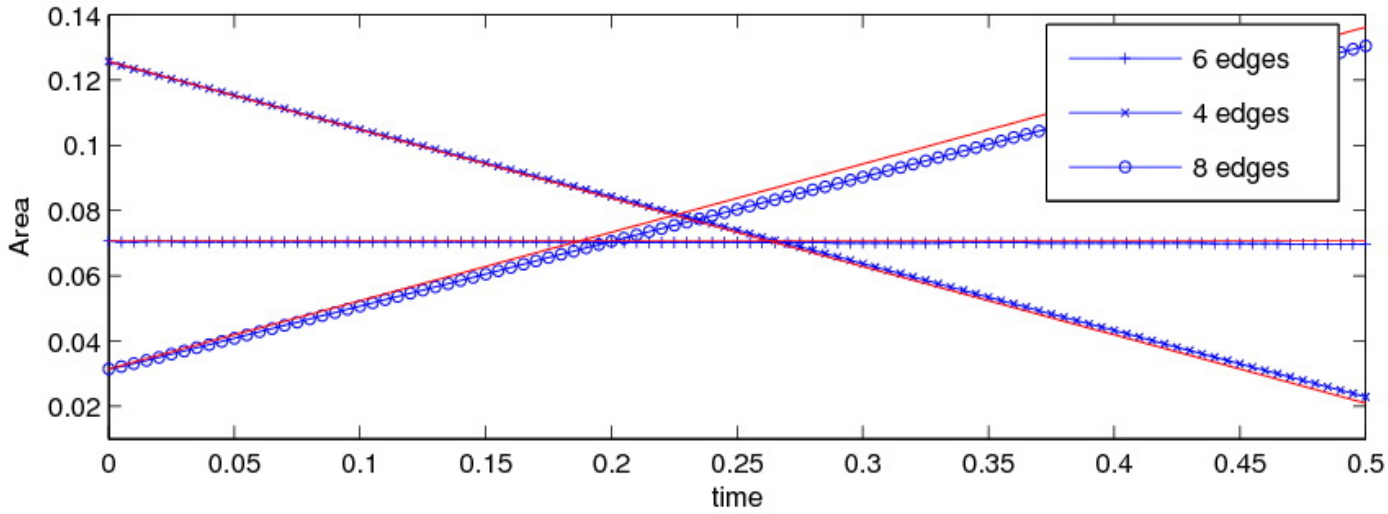
Foam with multiple inner cells



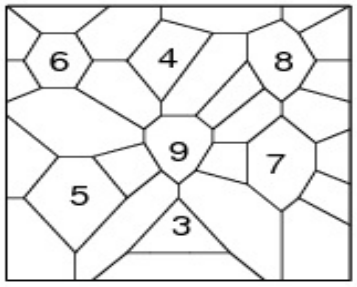


Foam with multiple inner cells under an oscillatory shear motion





Foam coarsening: surface energy minimization



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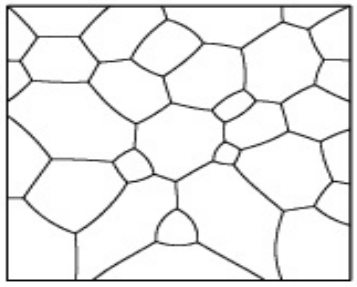
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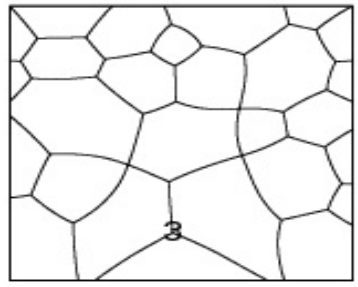

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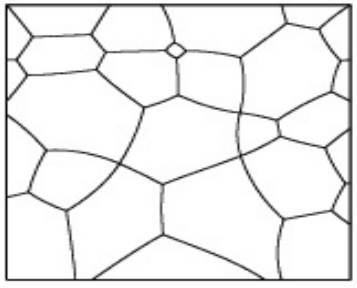
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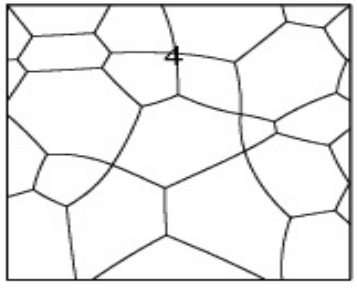

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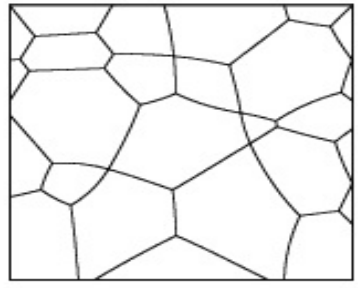
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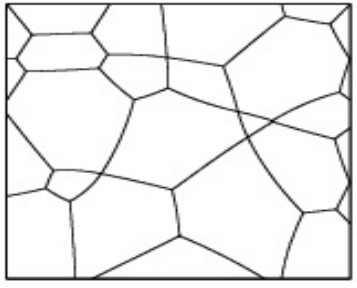
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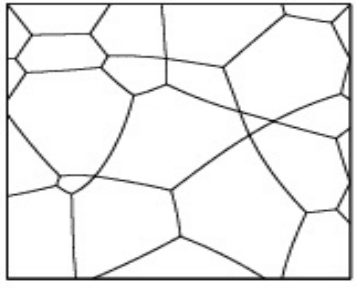
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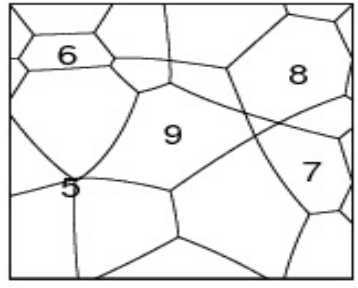

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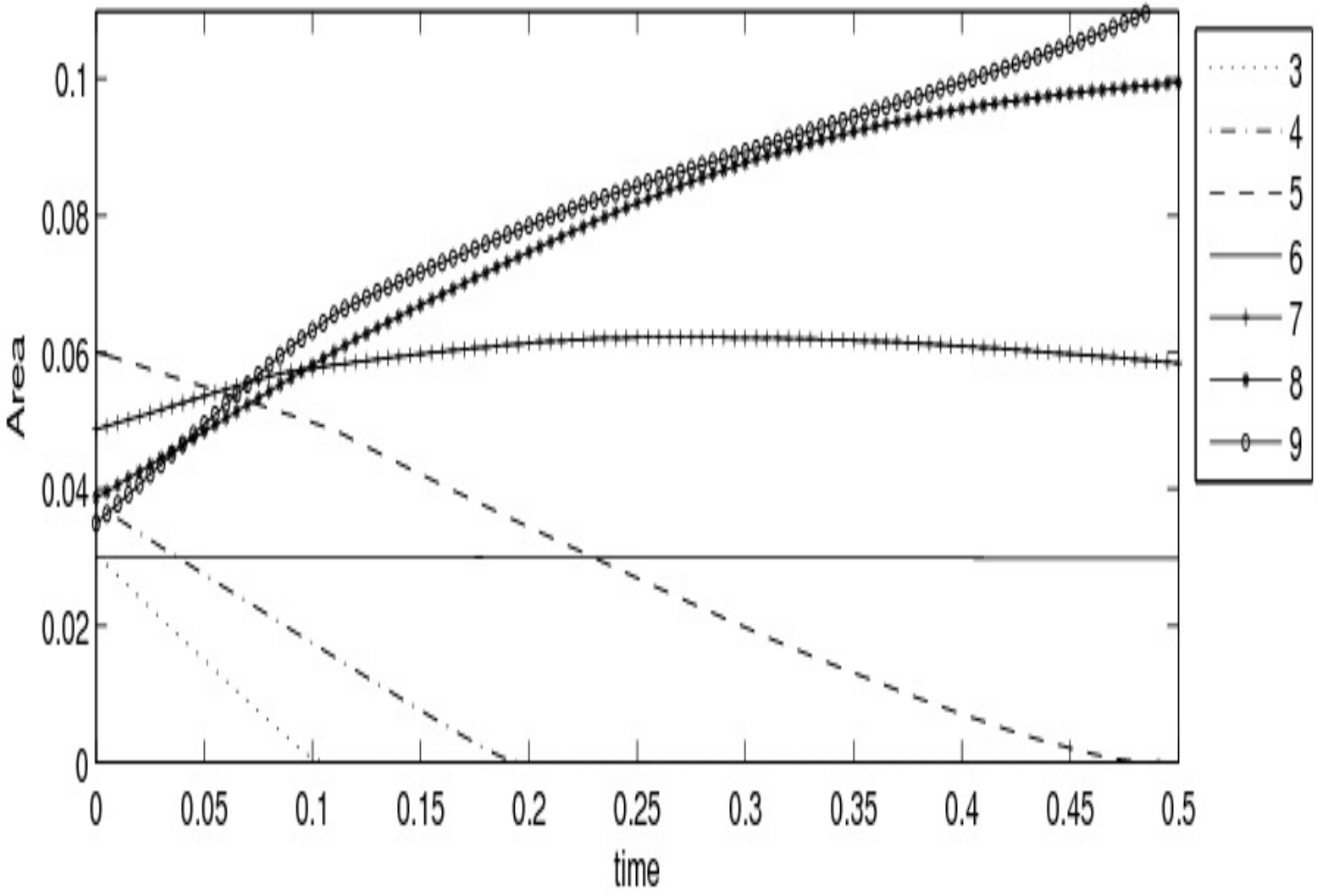
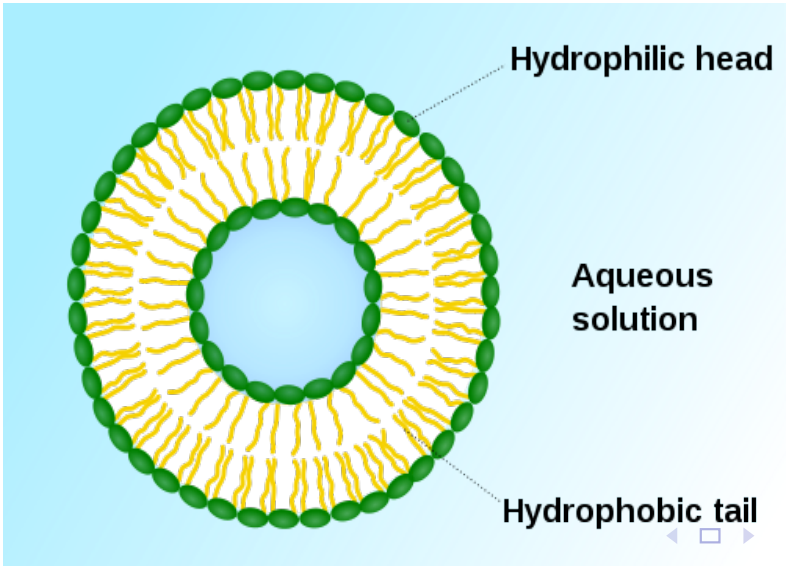


Figure: Area change for different cells

Dynamics of Inextensible vesicles

Some physics

- Vesicle can be visualized as a bubble of liquid within another liquid with a closed lipid membrane suspended in aqueous solution, size is about $10\mu m$
- Lipid membrane consists of tightly packed lipid molecules with hydrophilic heads facing the exterior and interior fluids and hydrophobic tails hiding in the middle, thickness is about $6nm$
- Cell membrane (or vesicle boundary) can deform but resist area dilation, that is inextensible or incompressible



Applications: Vesicles in shear flows

- Dynamical behavior of red blood cells, drug carrying capsules
- To understand rheological properties of vesicle solution flow

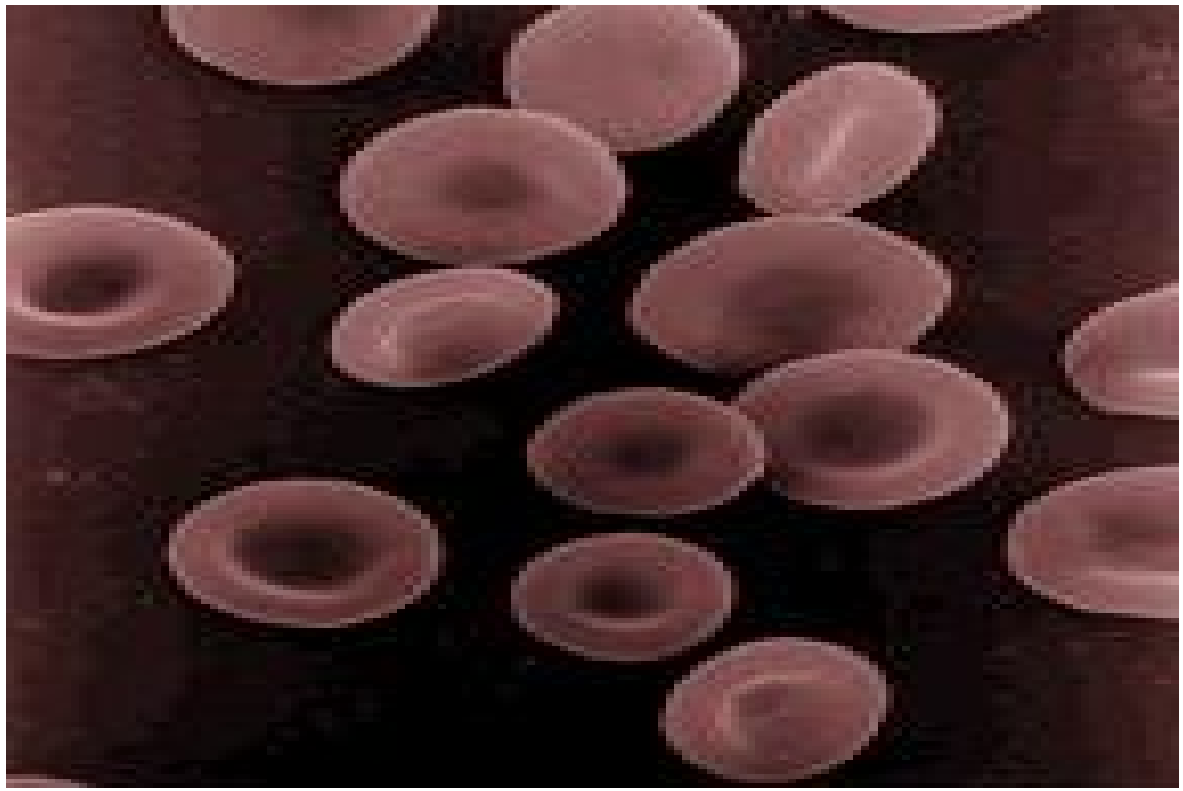


Figure: Red blood cells: flexible biconcave disks

Selected numerical works on inextensible vesicles with hydrodynamics

Numerical difficulties

- Coupled with fluid dynamics which vesicle boundary is moving with fluid and whose shape is not known *a priori*
- Both the volume and the surface area of the vesicle are conserved. How to maintain fluid and vesicle boundary incompressible simultaneously?

Boundary integral method

- Zhu & Pozrikidis 1995, incompressible interface without bending
- Kraus, Wintz, Seifert & Lipowsky 1996, incompressible interface with bending
- Veerapaneni, Gueyffier, Zorin & Biros 2009, 2D and 3D axisymmetric efficient solvers
- Sohn, Tseng, Li, Voigt & Lowengrub 2010, multi-component vesicles
- Others

Immersed boundary (IB) and immersed interface (IIM) methods

- Kim & Lai 2010, pIB for inextensible vesicles in Navier-Stokes flow, JCP 229 (2010), 4840-4853.
- Li & Lai 2010, IIM for inextensible interfaces in Navier-Stokes flow, preprint
- Tan, Le, Lim & Khoo 2010, IIM for inextensible interfaces in Stokes flow, preprint

Inextensible boundary with hydrodynamics

$$\rho(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u}) = -\nabla p + \mu \nabla^2 \mathbf{u} + \mathbf{f},$$

$$\nabla \cdot \mathbf{u} = 0,$$

$$\mathbf{f}(\mathbf{x}, t) = \int_\Gamma \mathbf{F}(s, t) \delta(\mathbf{x} - \mathbf{X}(s, t)) ds,$$

$$\mathbf{F}(s, t) = \frac{\partial}{\partial s}(\sigma(s, t)\, \boldsymbol{\tau}(s, t)) - \frac{\partial^2}{\partial s^2}\left(c_b \frac{\partial^2 \mathbf{X}(s, t)}{\partial s^2}\right)$$

$$\frac{\partial \mathbf{X}}{\partial t}(s, t) = \mathbf{U}(s, t) = \int \mathbf{u}(\mathbf{x}, t) \delta(\mathbf{x} - \mathbf{X}(s, t)) d\mathbf{x}$$

$$\boldsymbol{\tau}(s, t) = \frac{\partial \mathbf{X}}{\partial s} / \left| \frac{\partial \mathbf{X}}{\partial s} \right|$$

$$\frac{\partial \mathbf{U}}{\partial s} \cdot \frac{\partial \mathbf{X}}{\partial s} = 0 \quad \text{inextensibility on } \Gamma$$

Extra difficulty: $\sigma(s, t)$ is unknown and can be viewed as a Lagrange's multiplier that enforces the local inextensible constraint

Derivation of the forcing terms

Vesicle membrane energy:

$$E = E_e + E_b = \int_\Gamma \sigma \, ds + \int_\Gamma \frac{c_b}{2} \left| \frac{\partial^2 \mathbf{X}}{\partial s^2} \right|^2 ds$$

c_b is the bending rigidity, σ is the unknown tension
By taking the variational derivative, we have

$$\begin{aligned} \mathbf{F} &= \mathbf{F}_e + \mathbf{F}_b = -\left(\frac{\delta E_e}{\delta \mathbf{X}} + \frac{\delta E_b}{\delta \mathbf{X}} \right) \\ &= \frac{\partial}{\partial s}(\sigma(s,t)\,\boldsymbol{\tau}(s,t)) - \frac{\partial^2}{\partial s^2}\left(c_b \frac{\partial^2 \mathbf{X}(s,t)}{\partial s^2} \right) \end{aligned}$$

Inextensible constraint $\nabla_s \cdot \boldsymbol{u} = 0$

Local stretching factor of the vesicle is $\left|\frac{\partial \mathbf{X}}{\partial s}\right|$. The rate of the stretching factor is

$$\begin{aligned}
\frac{\partial}{\partial t}\left|\frac{\partial \mathbf{X}}{\partial s}\right| &= \frac{\frac{\partial X}{\partial s}\frac{\partial}{\partial s}\left(\frac{\partial X}{\partial t}\right)+\frac{\partial Y}{\partial s}\frac{\partial}{\partial s}\left(\frac{\partial Y}{\partial t}\right)}{\left|\frac{\partial \mathbf{X}}{\partial s}\right|} = \frac{\frac{\partial X}{\partial s}\frac{\partial U}{\partial s}+\frac{\partial Y}{\partial s}\frac{\partial V}{\partial s}}{\left|\frac{\partial \mathbf{X}}{\partial s}\right|} \\
&= \frac{\frac{\partial X}{\partial s}\left(\nabla u \cdot \frac{\partial \mathbf{X}}{\partial s}\right)+\frac{\partial Y}{\partial s}\left(\nabla v \cdot \frac{\partial \mathbf{X}}{\partial s}\right)}{\left|\frac{\partial \mathbf{X}}{\partial s}\right|} = \left(\frac{\partial \mathbf{u}}{\partial \boldsymbol{\tau}} \cdot \boldsymbol{\tau}\right)\left|\frac{\partial \mathbf{X}}{\partial s}\right| \\
&= (\nabla_s \cdot \boldsymbol{u})\left|\frac{\partial \mathbf{X}}{\partial s}\right|
\end{aligned}$$

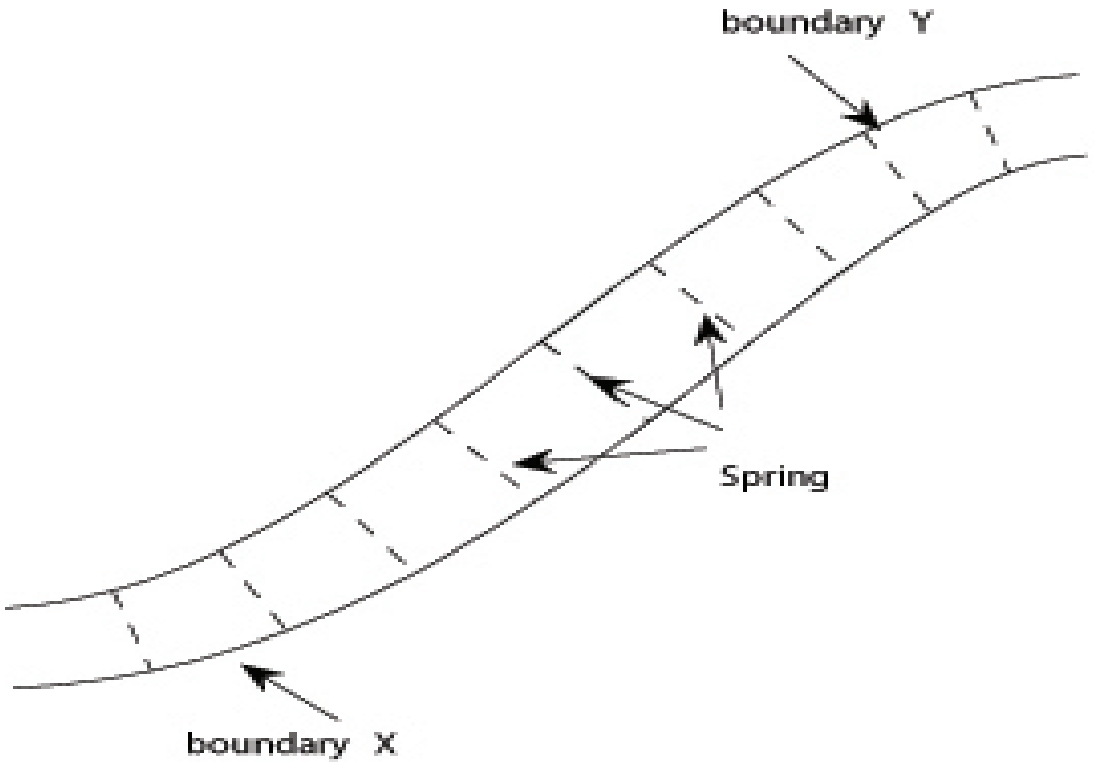
Since the vesicle is inextensible, we have $\frac{\partial}{\partial t}\left|\frac{\partial \mathbf{X}}{\partial s}\right| = 0$. Thus, we have

$$\frac{\partial \mathbf{U}}{\partial s} \cdot \frac{\partial \mathbf{X}}{\partial s} = 0$$

Penalty IB method

Idea: Try to decouple the fluid and vesicle computations by introducing a dual representation of the immersed boundary.

- $\boldsymbol{X}(s,t)$ interacts with the fluid and moves at the local fluid velocity, just as traditional IB
- $\boldsymbol{Y}(s,t)$ is linked to $\boldsymbol{X}$ by a system of stiff springs, and is not coupled directly to the fluid. The inextensibility is mainly enforced on $\boldsymbol{Y}$.



Previous idea similar to pIB

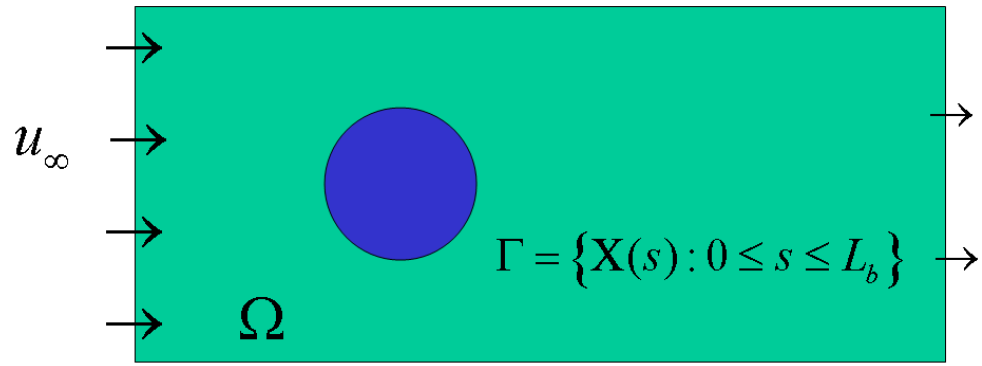


Figure: To introduce an unknown force $\boldsymbol{F}(s,t)$ along the cylinder surface so that the no-slip boundary condition $\boldsymbol{U}(s,t) = 0$ is satisfied.

- Virtual boundary method: Goldstein, Handler & Sirovich, 1993; Saiki & Biringen, 1996
- Feedback forcing approach: Lai & Peskin, 2000

Reformulate the equations

$$\rho(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u}) = -\nabla p + \mu \nabla^2 \mathbf{u} + \mathbf{f},$$

$$\nabla \cdot \mathbf{u} = 0,$$

$$\mathbf{f}(\mathbf{x}, t) = \int_\Gamma \mathbf{F}(s, t) \delta(\mathbf{x} - \mathbf{X}(s, t)) ds,$$

$$\mathbf{F} = K(\mathbf{Y}(s, t) - \mathbf{X}(s, t)) + R(\mathbf{V}(s, t) - \mathbf{U}(s, t)),$$

$$K(\mathbf{Y}(s,t)-\mathbf{X}(s,t))+R(\mathbf{V}(s,t)-\mathbf{U}(s,t)) = \frac{\partial}{\partial s}(\sigma(s,t)\,\boldsymbol{\tau}(s,t))-c_b\frac{\partial^4 \mathbf{Y}(s,t)}{\partial s^4},$$

$$\boldsymbol{\tau}(s, t) = \frac{\partial \mathbf{Y}}{\partial s} / \left| \frac{\partial \mathbf{Y}}{\partial s} \right|,$$

$$\frac{\partial \mathbf{V}}{\partial s} \cdot \frac{\partial \mathbf{Y}}{\partial s} = 0,$$

where $\mathbf{U} = \partial \mathbf{X}/\partial t$ and $\mathbf{V} = \partial \mathbf{Y}/\partial t$.

Numerical algorithm

Fluid part involving the immersed boundary $\boldsymbol{X}$

$$\mathbf{F}^n(s) = K(\mathbf{Y}^n(s) - \mathbf{X}^n(s)) + R(\mathbf{V}^n(s) - \mathbf{U}^n(s)),$$

$$\mathbf{f}^n(\mathbf{x}) = \sum_s \mathbf{F}^n(s)\delta_h(\mathbf{x} - \mathbf{X}^n(s))\Delta s,$$

$$\rho\Big(\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} + \frac{1}{2}\sum_{i=1,2}(u_i D_i^0 \mathbf{u} + D_i^0(u_i\mathbf{u}))^n\Big) + \mathbf{D}p^{n+1} = \mu L\mathbf{u}^{n+1} + \mathbf{f}^n,$$

$$\mathbf{D}\cdot\mathbf{u}^{n+1} = 0,$$

$$\mathbf{U}^{n+1}(s) = \sum_{\mathbf{x}} \mathbf{u}^{n+1}(\mathbf{x})\delta_h(\mathbf{x} - \mathbf{X}^n(s))h^2,$$

$$\mathbf{X}^{n+1}(s) = \mathbf{X}^n(s) + \Delta t\mathbf{U}^{n+1}(s)$$

Vesicle part involving the immersed boundary $\boldsymbol{Y}$

$$\tilde{\mathbf{Y}}^{n+1}(s) = \mathbf{Y}^{n}(s) + \frac{\Delta t}{2}\mathbf{V}^{n}(s), \qquad \tilde{\boldsymbol{\tau}}^{n+1}(s) = \frac{\partial \tilde{\mathbf{Y}}^{n+1}/\partial s}{|\partial \tilde{\mathbf{Y}}^{n+1}/\partial s|}$$

$$K(\mathbf{Y}^{n}(s) - \mathbf{X}^{n}(s)) + R(\mathbf{V}^{n+1}(s) - \mathbf{U}^{n+1}(s)) = \frac{\partial}{\partial s}(\tilde{\sigma}^{n+1}\tilde{\boldsymbol{\tau}}^{n+1}) - c_b \frac{\partial^4 \mathbf{Y}^{n}(s)}{\partial s^4}$$

$$\frac{\partial \mathbf{V}^{n+1}}{\partial s} \cdot \frac{\partial \tilde{\mathbf{Y}}^{n+1}}{\partial s} = 0$$

$$\mathbf{Y}^{n+1}(s) = \mathbf{Y}^{n}(s) + \Delta t \mathbf{V}^{n+1}(s).$$

Compute the unknown tension

$$\tilde{\mathbf{F}}^n = K(\mathbf{Y}^n - \mathbf{X}^n) - R\mathbf{U}^{n+1} + c_b \frac{\partial^4 \mathbf{Y}^n}{\partial s^4},$$

$$\frac{\partial}{\partial s}(\tilde{\sigma}^{n+1}\,\tilde{\boldsymbol{\tau}}^{n+1}) = R\mathbf{V}^{n+1} + \tilde{\mathbf{F}}^n.$$

$$\frac{\partial^2}{\partial s^2}(\tilde{\sigma}^{n+1}\,\tilde{\boldsymbol{\tau}}^{n+1}) \cdot \tilde{\boldsymbol{\tau}}^{n+1} = (R\frac{\partial \mathbf{V}^{n+1}}{\partial s} + \frac{\partial \tilde{\mathbf{F}}^n}{\partial s}) \cdot \tilde{\boldsymbol{\tau}}^{n+1}.$$

$$\frac{\partial^2}{\partial s^2}(\tilde{\sigma}^{n+1}\,\tilde{\boldsymbol{\tau}}^{n+1}) \cdot \tilde{\boldsymbol{\tau}}^{n+1} = \frac{\partial \tilde{\mathbf{F}}^n}{\partial s} \cdot \tilde{\boldsymbol{\tau}}^{n+1}.$$

More precisely, a modified Helmholtz equation must be solved to obtain σ.

Single vesicle in a shear flow

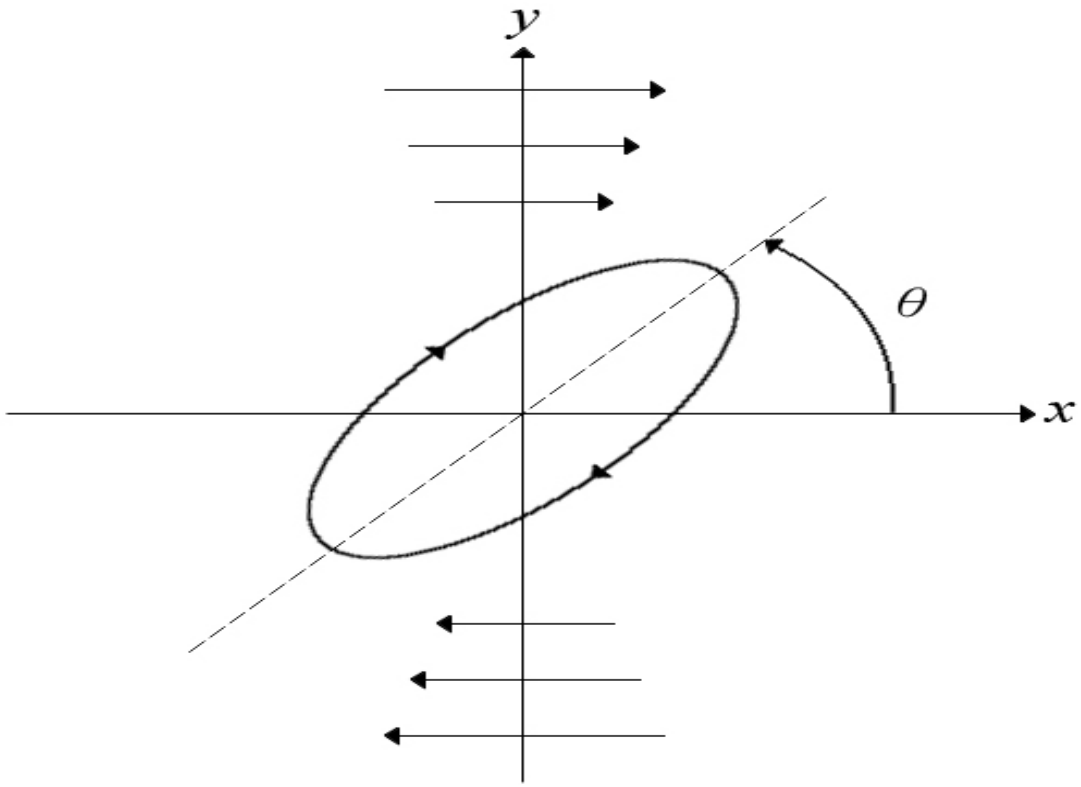


Figure: Inclination angle and tank-treading in a simple shear flow

Problem setup

- $\Omega = (0, D) \times (0, D)$ where $D = 80$ μm
- The fluid density $\rho = 1.0 g/cm^3$, the viscosity $\mu = 0.01 g/(cm - s)$, the bending coefficient $c_b = 10^{-10} dyne - cm$
- Periodic shear flow $\mathbf{u}_0(y) = \gamma(-\frac{D}{2\pi}\sin(2\pi y/D), 0)$, γ is the shear rate
- L is the perimeter of the vesicle boundary, A is the area of vesicle; $R_0 = L/2\pi = 10 \mu m$ is the characteristic length scale

Numerical parameters

- Spatial mesh width $h = \Delta x = \Delta y = 80/256 \mu$m
- $K = 2 \times 10^9 dyne/cm^3$ and $R = 4 \times 10^3 dyne - s/cm^3$
- Time step size $\Delta t < \frac{\sqrt{R^2 + 2KC} - R}{K}$, where C is a problem dependent constant of order one

Dimensionless parameters

- The reduced area $V = \frac{A}{\pi R_0^2} = \frac{4 A \pi}{L^2}$ ($V = 1$ is a circle), circularity, excess area
- The dimensionless shear rate $\chi = \gamma \mu R_0^3 / c_b = 0.1\gamma$

Interesting quantities

- Inclination angle
- Tank-treading velocity
- Membrane tension

Initial setup and tank-treading motion

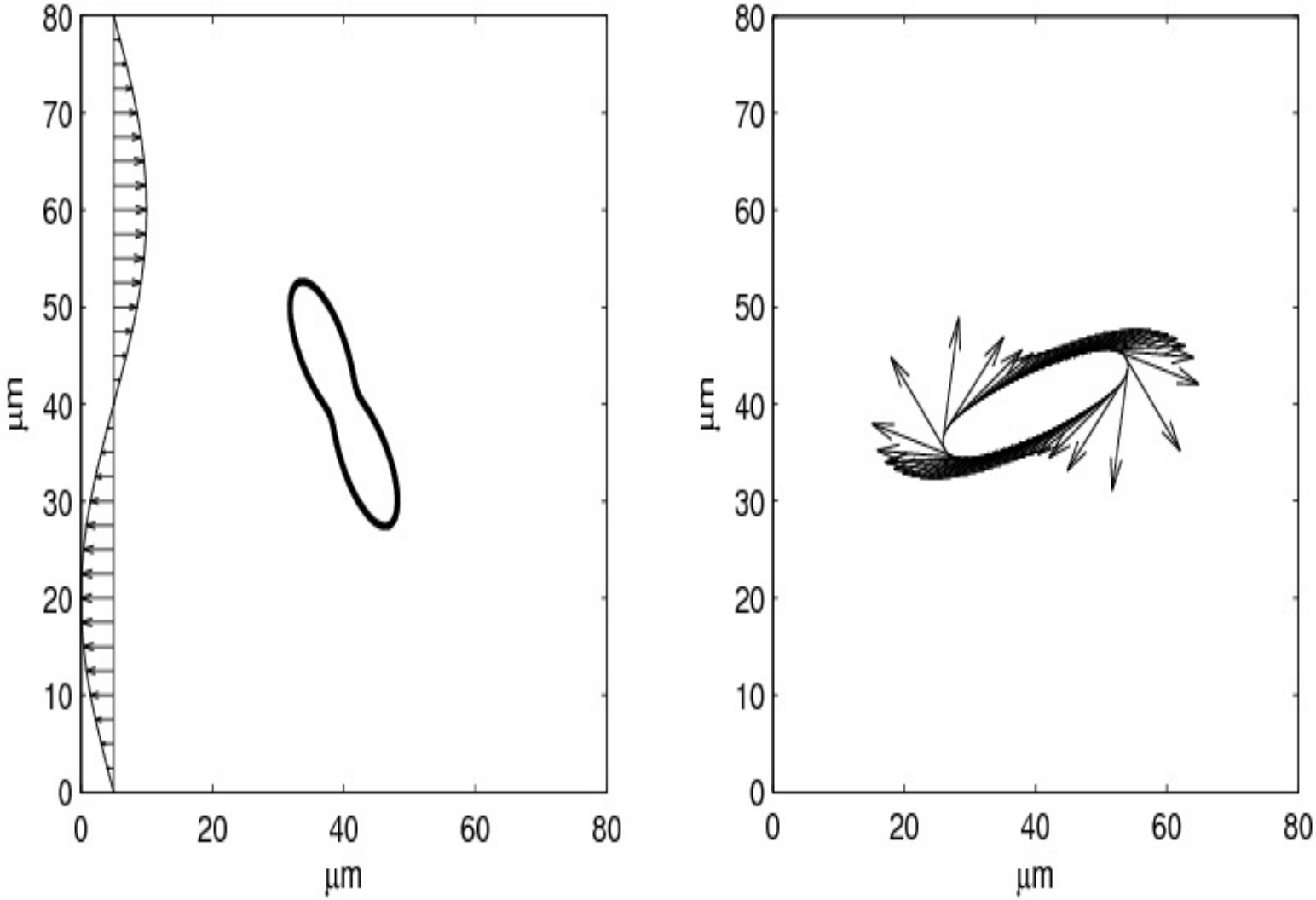
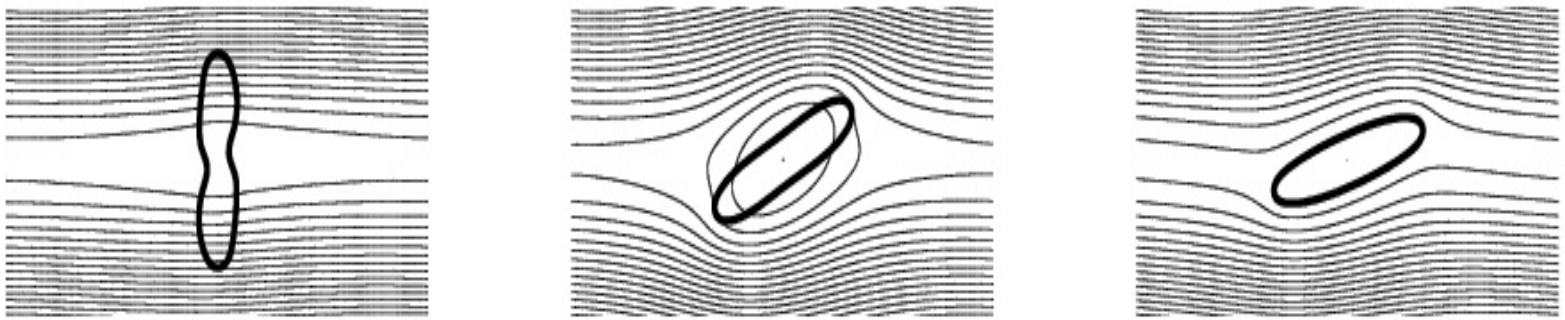


Figure: The configuration of a single vesicle suspended in the shear flow at $t = 0$ (left) and $t = 0.04$ (right) in dimensionless time. V=0.51, χ=250.



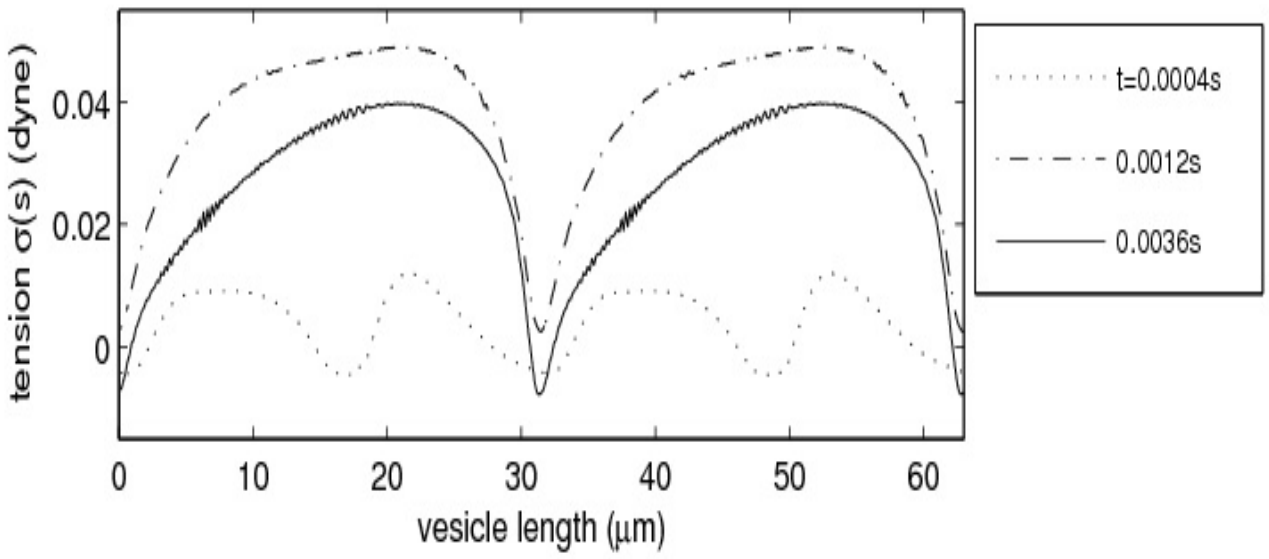


Figure: The motion of a single vesicle and streamlines (top) and the surface tension $\sigma(s,t)$ (bottom) along the vesicle at times 0.004, 0.012, and 0.036. $V = 0.51$, χ=250. The result is in agreement with Zhu & Pozrikidis 1995.

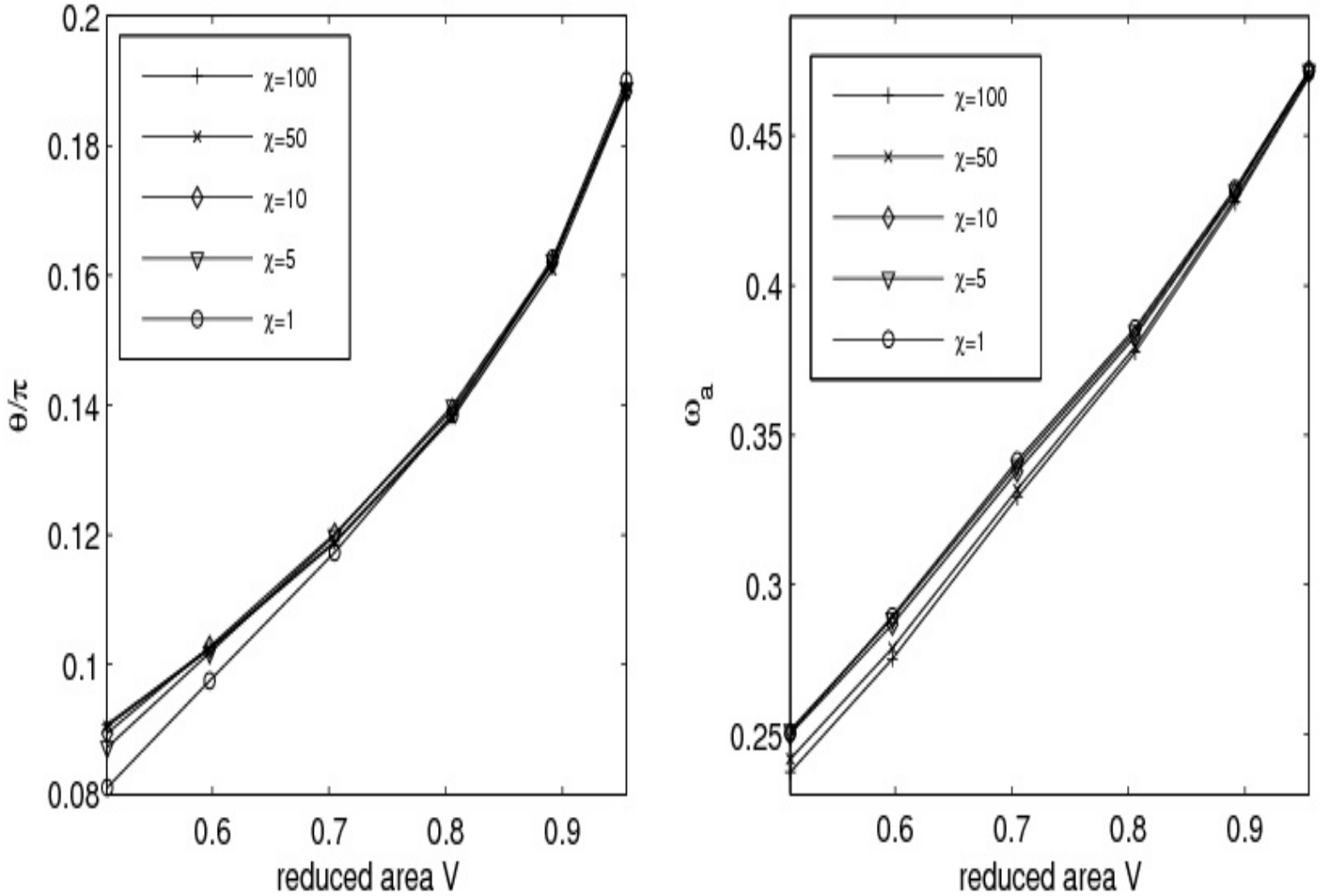


Figure: The inclination angles θ and the angular velocities ω_a of vesicles with different reduced areas V and different shear rates χ. $\omega_a = \frac{\sqrt{2}\overline{\omega}}{\gamma R_0}$, where $\overline{\omega}$ is the mean angular velocity over the vesicle boundary at the equilibrium configuration. The result is in agreement with Kraus et. al. 1996, and Veerapaneni et. al. 2009.

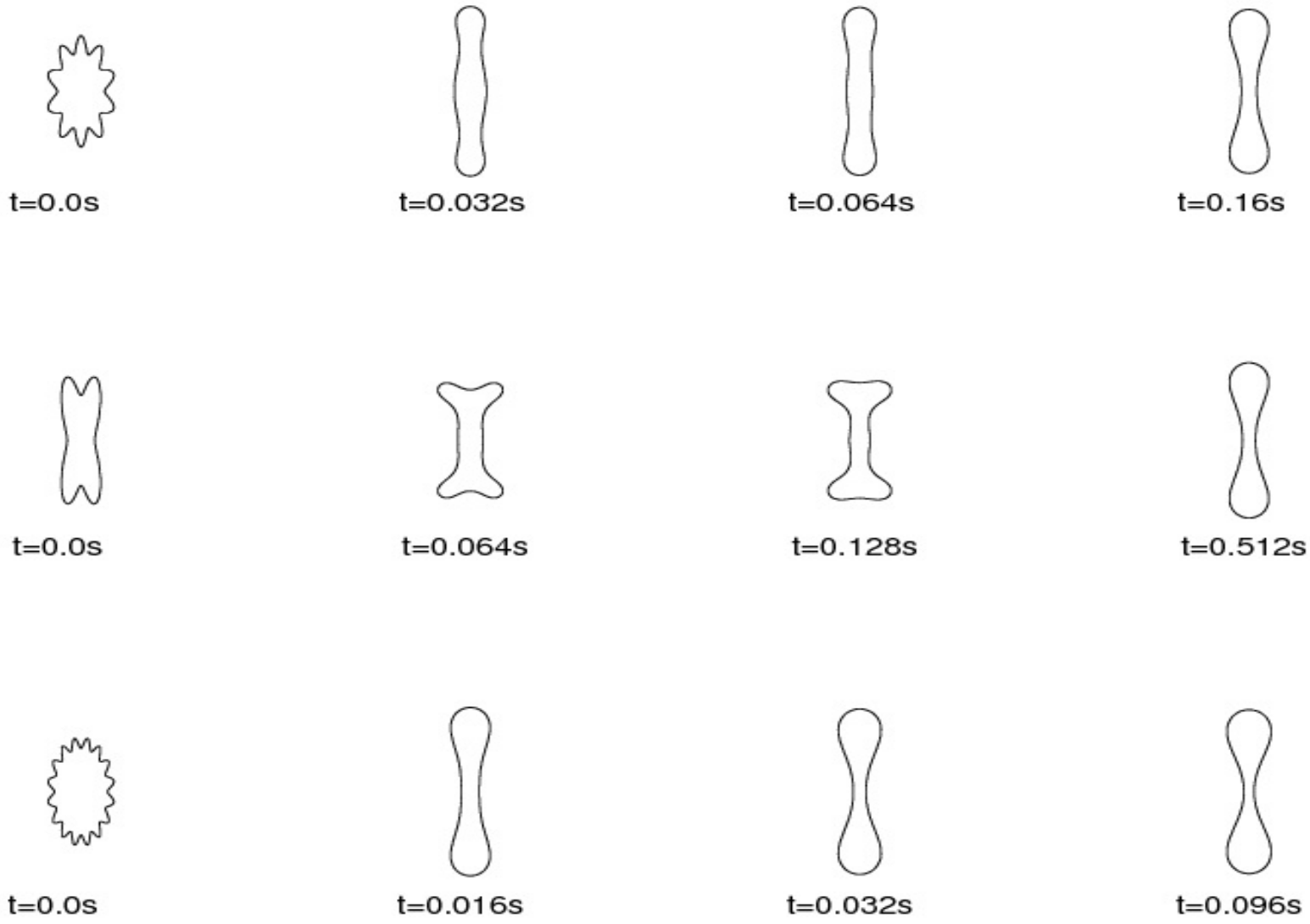


Figure: Same reduced area $V = 0.33$ with different bending rigidities and different fluid viscosities. The equilibrium shapes of the three vesicles are almost the same, i.e., it is independent of fluid viscosity and the material property.

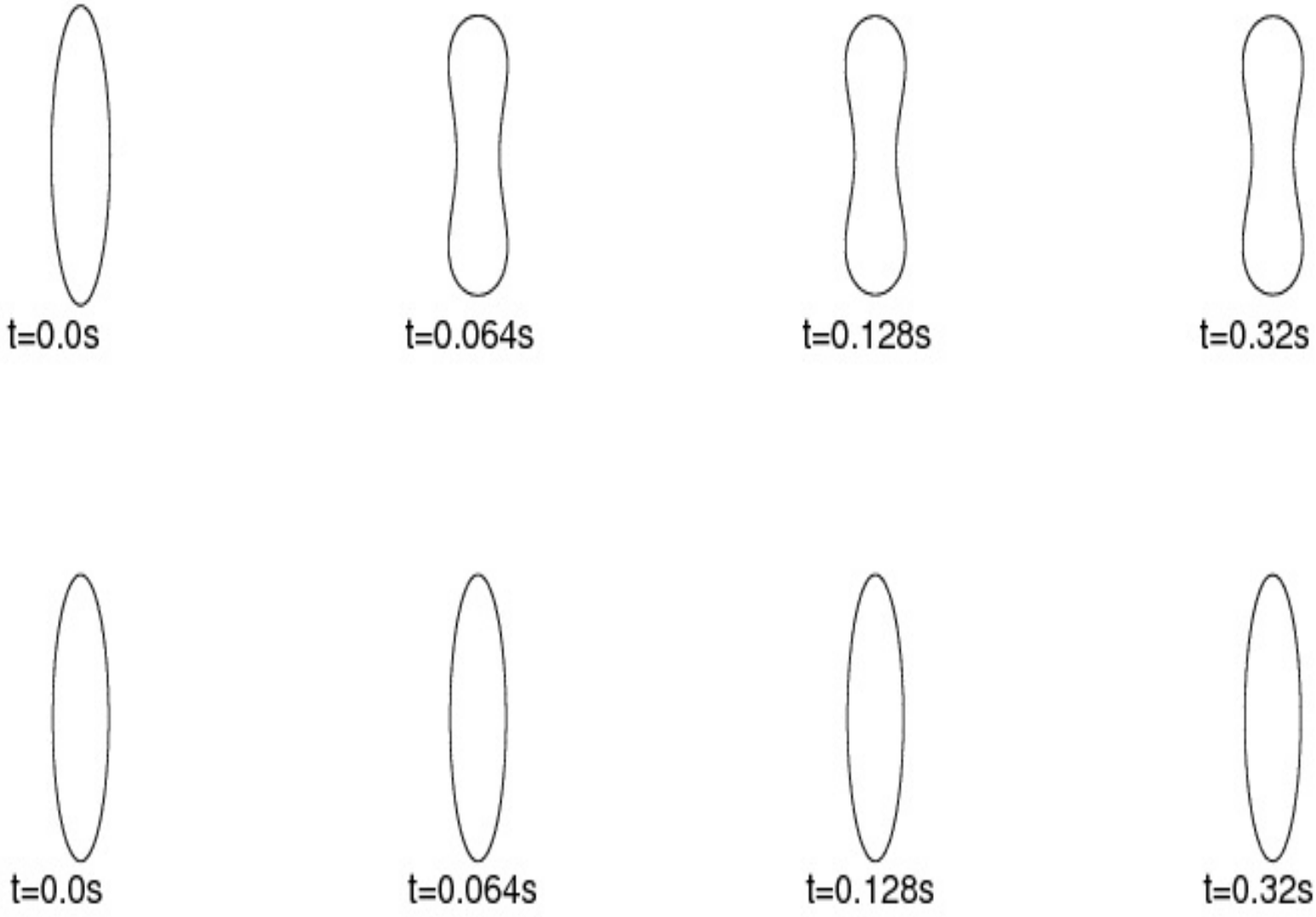


Figure: Different bending rigidity $c_b = 10^{-10}$ dyne-cm (top), $c_b = 10^{-14}$ dyne-cm (bottom).

Convergence study

N	$\lvert L_T - L_0\rvert / L_0(\mathbf{X})$	$\lvert A_T - A_0\rvert / A_0(\mathbf{X})$
128	1.13e-6	3.14e-5
256	7.12e-7	6.21e-6
512	4.05e-7	4.61e-7
1024	2.21e-7	2.17e-7

Table: The relative errors of the perimeter and the enclosed area measured at time 0.04. $\chi = 10$

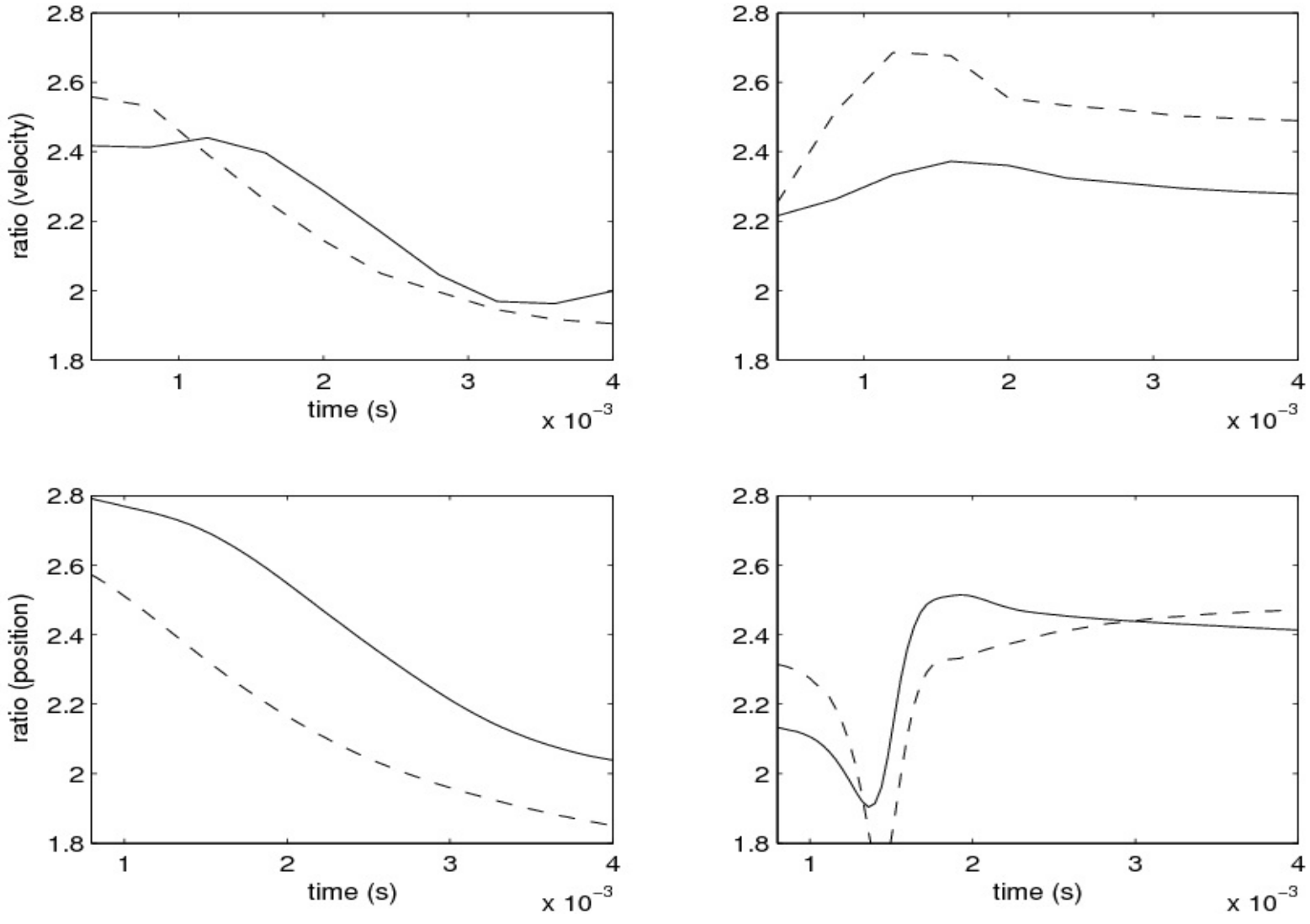


Figure: $\chi = 10$ (left) and $\chi = 250$ (right). Dashed line is the convergence ratio obtained using the grids $N = 128, 256, 512$, and the solid line is the ratio obtained with $N = 256, 512, 1024$. First-order convergence.

Multiple vesicles in a shear flow

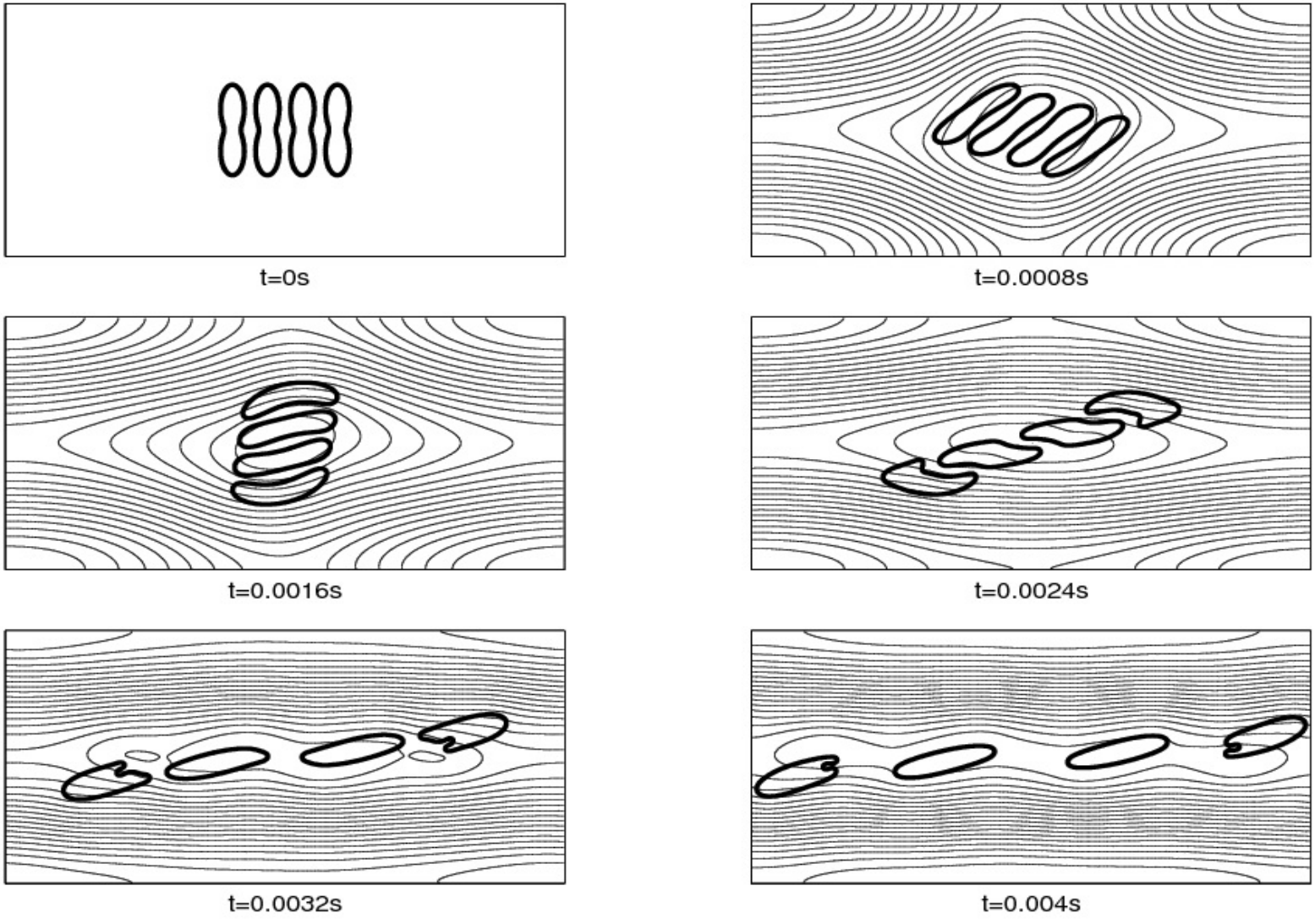


Figure: The motion of four vesicles in a shear flow at some chosen times.

Binary component vesicle

Mathematical formulation: a simplified model

- The bending rigidity and the spontaneous curvature depend on the concentration of the different lipid phases, liquid-ordered and liquid-disordered surface phases
- The mass concentration variable is defined as $\phi = \rho_B/(\rho_A + \rho_B)$ such that $\phi = 0$ and $\phi = 1$ represent the component A and B, respectively
- The bending energy

$$E_b = \int_\Gamma \frac{c_b(\phi)}{2} \left(\kappa - \kappa_0(\phi)\right)^2 \, ds,$$

where κ_0 is the spontaneous curvature which represents the asymmetry nature of the membrane

- The bending force

$$\mathbf{F}_b = -\frac{\delta E_b}{\delta \mathbf{X}} = \frac{\partial^2}{\partial s^2}\left(c_b(\phi)\left(\frac{\kappa_0(\phi)}{|\frac{\partial^2 \mathbf{X}}{\partial s^2}|} - 1\right)\frac{\partial^2 \mathbf{X}}{\partial s^2}\right)$$

Surface components equation

Phase field approach: Cahn & Hilliard 1958

$$\begin{aligned} \frac{\partial \phi}{\partial t} &= M_\phi \, \Delta_s \psi \\ \psi &= \frac{1}{\varepsilon} G'(\phi) - \varepsilon \, \Delta_s \phi, \end{aligned}$$

- The surface Laplacian is defined as $\Delta_s = \frac{\partial}{\partial s}\left(\frac{\partial}{\partial s}/|\frac{\partial \mathbf{X}}{\partial s}|\right)/|\frac{\partial \mathbf{X}}{\partial s}|$
- ψ represents the chemical potential
- $G(\phi) = \frac{1}{4}\phi^2(1-\phi)^2$ is a double well potential that describes the tendency of the phase concentration ϕ into the two stable phase separation $\phi = 0$ or $\phi = 1$
- M_ϕ is the mobility; ε is a small parameter that describes the thickness of the transitional layer on the membrane that separates the components A and B

pIB extension

Modify the feedback forcing term and solve the Cahn-Hilliard equation in $\boldsymbol{Y}$ representation

$$\frac{\partial \phi}{\partial t} = M_\phi \frac{\partial}{\partial s}\left(\frac{\partial \psi}{\partial s}/|\frac{\partial \mathbf{Y}}{\partial s}|\right)/|\frac{\partial \mathbf{Y}}{\partial s}|,$$

$$\psi = \frac{1}{\varepsilon} G'(\phi) - \varepsilon \frac{\partial}{\partial s}\left(\frac{\partial \phi}{\partial s}/|\frac{\partial \mathbf{Y}}{\partial s}|\right)/|\frac{\partial \mathbf{Y}}{\partial s}|,$$

$$\begin{aligned} & K(\mathbf{Y}(s,t) - \mathbf{X}(s,t)) + R(\mathbf{V}(s,t) - \mathbf{U}(s,t)) \\ = \quad & \frac{\partial}{\partial s}(\sigma(s,t)\,\boldsymbol{\tau}(s,t)) + \frac{\partial^2}{\partial s^2}\left(c_b(\phi)\left(\frac{\kappa_0(\phi)}{|\frac{\partial^2 \mathbf{Y}}{\partial s^2}|} - 1\right)\frac{\partial^2 \mathbf{Y}}{\partial s^2}\right). \end{aligned}$$

Numerical setup

- The spontaneous curvature $\kappa_0(\phi) = \frac{1}{R_0}(5(1-\phi) + 0.1\phi)$, where the length scale $R_0 = 10^{-3}$
- The bending rigidity is $c_b(\phi) = c_0((1-\phi) + 0.5\phi)$, where the coefficient c_0 is 10^{-10}
- $M_\phi = 10^{-6}$, and $\varepsilon = 10^{-4}$
- Initial surface concentration

$$\phi(s, 0) = \overline{\phi} + 0.001(\cos(2s) + \cos(4s) + \cos(6s)),$$

  where $\overline{\phi}$ is the average concentration
- How the values of $\overline{\phi}$ affect the vesicle configuration?

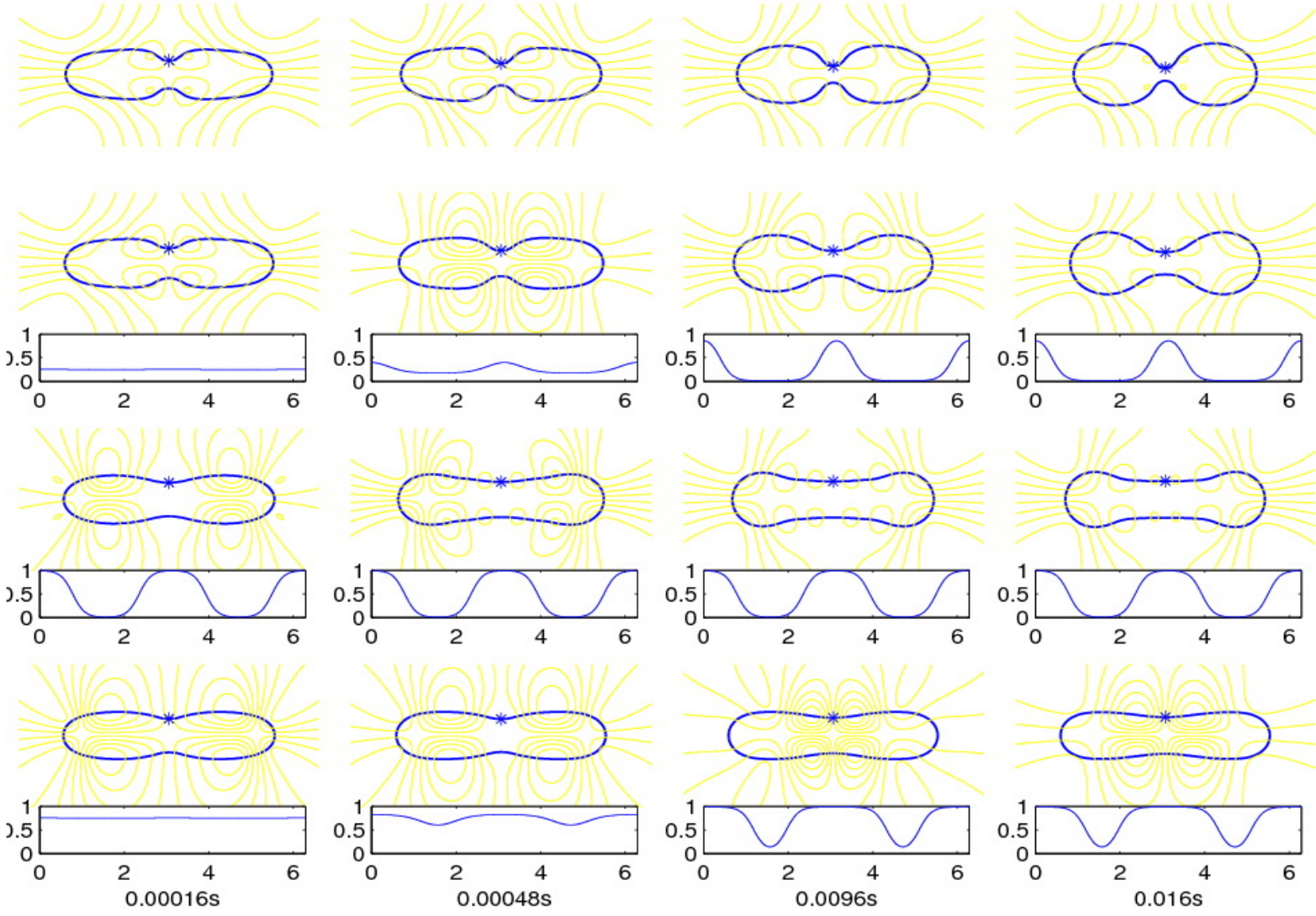


Figure: Four different concentration cases: constant concentration $\phi = 0$ (first row), $\overline{\phi} = 0.25$ (2nd-3th rows), $\overline{\phi} = 0.5$ (4th-5th rows) and $\overline{\phi} = 0.75$ (bottom two rows).