Vesicle electrohydrodynamic simulations by coupling immersed boundary and immersed interface method

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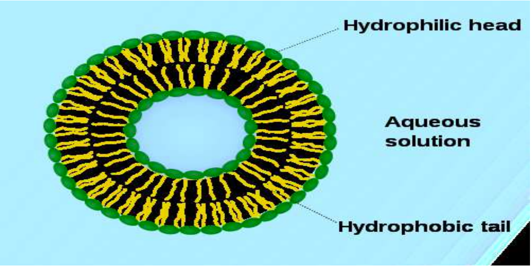
SIAM LS16, Celebrating Charles S. Peskin's 70th birthday: The Immersed Boundary Method and its Extensions, July 11-14, 2016

Vesice problem: Navier-Stokes + PDE constraint on the evolving surface

- 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 $6nm$ so we treat the membrane as a surface (3d) or a curve (2d)
- Lipid membrane (or vesicle boundary) can deform but resist area dilation, that is surface incompressible



Questions: How the vesicle behaves in fluid flows?

- To mimic some mechanical behavior of red blood cells (RBC), drug carrying capsules in capillary
- Amoeboid motion (active vesicle swimmer) in confined geometry, Wu et. al. Lai & Misbah, PRE-Rapid 2015
- In shear flow: Tank-treading (TT), Tumbling (TU), Trembling (TR), depend on the viscosity contrast $\lambda = \mu_{in}/\mu_{out}$; Keller & Skalak JFM, 1982 (theory), Deschamps et. al. PNAS, 2009 (experiment)

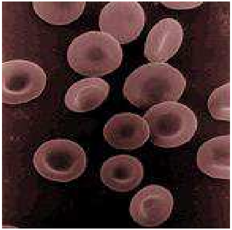
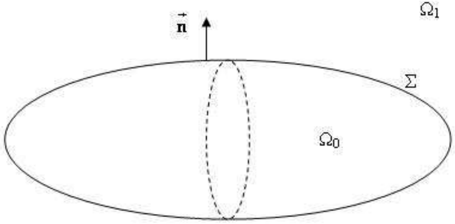


Figure: Red blood cells: flexible biconcave disks

Mathematical formulation for vesicle problem

- Vesicle: A liquid drop within another liquid with a closed lipid membrane
- Vesicle boundary Σ: fluid membrane can deform, but resist area dilation, i.e. Σ is surface incompressible
- The fluid-structure interaction is formulated by the stress balance condition on Σ



Immersed Boundary (IB) formulation: treat the vesicle boundary as a force generator

$$
\begin{aligned}
\rho\left(\frac{\partial \boldsymbol{u}}{\partial t}+\boldsymbol{u}\cdot\nabla\boldsymbol{u}\right)+\nabla p &= \mu\Delta\boldsymbol{u}+\boldsymbol{f} \qquad \text{in } \Omega \\
\nabla\cdot\boldsymbol{u} &= 0 \qquad \text{in } \Omega \\
\nabla_s\cdot\boldsymbol{U} &= 0 \qquad \text{on } \Sigma \\
\frac{\partial \mathbf{X}}{\partial t} &= \boldsymbol{U}=\int_\Omega \mathbf{u}(\mathbf{x},t)\delta(\mathbf{x}-\mathbf{X})d\mathbf{x}
\end{aligned}
$$

where the immersed boundary force

$$
\begin{aligned}
\boldsymbol{f} &= \int_\Sigma \boldsymbol{F}(\boldsymbol{X})\,\delta(\boldsymbol{x}-\boldsymbol{X})\,d\boldsymbol{X} \\
\boldsymbol{F} &= \boldsymbol{F}_b+\boldsymbol{F}_\sigma \qquad \text{on } \Sigma \\
\boldsymbol{F}_b &= c_b\left(\Delta_s H+2H(H^2-K)\right)\boldsymbol{n} \\
\boldsymbol{F}_\sigma &= \nabla_s\sigma-2\,H\,\sigma\boldsymbol{n}
\end{aligned}
$$

- H: mean curvature, K: Gaussian curvature,

$$\nabla_s = \nabla - \frac{\partial}{\partial \boldsymbol{n}}\boldsymbol{n}, \qquad \Delta_s = \nabla_s \cdot \nabla_s$$

- c_b: bending rigidity
- σ: unknown elastic tension to be introduced to enforce $\nabla_s \cdot \boldsymbol{U} = 0$
- It can be shown that the tension doesn't do extra work to the fluid; i.e. $< S(\sigma), \mathbf{u} >_\Omega = - < \sigma, \nabla_s \cdot \boldsymbol{U} >_\Gamma$
- The pressure and elastic tension have the same roles as Lagrange multipliers

Question: Where does the boundary force $\boldsymbol{F}$ come from?

Answer: Variational derivative of Helfrich energy

$$\begin{aligned} E &= \frac{c_b}{2}\int_\Sigma H^2 \, d\boldsymbol{S} + \int_\Sigma \sigma \, d\boldsymbol{S} \\ \Rightarrow \boldsymbol{F} &= -\frac{\delta E}{\delta \boldsymbol{X}} = \boldsymbol{F}_b + \boldsymbol{F}_\sigma \end{aligned}$$

Skew-adjoint operators

$$\langle \mathbf{u}, \mathbf{v} \rangle_\Omega = \int_\Omega \mathbf{u}(\mathbf{x}) \cdot \mathbf{v}(\mathbf{x}) \, \mathrm{d}\mathbf{x},$$
$$\langle f, g \rangle_\Gamma = \int_\Gamma f(S) \, g(S) \, \mathrm{d}S,$$

Define $S(\sigma) = \int_\Gamma (\nabla_s \sigma - 2\sigma H \mathbf{n}) \, |\mathbf{X}_\alpha \times \mathbf{X}_\beta| \, \delta(\mathbf{x} - \mathbf{X}(\alpha, \beta, t)) \, \mathrm{d}\alpha \mathrm{d}\beta$, then

$$
\begin{aligned}
& \langle S(\sigma), \mathbf{u} \rangle_\Omega \\
= \; & \int_\Omega \left[\int_\Gamma (\nabla_s \sigma - 2\sigma H \mathbf{n}) \, |\mathbf{X}_\alpha \times \mathbf{X}_\beta| \, \delta(\mathbf{x} - \mathbf{X}(\alpha, \beta, t)) \, \mathrm{d}\alpha \mathrm{d}\beta \right] \cdot \mathbf{u}(\mathbf{x}) \, \mathrm{d}\mathbf{x} \\
= \; & \int_\Gamma (\nabla_s \sigma - 2\sigma H \mathbf{n}) \cdot \mathbf{U}(\alpha, \beta, t) \, |\mathbf{X}_\alpha \times \mathbf{X}_\beta| \; \mathrm{d}\alpha \mathrm{d}\beta \\
= \; & \int_\Gamma \sigma_\alpha (\mathbf{X}_\beta \times \mathbf{n}) \cdot \mathbf{U} + \sigma_\beta (\mathbf{n} \times \mathbf{X}_\alpha) \cdot \mathbf{U} - 2\sigma H \mathbf{n} \cdot \mathbf{U} \, |\mathbf{X}_\alpha \times \mathbf{X}_\beta| \; \mathrm{d}\alpha \mathrm{d}\beta \\
= \; & \int_\Gamma (\sigma(\mathbf{X}_\beta \times \mathbf{n}))_\alpha \cdot \mathbf{U} + (\sigma(\mathbf{n} \times \mathbf{X}_\alpha))_\beta \cdot \mathbf{U} \\
& - [\sigma(\mathbf{X}_\beta \times \mathbf{n})_\alpha + \sigma(\mathbf{n} \times \mathbf{X}_\alpha)_\beta + 2\sigma H \mathbf{n} \, |\mathbf{X}_\alpha \times \mathbf{X}_\beta|] \cdot \mathbf{U} \, \mathrm{d}\alpha \mathrm{d}\beta \\
= \; & - \int_\Gamma \sigma(\mathbf{X}_\beta \times \mathbf{n}) \cdot \mathbf{U}_\alpha + \sigma(\mathbf{n} \times \mathbf{X}_\alpha) \cdot \mathbf{U}_\beta \, \mathrm{d}\alpha \mathrm{d}\beta \\
& (\text{since } \sigma(\mathbf{X}_\beta \times \mathbf{n})_\alpha + \sigma(\mathbf{n} \times \mathbf{X}_\alpha)_\beta + 2\sigma H \mathbf{n} \, |\mathbf{X}_\alpha \times \mathbf{X}_\beta| = 0) \\
= \; & - \int_\Gamma \sigma(\nabla_s \cdot \mathbf{U}) \, |\mathbf{X}_\alpha \times \mathbf{X}_\beta| \; \mathrm{d}\alpha \mathrm{d}\beta \\
= \; & -\langle \sigma, \nabla_s \cdot \mathbf{U} \rangle_\Gamma
\end{aligned}
$$

Numerical issues:

1. Coupled with fluid dynamics which vesicle boundary is moving with fluid and whose shape is not known *a priori*
2. Both the volume and the surface area of the vesicle are conserved. How to maintain fluid and vesicle boundary incompressible simultaneously?
3. Need to find H, $\Delta_s H$, $\boldsymbol{n}$, K on a moving surface Σ
4. In additional to the fluid incompressibility, we need extra constraint (surface incompressibility) on the surface
5. The role of pressure p on fluid equations is the same as the role of tension σ on $\nabla_s \cdot \boldsymbol{U} = 0$. Both conditions are local!
6. How to solve the above governing equations efficiently?
7. Boundary integral method, Immersed boundary (Front-tracking), Level-set, or Phase field method?

IB and IIM simulations for vesicle problems

- Kim & Lai JCP 2010, 2D penalty IB method
- Li & Lai EAJAM 2011, IIM for 2D inextensible interface
- Kim & Lai PRE 2012, study the inertial effect on tumbling inhibition
- Lai, Hu & Lin SISC 2012, a compound inextensible interface with a solid particle, skew-adjoint operators
- Hu, Kim & Lai JCP 2014, 3D axis-symmetric case, nearly incompressible approach
- Hsieh, Lai, Yang & You JSC 2015, an unconditionally energy stable IB method for a compound inextensible interface with a solid particle
- Wu, Fai, Atzberger & Peskin SISC 2015, SIBM for osmotic swelling of vesicles
- Seol, Hu, Kim & Lai JCP 2016, 3D vesicle simulations under shear flow

Nearly surface incompressibility approach

- $\nabla_s \cdot \mathbf{U} = 0$ means that $\frac{\partial}{\partial t}|\mathbf{X}_r \times \mathbf{X}_s| = 0$
- To avoid solving the extra unknown tension $\sigma(r, s, t)$, we alternatively use a spring-like elastic tension

$$\sigma = \sigma_0 \left(|\mathbf{X}_r \times \mathbf{X}_s| - |\mathbf{X}_r^0 \times \mathbf{X}_s^0| \right)$$

  where $\sigma_0 \gg 1$ and $|\mathbf{X}_r^0 \times \mathbf{X}_s^0|$ is the initial surface dilating factor
- Similar idea has been used in level set framework by Maitre, Misbah, Peyla & Raoult, Physica D 2012
- The modified elastic energy by

$$E_\sigma(\mathbf{X}) = \frac{\sigma_0}{2} \iint \left(|\mathbf{X}_r \times \mathbf{X}_s| - |\mathbf{X}_r^0 \times \mathbf{X}_s^0| \right)^2 \, drds$$

Derivation of modified elastic force by variational derivative

$$
\begin{aligned}
&\frac{d}{d\varepsilon}E_\sigma(\mathbf{X}+\varepsilon\mathbf{Y})\Big|_{\varepsilon=0}\\
&=\iint \sigma_0\left(|\mathbf{X}_r\times\mathbf{X}_s|-|\mathbf{X}_r^0\times\mathbf{X}_s^0|\right)\frac{\mathbf{X}_r\times\mathbf{X}_s}{|\mathbf{X}_r\times\mathbf{X}_s|}\cdot(\mathbf{Y}_r\times\mathbf{X}_s+\mathbf{X}_r\times\mathbf{Y}_s)\,drds\\
&=\iint \sigma\mathbf{n}\cdot(\mathbf{Y}_r\times\mathbf{X}_s+\mathbf{X}_r\times\mathbf{Y}_s)\,drds \quad \left(\text{by } \mathbf{n}=\frac{\mathbf{X}_r\times\mathbf{X}_s}{|\mathbf{X}_r\times\mathbf{X}_s|}\right)\\
&=\iint \sigma(\mathbf{X}_s\times\mathbf{n})\cdot\mathbf{Y}_r+\sigma(\mathbf{n}\times\mathbf{X}_r)\cdot\mathbf{Y}_s\,drds \quad (\text{by the scalar triple product formula})\\
&=-\iint(\sigma\mathbf{X}_s\times\mathbf{n})_r\cdot\mathbf{Y}+(\sigma\mathbf{n}\times\mathbf{X}_r)_s\cdot\mathbf{Y}\,drds \quad (\text{by integration by parts})\\
&=-\iint[\sigma_r\mathbf{X}_s\times\mathbf{n}+\sigma_s\mathbf{n}\times\mathbf{X}_r+\sigma(\mathbf{X}_s\times\mathbf{n})_r+\sigma(\mathbf{n}\times\mathbf{X}_r)_s]\cdot\mathbf{Y}\,drds\\
&=-\iint(\sigma_r\mathbf{X}_s\times\mathbf{n}+\sigma_s\mathbf{n}\times\mathbf{X}_r+\sigma\mathbf{X}_s\times\mathbf{n}_r+\sigma\mathbf{n}_s\times\mathbf{X}_r)\cdot\mathbf{Y}\,drds\\
&=-\iint(\nabla_s\sigma-2\sigma H\mathbf{n})\cdot\mathbf{Y}\,|\mathbf{X}_r\times\mathbf{X}_s|\,drds\\
&=-\int_\Gamma(\nabla_s\sigma-2\sigma H\mathbf{n})\cdot\mathbf{Y}\,\mathrm{d}A \quad (\text{since } \mathrm{d}A=|\mathbf{X}_r\times\mathbf{X}_s|\,drds)\\
&=-\int_\Gamma\mathbf{F}_\sigma\cdot\mathbf{Y}\,\mathrm{d}A \qquad \mathbf{F}_\sigma\ \text{are exactly identical !}
\end{aligned}
$$

Axis-symmetric case, Hu, Kim & Lai, JCP 2014

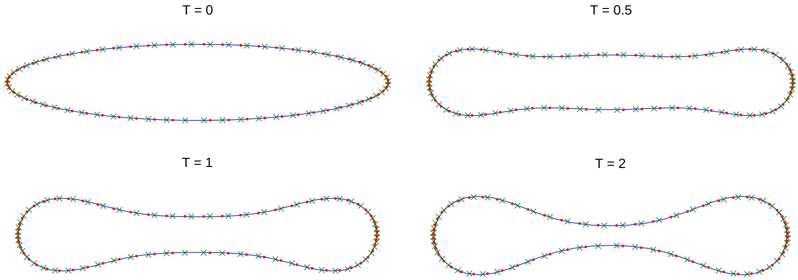


Figure: Freely suspended vesicles with different penalty number σ_0. Blue solid line: $\sigma_0 = 2 \times 10^3$; green marker "$\times$": $\sigma_0 = 2 \times 10^4$; red marker "$\cdot$": $\sigma_0 = 2 \times 10^5$.

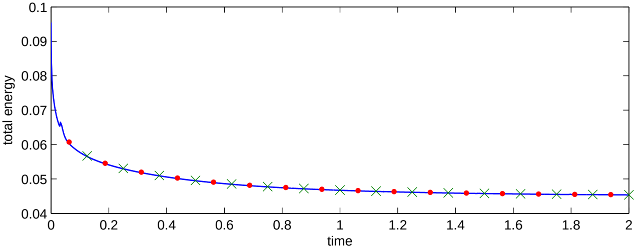


Figure: The corresponding evolution of total energy. Blue solid line: $\sigma_0 = 2 \times 10^3$; green marker "$\times$": $\sigma_0 = 2 \times 10^4$; red marker "$\cdot$": $\sigma_0 = 2 \times 10^5$

σ_0	$\\|R\,\|\mathbf{X}_s\| - R^0\,\|\mathbf{X}_s\|^0\,\\|_\infty$	$\|A_h - A_0\|/A_0$	$\|V_h - V_0\|/V_0$
2×10^3	2.988E-04	2.431E-03	9.391E-04
2×10^4	6.551E-05	2.060E-04	2.865E-04
2×10^5	2.903E-05	2.105E-05	2.657E-04

Table: The errors of the area dilating factor, the total surface area, and the volume.

Full 3D case: Seol, Hu, Kim & Lai JCP 2016

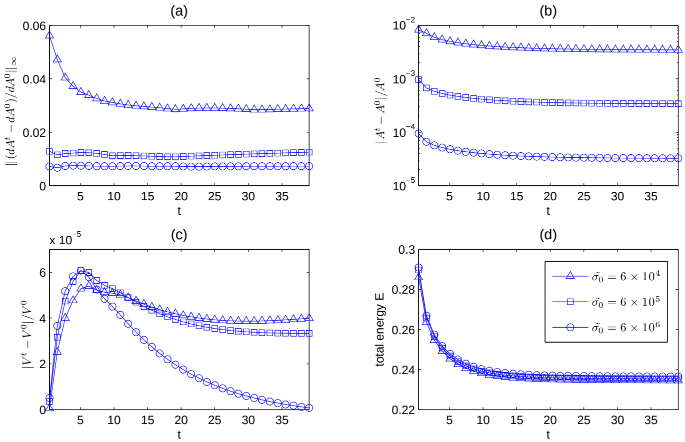


Figure: The comparison for three different stiffness parameters: $\tilde{\sigma_0} = 6 \times 10^4(\triangle)$, $6 \times 10^5(\square)$, and $6 \times 10^6(\bigcirc)$. (a) the maximum relative error of the local surface area; (b) the relative error of the global surface area; (c) the relative error of the global volume; (d) the total energy.

Vesicle under shear flow

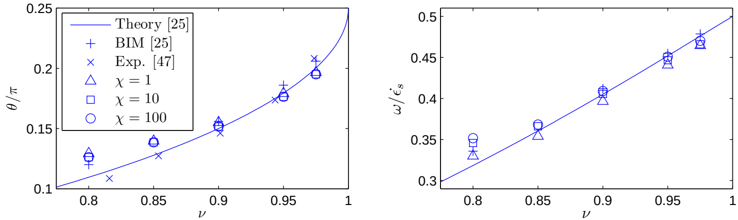
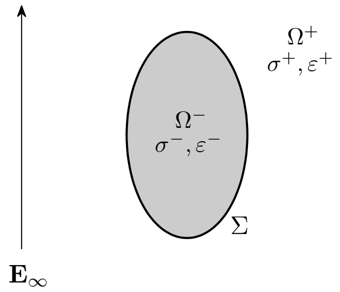


Figure: The plot of the inclination angle (left) and the scaled mean angular velocity (right) as functions of reduced volume ν for different dimensionless shear rate χ.

- The frequency ω can be computed using $\omega = \frac{1}{N_v}\sum_{i=1}^{N_v}\frac{|\mathbf{r}\times\mathbf{v}|}{|\mathbf{r}|^2}$, where $\mathbf{r}$ and $\mathbf{v}$ are the position and velocity of the vertices projected on the xz-plane, respectively.

A leaky dielectric vesicle under DC electric field



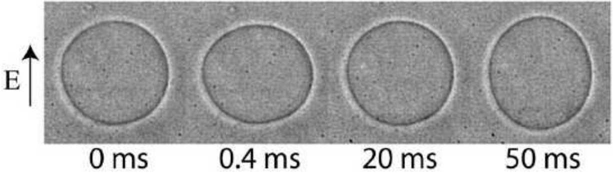
Questions:

- How the vesicle respond?
- How the electric field affects the vesicle dynamics in shear flow? eg. tank-treading, and tumbling

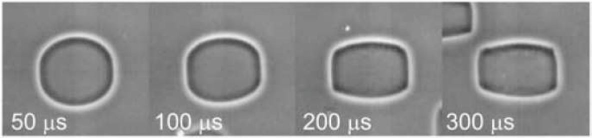
Conductivity σ: a measure of a material's ability to conduct an electric current

Permittivity ε: or dielectric constant, a measure of how easily a dielectric material polarizes in response to an electric field;

Vesicle electrohydrodynamics



(a)



(b)

Figure: (a) Prolate-oblate-prolate (POP) transition (Salipante & Vlahovska 2014); (b) Cylindrical electro-deformation (Riske & Dimova 2006)

Experiments:

- Electroporation, creating crack open, electrofusion
  - Dimova et al., Biophysical J. (2005), PNAS (2006), Soft Matter (2007, 2009, 2010)
- Electro-deformation
  - Salipante & Vlahovska, 2014

Theoretical analysis:

- A nearly spherical model in DC electric field, Schwalbe, Vlahovska, & Miksis, 2011;
- Long-wave approximation for planar membrane, Young, Veerapaneni, & Miksis, 2014

Numerical simulations:

- Boundary integral method: McConnell, Miksis, & Vlahovska, IMA J. Appl. Math. (2013), Soft Matter (2015)
- Level set method: Kolahdouz & Salac, SIAM J. Sci. Comput. (2015)
- A coupled immersed boundary and immersed interface method: Hu, Lai, Seol & Young, JCP 2016

Electric force field

Eulerian electric volume force

- Maxwell stress tensor $\mathbf{M}_E = \varepsilon\left(\mathbf{E}\mathbf{E} - \frac{1}{2}(\mathbf{E}\cdot\mathbf{E})I\right)$
- $\mathbf{f}_E = \nabla\cdot\mathbf{M}_E = -\frac{1}{2}(\mathbf{E}\cdot\mathbf{E})\nabla\varepsilon + \nabla\cdot(\varepsilon\mathbf{E})\mathbf{E}$
- Across the interface, $\mathbf{E}$ is not continuous
- Using smoothing numerical method, $\mathbf{E}$ has $O(1)$ error and $\mathbf{f}_E$ has $O(1/h)$ error near the interface

Lagrangian electric interfacial force

- $\mathbf{F}_E = [\mathbf{M}_E\cdot\mathbf{n}] = (\mathbf{M}_E^+ - \mathbf{M}_E^-)\cdot\mathbf{n}$; where $\mathbf{M}_E^\pm$: Maxwell stress tensor inside $(-)$ and outside $(+)$ of the drop
- Necessary to the Boundary Integral Method
- Compute $\mathbf{M}_E^\pm$ accurately
- Then $\mathbf{f}_E = \int_\Sigma \mathbf{F}_E(s,t)\,\delta(\mathbf{x}-\mathbf{X}(s,t))|\mathbf{X}_s|\,\mathrm{d}s$
- The interfacial electric force $\mathbf{F}_E$ can be distributed in an unified manner as the tension and bending forces

Leaky dielectric model, G. I. Taylor 1966

- The electric field $\mathbf{E}$ is irrotational; $\mathbf{E} = -\nabla\phi$, where the electric potential ϕ satisfies the Laplace equation

$$\Delta\phi = 0 \quad \text{in } \Omega \setminus \Sigma$$

- The vesicle membrane acts like a capacitor during the charging process, and thus forms a transmembrane potential V_m. That is,

$$[\phi] = \phi^+ - \phi^- = V_m(s,t) \quad \text{on } \Sigma$$

  where the bracket $[\cdot]$ stands for the jump

- The normal component of ohmic current $\mathbf{J} = \sigma\mathbf{E}$ is continuous across the membrane. Thus we have

$$[\sigma\phi_n] = \sigma^+\phi_n^+ - \sigma^-\phi_n^- = -(\mathbf{J}^+ - \mathbf{J}^-)\cdot\mathbf{n} = 0 \quad \text{on } \Sigma$$

- The transmembrane potential is calculated from the conservation law of current density across the membrane

$$C_m\frac{\partial V_m}{\partial t} + G_m V_m = \sigma^+\phi_n^+ = \sigma^-\phi_n^- \quad \text{on } \Sigma$$

  where C_m and G_m are the membrane capacitance and conductance, respectively

An immersed interface method for solving elliptic interface problem

Ref.: Li & Ito, SIAM (2006)

$$\Delta\phi = 0 \quad \text{in } \Omega \setminus \Sigma$$

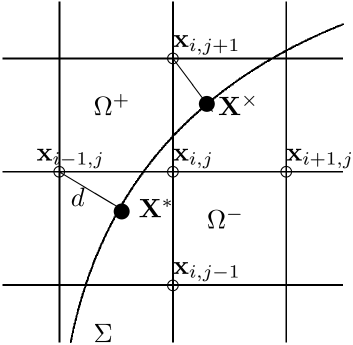
$$[\phi] = V_m, \quad \phi_n^- + \frac{\sigma^+}{[\sigma]}[\phi_n] = \frac{[\sigma\phi_n]}{[\sigma]} = 0 \quad \text{(with assumption } \sigma^- < \sigma^+\text{)} \quad \text{on } \Sigma$$

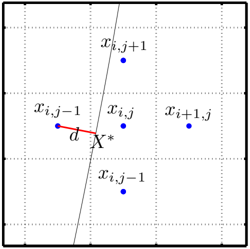
$$\left(1 - \frac{1}{\sigma_r}\right)\left(\frac{C_m}{\sigma^+}\frac{\partial V_m}{\partial t} + \frac{G_m}{\sigma^+}V_m\right) = [\phi_n] \quad \text{on } \Sigma$$

$\sigma_r = \sigma^-/\sigma^+$ is the conductivity ratio

Ref.: Tom Beale and collaborators (since 2001), Maximum norm error estimates on IIM, for elliptic, parabolic and Navier-Stokes with interfaces

Regular and irregular points for 5-point Laplacian





The discretized equation by finite difference method can be written as

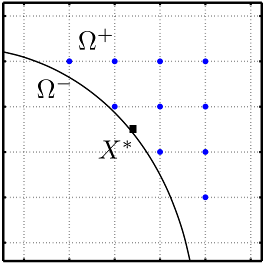
$$\Delta_h \phi_{ij} + \frac{\phi_{ij}^c}{h^2} = f_{ij}$$

Here $\phi_{ij}^c = 0$ at regular points, and at irregular points,

$$\phi_{ij}^c = [\phi]\mathbf{x}^* + d[\phi_n]\mathbf{x}^* + \frac{d^2}{2}\left([f]\mathbf{x}^* - \kappa\mathbf{x}^*[\phi_n]\mathbf{x}^* - \nabla_s^2[\phi]\mathbf{x}^*\right)$$

Reference: Russel & Wang (2003), Poisson equation; Lai & Tseng (2008), Stokes equations; Xu (2012), piecewise coefficient Poisson equation

Compute one-sided normal derivative along the interface by least square approximation



- $\phi_n^- + \frac{\sigma^+}{[\sigma]}[\phi_n] = \frac{[\sigma\phi_n]}{[\sigma]},$ if $\sigma^+ > \sigma^-$
- At each orthogonal projection $\mathbf{X}^*$, we use blue nodes to construct least squares polynomial $P(x,y) \Rightarrow \min \sum_{i,j}(P_{i,j} - \phi_{i,j})^2$
- Approximate $\phi_n^-(\mathbf{X}^*) \approx \nabla P(\mathbf{X}^*) \cdot \mathbf{n}(\mathbf{X}^*) = B^-\phi$
- $B^-\phi + \frac{\sigma^+}{[\sigma]}[\phi_n] = \frac{[\sigma\phi_n]}{[\sigma]} = 0$

Numerical discretizations

Let Φ, Ψ_1, and Ψ_2 be the solution vectors formed by ϕ, $[\phi]$, and $[\phi_n]$ respectively

Backward Euler:

$$\begin{aligned} \Delta_h \Phi + C_1 \Psi_1 + C_2 \Psi_2 &= F \\ B^- \Phi + \frac{\sigma^+}{[\sigma]} \Psi_2 &= 0 \\ \left(1 - \frac{1}{\sigma_r}\right) \left(\frac{C_m}{\sigma^+} \frac{\Psi_1 - \Psi_1^n}{\Delta t} + \frac{G_m}{\sigma^+} \Psi_1 \right) &= \Psi_2 \end{aligned}$$

Crank-Nicholson:

$$\begin{aligned} \Delta_h \Phi + C_1 \Psi_1 + C_2 \Psi_2 &= F \\ B^- \Phi + \frac{\sigma^+}{[\sigma]} \Psi_2 &= 0 \\ \left(1 - \frac{1}{\sigma_r}\right) \left(\frac{C_m}{\sigma^+} \frac{\Psi_1 - \Psi_1^n}{\Delta t} + \frac{G_m}{\sigma^+} \frac{\Psi_1 + \Psi_1^n}{2} \right) &= \frac{\Psi_2 + \Psi_2^n}{2} \end{aligned}$$

The resultant matrix can be written in the form of

$$\begin{bmatrix} A & C_1 & C_2 \\ B^- & 0 & \frac{\sigma^+}{[\sigma]}\mathbf{I} \\ 0 & \alpha\mathbf{I} & \beta\mathbf{I} \end{bmatrix} \begin{bmatrix} \Phi \\ \Psi_1 \\ \Psi_2 \end{bmatrix} = \begin{bmatrix} F \\ 0 \\ G \end{bmatrix}$$

where α and β are nonzero (if $\sigma_r \neq 1$) constant coefficients depending on the usage of BE or CN scheme. By using Schur complement technique, solving the above linear system can be split into four steps as follows

1. Apply one fast Poisson solver to solve Φ^* in

$$A\Phi^* = F - \frac{1}{\beta}C_2 G$$

2. Use GMRES iteration to solve Ψ_1 in

$$\left[B^- A^{-1}(C_1 - \frac{\alpha}{\beta}C_2) + \frac{\alpha}{\beta}\frac{\sigma^+}{[\sigma]}I\right]\Psi_1 = B^-\Phi^* + \frac{1}{\beta}\frac{\sigma^+}{[\sigma]}G$$

3. Update Ψ_2 explicitly by the transmembrane potential equation
4. Apply one fast Poisson solver to solve Φ in

$$A\Phi = F - C_1\,\Psi_1 - C_1\,\Psi_2$$

Convergence and efficiency study

Example 1

- Exact solution $\phi(x,y,t)$ in $\Omega = [-1,1]\times[-1,1]$ is defined by

$$\phi(x,y,t) = \begin{cases} \frac{e^{-t}}{\sigma^-}(x^2-y^2) & \mathbf{x}\in\Omega^- \\ \frac{e^{-t}}{\sigma^+}(x^2-y^2) & \mathbf{x}\in\Omega^+ \end{cases}, \qquad V_m = \left(1-\frac{1}{\sigma_r}\right)\frac{e^{-t}}{\sigma^+}(X(s)^2 - Y(s)^2)$$

- $\sigma_r = 0.1$, interface $\mathbf{X} = (0.5\cos s, 0.5\sin s)$, $C_m = 1, G_m = 4/(1-\sigma_r)+1$
- $h = 2/N, \Delta t = h/4$, terminal time $T = 0.2$

N	BE			CN		
	$\|\phi_h-\phi_e\|_\infty$	Rate	Iter.	$\|\phi_h-\phi_e\|_\infty$	Rate	Iter.
80	8.046E−04	-	3	2.128E−04	-	3
160	4.958E−04	0.69	3	3.168E−05	2.74	4
320	2.587E−04	0.93	3	7.959E−06	1.99	4
640	1.313E−04	0.97	3	1.994E−06	2.00	4

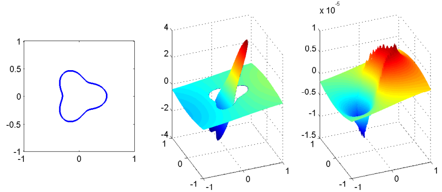
Example 2

- Exact solution $\phi(x,y,t)$ in $\Omega = [-1,1]\times[-1,1]$ is defined by

$$\phi(x,y,t) = \begin{cases} \frac{e^{-t}}{\sigma^-} e^x \cos y & \mathbf{x}\in\Omega^- \\ \frac{e^{-t}}{\sigma^+} e^x \cos y & \mathbf{x}\in\Omega^+ \end{cases}, \qquad V_m = \left(1-\frac{1}{\sigma_r}\right)\frac{e^{-t}}{\sigma^+} e^{X(s)} \cos Y(s)$$

- Interface $\mathbf{X} = (r(s)\cos s, r(s)\sin s)$, where $r(s) = 0.1(4+\cos 3s)$
- $\sigma_r = 0.1$, $C_m = 1, G_m = 0.1$, an extra term in transmembrane potential equation

N	BE			CN		
	$\Vert\phi_h-\phi_e\Vert_\infty$	Rate	Iter.	$\Vert\phi_h-\phi_e\Vert_\infty$	Rate	Iter.
80	8.299E−03	-	8	7.249E−04	-	9
160	4.033E−03	1.04	9	6.313E−05	3.52	10
320	2.017E−03	0.99	9	1.229E−05	2.36	9
640	1.010E−03	0.99	8	3.204E−06	1.93	8



Non-dimensionalization of vesicle EHD system

- All physical units: the vesicle radius $R \approx 10^{-5}$ m, the strength of electric field $E_\infty \approx 10^5$ V/m, the fluid viscosity $\mu \approx 10^{-3}$ Pa s, the fluid density $\rho \approx 10^3$ kg/m^3, the bulk fluid conductivity $\sigma^+ \approx 10^{-4}$ S/m, the permittivity $\varepsilon^+ \approx 10^{-10}$ F/m, and the membrane conductivity $C_m \approx 10^{-2}$ F/m^2.
- Characteristic scales: $t_{mm} = \frac{RC_m}{\sigma^+}\left(\frac{1}{2} + \frac{1}{\sigma_r}\right)$, $\mathbf{x}^* = \frac{\mathbf{x}}{R}$, $t^* = \frac{t}{t_{mm}}$, $p^* = \frac{t_{mm}^2}{\rho R^2} p$, $\gamma^* = \frac{R^2}{c_b}\gamma$, $\varepsilon^* = \frac{\varepsilon}{\varepsilon^+}$, $\sigma^* = \frac{\sigma}{\sigma^+}$, $\mathbf{E}^* = \frac{\mathbf{E}}{E_\infty}$
- Dimensionless numbers: $Re = \frac{\rho R^2}{\mu\, t_{mm}}$; the capillary number, $Ca = \frac{\mu R^3/c_b}{t_{mm}}$, measures the ratio of restoring bending and membrane charging timescale; the Mason number, $Mn = \frac{t_{mm}}{\mu/\varepsilon^+ E_\infty^2}$ measures the strength of the electric field; the dimensionless membrane capacitance, $C = \frac{RC_m/\sigma^+}{t_{mm}}$ measures the membrane charging rate; the dimensionless membrane conductivity, $G = RG_m/\sigma^+$ measures the ratio of charging and membrane conductivity rate

Hydrodynamical part:

$$
\begin{aligned}
&\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\nabla p + \frac{1}{Re}\Delta \mathbf{u} \\
&+ \int_\Sigma \left(\mathbf{F}_\gamma + \frac{1}{Re\,Ca}\mathbf{F}_b + \frac{Mn}{Re}\mathbf{F}_E \right) \delta(\mathbf{x} - \mathbf{X}) \left|\mathbf{X}_s\right| \; \mathrm{d}s \quad \text{in } \Omega \\
&\nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega \\
&\frac{\partial \mathbf{X}}{\partial t} = \int_\Omega \mathbf{u}(\mathbf{x}, t)\delta(\mathbf{x} - \mathbf{X}) \; \mathrm{d}\mathbf{x} \quad \text{on } \Sigma
\end{aligned}
$$

Electrical part:

$$
\begin{gathered}
\Delta \phi = 0 \quad \text{in } \Omega/\Sigma, \quad [\phi] = V_m, \quad [\sigma \phi_n] = 0 \quad \text{on } \Sigma \\
\left(1 - \frac{1}{\sigma_r}\right)\left(C\frac{\partial V_m}{\partial t} + G V_m\right) = [\phi_n] \quad \text{on } \Sigma
\end{gathered}
$$

Interfacial forces:

$$
\begin{aligned}
&\mathbf{F}_\gamma = \frac{1}{|\mathbf{X}_s|}\gamma_s \boldsymbol{\tau} - \gamma\kappa\mathbf{n}, \qquad \text{where } \gamma = \gamma_0(|\mathbf{X}_s| - |\mathbf{X}_s|^0) \\
&\mathbf{F}_b = \left(\Delta_s \kappa + \frac{\kappa^3}{2}\right)\mathbf{n}, \quad \mathbf{E} = -\nabla\phi \quad \mathbf{F}_E = \left(\mathbf{M}_E^+ - \mathbf{M}_E^-\right) \cdot \mathbf{n}
\end{aligned}
$$

Numerical algorithm

1. Solve the electric potential ϕ^n and the transmembrane potential (using Crank-Nicholson scheme) by the immersed interface method. Then we perform the one-sided difference by least squares polynomial approach to compute $\mathbf{E}^n = (-\phi_x^n, -\phi_y^n)$ at the Lagrangian markers and use them to compute the Maxwell stress tensor $\mathbf{M}_E^+$ and $\mathbf{M}_E^-$ to obtain the interfacial electric force $\mathbf{F}_E^n$ (also at Lagrangian markers)
2. Compute the tension force $\mathbf{F}_\gamma^n$ associated with the spring-like tension $\gamma^n = \gamma_0(|\mathbf{X}_s|^n - |\mathbf{X}_s|^0)$ and the bending force $\mathbf{F}_b^n$ (by Fourier spectral method)
3. Distribute the interfacial force terms $\mathbf{F}_E^n$, $\mathbf{F}_\gamma^n$ and $\mathbf{F}_b^n$ from the Lagrangian markers to the fluid grid points by using the discrete delta function as in traditional IB method
4. Solve the Navier-Stokes equations by the pressure-increment projection method to obtain new velocity field $\mathbf{u}^{n+1}$
5. Interpolate the new velocity on the fluid grid point to the marker points and then move the marker points to new positions $\mathbf{X}^{n+1}$

Numerical results

Parameter setting

- Put a prolate vesicle in $\Omega = [-4, 4] \times [-4, 4]$
- Fix the reduced area $\nu = 4\pi A_0/L_0^2 = 0.9$, where A_0 and L_0 are the area and perimeter of the vesicle respectively, the effect radius $R = \sqrt{A_0/\pi} = 1$,
- Choose the stiffness number $\gamma_0 = 2 \times 10^5$
- Unless otherwise stated, the Reynolds number $Re = 0.02$, the Capillary number $Ca = 10$, the Mason number $Mn = 20$, the membrane capacitance $C = 0.1$, the conductivity ratio $\sigma_r = 0.1$, the permittivity ratio $\varepsilon_r = 1$

Numerical study

- Convergence test for the fluid variables
- The prolate-oblate-prolate transition
- Effect of membrane conductance
- Effect of Reynolds number
- Combination of shear flow and electric field
- Unmatched viscosity

Convergence test for the fluid variables

- Take the membrane capacitance $C = 0.1$ and membrane conductance $G = 0.05$ with different grid sizes $N = 80, 160, 320, 640$
- The successive error $\|u_{2N} - u_N\|_\infty$, the Rate $= \log_2 \frac{\|u_N - u_{N/2}\|}{\|u_{2N} - u_N\|}$ (also for v and $\mathbf{X}$)

N	$\|u_{2N} - u_N\|_\infty$	Rate	$\|\mathbf{X}_{2N} - \mathbf{X}_N\|_\infty$	Rate	$\frac{\lvert A_N - A_0\rvert}{A_0}$
80	1.459E−01	-	1.006E−02	-	9.737E−05
160	4.407E−02	1.73	3.065E−03	1.72	2.090E−05
320	1.228E−02	1.84	8.545E−04	1.84	7.656E−06

Table: The mesh refinement analysis for the velocity component u, and the vesicle configuration $\mathbf{X}$, and the relative volume loss of the vesicle at $T = 0.1$

The prolate-oblate-prolate (POP) transition

- Take the membrane capacitance $C = 0.1$ and the membrane conductance $G = 0$ (perfect capacitor)

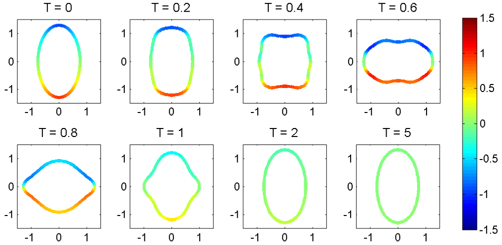


Figure: (a) The snapshots for the POP transition. The color indicates the density of surface charge $Q = [\varepsilon \mathbf{E} \cdot \mathbf{n}]$; $Ca = 10$

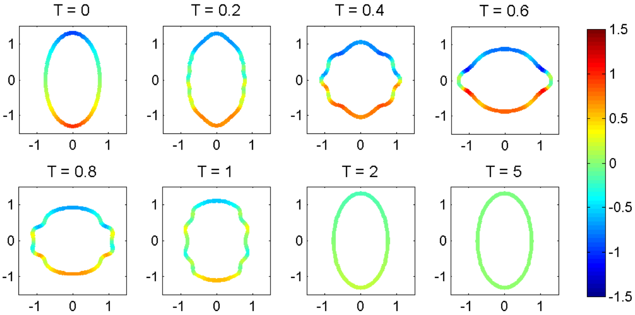


Figure: (a) The snapshots for the POP transition. The color indicates the density of surface charge $Q = [\varepsilon \mathbf{E} \cdot \mathbf{n}]$; $Ca = 1000$

Discussion: when the vesicle membrane capacitor is fully-charged $Q = 0$

- Recall the transmembrane potential equation

$$\left(1 - \frac{1}{\sigma_r}\right)\left(C\frac{\partial V_m}{\partial t} + GV_m\right) = [\phi_n] \Rightarrow [\phi_n] = 0 \text{ at equilibrium}$$

- By using the definition

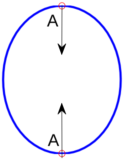
$$Q = [\varepsilon \mathbf{E} \cdot \mathbf{n}] = -[\varepsilon \phi_n] = -[\phi_n]$$

  we have $Q = 0$ at equilibrium state

Why POP transition?

Assume $\varepsilon^+ = \varepsilon^- = \varepsilon$ and denote $J_n = \sigma \mathbf{E} \cdot \mathbf{n}$, $E_\tau = \mathbf{E} \cdot \boldsymbol{\tau}$, the electric force can be alternatively written by

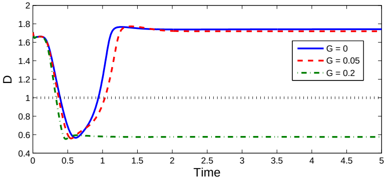
$$\mathbf{F}_E = \frac{\varepsilon}{2}\left(J_n^2\left(\frac{1}{(\sigma^+)^2} - \frac{1}{(\sigma^-)^2}\right) - ({E_\tau^+}^2 - {E_\tau^-}^2)\right)\mathbf{n} + J_n\,\varepsilon\left(\frac{E_\tau^+}{\sigma^+} - \frac{E_\tau^-}{\sigma^-}\right)\boldsymbol{\tau}$$



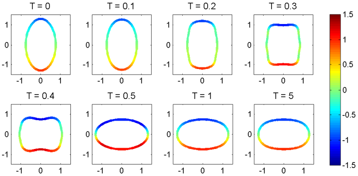
The electric force at A points inward if $\sigma_r < 1$

Effect of membrane conductance

- Fix $C = 0.1$ and vary the membrane conductance $G = 0, 0.05, 0.2$
- (a) The deformation number D versus time (b) The snapshots of the vesicle with $G = 0.2$. The color denotes the value of surface charge density Q.



(a)



(b)

Effect of Reynolds number

- Fix the membrane capacitance $C = 0.1$ and membrane conductance $G = 0$
- We run the simulations with $Re = 0.02, 0.2, 2$
- We attribute damping on POP transition $(Re = 2)$ by the effect of inertia

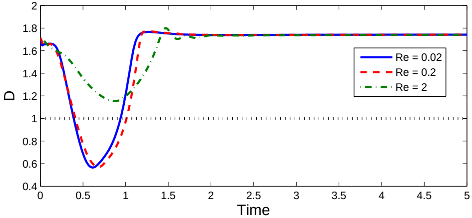
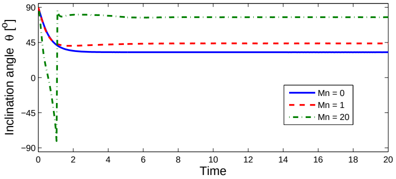


Figure: The time evolutional profile of deformation number D for $Re = 0.02, 0.2, 2$ with fixed $C = 0.1$ and $G = 0$

Combination of shear flow and electric field

- A normalized shear flow $\mathbf{u} = (y, 0)$ is imposed
- $C = 0.1$ and $G = 0$
- Choose $Mn = 0, 1, 20$ (no electric field applied for $Mn = 0$) and measure the inclination angle θ
- The larger electric field is applied, the larger inclination angle will be



(a)

Figure: (a) The inclination angles for $Mn = 0, 1, 20$

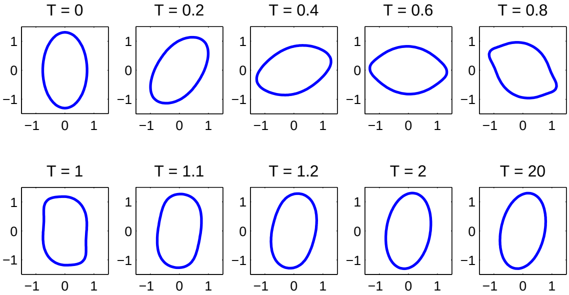


Figure: (b) the snapshots for vesicle under shear flow, $Mn = 20$

Unmatched viscosity

- The viscosity contrast $\mu_r = \frac{\mu^-}{\mu^+} = 20$ (to ensure the vesicle tumbles under shear flow but without the electrical field), $Re = 0.02$ (to avoid vesicle tumbling inhibited by inertia)
- $C = 0.1$ and $G = 0$
- Choose $Mn = 0, 1, 20$ (no electric field applied for $Mn = 0$) and measure the inclination angle θ
- Increasing the intensity of electrical field, the tumbling motion of vesicle under shear flow will be damped out

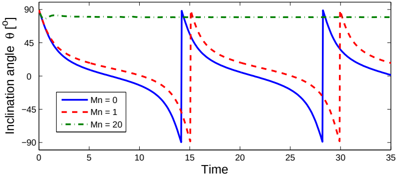


Figure: The inclination angles for $Mn = 0, 1, 20$;

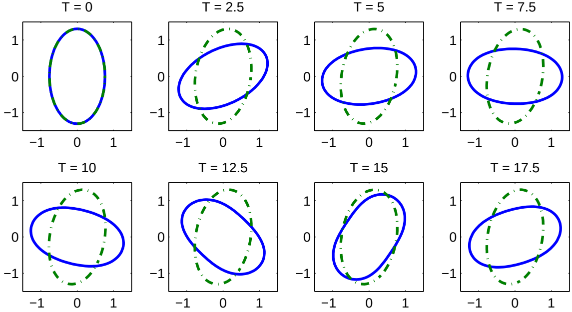


Figure: (b) the snapshots for vesicle under shear flow. Solid line '-': $Mn = 0$; dashed dotted line '-.-': $Mn = 20$