An immersed boundary method for simulating vesicle dynamics in three dimensions

Yunchang Seol
Mathematics Division
National Center for Theoretical Sciences (NCTS)
National Taiwan University, Taiwan

Collaborators: Wei-Fan Hu (NCHU, Taiwan),
Yongsam Kim (CAU, Korea),
Ming-Chih Lai (NCTU, Taiwan)

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Outline

What are Vesicles?

Vesicles are cellular organelles that are composed of a lipid bilayer.

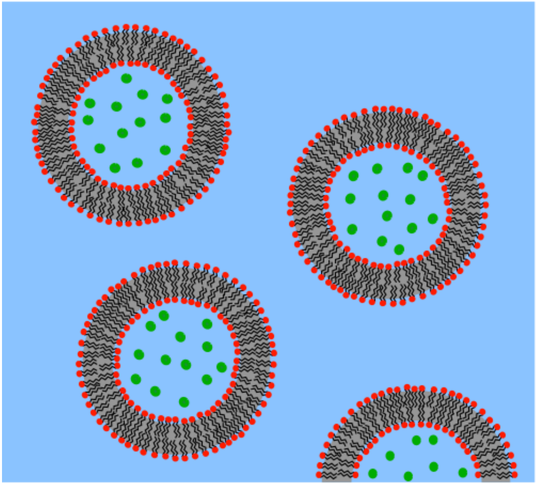


Figure: Diagram of lipid vesicles showing a solution of molecules (green dots) trapped in the vesicle interior. (Taken from Wikipedia.org)

Vesicle and Red Blood Cells (RBCs) both share similar mechanical behaviors.

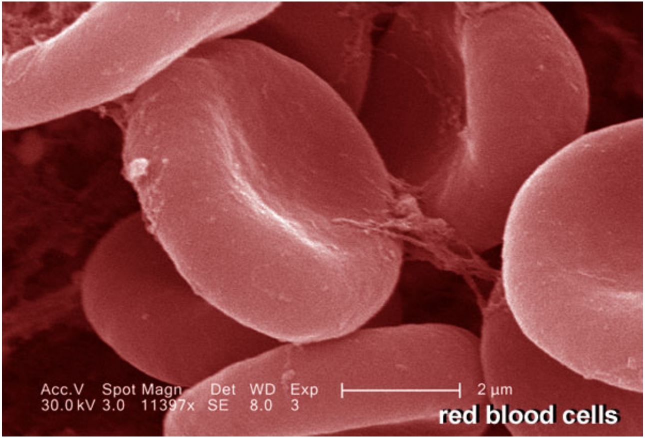


Figure: Red Blood Cells (Taken from Google Search)

Governing equations

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\nabla p + \frac{1}{Re}\Delta \mathbf{u} + \mathbf{f}, \tag{1}$$

$$\nabla \cdot \mathbf{u} = 0, \tag{2}$$

$$\mathbf{f}(\mathbf{x}) = \int_\Gamma \left(\mathbf{F}_\sigma + \frac{1}{ReCa}\mathbf{F}_b \right) \delta(\mathbf{x} - \mathbf{X}(r,s,t))\, \mathrm{d}A, \tag{3}$$

$$\mathbf{F}_\sigma = \nabla_s \sigma - 2H\sigma\mathbf{n}, \qquad \mathbf{F}_b = \frac{1}{2}\left(\Delta_s H + 2H(H^2 - K)\right)\mathbf{n}, \tag{4}$$

$$\frac{\partial \mathbf{X}}{\partial t}(r,s,t) = \mathbf{U}(r,s,t) = \int_\Omega \mathbf{u}(\mathbf{x},t)\delta(\mathbf{x} - \mathbf{X}(r,s,t))d\mathbf{x}, \tag{5}$$

$$\nabla_s \cdot \mathbf{U} = 0 \quad \text{on } \Gamma. \tag{6}$$

where $Re = \rho R_0^2/\mu t_c$ (the Reynolds number), $Ca = \mu R_0^3/c_b t_c$ (the capillary number), and $R_0 = \sqrt{A/4\pi} = (3V/4\pi)^{1/3}$ (effective radius).

$$\nu = \frac{3V}{4\pi(A/4\pi)^{3/2}} \tag{7}$$

The reduced volume ν represents the volume ratio between the vesicle and the sphere with the same surface area. ($\nu = 1$ for sphere)

Classical differential geometry

For the vesicle boundary $\mathbf{X}$, define the first fundamental coefficients as

$$E = \mathbf{X}_r \cdot \mathbf{X}_r, \quad F = \mathbf{X}_r \cdot \mathbf{X}_s, \quad \text{and} \quad G = \mathbf{X}_s \cdot \mathbf{X}_s,$$

then

- $\nabla_s \sigma = \dfrac{G\mathbf{X}_r - F\mathbf{X}_s}{EG - F^2}\sigma_r + \dfrac{E\mathbf{X}_s - F\mathbf{X}_r}{EG - F^2}\sigma_s$
- $\nabla_s \cdot \mathbf{U} = \dfrac{G\mathbf{X}_r - F\mathbf{X}_s}{EG - F^2} \cdot \mathbf{U}_r + \dfrac{E\mathbf{X}_s - F\mathbf{X}_r}{EG - F^2} \cdot \mathbf{U}_s$
- Using $\mathbf{a} \times (\mathbf{b} \times \mathbf{c}) = (\mathbf{a} \cdot \mathbf{c})\mathbf{b} - (\mathbf{a} \cdot \mathbf{b})\mathbf{c}$,
  we obtain two useful relations

$$\mathbf{X}_s \times \mathbf{n} = \frac{G\mathbf{X}_r - F\mathbf{X}_s}{|\mathbf{X}_r \times \mathbf{X}_s|}, \quad \mathbf{n} \times \mathbf{X}_r = \frac{E\mathbf{X}_s - F\mathbf{X}_r}{|\mathbf{X}_r \times \mathbf{X}_s|}$$

  which give

- $\nabla_s \sigma = \dfrac{(\mathbf{X}_s \times \mathbf{n})\sigma_r + (\mathbf{n} \times \mathbf{X}_r)\sigma_s}{|\mathbf{X}_r \times \mathbf{X}_s|}$ and
- $\mathbf{X}_s \times \mathbf{n}_r + \mathbf{n}_s \times \mathbf{X}_r = -2H\mathbf{n}|\mathbf{X}_r \times \mathbf{X}_s|$.

Nearly incompressible surface

To avoid solving the extra unknown tension $\sigma(r, s, t)$, we propose an alternative way to *approximate* the zero surface divergence. We use

$$\frac{\partial}{\partial t}|\mathbf{X}_r \times \mathbf{X}_s| = (\nabla_s \cdot \mathbf{U})|\mathbf{X}_r \times \mathbf{X}_s|$$

from which each surface dilating factor should maintain the initial profile during time integration whenever $\nabla_s \cdot \mathbf{U} = 0$. Therefore, we introduce a spring-like elastic tension as

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

where $\sigma_0 \gg 1$ and $|\mathbf{X}_r^0 \times \mathbf{X}_s^0|$ is the initial surface dilating factor. We also define the modified elastic energy by

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

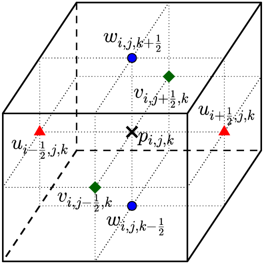
Derivation of the rate of change of surface dilation factor

$$
\begin{aligned}
\frac{\partial}{\partial t}|\mathbf{X}_r \times \mathbf{X}_s| &= \frac{\mathbf{X}_r \times \mathbf{X}_s}{|\mathbf{X}_r \times \mathbf{X}_s|} \cdot (\mathbf{X}_{rt} \times \mathbf{X}_s + \mathbf{X}_r \times \mathbf{X}_{st}) \\
&= \mathbf{n} \cdot (\mathbf{X}_{rt} \times \mathbf{X}_s) + \mathbf{n} \cdot (\mathbf{X}_r \times \mathbf{X}_{st}) \quad \left(\text{since } \mathbf{n} = \tfrac{\mathbf{X}_r \times \mathbf{X}_s}{|\mathbf{X}_r \times \mathbf{X}_s|}\right) \\
&= (\mathbf{X}_s \times \mathbf{n}) \cdot \mathbf{X}_{rt} + (\mathbf{n} \times \mathbf{X}_r) \cdot \mathbf{X}_{st} \quad (\text{using } (\mathbf{a} \times \mathbf{b}) \cdot \mathbf{c} = (\mathbf{b} \times \mathbf{c}) \cdot \mathbf{a}) \\
&= (\mathbf{X}_s \times \mathbf{n}) \cdot \mathbf{U}_r + (\mathbf{n} \times \mathbf{X}_r) \cdot \mathbf{U}_s \quad (\text{since } \mathbf{X}_t = \mathbf{U}) \\
&= \frac{G\mathbf{X}_r - F\mathbf{X}_s}{|\mathbf{X}_r \times \mathbf{X}_s|} \cdot \mathbf{U}_r + \frac{E\mathbf{X}_s - F\mathbf{X}_r}{|\mathbf{X}_r \times \mathbf{X}_s|} \cdot \mathbf{U}_s \quad (\text{using the two relations}) \\
&= (\nabla_s \cdot \mathbf{U})|\mathbf{X}_r \times \mathbf{X}_s| \quad (\text{by the definition of } \nabla_s \cdot \mathbf{U})
\end{aligned}
$$

Derivation of modified elastic force by variational derivative

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

Grid layouts for Eulerian and Lagrangian variables



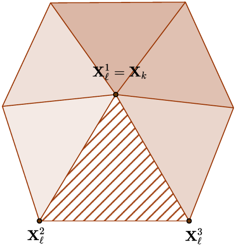


Figure: Fluid variables on a staggered MAC grid in 3D (left). Triangular surface patches that share the vertex $\mathbf{X}_k$ (right).

- The unit outward normal vector of the ℓ-th triangle is $\mathbf{n}_\ell = \frac{(\mathbf{X}_\ell^2 - \mathbf{X}_\ell^1)\times(\mathbf{X}_\ell^3 - \mathbf{X}_\ell^1)}{\left|(\mathbf{X}_\ell^2 - \mathbf{X}_\ell^1)\times(\mathbf{X}_\ell^3 - \mathbf{X}_\ell^1)\right|}$.
- The area of the ℓ-th triangle is $\mathrm{d}A_\ell = \left|(\mathbf{X}_\ell^2 - \mathbf{X}_\ell^1)\times(\mathbf{X}_\ell^3 - \mathbf{X}_\ell^1)\right|/2$.

Numerical algorithm

1. Compute the vesicle boundary forces.

   We find the tension $\mathbf{F}_\sigma(\mathbf{X}_k) = \nabla_s \sigma(\mathbf{X}_k) - \sigma(\mathbf{X}_k)\mathbf{H}(\mathbf{X}_k)$ using

   $\sigma_\ell = \tilde{\sigma}_0 \left(\mathrm{d}A_\ell - \mathrm{d}A_\ell^0 \right)$, where formally $\tilde{\sigma}_0 = \sigma_0/(drds)$,

   $$\sigma(\mathbf{X}_k) = \sum_{\ell \in T(\mathbf{X}_k)} \sigma_\ell/3,$$

   $$\nabla_s \sigma_\ell = \frac{(\mathbf{X}_\ell^3 - \mathbf{X}_\ell^1) \times \mathbf{n}_\ell}{2\,\mathrm{d}A_\ell}(\sigma_\ell^2 - \sigma_\ell^1) + \frac{\mathbf{n}_\ell \times (\mathbf{X}_\ell^2 - \mathbf{X}_\ell^1)}{2\,\mathrm{d}A_\ell}\left(\sigma_\ell^3 - \sigma_\ell^1\right),$$

   $$\nabla_s \sigma(\mathbf{X}_k) = \sum_{\ell \in T(\mathbf{X}_k)} \omega_\ell \nabla_s \sigma_\ell, \text{ where } \omega_\ell = \frac{\mathrm{d}A_\ell/3}{\mathrm{d}A(\mathbf{X}_k)},$$

   $$\mathbf{H}(\mathbf{X}_k) = \frac{1}{2\,\mathrm{d}A(\mathbf{X}_k)} \sum_{\ell \in T(\mathbf{X}_k)} \mathbf{n}_\ell \times \left(\mathbf{X}_\ell^3 - \mathbf{X}_\ell^2\right), \text{ where } \mathbf{H} = 2H\mathbf{n}.$$

   For a smooth surface patch S, the last formula is a discrete version of

   $$\int_S 2H\mathbf{n}\,\mathrm{d}A = \oint_{\partial S} \mathbf{n} \times \mathrm{d}\mathbf{X},$$ and equivalent to the cotangent formula.

From the discrete version of bending energy

$$E_b[\mathbf{X}] = \frac{c_b}{8} \sum_{k=1}^{N_v} |\mathbf{H}(\mathbf{X}_k)|^2 \, \mathrm{d}A(\mathbf{X}_k),$$

we obtain the bending force $\mathbf{F}_b(\mathbf{X}_k)\mathrm{d}A(\mathbf{X}_k) =$

$$\frac{c_b}{8} \sum_{\ell \in T(\mathbf{X}_k)} \left((H_\ell - \mathbf{n}_\ell \cdot \mathbf{C}_\ell) \left(\frac{1}{2} \mathbf{n}_\ell \times \mathbf{E}_\ell^k \right) + \frac{1}{2} \mathbf{C}_\ell \times \mathbf{E}_\ell^k + \mathbf{n}_\ell \times \mathbf{h}_\ell^k \right),$$

where

$$H_\ell = \frac{1}{3} \sum_{p \in V(\ell)} |\mathbf{H}(\mathbf{X}_p)|^2, \quad \mathbf{C}_\ell = \frac{1}{\mathrm{d}A_\ell} \sum_{p \in V(\ell)} \mathbf{E}_\ell^p \times \mathbf{H}(\mathbf{X}_p),$$

$$\mathbf{E}_\ell^k = \mathbf{X}_\ell^3 - \mathbf{X}_\ell^2, \quad \mathbf{h}_\ell^k = \mathbf{H}(\mathbf{X}_\ell^3) - \mathbf{H}(\mathbf{X}_\ell^2).$$

Thus, the boundary force becomes

$$\mathbf{F}(\mathbf{X}_k^n)\mathrm{d}A(\mathbf{X}_k^n) = \mathbf{F}_\sigma(\mathbf{X}_k^n)\mathrm{d}A(\mathbf{X}_k^n) + \mathbf{F}_b(\mathbf{X}_k^n)\mathrm{d}A(\mathbf{X}_k^n).$$

2. Solve the Navier-Stokes

$$\rho\left(\frac{3\mathbf{u}^* - 4\mathbf{u}^n + \mathbf{u}^{n-1}}{2\Delta t} + 2\left(\mathbf{u}^n \cdot \nabla_h\right)\mathbf{u}^n - \left(\mathbf{u}^{n-1} \cdot \nabla_h\right)\mathbf{u}^{n-1}\right)$$

$$= -\nabla_h p^n + \mu \Delta_h \mathbf{u}^* + \sum_{k=1}^{N_v} \mathbf{F}(\mathbf{X}_k^n)\, \mathrm{d}A(\mathbf{X}_k^n)\delta_h\left(\mathbf{x} - \mathbf{X}_k^n\right),$$

$$\Delta_h p^* = \frac{3\rho}{2\Delta t}\nabla_h \cdot \mathbf{u}^*, \quad \frac{\partial p^*}{\partial \mathbf{n}} = 0 \text{ on } \partial\Omega, \quad \mathbf{u}^* = \mathbf{u}^{n+1} \text{ on } \partial\Omega,$$

$$\mathbf{u}^{n+1} = \mathbf{u}^* - \frac{2\Delta t}{3\rho}\nabla_h p^*, \nabla_h p^{n+1} = \nabla_h p^* + \nabla_h p^n - \frac{2\mu\Delta t}{3\rho}\Delta_h(\nabla_h p^*).$$

3. Update the new position

$$\mathbf{X}_k^{n+1} = \mathbf{X}_k^n + \Delta t \sum_{\mathbf{x}} \mathbf{u}^{n+1}(\mathbf{x})\delta_h(\mathbf{x} - \mathbf{X}_k^n)h^3$$

Equivalence of the discrete mean curvature vector formula and the cotangent formula

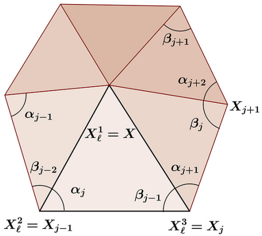


Figure: The notations for the computation of the mean curvature vector using two equivalent formulas.

We begin with the cotangent formula

$$\mathbf{H}(\mathbf{X})\mathrm{d}A(\mathbf{X}) = \frac{1}{2}\sum_{j=1}^{N}(\cot\alpha_j + \cot\beta_j)(\mathbf{X} - \mathbf{X}_j),$$

where $\mathbf{X}_j$ are the vertices within 1-ring of the vertex $\mathbf{X}$, and the angles α_j and β_j are the corresponding angles.

The righthand side becomes

$$
\begin{aligned}
&\frac{1}{2}\sum_{j=1}^{N}\left(\cot\alpha_j+\cot\beta_j\right)\left(\mathbf{X}-\mathbf{X}_j\right)\\
&=-\frac{1}{2}\sum_{j=1}^{N}\cot\alpha_j(\mathbf{X}_j-\mathbf{X})+\cot\beta_j(\mathbf{X}_j-\mathbf{X})\\
&=-\frac{1}{2}\sum_{j=1}^{N}\cot\alpha_j(\mathbf{X}_j-\mathbf{X})+\cot\beta_{j-1}(\mathbf{X}_{j-1}-\mathbf{X})\ \text{(using the periodicity of index)}\\
&=-\frac{1}{2}\sum_{j=1}^{N}\cot\alpha_j(\mathbf{X}_\ell^3-\mathbf{X}_\ell^1)+\cot\beta_{j-1}(\mathbf{X}_\ell^2-\mathbf{X}_\ell^1)\ \text{(denoting the vertices in the ℓ-th triangle)}\\
&=-\frac{1}{2}\sum_{j=1}^{N}\cot\alpha_j\mathbf{X}_{31}+\cot\beta_{j-1}\mathbf{X}_{21},\ \text{(where } \mathbf{X}_{ij}=\mathbf{X}_\ell^i-\mathbf{X}_\ell^j\text{)}.
\end{aligned}
\tag{8}
$$

Using the identity $\cot\theta=\frac{\mathbf{a}\cdot\mathbf{b}}{|\mathbf{a}\times\mathbf{b}|}=\frac{\mathbf{a}\cdot\mathbf{b}}{2\,\mathrm{d}A}$, where θ is the angle between the two vectors **a** and **b**, for the ℓ-th triangle with the vertices $\mathbf{X}_\ell^1$, $\mathbf{X}_\ell^2$, $\mathbf{X}_\ell^3$ and its area $\mathrm{d}A_\ell$, we obtain

$$\cot\alpha_j=\frac{\mathbf{X}_{12}\cdot\mathbf{X}_{32}}{2\,\mathrm{d}A_\ell},\quad \cot\beta_{j-1}=\frac{\mathbf{X}_{13}\cdot\mathbf{X}_{23}}{2\,\mathrm{d}A_\ell}.$$

Substituting these cotangents into Eq. (8) and summing all the triangles $T(\mathbf{X})$ within 1-ring around the vertex $\mathbf{X}$, we have

$$\frac{1}{2}\sum_{\ell\in T(\mathbf{X})}\frac{(\mathbf{X}_{21}\cdot\mathbf{X}_{32})\mathbf{X}_{31}-(\mathbf{X}_{31}\cdot\mathbf{X}_{32})\mathbf{X}_{21}}{2\,\mathrm{d}A_\ell},$$

which, using the vector triple product $(\mathbf{a}\times\mathbf{b})\times\mathbf{c}=(\mathbf{a}\cdot\mathbf{c})\mathbf{b}-(\mathbf{b}\cdot\mathbf{c})\mathbf{a}$, becomes

$$\begin{aligned}
& \frac{1}{2}\sum_{\ell\in T(\mathbf{X})}\frac{(\mathbf{X}_{21}\times\mathbf{X}_{31})\times\mathbf{X}_{32}}{2\,\mathrm{d}A_\ell} \\
= & \frac{1}{2}\sum_{\ell\in T(\mathbf{X})}\frac{(\mathbf{X}_{21}\times\mathbf{X}_{31})\times\mathbf{X}_{32}}{|\mathbf{X}_{21}\times\mathbf{X}_{31}|} \\
= & \frac{1}{2}\sum_{\ell\in T(\mathbf{X})}\mathbf{n}_\ell\times\mathbf{X}_{32}=\frac{1}{2}\sum_{\ell\in T(\mathbf{X})}\mathbf{n}_\ell\times(\mathbf{X}_\ell^3-\mathbf{X}_\ell^2).
\end{aligned}$$

Remesh of triangular surface

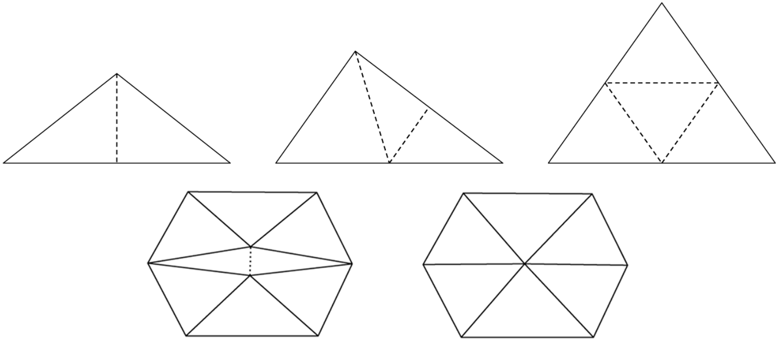


Figure: Re-meshing triangulation by edge addition (top) and deletion (bottom).

Mapping of local area during simulation

$$\sigma_\ell = \tilde{\sigma}_0 \left(dA_\ell^t - dA_\ell^0 \right)$$

X(0)

# Vertex	(x, y, z)
1	(0, 0, 0)
2	(0, 0, 1)
3	(0, 1, 1)
⋮	⋮

Index

# Triangle	(v_1, v_2, v_3)
1	(1, 2, 3)
2	(1, 4, 5)
3	(1, 6, 7)
⋮	⋮

X(t)

# Vertex	(x, y, z)
1	(0.1, 0, 0)
2	(0, 0, 2.1)
3	(1.2, 1, 2)
⋮	⋮

Figure: Mapping of triangular area.

Numerical results

Numerical issues

- Accuracy check for mean curvature and bending force
- Study on different stiffness parameter $\tilde{\sigma_0}$
- Convergence of vesicle configuration and fluid velocity
- Numerical experiments
  - A suspended vesicle in quiescent flow
  - A vesicle in shear flow
  - A vesicle under the gravity

Numerical parameters

Unless otherwise stated, we use

- $Re = 1, \; Ca = 50$
- $\sigma_0 = 6 \times 10^5$, grid width $h = 6/128$
- The initial number of triangles is either 81920 or 327680

Accuracy check for mean curvature and bending force

Using spherical parametric coordinates $(\theta, \phi) \in [0, 2\pi] \times [0, \pi]$,

- Unit sphere: $\mathbf{X}(\theta, \phi) = (\cos\theta \sin\phi, \sin\theta \sin\phi, \cos\phi)$,
- Ellipsoid: $\mathbf{X}(\theta, \phi) = (0.5\cos\theta \sin\phi, 0.5\sin\theta \sin\phi, \cos\phi)$,
- Biconcave surface: $\mathbf{X}(\theta, \phi) =$ $\left(\cos\theta \sin\phi, \sin\theta \sin\phi, (0.1242 + 0.8012\sin^2\phi - 0.4492\sin^4\phi)\cos\phi\right)$.

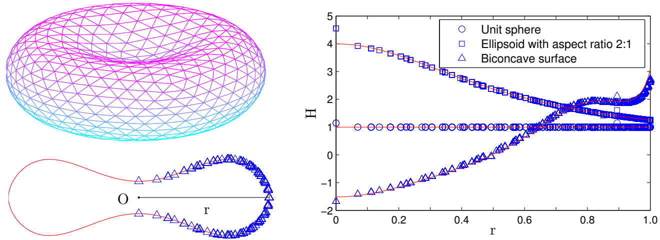


Figure: Left: A triangulated biconcave surface and its cross-sectional view. Right: The comparison of mean curvature between numerical values (symbols) and exact values (solid lines) for three different surfaces. Here, the number of vertices is $N_v = 2562$ corresponding to 5120 triangles used.

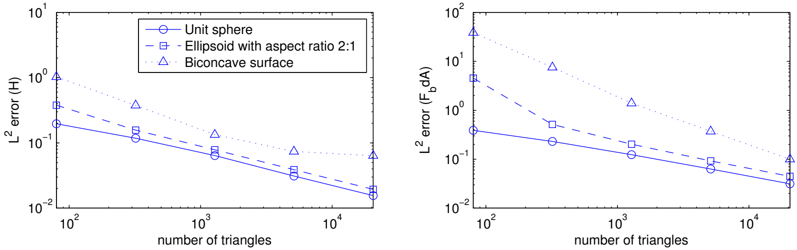


Figure: The L^2 errors for the mean curvature H (left) and the bending force $\mathbf{F}_b dA$ (right) as functions of the number of triangles.

The L^2 error of a function ψ is calculated as $\sqrt{\sum_{k=1}^{N_v} |\psi^e(\mathbf{X}_k) - \psi(\mathbf{X}_k)|^2 \, dA(\mathbf{X}_k)}$, where $\psi^e(\mathbf{X}_k)$ is the exact value and $\psi(\mathbf{X}_k)$ is the computed value.

Study on different stiffness parameter $\tilde{\sigma}_0$

In this test, we study how the stiffness number $\tilde{\sigma}_0$ affects the conservation of surface area and vesicle volume, and the total surface energy.

- Put an initially oblate vesicle $\mathbf{X}(\theta, \phi) = (\cos\theta \sin\phi, \sin\theta \sin\phi, \cos\phi/3.5)$ in quiescent flow
- Computational domain $\Omega = [-2, 2]^3$ with grid size 128^3
- Choose $\tilde{\sigma}_0 = 6 \times 10^4, 6 \times 10^5, 6 \times 10^6$
- The meshwidth $h = 1/32$ and the time step size $\Delta t = h/16$
- The number of triangles used in the initial vesicle surface is 81920 with 40962 number of vertices.

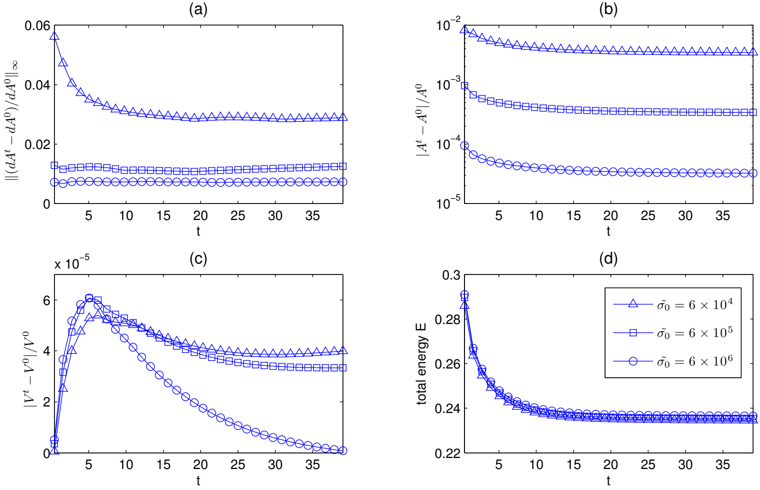


Figure: The comparison for three different stiffness parameters: $\tilde{\sigma_0} = 6 \times 10^4(\triangle)$, $6 \times 10^5(\square)$, and $6 \times 10^6(\bigcirc)$. (a) the maximum relative error of the local surface area; (b) the relative error of the global surface area; (c) the relative error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

Convergence of vesicle configuration and fluid velocity

- Relax the same oblate vesicle with $\nu = 0.643$ in a cube $[-2, 2]^3$
- The grid size $N = 32, 64, 128, 256$
- $\tilde{\sigma}_0 = (N/32)^2 10^4$ and $\Delta t = h/8$
- $ratio = \log_2(\|u_N - u_{2N}\|_\infty / \|u_{2N} - u_{4N}\|_\infty)$
- When $N = 32$, we use 5120 number of triangles which corresponds to 2562 number of vertices.

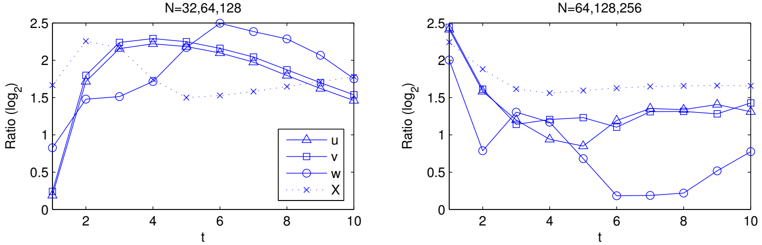


Figure: The ratios of convergence for the fluid velocity (u, v, w) and the vesicle configuration $\mathbf{X}$. Left: $N = 32$; Right: $N = 64$

Numerical experiments

A suspended vesicle in quiescent flow

- Oblate surface: $\mathbf{X}(\theta, \phi) = (\cos\theta \sin\phi, \sin\theta\sin\phi, \cos\phi/3.5)$
- Prolate surface: $\mathbf{X}(\theta, \phi) = (0.2\cos\theta \sin\phi, 0.2\sin\theta\sin\phi, \cos\phi)$
- Oscillatory surface: $\mathbf{X}(\theta, \phi) = \left(\frac{3}{20} r(\phi)\cos\theta\sin\phi, \frac{3}{20} r(\phi)\sin\theta\sin\phi, \frac{3}{25} r(\phi)\cos\phi\right)$, where $r(\phi) = \sqrt{\cos^2\phi + 9\sin^2\phi} + \cos^2(4\phi)$.
- $\Omega = [-2, 2]^3$, $c_b = 0.02$, $\tilde{\sigma_0} = 6 \times 10^5$, and $\Delta t = h/16$

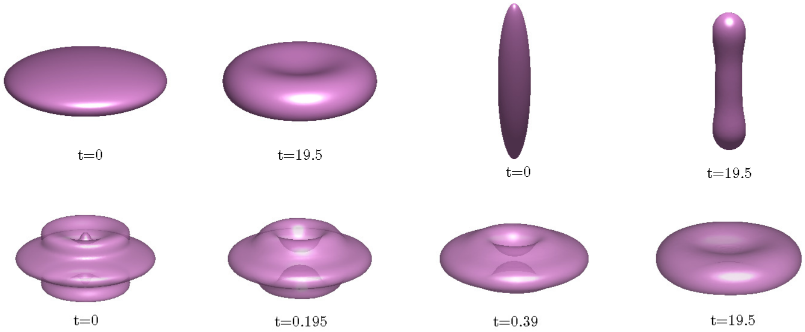


Figure: Suspended vesicles in quiescent flow. Oblate vesicle (two upper-left panels); Prolate vesicle (two upper-right panels); Oscillatory vesicle (lower panels)

A vesicle in shear flow

- Put a prolate vesicle in a simple shear flow $\mathbf{u} = (z, 0, 0)$
- The non-dimensional shear rate $\chi = \mu R_0^3 / c_b$
- $\Omega = [-3, 3]^3$ and a small Reynolds number $Re = 10^{-3} \ll 1$ (Stokes flow regime)
- The reduced volume $\nu = 0.8$, 0.85, 0.9, 0.95, and 0.975 by fixing the effective radius $R_0 = 1$

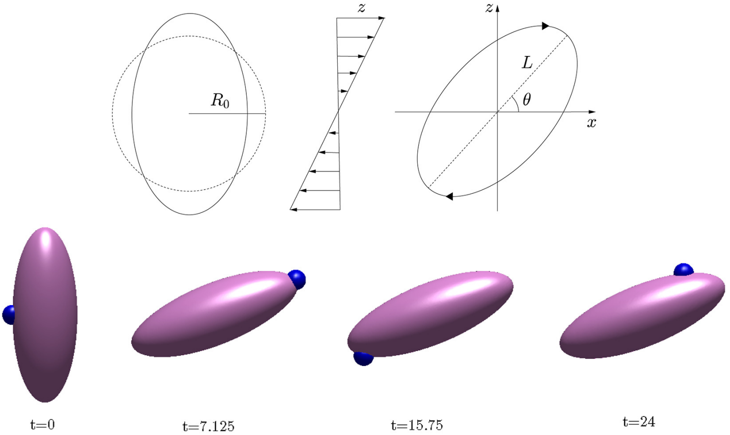


Figure: The simulation setup of a vesicle motion in a shear flow (top) and the tank-treading motion of a vesicle with $\nu = 0.8$ in a shear flow with $\chi = 100$ (bottom).

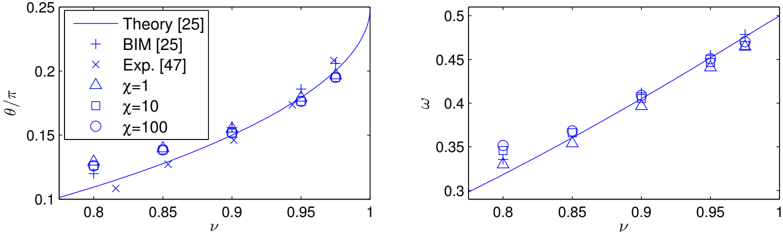


Figure: The plot of the inclination angle (left) and the scaled mean angular velocity (right) as functions of reduced volume ν for different dimensionless shear rate χ.

- 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 **r** and **v** are the position and velocity of the vertices projected on the xz-plane, respectively.

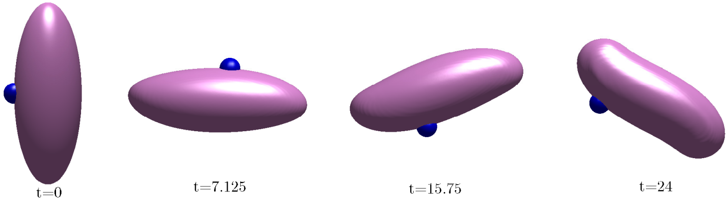


Figure: Tumbling motion of a vesicle with $\nu = 0.8$ and $\lambda = 40$ in a shear flow with $\chi = 100$. The computed time is up to $t = 24$.

To consider viscosity contrast between the interior and exterior of vesicle, instead of

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\nabla p + \frac{1}{Re}\Delta \mathbf{u} + \mathbf{f}, \tag{9}$$

we use

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\nabla p + \frac{1}{Re}\nabla \cdot \left[\mu(\mathbf{x})\left(\nabla \mathbf{u} + \nabla \mathbf{u}^T\right)\right] + \mathbf{f}, \tag{10}$$

where $\mu(\mathbf{x})$ is the dimensionless viscosity contrast.

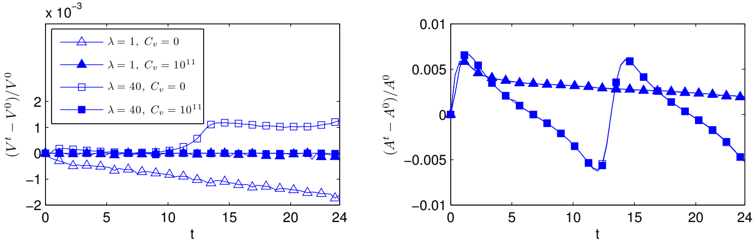


Figure: The volume relative errors (left) and the surface area relative errors (right) for the cases of with or without the penalty volume conservation term Eq. (11). Here, $\nu = 0.8$ and $\chi = 100$. The viscosity contrast $\lambda = 1$ and $\lambda = 40$, respectively.

To conserve the vesicle volume, we add

$$\mathbf{F}_v dA(\mathbf{X}) = -C_v \left(\frac{V^t - V^0}{V^0} \right) \mathbf{n}\, dA(\mathbf{X}), \tag{11}$$

where C_v is a sufficiently large constant called a penalty parameter, V^t is the global volume of vesicle at time t, and V^0 is the global volume of initially given vesicle.

A vesicle under the gravity

- Prolate: $\mathbf{X}(\theta, \phi) = (0.5 \cos\theta \sin\phi, 0.5 \sin\theta \sin\phi, \cos\phi)$
- Oblate: $\mathbf{X}(\theta, \phi) = (0.75 \cos\theta \sin\phi, 0.75 \sin\theta \sin\phi, 0.375 \cos\phi)$
- The prolate vesicle is placed at different tilted angles $\eta = 0, \pi/4$ and $\pi/2$ initially to see how the initial orientation affects the equilibrium shape
- To model this problem, simply add an interfacial force $\mathbf{F}_g dA(\mathbf{X}) = (\rho^i - \rho^e)(\mathbf{g} \cdot \mathbf{X}) dA(\mathbf{X})\mathbf{n}$ where ρ^i and ρ^e are interior and exterior fluid densities, respectively, and $\mathbf{g} = (0, 0, -1)$

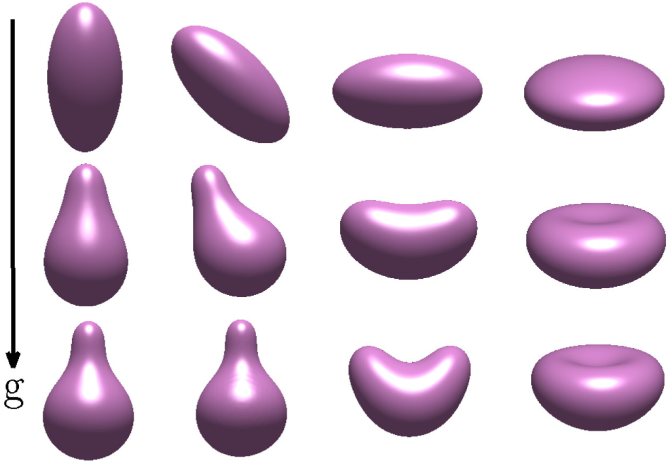


Figure: The prolate vesicle with three different tilted angles $\eta = 0, \pi/4, \pi/2$ (first to third column) and oblate (fourth column) vesicle under the gravity. All the snapshots are taken at the same time.

Future Works

- High-order scheme to compute the curvatures and the Laplace-Beltrami operator
- Vesicle dynamics in extensional flow or in Poiseuille flow
- Multi-vesicle problems to mimic the behaviors of RBCs in capillary
- Viscosity contrast effects on vesicle dynamics
- Reynolds number effects on vesicle dynamics

Thank you for your attention!