Numerical Simulation of 2D Fluid Membranes

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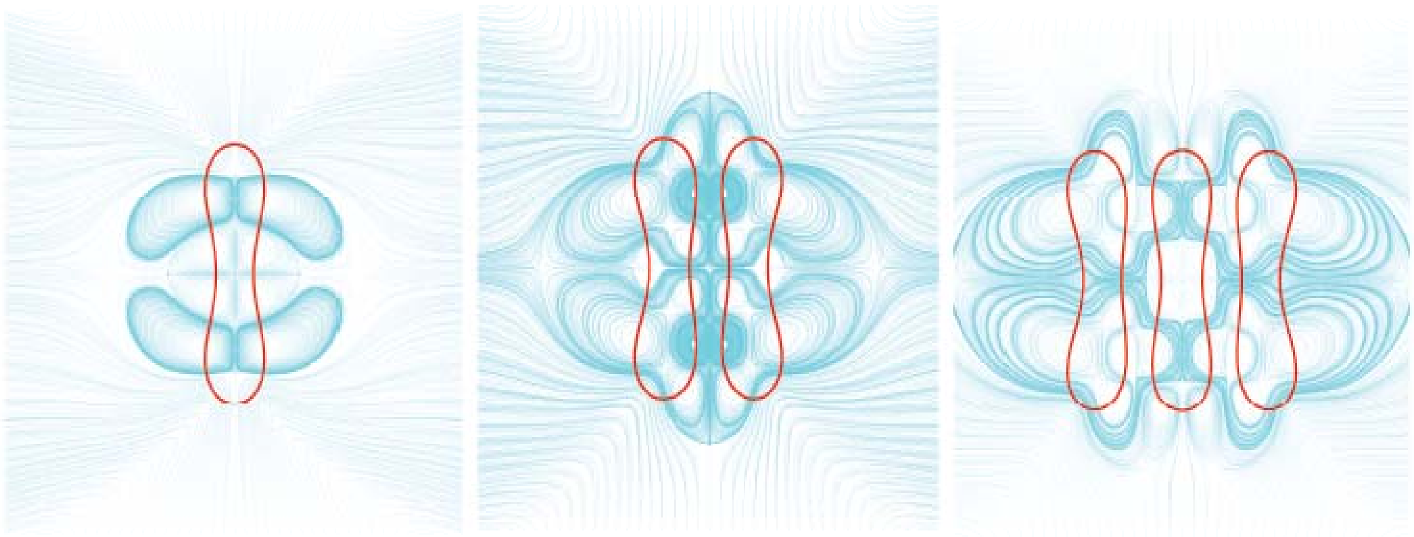

Collaborators/Support

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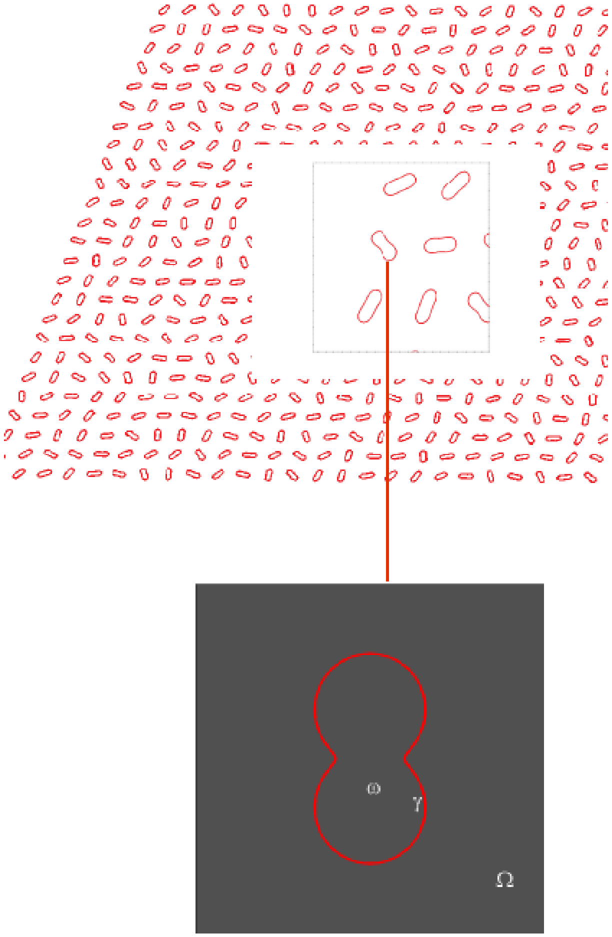
- Scott Diamond
  - *University of Pennsylvania*
- Denis Zorin, Denis Gueyffier
  - *New York University*

- NSF (DMS,OCI), DOE

Overview

- Motivation
- Vesicles and fluid membranes
  - Formulation
  - Numerics
  - Analytic solution
  - Simulations

Stokesian particulate flows



Fluid model:

$$\nabla p - \mathrm{div}(\mu \nabla \mathbf{v}) = \mathbf{F} \quad \text{in} \quad \Omega$$
$$\mathrm{div}\mathbf{v} = 0 \quad \text{in} \quad \Omega$$

Boundary Conditions:

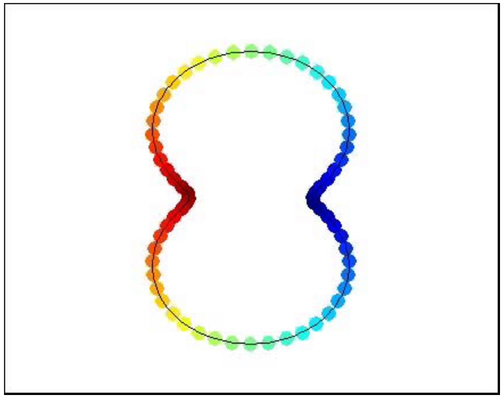
$$\mathbf{v} = \dot{\mathbf{x}} \quad \text{on} \quad \gamma \quad \text{and} \quad \lim_{\mathbf{x} \to \infty} \mathbf{v} = \mathbf{v}_\infty$$

Force:

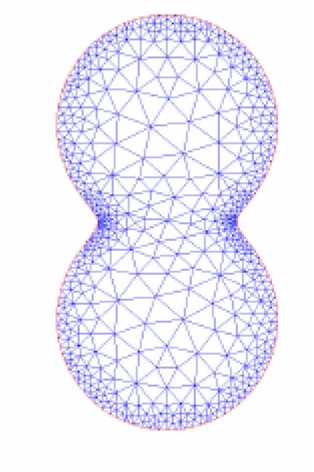
$$\mathbf{F}(\mathbf{x}) = \int_\gamma \delta(\mathbf{x} - \mathbf{y}) \mathbf{f}(\mathbf{y})\, d\gamma$$

Algorithmic challenges

- Moving interfaces, nonlinearity, complex geometries
- Algorithmic/Parallel scalability
  - Implicit time-stepping, Fast elliptic solvers
- High-order schemes
  - Faster running times for a few digits of accuracy
  - Long-time simulations

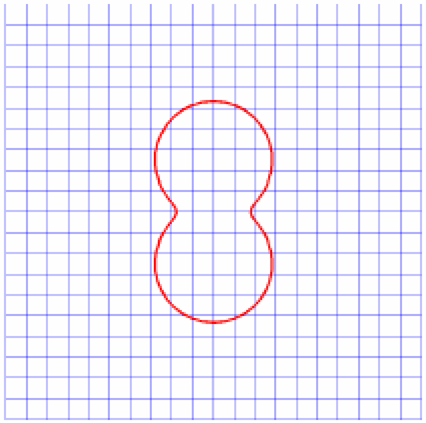


Problem: complex geometries



- Unstructured mesh generation
    - Sequential in 3D
    - Parallelizability
    - Preconditioners
        - Geometric coarsening algorithms
        - Algebraic multilevel methods
            - Do not work well for indefinite operators (Stokes, Helmholtz)
            - Large constants

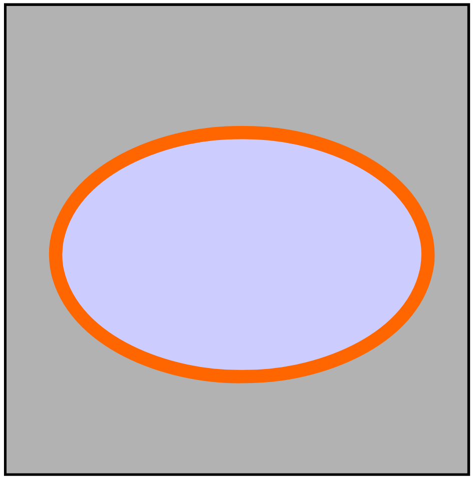
Cartesian grids



- Geometrically conforming grids
  - Expensive for moving boundaries
- Cartesian grids
  - Different stencils around the interface – typically modified finite volumes
- Regular grids
  - No modification on the regular grid operator, additional equations to satisfy jump conditions
- Advantages of regular grids
  - Fast solvers, phase field, level-set type problems

Interfacial flows/Integral equations for Re<<1

- Linear integral equation for exterior
- Linear integral equation for interior
- Nonlinear interface conditions
  - o Force balance
  - o Velocity continuity
- Nonlinearity on the interface only
- Can solve interfacial problem with a nonlinear system of equations on the **interface**



Vesicles

- Aqueous solution enclosed by lipid bilayer membrane
- Vanishing shear modulus; nearly inextensible

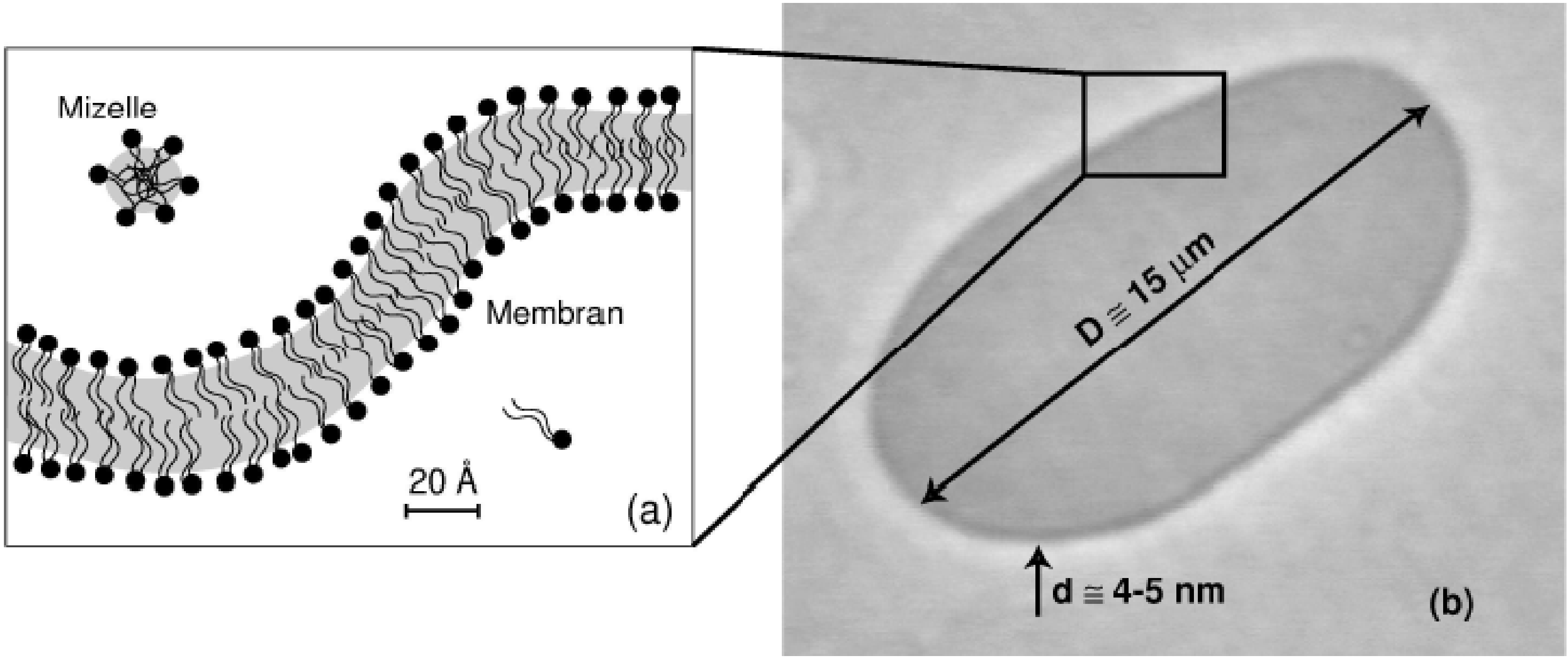


Image credit: Seifert' 98

A vesicle suspended in shear flow: experiment

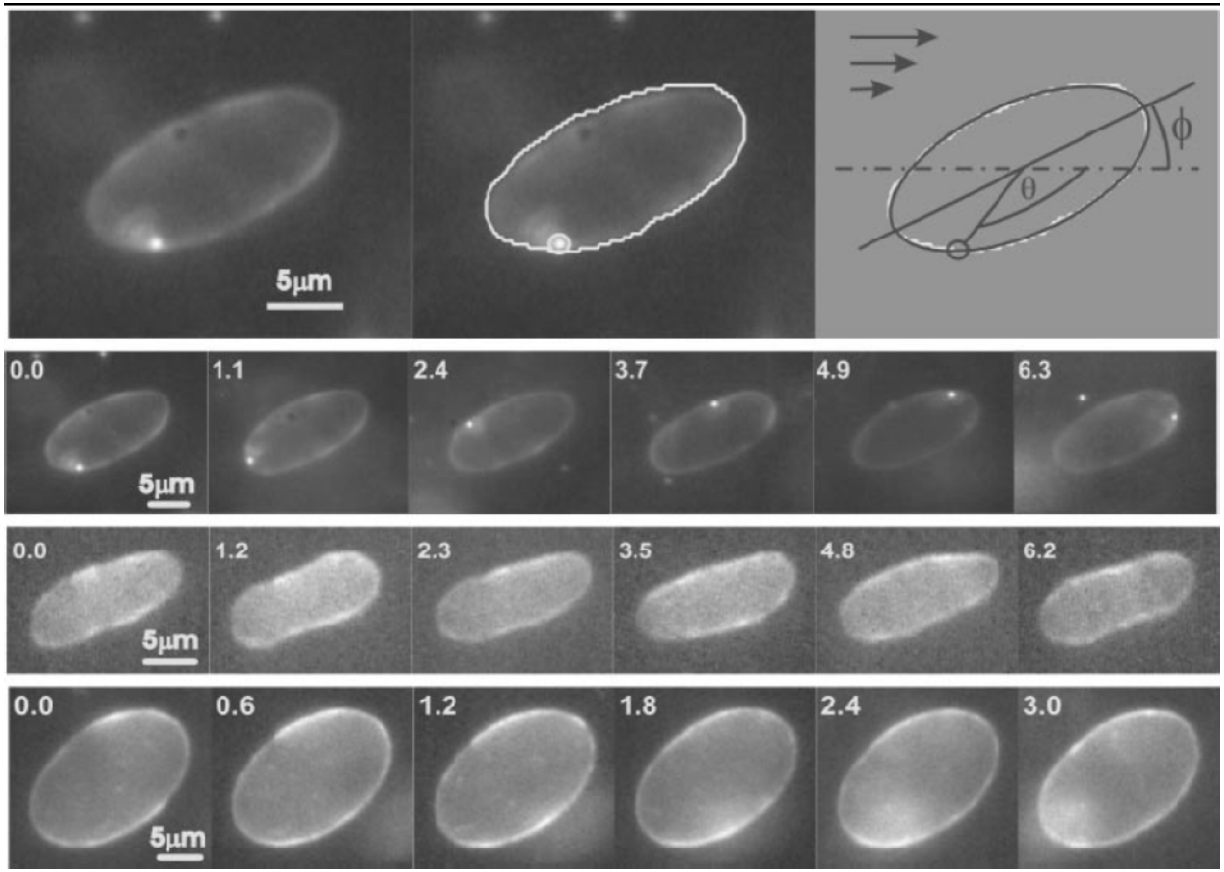
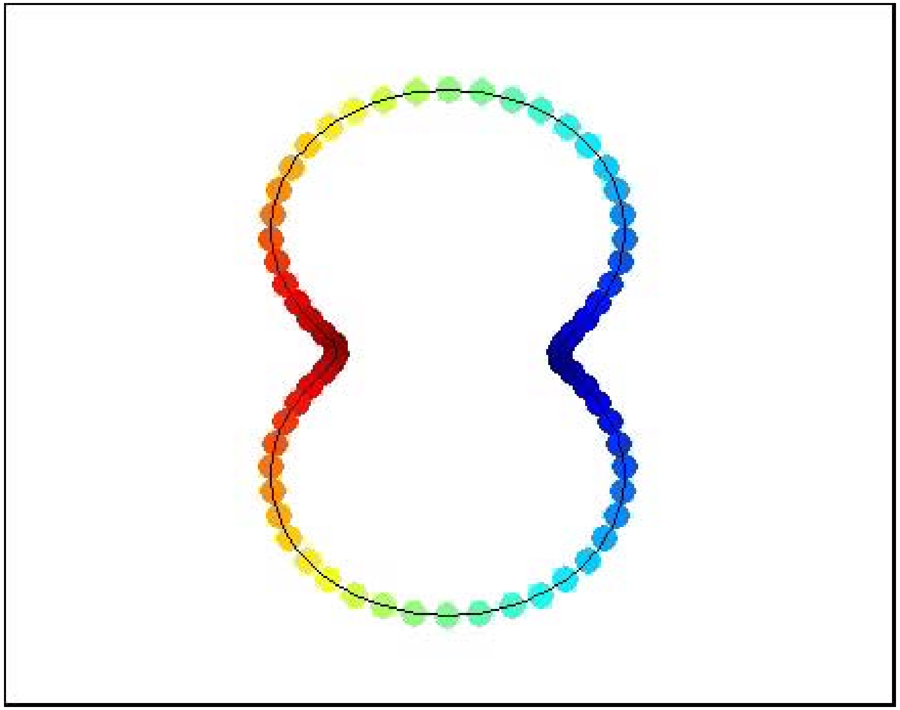
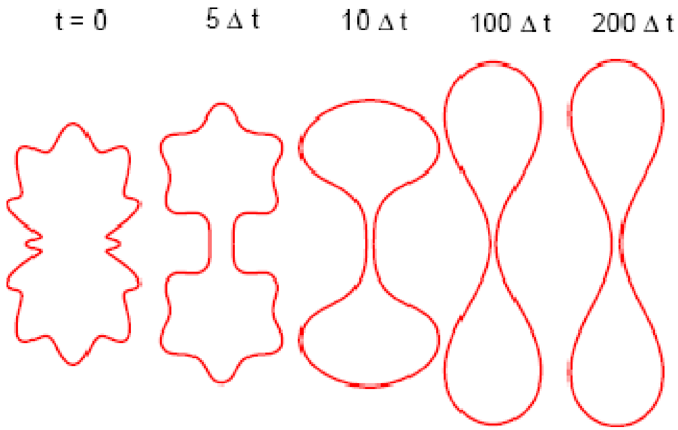


Image: Kanstler & Steinberg'05

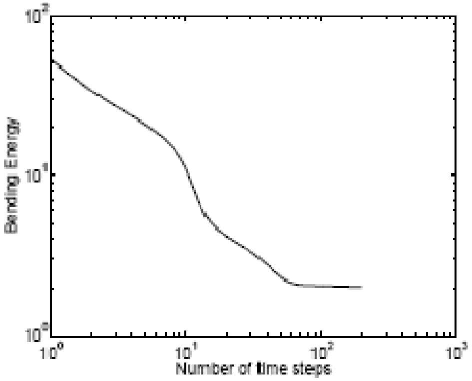
A vesicle suspended in shear flow: simulation



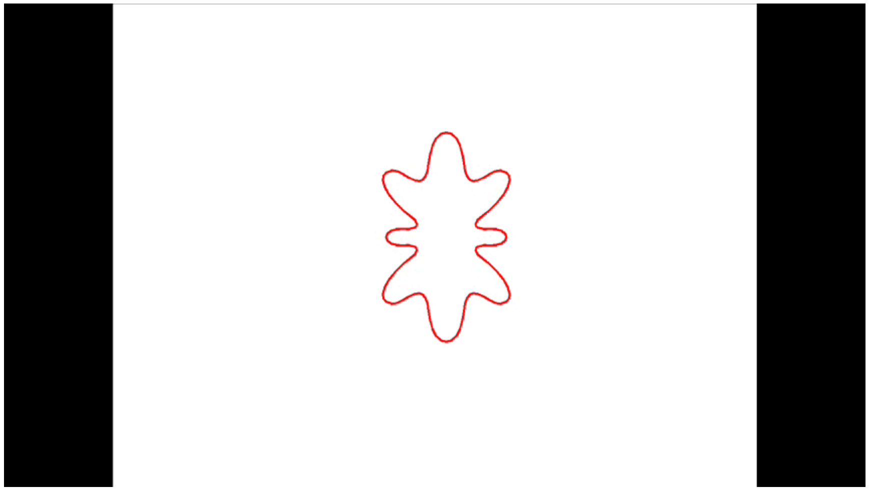
Freely suspended vesicle



(m) Relaxation



(n) Bending energy



Related work

Numerics for vesicles

- Zhou and Pozrikidis, 1995 - Inextensible vesicle in shear flow
- Cantat and Misbah, 1999 - Integral equations for vesicles
- Pozrikidis, 2001 - Global Cartesian coordinates
- Sukumaran and Seifert, 2001 - Adhesion of 3D vesicle
- Lowengrub, 2008 - Semi-implicit schemes for 2D vesicles

Closely related work

- Shelley and Ueda, 2000 - Stretching filaments
- Misbah et al, 2003 - Phase field methods
- Du et al, 2004 - Phase field method
- Tornberg and Shelley, 2003 - Inextensible filaments

Problem definition

Fluid model:

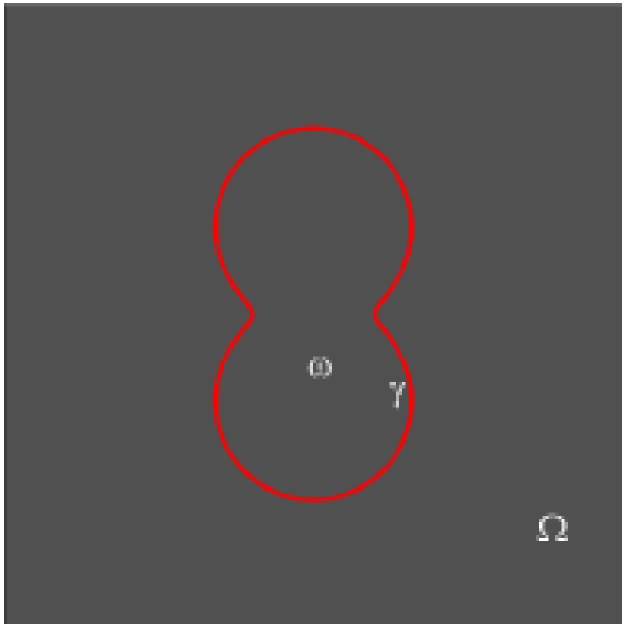
$$\begin{aligned} \nabla p - \mu \Delta \mathbf{v} = \mathbf{F} \quad & \text{in} \quad \Omega \\ \mathrm{div}\mathbf{v} = 0 \quad & \text{in} \quad \Omega \end{aligned}$$

Boundary Conditions:

$$\mathbf{v} = \dot{\mathbf{x}} \quad \text{on} \quad \gamma \quad \text{and} \quad \lim_{\mathbf{x}\to\infty} \mathbf{v} = \mathbf{v}_\infty$$

Force:

$$\mathbf{F}(\mathbf{x}) = \int_\gamma \delta(\mathbf{x} - \mathbf{y}) \mathbf{f}(\mathbf{y}) \, d\gamma$$



Jumps related to tension and bending

Jumps

$$\mathbf{f} = \nabla\left(\frac{1}{2}k_B\kappa^2 + \sigma\right)$$

$$\mathbf{f} = \mathbf{f}_\kappa + \mathbf{f}_\sigma$$

- $\mathbf{f}_\kappa = -k_B\left(\kappa\;\kappa_s\mathbf{t} + \kappa_{ss}\;\mathbf{n}\right)$
- $\mathbf{f}_\sigma = \sigma_s\mathbf{t} - \kappa\sigma\mathbf{n}$

Inextensibility constraint

$$\mathrm{div}_\gamma\dot{\mathbf{x}} = 0$$

σ membrane tension
κ curvature
k_B bending rigidity

Fluid model:

$$\begin{aligned} \nabla p - \mu\Delta\mathbf{v} &= \mathbf{F} \quad \text{in} \quad \Omega \\ \mathrm{div}\mathbf{v} &= 0 \quad \text{in} \quad \Omega \end{aligned}$$

Boundary Conditions:

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Force:

$$\mathbf{F}(\mathbf{x}) = \int_\gamma \delta(\mathbf{x}-\mathbf{y})\mathbf{f}(\mathbf{y})\,d\gamma$$

Integral equations

Governing equations for $\mathbf{x}$ and σ

$$\dot{\mathbf{x}} = \mathbf{v}_\infty(\mathbf{x}) + \mathcal{S}(\mathbf{x})[\mathbf{f}_\sigma(\mathbf{x}) + \mathbf{f}_\kappa(\mathbf{x})]$$

$$\mathrm{div}_{\gamma(\mathbf{x})}\mathcal{S}(\mathbf{x})[\mathbf{f}_\sigma(\mathbf{x}) + \mathbf{f}_\kappa(\mathbf{x})] = -\mathrm{div}_\gamma \mathbf{v}_\infty$$

Single-Layer Potential

$$\mathcal{S}[\mu](\mathbf{x}) = \int_\gamma G(\mathbf{x},\mathbf{y})\mu(\mathbf{y})\,ds(\mathbf{y})$$

$$G(\mathbf{x},\mathbf{y}) = \frac{1}{4\pi}\left(-\ln\rho\mathbf{I} + \frac{\mathbf{r}\otimes\mathbf{r}}{\rho^2}\right), \quad \mathbf{r} = \mathbf{x}-\mathbf{y}, \quad \rho = \|\mathbf{r}\|_2$$

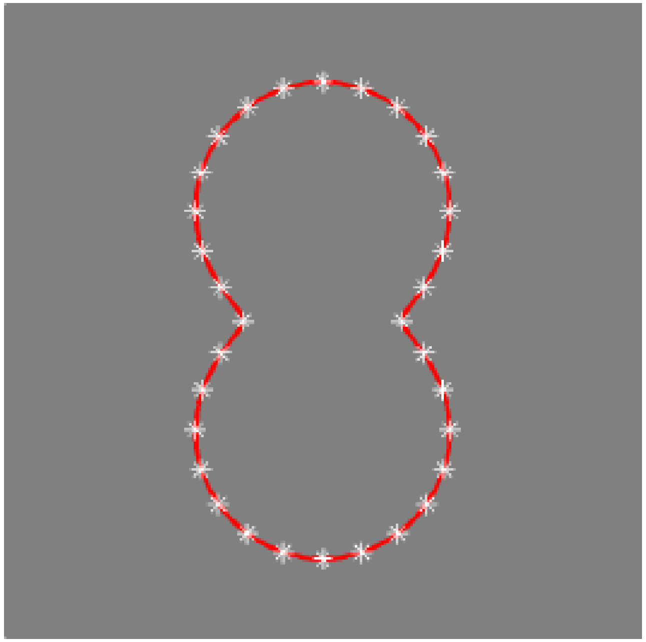
Discretization

- Time/space discretization
  - Existing implementations are RK4 explicit in time, and low-order accurate in space (discretization and quadratures)
  - Severe restrictions on time-step due to stiffness
  - long-time simulations, conservation of area/length are problematic
- Ill-conditioning and stability
  - No analysis of the operator
- Fast summation

Spatial discretization

$$\mathbf{x}(\alpha) = \sum_{k=-M/2}^{M/2-1} \hat{\mathbf{x}}(k) e^{-ik\alpha}, \quad \text{and} \quad \mathbf{x}_\alpha = \sum_{k=-M/2}^{M/2-1} (-ik)\hat{\mathbf{x}}(k) e^{-ik\alpha}$$

- Arc-length equispaced
- FFT for derivatives
- Corrected quadratures
  - o Alpert'99
- Nystrom for integral equation
- FMM for fast summation



Time-stepping scheme

IMEX scheme:

$$\frac{1}{\delta}\left(\mathbf{x}^n - \mathbf{x}^{n-1}\right) = -\mathbf{v}_\infty^n + \mathcal{S}[\mathbf{f}_\kappa^n + \mathbf{f}_\sigma^n],$$

$$\mathrm{div}_\gamma \mathcal{S}[\mathbf{f}_\sigma^n] = \mathrm{div}_\gamma \left(\mathbf{v}_\infty^n - \mathcal{S}[\mathbf{f}_\kappa^n]\right)$$

$$\mathbf{f}_\kappa^n = -k_B\left(\mathbf{x}_{ssss}^n + 2\kappa\kappa_s\mathbf{x}_s + \kappa^2\mathbf{x}_{ss}\right) \qquad \mathbf{f}_\sigma^n = \sigma_s^n\mathbf{t} - \sigma^n\kappa\mathbf{n}$$

$$\boxed{\mathbf{x}_s^n = \frac{\mathbf{x}_{s_0}^n}{s_{s_0}}}$$

Unknowns: $\mathbf{x}^n, \sigma^n$
Solve momentum for $\mathbf{x}^n$ (GMRES)
At each matvec, incompressibility for σ^n (GMRES)

Time-stepping scheme (details)

$$\frac{1}{\triangle t}\left(\mathbf{x}^{n+1}-\mathbf{x}^{n}\right)=\mathbf{v}_\infty+\mathcal{B}(\mathbf{x}^n)\mathbf{x}^{n+1}+\mathcal{T}(\mathbf{x}^n)\sigma^{n+1},$$

$$\mathcal{L}(\mathbf{x}^n)\sigma^{n+1}=-D(\mathbf{x}^n)\left[\mathbf{v}_\infty+\mathcal{B}(\mathbf{x}^n)\mathbf{x}^{n+1}\right],$$

$$\text{where}\quad \mathcal{B}(\mathbf{x}^n)\mathbf{x}^{n+1}=-\int_0^{2\pi}G(\mathbf{x}^n,\mathbf{y}^n)\left(\frac{1}{|\mathbf{y}^n_\alpha|}\left(\frac{1}{|\mathbf{y}^n_\alpha|}\left(\frac{\mathbf{y}^{n+1}_\alpha}{|\mathbf{y}^n_\alpha|}\right)_\alpha\right)_\alpha\right)_\alpha d\alpha,$$

$$\text{and}\quad \mathcal{T}(\mathbf{x}^n)\sigma^{n+1}=\int_0^{2\pi}G(\mathbf{x}^n,\mathbf{y}^n)\left(\sigma^{n+1}\frac{\mathbf{y}^n_\alpha}{|\mathbf{y}^n_\alpha|}\right)_\alpha d\alpha.$$

$$\mathcal{D}(\mathbf{x})\mathbf{f}:=\mathbf{x}_s\cdot\mathbf{f}_s;$$
$$\mathcal{L}(\mathbf{x}):=D(\mathbf{x})\mathcal{T}(\mathbf{x},\mathbf{x});$$

Spectral analysis

- Consider a single vesicle, the unit circle
- Write analytic expression for integral and differential operators
- 'Diagonalize' analytically
  - Pseudo-differential operators

- Example:

$$G(\mathbf{x},\mathbf{y}) = \frac{1}{4\pi\mu}\left(-\ln\rho\,1 + \frac{\mathbf{r}\otimes\mathbf{r}}{\rho^2}\right), \quad \mathbf{r} = \mathbf{x}-\mathbf{y}, \quad \rho = \|\mathbf{r}\|_2.$$

Single-layer potential and inextensibility operator

$$G(\mathbf{x},\mathbf{y}) = \frac{1}{4\pi\mu}\left(-\ln\rho\,1 + \frac{\mathbf{r}\otimes\mathbf{r}}{\rho^2}\right), \quad \mathbf{r} = \mathbf{x}-\mathbf{y}, \quad \rho = \|\mathbf{r}\|_2.$$

$$\log\rho = \frac{1}{2}\log(2-2\cos(s-t)) = -\sum_{|k|>0}\frac{1}{2|k|}e^{ik(t-s)},$$

and
$$\frac{\mathbf{r}\otimes\mathbf{r}}{\rho^2} = -\frac{1}{2}\begin{bmatrix}\cos(s+t)-1 & \sin(s+t)\\ \sin(s+t) & -1-\cos(s+t)\end{bmatrix}.$$

$$\boxed{\begin{aligned} S_1[\mathbf{f}] &= \sum_{|k|>0}\frac{1}{8\pi|k|}e^{iks}\int_0^{2\pi}\begin{bmatrix}e^{-ikt} & 0\\ 0 & e^{-ikt}\end{bmatrix}\sum_{m\in\mathbb{Z}}\begin{bmatrix}\hat{v}_{1m}\\ \hat{v}_{2m}\end{bmatrix}e^{imt}\,dt,\\ &= \sum_{|k|>0}\frac{1}{4|k|}e^{iks}\begin{bmatrix}\hat{v}_{1k}\\ \hat{v}_{2k}\end{bmatrix}.\end{aligned}}$$

$$(\sigma\mathbf{x}_s)_s = \sum_{k=-\infty}^{\infty}\hat{\sigma}_k e^{iks}\begin{bmatrix}-ik\sin s-\cos s\\ ik\cos s-\sin s\end{bmatrix} = -\hat{\sigma}_0\begin{bmatrix}\cos s\\ \sin s\end{bmatrix} + \sum_{|k|>0}\frac{k}{2}e^{iks}\begin{bmatrix}\hat{\sigma}_{k+1}-\hat{\sigma}_{k-1}\\ i(\hat{\sigma}_{k+1}+\hat{\sigma}_{k-1})\end{bmatrix}.$$

Spectral properties

$$
\begin{aligned}
&\textit{for } \mathcal{S} \textit{ (single-layer potential operator)}, && \mathcal{O}(|k|^{-1});\\
&\textit{for } \mathcal{L} \textit{ (inextensibility operator)}, && \mathcal{O}(-|k|);\\
&\textit{for } \mathcal{B} \textit{ (bending force potential operator)}, && \mathcal{O}(-|k|^{3});\\
&\textit{for } \mathcal{M} \textit{ (stretching operator)}, && \mathcal{O}(1).
\end{aligned}
$$

Inextensibility operator (inner iteration)

Inextensibility operator

$$\mathcal{L}^\gamma[\sigma] = f$$

$$\mathcal{L}^\gamma = \text{div}_\gamma \int_\gamma G(\mathbf{x},\mathbf{y}) \left(\mathbf{t}\frac{d}{ds} - \kappa\mathbf{n}\right)$$

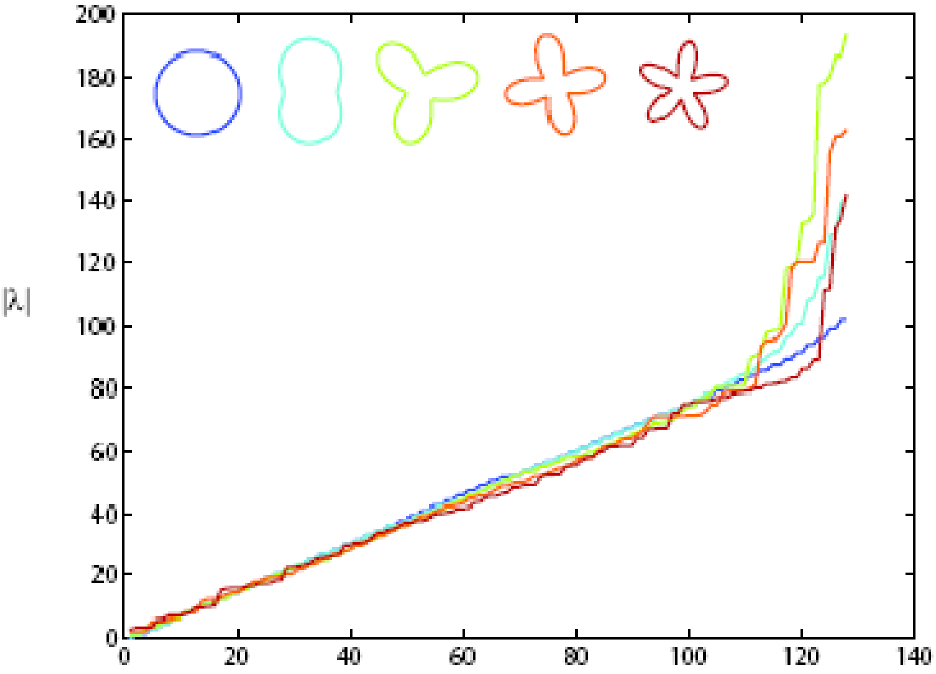
Spectral Analysis on unit circle

Null space of dimension one

Condition number of $\mathcal{L}^\gamma$ is $\mathcal{O}(N)$

Preconditioner

$$\mathcal{F}^{-1}\Lambda_c^{-1}\mathcal{F}$$



Time-marching scheme

for $n = 1 : N - 1$ **do**

  $\sigma = \texttt{ComputeTension}(\mathbf{x})$ *given positions* **x**, *compute tension*

  for k = 1 to K **do**

    $\mathbf{f}_k^b = -\kappa_B \texttt{ComputeDerivative}(\mathbf{x}_k, \mathbf{x}_k, 4)$ *traction jump due to bending*

    $\mathbf{t}_k = \texttt{ComputeDerivative}(\mathbf{x}_k, \mathbf{x}_k, 1)$ *tangent vector*

    $\mathbf{f}_k^\sigma = \texttt{ComputeDerivative}(\sigma_k \mathbf{t}_k, \mathbf{x}_k, 1)$ *traction jump due to tension*

  end for

  $\mathbf{F} = \mathbf{v}_\infty(\mathbf{x}) + \texttt{ComputeInteraction}(\mathbf{f}^\sigma + \mathbf{f}^b, \mathbf{x})$

  for k = 1 to K **do**

    $\mathbf{F}_k = \mathbf{F}_k - \texttt{ComputeInteraction}(\mathbf{f}_k^b, \mathbf{x}_k)$ *subtract the self-interaction due to bending*

    Solve: $(\mathbf{I} - \triangle t \mathcal{B}(\mathbf{x}_k))\mathbf{y}_k = \mathbf{x}_k + \triangle t \mathbf{F}_k$ *using preconditioned GMRES*

    $\mathbf{x}_k := \mathbf{y}_k$

  end for

end for

Algorithm for tension

Given positions, computes the tensions

$\mathbf{f}_k^b = -\kappa_B \texttt{ComputeDerivative}(\mathbf{x}_k, \mathbf{x}_k, 4), \quad k = 1, \ldots, K$ *traction jump due to bending*

$F = \texttt{ComputeInteraction}(\mathbf{f}^b, \mathbf{x})$ *velocity field due to bending*

$\mathbf{t}_k = \texttt{ComputeDerivative}(\mathbf{x}_k, \mathbf{x}_k, 1), \quad k = 1, \ldots K$ *tangent vector*

$F_k = -\mathbf{t}_k \cdot [F_k + \mathbf{v}_\infty(\mathbf{x}_k)], \quad k = 1, \ldots, K$ *surface divergence*

Solve for σ: $\texttt{TensionMatVec}(\sigma, \mathbf{x}) = F$ *using preconditioned GMRES*

Algorithm 3 TensionMatVec($\sigma, \mathbf{x}$)

Given tensions and positions, computes the left hand side of 24

for k = 1 to K **do**

  $\mathbf{t}_k = \texttt{ComputeDerivative}(\mathbf{x}_k, \mathbf{x}_k, 1)$ *tangent vector*

  $\mathbf{f}_k^\sigma = \texttt{ComputeDerivative}(\sigma_k \mathbf{t}_k, \mathbf{x}_k, 1)$ *traction jump due to tension*

end for

$F = \texttt{ComputeInteraction}(\mathbf{f}^\sigma, \mathbf{x})$

return $F_k = \mathbf{t}_k \cdot F_k, \quad k = 1, \ldots K$

Algorithms for integrals and differentiation

Algorithm 4 ComputeInteraction $(\mathbf{f}, \mathbf{x})$

Given jumps f across the vesicle boundaries x, computes $\sum_{k=1}^{K} \mathcal{S}_k[\mathbf{f}_k](\mathbf{x})$

$\phi_1 = \sum_{k=1}^{K} \int_{\gamma_k} \log|\mathbf{x} - \mathbf{y}| f_1(\mathbf{y})\, ds(\mathbf{y})$ *using trapezoidal rule and FMM*

$\phi_2 = \sum_{k=1}^{K} \int_{\gamma_k} \log|\mathbf{x} - \mathbf{y}| f_2(\mathbf{y})\, ds(\mathbf{y})$ *using trapezoidal rule and FMM*

$\phi_3 = \sum_{k=1}^{K} \int_{\gamma_k} \log|\mathbf{x} - \mathbf{y}| \left[f_1(\mathbf{y}) y_1 + f_2(\mathbf{y}) y_2\right] ds(\mathbf{y})$ *using trapezoidal rule and FMM*

$\mathbf{F} = \{\phi_1, \phi_2\} + x_1 \nabla_{\mathbf{x}} \phi_1 + x_2 \nabla_{\mathbf{x}} \phi_2 - \nabla_{\mathbf{x}} \phi_3$

Correct the trapezoidal rule to compute self interactions

Get the nodes and weights $\{\alpha_i^c, w_i\}_{i=1}^{m}$ corresponding to order q, that correct the trapezoidal rule [1].

for k = 1 to K **do**
  for j = 1 to M **do**
    for i = 1 to m **do**
      Compute $\mathbf{f}_k, \mathbf{x}_k$ at $\alpha_j + \alpha_i^c$ *using spline interpolation/nonuniform FFT*
      $F_{kj} = F_{kj} + w_i G(\mathbf{x}_{kj}, \mathbf{x}_k(\alpha_j + \alpha_i^c)) \mathbf{f}_k(\alpha_j + \alpha_i^c)$ *add the correction*
    end for
  end for
end for

Algorithm 5 ComputeDerivative $(\mathbf{f}, \mathbf{x}, m)$

Computes the mth derivative of a vector field f with respect to the arclength s. x is the position of the boundary.

$c = \left[-\frac{M}{2}, -\frac{M}{2} + 1, \ldots, \frac{M}{2} - 1\right]$ *coefficient vector*

Set $\mathbf{F} = \mathbf{f}$ *initialization*

$|\mathbf{x}_\alpha| = \sqrt{[\mathtt{IFFT}(ic\mathtt{FFT}(x_1))]^2 + [\mathtt{IFFT}(ic\mathtt{FFT}(x_2))]^2}$ *Jacobian*

for 1 to m **do**
  $\mathbf{F} = \left\{ \frac{\mathtt{IFFT}(ic\mathtt{FFT}(F_1))}{|\mathbf{x}_\alpha|}, \frac{\mathtt{IFFT}(ic\mathtt{FFT}(F_2))}{|\mathbf{x}_\alpha|} \right\}$ *differentiate once*
end for
return F

Time marching stability

	Explicit scheme			Semi-implicit scheme I			Semi-implicit scheme II		
M	$\chi = 0$	10	100	0	10	100	0	10	100
32	3.90e-03	7.81e-03	9.76e-04	∞	1.56e-02	9.76e-04	3.12e-02	1.56e-02	9.76e-04
64	9.76e-04	9.76e-04	4.88e-04	∞	1.56e-02	9.76e-04	1.56e-02	7.81e-03	9.76e-04
128	6.10e-05	3.05e-05	6.10e-05	∞	1.56e-02	9.76e-04	7.81e-03	7.81e-03	9.76e-04
256	3.81e-06	3.81e-06	3.81e-06	∞	1.56e-02	9.76e-04	7.81e-03	7.81e-03	9.76e-04
512	2.38e-07	2.38e-07	2.38e-07	∞	1.56e-02	9.76e-04	7.81e-03	7.81e-03	9.76e-04

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Preconditioning

Preconditioner	None			Q		
M	$\chi = 0$	10	100	0	10	100
32	16	20	11	11	14	10
64	43	48	25	14	16	16
128	111	121	65	14	16	21
256	282	300	163	14	16	23
512	701	731	442	14	16	23
1024	1656	1699	1095	14	16	23

Bending

Preconditioner	None		P	
M	$\epsilon = 10^{-6}$	$\epsilon = 10^{-12}$	$\epsilon = 10^{-6}$	$\epsilon = 10^{-12}$
64	21	35	12	22
128	30	55	13	25
256	41	74	12	28
512	59	102	11	30
1024	91	123	10	28

Tension

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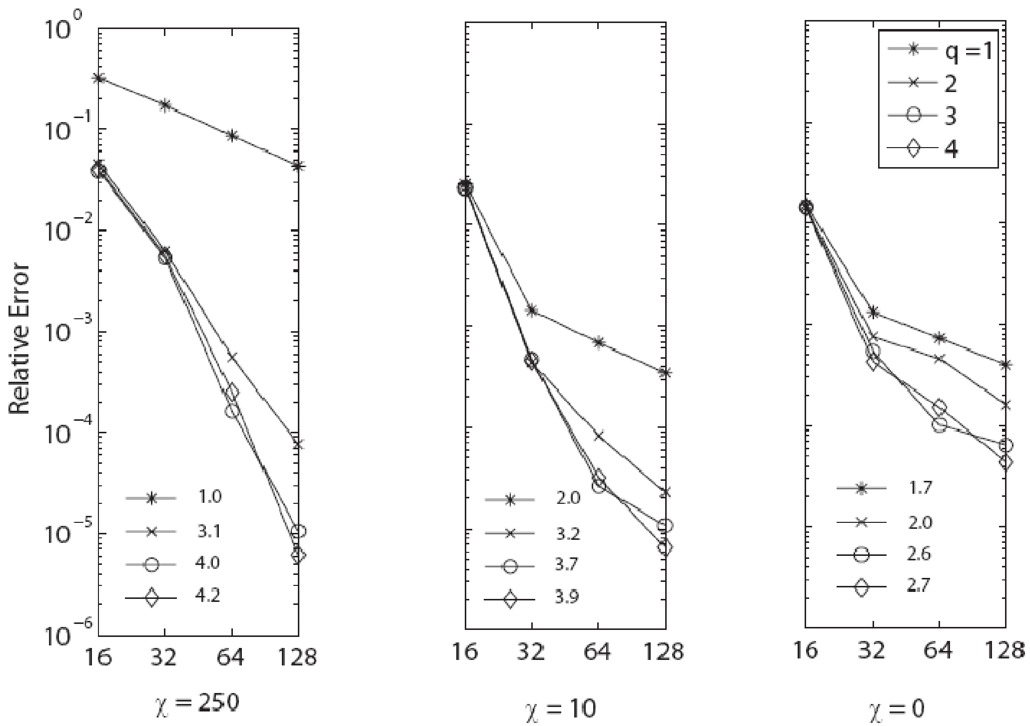
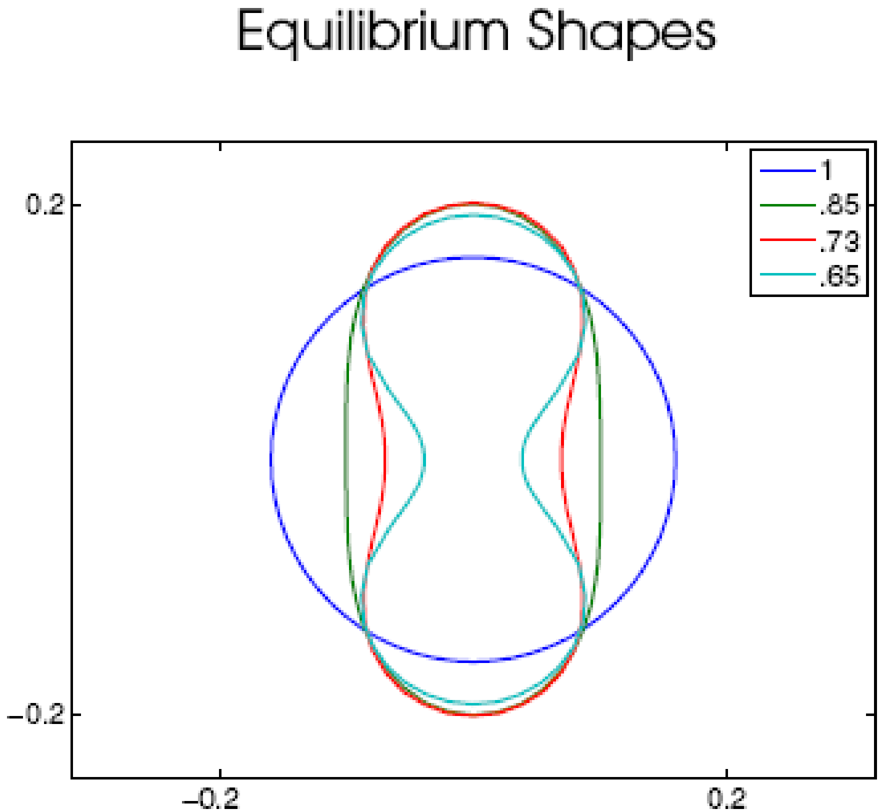
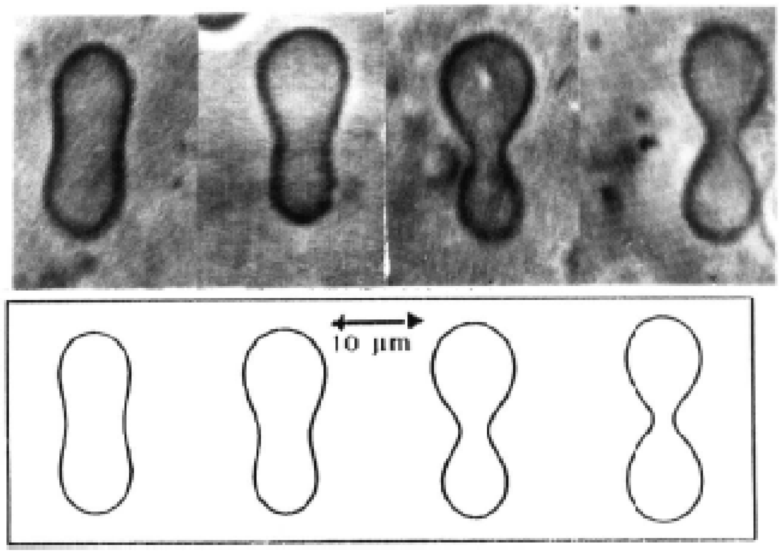
Suboptimal accuracy in time

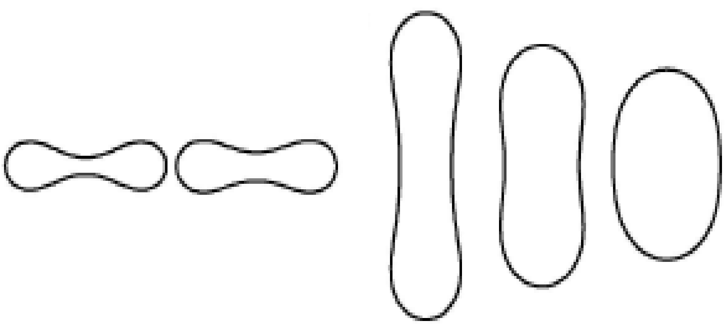
	$\lvert L - L_f \rvert / L$			$\lvert A - A_f \rvert / A$		
M	$q = 1$	2	3	1	2	3
32	5.36e-004	4.98e-004	4.98e-004	1.69e-004	3.50e-004	3.50e-004
64	4.28e-005	2.27e-005	2.28e-005	1.18e-004	8.67e-006	6.48e-006
128	1.01e-005	6.27e-008	2.73e-008	6.82e-005	2.20e-006	9.73e-007
256	5.02e-006	1.76e-008	4.72e-009	3.42e-005	6.60e-007	2.25e-007



Reduced Area Determines Equilibrium Shape







0.592 0.651 0.652 0.8 0.95

Eyeball validation with Seifert'97

reduced area = $\frac{4\pi A}{L^2}$

Penn

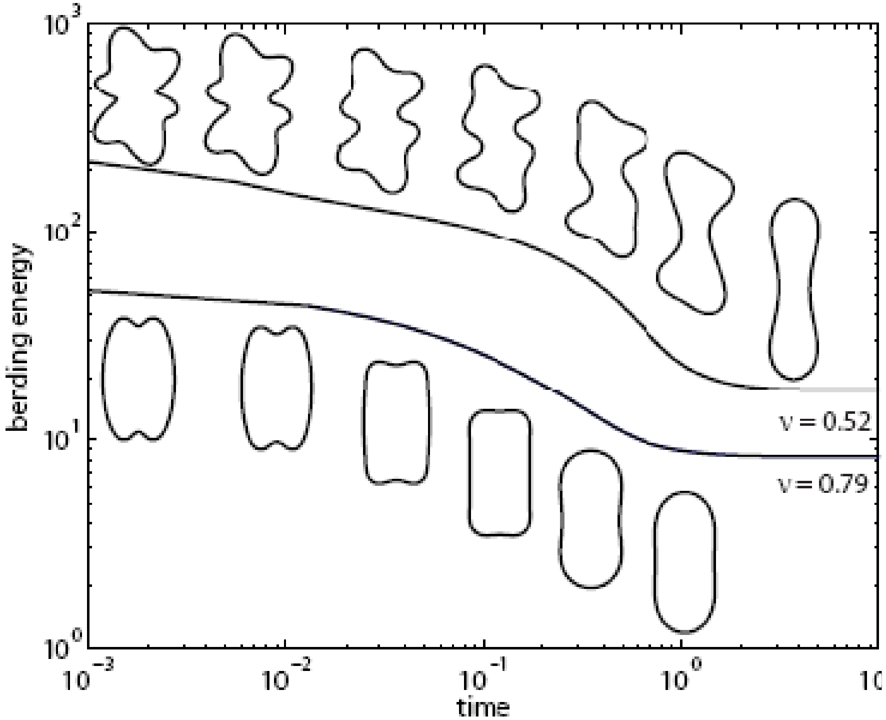
Analytical solutions, minimization approach

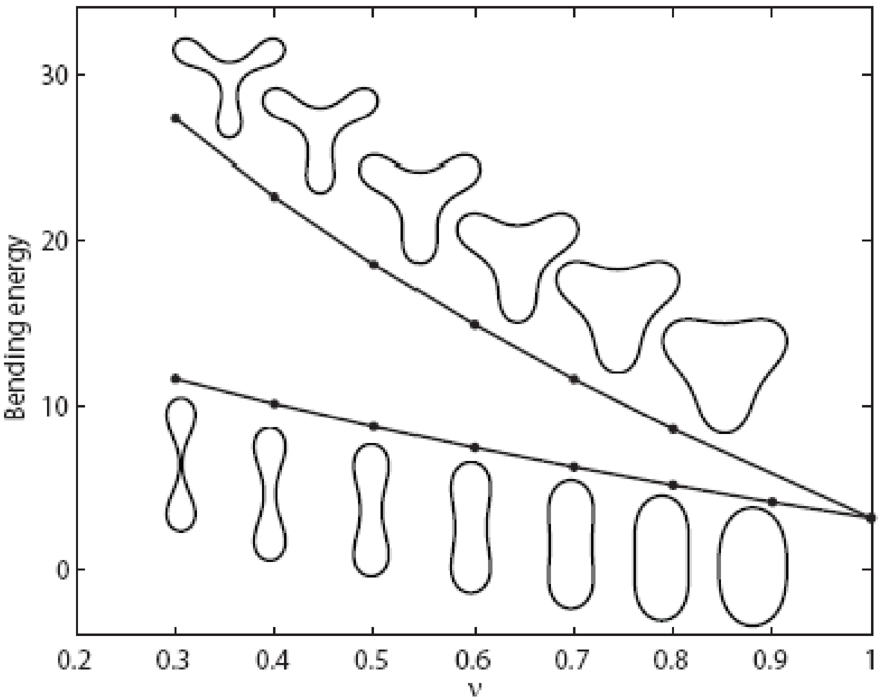
$$\int_\gamma \frac{\kappa^2}{2} d\gamma + \sigma \left(\int_\gamma d\gamma - L \right) + p \left(\int_\gamma \frac{1}{2} \mathbf{x} \cdot \mathbf{n} \, d\gamma - A \right),$$

$$\boxed{\kappa_{ss} + \frac{1}{2}\kappa^3 - \sigma\kappa + p = 0.}$$

Evolution/Multiple minima (analytic solutions)

M	16	32	64	128
$\|\mathbf{v}(\mathbf{x})\|_\infty$	4.32e-001	8.40e-004	7.79e-009	3.21e-010

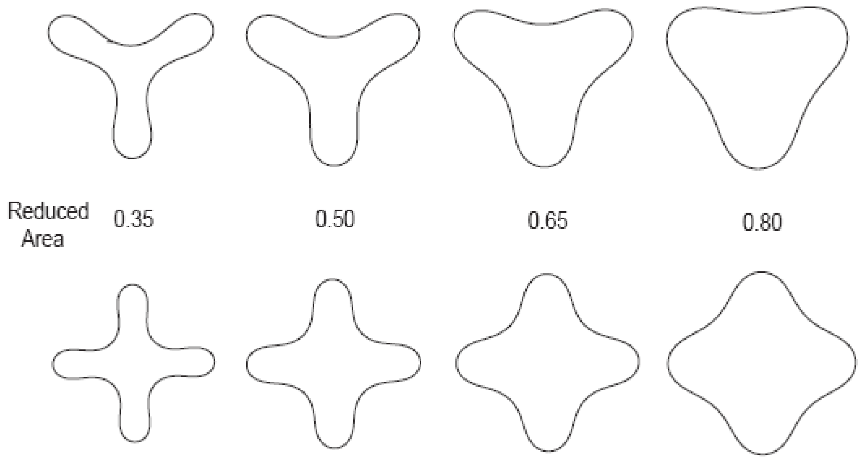


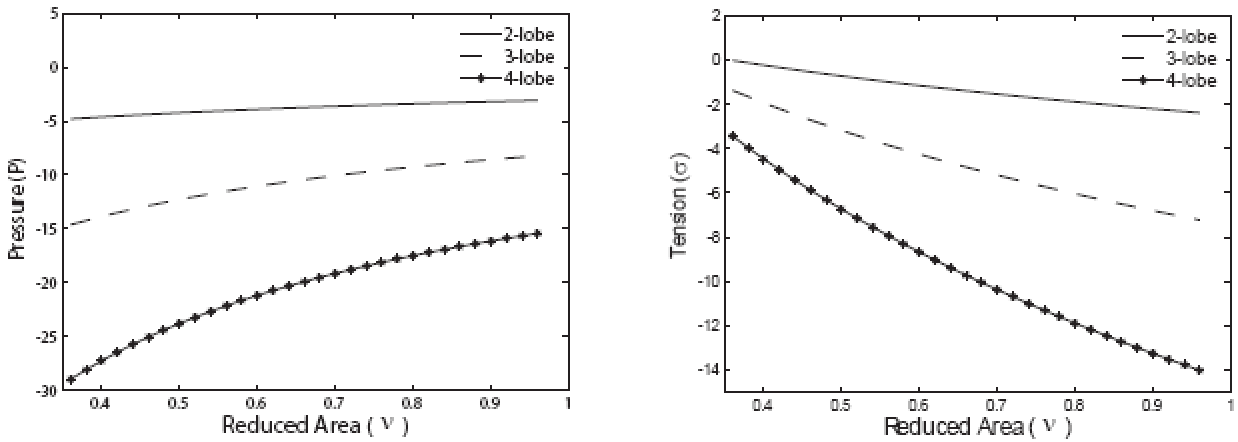


Using a variational formulation, can construct semi-analytic solutions for zero shear
Veerapaneni, Ritwik, B., Purohit'08

Penn

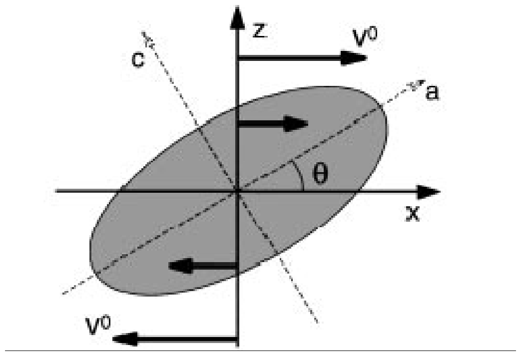
3- and 4-lobed vesicles





Shear flow

- Length scale $R_0 = L/2\pi$
- Time scale $\tau = \eta R_0^3/\kappa_B$
- Shear $\chi = \dot{\gamma}\eta R_0^3/\kappa_B$



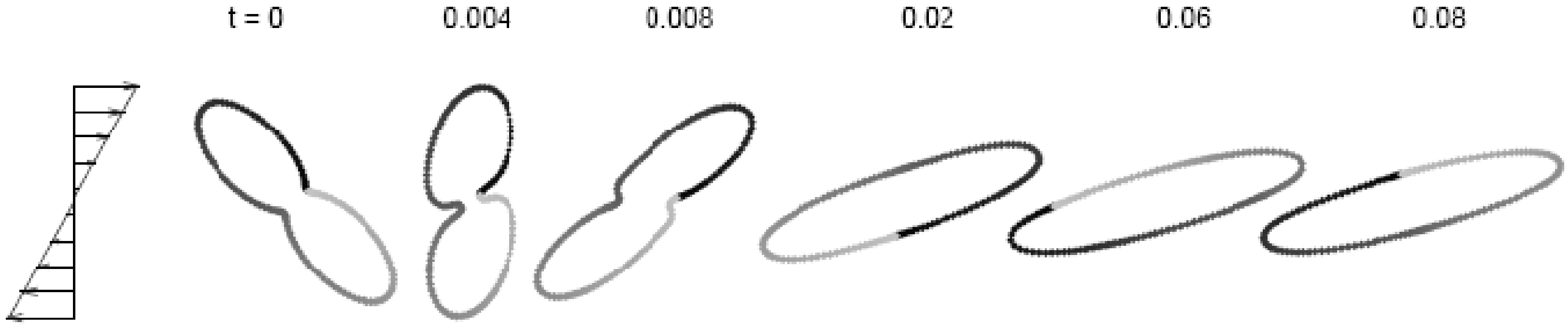
$$\dot{\gamma} = 1s^{-1},\ \kappa_B = 10^{-19}J,\ \eta = 10^{-3}Js/m^3,\ R_0 = 10\mu m$$

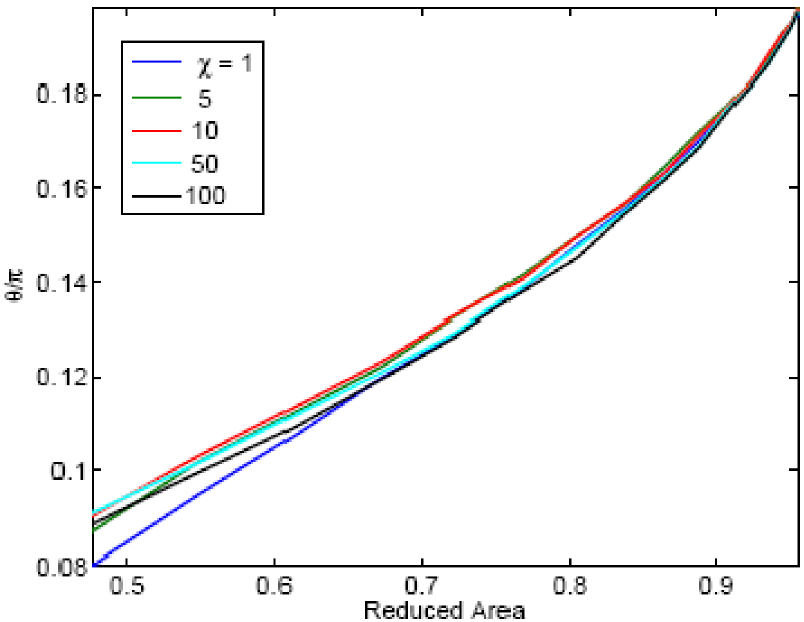
$$\tau = 0.1 \text{ and } \chi = 1$$

$$\frac{d\hat{\mathbf{x}}}{dt} = \chi\{x_2, 0\} + \tau\hat{\mathcal{S}}[\mathbf{f}_{\hat{\sigma}} + \mathbf{f}_{\hat{\kappa}}]$$

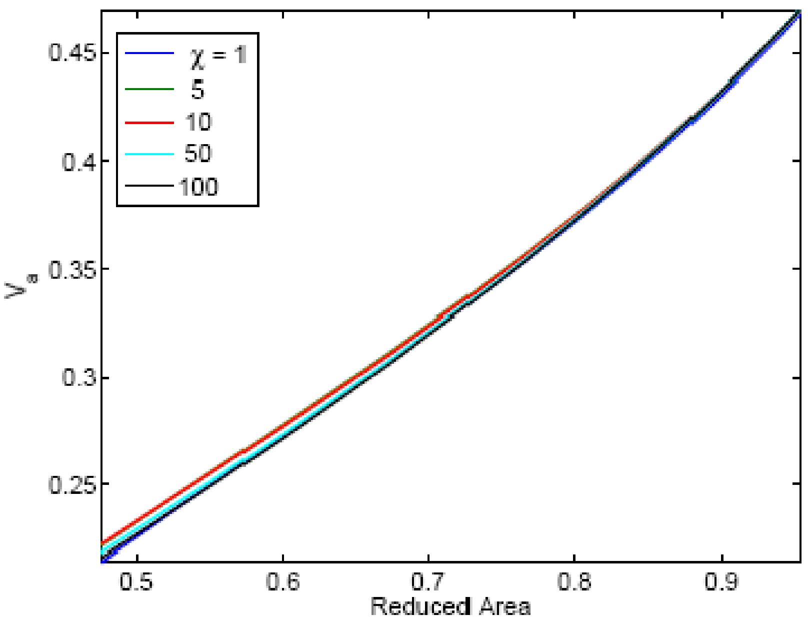
Kraus et al,'96

Shear validation with experimental results



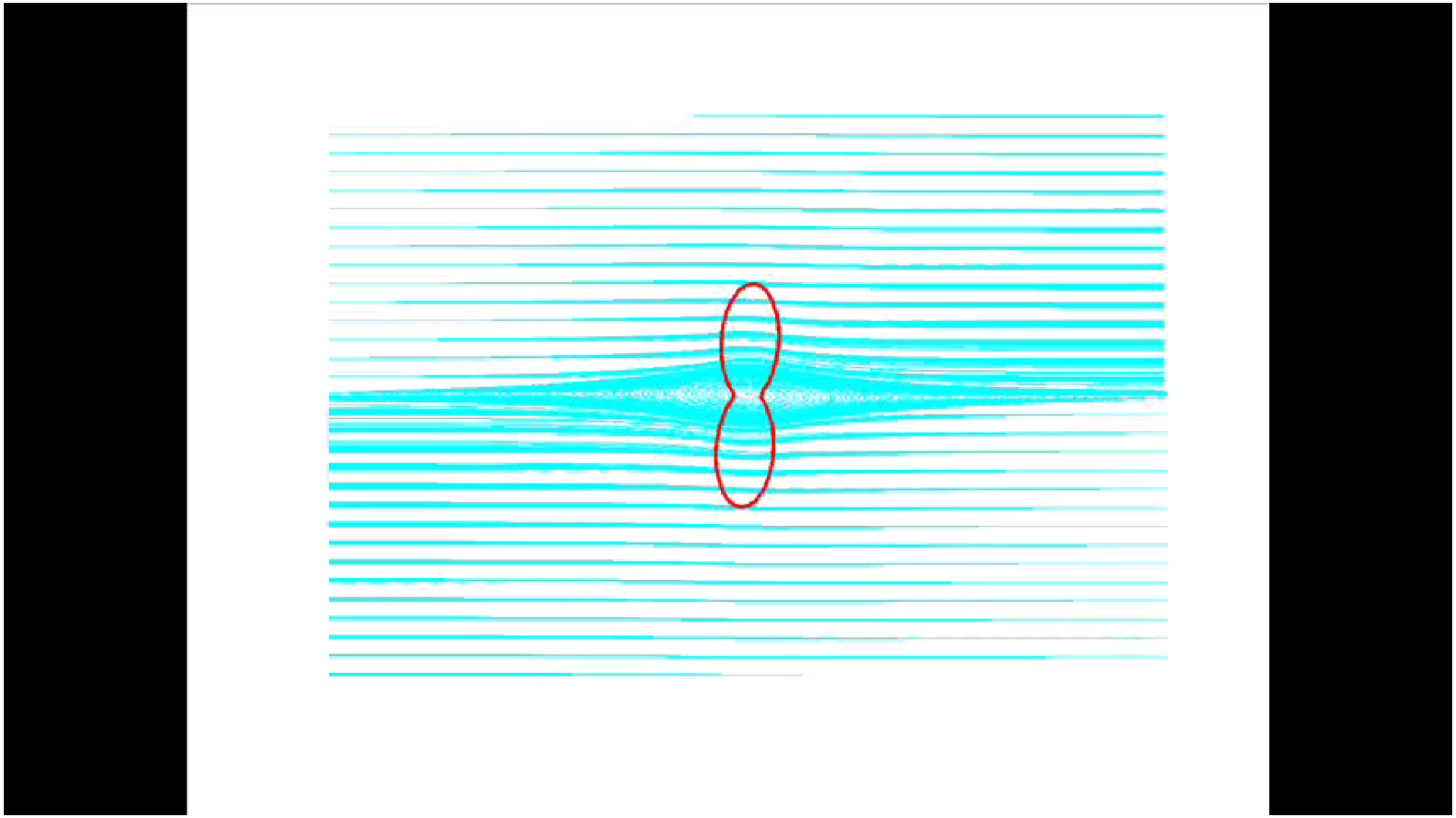


(a) Angle of inclination

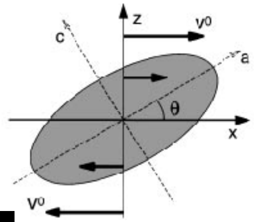


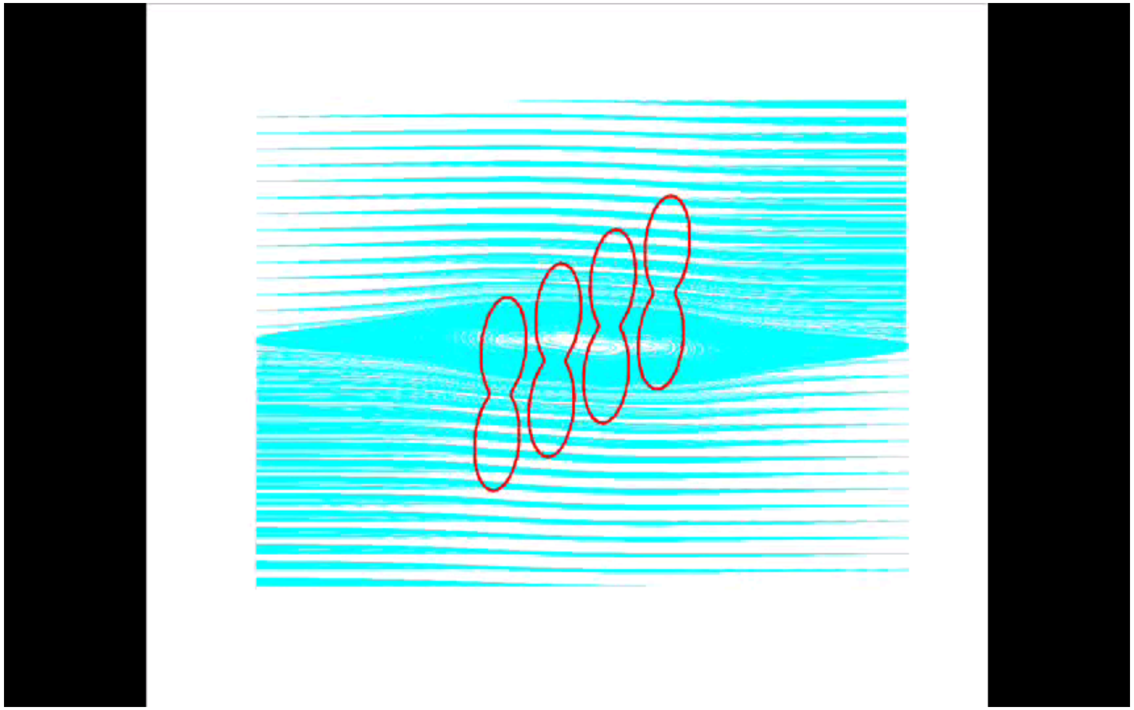
(b) Scaled average angular velocity

One vesicle—streamlines



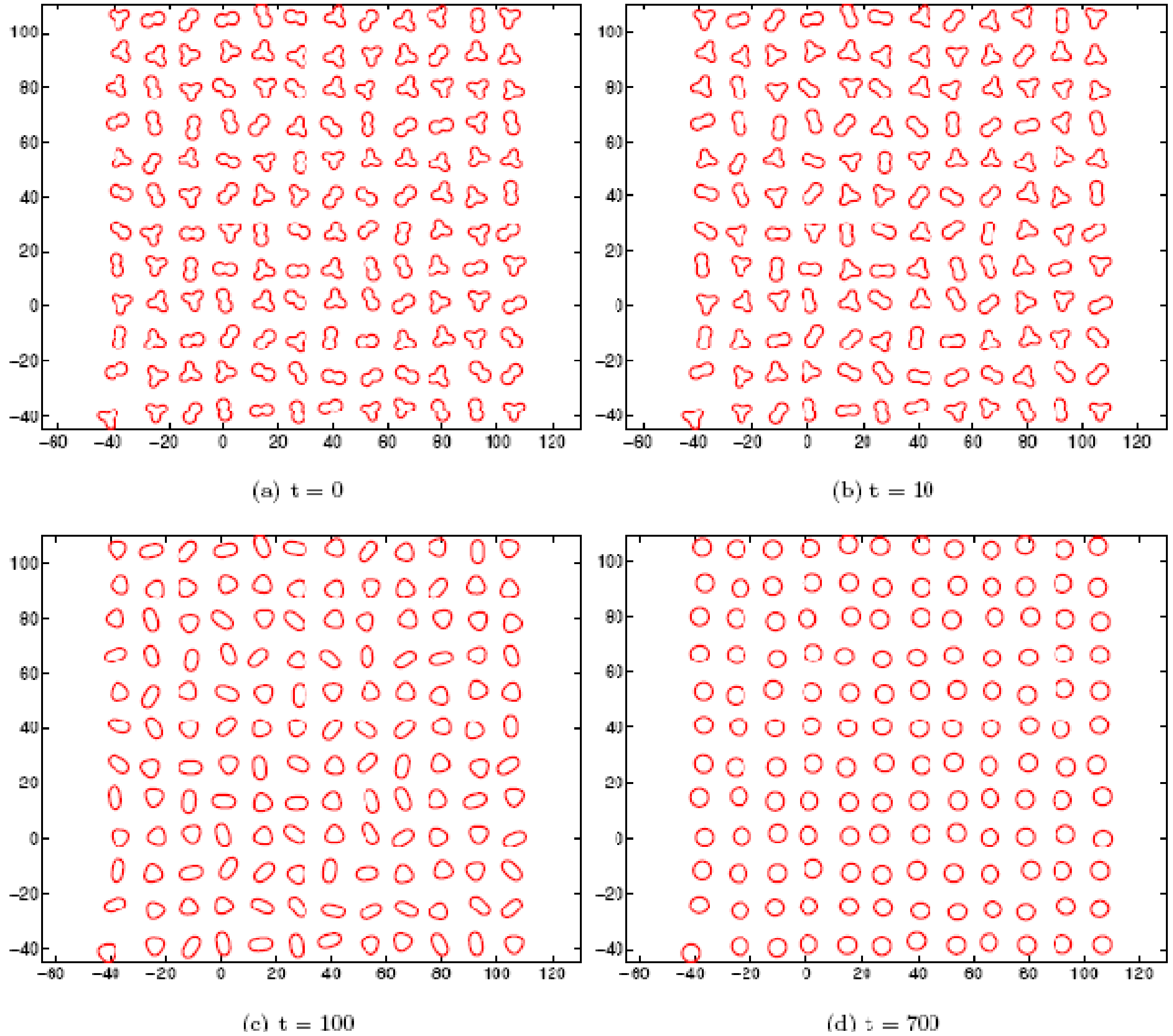
Multiple particles in shear flow



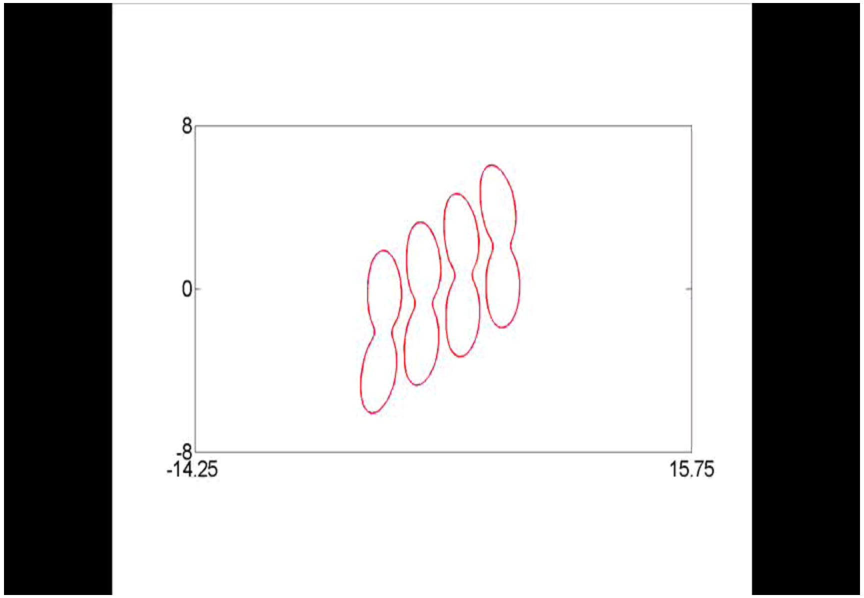


$$\frac{d\mathbf{x}_j}{dt} = -\mathbf{v}_\infty - \sum_{k=1}^{N_v} \mathcal{S}_k[\mathbf{f}_\sigma + \mathbf{f}_\kappa](\mathbf{x}_j); \quad \mathrm{div}_{\gamma_j}\mathbf{v}_\infty = \mathrm{div}_{\gamma_j}\mathcal{S}_j[\mathbf{f}_\sigma + \mathbf{f}_\kappa],$$

144 vesicles, relaxation (no incompressibility)



Vesicles in parabolic flow and in confined flows



computational science & engineering laboratory

Summary

- Particulate flows
- Integral equation formulation for fluid membranes
  - Bending and tension
- IMEX scheme, 3^{rd} order in time, spectral in space
  - Spectral analysis for unit circle
  - Lagrangian, no-reparametrization

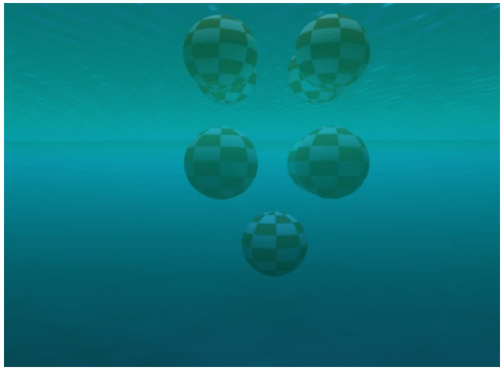
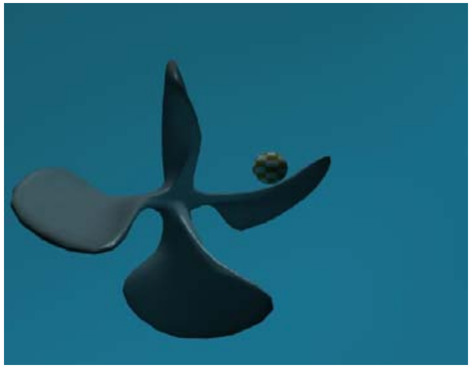
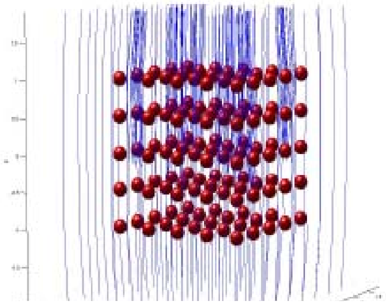
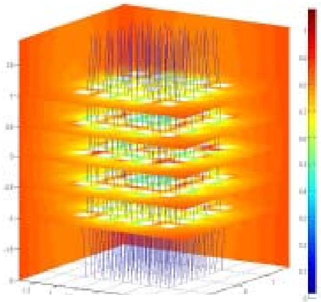
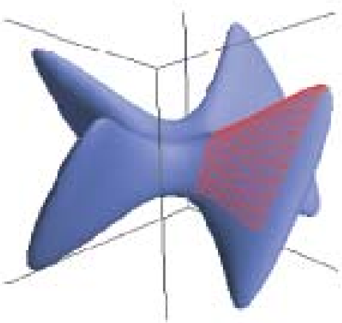
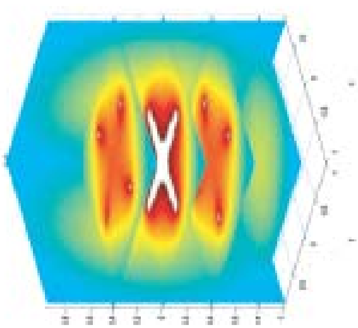
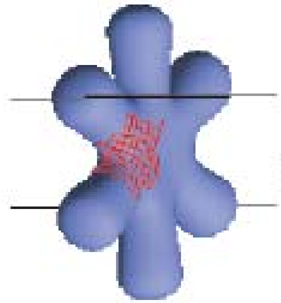
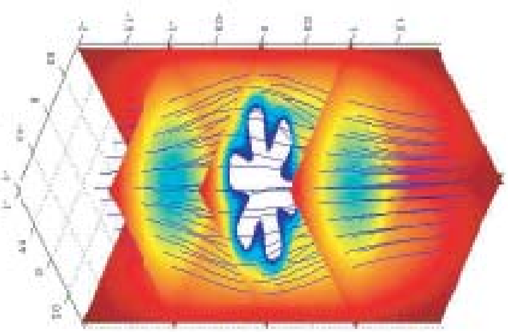
Limitations

- Piecewise-constant coefficients
- Only smooth surfaces
- No adaptivity (space or time)
- Need for preconditioning
- CFL time-step restrictions
- Arbitrary boundary conditions a challenge
    - Walls, arteries, periodic BCs
- Difficult to develop and maintain
- Concentrated suspensions
    - singularities

3D Simulations

- Stokes + rigid body dynamics
- Double-layer formulation
- Spectral algorithm for singularities
- Partition of unity/ manifold repres.
- Fast summation
- $O(N^{3/2})$, 4^{th} order

B. & Ying & Zorin, JCP'06

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  - o *New York University*

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