Surface Fluctuating Hydrodynamics Methods
Soft Materials with Fluid-Structure Interactions within Curved Fluid Interfaces

October 2020
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DOE ASCR CM4 DE-SC0009254
DOE ASCR PhILMS DE-SC0019246
NSF Grant DMS - 1616353
NSF CAREER Grant DMS-0956210
Lipid Bilayer Membranes

- Dynamic structures with diverse roles in cell biology.
- Fluid phase two-layered structures (bilayer).
- Mechanically behaves as a fluid-elastic sheet: in-plane flow, elastic responses to bending.

Experimental Assays

Single Particle Tracking

- Quantum Dots (QDs) conjugated to individual proteins.
- Image processing → QD location → protein positions.
- Trajectories measured over time-scales up to seconds.
- Protein diffusivity / kinetics depend on membrane mechanics.

Fluorescence Contrast Microscopy

- Lipids labeled and membrane configuration observed.
- Image processing → representation of shapes.
- Thermal undulations → mechanics (bending elasticity, …).

hydrodynamics, elasticity, geometry…

Motivations

- Hydrodynamic flows within curved fluid interfaces relevant in many problems.
- Soap films, bubbles, cellular mechanics.
- Geometry plays important role in hydrodynamic responses.
- Fluctuations important in many problems:
  - diffusive transport, osmotic swelling, fission/fusion.

Challenges

- Need good methods to formulate tractable hydrodynamic equations on manifolds.
- Approaches for performing analysis and reductions.
- Computational methods for efficient numerical approximation.
Classical Work: Saffman-Delbruck Theory 1975

Proteins in Bilayers

Membrane Protein Diffusion:
• Membrane treated as 2D fluid slab. \( V = MF \sim D = 2K_B TM \)
• Not pure 2D flow even though \( \mu_m \sim 100 \times \mu_f \), Stokes' Paradox!
• Must treat both 2D lipid flow + coupling to bulk 3D flow of solvent.

Saffman-Delbruck Theory (1975):
• Mobility / Diffusion as \( h \rightarrow 0 \),
  \[ V = M_{SD} F \sim D = 2K_B T M_{SD} \]
  \[ M_{SD} = \left( \frac{1}{4\pi \mu_m} \right) \left( \log\left( \frac{2L_{SD}}{a} \right) - \gamma \right), \quad L_{SD} = \frac{\mu_m}{2\mu_f} \]
• Predicts diffusion of proteins depends as log on size!
• \( L_{SD} \sim 1 \mu m, \ a \sim 10 \text{ nm} \), long-range coupling.
• Many membranes exhibit curvature over this length-scale.

How can we account for curvature, hydrodynamics, thermal fluctuations?
How does this affect transport?
Exterior Calculus Operators

\[ \begin{align*}
\text{d} & : \text{Exterior Derivative} \quad (k\text{-form} \to (k+1)\text{-form}) \\
\ast & : \text{Hodge Star} \quad \text{(k\text{-form} \to (n-k)\text{-form})} \\
\wedge & : \text{Wedge Product} \quad \text{(k}_1, k_2\text{-form} \to (k_1+k_2)\text{-form}).
\end{align*} \]

Vector Calculus Correspondence

\[ \begin{align*}
\text{grad}(f) & = [\text{df}]^\sharp \\
\text{div}(\mathbf{F}) & = -(*\text{d} * \mathbf{F}^b) = -\delta \mathbf{F}^b \\
\text{curl}(\mathbf{F}) & = [*\text{d} \mathbf{F}^b]^\sharp. \\
\text{div}(\mathbf{D}) & = -\delta \text{d} \mathbf{v}^b + 2K \mathbf{v}^b.
\end{align*} \]

Conservation Laws on Manifolds

\[ \begin{align*}
\int_{\partial \Omega} \omega & = \int_{\Omega} \text{d} \omega \quad \text{Stokes Theorem} \\
\int_{\partial \Omega} \ast \omega & = \int_{\Omega} \text{d} \ast \omega \quad \text{Divergence Theorem}
\end{align*} \]

Diffusion Equation / Laplace-Beltrami

\[ \frac{\partial}{\partial t} \int_{\Omega} \ast u = \int_{\partial \Omega} \ast \omega = \int_{\Omega} \text{d} \ast \omega. \quad \omega = \text{d} u. \quad \frac{\partial u}{\partial t} = -\ast \text{d} \ast \omega = -\delta \omega = -\delta \text{d} u. \]
Hydrodynamics on Manifolds

Rate-of-Deformation Tensor

\[ \mathbf{D} = \nabla \mathbf{v} + \nabla \mathbf{v}^T \quad \text{div}(\mathbf{D}) = -\delta \mathbf{v}^b + 2K \mathbf{v}^b \]

Momentum Equations

\[ \rho \left( \partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v} \right) = \text{div}(\sigma) + \mathbf{b} \]
\[ \partial_t \rho + \rho \text{div}(\mathbf{v}) = 0. \]

Stokes Equations (surface)

\[ \mu_m \left( -\delta \mathbf{v}^b + 2K \mathbf{v}^b \right) - dp + \mathbf{b}^b = 0 \]
\[ -\delta \mathbf{v}^b = 0 \]

Surface Hydrodynamic Equations

\[ \begin{cases} 
\rho \frac{D\mathbf{v}^b}{dt} = \mu_m (-\delta \mathbf{d} + 2K) \mathbf{v}^b - dp + \mathbf{b}^b \\
-\delta \mathbf{v}^b = 0
\end{cases} \]

Vector Potential Form:

\[ \mathbf{v}^b = -\star \mathbf{d} \Phi \]
\[ \mu_m (-\delta \mathbf{d})^2 \Phi - 2\mu_m (-\star \mathbf{d} (K(-\star \mathbf{d} \Phi)) = -\star \mathbf{d} \mathbf{b}^b \]
Lipid Bilayer Membranes
- Each leaflet treated as a 2D fluid.
- Hydrodynamic coupling:
  i. Intra-monolayer lipid flow.
  ii. Inter-monolayer slip.
  iii. Traction with bulk solvent fluid.

Bilayer Hydrodynamics

\[
\begin{align*}
\mu_m \left[ -\delta dv^b_+ + 2K_+ v^b_+ \right] + t^b_+ - \gamma (v^b_+ - v^b_-) \\
&= dp_+ - b^b_+ = -c^b_+, \quad x \in \Gamma_+ \\
\delta v^b_+ &= 0, \quad x \in \Gamma_+,
\end{align*}
\]

(outer layer)

\[
\begin{align*}
\mu_m \left[ -\delta dv^b_- + 2K_- v^b_- \right] + t^b_- - \gamma (v^b_- - v^b_+) \\
&= dp_- - b^b_- = -c^b_-, \quad x \in \Gamma_-
\delta v^b_- &= 0, \quad x \in \Gamma_-. 
\end{align*}
\]

(inner layer)

Solvent Hydrodynamics

\[
\begin{align*}
\mu \Delta u - \nabla p &= 0, \quad x \in \Omega \\
\nabla \cdot u &= 0, \quad x \in \Omega \\
u &= v, \quad x \in \partial \Omega \\
u_\infty &= 0. 
\end{align*}
\]

Traction coupling

\[
\begin{align*}
t^+ &= \sigma^+ \cdot n^+ \\
t^- &= \sigma^- \cdot n^- 
\end{align*}
\]
Immersed Boundary Methods on Manifolds

Leaflet Cases

Immersed Boundary Coupling

Particle Force

Particle Torque

Immersed Boundary Methods for Manifolds

Velocity-Averaging operator: \( \Gamma v = \int_\Omega W[v](y)dy \)

Force-Spreading operator: \( \Lambda F = W^*[F](x) \)

Adjoint condition: \( \langle v, \Lambda F \rangle = \int_\Omega v(x) \cdot (\Lambda F)(x)dx \)

\( \langle \Gamma v, F \rangle = \sum_i [\Gamma v]_i \cdot [F]_i \)

\( \langle \Gamma v, F \rangle = \langle v, \Lambda F \rangle \rightarrow \Gamma^T = \Lambda \)

Weight Tensor

\[ W[v] = \sum_i \left( \begin{array}{c} w[i] \alpha \\ w[i] \alpha \end{array} \right) \partial_\alpha x^{[i]} \]

Reference Fields \( \psi(r) = C \exp(-r^2/2\sigma^2) \)

\( q^\theta = \psi(x - X^{[i]}) \partial_\theta \)

\( q^\phi = \psi(x - X^{[i]})/\cos(\theta) \partial_\phi \)

\( q^n = \psi(x - X^{[i]}) (n \times (x - X^{[i]})) \)

Mobility Tensor

\[ \begin{bmatrix} V \\ \omega \end{bmatrix} = M \begin{bmatrix} F \\ \tau \end{bmatrix} \]

IB-Membrane Mobility

\( M_{ij} = \Gamma_i \delta_{ij} \)

S is fluid solution operator

2016 Atzberger & Sigurdsson

2019 Atzberger, Padidar, Rower

2016 Atzberger & Sigurdsson
Analytic Solutions and Lebedev Quadrature

Bilayer Hydrodynamics

\[
\begin{align*}
\mu_m \left[ -\delta \mathbf{v}_+^b + 2K_+ \mathbf{v}_+^b \right] + \mathbf{t}_+^b - \gamma (\mathbf{v}_+^b - \mathbf{v}_-^b) &= \mathbf{d}_+ - \mathbf{b}_+^b = -\mathbf{c}_+^b, \quad \mathbf{x} \in \Gamma_+ \\
\delta \mathbf{v}_+^b &= 0, \quad \mathbf{x} \in \Gamma_+ \\

\mu_m \left[ -\delta \mathbf{v}_-^b + 2K_- \mathbf{v}_-^b \right] + \mathbf{t}_-^b - \gamma (\mathbf{v}_-^b - \mathbf{v}_+^b) &= \mathbf{d}_- - \mathbf{b}_-^b = -\mathbf{c}_-^b, \quad \mathbf{x} \in \Gamma_- \\
\delta \mathbf{v}_-^b &= 0, \quad \mathbf{x} \in \Gamma_-.
\end{align*}
\]

L²-Orthogonal Projection

Spherical Harmonics

\[
P[f] = \tilde{f}(\theta, \phi) = \sum_i \hat{f}_i Y_i(\theta, \phi), \quad \hat{f}_i = \langle f, Y_i \rangle_Q
\]

Lebedev Nodes

Solution Spherical Harmonics

\[
\mathbf{v}_\pm = -\star \mathbf{d} \sum_s a_s^\pm \Phi_s, \quad c^b = -\star \mathbf{d} \sum_s c_s \Phi_s
\]

Flow Streamlines

\[
\begin{bmatrix}
a_s^+ \\ a_s^-
\end{bmatrix} = A_s^{-1} \begin{bmatrix}
-c_s^+ \\ -c_s^-
\end{bmatrix}
\]

\[
A_s = \begin{bmatrix}
A_1^\ell - \gamma & A_2^\ell - \gamma \\
\gamma & A_2^\ell - \gamma
\end{bmatrix}
\]

\[
A_1^\ell = \frac{\mu_m}{R_+^2} \left( 2 - \ell(\ell + 1) - \frac{R_+}{L}(\ell + 1) \right)
\]

\[
A_2^\ell = \frac{\mu_m}{R_-^2} \left( 2 - \ell(\ell + 1) - \frac{R_-}{L}(\ell - 1) \right)
\]

\[
L^\pm = \mu_\pm / 2 \mu_f
\]

2016 Atzberger & Sigurdsson
Many Particle Interactions

Collective Motions

\[ \frac{dX}{dt} = MF \]

Driving Force and Cross-Section

Mobility Response

Hydrodynamic Response

2016 Atzberger & Sigurdsson
Mobility for Spherical Vesicles

Mobility Response vs Membrane Viscosity

L/R = 0.13  L/R = 0.65  L/R = 52

Collective Motions

\[ \frac{dX}{dt} = MF \]

Vortex Location vs Membrane Viscosity

L/R = 0.13  L/R = 1.3  L/R = 13

2016 Atzberger & Sigurdsson
Surface Hydrodynamic Methods

Golestanian Swimmer

Golestanian Swimmer Flows

Active Swimmer and Mixing

Polymer Network Fluctuations

Hydrodynamics and Geometry
Spectral Solver for Surface Hydrodynamics

**L²-Orthogonal Projection**

\[ \mathcal{P} [f] = \bar{f}(\theta, \phi) = \sum_i \hat{f}_i Y_i(\theta, \phi), \]

\[ \hat{f}_i = \langle f, Y_i \rangle_Q \]

**Lebedev Quadrature**

**Spherical Harmonics**

**Spectral Approximation**

**L²-Projection:**

\[ \mathcal{P} [f] = \bar{f}(\theta, \phi) = \sum_i \hat{f}_i Y_i(\theta, \phi), \]

**Inner-Product:**

\[ \langle u, v \rangle_Q = \sum_{\ell} w_\ell u(x_\ell) v(x_\ell) \]

**Differential forms** \( v^b \) (0-forms, 1-forms, 2-forms).

Represented as scalar / vector fields \( v^# \) at the Lebedev nodes.

**Exterior Derivative:** \( d \) approximated by \( \overrightarrow{d} \)

\[ \bar{v}^b(\theta, \phi) = [\mathcal{P} \bar{v}^x, \mathcal{P} \bar{v}^y, \mathcal{P} \bar{v}^z] \]

**Hodge Star:** \( \star \) approximated by \( \overrightarrow{\star} \)

**Approximating PDEs on the Manifold:**

\[ \hat{\mathcal{L}} u = -g, \quad \langle \hat{\mathcal{L}} \bar{u}, Y_i \rangle_Q = -\langle \bar{g}, Y_i \rangle_Q \quad \rightarrow \quad K \hat{u} = -M \bar{g} \]

**Method can be used for approximating general PDEs on manifolds.**

2018 Gross & Atzberger.
Role of geometry in hydrodynamic flow responses

Flow transitions:

Manifold B Flow Response

Manifold C Flow Response

2018 Gross & Atzberger.
Role of geometry in hydrodynamic flow responses

Role of Geometry in Hydrodynamic Flows

![Diagram showing the role of geometry in hydrodynamic flows.](Image)
Role of geometry in hydrodynamic flow responses

Rayleigh Dissipation Rate:

\[
\text{RD}[\mathbf{v}^b] = \mu_m \langle d\mathbf{v}^b, d\mathbf{v}^b \rangle_M - 2\mu_m \langle K\mathbf{v}^b, \mathbf{v}^b \rangle_M + \gamma \langle \mathbf{v}^b, \mathbf{v}^b \rangle_M
\]

Rayleigh-Dissipation (Manifold B)

Rayleigh-Dissipation (Manifold C)
Thermal Fluctuations
Surface Fluctuating Hydrodynamics

Fluid-structure Interactions

Hydrodynamics

Fluctuating Fluid Velocity Fields

Surface Fluctuating Hydrodynamics (Inertial Regime)

Fluid
\[
\frac{d\mathbf{v}}{dt} = \mu_m \left( -\delta \mathbf{v} + 2K \mathbf{v} \right) - \mathbf{d} + \mathbf{t}^b + \Lambda \left[ \gamma \left( \mathbf{V} - \Gamma \mathbf{v} \right) \right] + \mathbf{F}_{\text{thm}}
\]

Microstructures
\[
\frac{d\mathbf{V}}{dt} = -\gamma \left( \mathbf{V} - \Gamma \mathbf{v} \right) - \nabla \phi + \mathbf{F}_{\text{thm}}
\]

Thermal Fluctuations
\[
\langle \mathbf{F}_{\text{thm}}(t) \mathbf{F}_{\text{thm}}(s)^T \rangle = -2k_B T \mathcal{L}_f \delta(t - s)
\]

\[
\langle \mathbf{F}_{\text{thm}}(t) \mathbf{F}_{\text{thm}}(s)^T \rangle = 2k_B T \gamma \mathcal{L}(t - s)
\]

\[
\langle \mathbf{F}_{\text{thm}}(t) \mathbf{F}_{\text{thm}}(s)^T \rangle = -2k_B T \gamma \mathcal{L}(t - s)
\]

Surface Fluctuating Hydrodynamics (Overdamped)

Microstructures
\[
\frac{d\mathbf{X}}{dt} = \mathbf{M} \mathbf{F} + k_B T \mathbf{V} \cdot \mathbf{M} + \mathbf{F}_{\text{thm}}
\]

Thermal Fluctuations
\[
\langle \mathbf{F}_{\text{thm}}(s) \mathbf{F}_{\text{thm}}(t)^T \rangle = 2k_B T M \delta(t - s)
\]

\[
\mathbf{M}_{ij} = \Gamma_i \mathcal{S} \Delta_j
\]

Fluid-structure Interactions
Hydrodynamics
Fluctuating Fluid Velocity Fields

Gibb-Boltzmann Distribution

Particle Diffusive Encounters

Two Particle Meeting Times

2019 Padidar, Rower, Atzberger, 2015 Tabak, Atzberger
Surface Fluctuating Hydrodynamics

Fluid-structure interactions for drift-diffusion dynamics

Surface Fluctuating Hydrodynamics (Overdamped)
Microstructures
\[
\frac{dX}{dt} = MF + k_B T \nabla \cdot M + F_{thm}
\]

Thermal Fluctuations
\[
\langle F_{thm}(s)F_{thm}(t)^T \rangle = 2k_B TM\delta(t-s)
\]

Immersed Boundary for Manifolds

Collective Diffusion

Collective Particle Drift-Diffusion

2019 Padidar, Rower, Atzberger
Surface Fluctuating Hydrodynamics

Fluid-structure Interactions

Fluctuating Fluid Velocity Fields

Velocity Autocorrelations

Surface Fluctuating Hydrodynamics (Inertial Regime)

Fluid

\[ \frac{d\mathbf{v}^b}{dt} = \mu_m \left( -\delta \mathbf{v}^b + 2K \mathbf{v}^b \right) - d\mathbf{p} + \mathbf{t} + \Lambda \left[ \gamma \left( \mathbf{V} - \Gamma \mathbf{v}^b \right) \right] + f_{thm} \]

\[ -\delta \mathbf{v}^b = 0. \]

Microstructures

\[ \frac{d\mathbf{v}}{dt} = -\gamma \left( \mathbf{V} - \Gamma \mathbf{v}^b \right) - \nabla \phi + F_{thm} \]

\[ \frac{d\mathbf{X}}{dt} = \mathbf{V}. \]

Thermal Fluctuations

\[ \langle f_{thm}(t) f_{thm}(s)^T \rangle = -2k_B T \mathcal{L}_f \delta(t-s) \]

\[ \langle F_{thm}(t) F_{thm}(s)^T \rangle = 2k_B T \gamma \Sigma \delta(t-s) \]

\[ \langle F_{thm}(t) f_{thm}(s) \rangle = -2k_B T \gamma \Gamma \delta(t-s) \]

\[ \mathcal{L}_f = \mathcal{L}_f - \gamma \Lambda \Gamma \]

\[ \mathcal{L}_f = \mu_m (-\delta \mathbf{d} + 2K) + T_f \]

2019 Padidar, Rower, Atzberger

exhibits \( \tau^{-1} \), \( \tau^{-2} \) power laws vs \( \tau^{-3/2} \) bulk fluids
Surface Fluctuating Hydrodynamics

Fluid-structure Interactions

Active Mixing: Drift-Diffusion

Golestanian Swim Cycle

2019 Padidar, Rower, Atzberger

2019 Padidar, Rower, Atzberger
PDEs on manifolds present challenges for discretization and solvers from geometric contributions.

\[
\mu_m (-\delta d)^2 \Phi - \gamma \delta d \Phi - 2 \mu_m (-\star d (K(-\star d \Phi)) = -\star d b^b
\]

Incompressible Hydrodynamic Surface Flow (vector-potential):

GMLS methods developed to obtain consistent high-order discretizations.

**Generalized Moving Least Squares:**

**Target operator:** \( \tau_{x_i} [u] \) with Banach space \( V \) and dual \( V^* \).

**Probing functionals:** \( \Lambda[u] = (\lambda_1[u], \lambda_2[u], \ldots, \lambda_N[u]) \)

Find best reconstruction of \( p^* \) in \( V_n \) of \( u \) in \( V \).

\[
p^* = \text{arg min}_{p \in V_n} \sum_{j=1}^{N} (\lambda_j[u] - \lambda_j[p])^2 \omega(\lambda_j, \tau_{x_i})
\]

Approximate target operator \( \tau_{x_i} [u] \) by

\[
\tilde{\tau}[u] := \tau[p^*]
\]

**PDEs on Manifolds:** GMLS both for geometric quantities and for operators acting on surface fields.
GMLS Gaussian Curvature Estimation:

Gaussian Curvature Accuracy

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2019 Gross, Trask, Atzberger

http://atzberger.org/
Regression for learning geometric operators and developing solvers for PDEs on surfaces (transport equations / hydrodynamic flows).

Fourth-order PDEs with non-linear coupling geometry and differentiation via exterior calculus operators. **Collocation Method.**

**High-order Convergence:** Biharmonic equation for hydrodynamics.

\[
\mu_m \left(-\delta d^2\right)^2 \Phi - \gamma\delta d\Phi - 2\mu_m \left(-\ast d \left(K(-\ast d\Phi)\right)\right) = -\ast db^b.
\]

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Conclusions

Summary

Extended Saffman-Delbruck Approach for hydrodynamics of curved membranes.
Exterior calculus formulations and solvers for mechanics on manifolds.
Surface Fluctuating Hydrodynamics for drift-diffusion dynamics of microstructures in membranes.
Potential applications: cell biology (vesicles, liposomes, organelles), solvers for other bio-problems.

Papers


UCSB Student Collaborators


Sandia Collaborators

N. Trask, P. Kuberry, J. Hu, C. Siefert, and others.

Funding

DOE ASCR CM4 DE-SC0009254
NSF Grant DMS - 1616353
DOE ASCR PhILMS DE-SC0019246

More information: http://atzberger.org/