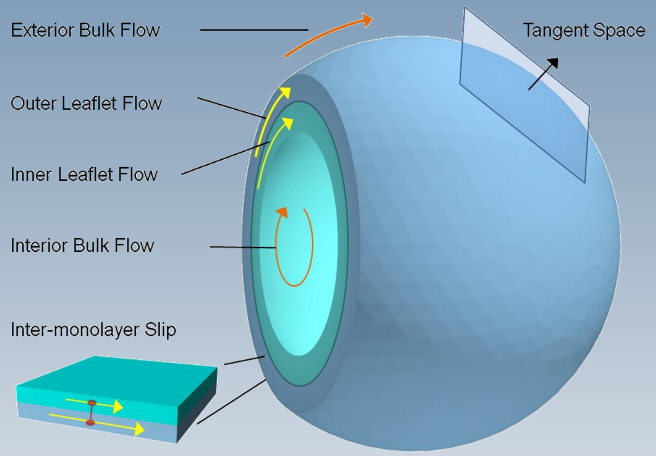
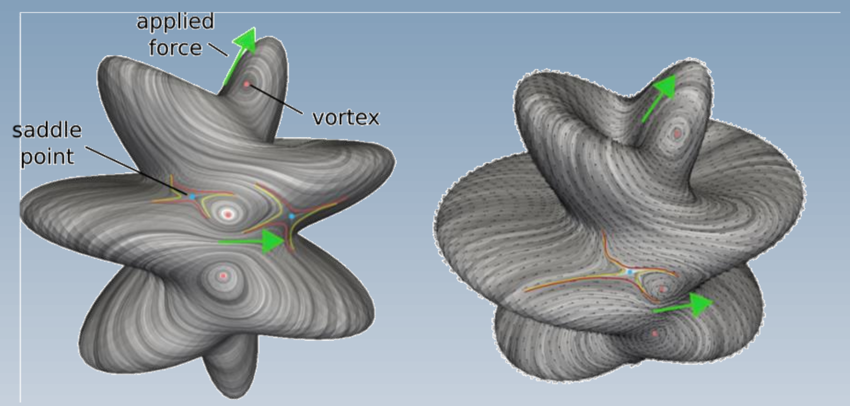
Surface Fluctuating Hydrodynamics Methods

Soft Materials with Fluid-Structure Interactions within Curved Fluid Interfaces





November 2020

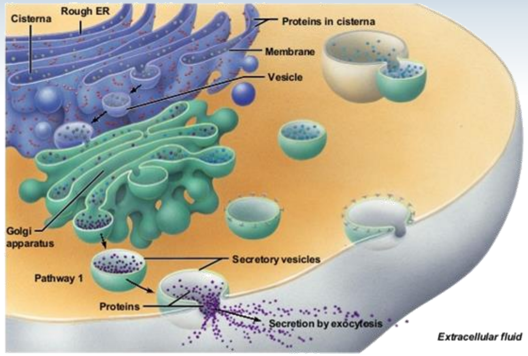
Paul J. Atzberger
University of California Santa Barbara

In collaboration: D. Rower, B. Gross, M. Padidar, N. Trask, P. Kuberry, and others.

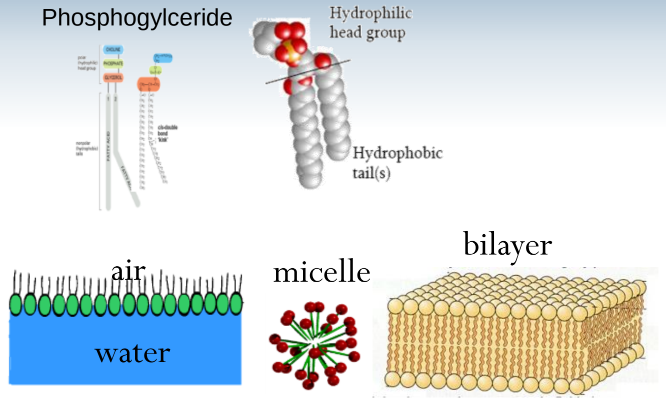
DOE ASCR CM4 DE-SC0009254
DOE ASCR PhILMS DE-SC0019246
NSF Grant DMS - 1616353
NSF CAREER Grant DMS-0956210

Lipid Bilayer Membranes

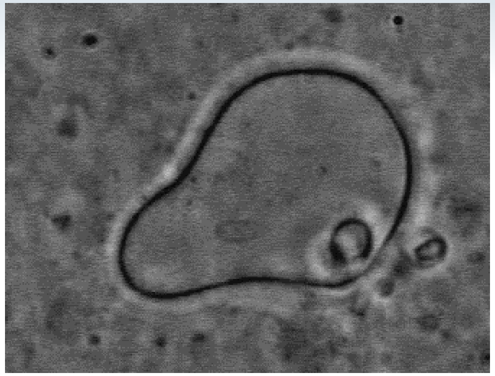
Cell Membranes



Phosphogylceride



Lipid Bilayer Configurations



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

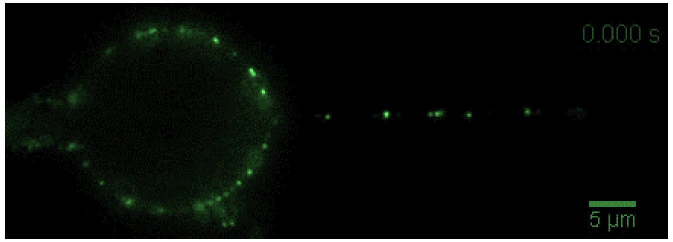
- Quantum Dots (QDs) conjugated to individual proteins.
- Image process --> QD location → protein positions.
- Trajectories measured over time-scales up to seconds.
- Protein diffusivity / kinetics depend on membrane mechanics.

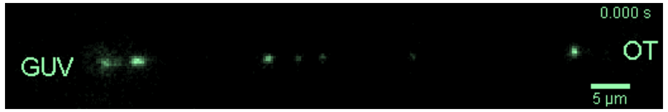
Fluorescence Contrast Microscopy

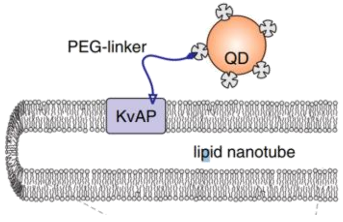
- Lipids labeled and membrane configuration observed.
- Image processing → representation of shapes.
- Thermal undulations → mechanics (bending elasticity, …).

hydrodynamics, elasticity, geometry…

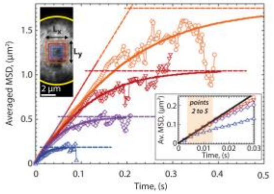
Single Particle Tracking of Proteins







Basserau 2011, 2016.

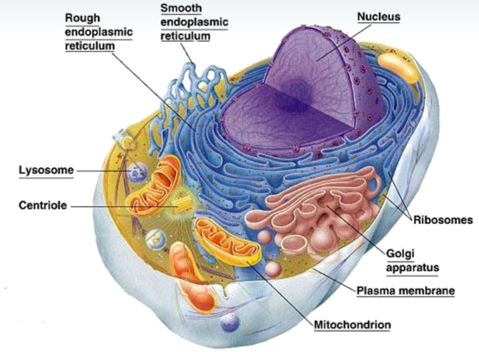


Basserau, Atzberger 2014.

Fluid Interfaces: General Motivations

soap films

red blood cells



cell mechanics

Motivations

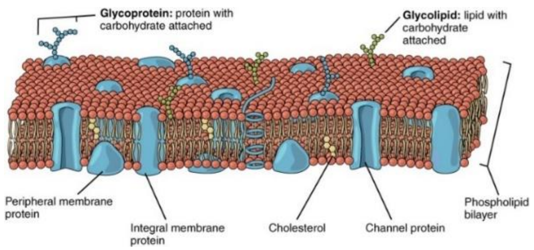
- Hydrodynamic flows within curved fluid interfaces relevant in many problems.
- Soap films, bubbles, cellular mechanics.
- Geometry plays important role in hydrodynamic responses.
- Fluctuations important in many problems:
    - diffusive transport, osmotic swelling, fission/fusion.

Challenges

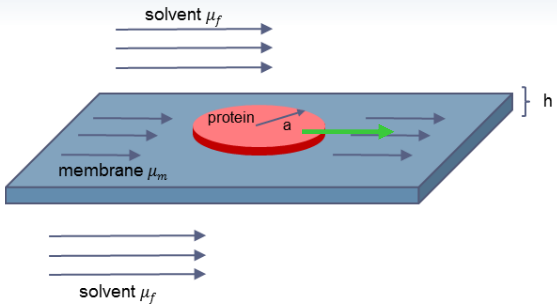
- Need good methods to formulate tractable hydrodynamic equations on manifolds.
- Approaches for performing analysis and reductions.
- Computational methods for efficient numerical approximation.

Classical Work: Saffman-Delbruck Theory 1975

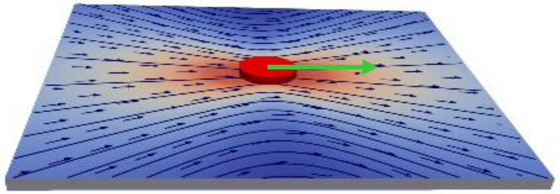
Proteins in Bilayers



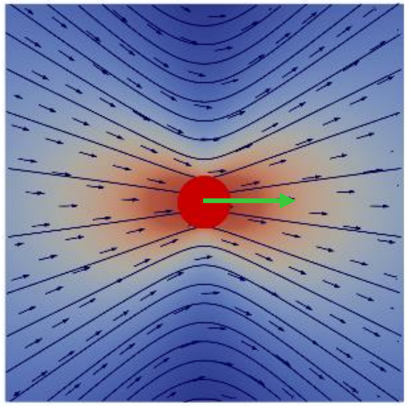
Saffman-Delbruck Theory



Immersed Boundary SD



(Atzberger & Sigurdsson, Soft Matter, 2016)



Membrane Protein Diffusion:

- Membrane treated as 2D fluid slab. V = MF ~ D = $2K_BTM$
- 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.

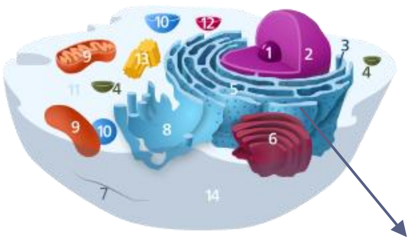
Saffman-Delbruck Theory (1975):

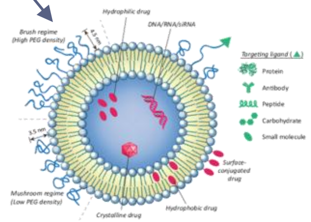
- Mobility / Diffusion as h → 0,

  $V = M_{SD}F \quad \sim \quad D = 2K_BTM_{SD}$

  $$M_{SD} = (1/4\pi\mu_m)\left(\log(2L_{SD}/a) - \gamma\right), \qquad L_{SD} = \mu_m/2\mu_f$$

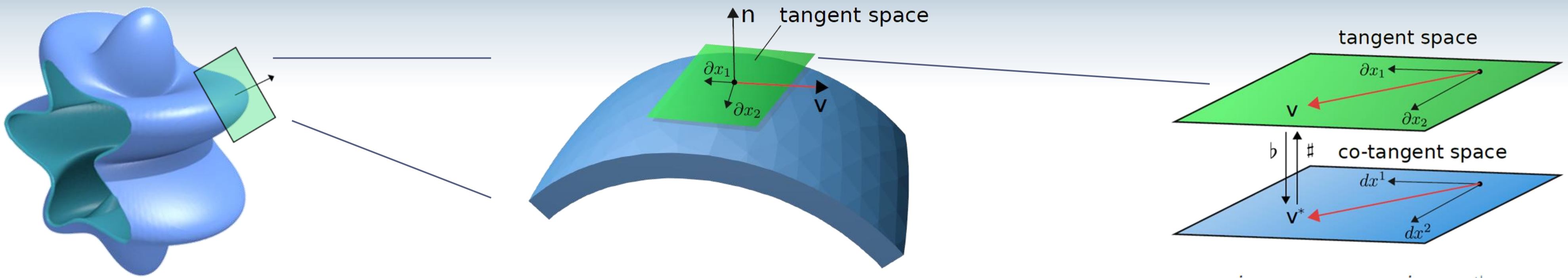
- Predicts diffusion of proteins depends as log on size!
- $L_{SD} \sim 1\ \mu m$, a ~ 10 nm, long-range coupling.
- Many membranes exhibit curvature over this length-scale.





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

Exterior Calculus Formulation of Mechanics



$$\flat \;:\; v^j \partial_{\mathbf{x}^j} \to v_i d\mathbf{x}^i \qquad \sharp \;:\; v_i d\mathbf{x}^i \to v^j \partial_{\mathbf{x}^j}.$$

Exterior Calculus Operators

d : **Exterior Derivative** (k-form → (k+1)-form)
***** : **Hodge Star** (k-form → (n-k)-form)
^ : **Wedge Product** (k_1,k_2-form → (k_1+k_2)-form).

Operators d and *

$$\mathbf{d}\alpha = \frac{1}{k!}\frac{\partial \alpha_{i_1\ldots i_k}}{\partial x^j}\mathbf{dx}^j \wedge \mathbf{dx}^{i_1} \wedge \cdots \wedge \mathbf{dx}^{i_k}$$

$$\star\alpha = \frac{\sqrt{|g|}}{(n-k)!k!}\alpha^{i_1\ldots i_k}\epsilon_{i_1\ldots i_k j_1 \ldots j_{n-k}} \cdot \mathbf{dx}^{j_1} \wedge \cdots \wedge \mathbf{dx}^{j_{n-k}}$$

Vector Calculus Correspondence

$$\begin{aligned}
\mathrm{grad}(f) &= [\mathbf{d}f]^\sharp \\
\mathrm{div}(\mathbf{F}) &= -(\star\mathbf{d}\star\mathbf{F}^\flat) = -\boldsymbol{\delta}\mathbf{F}^\flat \\
\mathrm{curl}(\mathbf{F}) &= \left[\star(\mathbf{d}\mathbf{F}^\flat)\right]^\sharp. \\
\mathrm{div}(\mathbf{D}) &= -\boldsymbol{\delta}\mathbf{d}\mathbf{v}^\flat + 2K\mathbf{v}^\flat
\end{aligned}$$

Conservation Laws on Manifolds

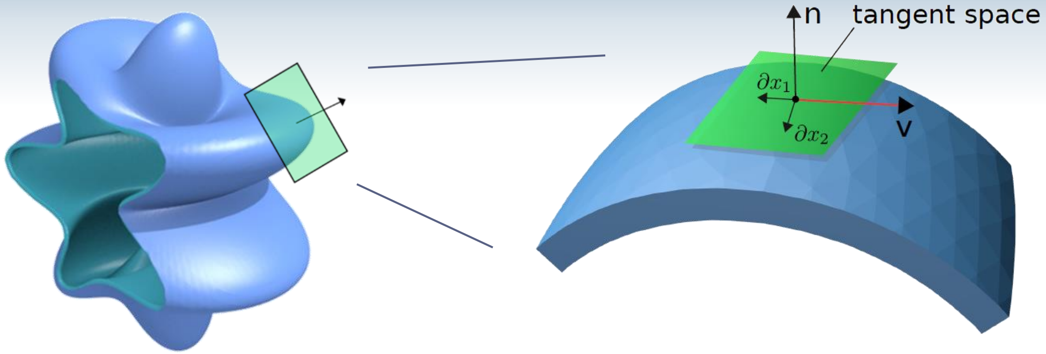
$$\int_{\partial\Omega}\omega = \int_\Omega \mathbf{d}\omega$$ Stokes Theorem

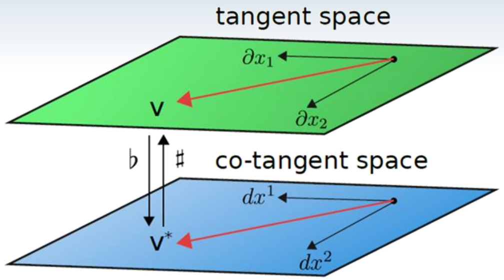
$$\int_{\partial\Omega}\star\omega = \int_\Omega \mathbf{d}\star\omega$$ Divergence Theorem

Diffusion Equation / Laplace-Beltrami

$$\frac{\partial}{\partial t}\int_\Omega \star u = \int_{\partial\Omega}\star\omega = \int_\Omega \mathbf{d}\star\omega. \xrightarrow{\omega = \mathbf{d}u} \frac{\partial u}{\partial t} = -\star\mathbf{d}\star\omega = -\boldsymbol{\delta}\omega = -\boldsymbol{\delta}\mathbf{d}u.$$

Exterior Calculus Formulation of Mechanics





$$\flat \; : \; v^j \partial_{\mathbf{x}^j} \rightarrow v_i d\mathbf{x}^i \qquad \sharp \; : \; v_i d\mathbf{x}^i \rightarrow v^j \partial_{\mathbf{x}^j}.$$

Hydrodynamics on Manifolds

Rate-of-Deformation Tensor

$$\mathbf{D} = \nabla \mathbf{v} + \nabla \mathbf{v}^T \longrightarrow \mathrm{div}(\mathbf{D}) = -\boldsymbol{\delta} \mathbf{d} \mathbf{v}^\flat + 2K \mathbf{v}^\flat$$

Momentum Equations

$$\begin{aligned} \rho \left(\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v} \right) &= \mathrm{div}(\boldsymbol{\sigma}) + \mathbf{b} \\ \partial_t \rho + \rho \mathrm{div}(\mathbf{v}) &= 0. \end{aligned}$$

Stokes Equations (surface)

$$\begin{aligned} \mu_m \left(-\boldsymbol{\delta} \mathbf{d} \mathbf{v}^\flat + 2K \mathbf{v}^\flat \right) - \mathbf{d}p + \mathbf{b}^\flat &= 0 \\ -\boldsymbol{\delta} \mathbf{v}^\flat &= 0. \end{aligned}$$

Surface Hydrodynamic Equations

$$\begin{cases} \rho \dfrac{D\mathbf{v}^\flat}{dt} = \mu_m \left(-\boldsymbol{\delta} \mathbf{d} + 2K \right) \mathbf{v}^\flat - \boldsymbol{d}p + \mathbf{b}^\flat \\ -\boldsymbol{\delta} \mathbf{v}^\flat = 0 \end{cases}$$

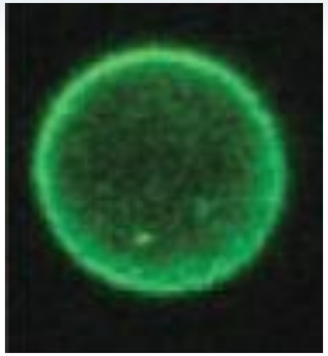
Vector Potential Form: $\mathbf{v}^\flat = - \star \mathbf{d} \Phi$

$$\mu_m \left(-\boldsymbol{\delta} \mathbf{d} \right)^2 \Phi - 2\mu_m \left(- \star \mathbf{d} \left(K \left(- \star \mathbf{d} \Phi \right) \right) \right) = - \star \mathbf{d} \mathbf{b}^\flat$$

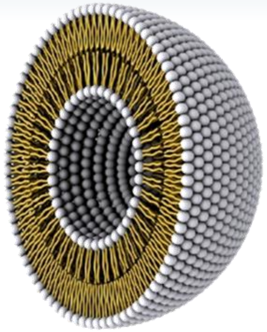
2016 Atzberger & Sigurdsson, 2018 Gross & Atzberger.

Lipid Bilayer Membranes: Spherical Vesicles

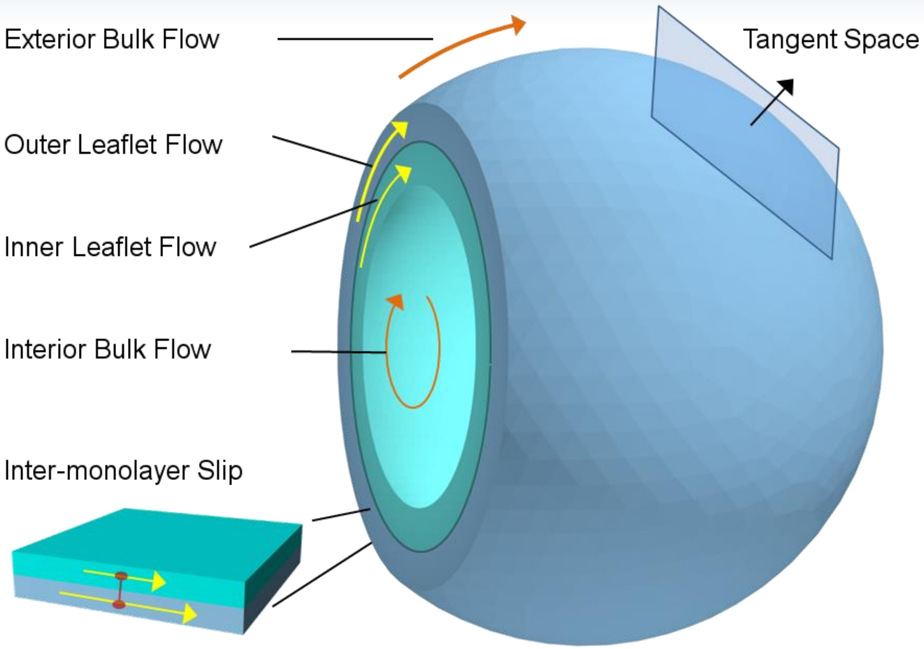
Vesicle



Lipid Bilayer



Bilayer Hydrodynamics



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

$$\begin{cases} \mu_m\left[-\boldsymbol{\delta}\mathbf{d}\mathbf{v}^\flat_+ + 2K_+\mathbf{v}^\flat_+\right] + \mathbf{t}^\flat_+ - \gamma\left(\mathbf{v}^\flat_+ - \mathbf{v}^\flat_-\right) \\ \quad = \mathbf{d}p_+ - \mathbf{b}^\flat_+ = -\mathbf{c}^\flat_+, \quad \mathbf{x}\in\Gamma_+ \\ \boldsymbol{\delta}\mathbf{v}^\flat_+ = 0, \qquad \mathbf{x}\in\Gamma_+, \\ \\ \mu_m\left[-\boldsymbol{\delta}\mathbf{d}\mathbf{v}^\flat_- + 2K_-\mathbf{v}^\flat_-\right] + \mathbf{t}^\flat_- - \gamma\left(\mathbf{v}^\flat_- - \mathbf{v}^\flat_+\right) \\ \quad = \mathbf{d}p_- - \mathbf{b}^\flat_- = -\mathbf{c}^\flat_-, \quad \mathbf{x}\in\Gamma_- \\ \boldsymbol{\delta}\mathbf{v}^\flat_- = 0, \qquad \mathbf{x}\in\Gamma_-. \end{cases}$$

(outer layer)

(inner layer)

Solvent Hydrodynamics

$$\begin{aligned} \mu\Delta\mathbf{u} - \nabla p &= 0, \quad \mathbf{x}\in\Omega \\ \nabla\cdot\mathbf{u} &= 0, \quad \mathbf{x}\in\Omega \\ \mathbf{u} &= \mathbf{v}, \quad \mathbf{x}\in\partial\Omega \\ \mathbf{u}_\infty &= 0. \end{aligned}$$

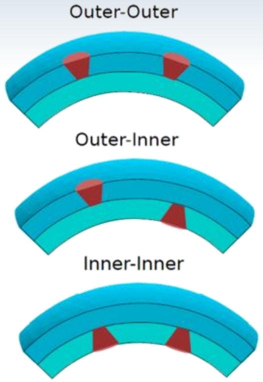
Traction coupling

$$\begin{aligned} \mathbf{t}^+ &= \boldsymbol{\sigma}^+\cdot\mathbf{n}^+ \\ \mathbf{t}^- &= \boldsymbol{\sigma}^-\cdot\mathbf{n}^- \end{aligned}$$

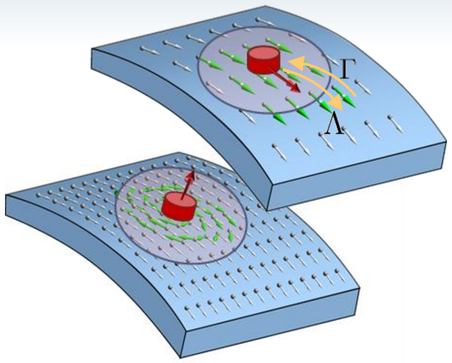
2016 Atzberger & Sigurdsson

Immersed Boundary Methods on Manifolds

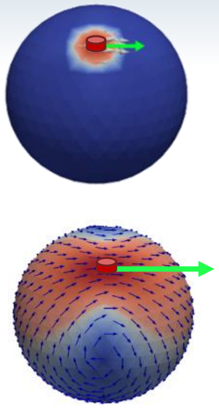
Leaflet Cases



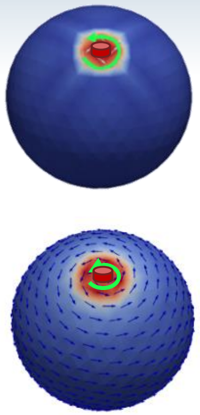
Immersed Boundary Coupling



Particle Force



Particle Torque



Immersed Boundary Methods for Manifolds

Velocity-Averaging operator: $\Gamma \mathbf{v} \;=\; \int_{\Omega} \mathbf{W}[\mathbf{v}](\mathbf{y}) d\mathbf{y}$

Force-Spreading operator: $\Lambda \mathbf{F} \;=\; \mathbf{W}^{*}[\mathbf{F}](\mathbf{x})$

Adjoint condition: $\langle \mathbf{v}, \Lambda \mathbf{F} \rangle \;=\; \int_{\Omega} \mathbf{v}(\mathbf{x}) \cdot (\Lambda \mathbf{F})(\mathbf{x}) d\mathbf{x}$

$$\langle \Gamma \mathbf{v}, \mathbf{F} \rangle \;=\; \sum_i [\Gamma \mathbf{v}]_i \cdot [\mathbf{F}]_i$$

$$\langle \Gamma \mathbf{v}, \mathbf{F} \rangle \;=\; \langle \mathbf{v}, \Lambda \mathbf{F} \rangle \longrightarrow \Gamma^{T} = \Lambda$$

Weight Tensor

$$\mathbf{W}[\mathbf{v}] = \sum_i \left(\left(w^{[i]} \right)^{\alpha}_{\beta} v^{\beta} \right) \partial_{\alpha} |_{\mathbf{X}^{[i]}}$$

$$\left(w^{[i],\alpha} \right)^{\gamma} \partial_{\gamma} \;=\; \mathbf{q}^{\alpha}$$

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

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

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

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

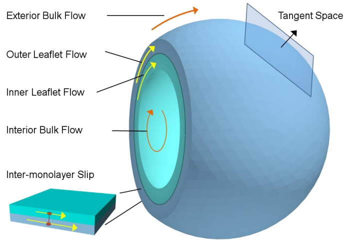
Mobility Tensor

$$\begin{bmatrix} \mathbf{V} \\ \boldsymbol{\omega} \end{bmatrix} = \mathbf{M} \begin{bmatrix} \mathbf{F} \\ \boldsymbol{\tau} \end{bmatrix}$$

IB-Membrane Mobility

$$M_{ij} = \Gamma_i \mathcal{S} \Lambda_j$$

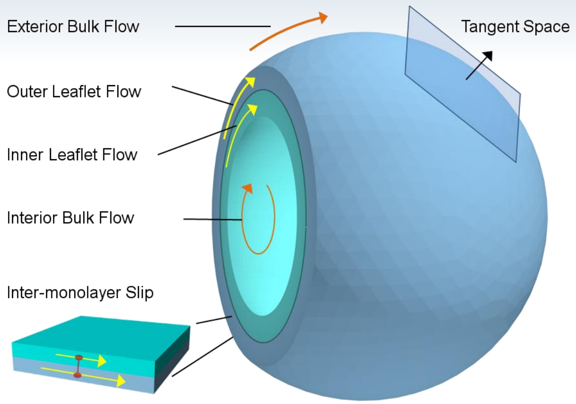
S is fluid solution operator



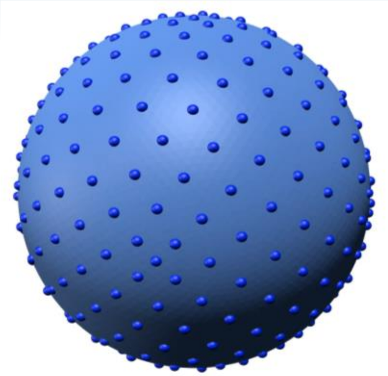
2019 Atzberger, Padidar, Rower
2016 Atzberger & Sigurdsson

Analytic Solutions and Lebedev Quadrature

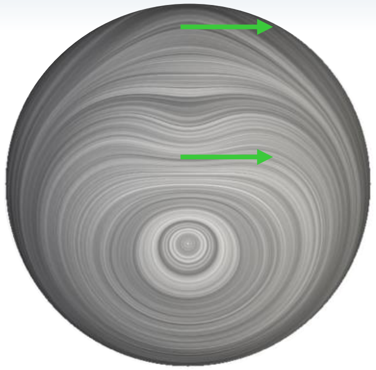
Bilayer Hydrodynamics



Lebedev Nodes



Flow Streamlines



Bilayer Hydrodynamics

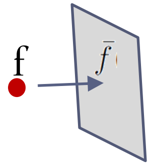
$$\begin{cases} \mu_m \left[-\boldsymbol{\delta}\mathbf{d}\mathbf{v}_+^\flat + 2K_+\mathbf{v}_+^\flat\right] + \mathbf{t}_+^\flat - \gamma\left(\mathbf{v}_+^\flat - \mathbf{v}_-^\flat\right) \\ \quad = \mathbf{d}p_+ - \mathbf{b}_+^\flat = -\mathbf{c}_+^\flat, \quad \mathbf{x} \in \Gamma_+ \\ \boldsymbol{\delta}\mathbf{v}_+^\flat = 0, \quad \mathbf{x} \in \Gamma_+, \\ \\ \mu_m \left[-\boldsymbol{\delta}\mathbf{d}\mathbf{v}_-^\flat + 2K_-\mathbf{v}_-^\flat\right] + \mathbf{t}_-^\flat - \gamma\left(\mathbf{v}_-^\flat - \mathbf{v}_+^\flat\right) \\ \quad = \mathbf{d}p_- - \mathbf{b}_-^\flat = -\mathbf{c}_-^\flat, \quad \mathbf{x} \in \Gamma_- \\ \boldsymbol{\delta}\mathbf{v}_-^\flat = 0, \quad \mathbf{x} \in \Gamma_-. \end{cases}$$

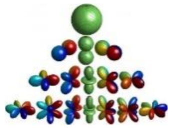
(outer layer)

(inner layer)

L^2-Orthogonal Projection

Spherical Harmonics





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

$$\hat{f}_i = \langle f, Y_i \rangle_Q$$

Solution Spherical Harmonics

$$\mathbf{v}_\pm^\flat = -\star\mathbf{d}\sum_s a_s^\pm \Phi_s\,, \quad \mathbf{c}^\flat = -\star\mathbf{d}\textstyle\sum_s c_s\Phi_s$$

$$\begin{bmatrix} a_s^+ \\ a_s^- \end{bmatrix} = \mathcal{A}_s^{-1}\begin{bmatrix} -c_s^+ \\ -c_s^- \end{bmatrix}$$

$$\mathcal{A}_s = \begin{bmatrix} A_1^\ell - \gamma & \gamma \\ \gamma & A_2^\ell - \gamma \end{bmatrix}$$

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

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

$$L^\pm = \mu_\pm/2\mu_f$$

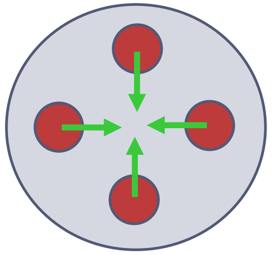
2016 Atzberger & Sigurdsson

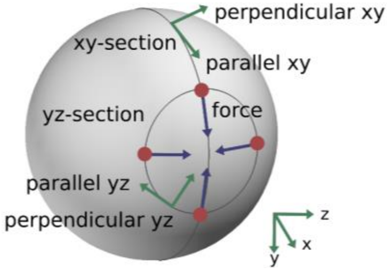
Many Particle Interactions

Collective Motions

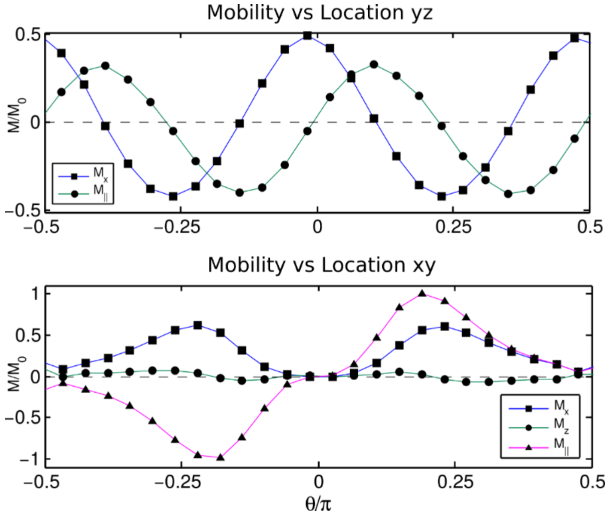
$$\frac{d\mathbf{X}}{dt} = \mathbf{MF}$$

Driving Force and Cross-Section

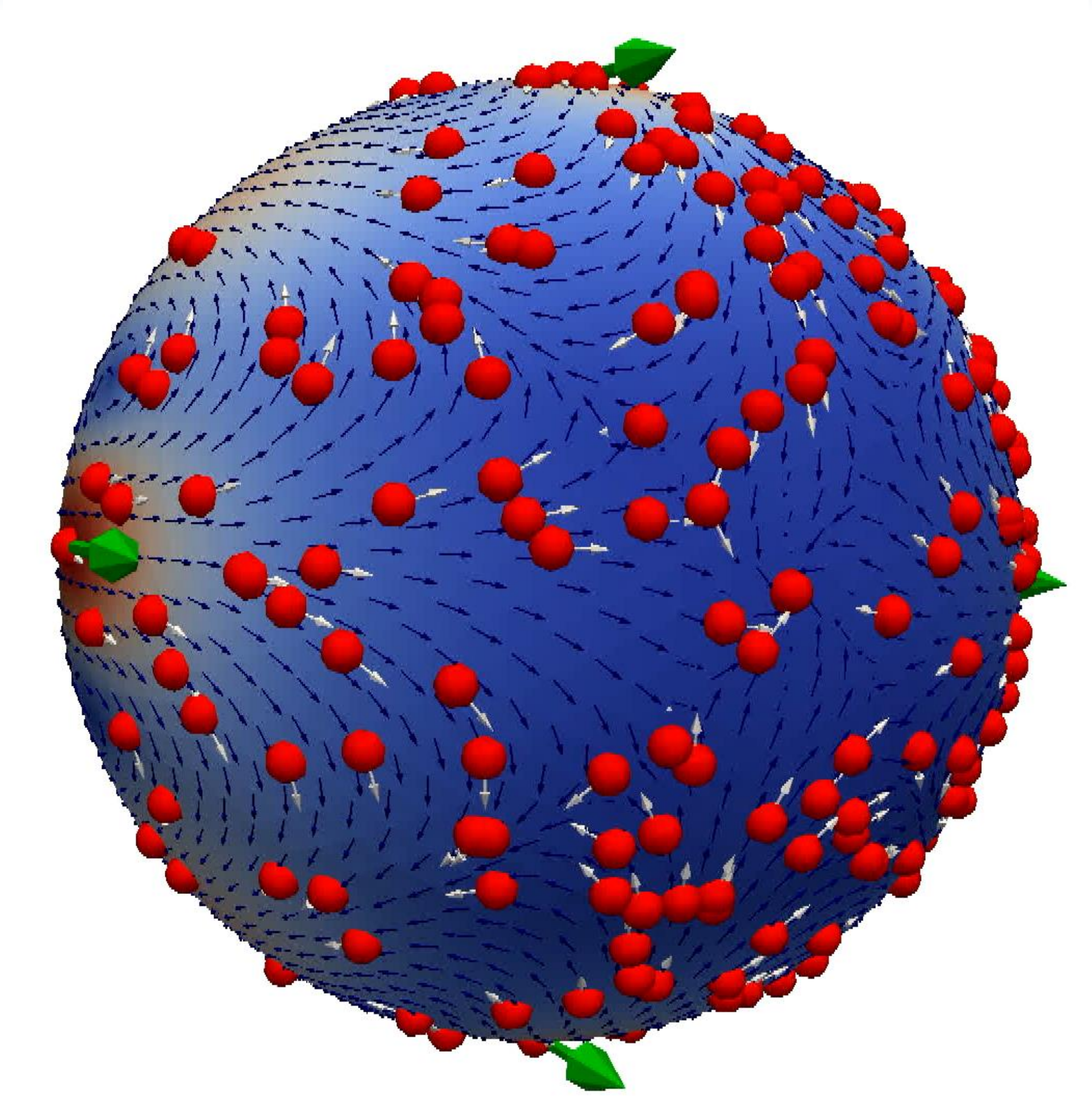




Mobility Response



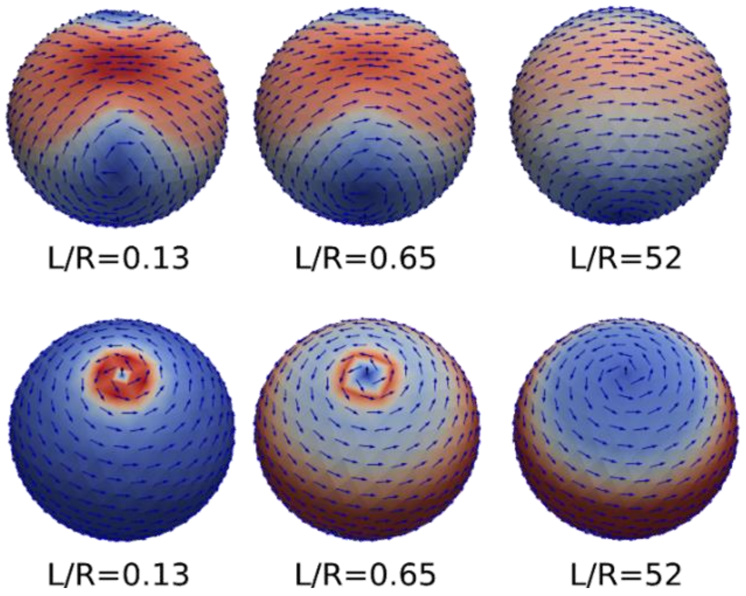
Hydrodynamic Response



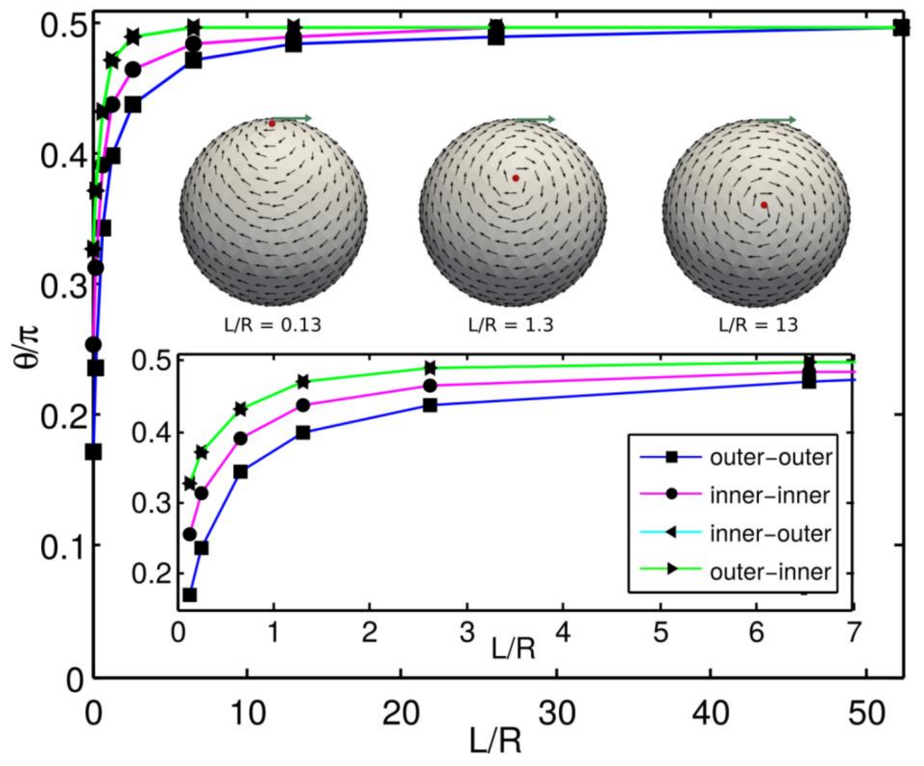
2016 Atzberger & Sigurdsson

Mobility for Spherical Vesicles

Mobility Response vs Membrane Viscosity

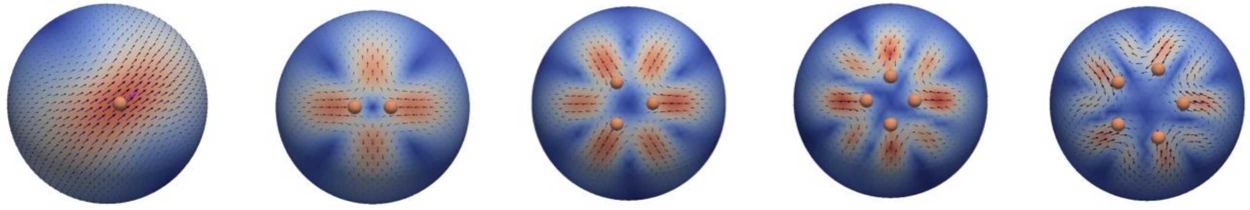


Vortex Location vs Membrane Viscosity



Collective Motions

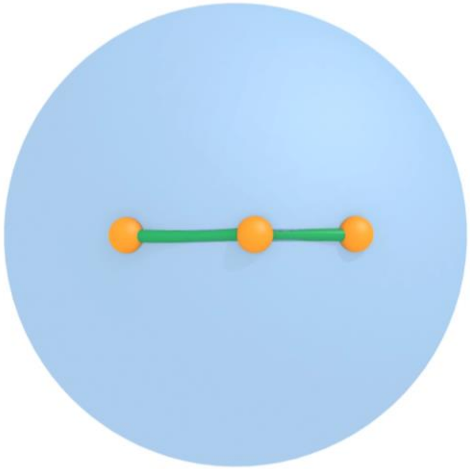
$$\frac{d\mathbf{X}}{dt} = \mathbf{MF}$$



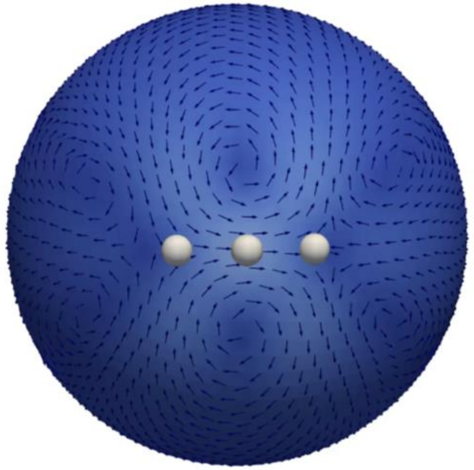
2016 Atzberger & Sigurdsson

Surface Hydrodynamic Methods

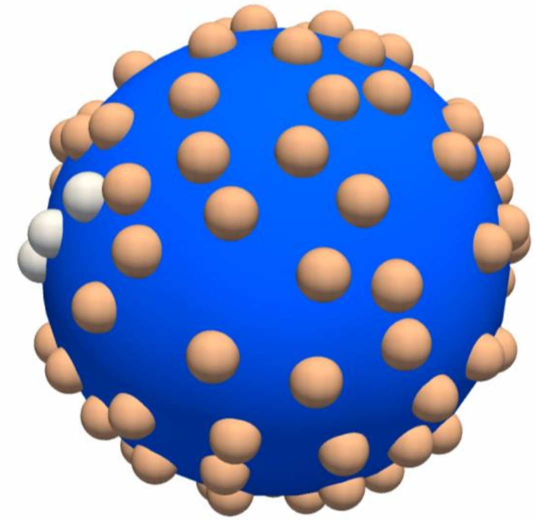
Golestanian Swimmer



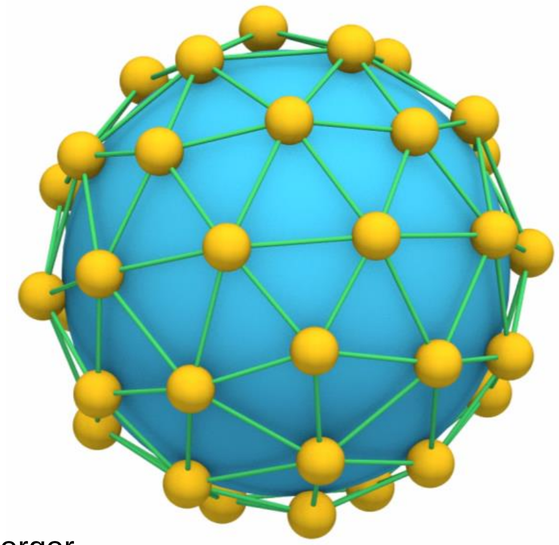
Golestanian Swimmer Flows



Active Swimmer and Mixing



Polymer Network Fluctuations

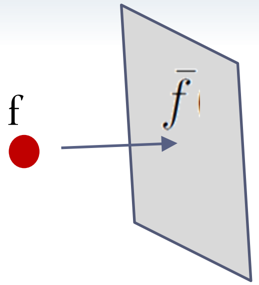


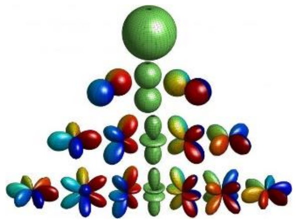
2016 Atzberger & Sigurdsson, 2019 Padidar, Rower, & Atzberger.

Hydrodynamics and Geometry

Spectral Solver for Surface Hydrodynamics

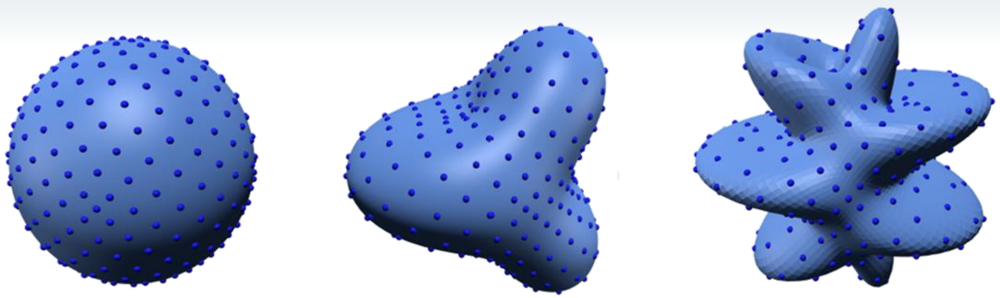
L^2-Orthogonal Projection





Spherical Harmonics

Lebedev Quadrature



Spectral Approximation

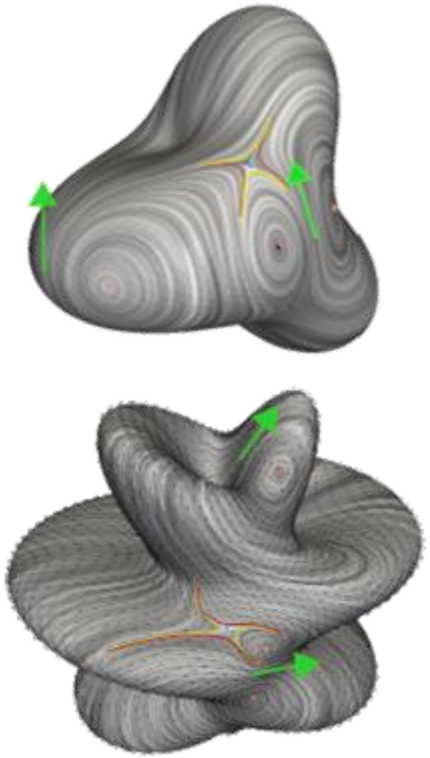
L^2-Projection:

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

$$\hat{f}_i = \langle f, Y_i \rangle_Q$$

Inner-Product:

$$\langle u, v \rangle_Q = \sum_\ell w_\ell u(\mathbf{x}_\ell) v(\mathbf{x}_\ell)$$



Differential forms $\mathbf{v}^\flat$ (0-forms, 1-forms, 2-forms).
Represented as scalar / vector fields $\mathbf{v}^\#$ at the Lebedev nodes.

Exterior Derivative: **d** approximated by $\bar{\mathbf{d}}$ $\longleftarrow$ $\bar{\mathbf{v}}^\sharp(\theta,\phi) = [\mathcal{P}\bar{v}^x, \mathcal{P}\bar{v}^y, \mathcal{P}\bar{v}^z]$

Hodge Star: ***** approximated by $\bar{\star}$

Approximating PDEs on the Manifold: $\tilde{\mathcal{L}} = -\bar{\boldsymbol{\delta}}\bar{\mathbf{d}} = -\bar{\star}\,\bar{\mathbf{d}}\,\bar{\star}\,\bar{\mathbf{d}}.$ $\bar{u} = \sum_j \hat{u}_j Y_j,\ \bar{g} = \sum_j \hat{g}_j Y_j$

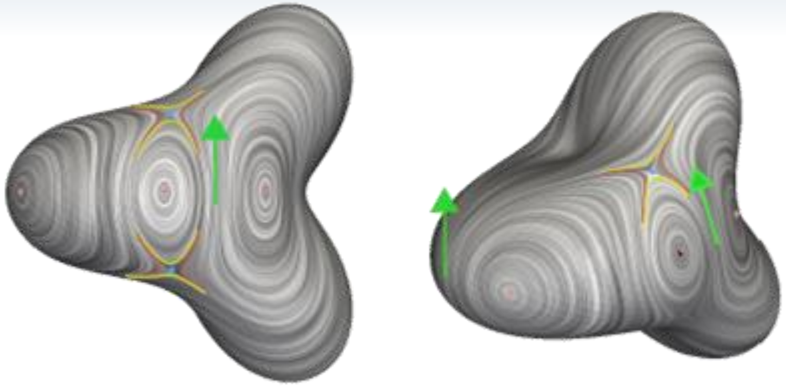
$$\mathcal{L}u = -g \longrightarrow \langle \tilde{\mathcal{L}}\bar{u}, Y_i \rangle_Q = -\langle \bar{g}, Y_i \rangle_Q \longrightarrow K\hat{\mathbf{u}} = -M\hat{\mathbf{g}}$$

Method can be used for approximating general PDEs on manifolds.

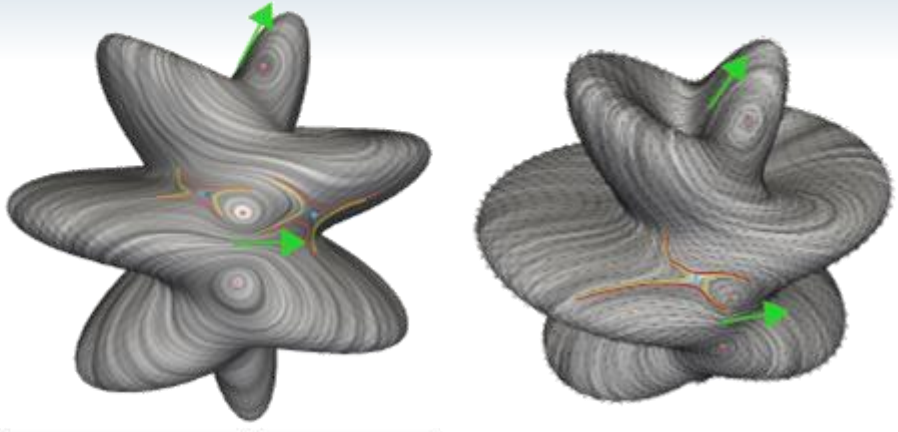
2018 Gross & Atzberger.

Role of geometry in hydrodynamic flow responses

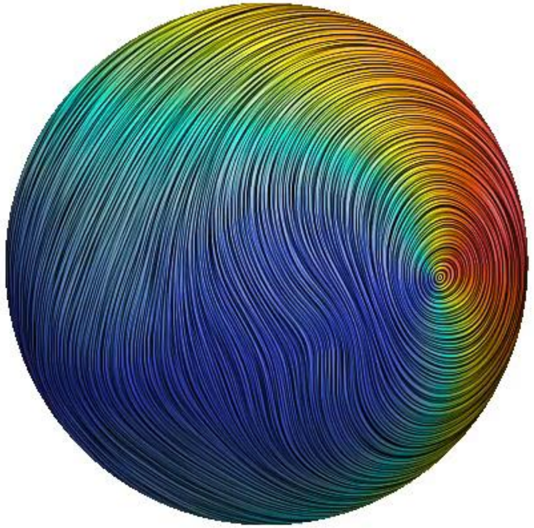
Manifold B Flow Response

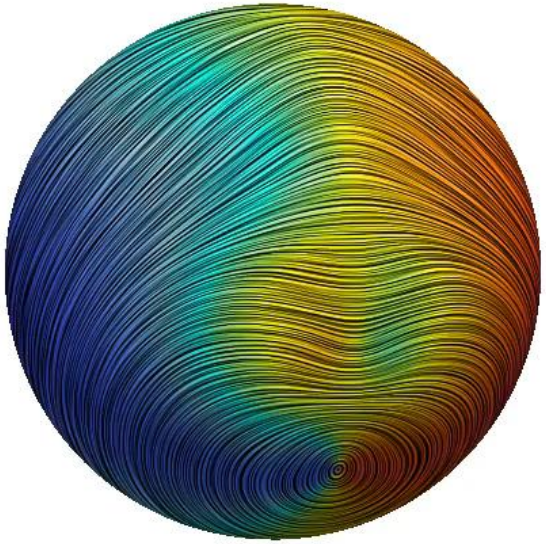


Manifold C Flow Response



Flow transitions:

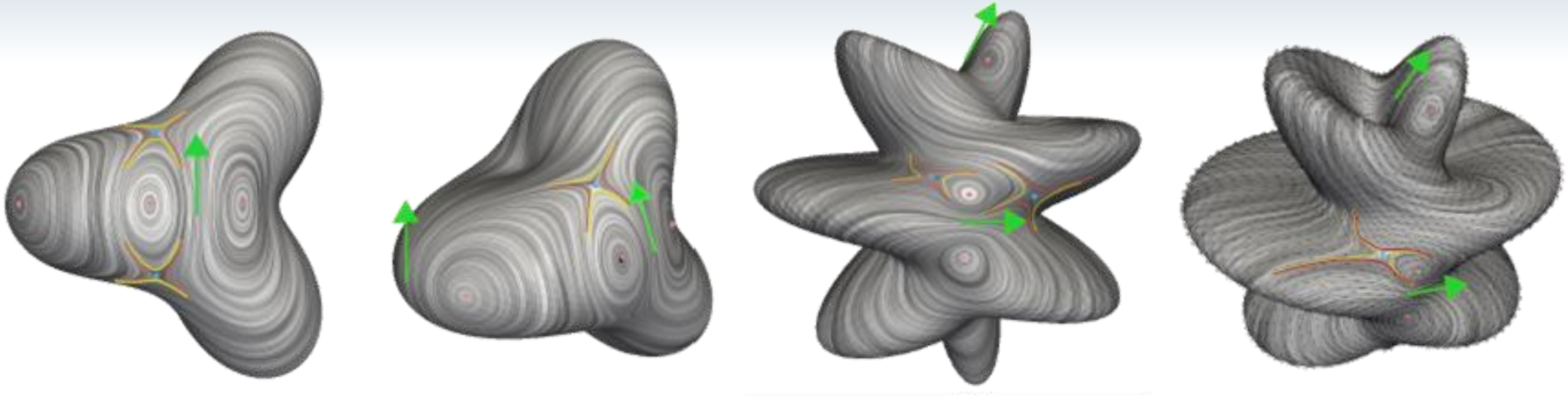


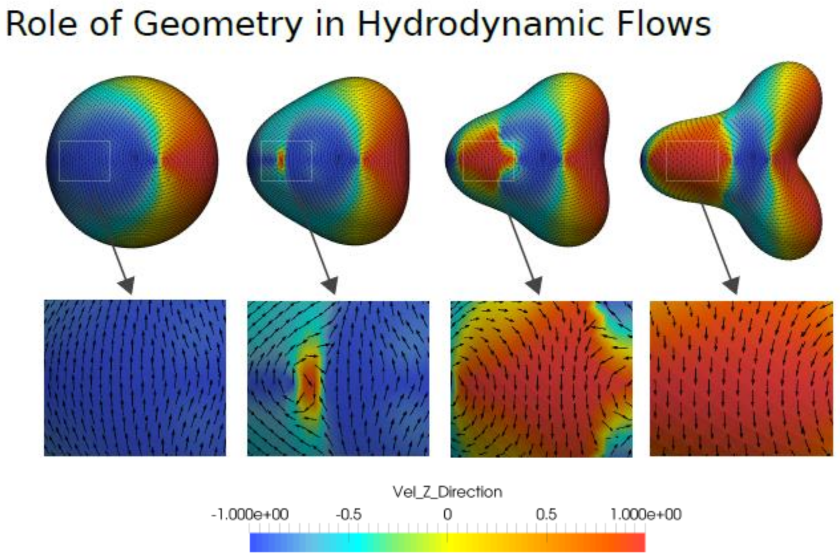


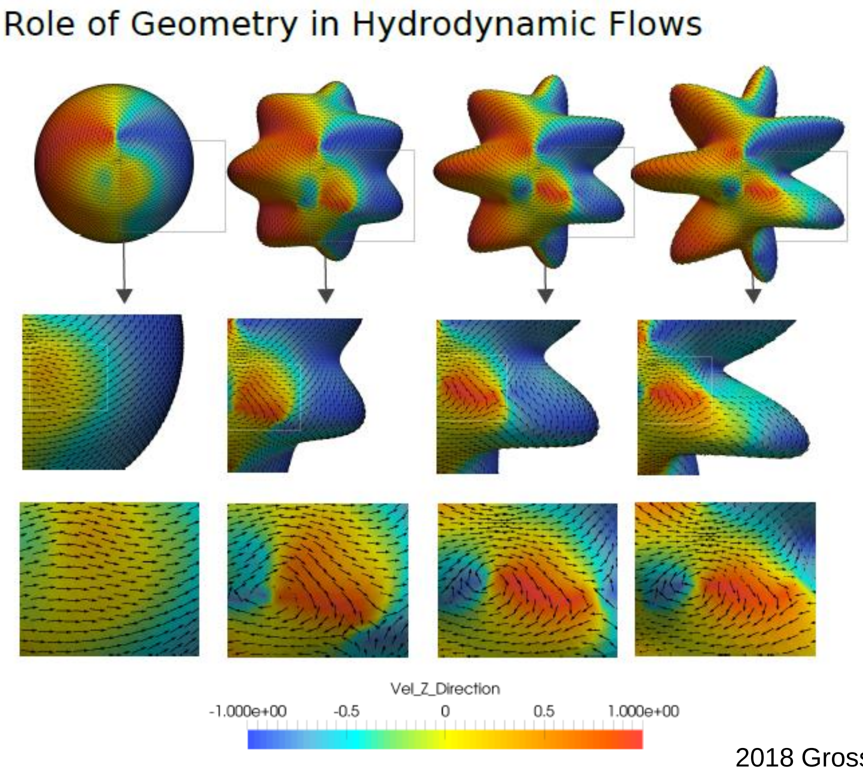
2018 Gross & Atzberger.

2018 Gross & Atzberger

Role of geometry in hydrodynamic flow responses

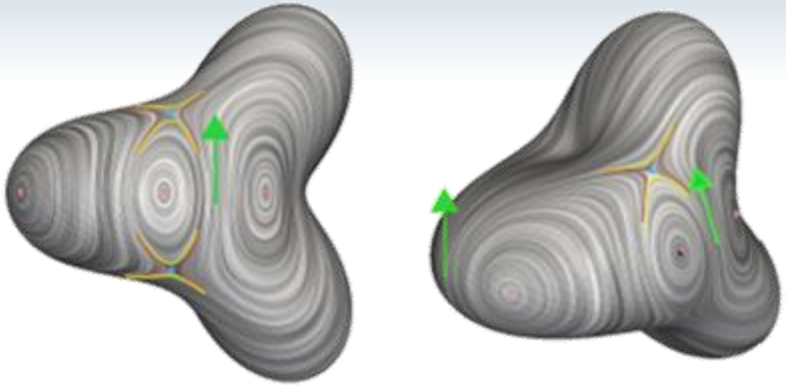


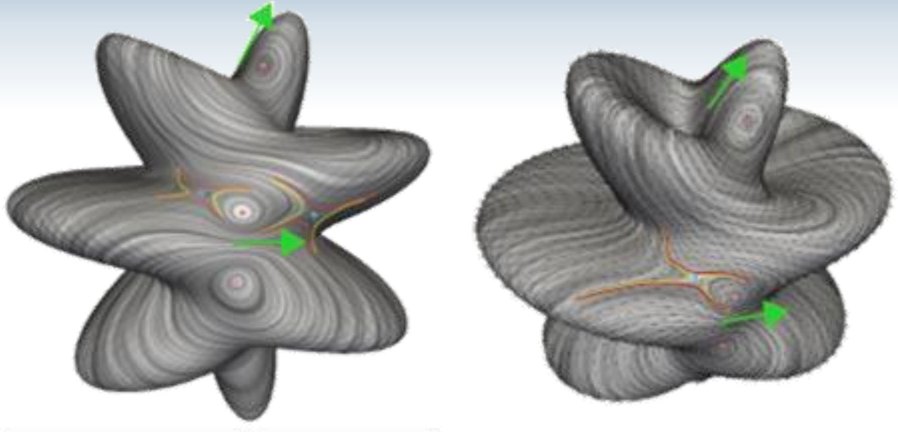




2018 Gross & Atzberger.

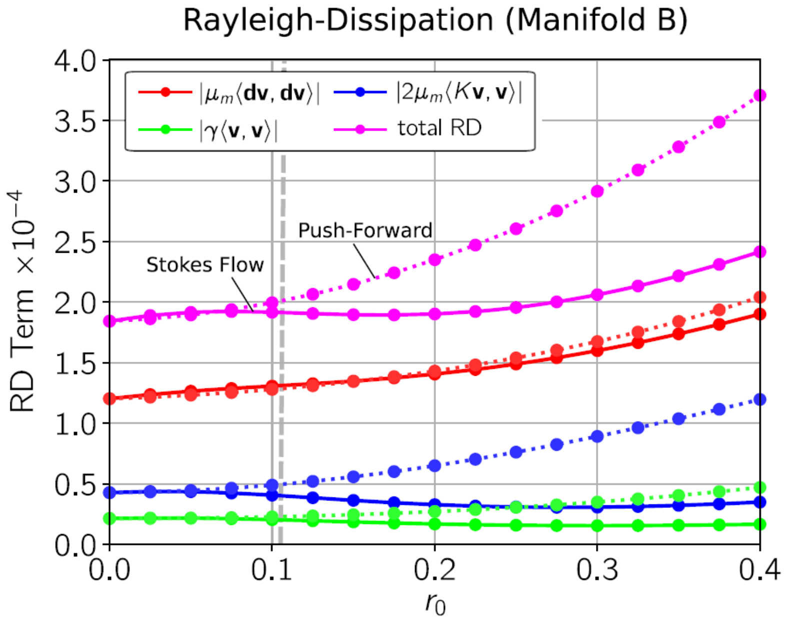
Role of geometry in hydrodynamic flow responses

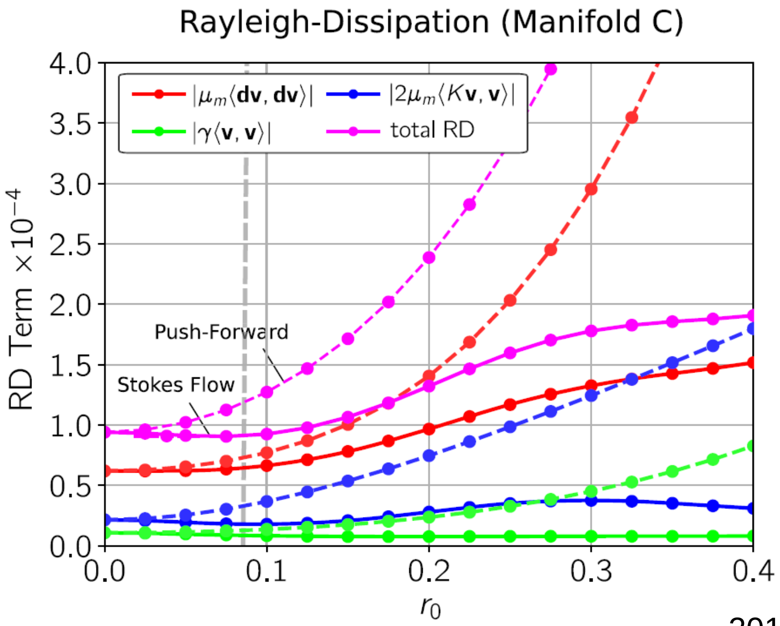




Rayleigh Dissipation Rate:

$$\mathrm{RD}[\mathbf{v}^\flat] \quad = \quad \mu_m\langle \mathbf{d}\mathbf{v}^\flat, \mathbf{d}\mathbf{v}^\flat\rangle_{\mathcal{M}} - 2\mu_m\langle K\mathbf{v}^\flat, \mathbf{v}^\flat\rangle_{\mathcal{M}} + \gamma\langle \mathbf{v}^\flat, \mathbf{v}^\flat\rangle_{\mathcal{M}}$$



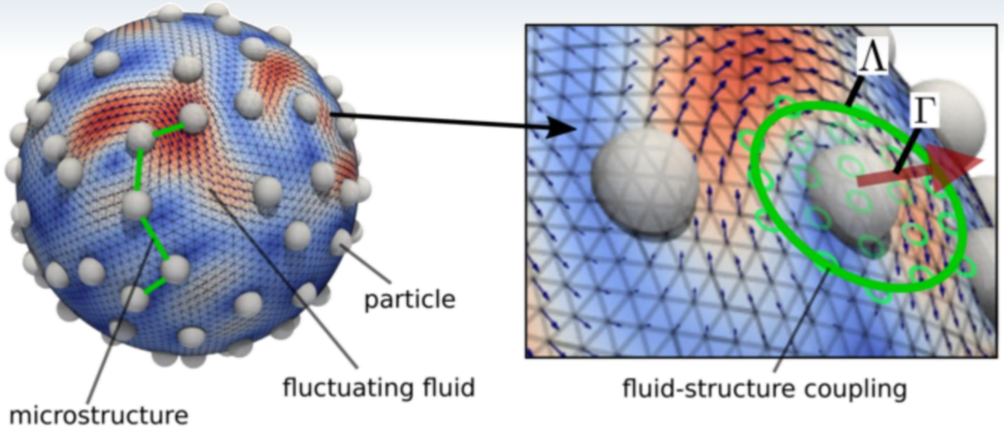


2018 Gross & Atzberger

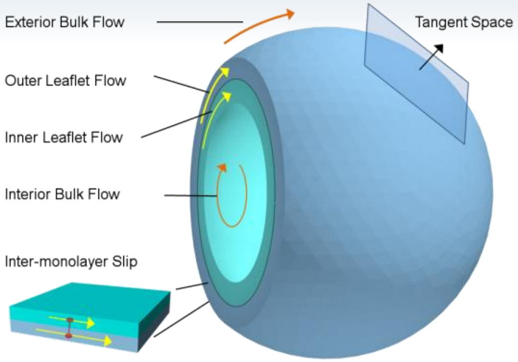
Thermal Fluctuations

Surface Fluctuating Hydrodynamics

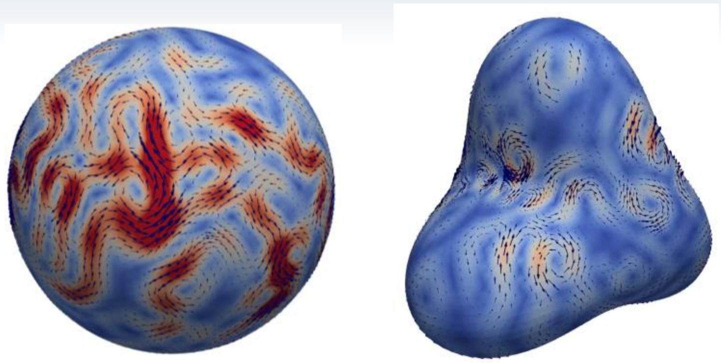
Fluid-structure Interactions



Hydrodynamics



Fluctuating Fluid Velocity Fields



Surface Fluctuating Hydrodynamics (Inertial Regime)

Fluid

$$\rho \frac{d\mathbf{v}^\flat}{dt} = \mu_m\left(-\boldsymbol{\delta}\mathbf{d}\mathbf{v}^\flat + 2K\mathbf{v}^\flat\right) - \mathbf{d}p + \mathbf{t}^\flat + \Lambda\left[\gamma\left(\mathbf{V} - \Gamma\mathbf{v}^\flat\right)\right] + \mathbf{f}^\flat_{thm}$$

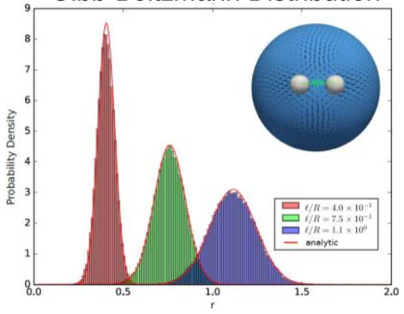
$$-\boldsymbol{\delta}\mathbf{v}^\flat = 0.$$

Microstructures

$$m\frac{d\mathbf{V}}{dt} = -\gamma\left(\mathbf{V} - \Gamma\mathbf{v}^\flat\right) - \nabla\phi + \mathbf{F}_{thm}$$

$$\frac{d\mathbf{X}}{dt} = \mathbf{V}.$$

Gibb-Boltzmann Distribution



Thermal Fluctuations

$$\langle \mathbf{f}_{thm}(t)\mathbf{f}_{thm}(s)^T\rangle = -2k_BT\mathcal{L}_{ff}\delta(t-s)$$

$$\langle \mathbf{F}_{thm}(t)\mathbf{F}_{thm}(s)^T\rangle = 2k_BT\gamma\mathcal{I}\delta(t-s)$$

$$\langle \mathbf{F}_{thm}(t)\mathbf{f}_{thm}(s)^T\rangle = -2k_BT\gamma\Gamma\delta(t-s).$$

$$\mathcal{L}_{ff} = \mathcal{L}_f - \gamma\Lambda\Gamma$$

$$\mathcal{L}_f = \mu_m\left(-\boldsymbol{\delta}\mathbf{d} + 2K\right) + \mathcal{T}_f$$

Surface Fluctuating Hydrodynamics (Overdamped)

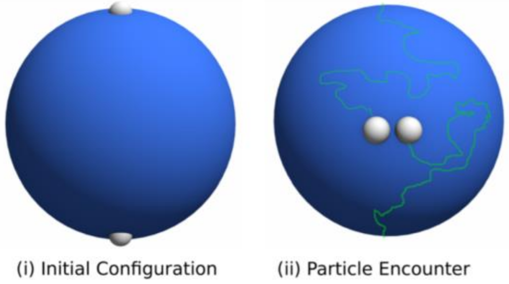
Microstructures

$$\frac{d\mathbf{X}}{dt} = \mathbf{MF} + k_BT\nabla\cdot\mathbf{M} + \mathbf{F}_{thm}$$

Thermal Fluctuations

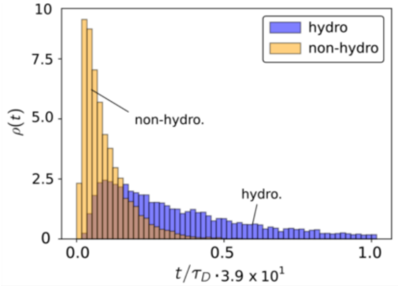
$$\langle \mathbf{F}_{thm}(s)\mathbf{F}_{thm}(t)^T\rangle = 2k_BT\mathbf{M}\delta(t-s) \qquad M_{ij} = \Gamma_i\mathcal{S}\Lambda_j$$

Particle Diffusive Encounters



(i) Initial Configuration (ii) Particle Encounter

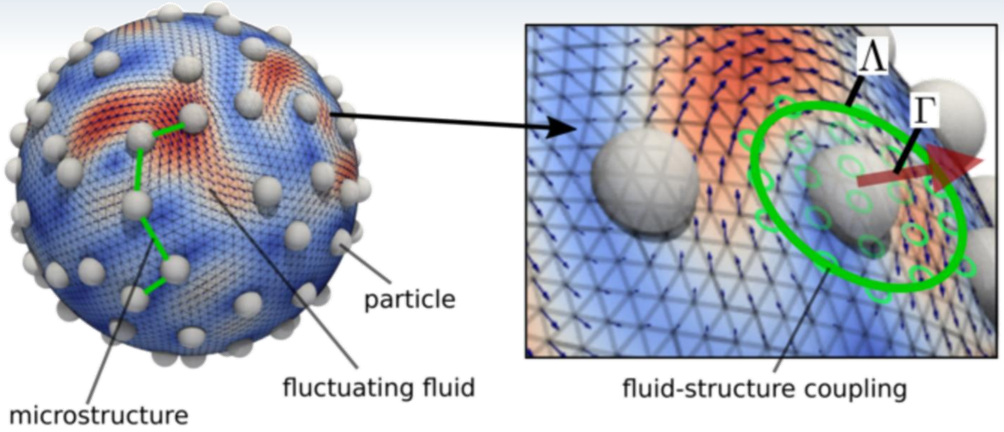
Two Particle Meeting Times



2019 Padidar, Rower, Atzberger, 2015 Tabak, Atzberger

Surface Fluctuating Hydrodynamics

Fluid-structure interactions for drift-diffusion dynamics



Surface Fluctuating Hydrodynamics (Overdamped)

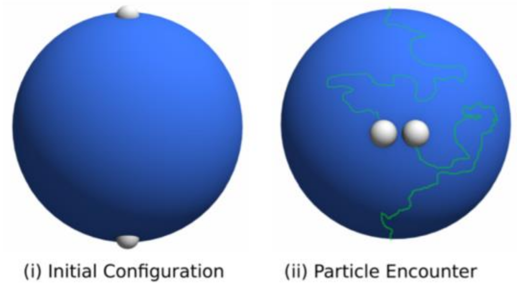
Microstructures

$$\frac{d\mathbf{X}}{dt} = \mathbf{M}\mathbf{F} + k_B T \nabla \cdot \mathbf{M} + \mathbf{F}_{thm}$$

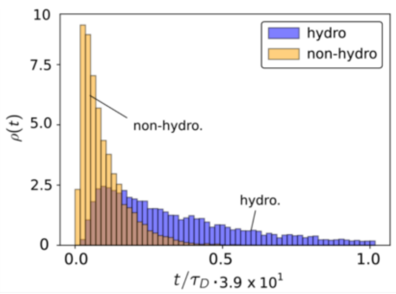
Thermal Fluctuations

$$\langle \mathbf{F}_{thm}(s)\mathbf{F}_{thm}(t)^T \rangle = 2k_B T \mathbf{M}\delta(t-s)$$

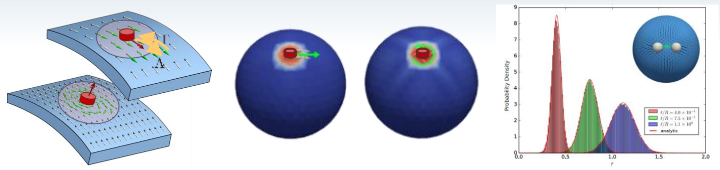
Particle Diffusive Encounters



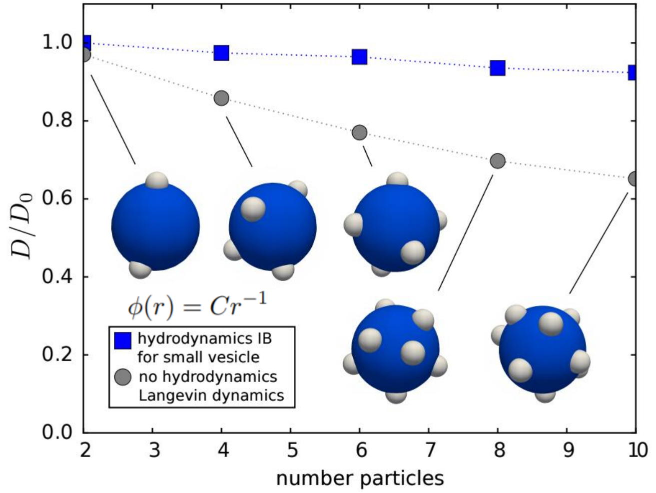
Two Particle Meeting Times



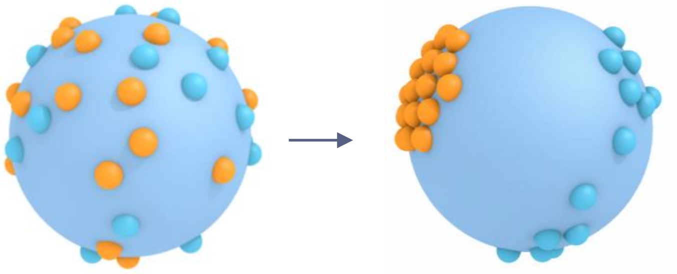
Immersed Boundary for Manifolds



Collective Diffusion



Collective Particle Drift-Diffusion

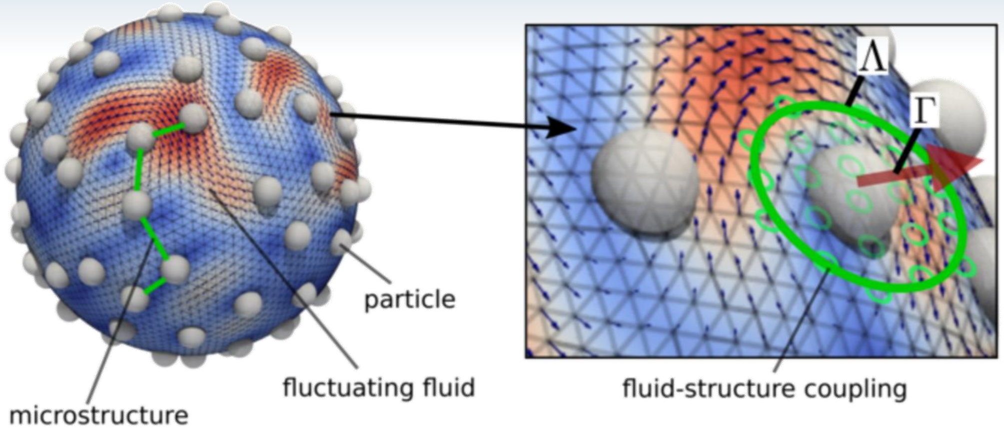


2019 Padidar, Rower, Atzberger

small λ^{-1} intermediate λ^{-1}

Surface Fluctuating Hydrodynamics

Fluid-structure Interactions



Surface Fluctuating Hydrodynamics (Inertial Regime)

Fluid

$$\rho \frac{d\mathbf{v}^\flat}{dt} = \mu_m\left(-\boldsymbol{\delta}\mathbf{d}\mathbf{v}^\flat + 2K\mathbf{v}^\flat\right) - \mathbf{d}p + \mathbf{t}^\flat + \Lambda\left[\gamma\left(\mathbf{V} - \Gamma\mathbf{v}^\flat\right)\right] + \mathbf{f}^\flat_{thm}$$

$$-\boldsymbol{\delta}\mathbf{v}^\flat = 0.$$

Microstructures

$$m\frac{d\mathbf{V}}{dt} = -\gamma\left(\mathbf{V} - \Gamma\mathbf{v}^\flat\right) - \nabla\phi + \mathbf{F}_{thm}$$

$$\frac{d\mathbf{X}}{dt} = \mathbf{V}.$$

Thermal Fluctuations

$$\left\langle \mathbf{f}_{thm}(t)\mathbf{f}_{thm}(s)^T \right\rangle = -2k_BT\mathcal{L}_{ff}\delta(t-s)$$

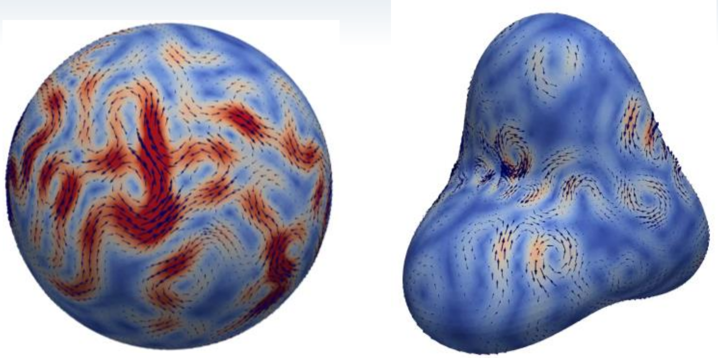
$$\left\langle \mathbf{F}_{thm}(t)\mathbf{F}_{thm}(s)^T \right\rangle = 2k_BT\gamma\mathcal{I}\delta(t-s)$$

$$\left\langle \mathbf{F}_{thm}(t)\mathbf{f}_{thm}(s)^T \right\rangle = -2k_BT\gamma\Gamma\delta(t-s).$$

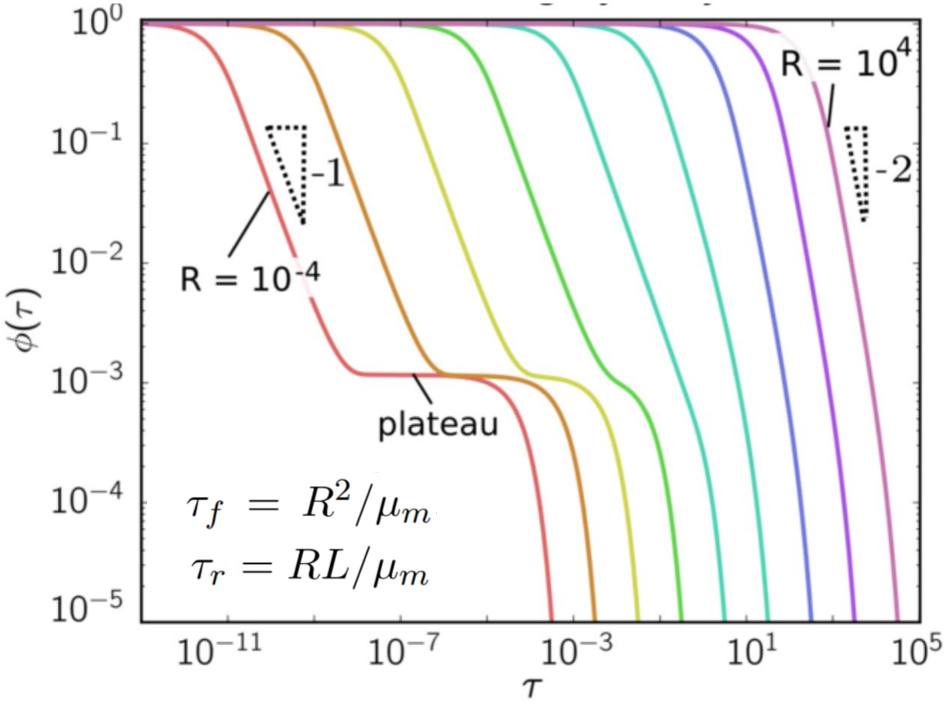
$$\mathcal{L}_{ff} = \mathcal{L}_f - \gamma\Lambda\Gamma$$

$$\mathcal{L}_f = \mu_m\left(-\boldsymbol{\delta}\mathbf{d} + 2K\right) + \mathcal{T}_f$$

Fluctuating Fluid Velocity Fields



Velocity Autocorrelations

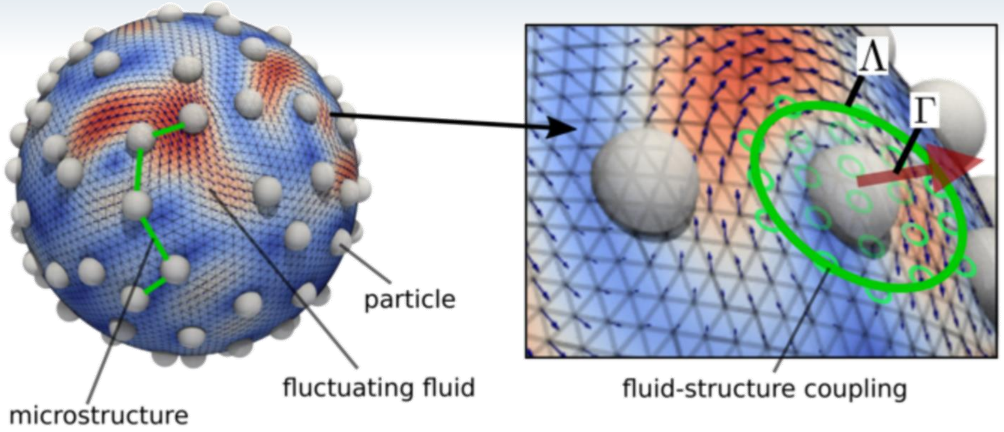


exhibits τ^{-1}, τ^{-2} power laws vs $\tau^{-3/2}$ bulk fluids

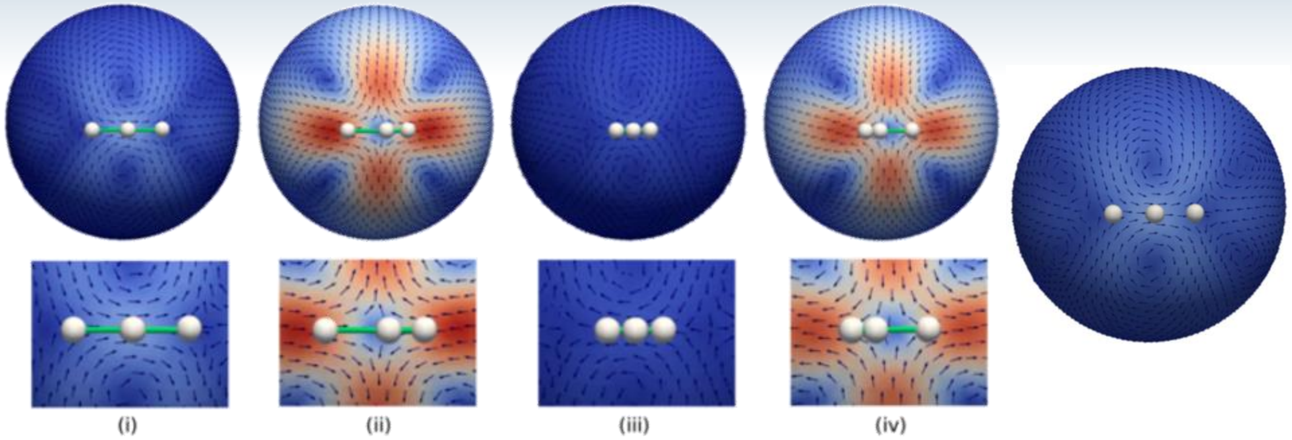
2019 Padidar, Rower, Atzberger

Surface Fluctuating Hydrodynamics

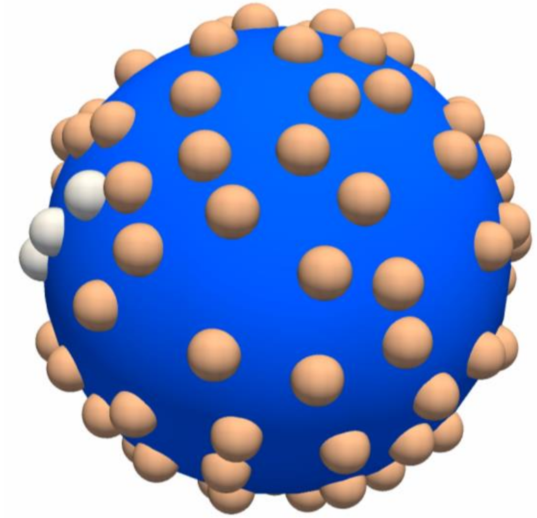
Fluid-structure Interactions

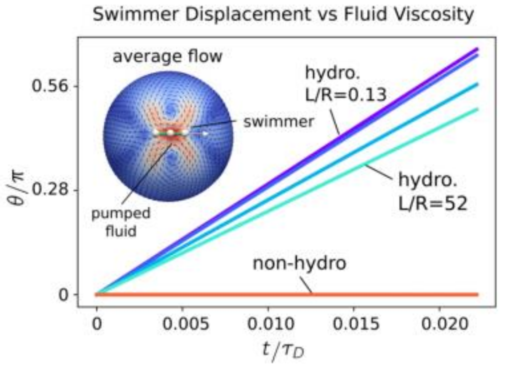


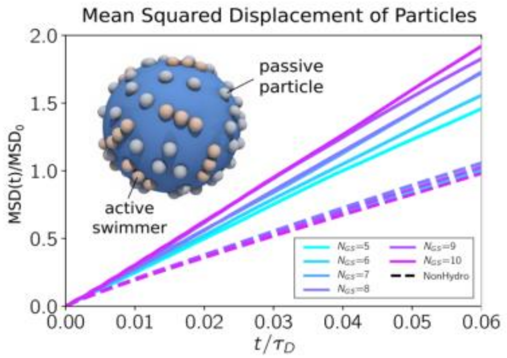
Golestanian Swim Cycle

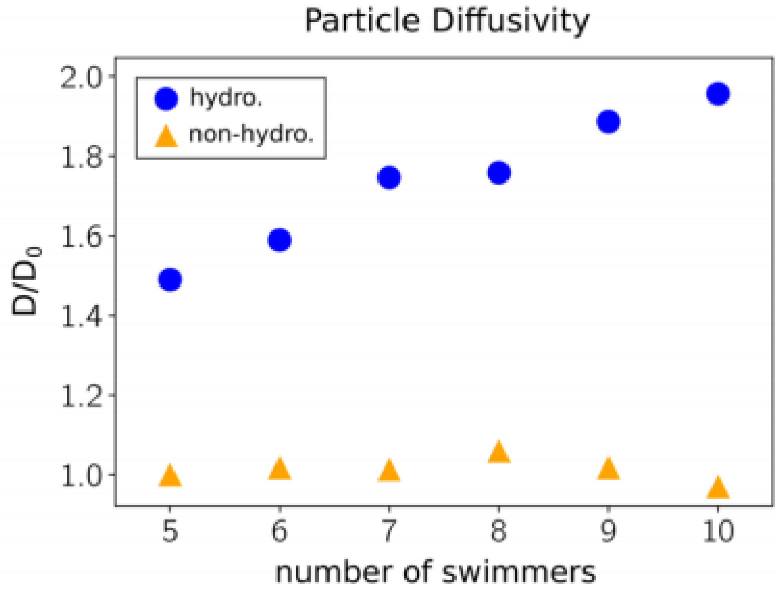


Active Mixing: Drift-Diffusion









2019 Padidar, Rower, Atzberger

Meshless Methods: Generalized Moving Least Squares (GMLS)

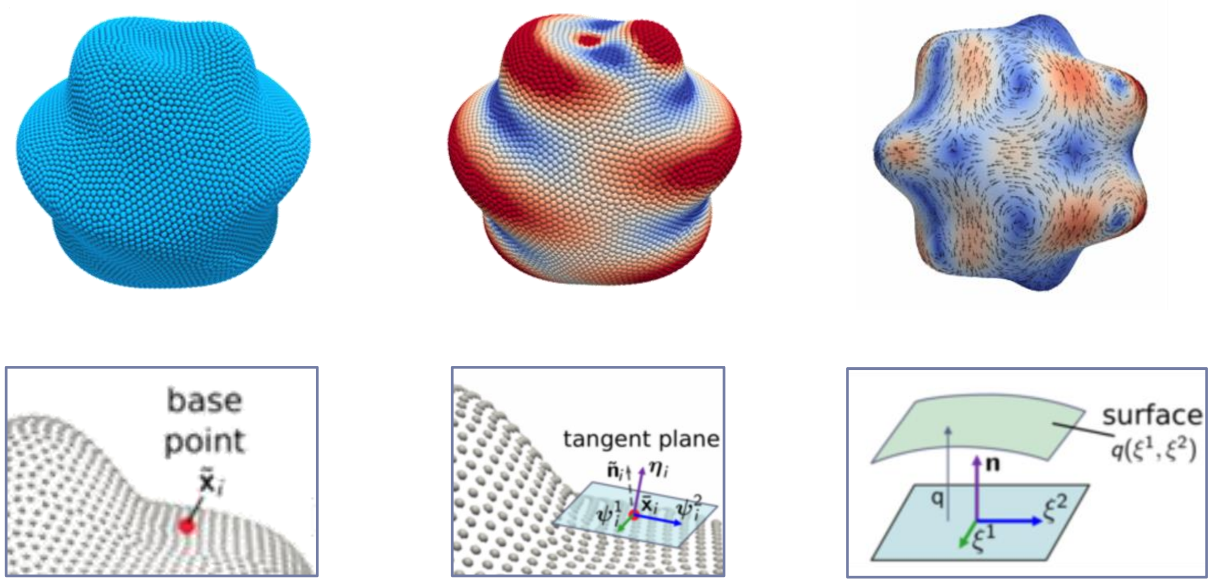
PDEs on manifolds present **challenges for discretization** and solvers from geometric contributions.

Incompressible Hydrodynamic Surface Flow (vector-potential):

$$\mu_m \left(-\boldsymbol{\delta}\mathbf{d}\right)^2 \Phi - \gamma \boldsymbol{\delta}\mathbf{d}\Phi - 2\mu_m \left(-\star\,\mathbf{d}\left(K(-\star\,\mathbf{d}\Phi)\right)\right) = -\star\,\mathbf{d}\mathbf{b}^\flat.$$

GMLS methods developed to obtain consistent high-order discretizations.

manifold representation | geometric quantities | surface fields



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.

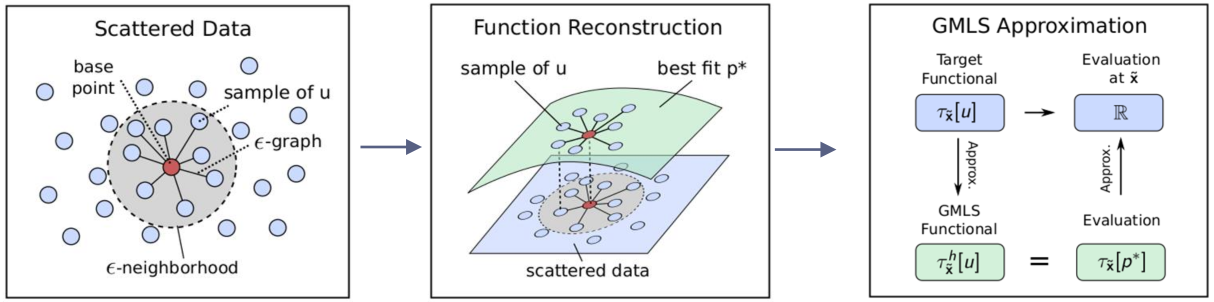
$$p^* = \arg\min_{p \in \mathbb{V}_n} \sum_{j=1}^{N} \left(\lambda_j[u] - \lambda_j[p]\right)^2 \omega(\lambda_j, \tau_{x_i})$$

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.

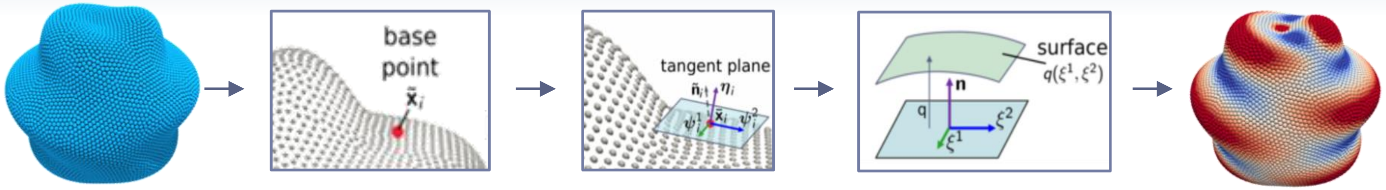
GMLS Approximation for PDEs on Manifolds



2020 Gross, Trask, Atzberger

Gaussian Curvature: GMLS Estimation

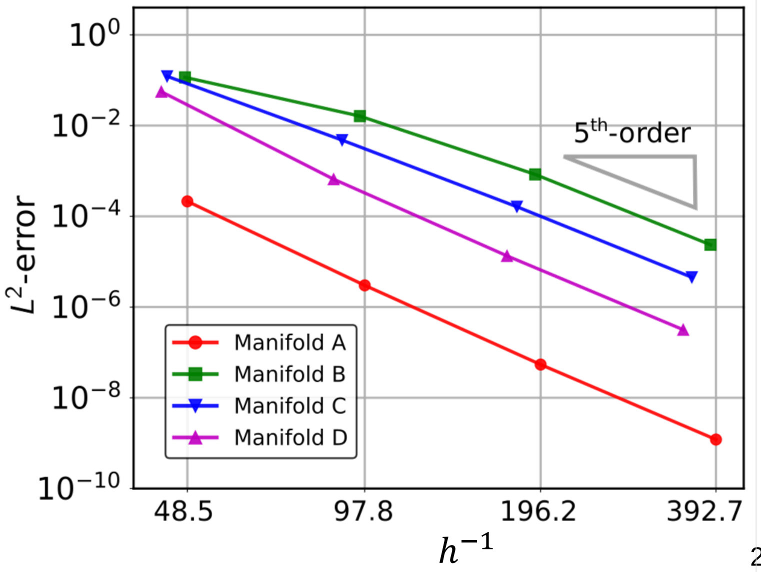
GMLS Gaussian Curvature Estimation:



Gaussian Curvature Accuracy

h	Manifold A ℓ_2-error	Manifold A Rate	Manifold B ℓ_2-error	Manifold B Rate	Manifold C ℓ_2-error	Manifold C Rate
0.1	2.1351e-04	-	1.1575e-01	-	1.2198e-01	-
0.05	3.0078e-06	6.07	1.6169e-02	2.84	4.7733e-03	4.67
0.025	5.3927e-08	5.77	8.3821e-04	4.26	1.6250e-04	4.88
0.0125	1.1994e-09	5.48	2.3571e-05	5.14	4.5204e-06	5.17

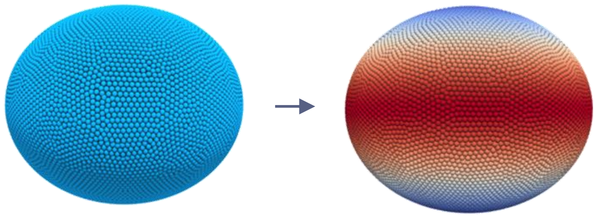
h	Manifold D ℓ_2-error	Manifold D Rate
.08	5.5871e-02	-
.04	6.5739e-04	6.51
.02	1.3418e-05	5.67
.01	3.1631e-07	5.37



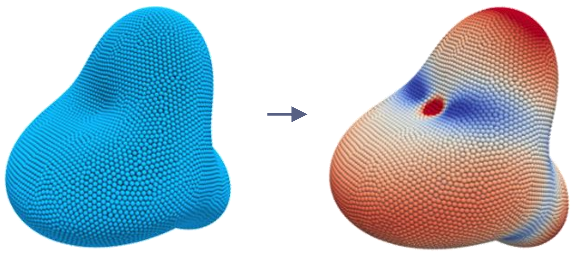
2019 Gross, Trask, Atzberger

Point Set **Curvature**

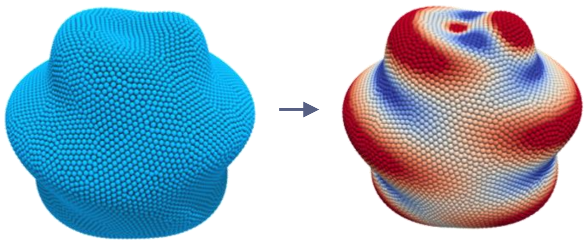
Manifold A



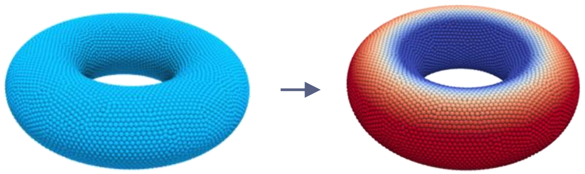
Manifold B



Manifold C

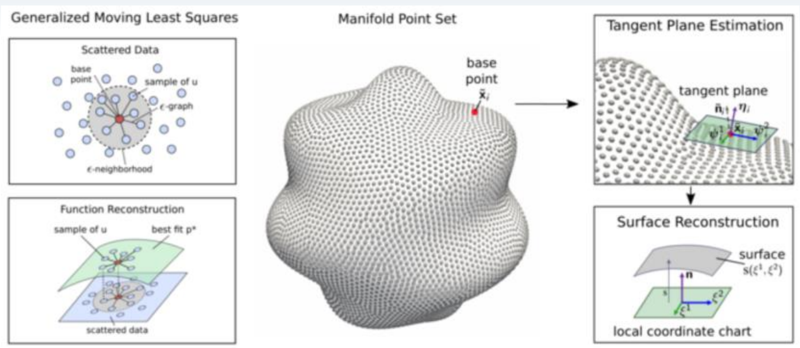


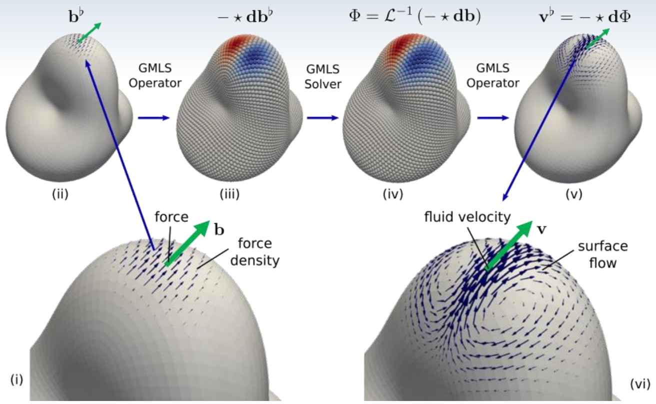
Manifold D

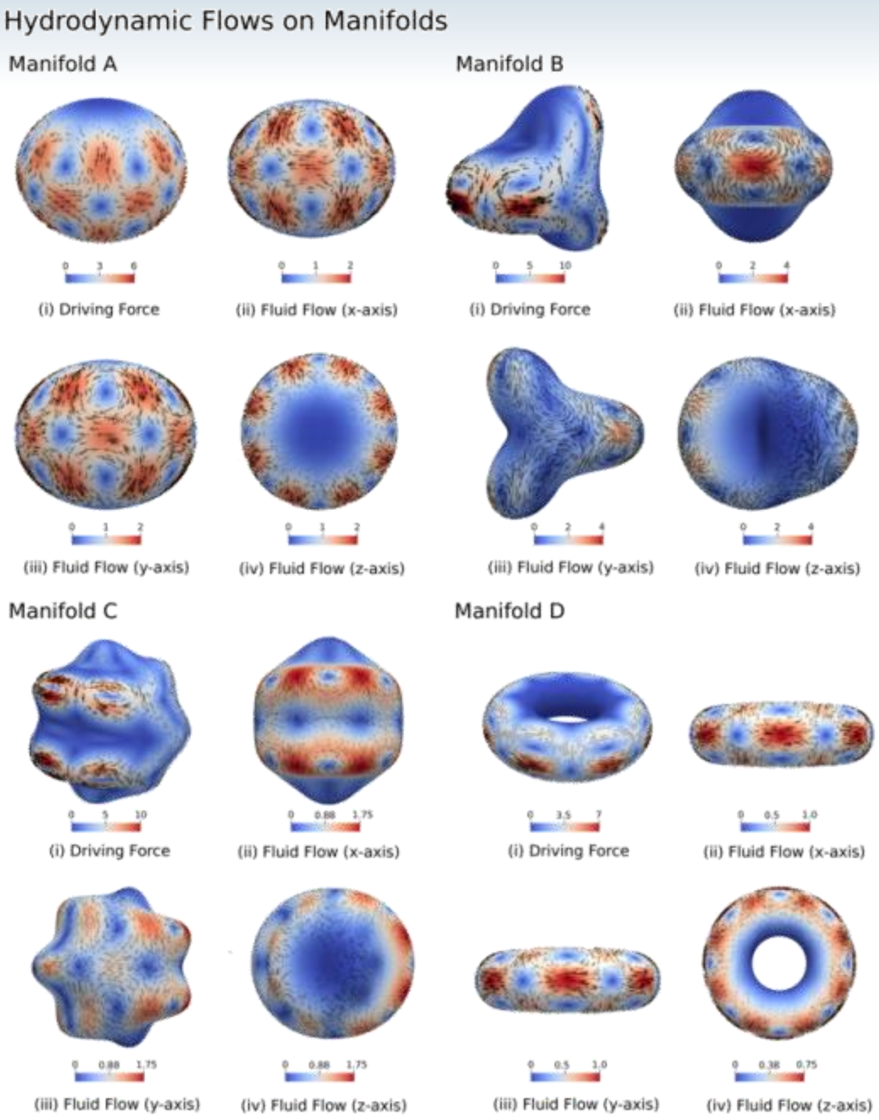


GMLS Solvers for PDEs on Manifolds

PDEs on Manifolds and Solvers







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.

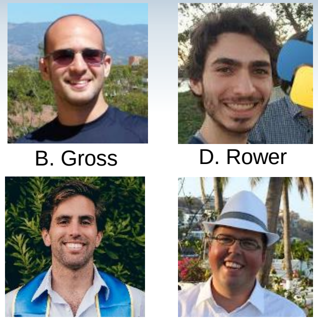
$$\mu_m \left(-\boldsymbol{\delta}\mathbf{d}\right)^2 \Phi - \gamma\boldsymbol{\delta}\mathbf{d}\Phi - 2\mu_m\left(-\star\mathbf{d}\left(K(-\star\mathbf{d}\Phi)\right)\right) = -\star\mathbf{d}\mathbf{b}^\flat.$$

	m = 4		m = 6		m = 8	
h	ℓ_2-error	Rate	ℓ_2-error	Rate	ℓ_2-error	Rate
0.1	9.7895e-02	-	6.5222e-02	-	2.8024e-01	-
0.05	1.4383e-02	2.77	2.8402e-03	4.52	1.2100e-02	4.53
0.025	3.6243e-03	1.98	3.9929e-04	2.82	4.9907e-04	4.59
0.0125	7.8747e-04	2.20	1.2357e-05	5.00	5.7023e-06	6.44

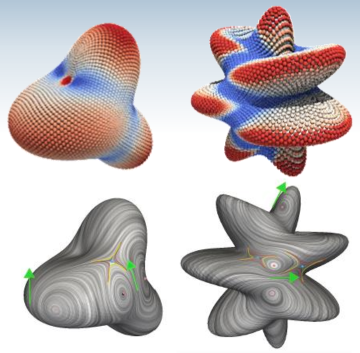
Meshfree Methods on Manifolds for Hydrodynamic Flows on Curved Surfaces: A Generalized Moving Least Squares (GMLS) Approach, B.J. Gross, N. Trask,, P. Kuberry, and P J. Atzberger, Journal of Computational Physics, Vol. 409, 15 May (2020) https://doi.org/10.1016/j.jcp.2020.109340

Conclusions

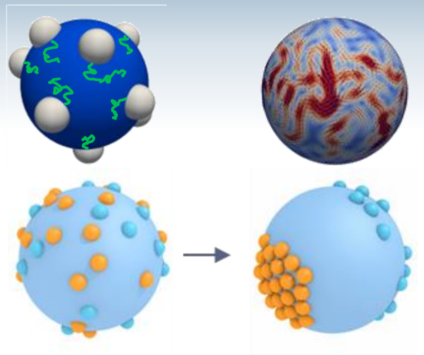
Conclusions



B. Gross D. Rower
M. Padidar J. Sigurdsson
UCSB Student Collaborators



Meshless and Spectral Methods for Hydrodynamic Flow on Surfaces



Stochastic Drift-Diffusion Dynamics Hydrodynamic Coupling

Paper
2016 Atzberger & Sigurdsson

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

Surface Fluctuating Hydrodynamics Methods for the Drift-Diffusion Dynamics of Particles and Microstructures within Curved Fluid Interfaces,
D. Rower, M. Padidar, and P. J. Atzberger, arXiv:1906.01146, (2019).

Hydrodynamic Coupling of Particle Inclusions Embedded in Curved Lipid Bilayer Membranes
J.K. Sigurdsson and P. J. Atzberger, 12, 6685-6707, Soft Matter, The Royal Society of Chemistry, (2016).

Hydrodynamic Flows on Curved Surfaces: Spectral Numerical Methods for Radial Manifold Shapes,
B. Gross, P. J. Atzberger, J. Comp. Phys, 371, 663-689 (2018).

Meshfree Methods on Manifolds for Hydrodynamic Flows on Curved Surfaces: A Generalized Moving Least-Squares (GMLS) Approach,
Gross B. J., Kuberry P. A., Trask N., Atzberger P. J., J. Comp. Phys., 409, 15 May (2020).

UCSB Student Collaborators

B. Gross, M. Padidar, D. Rower, J. K. Sigurdsson.

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/