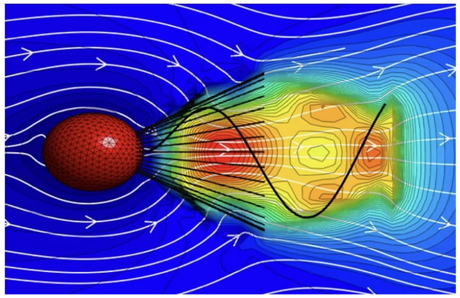
Mathematical Modeling, Computational Methods, and Biological Fluid Dynamics: Research and Training



Method of Regularized Stokeslets Tutorial: Part II

Sarah Olson and Dana Ferranti

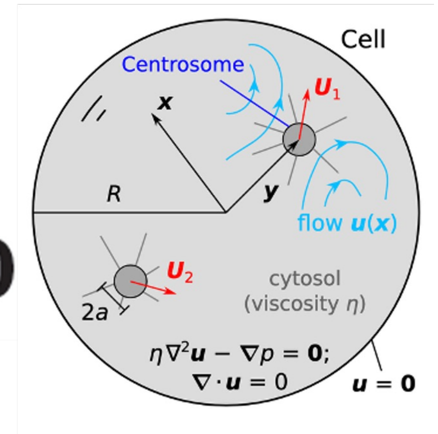
WPI

Department of Mathematical Sciences

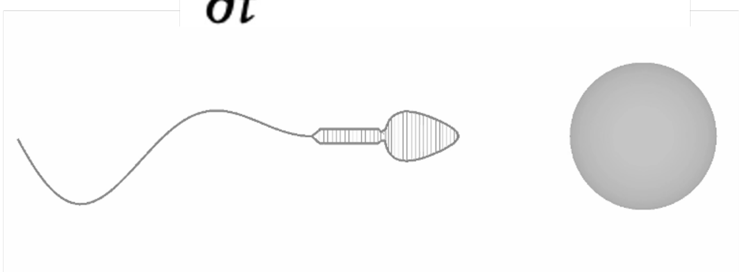
Worcester Polytechnic Institute

Biological Flows, Elastic Structures, and Rigid Boundaries

$$\mu\nabla^2 \boldsymbol{u} - \boldsymbol{\nabla} p = -\boldsymbol{f}(\boldsymbol{x}, t), \quad \boldsymbol{\nabla}\cdot\boldsymbol{u} = \boldsymbol{0}$$



$$\frac{\partial \mathbf{X}}{\partial t} = \mathbf{u}\left(\mathbf{X}(q, s, t)\right)$$



- Complex motion of boundaries
- Fluid-structure interactions
- Very low Reynolds number

Lefebvre et al. 1995. *Biol Reprod*

Today’s Topics

- Choice of regularization or blob function
- Modeling different fluids / different domains
  - Brinkman
  - Viscoelastic networks
- Approaches to reduce computational complexity
  - Time stepping approaches
  - KIFMM
  - Image systems
  - Reduced models of structures
  - Time steps
- Decoupling regularization parameter and discretization length

Choice of Blob Function in 3D

$$\phi_\epsilon(r) = \frac{15\epsilon^4}{8\pi(r^2+\epsilon^2)^{7/2}}$$ **" the 7/2 blob "**

Satisfies

1) $\iiint_{\mathbb{R}^3} \phi_\epsilon(r)dV = 1$

2) $\lim_{\epsilon\to 0} \phi_\epsilon(r) = \delta(r)$ (in the sense of distributions)

What might motivate the choice of a different blob function?

Choice of Blob Function in 3D

$$\phi_\epsilon(r) = \frac{15\epsilon^4}{8\pi(r^2+\epsilon^2)^{7/2}}$$

Regularization Error

Depends on

ϕ_ϵ, ϵ

Discretization/Quadrature Error

Depends on quadrature choice, discretization length h, and ϵ

Choice of Blob Function in 3D

$$\phi_\epsilon(r) = \frac{15\epsilon^4}{8\pi(r^2+\epsilon^2)^{7/2}}$$

Focus on this for now

Regularization Error

Depends on

ϕ_ϵ, ϵ

Discretization/Quadrature Error

Depends on quadrature choice, discretization length h, and ϵ

What do we mean by regularization error?

Regularized Velocity Field

$$\mathbf{u}_\epsilon(\mathbf{x}) = \iint_{\partial D} \mathcal{S}_\epsilon(\mathbf{x},\mathbf{y}) \cdot \mathbf{f}(\mathbf{y})\, dS(\mathbf{y})$$

Regularized Stokeslet

Singular Velocity Field

$$\mathbf{u}_0(\mathbf{x}) = \iint_{\partial D} \mathcal{S}_0(\mathbf{x},\mathbf{y}) \cdot \mathbf{f}(\mathbf{y})\, dS(\mathbf{y})$$

Singular Stokeslet

$$\text{Error} = \mathbf{u}_\epsilon(\mathbf{x}) - \mathbf{u}_0(\mathbf{x}) = \iint_{\partial D} [\mathcal{S}_\epsilon(\mathbf{x},\mathbf{y}) - \mathcal{S}_0(\mathbf{x},\mathbf{y})] \cdot \mathbf{f}(\mathbf{y})\, dS(\mathbf{y})$$

Regularization Error for Spherically Symmetric Blobs

Near-field Error

Under a few technical conditions, it can be shown that the near-field regularization error is (for almost any spherically symmetric blob),

$$\text{Near-field error} \sim \mathcal{O}(\epsilon)$$

(Nguyen H.-N, Cortez 2014, Commun. Comput. Phys.)

Far-field Error

The asymptotic form for the far-field error is related to the moments of the blob. In the case of the 7/2 blob, we have

$$\text{Far-field error} \sim \mathcal{O}(\epsilon^2)$$

(Cortez, Fauci, Medovikov 2005, Phys. of Fluids)

Regularization Error for Spherically Symmetric Blobs

Near-field Error

Under a few technical conditions, it can be shown that the near-field regularization error is (for almost any spherically symmetric blob),

$$\text{Near-field error} \sim \mathcal{O}(\epsilon)$$

(Nguyen H.-N, Cortez 2014, Commun. Comput. Phys.)

Far-field Error

However:
If the blob has zero second moment, i.e.

$$\iiint_{\mathbb{R}^3} s^2 \phi_\epsilon(s) dV = 0)$$

$$(\text{equivalent to } \int_0^\infty s^4 \phi_\epsilon(s) ds = 0$$

$$\text{Far-field error} \sim \mathcal{O}(\epsilon^k), k > 2$$

Nguyen H.-N, Cortez 2014, Commun. Comput. Phys.)

Constructing a blob with zero second moment

$$\phi_\epsilon(r) = \frac{15\epsilon^4}{8\pi(r^2+\epsilon^2)^{7/2}}$$

Exercise:

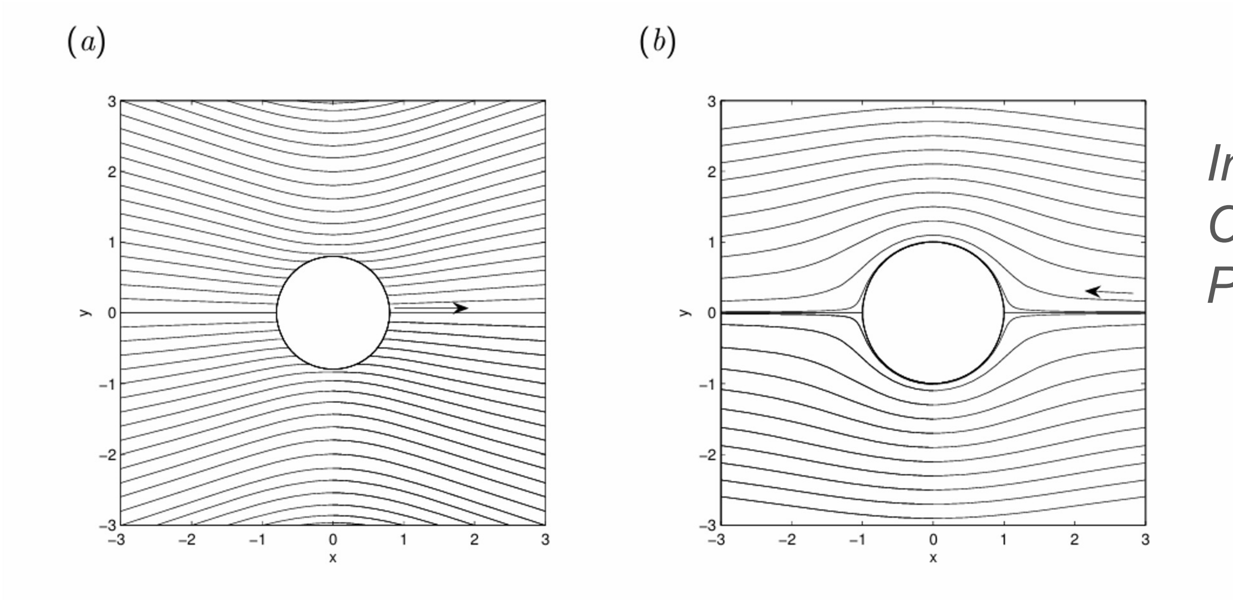
Let $\psi_\epsilon(r) = A\phi_\epsilon(r) + Br\phi'_\epsilon(r)$

Derive a system of equations for A, B using the conditions that

$$\int_0^\infty s^2\psi_\epsilon(s)\,ds = 1/4\pi$$

$$\int_0^\infty s^4\psi_\epsilon(s)\,ds = 0$$ and show that $A = 1/2, B = 5/2$

Test Problem: Translating Sphere or Spheroid



Intro. To Theor. And Comput. Fluid Dynamic Pozrikidis

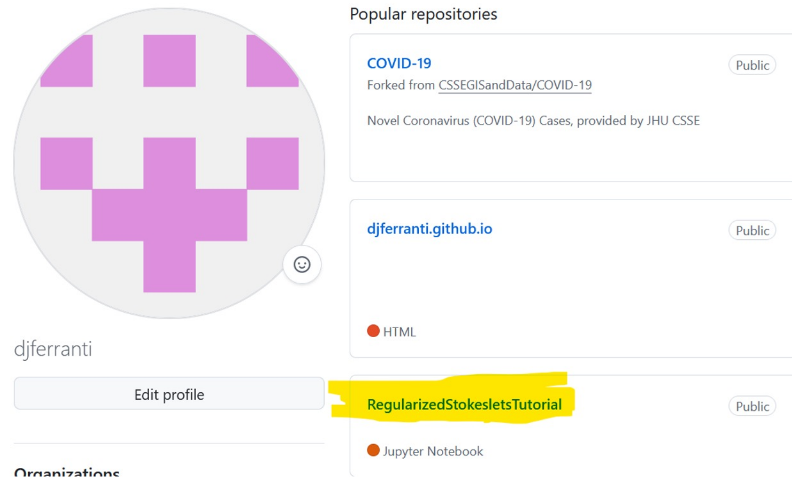
(a) Streamlines in fixed frame (b) Streamlines in co-moving frame

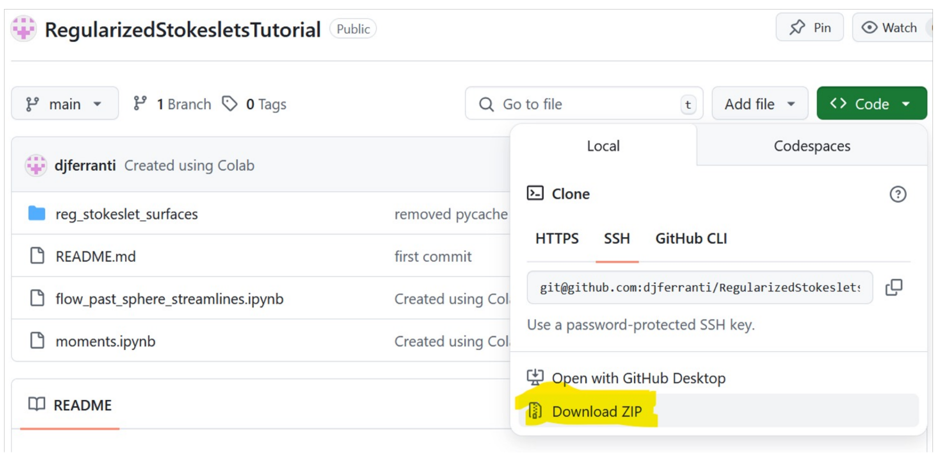
Sphere of radius a translates uniformly in fluid with velocity $\mathbf{U}$

www.github.com/djferranti -> Code to follow along

Steps to Follow Along

1) Click on “Regularized Stokeslets Tutorial”

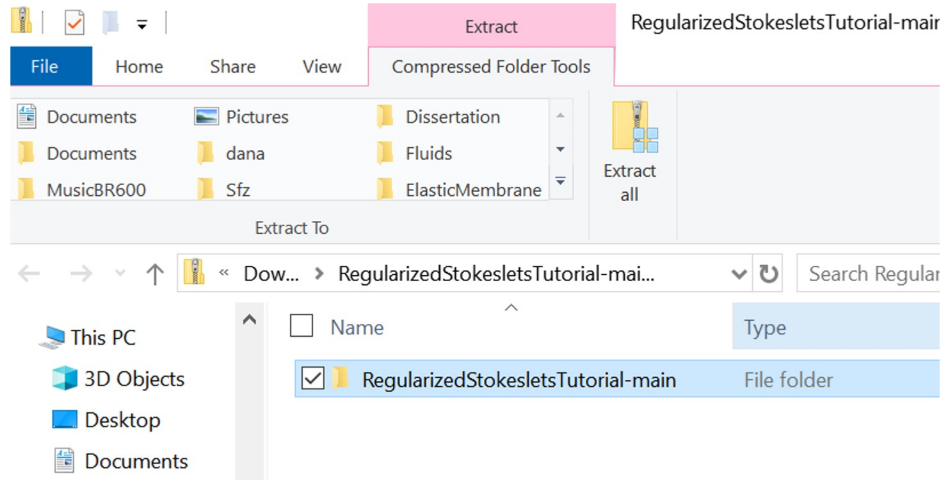


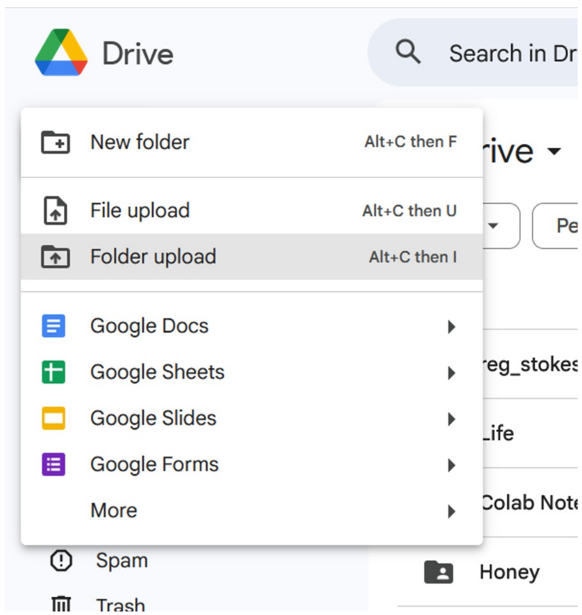


2) Look for green button that says “Code,” click on down arrow, then “Download ZIP”

Steps to Follow Along

3) Extract the contents of the folder on your computer to your “Downloads” folder.

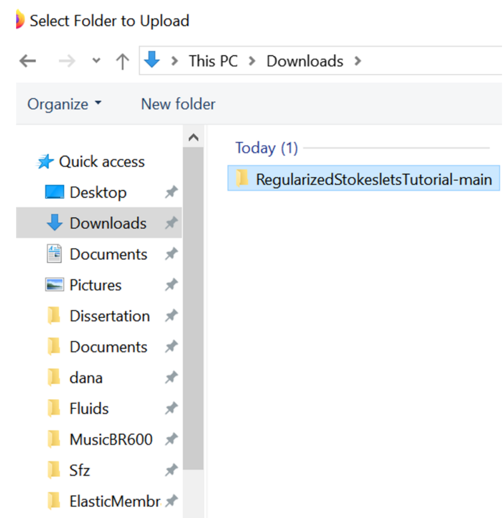


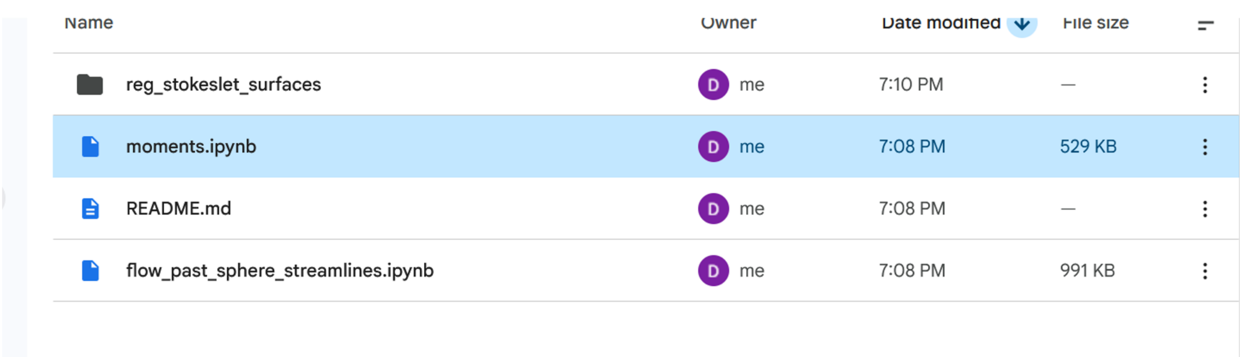


4) Go to your Google Drive account (drive.google.com). Click the “My Drive” button on the left. Then click the “+ New” button and choose “Folder upload”

Last steps

5) On your file manager, go to “Downloads”, click on the “RegularizedStokesletsTutorial-main” folder to upload to Google Drive.

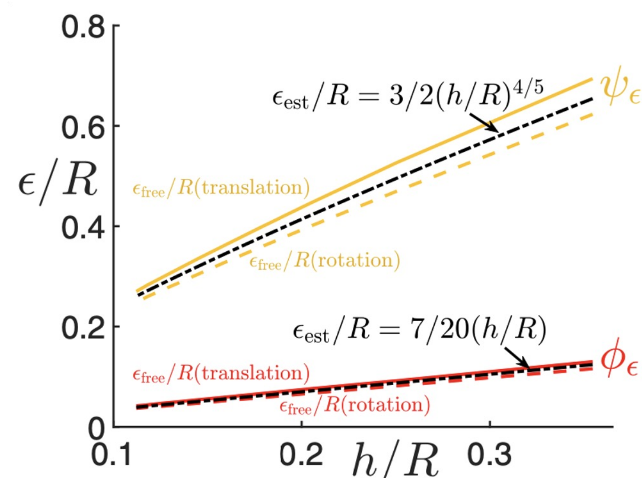




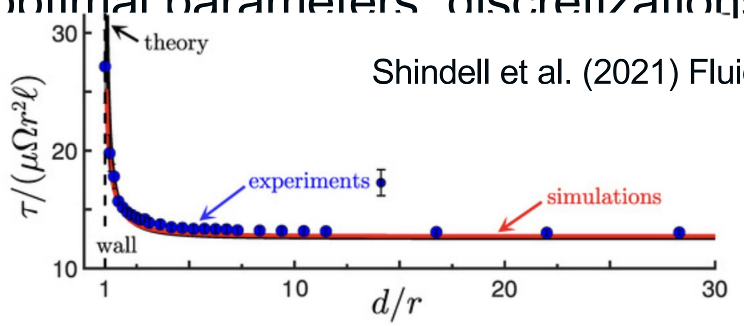
6) Go to the folder in Google Drive and click on “moments.ipynb.” Then click “Open in CoLab.”

Experimentally Calibrated Regularized Stokeslets

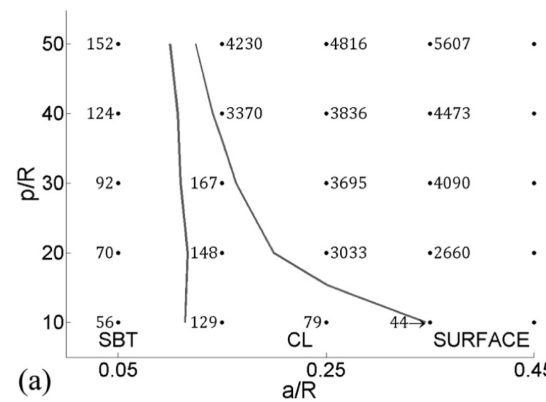
- Regularization parameter
  - often coupled to the surface discretization
  - Numerical and physical meaning
- Error between experiments depends on regularization function and regularization parameter, surface representation, …
- Guidance for optimal parameters, discretizations, and method



Nguyen et al. (2025) Phys Rev Fluids

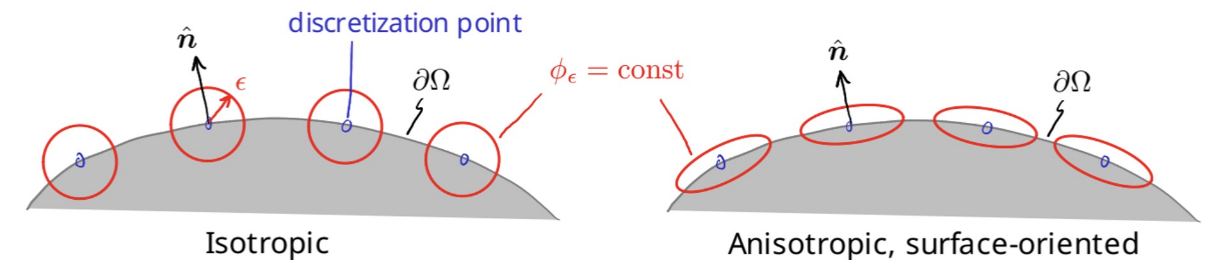


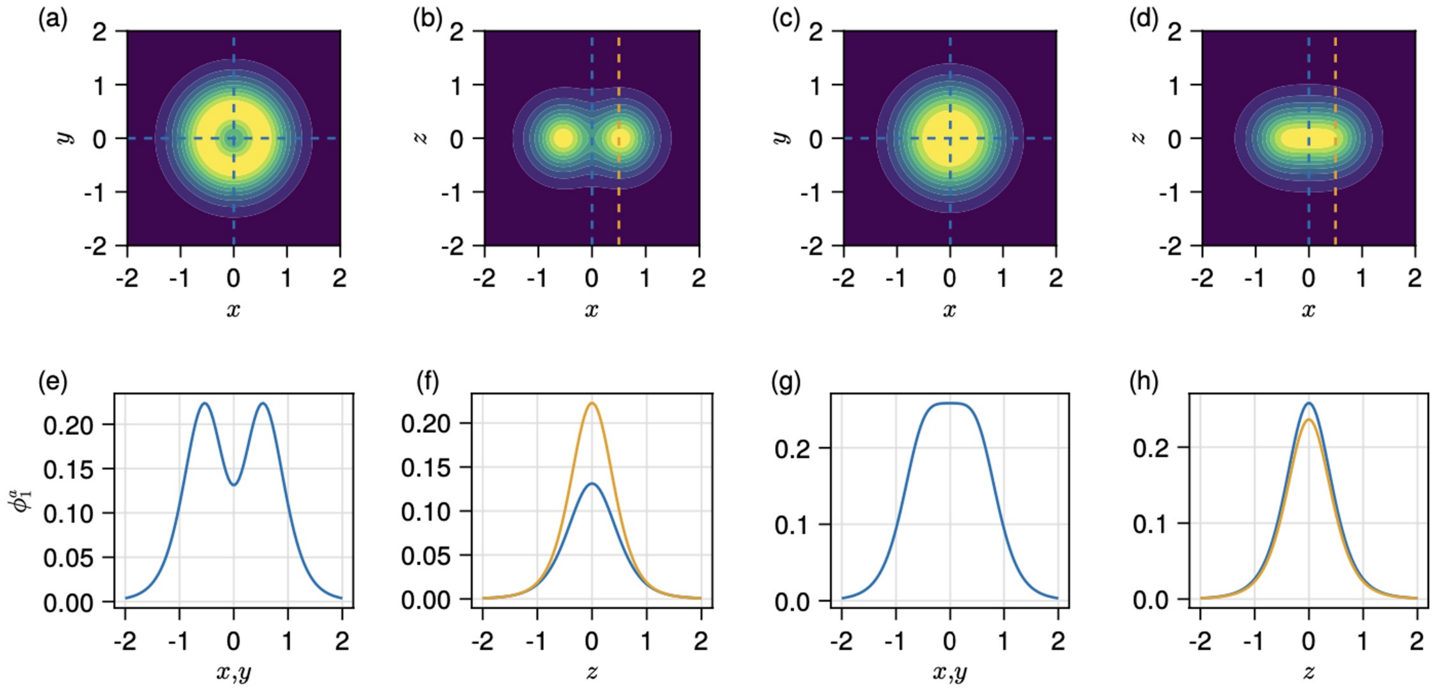
Shindell et al. (2021) Fluids



Martindale, Jabbarzadeh, and Fu. (2016) Phys Fluids

Surface Oriented Regularizations

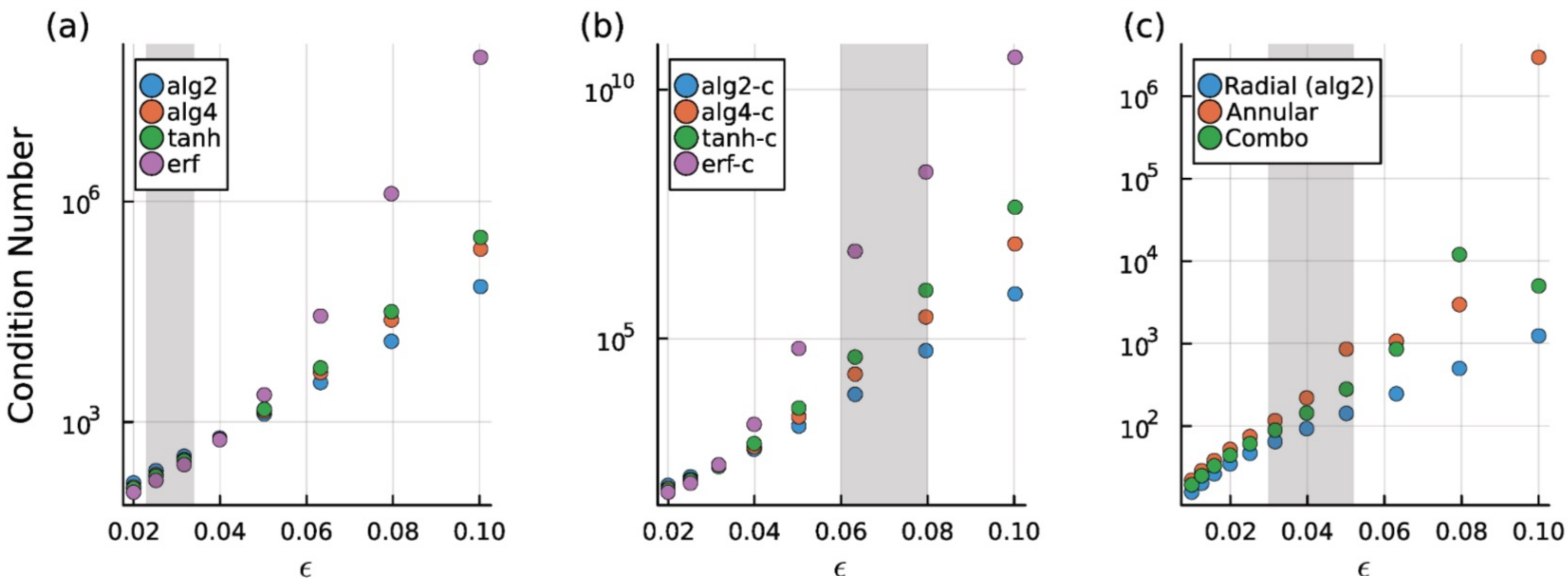




$$B_\epsilon^a(\boldsymbol{r}) = \frac{1}{16\pi}\left(\sqrt{z^2 + (\rho - a\epsilon)^2 + \epsilon^2} + \sqrt{z^2 + (\rho + a\epsilon)^2 + \epsilon^2}\right)$$

Chisholm and Olson. Fluids (2022)

Figure A1. Skeel's condition number for the inverse problem of a translating sphere described in **Section 2.5** using (**a**) uncorrected radial, (**b**) corrected radial, and (**c**) surface-oriented regularizations. For the radial (**a**,**b**) and surface-oriented (**c**) regularizations, $n = 4096$ and $n = 1024$ discretization points are used, respectively. The shaded regions indicate the values of ϵ where the error in the drag is approximately minimized.



near-field error can be reduced to $O(\epsilon^3)$ with a correction to the blob function

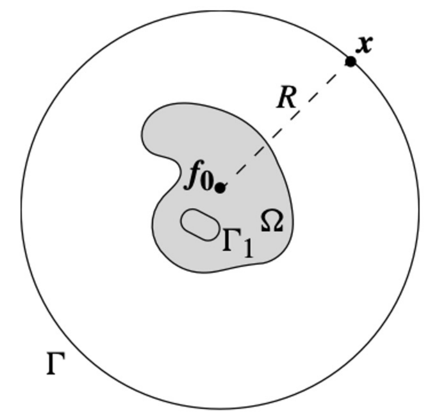
Exploring Different Fluid Domains, Fluid Types, and Boundaries

A note on 2D, $\mathbf{x} \in \mathbb{R}^2$

$$\text{IF} \sum_k f_k = 0, \text{ then } \mathbf{u} \to \mathbf{0}, p \to 0 \text{ as } |\mathbf{x}| \to \infty$$

$$\mathbf{u}(\mathbf{x}) = \sum_{k=1}^{N} \frac{-\mathbf{f}_k}{4\pi\mu} \left[\ln\left(\sqrt{r_k^2+\epsilon^2}+\epsilon\right) - \frac{\epsilon\left(\sqrt{r_k^2+\epsilon^2}+2\epsilon\right)}{\left(\sqrt{r_k^2+\epsilon^2}+\epsilon\right)\sqrt{r_k^2+\epsilon^2}} \right]$$
$$+ \frac{1}{4\pi\mu}[\mathbf{f}_k \cdot (\mathbf{x}-\mathbf{x}_k)](\mathbf{x}-\mathbf{x}_k) \left[\frac{\sqrt{r_k^2+\epsilon^2}+2\epsilon}{\left(\sqrt{r_k^2+\epsilon^2}+\epsilon\right)^2 \sqrt{r_k^2+\epsilon^2}} \right]$$

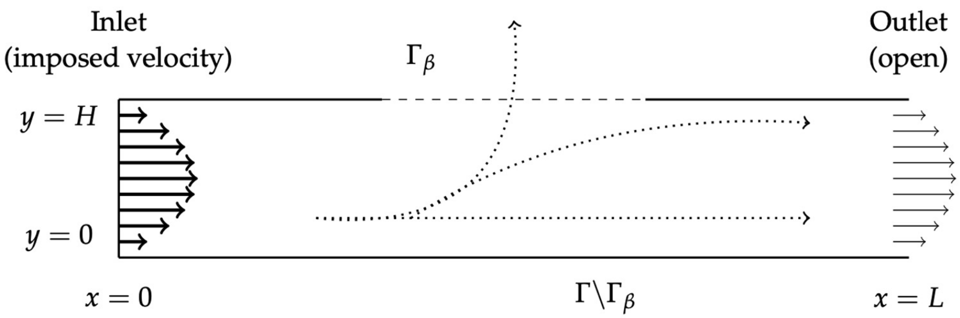
Modifications for nonzero net force: $\langle \boldsymbol{u} \rangle|_\Gamma = \mathbf{0}$.

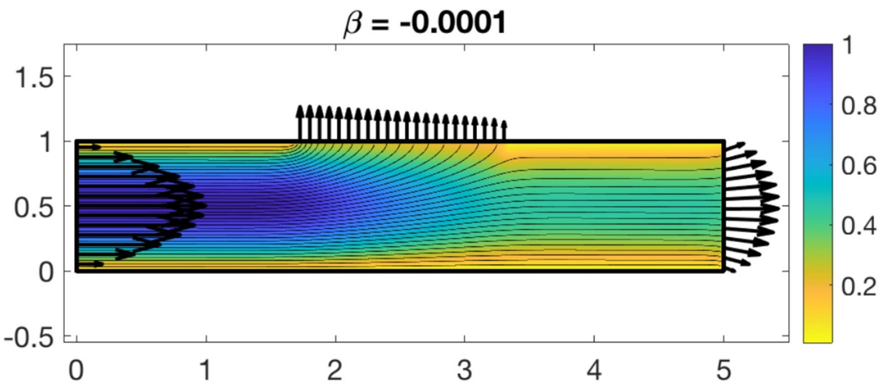


$$\boldsymbol{u}^{\boldsymbol{R}}(t) = \sum_{k=1}^{N} \boldsymbol{u}^{\boldsymbol{R}}(\boldsymbol{f}_k(t)) = \sum_{k=1}^{N} -\frac{\boldsymbol{f}_k(t)}{4\pi\mu}\left(\tfrac{1}{2} - \ln R\right)$$

Maxian and Strychalski (2019) Comm App Math and Comp Sci

Stokes Flow with a Permeable Boundary (2D)





$$\mu \Delta \mathbf{u} = \nabla p - \mathbf{F}, \qquad \nabla \cdot \mathbf{u} = 0 \text{ in } \mathbb{R}^2/\Gamma$$

$$\mathbf{F}(\mathbf{x}) = \int_\Gamma \mathbf{f}(s)\phi_\delta(\mathbf{x} - \mathbf{X}(s))ds \text{ for } \mathbf{x} \in \mathbb{R}^2$$

$$\mu \Delta \mathbf{v} = \nabla q, \qquad \nabla \cdot \mathbf{v} = A \qquad \text{in } \mathbb{R}^2$$

$$A(\mathbf{x}) = -\int_\Gamma \frac{b(s)}{\mu} \hat{\mathbf{n}}(s) \cdot \nabla \phi_\delta(\mathbf{x} - \mathbf{X}(s))ds \quad \text{for } \mathbf{x} \in \mathbb{R}^2$$

$$b(s) = \beta(\mathbf{f} \cdot \hat{\mathbf{n}})$$

Fluid particles move at $d\mathbf{x}/dt = \mathbf{u}(\mathbf{x})$

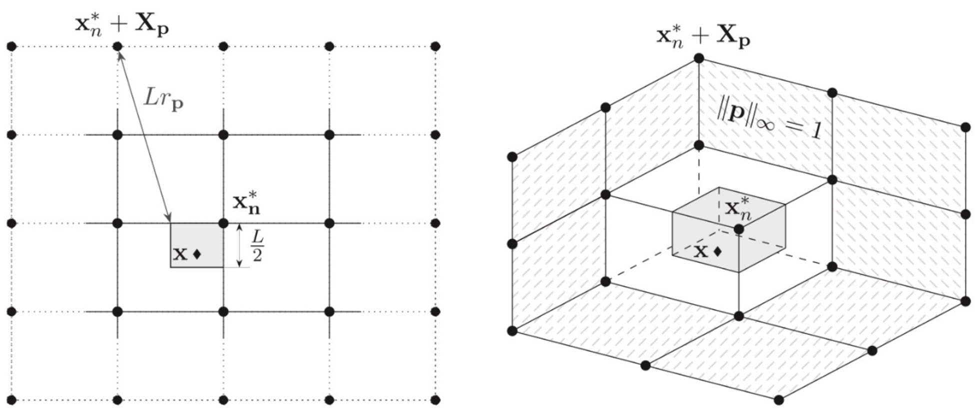
Membrane moves at $d\mathbf{X}/dt = \mathbf{u}(\mathbf{X}) + \mathbf{v}(\mathbf{X})$

3D

Tutorial has focused on free space:

$$\mathbf{x} \in \mathbb{R}^3 \text{ where } \mathbf{u} \to \mathbf{0}, p \to 0 \text{ as } |\mathbf{x}| \to \infty$$

Periodic domains: Flow is always a summation over all the point forces (and their periodic copies). The direct sum over the lattice is divergent (due to 1/r slow decay). Can decompose or split.



$$\mathcal{S}(\hat{\mathbf{x}}) = 8\pi(-\Delta\mathbf{I} + \nabla\nabla)B(r) = \Theta(\hat{\mathbf{x}}) + \Phi(\hat{\mathbf{x}})$$

$$\Theta(\hat{\mathbf{x}}) = 8\pi(-\mathbf{I}\Delta + \nabla\nabla)[B(r)\,\mathrm{erfc}(\xi r)],$$

$$\Phi(\hat{\mathbf{x}}) = 8\pi(-\mathbf{I}\Delta + \nabla\nabla)[B(r)\,\mathrm{erf}(\xi r)],$$

Fig. 3. Illustration of real space sum's layers. Left: slice of 3D box where x_n^* is a periodic image of the point force x_n that is closest to x. The center shaded square is the cube $\Omega_0 L = \{\mathbf{x} \in \mathbb{R}^3 | (\mathbf{x} - \mathbf{x}_n^*)/L \in \Omega_0\}$. Right: 3D domain, the center shaded box is the cube $\Omega_0 L$.

Periodic Regularized Stokeslets

- Triply Periodic - Leiderman, Bouzarth, Cortez, Layton (2013) J Comp Phys
- Doubly Periodic in 2D - Cortez and Hoffmann (2014) J Comp Phys ,
- …

$$B_{\Phi_\varepsilon}(r) = \underbrace{B(r)\,\mathrm{erf}\left(\frac{r}{\xi}\right)}_{\text{regular}} + \underbrace{B_{\Phi_\varepsilon}(r) - B(r)\,\mathrm{erf}\left(\frac{r}{\xi}\right)}_{\text{regular and fast decaying}}$$

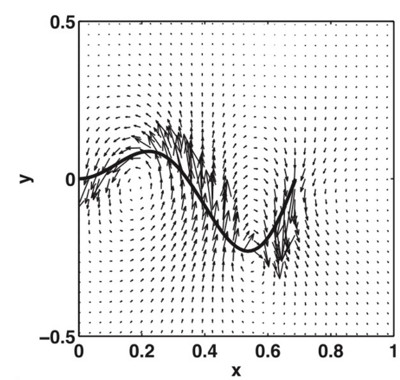
Note: careful selection of blobs to ensure required decay rates and existence of Fourier transforms

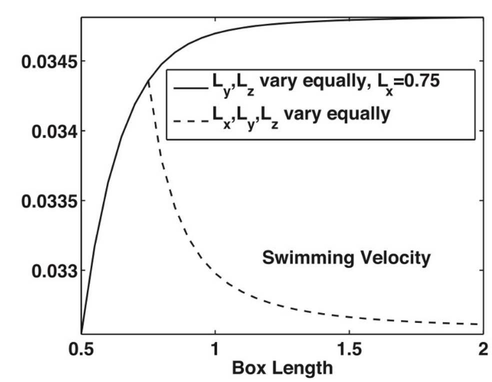
$$-\nabla p_1 + \mu\Delta \mathbf{u}_1 = -\sum_{\mathbf{n}} \mathbf{g}\delta(\hat{\mathbf{x}}_{\mathbf{n}}),$$

$$\nabla \cdot \mathbf{u}_1 = 0,$$

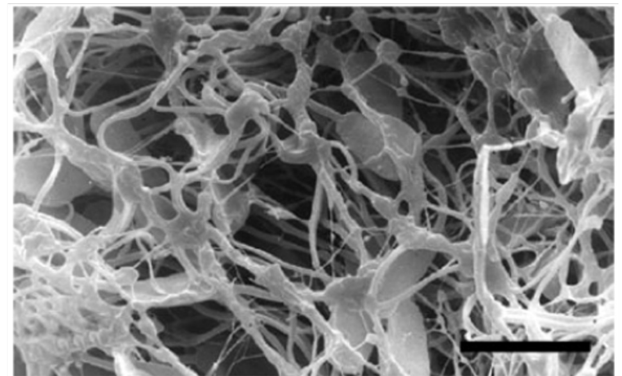
$$-\nabla p_2 + \mu\Delta \mathbf{u}_2 = -\sum_{\mathbf{n}} \mathbf{g}[\phi_\epsilon(\hat{\mathbf{x}}_{\mathbf{n}}) - \delta(\hat{\mathbf{x}}_{\mathbf{n}})],$$

$$\nabla \cdot \mathbf{u}_2 = 0.$$





Brinkman Equation



Ruttlant et al. (2015)

$$\nabla p = \mu \Delta \mathbf{u} - \mu \alpha^2 \mathbf{u} + \mathbf{f}, \qquad \nabla \cdot \mathbf{u} = 0$$

- Effective medium approach modeling Stokes flow through sparse, stationary objects
- $\alpha = 1/\sqrt{\gamma}$ is the resistance and γ is the permeability
- Assume pores are large enough

Permeability and Resistance

- Assuming randomly oriented fibers: a_f is fiber radius, φ is volume fraction of fibers

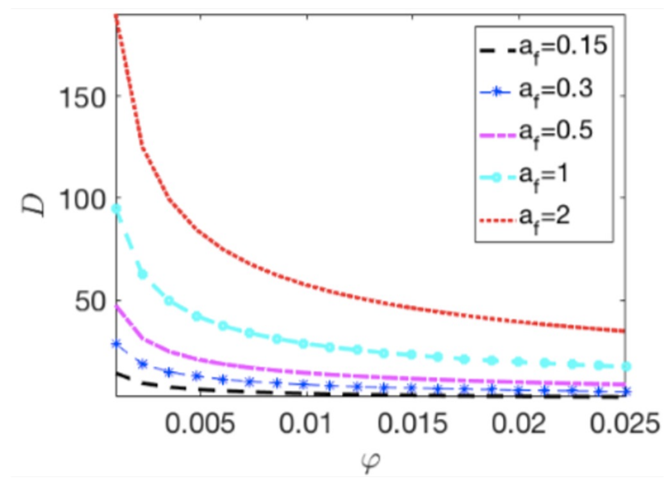
$$\frac{a_f^2}{\gamma} = 4\varphi\left[\frac{1}{3}\frac{a_f^2}{\gamma} + \frac{5}{6}\frac{a_f}{\sqrt{\gamma}}\frac{K_1\left(a_f/\sqrt{\gamma}\right)}{K_o\left(a_f/\sqrt{\gamma}\right)}\right]$$

Spielman & Goren (1968)

- Average fiber separation

$$D \approx 2a_f\left[\frac{1}{2}\sqrt{\frac{3\pi}{\varphi}} - 1\right]$$

Ho, Leiderman, Olson (2016)
Leiderman and Olson (2016)
Ho, Leiderman, Olson (2019)



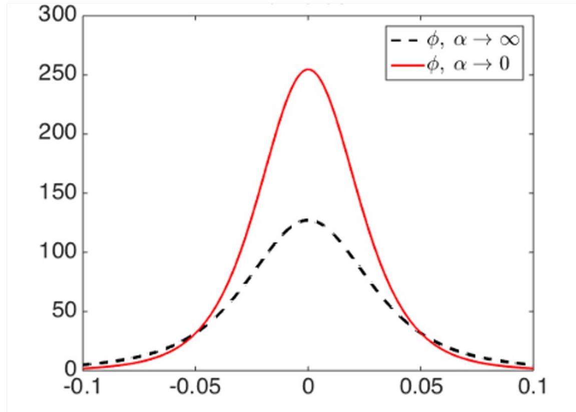
2D Regularized Brinkmanlet

- Brinkmanlet (singular point force)

$$\mathbf{u}(\mathbf{x}) = (\mathbf{f_o} \cdot \nabla)(\nabla B) - \mathbf{f_o}\Delta B \quad B(r) = -\frac{K_0(\alpha r) + \ln(r)}{2\alpha^2\pi}$$

- Regularized point force $\mathbf{f}_i = \mathbf{F}_i \psi_\varepsilon(\mathbf{x} - \mathbf{X}_i)$ for radially symmetric ψ_ε where $R = \sqrt{r^2 + \varepsilon^2}$ and choose $B_\varepsilon(R)$
- Implicitly define $(\Delta - \alpha^2)B_\varepsilon = G_\varepsilon$ and solve for $\psi_\varepsilon = \Delta G_\varepsilon$

2D Regularized Brinkmanlet



- Regularization function
- Ensuring the right limits are obtained
  - Recover Singular Brinkmanlet as $\varepsilon \to 0$
  - Recover Regularized Stokeslet as $\alpha \to 0$

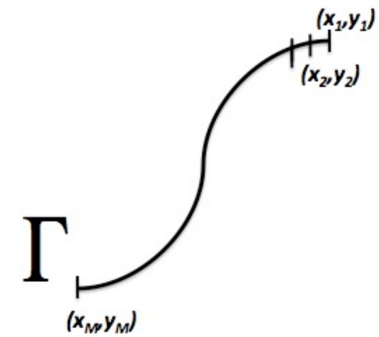
$$\mathbf{u}(\mathbf{x}) = \sum_{i=1}^{N} [\mathbf{F}_i H_1 + [\mathbf{F}_i \cdot (\mathbf{x} - \mathbf{X}_i)](\mathbf{x} - \mathbf{X}_i)\ H_2]$$

$$H_1 = -(B''_\varepsilon(r) + c_\alpha + c_S) \quad H_2 = \frac{B''_\varepsilon - B'_\varepsilon}{r^3}$$

$$c_\alpha = \frac{-\gamma_e - \log(\alpha/2)}{4\pi}, \quad c_S = -\frac{1}{8\pi}$$

3D: Cortez, Cummins, Leiderman, and Varela. J Comp Phys. 2010.
2D: Leiderman and Olson. Phys Fluids. 2016
3D KR: Ho, Leiderman, and Olson. J Fluid Mech. 2019.
Boundary Integral: Ahmadi, Cortez, and Fujioka. J Fluid Mech. 2017.

Planar: Euler Elastica



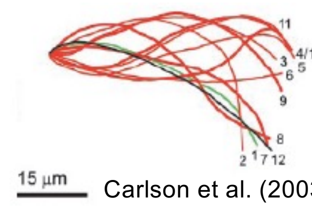
- Energy

$$E = \int_\Gamma S_1 \left[\left\| \frac{d\mathbf{X}}{ds} \right\| - 1 \right]^2 ds + \int_\Gamma S_2 \left[\frac{\partial \Theta}{\partial s} - \zeta(s,t) \right]^2 ds$$

$\Theta =$ Shear angle $\qquad \zeta =$ Preferred curvature

- Assume flagellum will bend as a small amplitude sine wave

$$\zeta(s,t) = -\kappa^2 b \sin(\kappa s - \omega t)$$

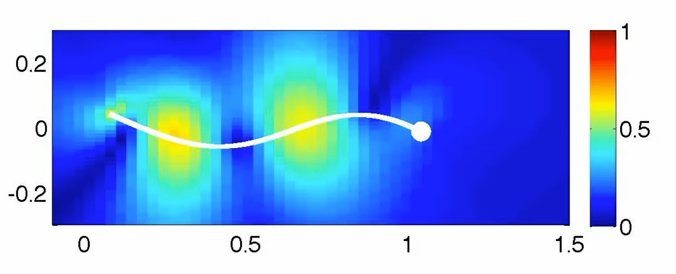


Carlson et al. (2003) PNAS

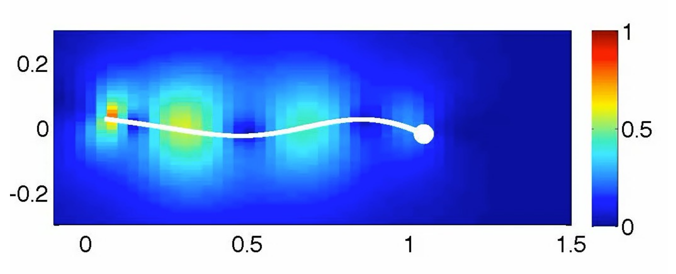
- Force: $\mathbf{F} = -\dfrac{\delta E}{\delta \mathbf{X}}$

Single Swimmer

$$\alpha = 1$$

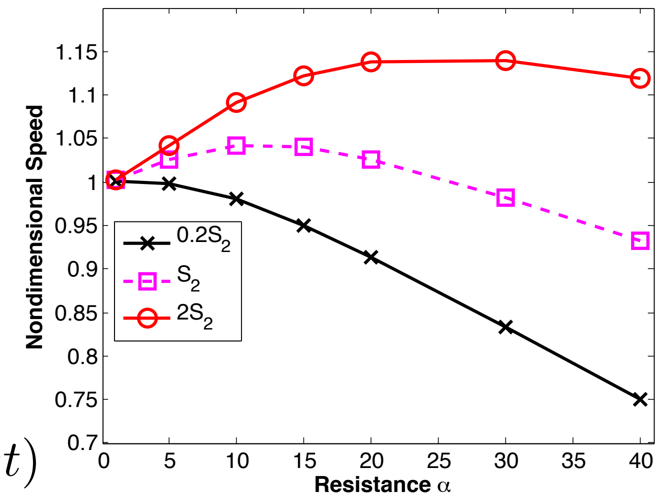


$$\alpha = 10$$



Same preferred curvature function

$$\zeta(s,t) = -\kappa^2 b \sin(\kappa s - \omega t)$$

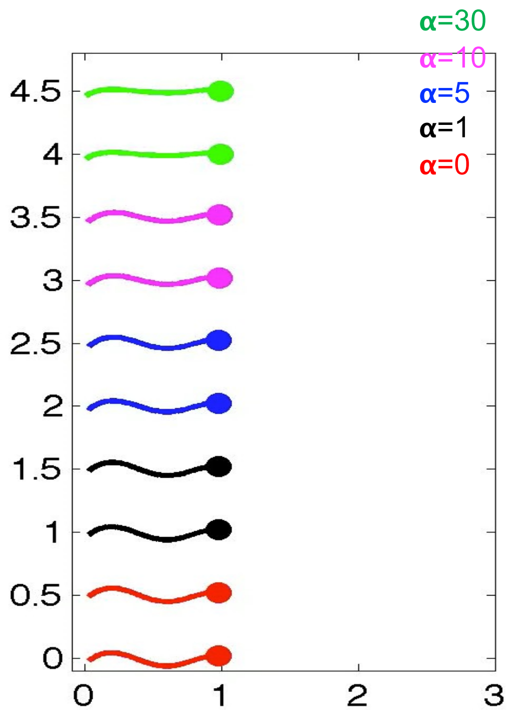


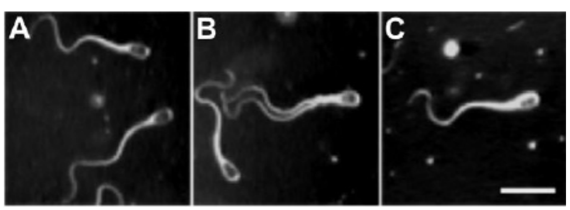
$$u_\infty = \frac{b^2 \kappa \omega}{2} \sqrt{1 + \left(\frac{\alpha}{\kappa}\right)^2}$$

Cortez et al. (2010) J Comp Phys
Olson and Leiderman (2015)
Leiderman and Olson (2016)
Leshansky (2009)

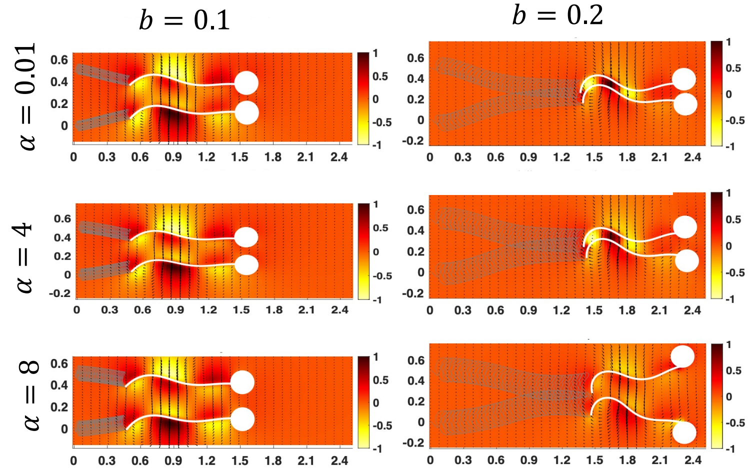
S. Olson (WPI)

Pairs of Swimmers





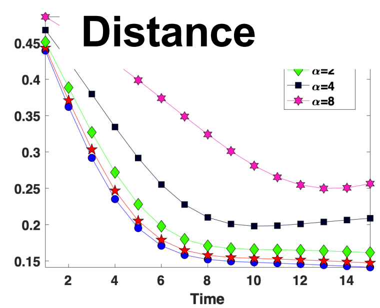
Woolley et al. 2009. J Exp Biol.

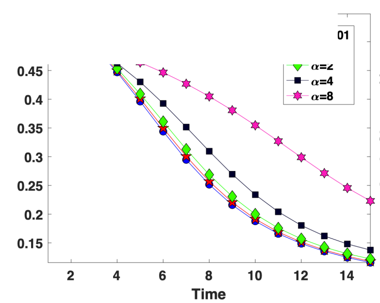


Head Distance

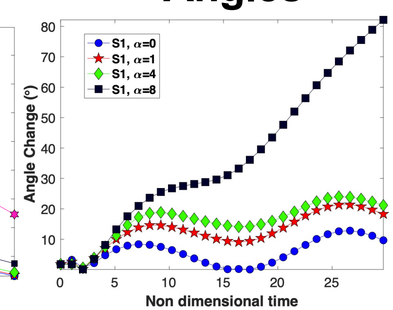
Tail

Distance



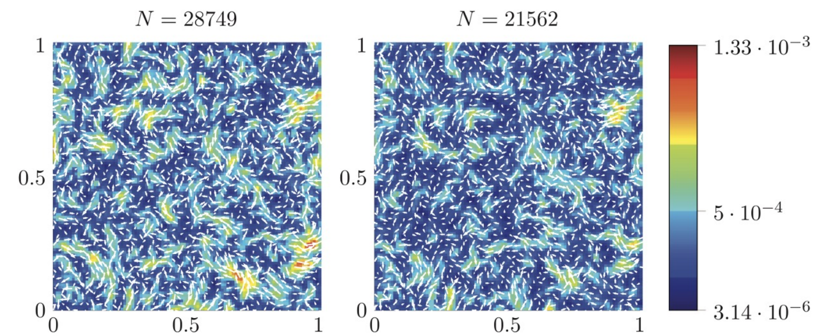


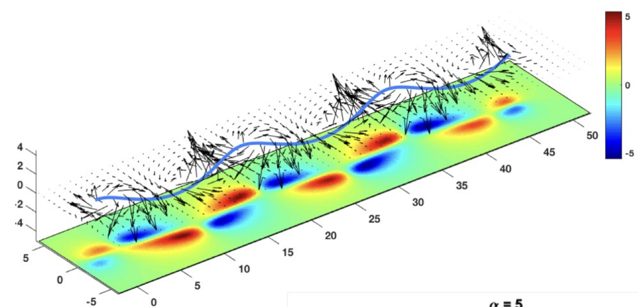
Angles

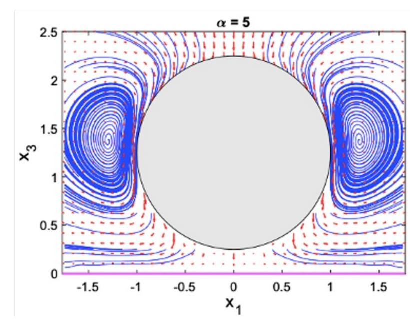


Brinkman

- 3D with point forces (Cummins, Cortez, Leiderman, Varela (2013) J Comp Phys)
- 3D with point forces and torques (Ho, Leiderman, Olson)
- 3D Triply Periodic (Nguyen, Olson, Leiderman)
- 3D with a wall (Nguyen, Olson, Leiderman)
- Comparison of point forces of different density from fibers or rigid spheres compared to Brinkmanlets solution (Kamarapu, Jabarzedeh, HC Fu (2022) Phys Fluids)
- Boundary integral formulation for interface between two porous media (Ahmadi, Cortez, Fujioka (2017) J Fluid Mech)







Viscoelastic Networks

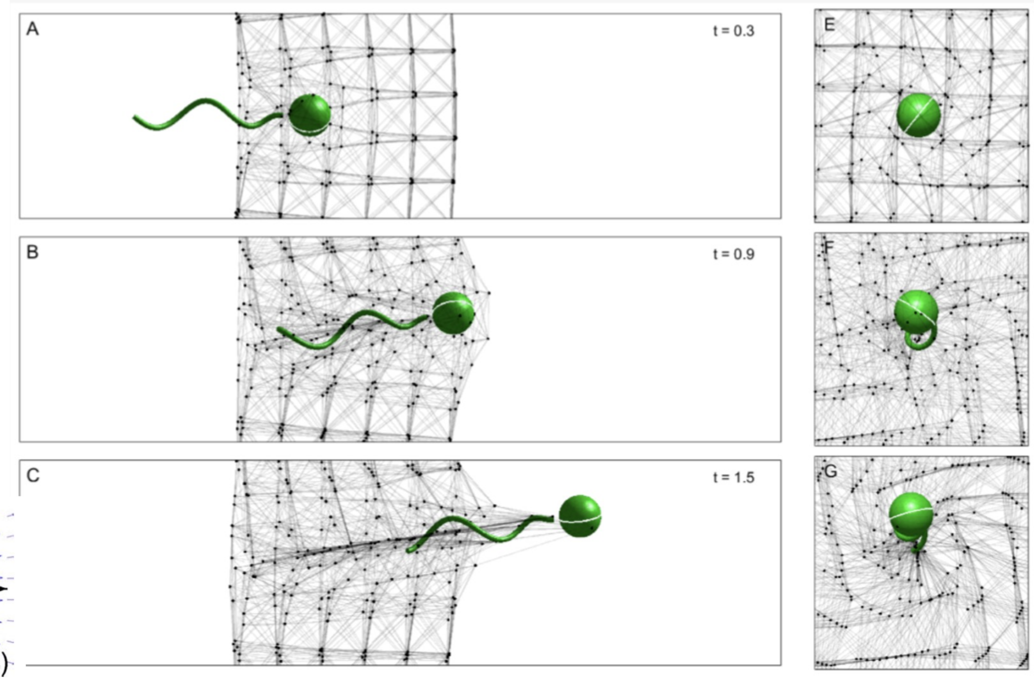
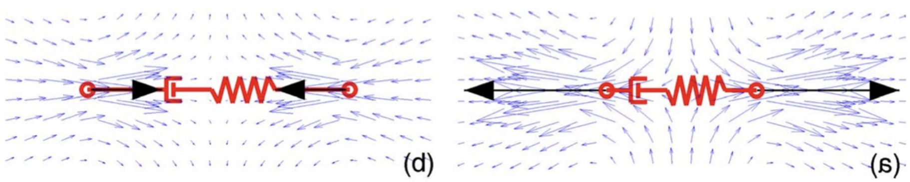
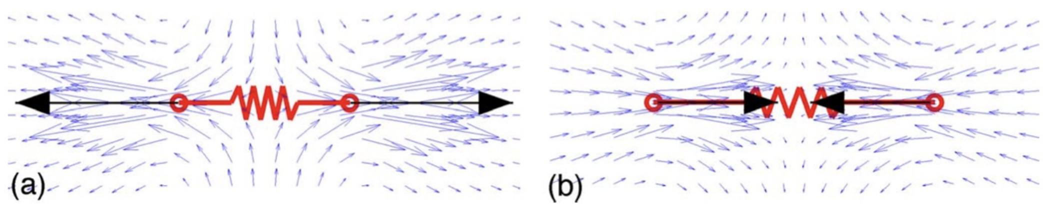


FIG. 9. Schematic Stokes-Maxwell element.



Schuech, Cortez, Fauci. (2022) Fluids

FIG. 6. Schematic Stokes-spring element.



Wrobel, Cortez, Fauci. (2014) Phys Fluids

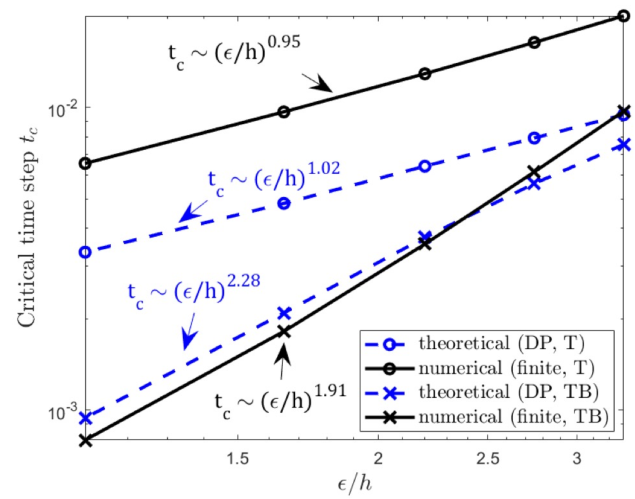
Updating the Structure

$$\frac{\partial \mathbf{X}}{\partial t} = \mathbf{u}\left(\mathbf{X}(q,s,t)\right)$$

- Explicit time-stepping methods (conditionally stable)
  - Stiffness of the elastic structure necessitates small time steps
  - Linear Stability Analysis in doubly periodic case (Ferranti and Olson) for surface with tension and bending forces
    - Stability and critical time step will depend on: regularization function, regularization parameter, force model and parameters, …

$$\lambda_{\alpha,\beta}\widehat{\mathbf{X}}_{\alpha,\beta} = \frac{K_{\alpha,\beta}}{8\pi\mu}\widehat{\boldsymbol{\mathcal{S}}}^{DP}_{\phi_\epsilon}(0;\alpha,\beta)\cdot\widehat{\mathbf{X}}_{\alpha,\beta}$$

Euler $t_c = \left|2/\min_{\alpha,\beta}(\lambda_1,\lambda_2,\lambda_3)\right|$

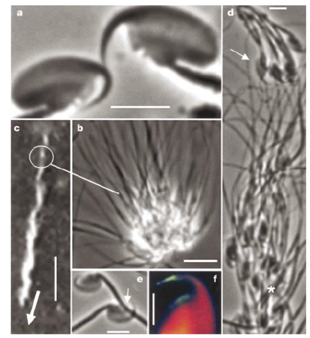


Updating the Structure

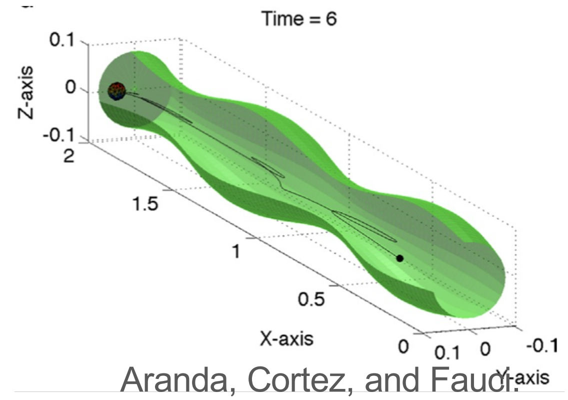
$$\frac{\partial \mathbf{X}}{\partial t} = \mathbf{u}\left(\mathbf{X}(q, s, t)\right)$$

- Multirate time integrator for regularized Stokeslets (Bouzarth and Minion, 2010, *J Comp Phys*)
- Parallel in time methods (Liu and Rostami, 2022, *J Comp Phys*)
- Implicit methods are solving nonlinear equations at each time step. Rosenbrock and Implicit-Explicit Methods now being studied by Uddin, Fauci, Cortez, Buvoli
- ….

Collective Motion: N-Body Problem



Moore et al. 2002. Nature.



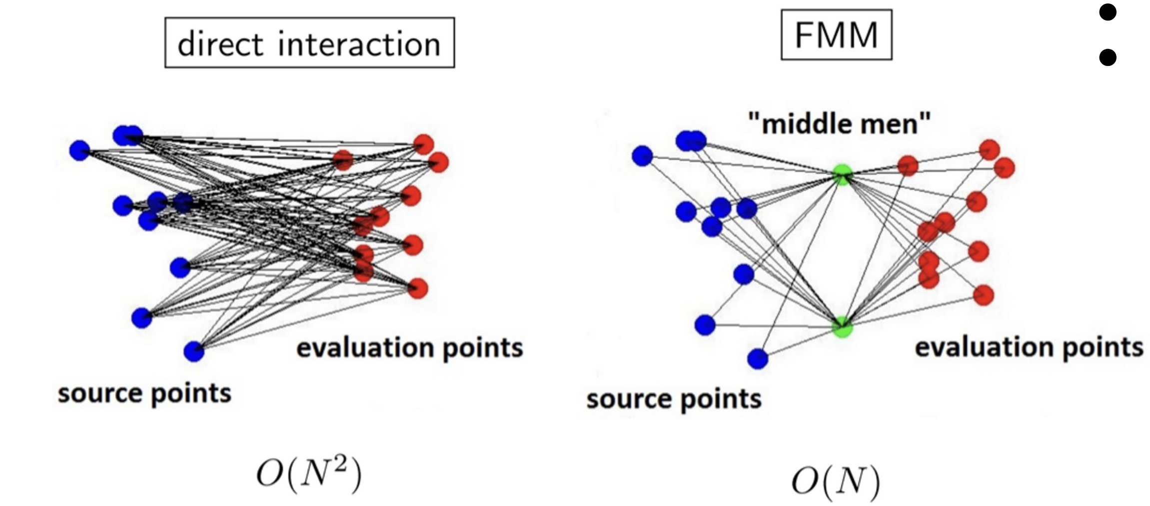
Aranda, Cortez, and Fauci. (2015) J Biomech

Assume there are N particles $\{\mathbf{x_1}, \mathbf{x_2}, \cdots, \mathbf{x_N}\}$ immersed in the fluid.

$$\begin{bmatrix} \mathbf{U} \\ \mathbf{W} \end{bmatrix} = \frac{1}{8\pi\mu} \underbrace{\begin{bmatrix} \mathbf{S} & \mathbf{R} \\ \mathbf{R} & \mathbf{D} \end{bmatrix}}_{\text{A } 6N \times 6N \text{ dense matrix}} \begin{bmatrix} \mathbf{F} \\ \mathbf{N} \end{bmatrix}$$

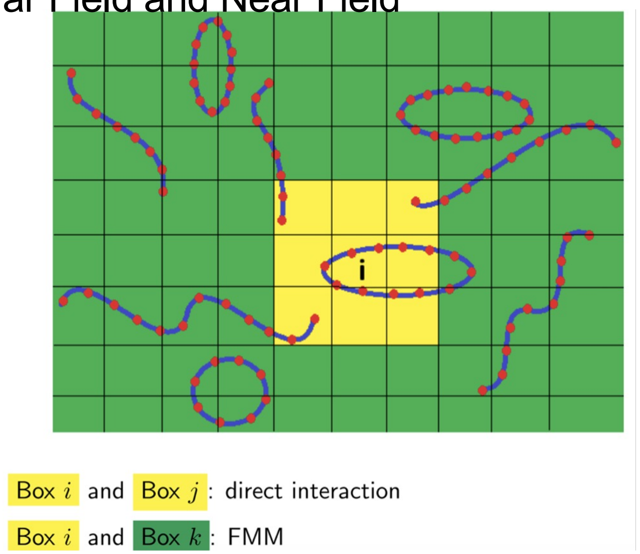
Fast Multipole Method (FMM)

The basic idea: to reduce direct interaction among particles



To achieve $O(N)$: need "middle men", a way to translate from one "middle man" to another, and a clever data structure (octant tree).

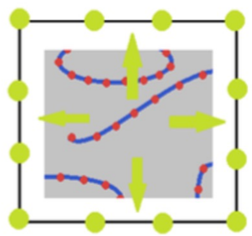
- Error with factorization
- Solution: divide up the domain (tree code)
- Far Field and Near Field

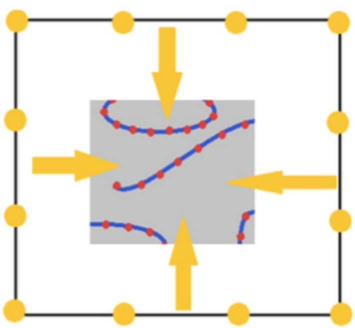


J. Barnes and P. Hut. A hierarchical O(NlogN) force-calculation algorithm. *Nature*, 324:446–449, 1986.
R. Beatson and L. Greengard. A short course on fast multipole methods.
L. Greengard and V. Rokhlin. A Fast Algorithm for Particle Simulations. *J. Comput. Phys.*, 73(2):325–348, 1987.

Kernel Independent Fast Multipole Method (KIFMM)

Upward and downward "equivalent surfaces" are introduced for each box:





Upward equivalent surface: a proxy for the particles inside the box

Downward equivalent surface: a proxy for the particles in the far field

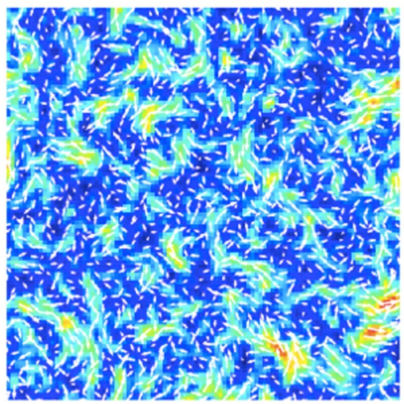
- Fictitious force and torque fields are imposed onto each surface.
- They are computed by solving integral equations, which entails solving small linear systems in the form of

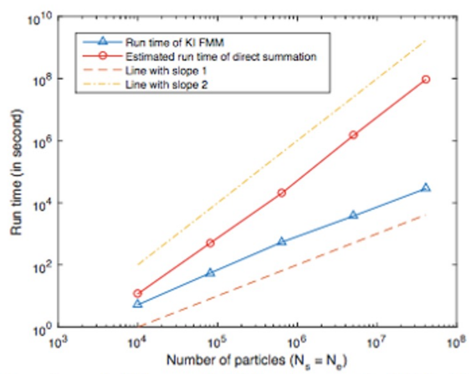
$$\begin{bmatrix} \mathbf{U}_\mathbf{s} \\ \mathbf{W}_\mathbf{s} \end{bmatrix} = \frac{1}{8\pi\mu} \begin{bmatrix} \mathbf{S}_\mathbf{sq} & \mathbf{R}_\mathbf{sq} \\ \mathbf{R}_\mathbf{sq} & \mathbf{D}_\mathbf{sq} \end{bmatrix} \begin{bmatrix} \mathbf{F}_\mathbf{q} \\ \mathbf{N}_\mathbf{q} \end{bmatrix}.$$

(Compute the linear and angular velocities for some sample points and then back out the forces and torques at the quadrature points.)

Collective Motion - KIFMM

"Dumbbell Model" - interactions of a large number of swimmers





Rostami and Olson. 2016. Journal of Fluids and Structures.

Relative error and run time of the KIFMM.

Cartesian grid	N_q	T_{fmm}	$E_{\mathbf{u}}$
$4 \times 4 \times 4$	64	537	7.33 10^{-4}
$5 \times 5 \times 5$	124	1145	2.95 10^{-4}
$6 \times 6 \times 6$	208	2485	1.07 10^{-4}

Run time of KIFMM for multiple cores.

N_c	Strong scaling efficiency
1	100%
2	87%
4	76%
8	67%

In upward/downward pass, loop over boxes on the same level is parallelizable.

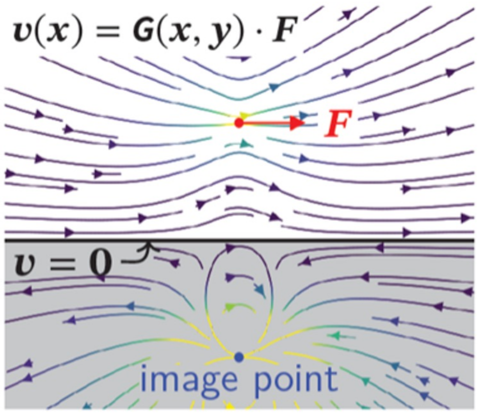
Additional Approaches

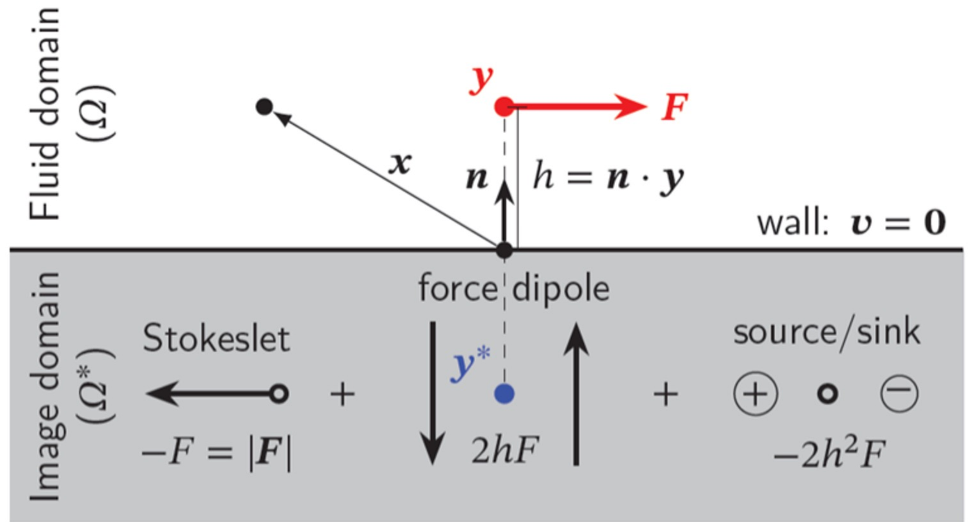
- Kernel independent tree code - barycentric Lagrange interpolation at Chebyshev points to approximate the well-separated particle-cluster interactions

L. Wang, R. Krasny, and S. Tlupova. A kernel-independent treecode algorithm based on barycentric Lagrange interpolation. *Commun. Comput. Phys.*, 28(4):1415–1436, 2020.

- If solving the linear system for forces
  - KIFMM based preconditioners can be utilized (Rostami and Olson (2019) J Comp Phys)
  - Multigrid approach utilizing decay of kernel function (Liu and Rostami (2023) J Comp Phys)
- Determining ways to minimize the number of points *N*

Blake's Image System
1971, Applied to a Stokeslet





$$G(x, y) = \overbrace{S(x - y)}^{\text{Stokeslet}} + \underbrace{S^*(x, y)}_{\text{images}} \quad \text{(Green's function)}$$

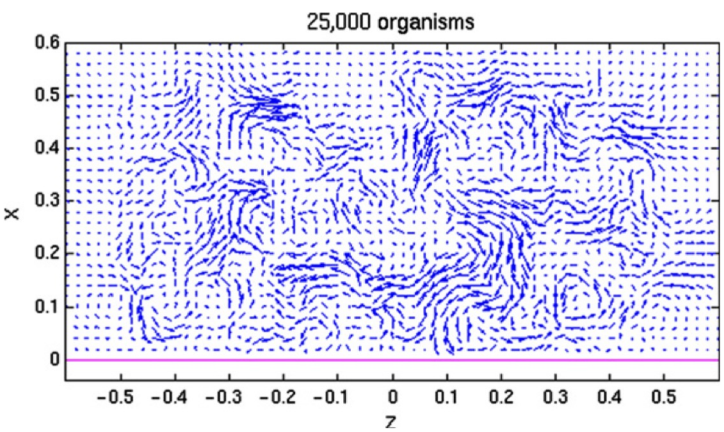
$$\delta^*_{jk} = (\delta_{jk} - 2n_j n_k)$$

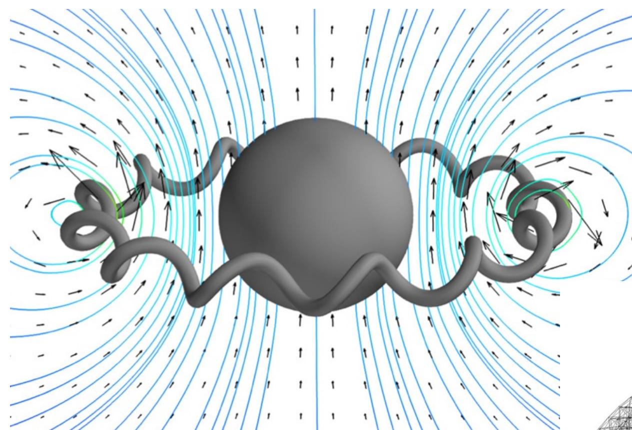
$$S^*_{ij}(x, y) = -\underbrace{S_{ij}(x - y^*)}_{\text{point force}} - 2(n \cdot y)\underbrace{\delta^*_{jl} n_k \nabla_l S_{ik}(x - y^*)}_{\text{force dipole}} + (n \cdot y)^2 \underbrace{\delta^*_{jk} \nabla^2 S_{ik}(x - y^*)}_{\text{source/sink}}$$

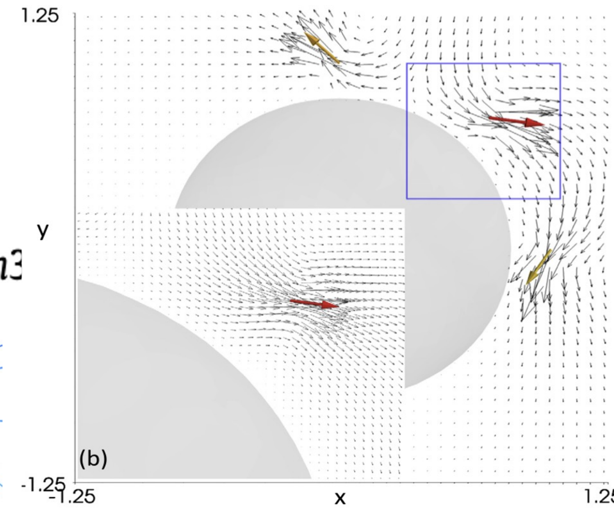
Blake (1971). "A Note on the Image System for a Stokeslet in a No-Slip Boundary".

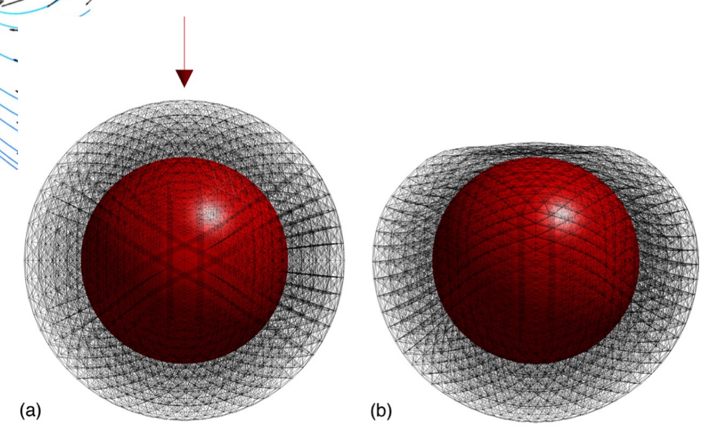
Regularized Image Systems

$$S_{ij}^{IM} = \left(S_{ij}^{*} - S_{ij}\right) - 2h\rho_{mj}\left(\Delta_{i3m} + \frac{h}{2}D_{im}\right) - 2h(\mathcal{R}_d - \mathcal{R}_s)_{im}\epsilon_{jm3}$$





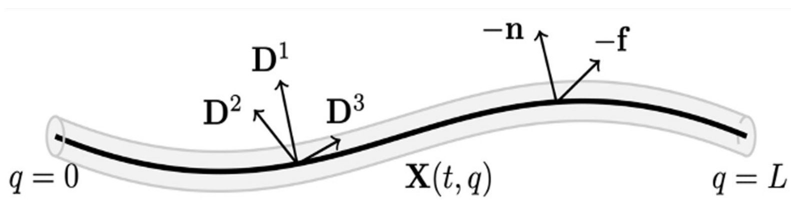


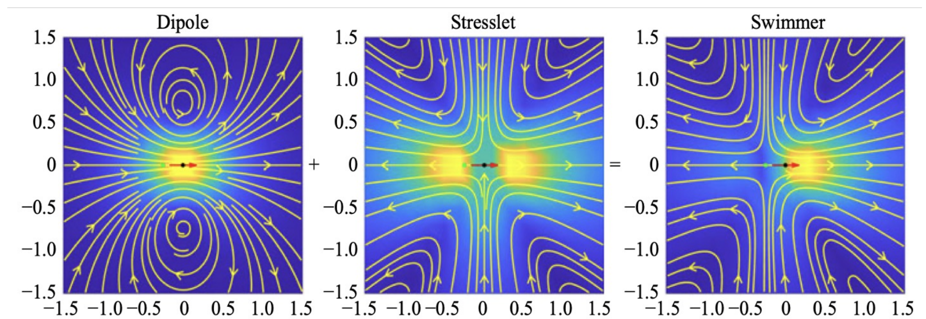


Ainley et al. J Comp Phys (2008)
Cortez et al. J Comp Phys (2015)
Wrobel et al. J Comop Phys (2016)
Mitchell and Pantova arXiv (2019)

Minimal Representations of Structures

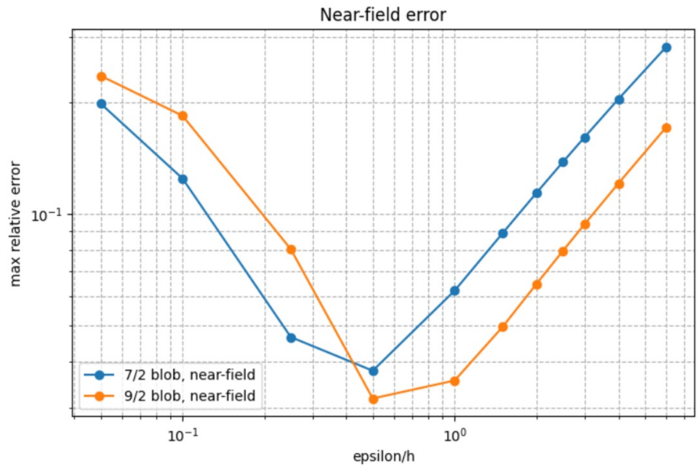
- Single particle representation of self propelled micro-swimmer as a force-doublet (Hoover, Boindala, Cortez (2024) J Fluid Mech)
- Representing thin elastic structures
  via a centerline (Olson, Lim, Cortez (2013) J Fluid Mech)
- ……





Regularized Stokeslet Segments/Surfaces

- Segments - integrate Stokeslet kernel over continuous piecewise linear segments - decouples ϵ, h for 1D models in 3D fluid (Cortez (2018) J Comp Phys)
- Surfaces - integrate Stokeslets kernel over triangles - decouples ϵ, h for 2D surfaces in fluid (Ferranti and Cortez (2024) J Comp Phys)



Discretization/Quadrature Error

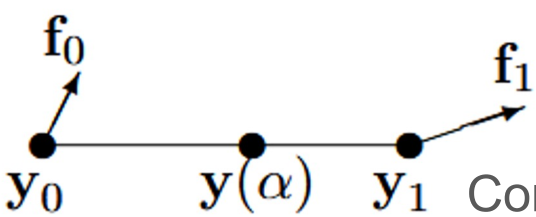
Depends on quadrature choice, discretizatio length, as well as regularization.

Issue: Nearly-singular kernel.

$\text{Error} \sim \mathcal{O}(h^2/\epsilon^3)$ for trap. quad.

Key idea: analytic integration

Linear forces over segments.



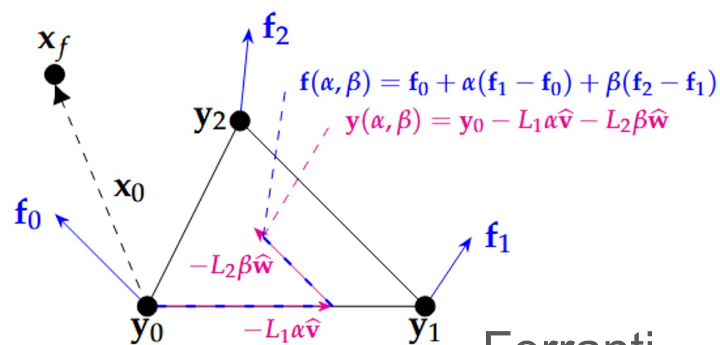
Cortez, 2018

Integrate

$$\int_{\text{seg.}} \mathcal{S}_\epsilon(\mathbf{x}, \mathbf{y}(\alpha)) \cdot (\mathbf{f}_0 + \alpha(\mathbf{f}_1 - \mathbf{f}_0)) \ d\alpha$$

analytically.

Linear forces over triangles



Integrate

Ferranti, Cortez, 2024

$$\iint_{\text{tri.}} \mathcal{S}_\epsilon(\mathbf{x}, \mathbf{y}(\alpha, \beta))$$
$$\cdot (\mathbf{f}_0 + \alpha(\mathbf{f}_1 - \mathbf{f}_0) + \beta(\mathbf{f}_2 - \mathbf{f}_1)) \ d\alpha \, d\beta$$

analytically.

Takeaway

Regularization parameter/discretization length have to be chosen in tandem for traditional MRS implementations (usually ϵ is a small multiple of h)

However, with regularized Stokeslet segments/surfaces, it is ok to have $\epsilon \ll h$.

Example

Open the *flow_past_sphere_streamlines.ipynb* in your Google Drive.

Thank you for your attention!