Computing the motion and fluid flow around cilia & microorganisms

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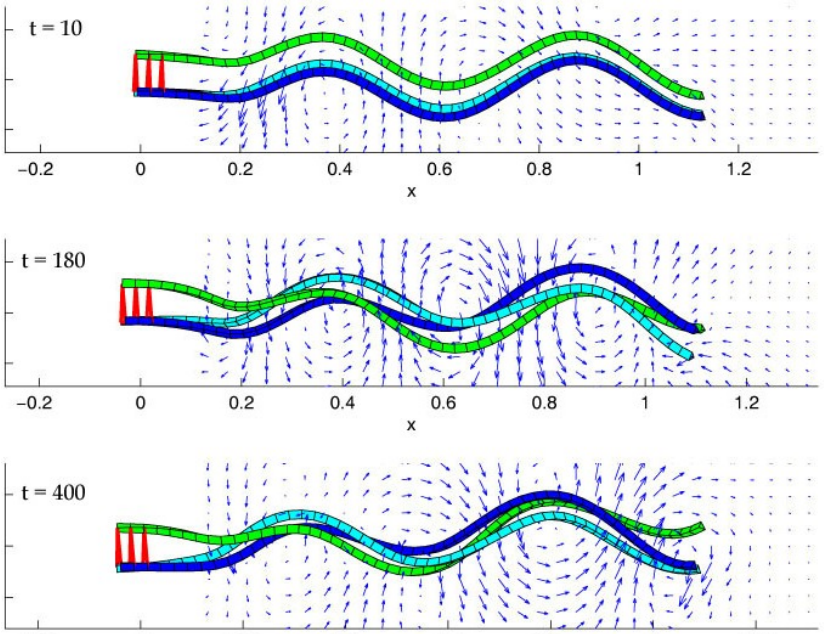

Ricardo Cortez, PI

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Priya Boindala, Math grad student

Marian Hernandez-Viera, Math grad student

The problem & challenges

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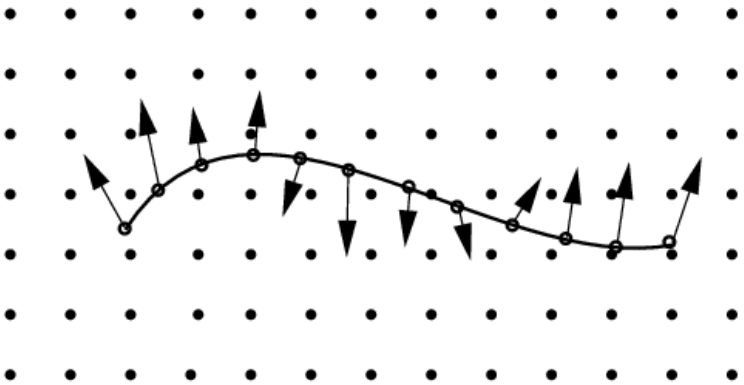
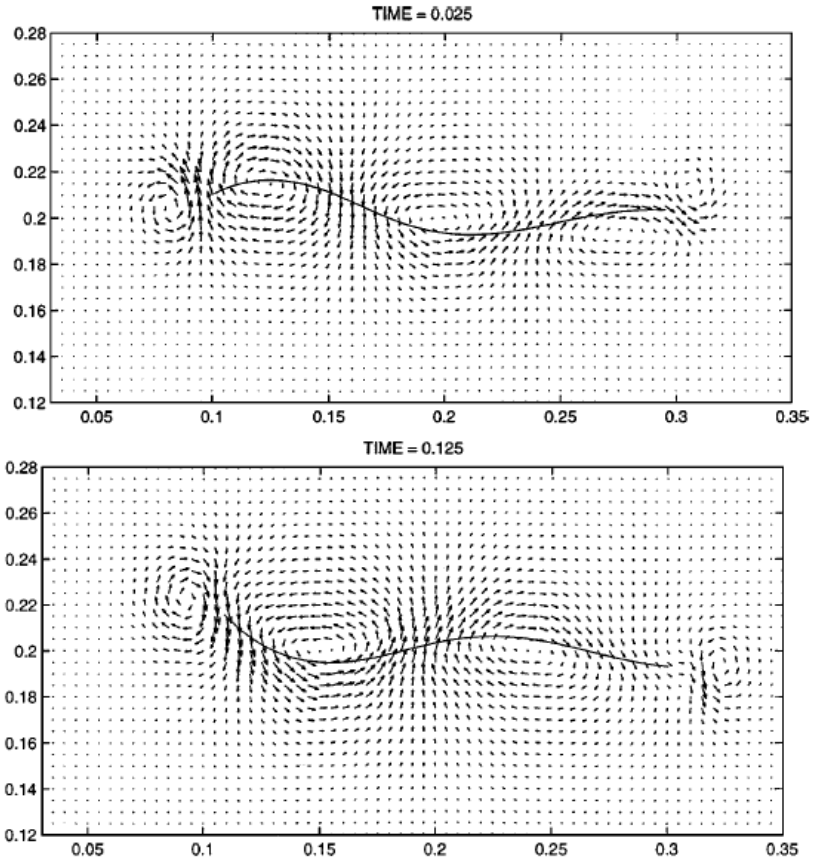
Microorganisms, flagella, cilia and other small scale bodies are flexible and elastic. They have internal mechanisms that generate forces on the fluid. In turn, the fluid motion they generate affects the motion of the organisms.

We are interested in understanding the interaction between the forces exerted by the bodies on the fluid, the fluid motion and the feedback to the organism motion. Both the fluid motion and the organism motion are unknown.





(Singular) Stokeslets

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$$\nabla p = \mu \Delta \mathbf{u} + \mathbf{F}, \qquad \nabla \cdot \mathbf{u} = 0$$

Suppose that $\mathbf{F}(\mathbf{x}) = \mathbf{f}\,\delta(\mathbf{x})$ and $r = |\mathbf{x}|$.

$$8\pi\mu\mathbf{u}(\mathbf{x}) = \frac{\mathbf{f}}{r} + \frac{(\mathbf{f}\cdot\mathbf{x})\mathbf{x}}{r^3} \sim \frac{1}{r} \qquad \textit{(Stokeslet)}$$

Can use superposition due to linearity!

Regularized Stokeslets

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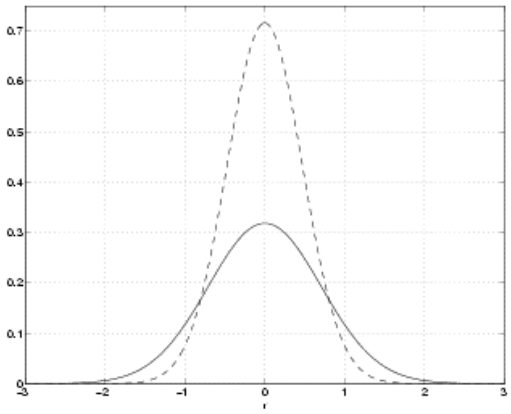
Replacing the delta function with the blob

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



Gives the regularized Stokeslet

$$8\pi\mu\mathbf{u}(\mathbf{x}) = \mathbf{f}\left[\frac{1}{\sqrt{r^2+\delta^2}} + \frac{\delta^2}{(r^2+\delta^2)^{3/2}}\right] + \frac{(\mathbf{f}\cdot\mathbf{x})\mathbf{x}}{(r^2+\delta^2)^{3/2}}$$

For multiple forces at different locations:

$$\mathbf{u}(\mathbf{x}) = \frac{1}{8\pi\mu}\sum_k S_\delta(\mathbf{y}_k - \mathbf{x})\mathbf{f}_k$$

Streamlines around organisms

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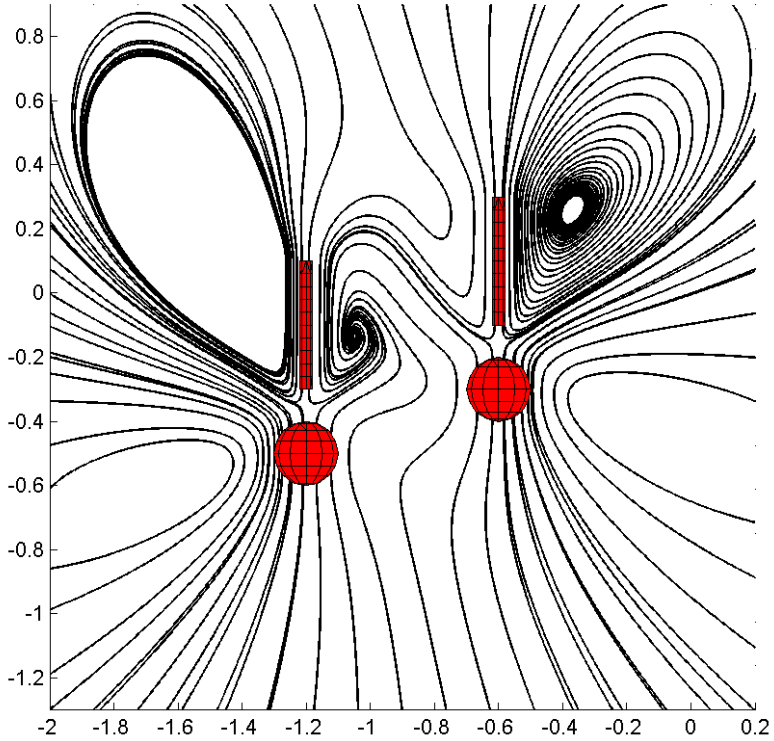

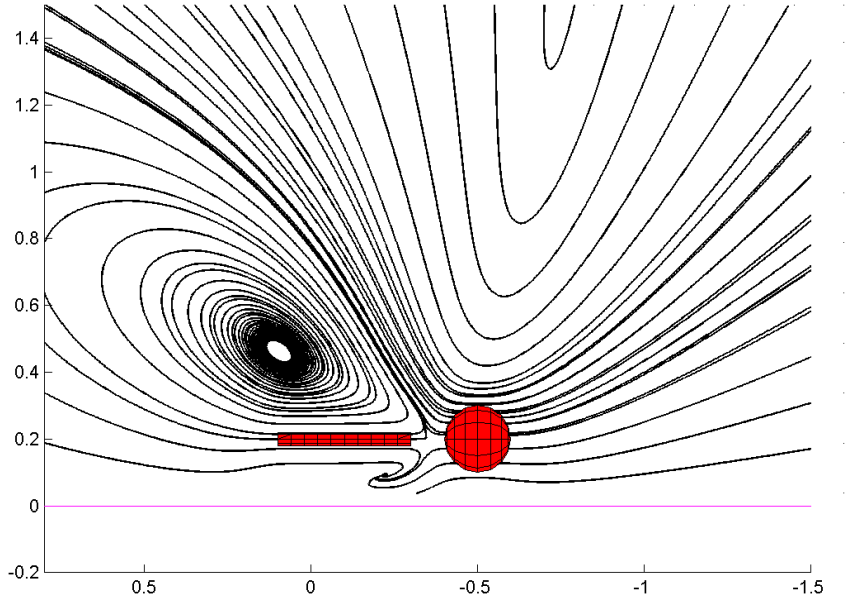

Instantaneous velocity streamlines around virtual microorganisms near a wall. No-flow boundary conditions are enforced using a method of images.

Flow around a cilium

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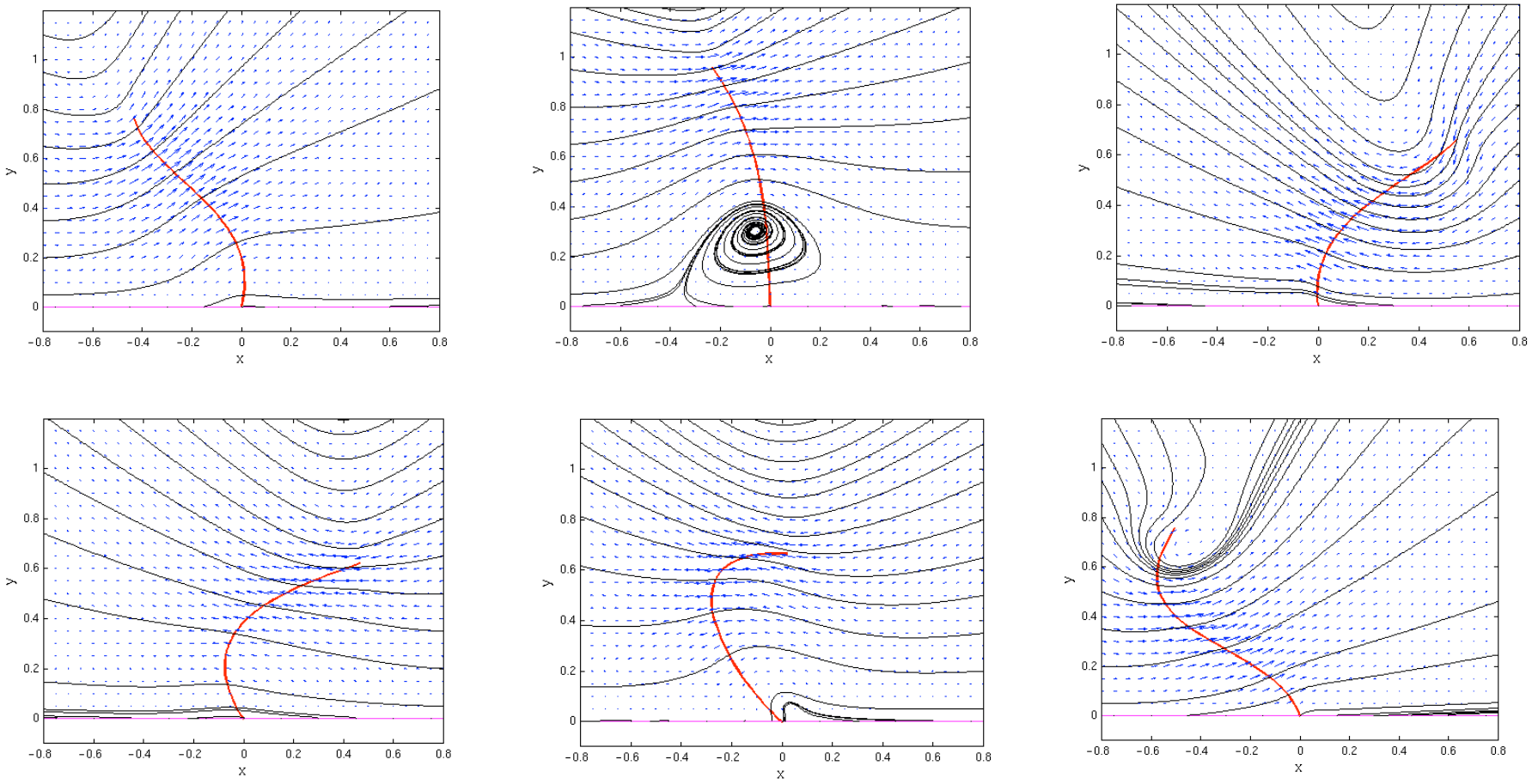
Velocity field generated during a cilium beat. Cilium shapes were taken from published data. Forces along the cilium and velocity fields were reconstructed using regularized Stokeslets.



Lamprey Swimming Project

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Postdoc

Lisa Fauci
Professor

CCS, Mathematics, Tulane University

Goal of the lamprey project

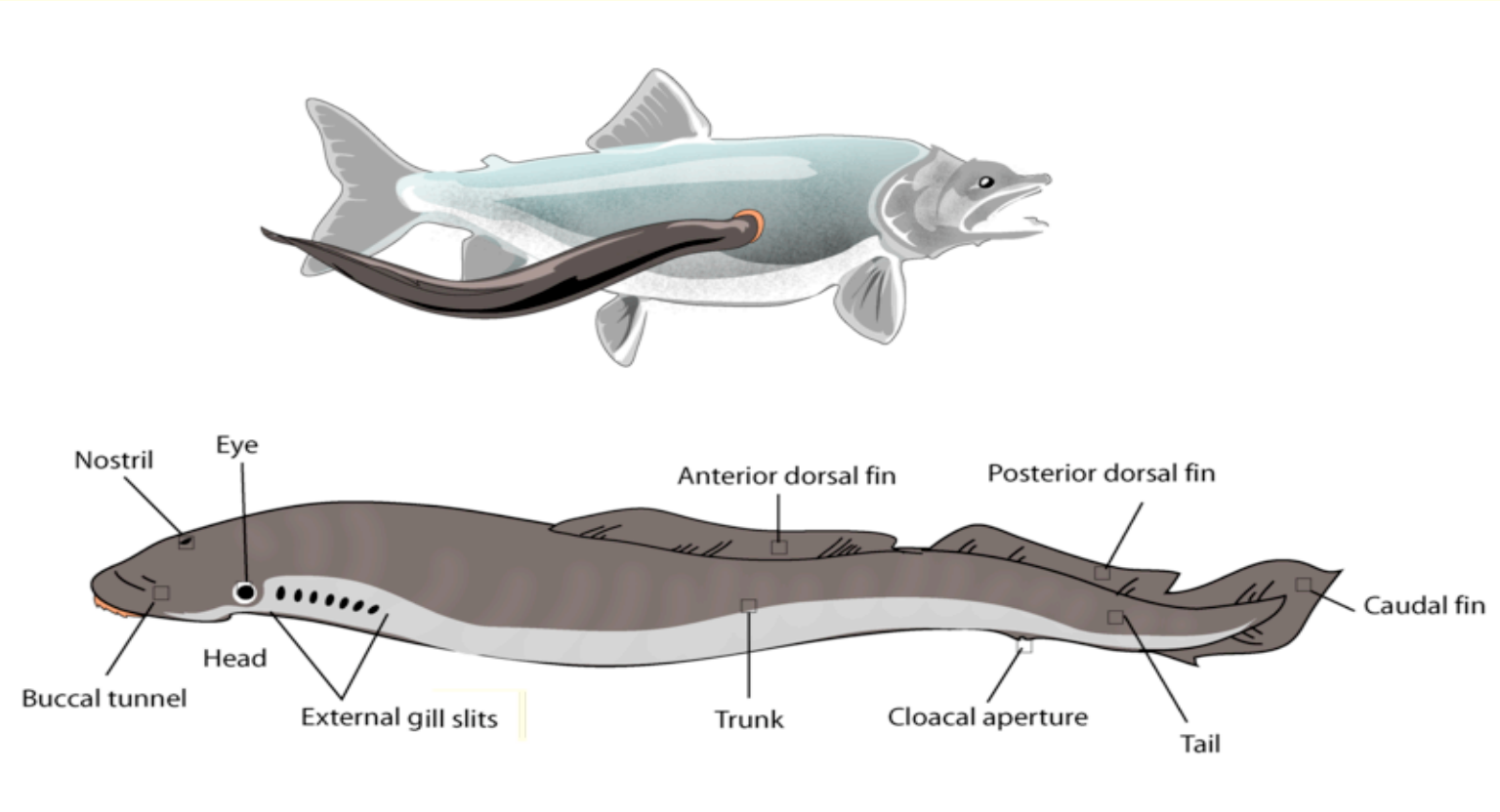
- To simulate the lamprey swimming with the muscle contraction by the internal activation of calcium ion flow and also the interaction of the external hydrodynamics.

What is the lamprey ?

Parasitical lamprey eel

- http://www.ucmp.berkeley.edu/vertebrates/basalfish/petro.html

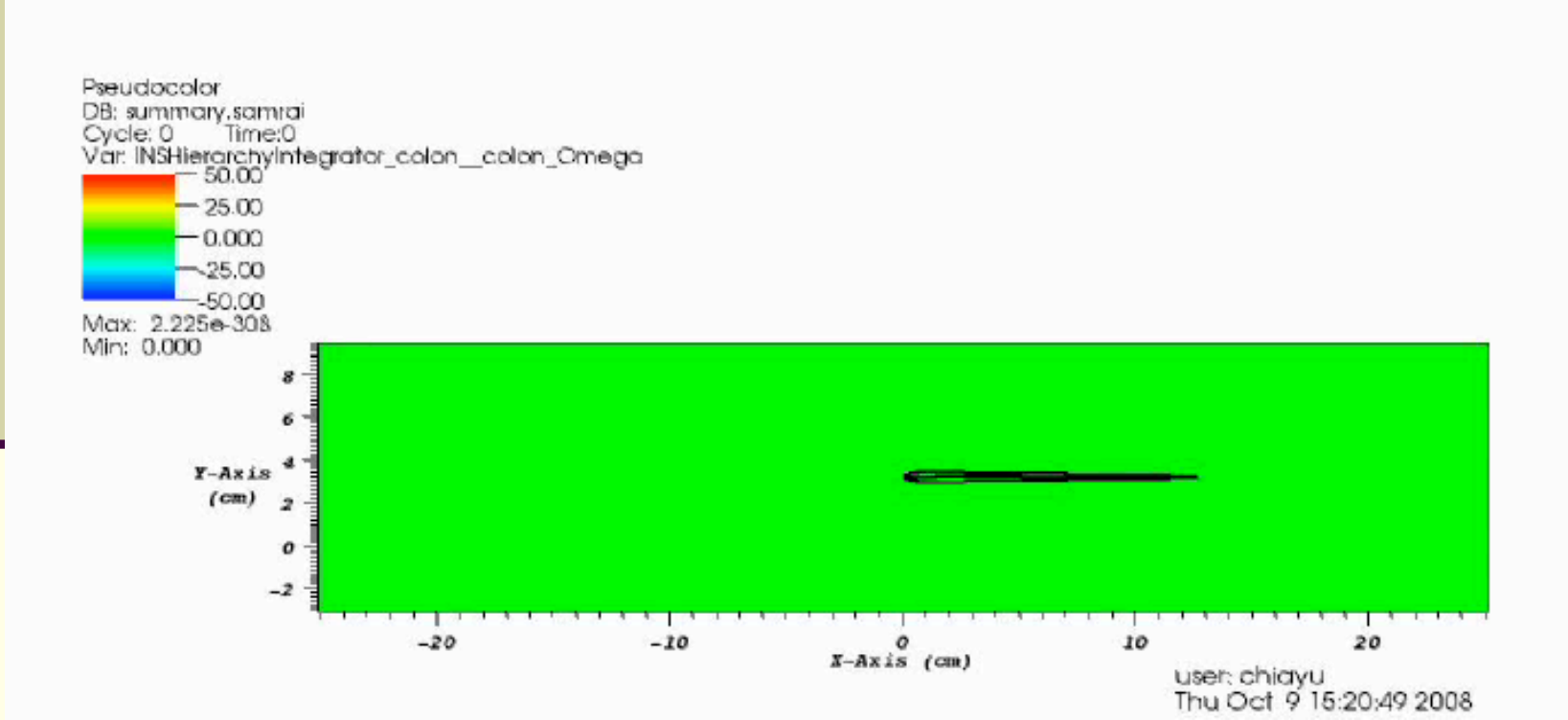
Lamprey illustration



- Picture from wikipedia

Progress on 2D

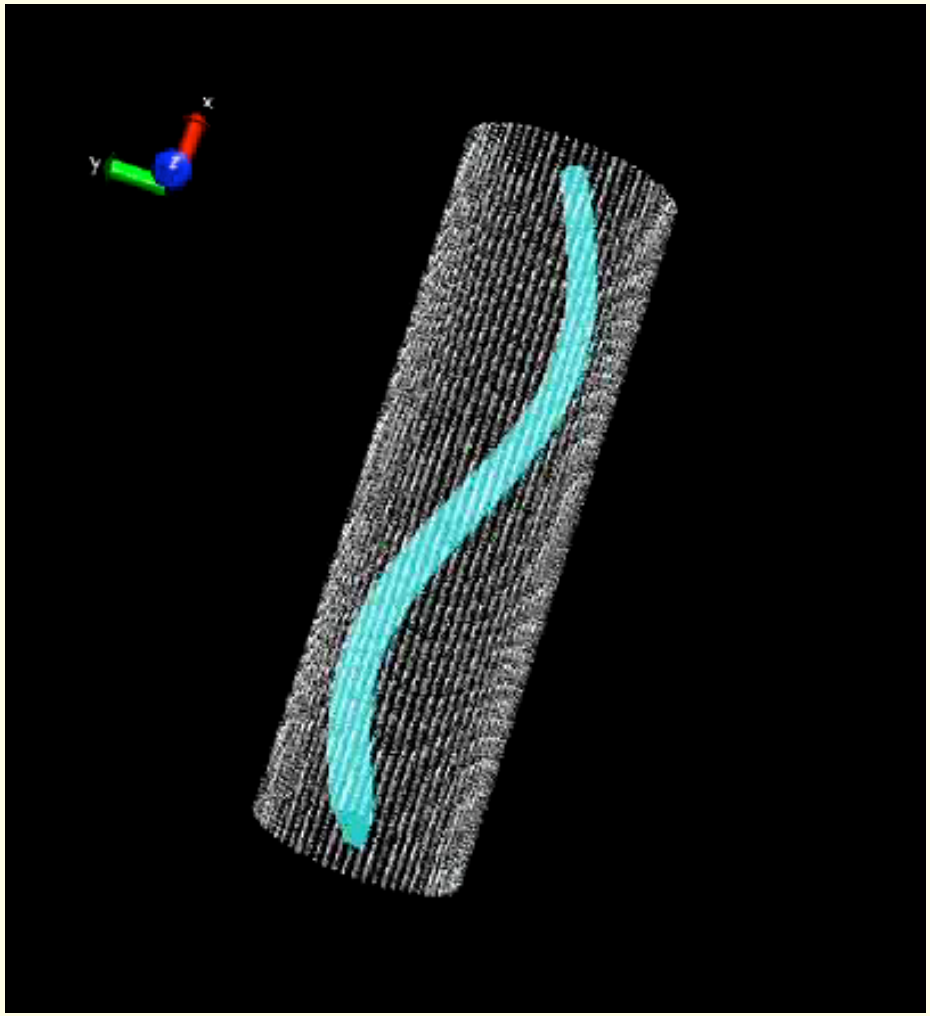
- 2D swimming simulation under simple muscle contraction function and the external hydrodynamics.



Progress on 3D

- 3D swimming simulation under simple sinusoidal wave propagation

  function and the external hydrodynamics



Project on going

- To import the muscle-calcium activation ODE model on this model.

Collaboration

- Dr.Tyler McMillen

  (Mathematics, California State University)
- Dr.Thelma Williams

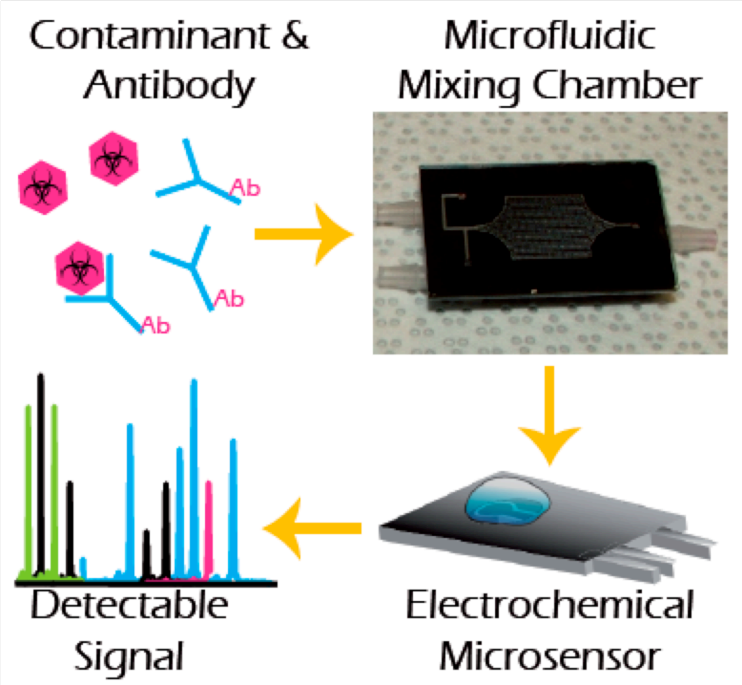
  (Physiology, St. George's Hospital Medical School,London, Retired)
- Dr.Eric Tytell

  (Biology, U. of Maryland, College Park)
- Dr. Avis Cohen

  (Institute for System Reseach, U. of Maryland, College Park)

Design and Optimization of a Microfluidic Mixing Chamber for an Immunosensor Device

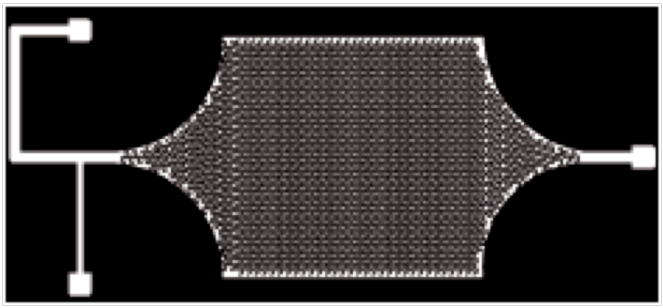
- *Miniaturized Immunosensor Devices*
  - Detect biological or chemical agents by analyte-antibody binding, enzyme activity, and electrochemical signal transduction
- *The Mixing Challenge*
  - Analyte and antibody must mix and bind for signal detection
  - Fluid flow is purely laminar (non-turbulent) at the microscale
  - Mixing occurs primarily due to diffusion, requiring long length- and time-scales, but may be enhanced by convection

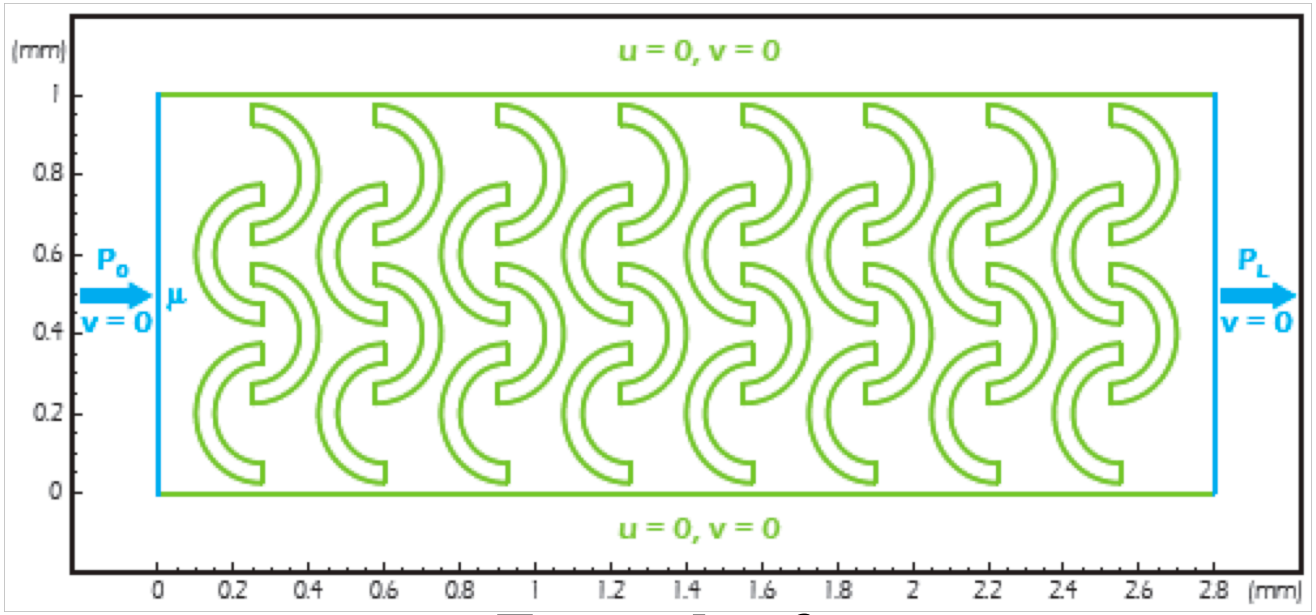


Goal: Determine the optimal geometric configuration of the microfluidic mixing chamber to enhance mixing of the analyte and antibody through numerical simulation.

Computational Model of Mixing Chamber: *Omega Channel Domain*

- 'Omega Channel' mixing chamber designed by colleagues at Louisiana Tech may promote mixing by inducing circulatory flows
- Modification of this design based on computational results will reduce number of mixing chambers to be manufactured and experimentally tested





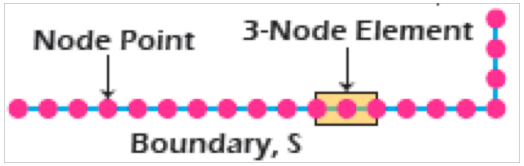
Example of Computational Domain

Computational Model of Mixing Chamber: *Convection Field*

- Incompressible flow is governed by the continuity and Stokes equations; Re << 1 at microscale

$$\nabla P = \mu \nabla^2 \mathbf{u}$$
$$\nabla \cdot \mathbf{u} = 0$$

  - Pressure difference placed across the channel length
  - No slip & no penetration boundary conditions imposed on upper and lower walls and obstructions
- Velocities obtained using Boundary Element Method
  - Grid-free approach; only boundaries must be discretized

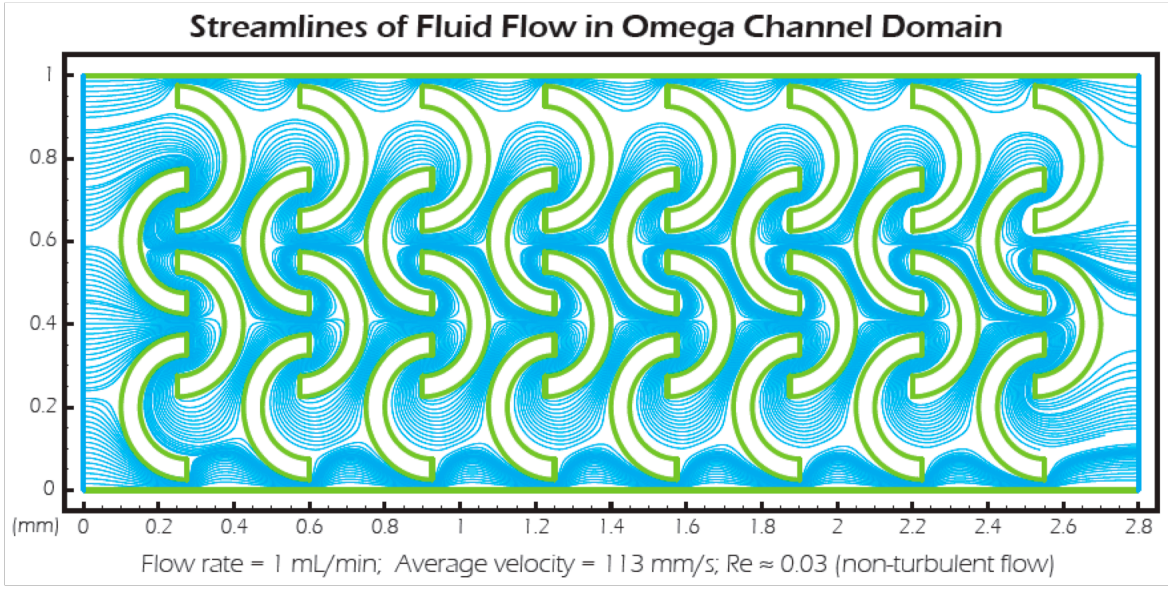


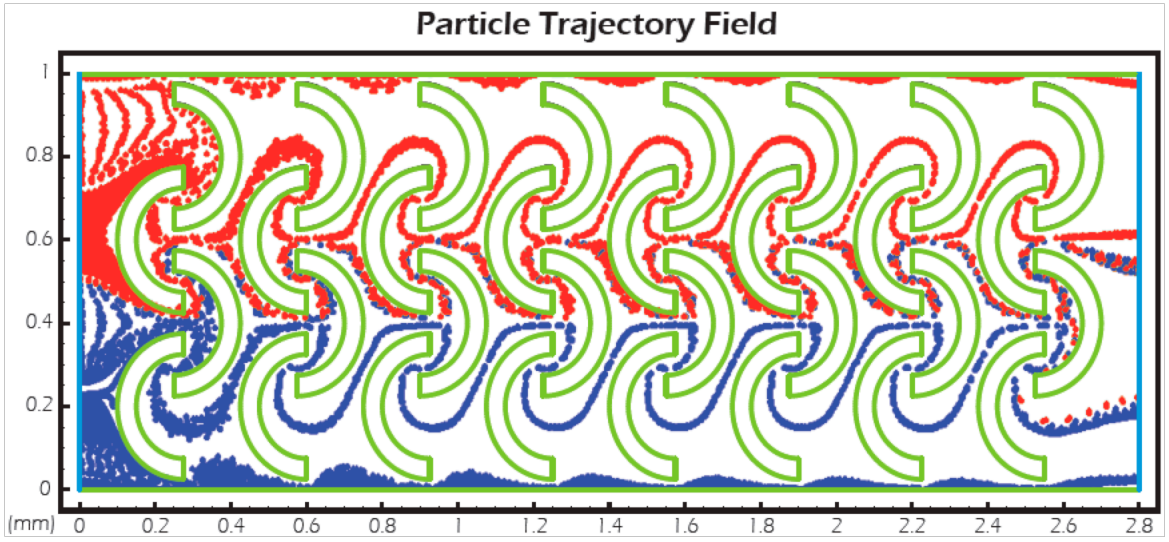
  - Boundary integral equation linking surface velocities and stresses computed by solving system of linear equations

$$\mathbf{C}_{ki} u_i(\mathbf{x}) + \int_S \mathbf{T}_{ik}(\mathbf{x},\mathbf{y}) u_i(\mathbf{y}) dS_y = \frac{1}{\mu} \int_S \mathbf{U}_{ik}(\mathbf{x},\mathbf{y}) \tau_i(\mathbf{y}) dS_y$$
$$H\mathbf{u} = G\tau$$

  - Parallelization allows computation of very large domains

Computational Model of Mixing Chamber:
Convection Field Visualization





I. Applying Density Functional Theory for Atomic Vacancies in Solids.

"Density functional theory (DFT) is among the most popular and versatile methods available in condensed matter physics, computational physics, and computational chemistry. It is a quantum mechanical method used in physics and chemistry to investigate the electronic structure of many-body systems, in particular molecules and the condensed phases." However, most DFT approximations are not very reliable for the formation energy of an atomic vacancy (missing atom) in a solid.

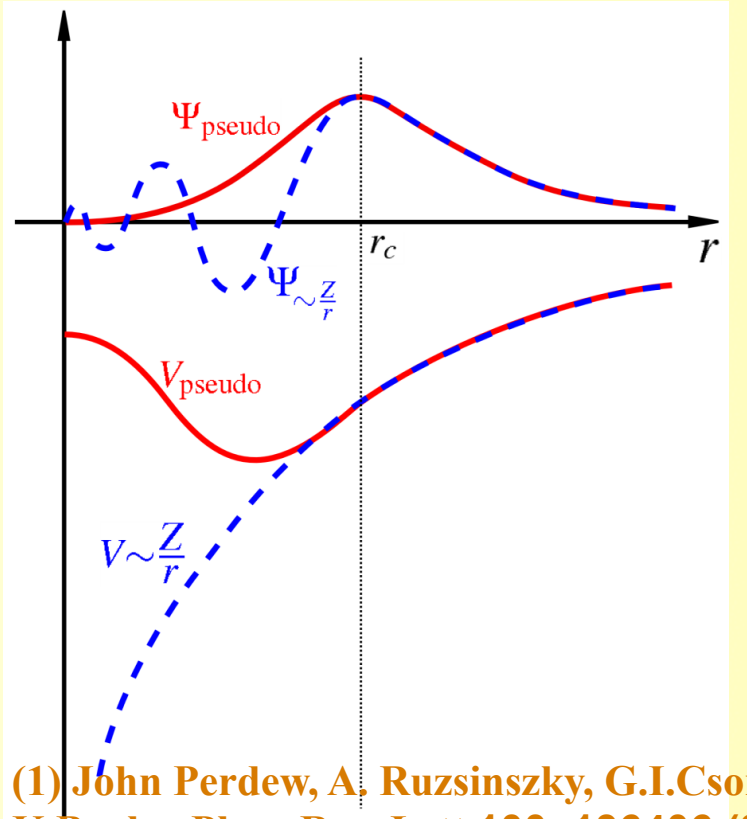
We have recently designed a "Restoring the density-gradient expansion for exchange in solids and surfaces.", which yields accurate metal surface energies. Vacancies are the simplest lattice defects and play an important role for various properties of materials. Since a vacancy in a metal is a kind of interior surface, we expect to be able to predict vacancy formation energies accurately, even for metals.

II. Method

1. Functional – PBEsol(1)

A revised Perdew-Burke Ernzerhof GGA. The main idea of it is to restore the first –principles gradient expansion(μ) for exchange over a wide range of density gradients in solids and surfaces. It improves equilibrium properties of densely-packed solids and their surfaces.

2. Pseudopotential



The pseudopotential approximation is an method to replace the core electrons and the strong nucleus with an effective potential, so that the Schrodinger equation contains a modified effective potential term instead of the Coulombic potential term for core electrons.

3. Software: ABINIT

Formation energy :

$$H_v^F = E_v^{tot}(N-1) - E^{tot}(N)*(N-1)/N$$

(1) John Perdew, A. Ruzsinszky, G.I.Csonka, O.A.Vydrov, G.E.Scuseria, L.A.Constantin, X.Zhou, K.Burke. Phys. Rev. Lett 100, 136406 (2008)

III. Result (formation energy of vacancy)

	supercell	LDA (eV)	PBE (eV)	PBE-sol (eV)	Expt.[2](ev)
Al:	8 atoms	0.57	0.55	0.61	
	27 atoms	0.71	0.63	0.74	
	64 atoms	0.729	0.65	0.76	
	Ref[2](80 cells)	***0.67***	***0.61***	***0.84 (AM05)***	0.68±0.03
	Ref[1](64atoms)	***0.70***	***0.55(PW91)***		
	125 atoms	0.724	0.64		
Si:	8 atoms	2.91	3.04	3.10	3.6
	Ref[2]	*3.58*	*3.65*	*3.59(AM05)*	

(1)K. Carling, G. Wahnstrom,etc, Phys.Rev. Lett.85,3862(2000)

(2)R.Armiento,A.E.Mattsson, Phys. Rev.B 72,085108(2005)

IV. Conclusion

PBEsol result here is not as good as that of PBE and LDA so far. But we have only looked at one case (Al), and need to calculate others. Possibly the experimental value is not as precise as it is claimed to be, or our calculation needs to be made more accurate. Alternatively, it could be that PBEsol gives a good surface energy but not a good curvature energy.

MetaGGA[1] is also good for surface energy, maybe we can try that one also.

The softeware ABINIT is slow for Silicon, we are also trying another software VASP.

(1) Jianmin Tao, John P. Perdew, Viktor N. Staroverov and Gustavo E. Scuseria.

Phys. Rev. Lett 91, 146401, (2003)

Design of powerful black-box solver for multidimensional conservative laws

Problem and Significance

- **Conservative hyperbolic equations are numerous. We want to solve them.**
- **We wish to capture discontinuities sharply and in a non-oscillatory way, while achieving high-order accuracy at the smooth parts of the solution.**

Methods

- **Central-upwind schemes have been successfully applied to hyperbolic conservation equations.**
- **A brute force upwind approach is much too intensive to get the results desired.**
- **Smoothness indicators allow scheme adaption and mesh adaption .**
- **Adaption allows to minimize the cost of nonlinear limiters that would be required to be used everywhere for an unadapted approach.**

Difficulties

- **Smoothness indicators attempt to point out discontinuities in our solution.**
- **Some of these are self-sharpening -- shock waves -- others are not -- contact waves.**
- **Using a limited scheme, we can deal with shock waves, however,**
- **We wish to use a high order scheme to preserve the quality of the contact wave, as these discontinuities do not sharpen themselves every time step.**

Outcomes, extensions, future work, etc.

- **Currently, we have a functional indicator in 2D for the Euler gas dynamics, but the indicator is specific to that set of equations.**
- **We are working towards extending from gas dynamics to a wider class of hyperbolic problems .**
- **Ultimately, a good smoothness indicator allows for a black box solver.**