Immersed boundary method:

Recent developments in analysis, algorithms and applications

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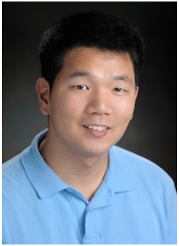
Acknowledgments

Many of the results I present are the work of recent PhD students:

Sudeshna Ghosh
India

Jeffrey Wiens
MDA Corp.

Will Ko
U. Cincinnati



Bamdad Hosseini
PhD, SFU

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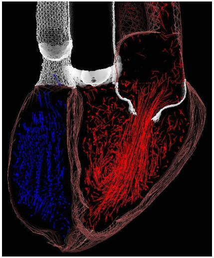
What is an immersed boundary?

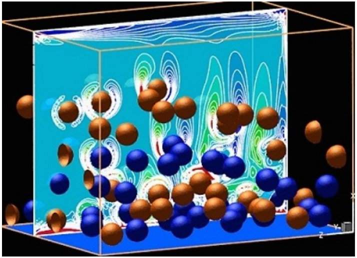
Immersed boundary or IB:

. . . a solid, moving and/or deformable object that is immersed within an incompressible fluid

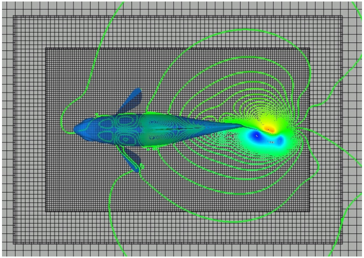
Beating heart
(Peskin & McQueen, NYU)



Particle suspension
(H. Nishida, Kyoto Inst Tech)



Swimming fish
(A*Star, Singapore)



Purpose

The purpose of this talk is . . .

- to provide a brief overview of the immersed boundary method, both mathematical formulation and numerial scheme.
- to summarize recent advances (last 10 years) in
  - analysis,
  - algorithms,
  - applications and extensions.
- to highlight several recent results by SFU students.

> "The IB method is both a mathematical formulation and a numerical scheme." (Peskin, 2002)

Outline

1. Overview of the Immersed Boundary Method
    - Mathematical formulation
    - Numerical scheme
    - Applications in biology and engineering
2. Recent advances: Analysis of IB problems
3. Recent advances: Algorithmic improvements, parallel computing
4. Recent advances: Extensions and applications
5. Closing remarks

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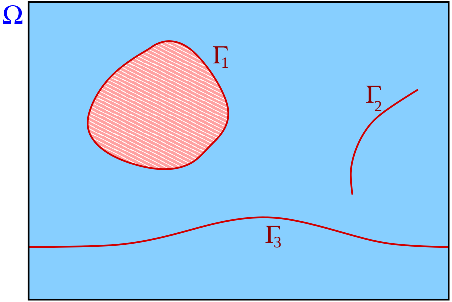
Outline

Geometry and assumptions

Ω: fluid domain, $\mathbf{x} \in \mathbb{R}^2$

Γ: immersed boundaries, parameterized by $q \in \mathbb{R}$ (fiber) or $\mathbf{q} \in \mathbb{R}^2$ (region)



Fundamental principle: Effect of solid structures can be captured by distributing appropriate forces onto the fluid.

Three main assumptions: (for simplicity, easily relaxed)

- Rectangular 2D domain with doubly periodic boundary conditions.
- IBs have zero mass and are permeated by fluid (neutrally buoyant).
- Fluid is incompressible.

Governing equations

Variables: $\mathbf{u}(\mathbf{x},t)$ = velocity, $p(\mathbf{x},t)$ = pressure
$\mathbf{X}(\mathbf{q},t)$ = IB position, $\mathbf{F}(\mathbf{q},t)$ = IB force density

Parameters: ρ = density, μ = viscosity

Incompressible Navier-Stokes equations:

$$\rho\frac{\partial \mathbf{u}}{\partial t} + \rho\mathbf{u}\cdot\nabla\mathbf{u} = \mu\nabla^2\mathbf{u} - \nabla p + \mathbf{f}$$

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

IB elastic force (IB → fluid):

$$\mathbf{f}(\mathbf{x},t) = \int_\Gamma \mathbf{F}(\mathbf{q},t)\,\delta(\mathbf{x}-\mathbf{X}(\mathbf{q},t))\,d\mathbf{q} \qquad \text{"force spreading"}$$

IB evolution equation (fluid → IB): no-slip condition

$$\frac{\partial \mathbf{X}}{\partial t} = \int_\Omega \mathbf{u}(\mathbf{x},t)\,\delta(\mathbf{x}-\mathbf{X}(\mathbf{q},t))\,d\mathbf{x} \qquad \text{"velocity interpolation"}$$

Fluid-structure interaction is mediated by delta functions!

Governing equations

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Fluid-structure interaction is mediated by delta functions!

Elastic forces

The heart of any IB model is the elastic force density $\mathbf{F}(\mathbf{q}, t)$:

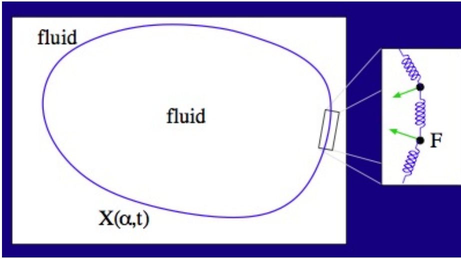
- IB configuration $\mathbf{X}(\mathbf{q}, t)$ determines the stressed elastic state.
- Formulate in terms of an elastic energy functional $E[\mathbf{X}]$.
- Principle of virtual work: $\mathbf{F} = -\dfrac{\wp E}{\wp \mathbf{X}}$ (Fréchet derivative).

Simple case: Elastic fiber with tension $T(q, t)$, tangent vector $\boldsymbol{\tau}(q)$:

$$\mathbf{F} = \frac{\partial}{\partial q}(T\boldsymbol{\tau}) \quad \text{with} \quad \boldsymbol{\tau} = \frac{\mathbf{X}_q}{|\mathbf{X}_q|}$$

Even simpler: Hookean springs, zero rest-length, $T(q) = \sigma|X_q|$:

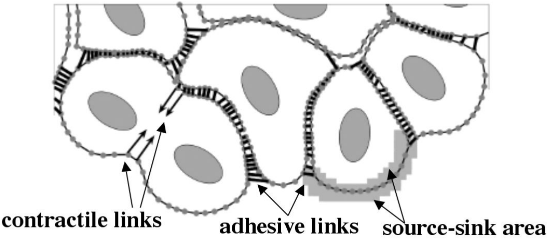
$$\mathbf{F} = \frac{\partial^2 \mathbf{X}}{\partial q^2} \qquad \text{(linear)}$$



Source: Guy & Hartenstine

Other types of forces

- Resistance to bending
- Resistance to torque in flexible rods
- "Tether" points for solid boundaries or other objects with an imposed location or motion
- Active contractile forces (e.g., muscles)
- Attraction/repulsion due to adhesion, contact or lubrication
- Electrochemical forces in ionic solutions
- Thermal fluctuations in microscale systems



Source: Rejniak (2007)

Alternate formulation: Jump conditions

- Solve Navier-Stokes equations away from Γ (where $\mathbf{f} = 0$):

$$\left.\begin{aligned} \rho\frac{\partial \mathbf{u}}{\partial t} + \rho\mathbf{u}\cdot\nabla\mathbf{u} &= \mu\nabla^2\mathbf{u} - \nabla p \\ \nabla\cdot\mathbf{u} &= 0 \end{aligned}\right. \qquad \text{on } \Omega \setminus \Gamma$$

- Eliminate delta functions and singular force term in favour of jumps across Γ:

$$\begin{aligned} [\![\mathbf{u}]\!] &= 0 \\ [\![p]\!] &= \frac{\mathbf{F}\cdot\mathbf{n}}{|\mathbf{X}_q|} \\ \mu\boldsymbol{\tau}\cdot\left[\!\!\left[\frac{\partial \mathbf{u}}{\partial \mathbf{n}}\right]\!\!\right] &= -\frac{\mathbf{F}\cdot\boldsymbol{\tau}}{|\mathbf{X}_q|} \end{aligned}$$

References: Peskin & Printz (1993), Lai & Li (2001)

This "jump formulation" is the basis for the Immersed Interface Method (LeVeque & Li, 1994), (Li & Ito, 2006) `MS-{We,Th}-*-26`

Dual philosophy

"Original" IB method:

- Ideally suited to biofluid problems with dynamically deforming structures.
- External boundaries are not so important – commonly assume an infinite or periodic fluid domain.
- When rigid boundaries or objects are present, treat them as "tethered" IBs with a very large elastic stiffness.

"Direct (or discrete) forcing" IB method: (Mittal & Iaccarino, 2005)

- Originally developed for IBs that are either stationary or have a prescribed motion, $\mathbf{U}_b$.
- Idea: apply a fictitious body force whose sole purpose is to bring the velocity to $\mathbf{U}_b$.
- Much more common in the engineering literature.

Our focus is on the first class of problems . . .

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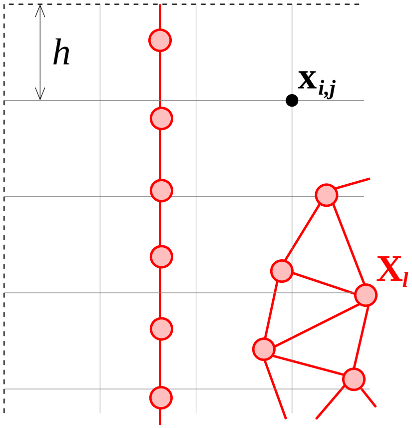
Spatial discretization

- Fluid domain Ω is divided into a rectangular grid $\mathbf{x}_{i,j} = (ih, jh)$ with cells of size $h \times h$.
- Immersed boundary Γ is discretized at Lagrangian points $\mathbf{X}_\ell(t)$ that move relative to the underlying fluid grid.



Simple case:
IB points connected
by springs

Algorithm outline

Replace delta function by a smooth regularization $\delta_h(\mathbf{x}) = d_h(x)\, d_h(y)$

$$\text{e.g.,} \quad d_h(x) = \frac{1}{4h}\left(1 + \cos\left(\frac{\pi x}{2h}\right)\right)$$

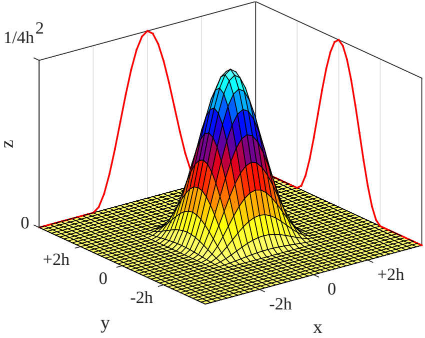
Then, within each time step:

1. Compute discrete "spring" forces, $\mathbf{F}_\ell^n$
2. Approximate force spreading integral:

$$\mathbf{f}_{i,j}^n = \sum_\ell \mathbf{F}_\ell^n\, \delta_h(\mathbf{x}_{i,j} - \mathbf{X}_\ell^n) \cdot h_b$$

3. Step velocity/pressure using your "favourite" fluid solver $\longrightarrow \mathbf{u}_{i,j}^{n+1}, p_{i,j}^{n+1}$
4. Update IB configuration:

$$\mathbf{X}_\ell^{n+1} = \mathbf{X}_\ell^n + \Delta t \sum_{i,j} \mathbf{u}_{i,j}^{n+1}\, \delta_h(\mathbf{x}_{i,j} - \mathbf{X}_\ell^n) \cdot h^2$$



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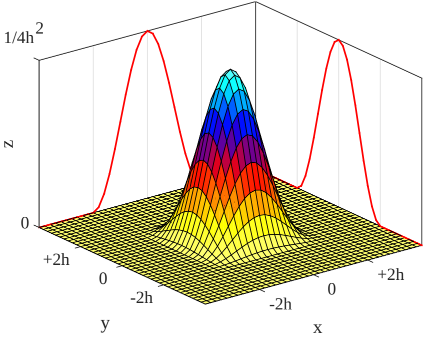

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Pros and cons

Advantages:

- Flexible: handles complex IBs with nearly arbitrary elastic forcing.
- Simple: explicit algorithm on a fixed Cartesian mesh is very easy to implement.
- Robust: relatively insensitive to changes in geometry, IB forcing, fluid properties, etc.

Disadvantages:

- Numerical stiffness: can be severe owing to large elastic forces.
- Nonlinearity and non-locality: make implementing an implicit solver extremely difficult.
- First-order: accuracy drops near the IB because interpolated fluid velocity field ($\frac{\partial \mathbf{X}}{\partial t}$) is not div-free. (Newren, 2007 thesis)

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Applications in biology and engineering

Biology:

- blood in heart and arteries: Peskin–McQueen, Griffith, Fogelson, Glowinski
- cilia and flagella: Fauci, Dillon, Kim–Lim–Peskin
- cell growth and locomotion: Bottino, Dillon, Rejniak, Strychalski–Guy, Vanderlei–Feng–Keshet
- swimming organisms: Fauci, Miller, Bhalla, Lushi–Peskin, Guy, Khatri
- vesicles and membrane transport: Huang, Kim–Lai
- viscoelastic biofluids: Chrispell, Strychalski–Guy, Devendran
- cochlear dynamics: Peskin–LeVeque–Lax, Beyer, Givelberg, Edom, Ko–JS
- biofilms: Klapper, Dillon–Fauci, Bortz et al., Sudarsan–Ghosh–JS
- aerodynamics and flying: Miller, Zhao

Engineering:

- particle suspensions: Fauci, Pan–Glowinski, Wang–Layton, Breugem, Ghosh–JS
- parachutes and flags: Kim–Peskin, Zhu
- foams: Kim–Lai–Peskin
- electrohydrodynamics: Bhalla et al.
- fishing nets: Takagi et al.

Speakers in this and related sessions:

`Invited Tu 11:10`
`MS-{We,Th}-*-26`
`MS-We-D-55`

Seminal reference

Acta Numerica (2002), pp. 479–517
DOI: 10.1017/S0962492902000077

The immersed boundary method

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New York University, 251 Mercer Street,
New York, NY10012-1185, USA
E-mail: peskin@cims.nyu.edu

Peskin has posted lecture notes and code at

http://www.math.nyu.edu/faculty/peskin/ib_lecture_notes

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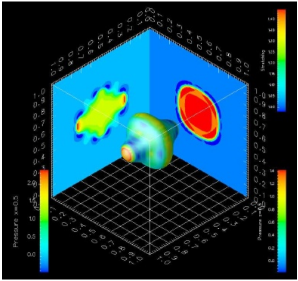
Analytical results

- Rigorous derivation of IB formulation from first principles: Peskin (2002, 2011 notes)
- Analysis of numerical stiffness, stability and time-step restrictions: Gong, Huang & Lu (2008), Hou & Shi (2008), Boffi, Gastaldi & Heltai (2007)
- Proof of pointwise and L^p convergence in $\mathbf{u}$ and p for Stokes flow with stationary IB: Mori & Liu (2008–2014) (beautiful!)
- Stability analysis for internally-forced spherical membranes: Ko & JS (2015)
- Regularized delta functions: Bringley (2008 thesis), Liu & Mori (2012), Hosseini et al. (2015), Bao et al. (2015), ...

Parametrically-forced oscillations in spherical membranes

Ko & JS, *SIAM J. Appl. Math.*, submitted, arXiv:1411.1345



- Extends earlier work on parametric resonance for internally-forced 2D membranes by Cortez et al. (2004).
- Aims also to explain instabilities in 3D computations of Maitre & Cottet (2006).
- Take linear elastic membrane with periodic forcing:

$$\mathbf{F}(\mathbf{X}, t) = \sigma(1 + 2\tau \sin(\omega t))\Delta_S \mathbf{X}$$

- Look for a Floquet series solution in vector spherical harmonics:

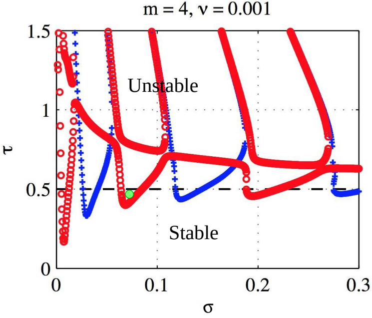
$$\mathbf{u}(r, \theta, \phi, t) = e^{\gamma t} \sum_{n=-\infty}^{\infty} e^{int} \left(u_n^r(r)\, \mathbf{Y}_{m,k} + u_n^{\Psi}(r)\, \mathbf{\Psi}_{m,k} + u_n^{\Phi}(r)\, \mathbf{\Phi}_{m,k} \right)$$

and similarly for p and $\mathbf{X}$.

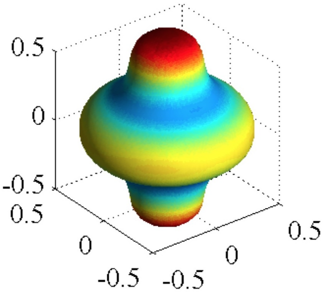
Stability results

- Finding neutrally stable solutions ($\mathrm{Re}\,\gamma = 0$) reduces to a large eigenvalue problem.
- Plotting stability regions in parameter space clearly identifies unstable modes.
- IB simulations verify that instabilities occur for the same parameters.

Stability boundaries, $\tau \leqslant \frac{1}{2}$



Unstable 4-mode



Outline

Algorithm improvements and extensions

- Adaptive mesh refinement yields practical second-order accuracy: Griffith et al. (2007)
- Various approaches to reducing volume conservation errors: Newren (2007), Griffith (2012), Li et al. (2012)
- Implicit treatment of the IB evolution equation: Mori & Peskin (2008), Newren et al. (2008), Hou & Shi (2008), Guy & Philip (2012) – multigrid
- Lattice-Boltzmann fluid solver: Crowl & Fogelson (2010), Hao & Zhu (2010)
- Finite element formulation: Boffi, Gastaldi & Heltai (2004–), Griffith & Luo (2014)
- IB benchmark problems: Roy, Heltai & Costanzo (2015)
- Other closely related methods:
  - regularized Stokeslets: Cortez, Olson, Huang
  - embedded boundary method: Stein, Guy & Thomases (2015)
  - ...

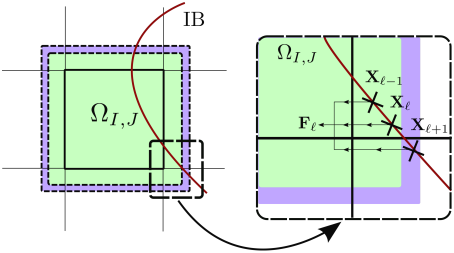
Parallel implementations

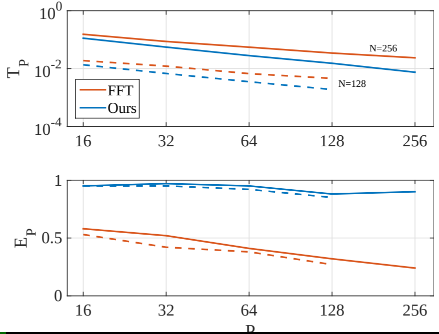
- IBAMR: Griffith et al. (2009) + very active user group
- Titanium: Givelberg & Yelick (2006)
- Direct-forcing IB method on GPUs: Layton et al. (2011)
- Pseudo-compressible fluid solver for distributed-memory clusters: Wiens & JS (2015)

An (optimally) scalable parallel IB solver

Wiens & JS, *J. Comput. Phys.*, 281:917–941, 2015

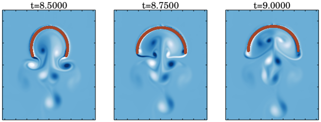
- Pseudo-compressibility method (Guermond & Minev, 2011): Navier-Stokes solve reduces to tridiagonal linear systems.
- Use parallel domain decomposition, exploit rectangular geometry, communicate IB data between subdomains via ghost cells.
- Extensively tested on a variety of "standard" 2D/3D problems.
- Numerical simulations demonstrate exceptional parallel scaling and near optimal efficiency ($E_P = \frac{T_1}{PT_P}$ on P processors)

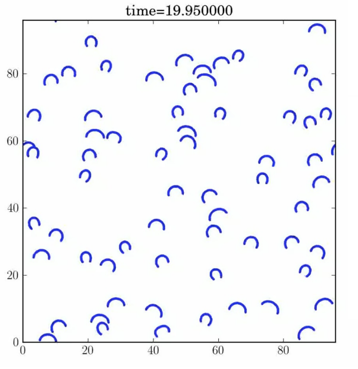




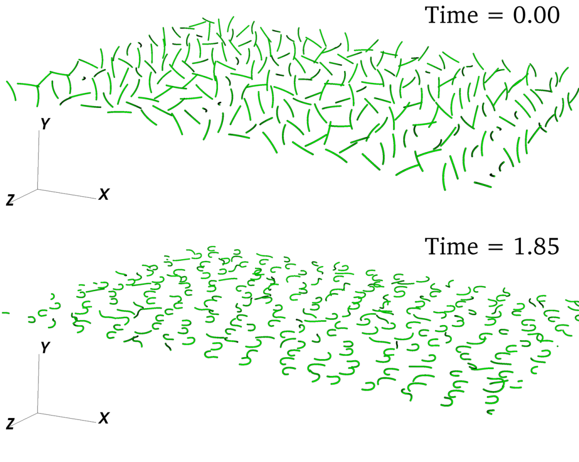
Two examples of illustrations

Jellyfish swimming (2D)





Flexible fiber suspension (3D)



Wiens & JS, *Comput. Meth. Appl. Mech. Eng.* 290:1–18, 2015

. . . it's possible to simulate suspensions of 100's to 1000's of objects!

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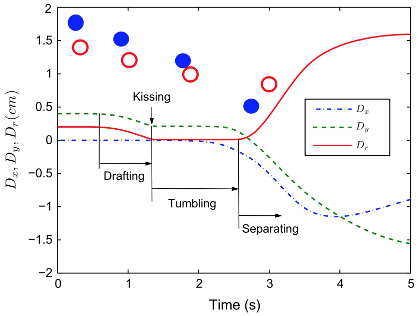
Extensions to the IB formulation

The IB formuation has been extended to handle much more than just the simple massless elastic membrane problem:

- Massive boundaries using penalty IB method (Kim & Peskin, 2007) or D'Alembert force (Mori & Peskin, 2008)
- Porous boundaries: Kim & Peskin (2006), JS (2009)
- Generalized IB method for torque in flexible rods: Lim et al. (2008)
- Membrane transport and osmosis: Atzberger & Peskin (2006), Huang et al. (2009), Gong, Gong & Huang (2014)
- Stochastic IB method: Atzberger, Kramer & Peskin (2007, 2008)
- Variable density and viscosity fluids: Fai et al. (2013, 2014)
- Arbitary linearly elastic materials: Mori & Peskin (2009)

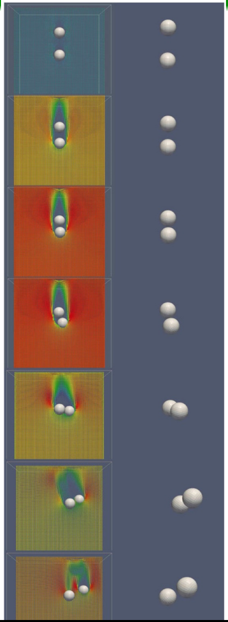
Gravitational settling in particle suspensions

- Rigid particles in suspension settle due to gravity, interacting in complex ways with each other and with surrounding walls.
- Pairs of particles undergo drafting–kissing–tumbling (DKT).
- This problem has been very well-studied in both experimentally numerically.



Wang et al. (2014) ⟵

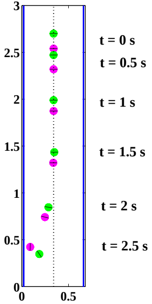
Münster et al. (2012) ⟶



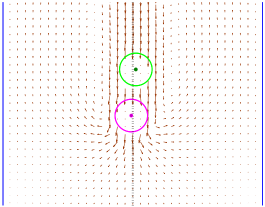
IB simulations of sedimentation

Ghosh & JS, *Commun. Comput. Phys.*, 18(2):380-416, 2015

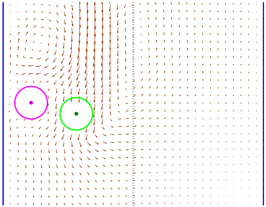
- We aim to perform IB simulations that reproduce observed DKT dynamics and wall-particle interactions.
- Added mass incorporated using a D'Alembert forcing approach.



Drafting/kissing



Tumbling

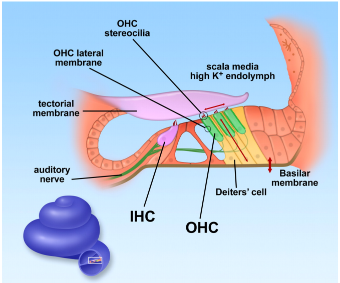


- Ongoing work: extension to irregular, deformable particles.

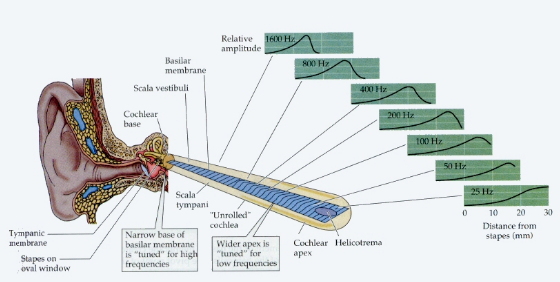
The "active" cochlea

- The cochlea or inner ear is capable of amplifying very weak signals and fine-tuning over an enormous frequency range.
- The basilar membrane (BM) is immersed in fluid and has been well-studied with IB methods. (LeVeque, Peskin & Lax, 1985, 1988)
- Outer hair cells (OHC) oscillate in response to sound, and in turn modulate the BM elastic stiffness. (Mammano & Ashmore, 1993)

BM cross-section



Cochlea unrolled

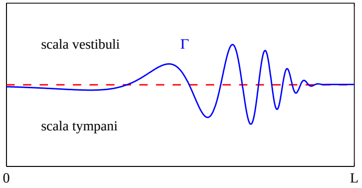


Parametric forcing: A new mechanism?

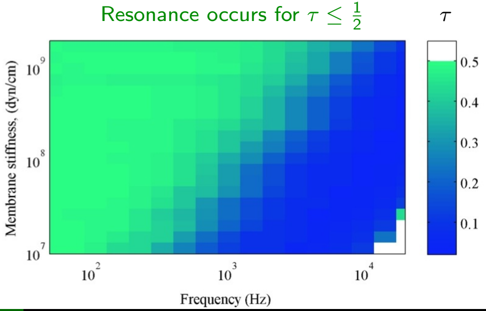
Ko & JS, *SIAM J. Appl. Math*, 75(3):1065-1089, 2015

- We hypothesize that parametric resonance, driven by OHC oscillations, may contribute to cochlear function.
- Using a simple 2D BM geometry (below) we show that:
  - a Floquet stability analysis yields resonant modes of oscillation within the parameter range relevant to human hearing.
  - numerical simulations produce travelling wave solutions that are similar to those observed in passive BM models.

2D BM model



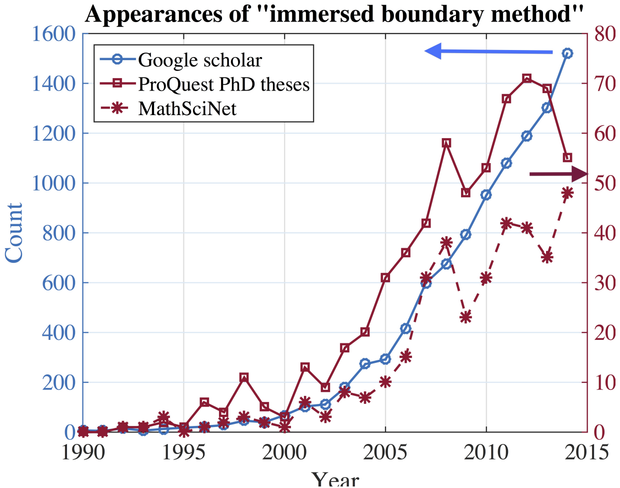
Resonance occurs for $\tau \leq \frac{1}{2}$



Outline

A flurry of recent activity

There has been a very rapid growth in recent study of IB problems:



Progress on many fronts

Most of the research challenges identified in Peskin's *Acta Numerica* paper in 2002 have been met:

- implicit and semi-implicit versions of the IB method, and associated stability analysis
- adaptive mesh refinement
- second order accuracy for "thick" elastic shells, but still not for thin membranes
- several approaches for obtaining better volume conservation
- parallel implementations
- variable viscosity and anisotropic viscoelastic materials
- convergence proof for the IB method
- turbulent flows (handled in the direct-forcing framework)

Opportunities

- Extend Mori's convergence proof to Navier–Stokes with a moving boundary.
- Fluid structure interaction coupled with other physical processes
- Multiscale numerical approaches
- Other algorithmic improvements
- Many more applications in biology, engineering, ...

Thank-you!

http://www.math.sfu.ca/~stockie

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