Lagrangian blob methods applied to biological fluid flow problems

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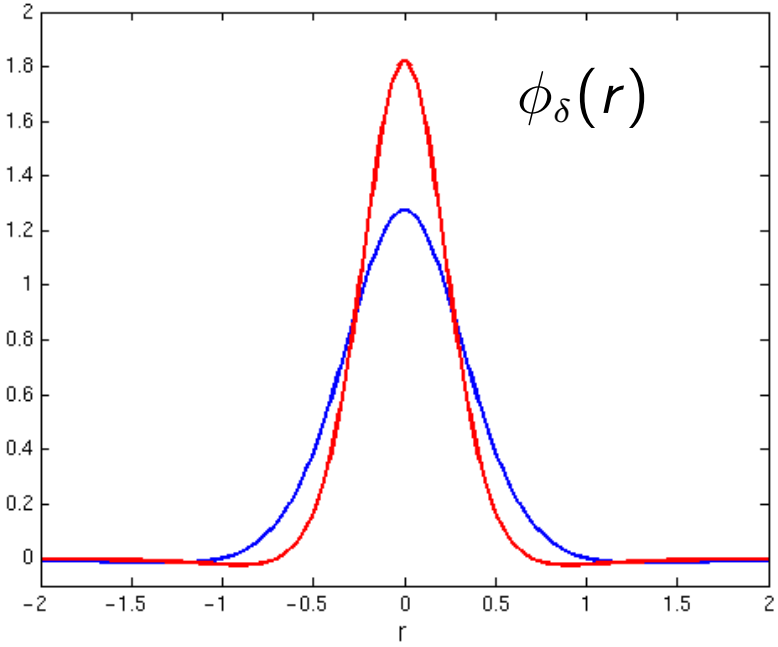
Idea of blob methods

The idea is motivated by the vortex blob method.

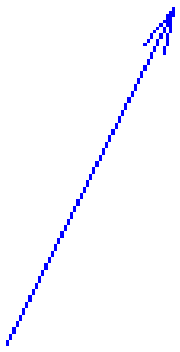
- Key: Develop a *regularized* version of the fundamental solutions by designing smooth approximations of Delta functions
- Do not simply modify final expressions

Blobs

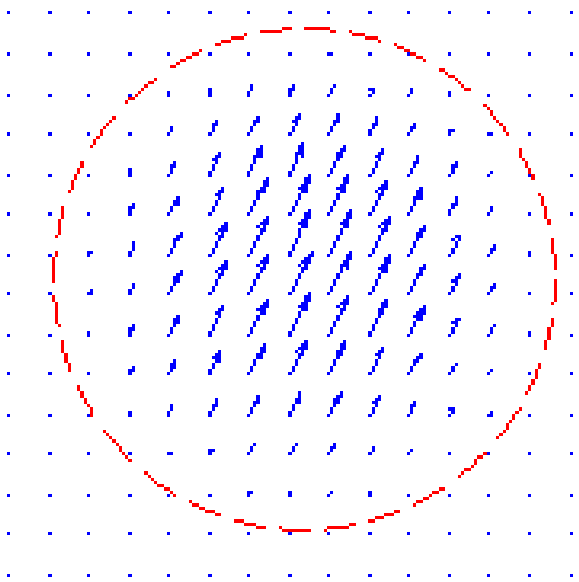


- ◇ unit mass
- ◇ radially symmetric
- ◇ concentrated near $\mathbf{x} = 0$
- ◇ decay properties
- ◇ scalable: $\phi_\delta(\mathbf{x}) = \frac{1}{\delta^n}\ \phi(\mathbf{x}/\delta)$

Singular vs. Regularized Forces



$\mathbf{f}\delta(\mathbf{x})$



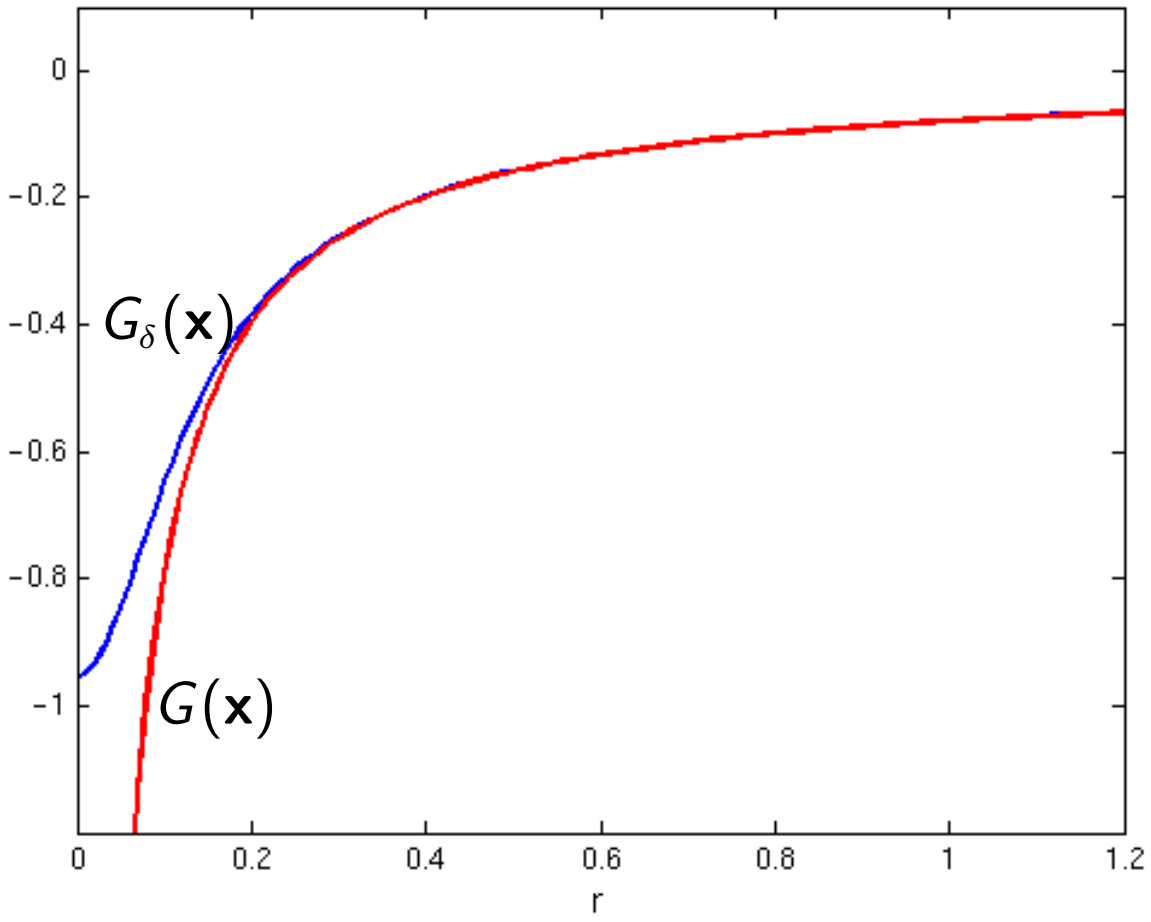
$\mathbf{f}\phi_\delta(\mathbf{x})$

Fundamental solution of Laplace's equation (3D)

Singular	Regularized
$\Delta u = a\ \delta(\mathbf{x})$	$\Delta u = a\ \phi_\delta(\mathbf{x})$
$\Rightarrow\ u(\mathbf{x}) = a\ G(\mathbf{x}) = \dfrac{-a}{4\pi r}$	$\Rightarrow\ u(\mathbf{x}) = a\ [G * \phi_\delta](\mathbf{x})$ $= a\ G_\delta(\mathbf{x}) = \dfrac{-a\ H_0(r)}{4\pi r}$

where $r = |\mathbf{x}|$.

Singular vs. Regularized Green's functions



Comments

◇ The regularized expressions are exact solutions of the given equations for regularized forces. No approximations.

◇ The spread of the force depends on the parameter δ

◇ $\lim_{\delta \to 0} \phi_\delta(\mathbf{x}) = \delta(\mathbf{x})$

◇ For $\delta \ll r$, $G_\delta(r) \approx G(r)$

◇ $\lim_{\delta \to 0} G_\delta(r) = G(r)$

Impulse blob method

Euler equations in two dimensions

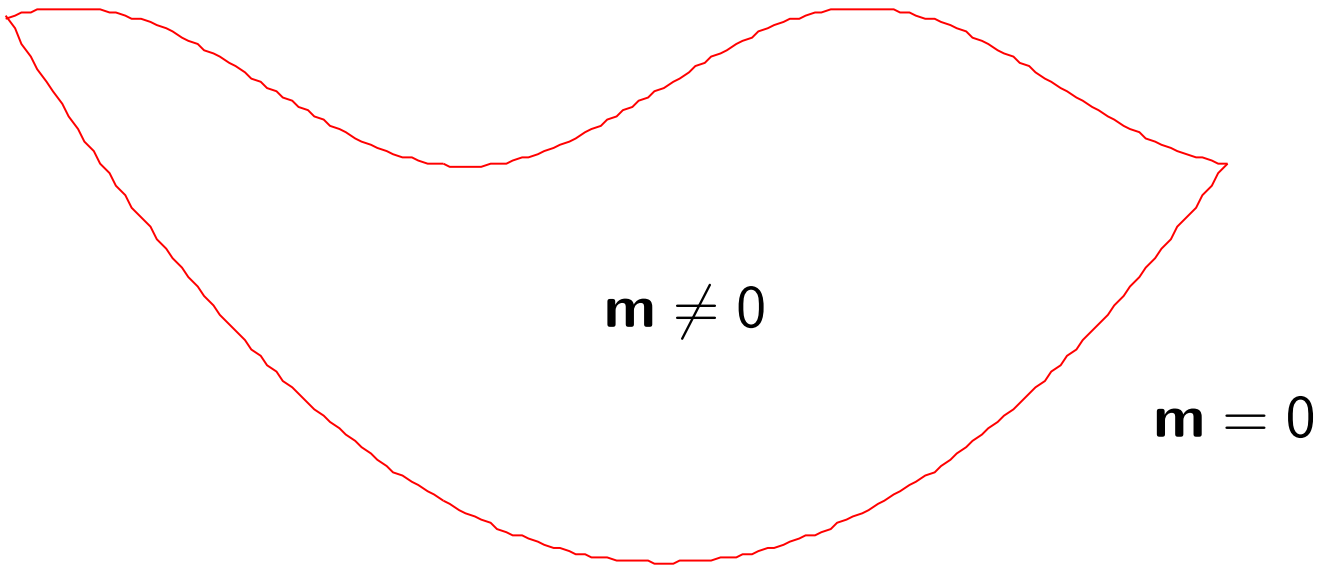
$$\mathbf{u}_t + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \mathbf{F}, \qquad \nabla \cdot \mathbf{u} = 0$$

Define a new vector field as $\mathbf{m} = \mathbf{u} + \nabla \chi$.
We can rewrite Euler's equations as

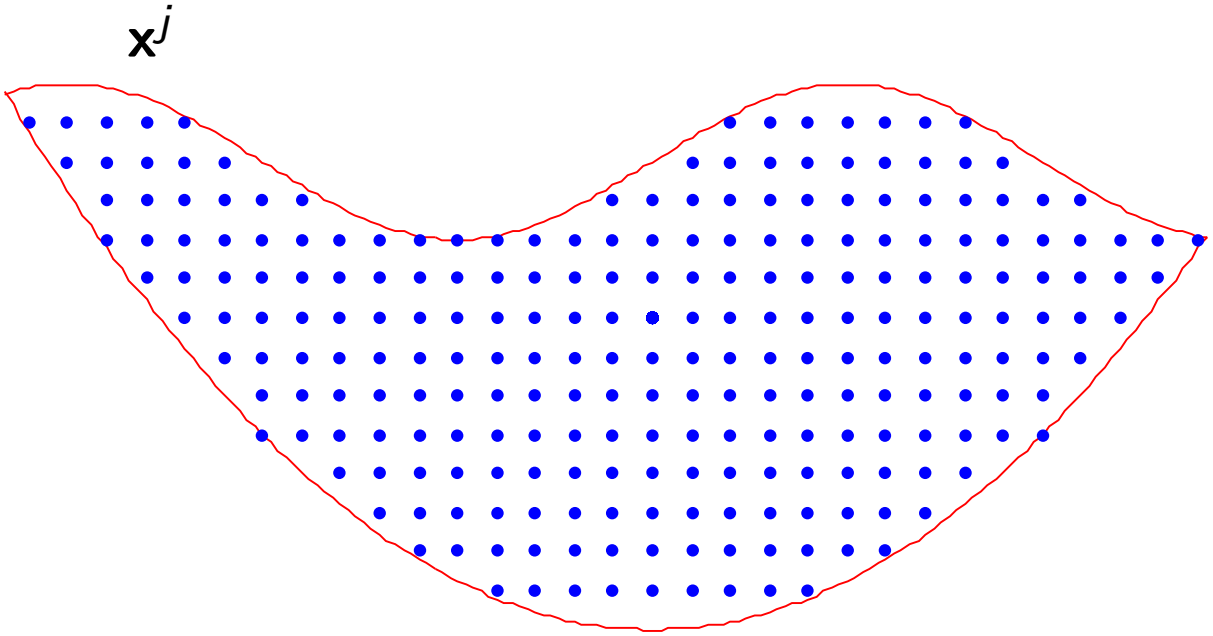
$$\mathbf{m}_t + \mathbf{u} \cdot \nabla \mathbf{m} = -\left(\nabla \mathbf{u}\right)^T \mathbf{m} + \mathbf{F}$$

where $(\nabla \mathbf{u})_{ij} = \partial u_i / \partial x_j$.

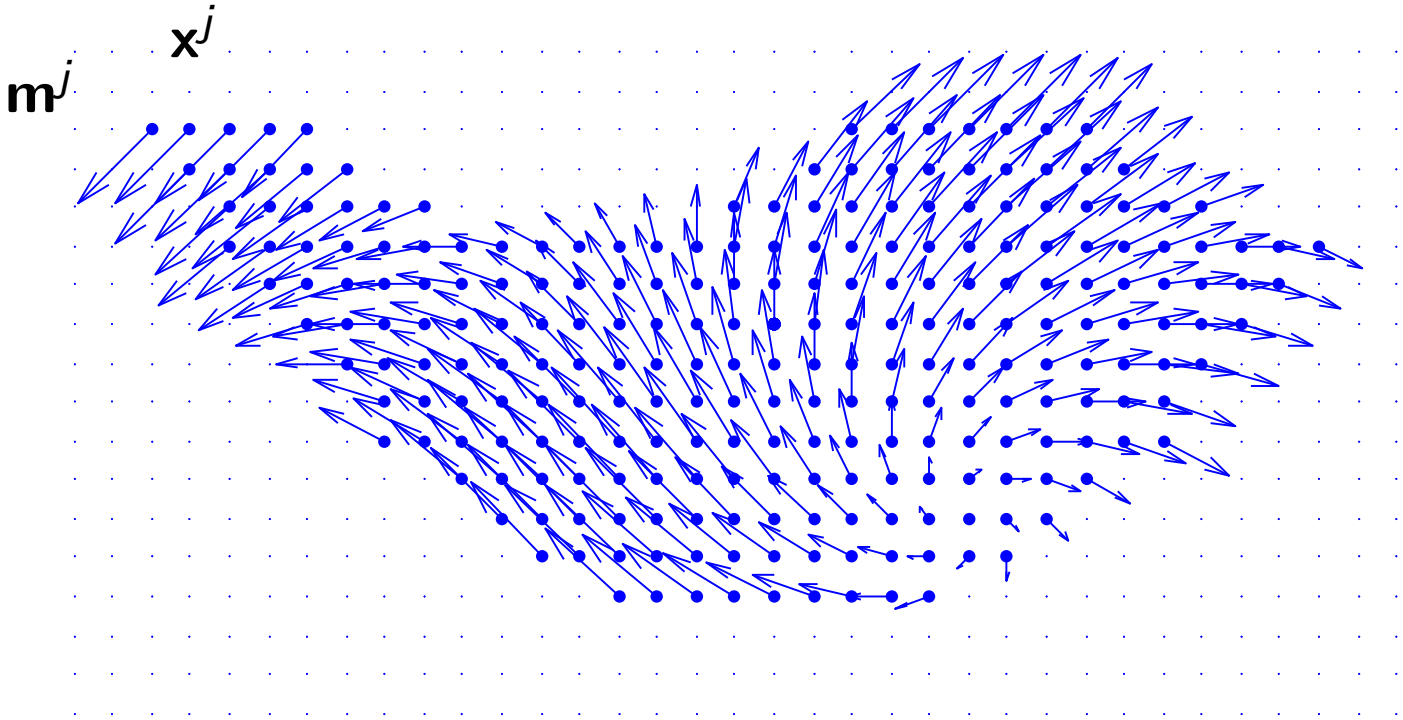
Impulse blob method: compact support



Impulse blob method: discretization



Impulse blob method: strengths



Impulse blob method

In a Lagrangian method, the particle $\mathbf{x}^j$ carries impulse $\mathbf{m}^j$. The particles move according to

$$\frac{d}{dt}\mathbf{x}^j = \mathbf{u}(\mathbf{x}^j)$$

where $\mathbf{u}$ is the incompressible component of $\mathbf{m}$, which evolves with

$$\frac{d}{dt}\mathbf{m}^j = -\left(\nabla\mathbf{u}\right)^T \mathbf{m}^j + \mathbf{F}(\mathbf{x}^j)$$

based on $\mathbf{m}_t + \mathbf{u}\cdot\nabla\mathbf{m} = -\left(\nabla\mathbf{u}\right)^T \mathbf{m} + \mathbf{F}$.

Impulse blob method

A Lagrangian blob method:

1. approximate the impulse field $\mathbf{m}$ using the discretization

$$\mathbf{m}(\mathbf{x}) = \int_{\mathbb{R}^2} \mathbf{m}(\mathbf{y})\delta(\mathbf{x}-\mathbf{y})d\mathbf{y} \approx \sum_{j=1}^{j=N} \mathbf{m}^j(t)\ \phi_\delta(\mathbf{x}-\mathbf{x}^j)A_j$$

2. find $\mathbf{u}$ from $\mathbf{m}$ via a projection $\mathbf{m} = \mathbf{u} + \nabla\chi$

$$\mathbf{u} = \left(I - \nabla\Delta^{-1}\nabla\cdot\right)\mathbf{m}$$

3. advance the particle position using $\dot{\mathbf{x}}^j = \mathbf{u}(\mathbf{x}^j)$
4. update the impuse strengths using $\dot{\mathbf{m}}^j = -\left(\nabla\mathbf{u}\right)^T\mathbf{m}^j + \mathbf{F}(\mathbf{x}^j)$

Impulse blob method

If $\mathbf{m}(\mathbf{x})$ occupies an area (in 2D), then A_j is an area element and an ℓ-th order blob $\phi_\delta(\mathbf{x})$ is chosen to satisfy the moment conditions

$$\int_{\mathbb{R}^2} \phi_\delta(\mathbf{x}) d\mathbf{x} = 1, \qquad \phi_\delta(r) = \delta^{-2}\phi_1(r/\delta)$$

$$\int_{\mathbb{R}^2} \mathbf{x}^\alpha \ \phi_\delta(\mathbf{x}) d\mathbf{x} = 0, \quad \text{for } 0 < |\alpha| < \ell - 1$$

$$\int_{\mathbb{R}^2} |\mathbf{x}|^\ell \ \phi_\delta(\mathbf{x}) d\mathbf{x} < \infty$$

An example of a 6th order blob is

$$\phi_1^{(6)}(r) = \frac{1}{2\pi}(r^4 - 6r^2 + 6)e^{-r^2}.$$

Old and New(er) blobs

For a radially symmetric blob $\phi_\delta(\mathbf{x})$ consider

$$\mathbf{m}(\mathbf{x}) = \mathbf{m}_o \phi_\delta(\mathbf{x} - \mathbf{x}_o)$$

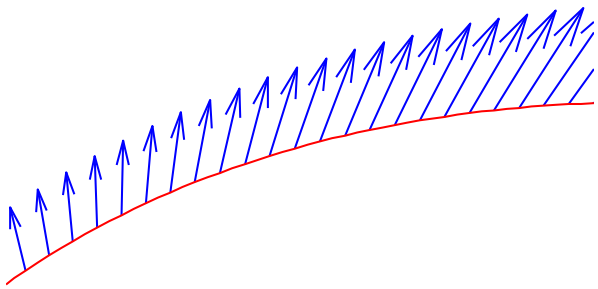
and define

$$\Delta G = \delta \quad \text{and} \quad \Delta G_\delta = \phi_\delta \qquad \Rightarrow G_\delta = G * \phi_\delta$$

in $\mathbb{R}^2$. Then $\mathbf{u} = \left(I - \nabla \Delta^{-1} \nabla \cdot\right) \mathbf{m}$ is

$$\frac{d\mathbf{x}}{dt} = \mathbf{u}_\delta(\mathbf{x}) = \mathbf{m}_o \phi_\delta(\mathbf{x} - \mathbf{x}_o) - (\mathbf{m}_o \cdot \nabla) \nabla G_\delta(\mathbf{x} - \mathbf{x}_o).$$

Old and New(er) blobs



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If $\mathbf{m}(\mathbf{x})$ is supported on a curve Γ in 2D or a surface in 3D, then

$$\mathbf{m}(\mathbf{x}) = \int_\Gamma \mathbf{m}(\mathbf{y})\delta(\mathbf{x}-\mathbf{y})dS(\mathbf{y}) \approx \sum_{j=1}^{j=N} \mathbf{m}^j(t)\ \phi_\delta(\mathbf{x}-\mathbf{x}^j)S_j$$

is not a convolution and moment conditions do not help.

Beale's result

In the context of single-layer potentials, Beale showed that in 3D for a homogeneous polynomial $p_n(\mathbf{x})$,

$$\iint_\Gamma [G_\delta(\mathbf{x}) - G(\mathbf{x})]\ p_n(\mathbf{x})\ d\mathbf{x} = C_n\ \delta^{n+1} \int_0^\infty [F(r) - 1]\ r^n\ dr$$

where Γ is a plane and $F(r) = 2\pi \int_0^r \phi_1(s)\ s\ ds$. The leading error term ($n = 0$) can be eliminated with the shape factor condition

$$\int_0^\infty [F(r) - 1] dr = 0$$

yielding to a regularization error of $O(\delta^3)$.

Extending Beale's result

This velocity $\mathbf{u}_\delta(\mathbf{x}) = \mathbf{m}_o \phi_\delta(\mathbf{x} - \mathbf{x}_o) - (\mathbf{m}_o \cdot \nabla)\nabla G_\delta(\mathbf{x} - \mathbf{x}_o)$ can also be written as

$$\mathbf{u}_\delta(\mathbf{x}) = \mathbf{m}_o \left(\frac{-1}{2\pi r^2}\right) s_1(r/\delta) + \frac{(\mathbf{m}_o \cdot \hat{\mathbf{x}})\hat{\mathbf{x}}}{r^2} \left(\frac{2}{2\pi r^2}\right) s_2(r/\delta)$$

where $\hat{\mathbf{x}} = \mathbf{x} - \mathbf{x}_o$ and $r = |\hat{\mathbf{x}}|$. The smoothing functions s_1 and s_2 are given by

$$s_1(r) = F(r) - rF'(r) \quad \text{and} \quad s_2(r) = F(r) - \frac{1}{2} rF'(r).$$

where F is the shape factor associated with the blob ϕ_δ:

$$F(r/\delta) = 2\pi \int_0^r \phi_\delta(s)\ s\ ds$$

Extending Beale's result

One can show that the condition

$$\int_0^\infty [F(r) - 1]\, dr = 0$$

implies that

$$\int_0^\infty [s_1(r) - 1]\, dr = \int_0^\infty [s_2(r) - 1]\, dr = 0$$

so that

$$\mathbf{u}_\delta(\mathbf{x}) = \mathbf{m}_o \left(\frac{-1}{2\pi r^2}\right) s_1(r/\delta) + \frac{(\mathbf{m}_o \cdot \hat{\mathbf{x}})\hat{\mathbf{x}}}{r^2} \left(\frac{2}{2\pi r^2}\right) s_2(r/\delta)$$

may exhibit 3-rd order convergence.

$$\text{Example: } \phi_1(r) = \frac{1}{\pi}(3 - 2r^2)e^{-r^2}$$

Example

Initial curve (in 2D) is a perturbed circle

$$r(\theta) = \sqrt{1 - \epsilon^2/2} + \epsilon \ \cos(2\theta)$$

Initial impulse: $\mathbf{m}(\theta) = \mathbf{0}$. The force at $\mathbf{x}(\theta, t)$ is given by the curve total arc length at t times the curvature at $\mathbf{x}(\theta, t)$. Asymptotically, the solution is

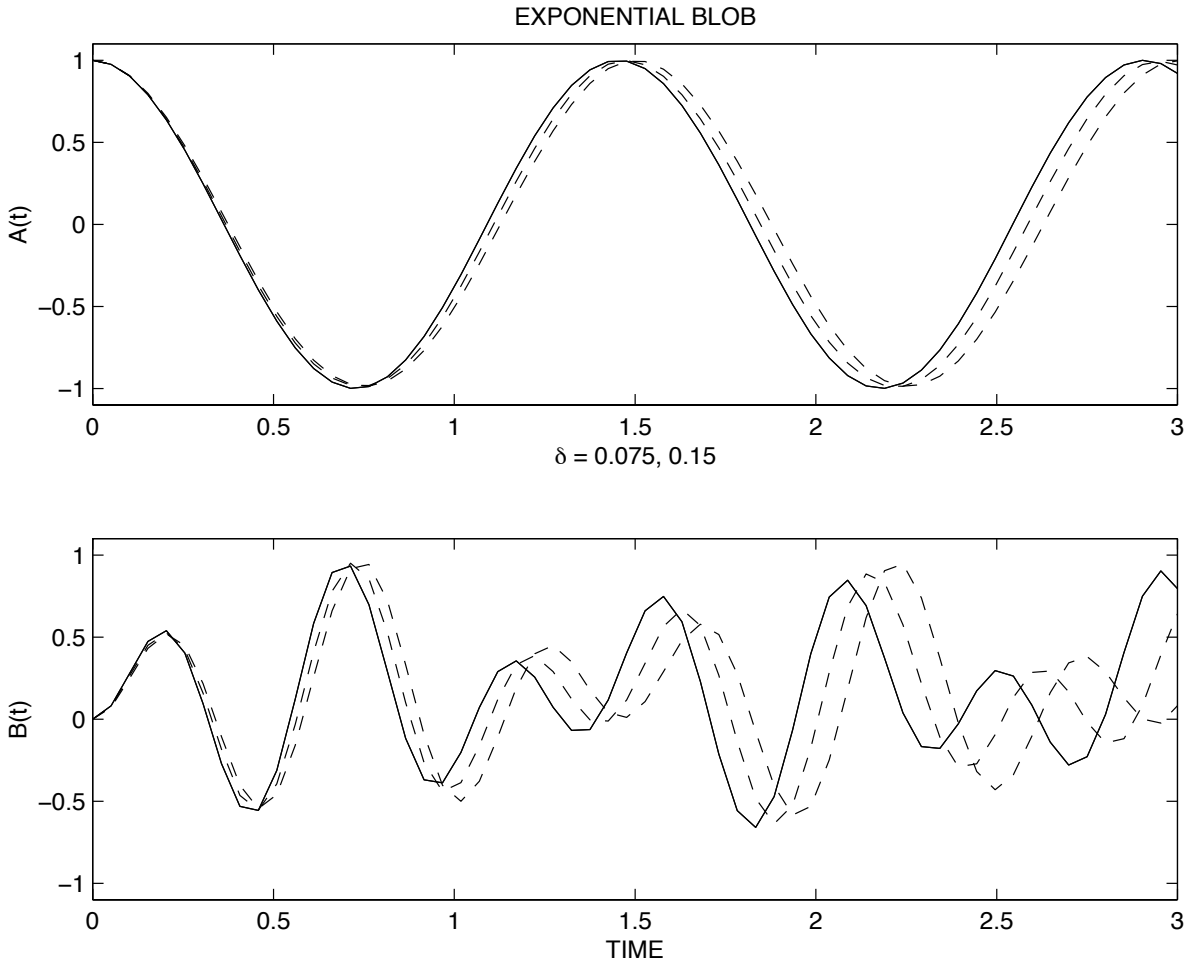
$$r(\theta, t) = \left[1 - \frac{\epsilon^2}{4} A^2(t)\right] + \epsilon A(t) \cos(2\theta) + \epsilon^2 B(t) \cos(4\theta) + O(\epsilon^4)$$

where

$$\begin{aligned} A(t) &= \cos\left(\sqrt{6\pi}\left(1 - \frac{223}{480}\epsilon^2\right) t\right) \\ B(t) &= \frac{3}{20} + \frac{1}{3}\cos(2\sqrt{6\pi}\ t) - \frac{29}{60}\cos(\sqrt{60\pi}\ t). \end{aligned}$$

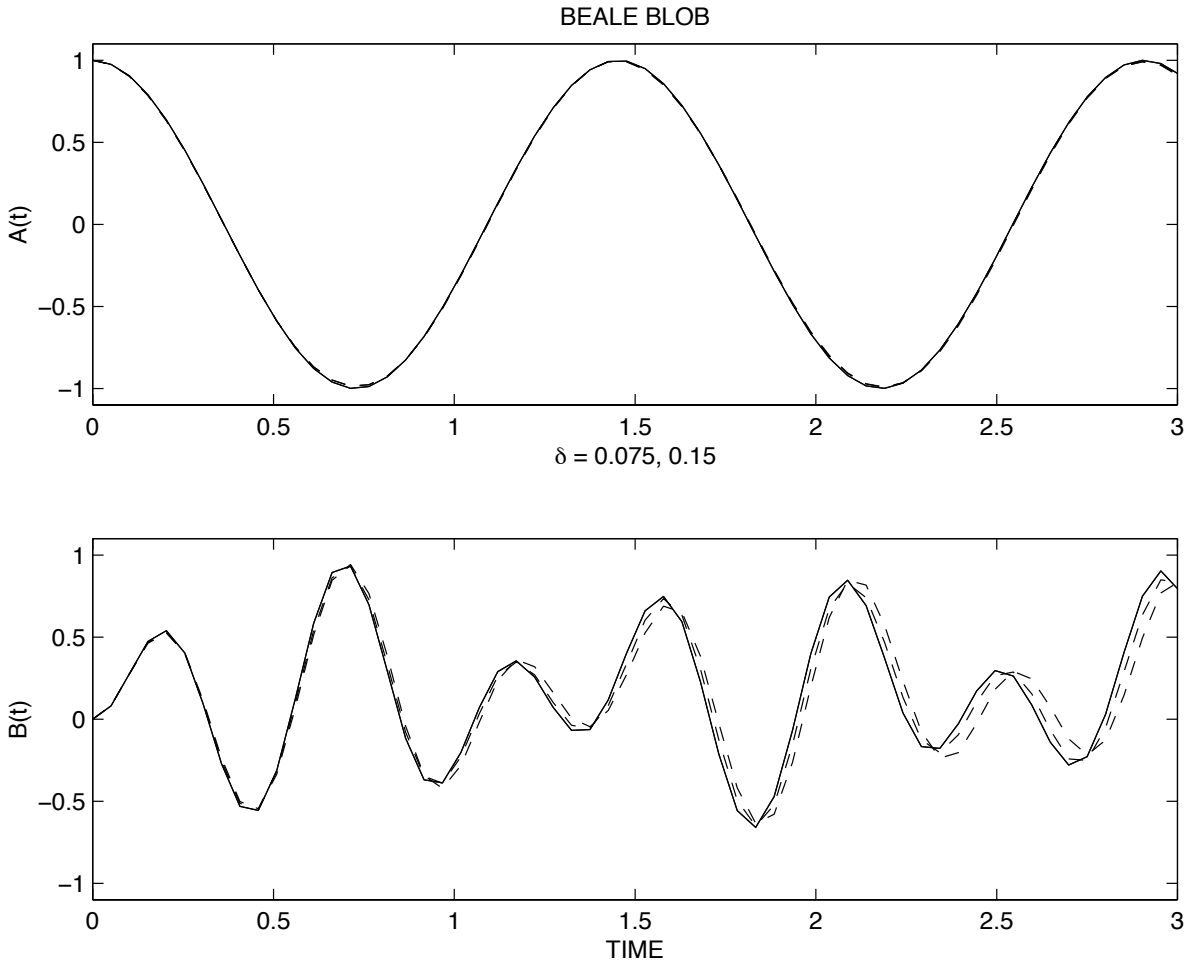
Results from exponential blob

Parameter: $\delta = 0.075$ and $\delta = 0.15$



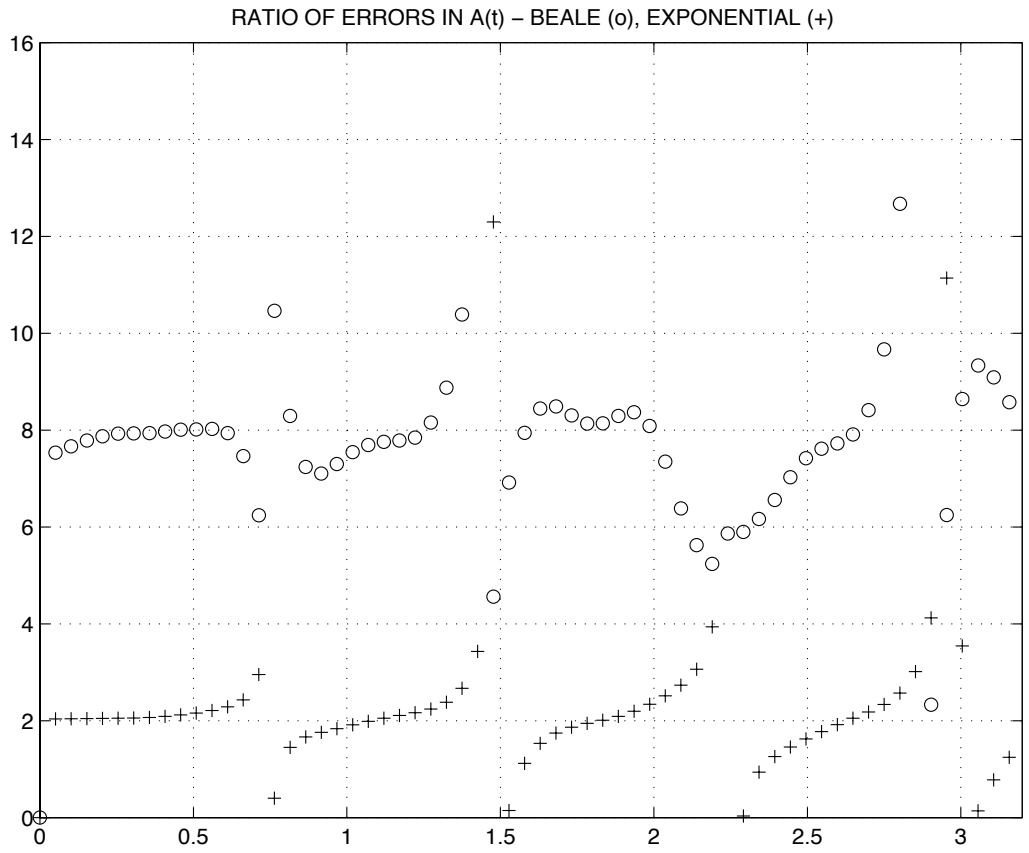
Results from Beale blob

Parameter: $\delta = 0.075$ and $\delta = 0.15$



Error comparison

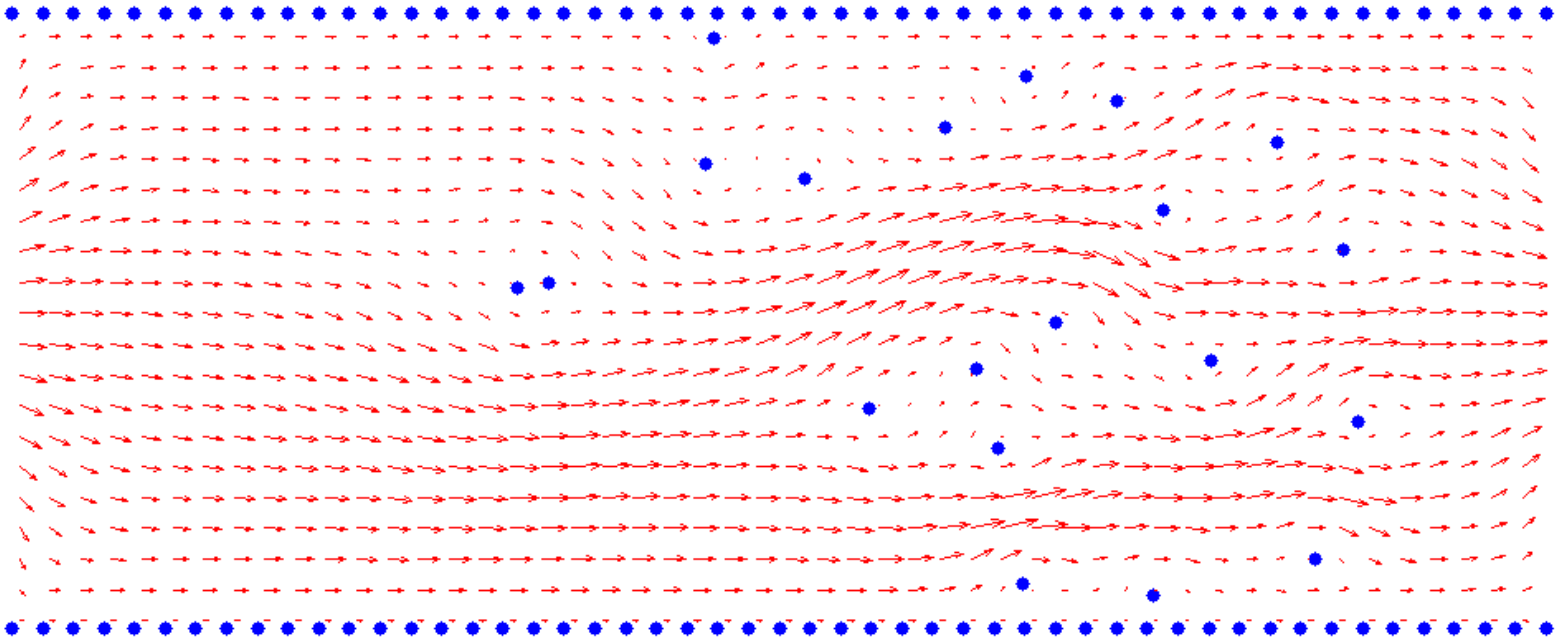
Ratio of errors in $A(t)$ between consecutive numerical solutions using $\delta = 0.075$, 0.15 and 0.3.



Change gears

New example

Example 1: Stokes flow past point obstacles in 2D



Example 2: Stokes flow around a cilium in 3D

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Fundamental solution of Stokes equations

$$\nabla p = \mu \Delta \mathbf{u} + \mathbf{f}\ \delta(\mathbf{x}), \qquad \nabla \cdot \mathbf{u} = 0$$

Suppose that $\mathbf{f}$ is constant and $r = |\mathbf{x}|$. Then formally,

$$\Delta p = \nabla \cdot [\mathbf{f}\ \delta(\mathbf{x})]$$

$$\Rightarrow\ p(\mathbf{x}) = \mathbf{f} \cdot \nabla G(\mathbf{x}) = \frac{\mathbf{f} \cdot \mathbf{x}}{4\pi r^3}$$

And finally,

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

Regularized solution of Stokes equations: *Stokeslet*

$$\nabla p = \mu \Delta \mathbf{u} + \mathbf{f}\ \phi_\delta(\mathbf{x}), \qquad \nabla \cdot \mathbf{u} = 0$$

Then, define G_δ by $\Delta G_\delta(\mathbf{x}) = \phi_\delta(\mathbf{x})$.

$$\Delta p = \nabla \cdot [\mathbf{f}\ \phi_\delta(\mathbf{x})] \qquad \Rightarrow \qquad p(\mathbf{x}) = \mathbf{f} \cdot \nabla G_\delta(\mathbf{x})$$

Now the velocity satisfies $\mu \Delta \mathbf{u} = (\mathbf{f} \cdot \nabla) \nabla G_\delta - \mathbf{f}\ \phi_\delta$ so that

$$\mu \mathbf{u}(\mathbf{x}) = -\mathbf{f}\ G_\delta(\mathbf{x}) + (\mathbf{f} \cdot \nabla) \nabla B_\delta(\mathbf{x})$$

where $\Delta B_\delta(\mathbf{x}) = G_\delta(\mathbf{x})$.

Summary of Stokes Flow due to a force at the origin

Singular Stokeslet:

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

Regularized Stokeslet [R. C., 2001]:

$$8\pi\mu\mathbf{u}(\mathbf{x}) = \frac{\mathbf{f}}{r}H_1(r) + \frac{(\mathbf{f}\cdot\mathbf{x})\mathbf{x}}{r^3}H_2(r)$$

where $H_1(r) = B_\delta{}'(r) - rG_\delta(r)$ and $H_2(r) = rB_\delta{}''(r) - B_\delta{}'(r)$.

◇ Note: $\lim_{\delta\to 0} H_1(r) = \lim_{\delta\to 0} H_2(r) = 1$

General formulation of regularized Stokeslets

[R. C., L. Fauci & A. Medovikov, 2005]

One can derive the expression

$$\int_{\mathbb{R}^3} \mathbf{u}(\mathbf{y})\phi_\delta(\mathbf{y}-\mathbf{x})d\mathbf{y} = \frac{1}{8\pi\mu}\int_{\partial D} S_\delta(\mathbf{y}-\mathbf{x})\mathbf{f}(\mathbf{y})\ ds(\mathbf{y})$$

leads to the *Method of Regularized Stokeslets:*

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

where

$$S_\delta(\mathbf{x})\mathbf{f} = \frac{\mathbf{f}}{r}H_1(r) + \frac{(\mathbf{f}\cdot\mathbf{x})\mathbf{x}}{r^3}H_2(r), \qquad r = |\mathbf{x}|$$

Biological applications

- microorganism swimming, sperm motility
- collective motion of bacteria and algae
- flow in arteries or channels
- dynamics of cells

Goal: compute simultaneously the motion of the fluid and the elastic structure

Questions: why are organisms designed as they are? How do cilia orchestrate collective motion? What are the consequences of defects in organism design?

Motion of headless helical organism

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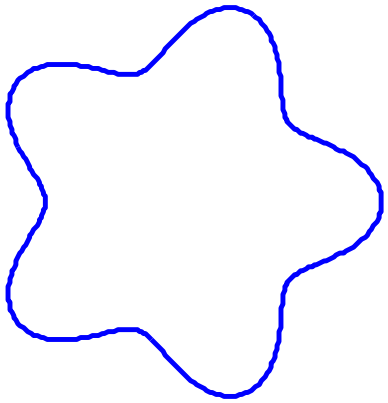
Improvement for closed boundaries

Velocity computation *on the boundary* or *far from the boundary* is not problematic. Very near the boundary, it is challenging (nearly-singular integrals) with fixed discretizations.

Consider a closed boundary parametrized by $\mathbf{x}(s)$ for $0 \leq s \leq L$.
Strategy: write the Stokeslet formula in terms of



$$I_1(\mathbf{x}, f) = \int_0^L f(s)\, \mathbf{x}'(s) \times \nabla G(\mathbf{x} - \mathbf{x}(s)) ds$$

$$I_2(\mathbf{x}, g) = \int_0^L g(s)\, \mathbf{x}'(s) \cdot \nabla G(\mathbf{x} - \mathbf{x}(s)) ds$$

Single and double layer potentials

Beale and Lai developed correction terms for the trapezoid rule on the regularized Green's functions that guarantee second-order accuracy. Use the identities

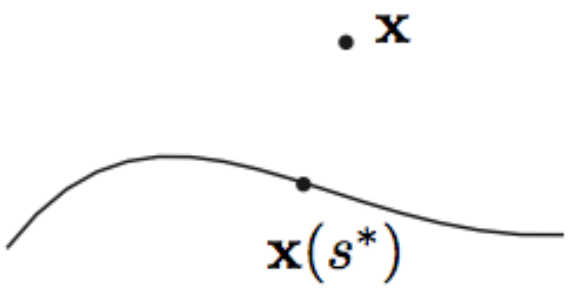
$$I_1(\mathbf{x},1) = \int_0^L \mathbf{x}'(s) \times \nabla G(\mathbf{x} - \mathbf{x}(s))ds = \begin{cases} 1, & \text{for } \mathbf{x} \text{ inside} \\ 0, & \text{for } \mathbf{x} \text{ outside} \end{cases}$$

$$I_2(\mathbf{x},1) = \int_0^L \mathbf{x}'(s) \cdot \nabla G(\mathbf{x} - \mathbf{x}(s))ds = 0$$

Single and double layer potentials

For example

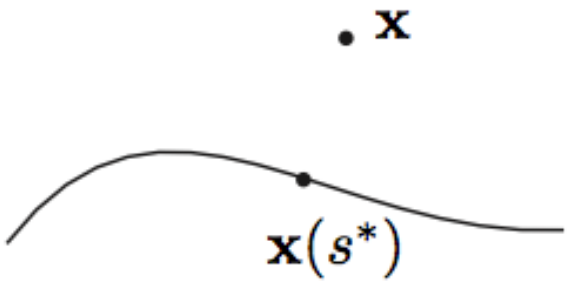
$$
\begin{aligned}
I_1(\mathbf{x}, f) &= \int_0^L f(s)\, \mathbf{x}'(s) \times \nabla G(\mathbf{x} - \mathbf{x}(s)) ds \\
&= f(s^*)\, \chi(\mathbf{x}) + \int_0^L [f(s) - f(s^*)]\, \mathbf{x}'(s) \times \nabla G(\mathbf{x} - \mathbf{x}(s)) ds
\end{aligned}
$$



Single and double layer potentials

For example

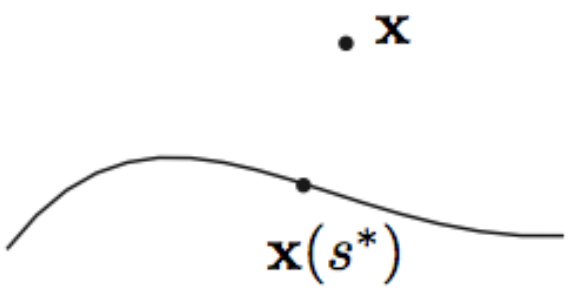
$$
\begin{aligned}
I_1(\mathbf{x}, f) &= \int_0^L f(s)\, \mathbf{x}'(s) \times \nabla G(\mathbf{x} - \mathbf{x}(s)) ds \\
&= f(s^*)\, \chi(\mathbf{x}) + \int_0^L [f(s) - f(s^*)]\, \mathbf{x}'(s) \times \nabla G(\mathbf{x} - \mathbf{x}(s)) ds \\
S_1(\mathbf{x}, f) &= f(s^*)\, \chi(\mathbf{x}) + \sum_k [f_k - f(s^*)]\, \mathbf{x}'(s_k) \times \nabla G_\delta(\mathbf{x} - \mathbf{x}_k)) \Delta s
\end{aligned}
$$



Single and double layer potentials

For example

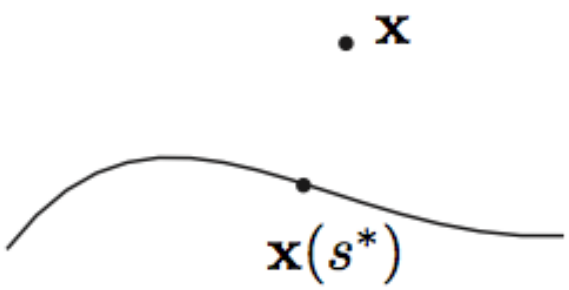
$$
\begin{aligned}
I_1(\mathbf{x}, f) &= \int_0^L f(s)\, \mathbf{x}'(s) \times \nabla G(\mathbf{x} - \mathbf{x}(s)) ds \\
&= f(s^*)\, \chi(\mathbf{x}) + \int_0^L [f(s) - f(s^*)]\, \mathbf{x}'(s) \times \nabla G(\mathbf{x} - \mathbf{x}(s)) ds \\
S_1(\mathbf{x}, f) &= f(s^*)\, \chi(\mathbf{x}) + \sum_k [f_k - f(s^*)]\, \mathbf{x}'(s_k) \times \nabla G_\delta(\mathbf{x} - \mathbf{x}_k)) \Delta s \\
I_1(\mathbf{x}, f) &= S_1(\mathbf{x}, f) + T_1^{(n)}(\mathbf{x}) + T_2^{(n)}(\mathbf{x}) + O(\Delta s^2) + O(\delta^3)
\end{aligned}
$$



Single and double layer potentials

Similarly

$$
\begin{aligned}
I_2(\mathbf{x}, g) &= \int_0^L g(s)\, \mathbf{x}'(s) \cdot \nabla G(\mathbf{x} - \mathbf{x}(s)) ds \\
&= \int_0^L [g(s) - g(s^*)]\, \mathbf{x}'(s) \times \nabla G(\mathbf{x} - \mathbf{x}(s)) ds \\
S_2(\mathbf{x}, g) &= \sum_k [g_k - g(s^*)]\, \mathbf{x}'(s_k) \cdot \nabla G_\delta(\mathbf{x} - \mathbf{x}_k)) \Delta s \\
I_2(\mathbf{x}, g) &= S_2(\mathbf{x}, g) + T_1^{(t)}(\mathbf{x}) + T_2^{(t)}(\mathbf{x}) + O(\Delta s^2) + O(\delta^3)
\end{aligned}
$$



Comments

- $T_1^{(n)}$ and $T_1^{(t)}$ are corrections due to the regularization of G with a Gaussian blob
- $T_2^{(n)}$ and $T_2^{(t)}$ are corrections to the quadrature
- In 2D

$$4\pi\mu\mathbf{u}(\mathbf{x}) = \int_\Gamma \mathbf{f}(s)\log|\mathbf{x}-\mathbf{x}(s)| + \frac{[\mathbf{f}\cdot(\mathbf{x}-\mathbf{x}(s))](\mathbf{x}-\mathbf{x}(s))}{|\mathbf{x}-\mathbf{x}(s)|^2}ds$$

must be written in terms of single and double-layer potentials.

Formulation

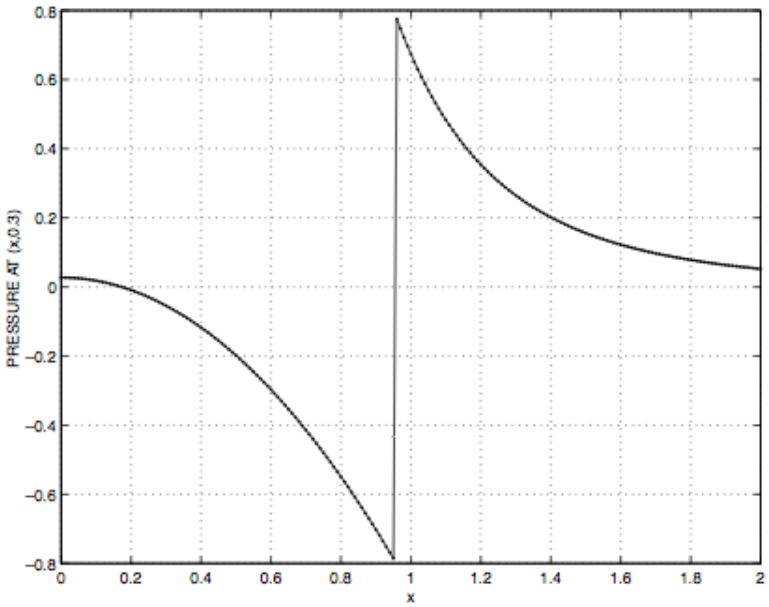
$$
\begin{aligned}
p(\mathbf{x}) &= \int_\Gamma \mathbf{f}(s)\cdot\nabla G(\mathbf{x}-\mathbf{x}(s))ds = I_2(\mathbf{x},\mathbf{f}) \\
4\pi\mu\mathbf{u}(\mathbf{x}) &= \int_\Gamma \mathbf{f}(s)\log|\mathbf{x}-\mathbf{x}(s)| + \frac{[\mathbf{f}\cdot(\mathbf{x}-\mathbf{x}(s))](\mathbf{x}-\mathbf{x}(s))}{|\mathbf{x}-\mathbf{x}(s)|^2}ds \\
&= I_2(\mathbf{x},\mathbf{F}) + I_1(\mathbf{x},\mathbf{Q^n}) + I_2(\mathbf{x},\mathbf{Q^t})
\end{aligned}
$$

where

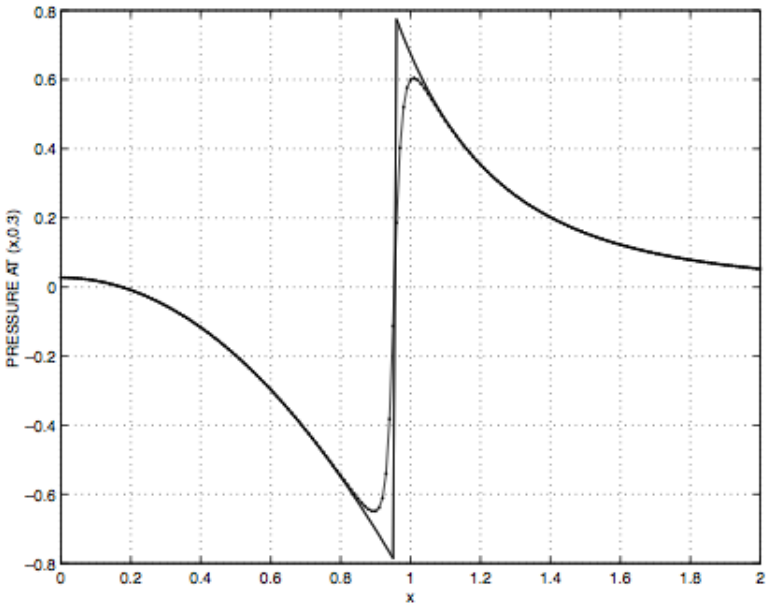
$$
\begin{aligned}
\mathbf{F}(s) &= -2\pi\int_0^s \mathbf{f}(\alpha)d\alpha, \\
\mathbf{Q^n}(s) &= -2\pi(\mathbf{x}-\mathbf{x}(s))\ \mathbf{f}(s)\cdot\hat{n}(s), \\
\mathbf{Q^t}(s) &= -2\pi(\mathbf{x}-\mathbf{x}(s))\ \mathbf{f}(s)\cdot\mathbf{x}'(s)
\end{aligned}
$$

Example: Circle with $\mathbf{f}(\theta) = 2\sin(3\theta)\mathbf{x}(\theta)$

Pressure



(a)



(b)

Corrected

Uncorrected/Exact

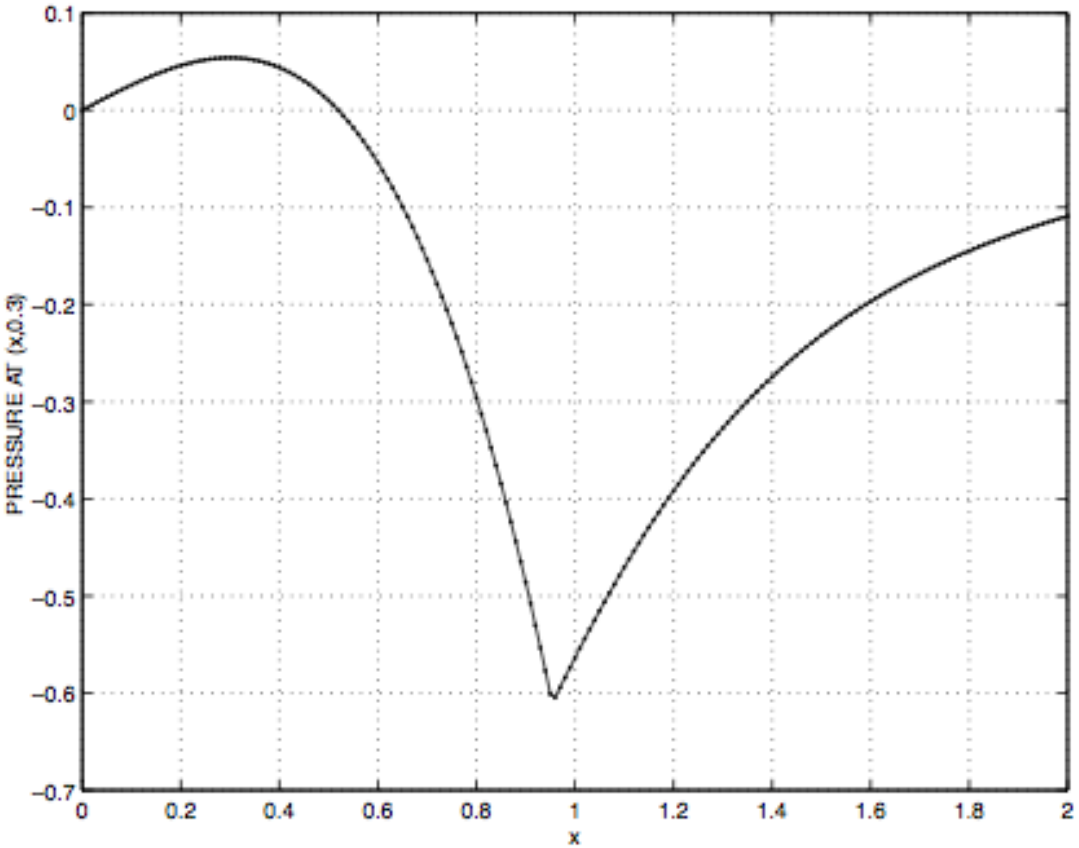
Example: Circle with $\mathbf{f}(\theta) = 2\sin(3\theta)\mathbf{x}(\theta)$

Errors as a function of discretization

N	Error in p	Error in u	Error in v
100	25.35×10^{-4}	4.603×10^{-4}	4.656×10^{-4}
200	6.023×10^{-4}	0.781×10^{-4}	1.052×10^{-4}
400	1.468×10^{-4}	0.200×10^{-4}	0.248×10^{-4}

Example: Circle with $\mathbf{f}(\theta) = 2\sin(3\theta)\mathbf{x}'(\theta)$

Pressure



Example: Circle with $\mathbf{f}(\theta) = 2\sin(3\theta)\mathbf{x}'(\theta)$

Velocities

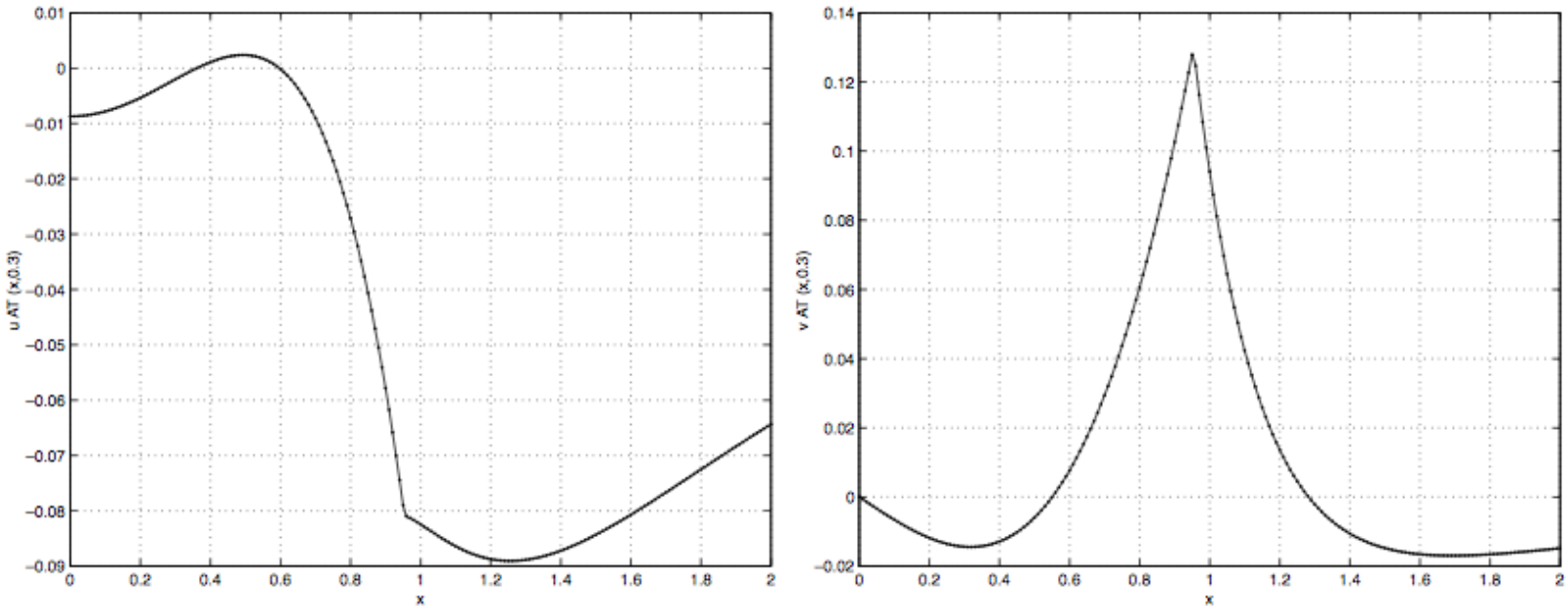


FIG. 13. *Computed velocity components u (left) and v (right) along the line $(x, 3/10)$ for $N = 100$ (dots). Also plotted is the exact solution (solid).*

Final Remarks

- The method of Regularized Stokeslet provides smoothing for force distributions at points or filaments. The integrability of Stokeslets over surfaces allows modifications (jump conditions) for increased accuracy. Thanks Tom.
- The regularization approach can be applied to single- and double-layer potentials. This allows derivatives of the potentials to be computed similarly [S. Tlupova's]. Thanks Tom.
- Current applications for Stokes flows: cilia, spirochetes, other organisms, individual and collective motion; extensions to Darcy's law and Brinkman flows.

Final Remarks

- Does the methodology extend to other fluids (viscoelastic, complex)?
- Regularized slender body theory
- Properties of the matrix relating the velocity to the force is geometry-dependent. Sometimes there is a non-trivial null space. Invertibility questions remain.
- Modifications for bounded flows

Thank you

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