Lagrangian blob methods applied to biological fluid flow problems

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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
Lagrangian blob methods applied to biological fluid flow problems

Blob methods in general

**Blobs**

- unit mass
- radially symmetric
- concentrated near \( x = 0 \)
- decay properties
- scalable: \( \phi_\delta(x) = \frac{1}{\delta^n} \phi(x/\delta) \)
Lagrangian blob methods applied to biological fluid flow problems
Blob methods in general

Singular vs. Regularized Forces

\[ f_\delta(x) \]

\[ f_{\phi_\delta}(x) \]
Fundamental solution of Laplace’s equation (3D)

<table>
<thead>
<tr>
<th>Singular</th>
<th>Regularized</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta u = a \delta(x)$</td>
<td>$\Delta u = a \phi_\delta(x)$</td>
</tr>
<tr>
<td>$\Rightarrow u(x) = a G(x) = \frac{-a}{4\pi r}$</td>
<td>$\Rightarrow u(x) = a \ <a href="x">G * \phi_\delta</a>$</td>
</tr>
<tr>
<td></td>
<td>$= a \ G_\delta(x) = \frac{-a H_0(r)}{4\pi r}$</td>
</tr>
</tbody>
</table>

where $r = |x|$. 
Lagrangian blob methods applied to biological fluid flow problems
Blob methods in general

Singular vs. Regularized Green’s functions

\[ G_\delta(x) \]
\[ G(x) \]
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 $\delta$

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

- 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

\[ u_t + u \cdot \nabla u = -\nabla p + F, \quad \nabla \cdot u = 0 \]

Define a new vector field as \( m = u + \nabla \chi \). We can rewrite Euler’s equations as

\[ m_t + u \cdot \nabla m = - (\nabla u)^T m + F \]

where \( (\nabla u)_{ij} = \partial u_i / \partial x_j \).
Example 1: Impulse blob method

Impulse blob method: compact support

\[ m \neq 0 \]

\[ m = 0 \]
Lagrangian blob methods applied to biological fluid flow problems

Example 1: Impulse blob method

Background

Impulse blob method: discretization
Impulse blob method: strengths
In a Lagrangian method, the particle $x^j$ carries impulse $m^j$. The particles move according to

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

where $u$ is the incompressible component of $m$, which evolves with

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

based on $m_t + u \cdot \nabla m = - (\nabla u)^T m + F$. 

Impulse blob method
Impulse blob method

A Lagrangian blob method:

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

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

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

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

3. advance the particle position using $\dot{x}^j = \mathbf{u}(x^j)$

4. update the impulse strengths using $\dot{m}^j = -(\nabla \mathbf{u})^T m^j + \mathbf{F}(x^j)$
Impulse blob method

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

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

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

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

An example of a 6th order blob is

$$
\phi^{(6)}_1(r) = \frac{1}{2\pi} (r^4 - 6r^2 + 6) e^{-r^2}.
$$
Old and New(er) blobs

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

$$m(x) = m_o \phi_\delta(x - x_o)$$

and define

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

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

$$\frac{dx}{dt} = u_\delta(x) = m_o \phi_\delta(x - x_o) - (m_o \cdot \nabla) \nabla G_\delta(x - x_o).$$
If $m(x)$ is supported on a curve $\Gamma$ in 2D or a surface in 3D, then

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

is not a convolution and moment conditions do not help.
In the context of single-layer potentials, Beale showed that in 3D for a homogeneous polynomial $p_n(x)$,

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

where $\Gamma$ 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 $u_\delta(x) = m_o \phi_\delta(x - x_o) - (m_o \cdot \nabla) \nabla G_\delta(x - x_o)$ can also be written as

$$u_\delta(x) = m_o \left( \frac{-1}{2\pi r^2} \right) s_1(r/\delta) + \frac{(m_o \cdot \hat{x})\hat{x}}{r^2} \left( \frac{2}{2\pi r^2} \right) s_2(r/\delta)$$

where $\hat{x} = x - x_o$ and $r = |\hat{x}|$. 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 $\phi_\delta$: 

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

\[ u_\delta(x) = m_o \left( \frac{-1}{2\pi r^2} \right) s_1(r/\delta) + \frac{(m_o \cdot \hat{x}) \hat{x}}{r^2} \left( \frac{2}{2\pi r^2} \right) s_2(r/\delta) \]

may exhibit 3-rd order convergence.

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: \( m(\theta) = 0 \). The force at \( x(\theta, t) \) is given by the curve total arc length at \( t \) times the curvature at \( x(\theta, t) \).

Asymptotically, the solution is

\[
\begin{aligned}
 r(\theta, t) &= \left[ 1 - \frac{\epsilon^2}{4} A^2(t) \right] + \epsilon A(t) \cos(2\theta) + \epsilon^2 B(t) \cos(4\theta) + O(\epsilon^4) \\
 A(t) &= \cos \left( \sqrt{6\pi} \left( 1 - \frac{223}{480} \epsilon^2 \right) t \right) \\
 B(t) &= \frac{3}{20} + \frac{1}{3} \cos(2\sqrt{6\pi} \ t) - \frac{29}{60} \cos(\sqrt{60\pi} \ t).
\end{aligned}
\]
Results from exponential blob

Parameter: $\delta = 0.075$ and $\delta = 0.15$
Results from Beale blob

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

Change gears

New example
Lagrangian blob methods applied to biological fluid flow problems

Example 2: Regularized Stokeslets

Background

Example 1: Stokes flow past point obstacles in 2D
Example 2: Stokes flow around a cilium in 3D
Lagrangian blob methods applied to biological fluid flow problems

Example 2: Regularized Stokeslets

Background

Fundamental solution of Stokes equations

\[ \nabla p = \mu \Delta u + f \delta(x), \quad \nabla \cdot u = 0 \]

Suppose that \( f \) is constant and \( r = |x| \). Then formally,

\[ \Delta p = \nabla \cdot [f \delta(x)] \]

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

And finally,

\[ 8\pi \mu u(x) = \frac{f}{r} + \frac{(f \cdot x)x}{r^3} \sim \frac{1}{r} \]
Regularized solution of Stokes equations: **Stokeslet**

\[ \nabla p = \mu \Delta u + f \phi_\delta(x), \quad \nabla \cdot u = 0 \]

Then, define \( G_\delta \) by \( \Delta G_\delta(x) = \phi_\delta(x) \).

\[ \Delta p = \nabla \cdot [f \phi_\delta(x)] \quad \Rightarrow \quad p(x) = f \cdot \nabla G_\delta(x) \]

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

\[ \mu u(x) = -f G_\delta(x) + (f \cdot \nabla) \nabla B_\delta(x) \]

where \( \Delta B_\delta(x) = G_\delta(x) \).
Lagrangian blob methods applied to biological fluid flow problems

Example 2: Regularized Stokeslets

Background

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 \( H_2(r) = rB_\delta''(r) - B_\delta'(r) \).

\( \diamond \) 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

\[ \int_{\mathbb{R}^3} u(y) \phi_\delta(y - x) dy = \frac{1}{8\pi \mu} \int_{\partial D} S_\delta(y - x)f(y) \, ds(y) \]

leads to the **Method of Regularized Stokeslets**:

\[ u(x) = \frac{1}{8\pi \mu} \sum_k S_\delta(y_k - x)f_k A_k \]

**where**

\[ S_\delta(x)f = \frac{f}{r}H_1(r) + \frac{(f \cdot x)x}{r^3}H_2(r), \quad r = |x| \]
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?
Lagrangian blob methods applied to biological fluid flow problems
Example 2: Regularized Stokeslets

Background

Motion of headless helical organism
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 $x(s)$ for $0 \leq s \leq L$. **Strategy:** write the Stokeslet formula in terms of

\[
I_1(x, f) = \int_0^L f(s) \, x'(s) \times \nabla G(x - x(s)) \, ds
\]

\[
I_2(x, g) = \int_0^L g(s) \, x'(s) \cdot \nabla G(x - x(s)) \, ds
\]
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

\[ l_1(x, 1) = \int_0^L x'(s) \times \nabla G(x - x(s)) ds = \begin{cases} 1, & \text{for } x \text{ inside} \\ 0, & \text{for } x \text{ outside} \end{cases} \]

\[ l_2(x, 1) = \int_0^L x'(s) \cdot \nabla G(x - x(s)) ds = 0 \]
Lagrangian blob methods applied to biological fluid flow problems

Example 2: Regularized Stokeslets

Background

Single and double layer potentials

For example

\[ l_1(x, f) = \int_0^L f(s) \mathbf{x}'(s) \times \nabla G(x - x(s)) \, ds \]

\[ = f(s^*) \chi(x) + \int_0^L [f(s) - f(s^*)] \mathbf{x}'(s) \times \nabla G(x - x(s)) \, ds \]
Example 2: Regularized Stokeslets

Background

Single and double layer potentials

For example

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

\[ = f(s^*) \chi(x) + \int_0^L [f(s) - f(s^*)] \mathbf{x}'(s) \times \nabla G(x - x(s)) ds \]

\[ S_1(x, f) = f(s^*) \chi(x) + \sum_k [f_k - f(s^*)] \mathbf{x}'(s_k) \times \nabla G_\delta(x - x_k) \Delta s \]
Example 2: Regularized Stokeslets

Background

Single and double layer potentials

For example

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

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\[ S_1(x, f) = f(s^*) \chi(x) + \sum_k [f_k - f(s^*)] \mathbf{x}'(s_k) \times \nabla G_\delta(x - x_k) \, \Delta s \]

\[ I_1(x, f) = S_1(x, f) + T_1^{(n)}(x) + T_2^{(n)}(x) + O(\Delta s^2) + O(\delta^3) \]

\[ \cdot x \]

\[ x(s^*) \]
Lagrangian blob methods applied to biological fluid flow problems

Example 2: Regularized Stokeslets

Background

Single and double layer potentials

Similarly

\[
l_2(x, g) = \int_0^L g(s) \ x'(s) \cdot \nabla G(x - x(s)) ds
\]

\[
= \int_0^L [g(s) - g(s^*)] \ x'(s) \times \nabla G(x - x(s)) ds
\]

\[
S_2(x, g) = \sum_k [g_k - g(s^*)] \ x'(s_k) \cdot \nabla G_\delta(x - x_k)) \Delta s
\]

\[
l_2(x, g) = S_2(x, g) + T_1^{(t)}(x) + T_2^{(t)}(x) + O(\Delta s^2) + O(\delta^3)
\]
Example 2: Regularized Stokeslets

Background

- $T^{(n)}_1$ and $T^{(t)}_1$ are corrections due to the regularization of $G$ with a Gaussian blob
- $T^{(n)}_2$ and $T^{(t)}_2$ 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.
Example 2: Regularized Stokeslets

Background

\[ p(x) = \int_{\Gamma} f(s) \cdot \nabla G(x - x(s)) \, ds = l_2(x, f) \]

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

\[ = l_2(x, F) + l_1(x, Q^n) + l_2(x, Q^t) \]

where

\[ F(s) = -2\pi \int_{0}^{s} f(\alpha) \, d\alpha, \]

\[ Q^n(s) = -2\pi (x - x(s)) \cdot f(s) \cdot \hat{n}(s), \]

\[ Q^t(s) = -2\pi (x - x(s)) \cdot f(s) \cdot x'(s) \]
Example: Circle with $f(\theta) = 2\sin(3\theta)x(\theta)$

Pressure

Corrected

Uncorrected/Exact
Example: Circle with $f(\theta) = 2 \sin(3\theta) x(\theta)$

Errors as a function of discretization

<table>
<thead>
<tr>
<th>$N$</th>
<th>Error in $p$</th>
<th>Error in $u$</th>
<th>Error in $v$</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>$25.35 \times 10^{-4}$</td>
<td>$4.603 \times 10^{-4}$</td>
<td>$4.656 \times 10^{-4}$</td>
</tr>
<tr>
<td>200</td>
<td>$6.023 \times 10^{-4}$</td>
<td>$0.781 \times 10^{-4}$</td>
<td>$1.052 \times 10^{-4}$</td>
</tr>
<tr>
<td>400</td>
<td>$1.468 \times 10^{-4}$</td>
<td>$0.200 \times 10^{-4}$</td>
<td>$0.248 \times 10^{-4}$</td>
</tr>
</tbody>
</table>
Example: Circle with \( f(\theta) = 2 \sin(3\theta)x'(\theta) \)

Pressure

![Graph](image_url)
Example: Circle with $f(\theta) = 2 \sin(3\theta)x'(\theta)$

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).
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
Lagrangian blob methods applied to biological fluid flow problems

Example 2: Regularized Stokeslets

Background

Thank you

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