In Pursuit of a Fast High-order Poisson Solver: Volume Potential Evaluation

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Introduction: Physical Examples and Motivating Problems
What is Vorticity?

\[ \omega = \nabla \times \mathbf{u} \]  \hspace{1cm} (1)

\[ \Gamma = \oint_{\partial S} \mathbf{u} \cdot d\mathbf{l} = \iint_{S} \omega \cdot dS \]  \hspace{1cm} (2)

\(^0\)https://commons.wikimedia.org/wiki/File:Generalcirculation-vorticitydiagram.svg
Some Brief Theory

Navier-Stokes momentum equation

\[ \rho \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \mu \nabla^2 \mathbf{u} + \frac{1}{3} \mu \nabla (\nabla \cdot \mathbf{u}) \]  \hspace{1cm} (3)

where \( \mathbf{u} \) is the velocity field, \( p \) is the pressure field, and \( \rho \) is the density. Navier-Stokes can be recast as

\[ \frac{\partial \omega}{\partial t} + \mathbf{u} \cdot \nabla \omega - \omega \cdot \nabla \mathbf{u} = S(x, t) \]  \hspace{1cm} (4)

viscous generation of vorticity, \( S \) For incompressible flows velocity related to vorticity by

\[ \nabla^2 \mathbf{u} = -\nabla \times \omega \]  \hspace{1cm} (5)

Invert to obtain Biot-Savart integral

\[ \mathbf{u}(x) = \int_{\Omega} K(x, y) \times \omega(y) \, dx \]  \hspace{1cm} (6)

\( x \) is velocity eval point, \( y \) is non-zero vorticity domain, \( K(x, y) \) singular Biot-Savart kernel.
Why Integral Equation Methods?

- Low-order solvers common (for both Lagrangian\textsuperscript{1} and Eulerian\textsuperscript{2} approaches)
- Some “high”-order work exists\textsuperscript{3}, but is special purpose
- Ultimately, choice must be made between what form of Poisson equation is most useful
- Integral equations offer robust and flexible way, especially for complex geometries and for high-order

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Methodology: Evaluation approach

- Volume potential share similarities to layer potentials
- Same main challenge: devising quadrature to handle singularity
- Take same approach: QBX
- But where do we put our expansion center, fictitious dimension?
- Off-surface: layer potential physically defined, off-volume has no requirements
Absent any compelling choice for off-volume potential, choose obvious one:

Consider 3D Poisson scheme: approximate $\frac{1}{r}$ kernel with $\frac{1}{\sqrt{r^2 + a^2}}$

Effectively $a$ parameter is the distance from expansion center to eval point in the fictitious dimension, and kernel is no longer singular

Choose a “good” $a$ so the kernel is smooth and take QBX approach of evaluating Taylor expansion of de-singularized kernel back at desired eval point
Is trial scheme high-order?

- No, in fact seems to be limited to second order regardless of expansion order.
- Consider example results in figure below for 5th order expansion.
- Why only second order?
Preliminary Error Analysis

- We would like to examine the error $\epsilon = |\text{Exact potential - QBX computed potential}|$ and it’s dependence on $a$
- Call $G(r) = \frac{1}{r}$, $f(r, a) = \frac{1}{\sqrt{r^2 + a^2}}$, and the $k$-th order Taylor series expansion about $d$ and evaluated at $a = 0$:

$$T_k(r, d) = \sum_{n=0}^{k} \frac{(-d)^n}{n!} f^{(n)}(r, d)$$

- So our error is:

$$\epsilon = \int_{\Omega} G(r) \sigma(r) \, dr - \int_{\Omega} T(r, d) \sigma(r) \, dr$$

where $\sigma(r)$ is the density (vorticity in our physical example).
- This form seems complicated to inspect, is there a way to avoid the integrals and factor out the density?
Error in Fourier Space

Consider the action of the Fourier transform on the error:

\[ \mathcal{F}[\epsilon] = \mathcal{F} \left( \int G \sigma \, dr \right) - \mathcal{F} \left( \int T \sigma \, dr \right) \]

and by the convolution theorem:

\[ = \mathcal{F}[G] \mathcal{F}[\sigma] - \mathcal{F}[T] \mathcal{F}[\sigma] = \mathcal{F}[\sigma] (\mathcal{F}[G] - \mathcal{F}[T]) \]

\[ \mathcal{F}[T_k] = \sum_{n=0}^{k} \frac{(-d)^n}{n!} \mathcal{F}[f^{(n)}(r, d)] \]

This looks more reasonable, let’s examine the behavior of \( \mathcal{F}[G] - \mathcal{F}[T] \) with respect to \( d \).
Fourier Transform Particulars

- Need 3D Fourier transform; both $G$ and $T$ are radially symmetric, so simplifications can be made: transforms can be given in terms of the scalar $k$ in Fourier space.

- It is known that $\mathcal{F}[1/r] = 1/\pi k^2$

- With some work one can show:

  $$\mathcal{F}\left[\frac{1}{\sqrt{r^2 + a^2}}\right] = \frac{2a}{k} K_1(2\pi ak)$$

  where $K_1(x)$ is the modified Bessel function of second kind

- Reduces to expected form for $\lim_{a \to 0} \frac{2a}{k} K_1(2\pi ak) = 1/\pi k^2$

- Without concerning ourselves with details, in general we find:

  $$\mathcal{F}[T_k] = \sum_{n=-1}^{k} C_n d^{n+2} k^n K_n(2\pi kd)$$
Fourier Space Behavior

- How well does $T_k$ approximate $G$ in Fourier space?
- Example figure shows $G$ vs $T_k$ for $d = 0.2$, higher order expansions do reasonably well qualitatively.
- One issue: modified Bessel function of second kind have log($k$)-type singularities at 0, while $G$ has a $k^{-2}$ singularity.
Examination of error: k dependence

- k dependence tells us how well the expansion preserves low vs high modes in real space
- Example figure shows k dependence for $d = 0.2$
- One way of thinking about the error quantitatively would be $\int (\mathcal{F}[G] - \mathcal{F}[T])^2 dk$, we would like to minimize this.
- Spoiler: closed form expression 2 slides away
Examination of error: d dependence

- Ultimately, a k-th order method should have the error be proportional to \( d^k \)
- However examine example figure for \( |G - T_5|/d \) for \( k = 5 \) (we saw that a moderate order expansion only weakly depended on \( k \), holds for other choice of \( k \))
- Looks linear! Add back in factor of \( d \), error seems to go as \( d^2 \). Looks linear at any zoom range of \( d \).
Closed form expression for error

- While $|\mathcal{F}[G] - \mathcal{F}[T]|$ is messy, as it turns out
  $\int (\mathcal{F}[G] - \mathcal{F}[T])^2 \, dk$ reduces concisely.

- For $T_3 : \frac{3\pi^3 d^3}{256}$, $T_4 : \frac{175\pi^3 d^3}{32768}$, $T_5 : \frac{3059\pi^3 d^3}{1048576}$

- Pick up extra power of $d$ due to integration across all $k$
  compared to at a particular $k$

- Alternately, consider Taylor series expansion of $T_5$ in Fourier space with respect to $d$:

  $$\frac{1}{\pi k^2} + \frac{\pi d^2}{10} + \frac{1}{20} \pi^3 d^4 k^2 + \mathcal{O}(d^6)$$
Future effort

- Suggests need for alternate basis in Fourier space more able to represent $k^{-2}$ singularity
- Alternate basis in turn would suggest appropriate de-singularized kernel in real space
- Caveat: If an inverse Fourier transform exists and the result is smooth enough!