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

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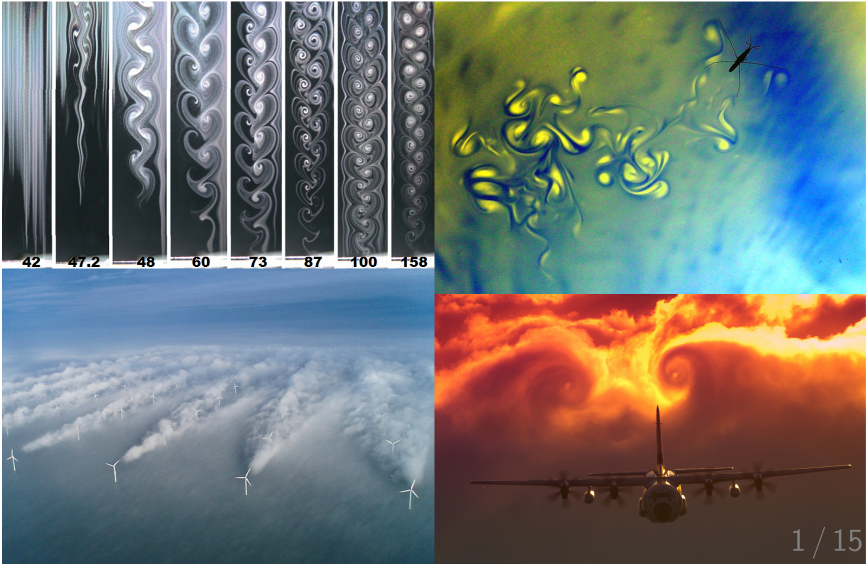
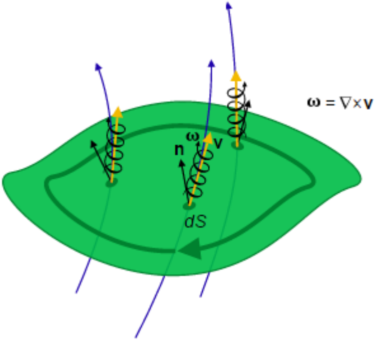
Introduction: Physical Examples and Motivating Problems



What is Vorticity?

$$\omega = \nabla \times \mathbf{u} \tag{1}$$

$$\Gamma = \oint_{\partial S} \mathbf{u} \cdot d\mathbf{l} = \iint_S \omega \cdot d\mathbf{S} \tag{2}$$



[0] https://commons.wikimedia.org/wiki/File:Generalcirculation-vorticitydiagram.svg

Some Brief Theory

Navier-Stokes momentum equation

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t}+\mathbf{u}\cdot\nabla\mathbf{u}\right)=-\nabla p+\mu\nabla^2\mathbf{u}+\tfrac{1}{3}\,\mu\nabla(\nabla\cdot\mathbf{u}) \tag{3}$$

where u is the velocity field, p is the pressure field, and ρ is the density. Navier-Stokes can be recast as

$$\frac{\partial \omega}{\partial t}+\mathbf{u}\cdot\nabla\omega-\omega\cdot\nabla\mathbf{u}=S(x,t) \tag{4}$$

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

$$\nabla^2\mathbf{u}=-\nabla\times\omega \tag{5}$$

Invert to obtain Biot-Savart integral

$$\mathbf{u}(x)=\int_\Omega K(x,y)\times\omega(y)dx \tag{6}$$

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[1] and Eulerian[2] approaches)
- Some "high"-order work exists[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

[1] Moussa, C., Carley, M. J. (2008). A Lagrangian vortex method for unbounded flows. International journal for numerical methods in fluids, 58(2), 161-181.

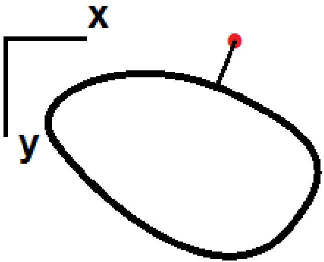
[2] R.E. Brown. Rotor Wake Modeling for Flight Dynamic Simulation of Helicopters. AIAA Journal, 2000. Vol. 38(No. 1): p. 57-63.

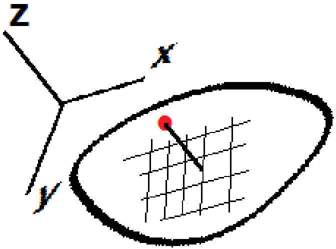
[3] J. Strain. Fast adaptive 2D vortex methods. Journal of computational physics 132.1 (1997): 108-122.

[4] Gholami, Amir, et al. "FFT, FMM, or Multigrid? A comparative Study of State-Of-the-Art Poisson Solvers for Uniform and Nonuniform Grids in the Unit Cube." SIAM Journal on Scientific Computing 38.3 (2016): C280-C306.

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



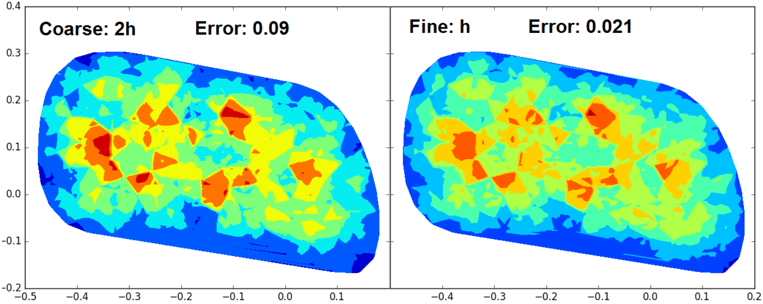


Trial Scheme

- Absent any compelling choice for off-volume potential, choose obvious one:
- Consider 3D Poisson scheme: approximate $1/r$ kernel with $1/\sqrt{r^2 + a^2}$
- 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 $\epsilon =$ |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:

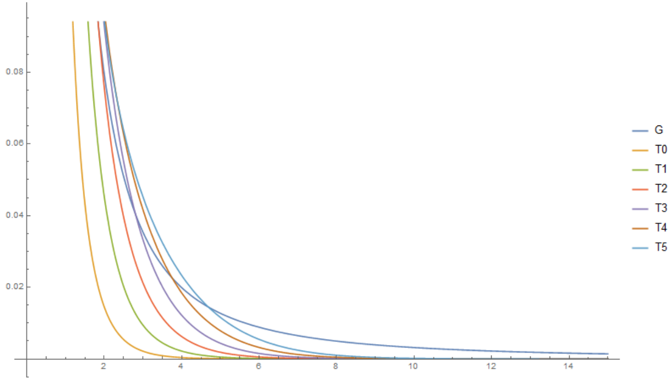
$$\mathcal{F}[\frac{1}{\sqrt{r^2 + a^2}}] = \frac{2a}{k} K_1(2\pi a k)$$

  where $K_1(x)$ is the modified Bessel function of second kind
- Reduces to expected form for $\lim_{a \to 0} \frac{2a}{k} K_1(2\pi a k) = 1/\pi k^2$
- Without concerning ourselves with details, in general we find:

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

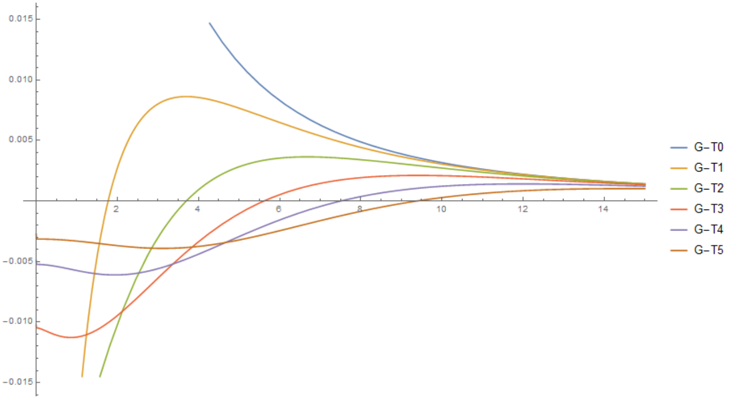
Fourier Space Behavior

- 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



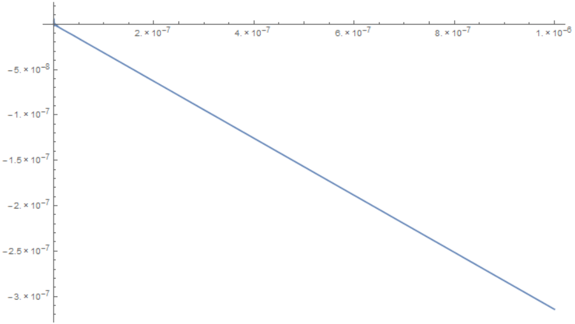
Examination of error: k dependence

- 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!