High-order Volume Potential Evaluation

+ in complex geometry?

J. Bevan, UIUC

(contextualize vs. Xiaoyu's talk)

CS591
March 9, 2018

Very texty overall

→ try to use figures and not write whole sentences

Introduction: Volume Potentials are Everywhere

[0]iter.org/sci/plasmaconfinement, www-math.mit.edu/dhu/Striderweb/striderweb.html, noaanews.noaa.gov/stories2011/20110426_windwakes.html, nasa.gov/spitzer-20070604.html

What is an Integral Equation?

- Integral equations one way of solving PDEs, can involve operations like solution of integral equations:

$$\int_\Omega K(\mathbf{x},\mathbf{y})\,\sigma(\mathbf{y})\,d\mathbf{y} = f(\mathbf{x}) \tag{1}$$

(where K is a kernel function and $\sigma(\mathbf{y})$ is unknown)

- Or evaluation of integrals:

$$\phi(\mathbf{x}) = \int_\Omega K(\mathbf{x},\mathbf{y})\,\sigma(\mathbf{y})\,d\mathbf{y} \tag{2}$$

- Central idea is solution of PDE is composed of sum of a "fundamental solution" G that solves PDE for point source:

$$\mathcal{L}G(x,y) = \delta(y-x) \qquad \text{(weakly)} \tag{3}$$

where $\mathcal{L}$ is a linear differential operator associated with the PDE, G is called the Green's function, and δ is the Dirac delta.

How are They Useful?

missing scaling

- Consider for example Poisson equation:

$$\nabla^2 \phi = f \tag{4}$$

- Solution is given by integral equation methods by evaluating

$$\phi(\mathbf{x}) = \int_\Omega G(\mathbf{x}, \mathbf{y})\, f(\mathbf{y})\, d\mathbf{y} \tag{5}$$

where 3D Laplace Green's function is $G(\mathbf{x}, \mathbf{y}) = \frac{1}{|\mathbf{x}-\mathbf{y}|}$.

\frac only in display math

- Integral equation methods within a fast algorithm are competitive efficiency-wise with other approaches[1], and have excellent conditioning

define

- However evaluation of the integrals can pose challenges

[1] 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.

Numerical Integral Evaluation

Ω discretized how?

$$\int_{\Omega} K(\mathbf{x},\mathbf{y})\,\sigma(\mathbf{y})\,d\mathbf{y}$$

text

- These type of integrals can be challenging to evaluate, especially if one wants high-order convergence.
- Traditional numerical quadrature (e.g. Gauss-Legendre) assumes integrand well-approximated by polynomials
- Poor assumption since K is usually singular or near singular, G-L converges very slowly and with large error

relate to err est.

- Usual approaches involve specialized quadrature rules[2], transformation of the integral[3], or adaptive quadrature

longer

- We want a high-order general purpose quadrature method that works for unstructured meshes and complex geometries: Quadrature by Expansion (QBX)[4]

almost certainly different from final

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

[3] Huybrechs, Cools. "On generalized Gaussian quadrature rules for singular and nearly singular integrals." SIAM Journal on Numerical Analysis 47.1 (2009): 719-739.

[4] Klöckner, et al. "Quadrature by expansion: A new method for the evaluation of layer potentials." Journal of Computational Physics 252 (2013): 332-349.

(but we use the nice things in QBX as inspiration:

- generality
- geom. flexibility
- high ord.)

Compare/contrast to box scheme

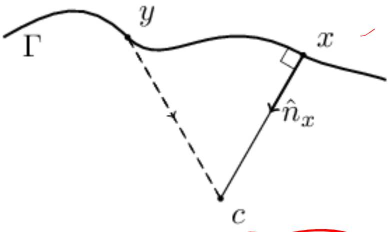
expected cost/accuracy tradeoff.

Methodology: Quadrature by Expansion

- Consider computing a *layer potential*
- Computing potential (at x) on surface Γ means evaluation of singular integral
- Idea: evaluate potential at a point off surface: c, no longer singular; in fact, far enough away: smooth
- Smooth potential means we can approximate near c with Taylor series expansion
- Use expansion to compute potential back at x

undefined

Is talking about lpots helpful?



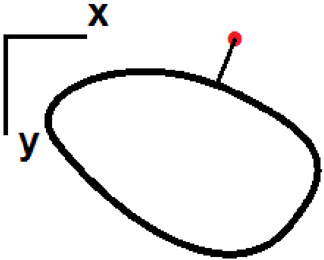
[0] https://relate.cs.illinois.edu/course/cs598apk-f17/flow-session/388695/1/

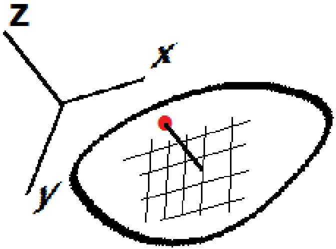
not a public URL – that's your session

QBX for Volume Potentials

think of different "branding"

- Volume potential share similarities to layer potentials ← be precise
- Same main challenge: devising quadrature to handle singularity
- Take same approach: QBX → similar?
- 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 $G = 1/r$ kernel with $\hat{G} = 1/\sqrt{r^2 + a^2}$
- ~~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

define

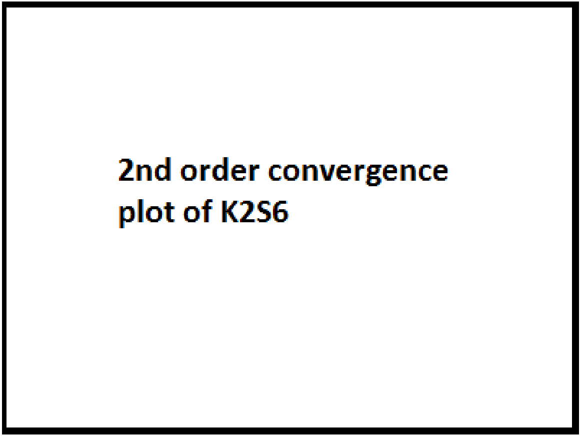
to what end?

→ "just a regularization scheme"

can now use smooth quad rule

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 6th 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 (Assumption: a correlates with req. quad. res.)
- Call T_k the k-th order Taylor series expansion of $\hat{G}$ about d and evaluated at $a = 0$:

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

- So our error is:

$$\epsilon_k = \int_\Omega G(r)\sigma(r)\, dr - \int_\Omega T_k(r, d)\sigma(r)\, dr$$

- 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:

$$\mathcal{F}[\epsilon] = \mathcal{F}\left[\int G\,\sigma\,dr\right] - \mathcal{F}\left[\int T_k\,\sigma\,dr\right]$$

  and by the convolution theorem:

$$= \mathcal{F}[G]\,\mathcal{F}[\sigma] - \mathcal{F}[T_k]\,\mathcal{F}[\sigma] = \mathcal{F}[\sigma]\,(\mathcal{F}[G] - \mathcal{F}[T_k])$$

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

- This looks more reasonable, let's examine the behavior of $\mathcal{F}[G] - \mathcal{F}[T_k]$ with respect to d.

avoid being colloquial in writing

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 $\mathcal{F}[1/r] = 1/\pi k^2$

(using scary integral shortcuts – actually defined in what sense?)

- With some work one can show:

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

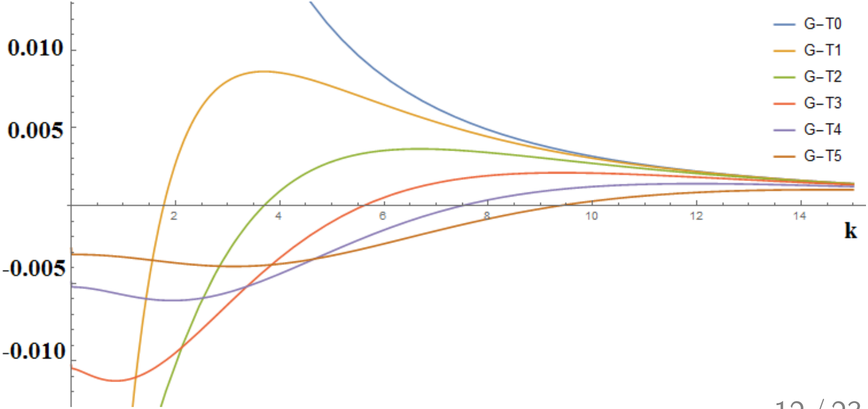
  where $K_n(x)$ is the modified Bessel function of second kind
- Reduces to expected form for $\lim_{a \to 0} \frac{2a}{k} K_1(2\pi a k) = 1/\pi k^2$
- Without concerning ourselves with details, in general we find:

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

Examination of Error

- k dependence tells us how well the expansion preserves low vs high modes in real space (in figure below $d = 0.2$)
- Taylor expansion of $\mathcal{F}[T_5]$ wrt d about 0:

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



Cause: Approximation Error

- It seems there is some additional approximation error that limits convergence, truncation error from Taylor series not the issue
- We replaced Green's function with de-singularized approximation, what does approximate kernel correspond to?
- Remember that for our Laplace equation

$$\nabla^2 G(x, y) = \delta(y - x) \tag{6}$$

- However our de-singularized Green's function doesn't satisfy this, instead of solving for a point source it solves for a blob source: ζ

$$\nabla^2 \hat{G}(x, y) = \zeta(y - x) \tag{7}$$

Dirac Delta Approximation and Moment Conditions

- The quality of our Green's function approximation then depends upon the quality of our Dirac delta approximation from our choice of a blob
- The order of convergence of this approximation can be shown[5,6] to depend upon the *moment conditions*, where for a s order accurate approximation we require:

In what sense?

$$\int \zeta(\mathbf{x})\, d\mathbf{x} = 1 \tag{8}$$

What converges?

$$\int \mathbf{x}^{\mathbf{i}}\, \zeta(\mathbf{x})\, d\mathbf{x} = 0\,,\ |\mathbf{i}| < s - 1 \tag{9}$$

$$\int \mathbf{x}^{s}\, \zeta(\mathbf{x})\, d\mathbf{x} < \infty \tag{10}$$

[5] Cottet, Koumoutsakos. Vortex methods: theory and practice. Cambridge University Press, 2000.

[6] Liu, Mori. "Properties of discrete delta functions and local convergence of the immersed boundary method." SIAM Journal on Numerical Analysis 50.6 (2012): 2986-3015.

High Order De-singularized Kernels

- We can see that $1/\sqrt{r^2 + a^2}$ is actually 0th order approximation (the third condition isn't totally satisfied for $s = 2$) ? is or is not ?
- This approximation error in turn bounds our overall error and limits convergence rate to at best 2nd order
- Why better convergence than expected from kernel? Postulated QBX expansion satisfies moment conditions for $s = 2$, remains to be verified
- Possible to construct higher-order kernels by satisfying moment conditions[7] for larger s
- For example consider the 2nd order kernel (i.e. satisfies moment conditions for $s = 2$:

Plot? Compare to orig?

$$\zeta = \frac{15/2}{(r^2 + a^2)^{7/2}} \rightarrow \hat{G} = \frac{r^2 + \frac{3}{2}a^2}{(r^2 + a^2)^{3/2}} \tag{11}$$

[7] Winckelmans, Leonard. "Contributions to vortex particle methods for the computation of three-dimensional incompressible unsteady flows." Journal of Computational Physics 109.2 (1993): 247-273.

Fourier Space Error Analysis of High Order Kernels

- Define $T_{s,k}$ to be similar to our T_k from before, but now for $\hat{G}_s$ the sth order algebraic approximate kernel
- We can examine again the error in our computed integral in Fourier space, but now for our higher order kernel
- We find that in general:

$$\mathcal{F}[T_{s,k}] = \frac{2}{(\frac{s}{2})!} d^n k^{n-2} \pi^{n-1} K_{\frac{s}{2}+1}(2\pi kd) + \sum_{n=\frac{s}{2}-1}^{k} C_n \, d^{n+2} \, k^n \pi^{n+1} K_n(2\pi kd) \tag{12}$$

- For example, consider the Taylor expansion of higher order kernels wrt d about 0:

$$\mathcal{F}[T_{2,5}] \rightarrow \frac{1}{\pi k^2} + \frac{k^2 \pi^3 d^4}{20} + \mathcal{O}(d^6) \; , \; \mathcal{F}[T_{4,7}] \rightarrow \frac{1}{\pi k^2} + \frac{k^4 \pi^5 d^6}{252} + \mathcal{O}(d^8)$$

Results: Test Setup

of what?

- Theoretical computed convergence rates were verified empirically
- Integral evaluated for 3D Laplace Green's function with constant density in domain ? $[-0.5, 0.5]^{3}\cancel{\times [-0.5, 0.5] \times [-0.5, 0.5]}$
- Possible to compute exact analytical expression for any target in domain
- Domain split into cube elements and tensor product Gauss-Legendre quadrature of varying order was used
- Computed result compared with exact result to determine error, and with h refinement the order of convergence

Required Minimum Quadrature Order

- Accuracy of result dependent on choice of quadrature order q and value chosen for d
- Min required quadrature order to accurately evaluate integral, smaller d less smooth kernel and higher required q
- Past min q, error dominated by truncation error in expansion

Error of result
compared to q for
a particular d
K6S7, d=0.01

Observed Convergence

K4S5 covergence plot in h

K6S7 convergence plot in h

Quadrature Error Bounds

- Content dependent on how far I get with TV error estimate by Thurs night

ok

- Explanation of bounding quadrature error[8] in terms of
- Analytic continuability
- and Total Variation (TV)

title case

of what series?

[8] Trefethen, Lloyd N. Approximation theory and approximation practice. Vol. 128. Siam, 2013.

Rough TV Bound Behavior

- Relate bound on required q and d, and behavior wrt h refinement

Observed Error Correctly Bounded by Estimate

- Hopefully show here that observed *quadrature error* (not *total error*) is properly bounded by the TV estimate

Conclusion