Towards High-order Volume Potential Evaluation for Unstructured Meshes

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CS591
March 9, 2018

Introduction: Volume Potentials are Everywhere

[1]

What is an Integral Equation?

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

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

  (K is a kernel function and $\sigma(\mathbf{y})$ 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: solution of PDE sum of "fundamental solutions" G that solve PDE for point source (in the weak sense):

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

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

How are They Useful?

- Example: Poisson equation:

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

- Solution given by evaluating:

$$\phi(\mathbf{x}) = \int_{\Omega} G(\mathbf{x}, \mathbf{y}) \, f(\mathbf{y}) \, d\mathbf{y} \qquad G(\mathbf{x}, \mathbf{y}) = \frac{1}{4\pi |\mathbf{x} - \mathbf{y}|} \tag{5}$$

- Integral equation methods evaluated with FMM competitive efficiency-wise with other approaches[2], and have excellent conditioning
- Evaluation of the integrals can pose challenges

Numerical Integral Evaluation

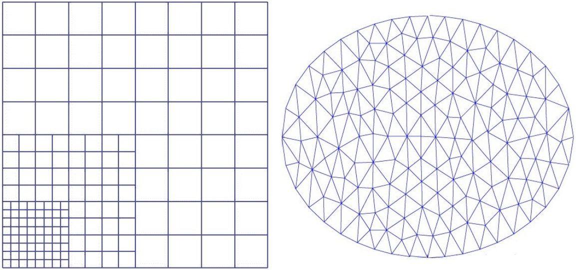
- Issue: Gaussian quadrature assumes integrand approximated well by polynomials
- Poor assumption since K is usually singular or near singular
- Consider common singularity, quadrature converges[3] slowly:

$$y \in [-1, 1],\ I(y) = \int_{-1}^{1} |x - y|^{-\delta} dx\,,\ \ |I - I_n| < \mathcal{O}(n^{-1+\delta}) \quad (6)$$

- Approaches include: product integration rules[4]; compute offline, weights that exactly integrate up to a polynomial order
- Transformation of the integral[5](e.g. to a semi-infinite domain), causes singularity to vanish
- Adaptive quadrature; adaptively divide domain based on error estimate, compute on each subdomain

More General Scheme for Unstructured Meshes

- Mentioned approaches lack generality: tied to specific integrand and/or for unmapped/structured meshes
- We want a high-order general purpose quadrature method that works for unstructured meshes and complex geometries
- For inspiration look to QBX (Quadrature by Expansion)[6]: high-order, geometric flexibility

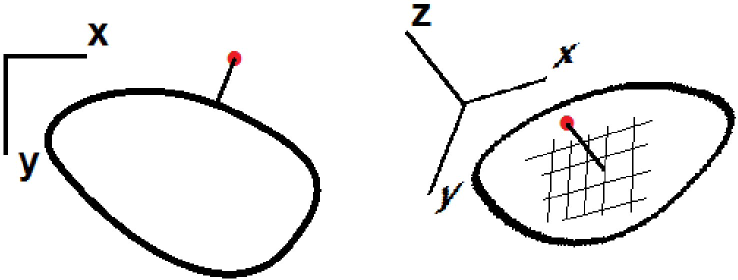


[7]

Methodology: Approximations for Volume Potential Kernels

- Use QBX-like ideas: add smoothing parameter a in Green's function approximation $\hat{G}$, Taylor expand in a, evaluate back at target
- Call T_k the k-th order Taylor series expansion of $\hat{G}$ about d and evaluate at $a = 0$:

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

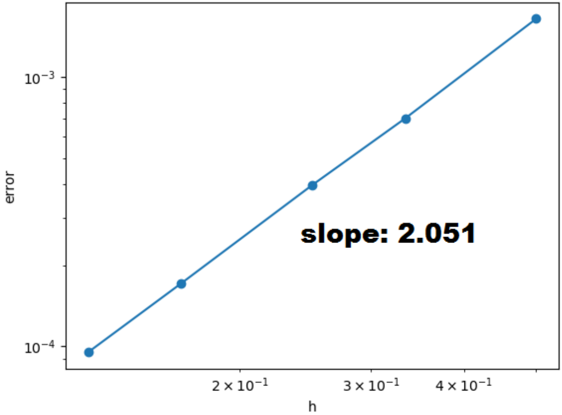


To Start: A Simple Choice for $\hat{G}$

- To start consider a simple smoothing scheme:
- 3D Poisson scheme: approximate $G = 1/r$ kernel with $\hat{G} = 1/\sqrt{r^2 + a^2}$
- Parameter a 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 evaluate Taylor expansion
- Our integrand is now smooth, and so we can use Gaussian quadrature

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

$$\epsilon = |\text{Exact potential - QBX computed potential}| \tag{7}$$

  and it's dependence on a
- 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:

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

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

- More reasonable, examine the behavior of $\mathcal{F}[G] - \mathcal{F}[T_k]$ 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:

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

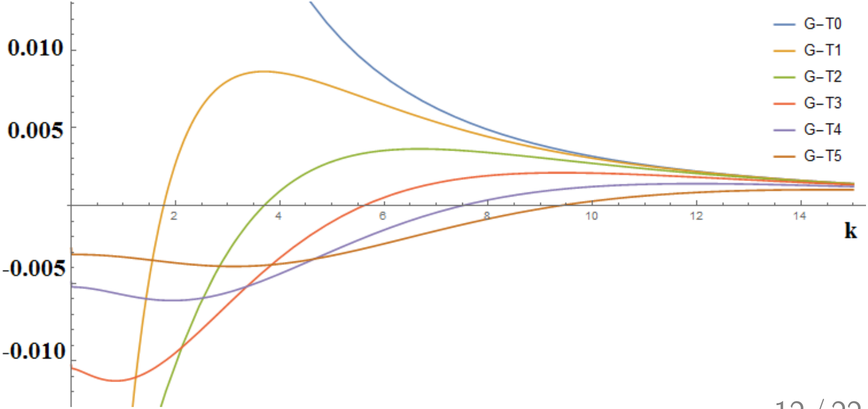
  where $K_n(x)$ is the modified Bessel function of second kind
- Reduces to expected form for $\lim_{a \to 0} \frac{2a}{k} K_1(2\pi a k) = 1/\pi k^2$
- Without concerning ourselves with details, in general we find:

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

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

$$\nabla^2 G(x, y) = \delta(y - x) \tag{8}$$

- 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

$$\nabla^2 \hat{G}(x, y) = \zeta(y - x) \tag{9}$$

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[8,9] to depend upon the *moment conditions*, where for a s order accurate approximation we require:

$$\int \zeta(\mathbf{x})\, d\mathbf{x} = 1 \tag{10}$$

$$\int \mathbf{x}^{\mathbf{i}}\, \zeta(\mathbf{x})\, d\mathbf{x} = 0\,,\ |\mathbf{i}| < s - 1 \tag{11}$$

$$\int \mathbf{x}^{s}\, \zeta(\mathbf{x})\, d\mathbf{x} < \infty \tag{12}$$

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 $s=2$)
- 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[10]for larger s
- For example consider the 2nd order kernel (i.e. satisfies moment conditions for $s=2$:

$$\zeta = \frac{15/2}{(r^2+a^2)^{7/2}} \rightarrow \hat{G} = \frac{r^2+\frac{3}{2}a^2}{(r^2+a^2)^{3/2}} \tag{13}$$

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:

$$\mathcal{F}[T_{s,k}] = \frac{2}{(\frac{s}{2})!} d^n k^{n-2} \pi^{n-1} K_{\frac{s}{2}+1}(2\pi k d) + \sum_{n=\frac{s}{2}-1}^{k} C_n \, d^{n+2} \, k^n \pi^{n+1} K_n(2\pi k d) \tag{14}$$

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

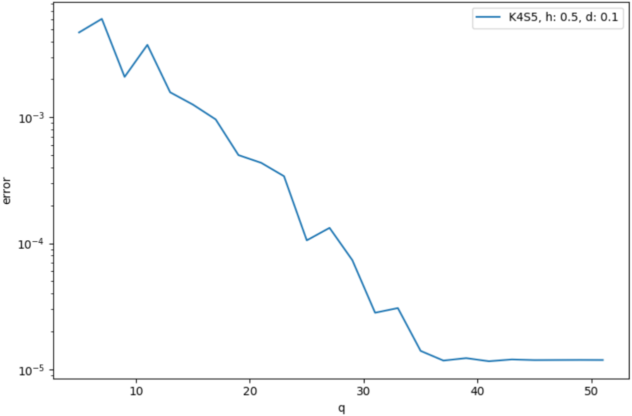
$$\mathcal{F}[T_{2,5}] \to \frac{1}{\pi k^2} + \frac{k^2 \pi^3 d^4}{20} + \mathcal{O}(d^6) \ , \ \mathcal{F}[T_{4,7}] \to \frac{1}{\pi k^2} + \frac{k^4 \pi^5 d^6}{252} + \mathcal{O}(d^8)$$

Results: Test Setup

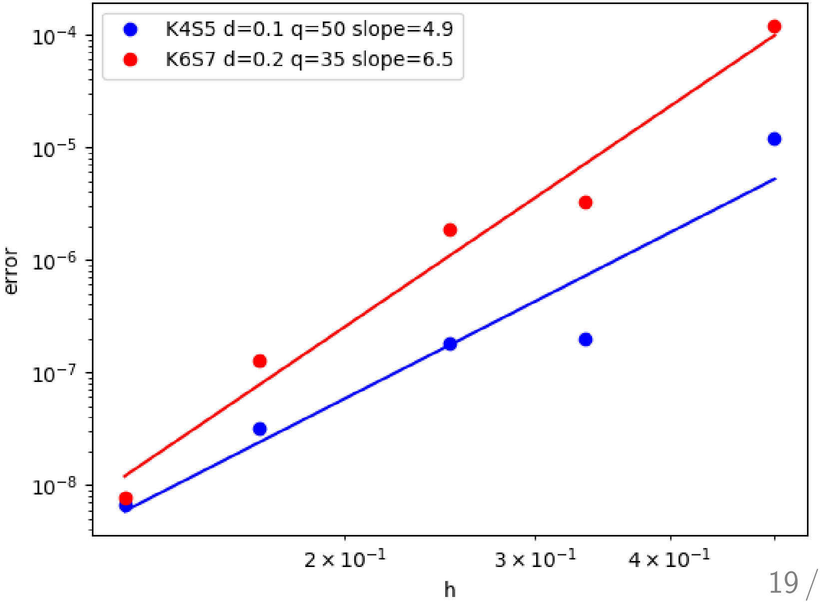
- Theoretical computed convergence rates were verified empirically
- Integral evaluated for 3D Laplace Green's function with constant density in domain $[-0.5, 0.5]^3$
- Possible to compute exact analytical expression for any target in domain
- Domain split into cube elements and tensor product Gauss-Legendre 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



Observed Convergence



Next Steps: Quadrature Error Bounds

- We would like some way of bounding the quadrature error in our computed integral
- Several ways of finding such bounds[11]in terms of analytic continuability and total variation (TV)
- Total variation bound:

$$|I - I_n| = \frac{32}{15} \frac{V}{\pi\nu(n - 2\nu - 1)^{2\nu+1}} \tag{15}$$

- where V is bounded variation of $f^{(\nu)}$
- Order of magnitude estimate at least provides useful metric for proportionality between d, q, and h

Conclusion

- High-order evaluation scheme for volume potentials on unstructured meshes in works
- Choice of smoothed kernel arbitrary, but important
- High-order convergence depends upon interplay between d, q, and h
- Still in development

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