Today

- Other PDEs
- Quadrature

Announcements

- Extra Office Hours
- Presentations
- Projection methods section rewritten

‘Off-the-shelf’ ways to compute integrals

How do I compute an integral of a nasty singular kernel?

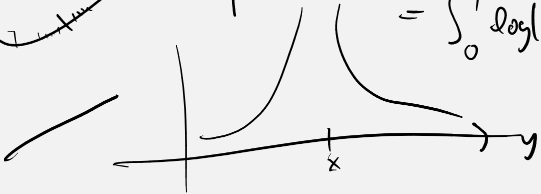
Symbolic integration

brittle

Why not Gaussian?

nphi $\left|\int f - \sum \omega f(\ldots)\right| \le C h^{2n} \|f^{(2n)}\|_\infty$

$$\int_\Gamma \log(|x-y|)\,\sigma(y)\,dy = \int_0^1 \log|x-\gamma(t)|)\,\sigma(\gamma(t))|\gamma'(t)|$$



Singular and Near-Singular Quadrature

$$\int_0^1 \log(x-\gamma(t))\,\sigma(\gamma(t))|\gamma'(t)|$$

Numerically distinct scenarios:

- Near-Singular quadrature
  - Integrand nonsingular
  - But may locally require lots of
  - Adaptive quadrature works, but. . .
- Singular quadrature
  - Integrand singular
  - Conventional quadrature fails

Kussmaul-Martensen quadrature

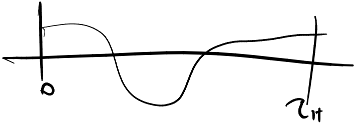
$$\int_0^1 \log(x-\gamma(t))\,\sigma(\gamma(t))|\gamma'(t)|$$

Theorem (A special integral [Kress LIE Lemma 8.21])

$$\frac{1}{2\pi}\int_0^{2\pi} \log\left(4\sin^2\frac{t}{2}\right) e^{imt}\,dt = \begin{cases} 0 & m = 0, \\ -\frac{1}{|m|} & m = \pm 1, \pm 2 \ldots. \end{cases}$$

Why is that exciting?

Demo: Kussmaul-Martensen quadrature



$$\sigma(t) \approx \sum_{-n}^{n} \alpha_m e^{imt}$$

Singularity Subtraction

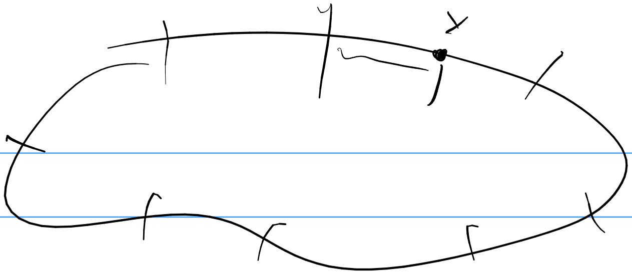
$$\int \langle \text{Thing } X \text{ you would like to integrate} \rangle$$

$$= \int \langle \text{Thing } Y \text{ you } \textit{can} \text{ integrate} \rangle$$

$$+ \int \langle \text{Difference } X - Y \text{ which } \underbrace{\text{is easy to integrate (numerically)}}_{\text{smooth}} \rangle$$

Give a typical application.

Drawbacks?



High-Order Corrected Trapezoidal Quadrature

- Conditions for new nodes, weights
  ($\rightarrow$ linear algebraic system, dep. on n)
  to integrate
  $$\langle\text{smooth}\rangle \cdot \langle\text{singular}\rangle + \langle\text{smooth}\rangle$$
- Allowed singularities: $|x|^{\lambda}$ (for $|\lambda| < 1$), $\log |x|$
- Generic nodes and weights for log singularity
- Nodes and weights copy-and-pasteable from paper

[Kapur, Rokhlin '97]

Alpert '99 conceptually similar:

Generalized Gaussian

- "Gaussian":
  - Integrates $2n$ functions exactly with n nodes
  - Positive weights
- Clarify assumptions on system of functions ("Chebyshev system") for which Gaussian quadratures exist
- When do (left/right) singular vectors of integral operators give rise to Chebyshev systems?
  - In many practical cases!
- Find nodes/weights by Newton's method
  - With special starting point
- Very accurate
- Nodes and weights for download

[Yarvin/Rokhlin '98]

Singularity cancellation: Polar coordinate transform

$$\int \int_{\partial\Omega} K(\mathbf{x}, \mathbf{y}) \phi(y) ds_y$$

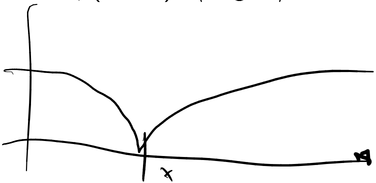
$$=$$

$$\int_0^R \int_{\mathbf{x}+\mathbf{r}\in\partial\Omega\cap\partial B(\mathbf{x},r)} K(\mathbf{x}, \mathbf{x}+\mathbf{r})\phi(\mathbf{x}+\mathbf{r}) d\langle \text{angles} \rangle \, r \, dr$$

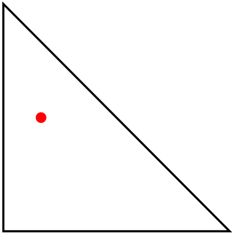
$$=$$

$$\int_0^R \int_{\mathbf{x}+\mathbf{r}\in\partial\Omega\cap\partial B(\mathbf{x},r)} \frac{K_{\text{less singular}}(\mathbf{x}, \mathbf{x}+\mathbf{r})}{r} \phi(\mathbf{x}+\mathbf{r}) d\langle \text{angles} \rangle \, r \, dr$$

where $K_{\text{less singular}} = K \cdot r$.

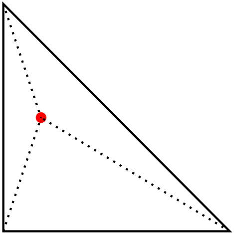


Quadrature on Triangles



Problem: Singularity can sit *anywhere* in triangle
$\rightarrow$ need *lots* of quadrature rules (one per target)

Quadrature on Triangles



Problem: Singularity can sit *anywhere* in triangle
$\rightarrow$ need *lots* of quadrature rules (one per target)

Kernel regularization

Singularity makes integration troublesome: *Get rid of it!*

$$\frac{\cdots}{\sqrt{(x-y)^2}} \quad \to \quad \frac{\cdots}{\sqrt{(x-y)^2+\epsilon^2}}$$

Use Richardson extrapolation to recover limit as $\epsilon \to 0$.

(May also use geometric motivation: limit along line towards singular point.)

Primary drawbacks:

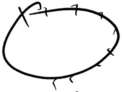
- Low-order accurate
- Need to make ϵ smaller (i.e. kernel more singular) to get better accuracy

Can take many forms–for example:

- Convolve integrand to smooth it
  ($\to$ remove/weaken singularity)
- Extrapolate towards no smoothing

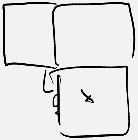
Related: [Beale/Lai '01]

Acceleration and Quadrature

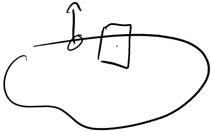


$$(\pm \tfrac{1}{2} I + D)\,\sigma(x) = \int_\Gamma \partial_n G(x-y)\,\sigma(y)\,dy$$

How can singular quadrature and FMM acceleration be made compatible?



FMMs and other Layer Potentials



How does an FMM evaluate a double layer?

compute mpoles of d/p kernel

How does an FMM evaluate S'?

eval ∇ of local expansions at the end

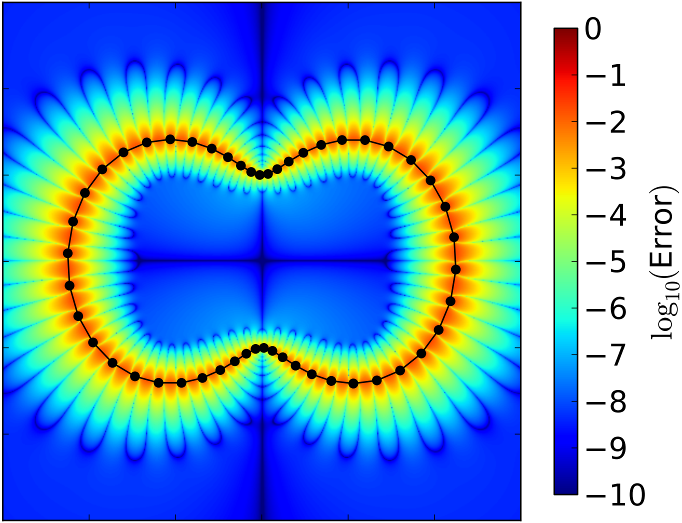
What effect does this have on accuracy?

D does not lose an order

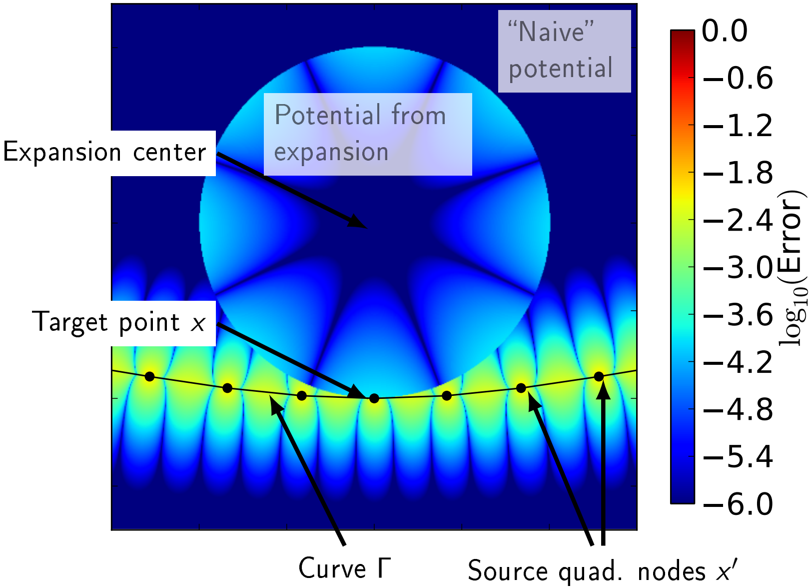
S' loses an order

Outline

Layer Potential Evaluation: Some Intuition

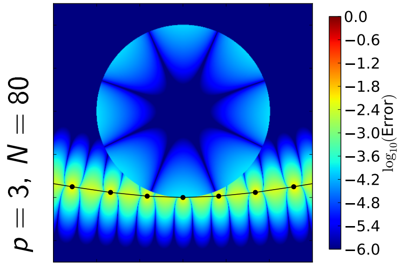


QBX: Idea

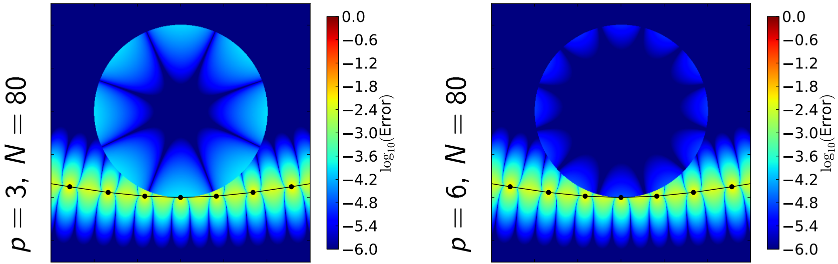


"Naive" potential
Potential from expansion
Expansion center
Target point x
Curve Γ
Source quad. nodes x'
0.0
−0.6
−1.2
−1.8
−2.4
−3.0
−3.6
−4.2
−4.8
−5.4
−6.0
$\log_{10}$(Error)

QBX: An Experiment



QBX: An Experiment



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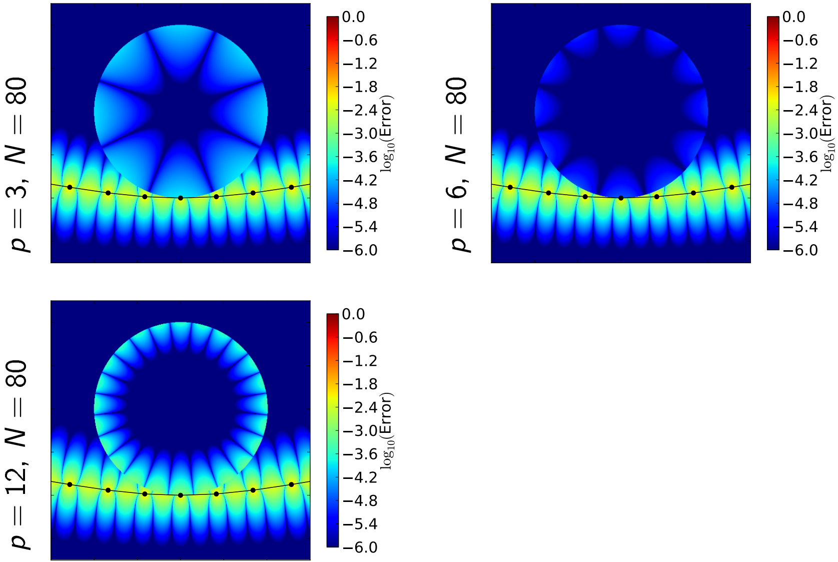
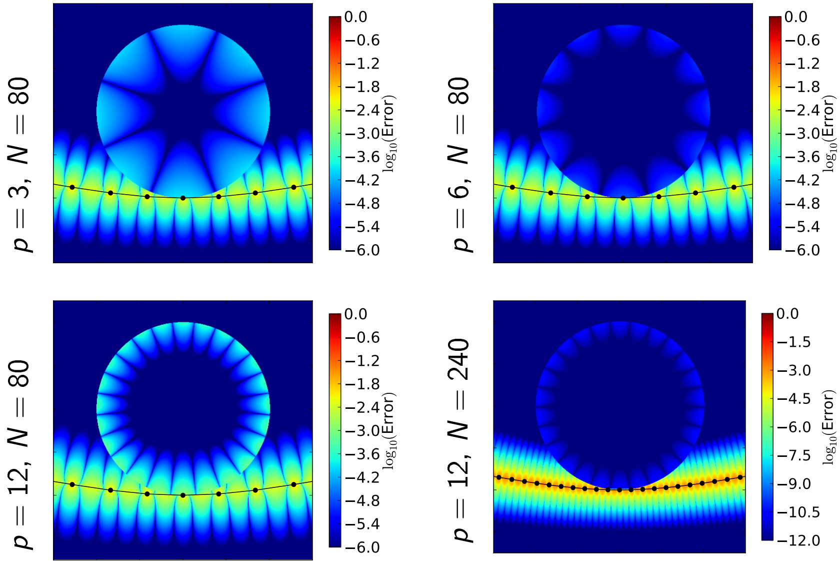
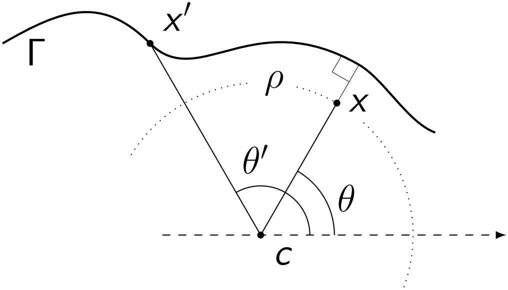


QBX: An Experiment



QBX: Notation, Basics

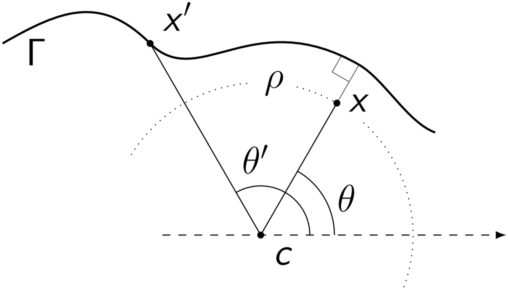
Graf's addition theorem



QBX: Notati

Graf's ad

> Requires: $|x - c| < |x' - c|$ ("local expansion")



$$H_0^{(1)}(k|x - x'|) = \sum_{l=-\infty}^{\infty} H_l^{(1)}(k|x' - c|)e^{il\theta'} J_l(k|x - c|)e^{-il\theta}$$

QBX: Formulation, Discretization

Compute layer potential on the disk as

$$S_k\sigma(x) = \sum_{l=-\infty}^{\infty} \alpha_l J_l(k\rho)e^{-il\theta}$$

with

$$\alpha_l = \frac{i}{4}\int H_l^{(1)}(k|x'-c|)e^{il\theta'}\sigma(x')\,\mathrm{d}x' \quad (l=-\infty,\dots,\infty)$$

$S\sigma$ is a smooth function *up to* Γ.

QBX: Formulation, Discretization

$$S_{QBX} = \sum \int H_l(\ldots)\,\sigma(y)\,dy = \int \sum H_l(\ldots)\,\sigma(y)\,dy$$

continuous

$A\sigma = f$

Compute layer potential on the disk as

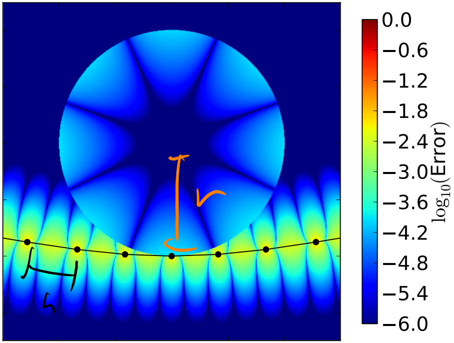
$$S_k\sigma(x) = \sum_{l=-p}^{p} \alpha_l J_l(k\rho)e^{-il\theta}$$

with

$$\alpha_l = \frac{i}{4} T_N\left(\int_\Gamma H_l^{(1)}(k|x' - c|)e^{il\theta'}\sigma(x')\,\mathrm{d}x' \right) \quad (l = -\infty, \ldots, \infty)$$

$S\sigma$ is a smooth function *up to* Γ.

Quadrature by Expansion (QBX)



$r \sim h$

$r = 2h$

$$\text{Error} \leq \left(C \underbrace{r^{p+1}}_{\text{Truncation error}} + C \underbrace{\left(\frac{h}{r}\right)^{q}}_{\text{Quadrature error}} \right) \|\sigma\|$$

h^{p+1} $\quad (\frac{1}{2})^q$ $\quad + \varepsilon$

[K, Barnett, Greengard, O'Neil JCP '13]

Achieving high order

$$\text{Error} \le \left(C \underbrace{r^{p+1}}_{\text{Truncation error}} + C \underbrace{\left(\frac{h}{r}\right)^q}_{\text{Quadrature error}} \right) \|\sigma\|$$

Two approaches:

- *Asymptotically convergent*: $r = \sqrt{h}$
  - ⊕ Error $\to 0$ as $h \to 0$
  - ⊖ Low order: $h^{(p+1)/2}$
- *Convergent with controlled precision*: $r = 5h$
  - ⊖ Error $\not\to 0$ as $h \to 0$
  - ⊕ High order: h^{p+1} to controlled precision $\epsilon := (1/5)^q$

Other layer potentials

Can't just do single-layer potentials:

$$\alpha_l^D = \frac{i}{4} \int_\Gamma \frac{\partial}{\partial \hat{n}_{x'}} H_l^{(1)}(k|x' - c|)e^{il\theta'} \mu(x') \, \mathrm{d}x'.$$

Even easier for target derivatives (S' et al.): Take derivative of local expansion.
Analysis says: Will lose an order.
Slight issue: QBX computes one-sided limits.
Fortunately: Jump relations are known–e.g.

$$(PV) D^* \mu(x)|_\Gamma = \lim_{x^\pm \to x} D\mu(x^\pm) \mp \frac{1}{2}\mu(x).$$

Alternative: Two-sided average → Preferred because of conditioning