

High-order quadratures for boundary integral equations: a tutorial

CBMS conference on fast direct solvers

6/23/14

Alex Barnett (Dartmouth College)

Slides accompanying a partly chalk talk.

Certain details, references, codes, exercises: download `quadrut.zip`



Representing PDE solns: potential theory

‘charge’ (source of waves) distributed along curve Γ w/ density func.

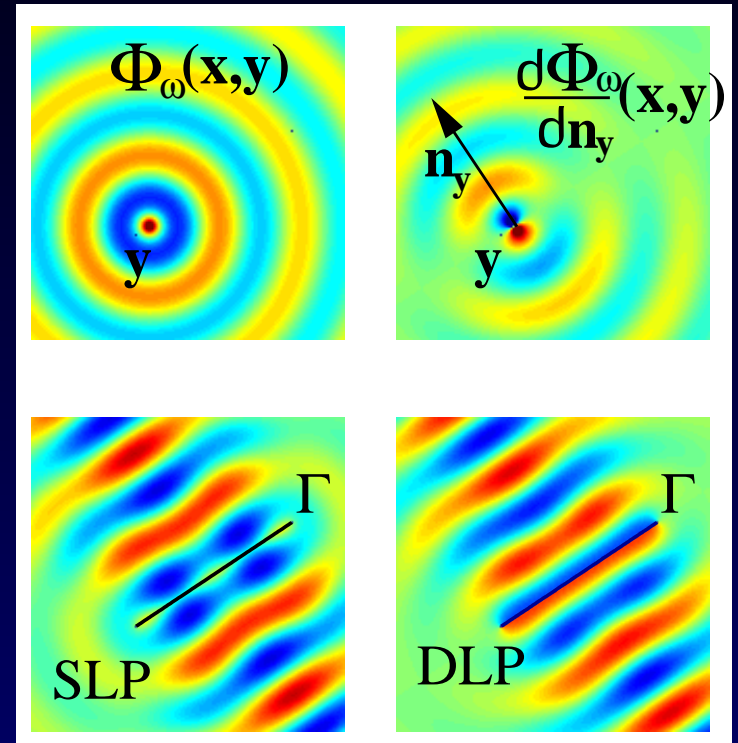
Single-, double-layer potentials, $\mathbf{x} \in \mathbb{R}^2$

$$v(\mathbf{x}) = \int_{\Gamma} \Phi(\mathbf{x}, \mathbf{y}) \sigma(\mathbf{y}) ds_{\mathbf{y}} := (\mathcal{S}\sigma)(\mathbf{x})$$

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$$\Phi(\mathbf{x}, \mathbf{y}) := \Phi(\mathbf{x} - \mathbf{y}) = \frac{i}{4} H_0^{(1)}(\omega |\mathbf{x} - \mathbf{y}|)$$

kernel is Helmholtz fundamental soln
a.k.a. free space Greens func



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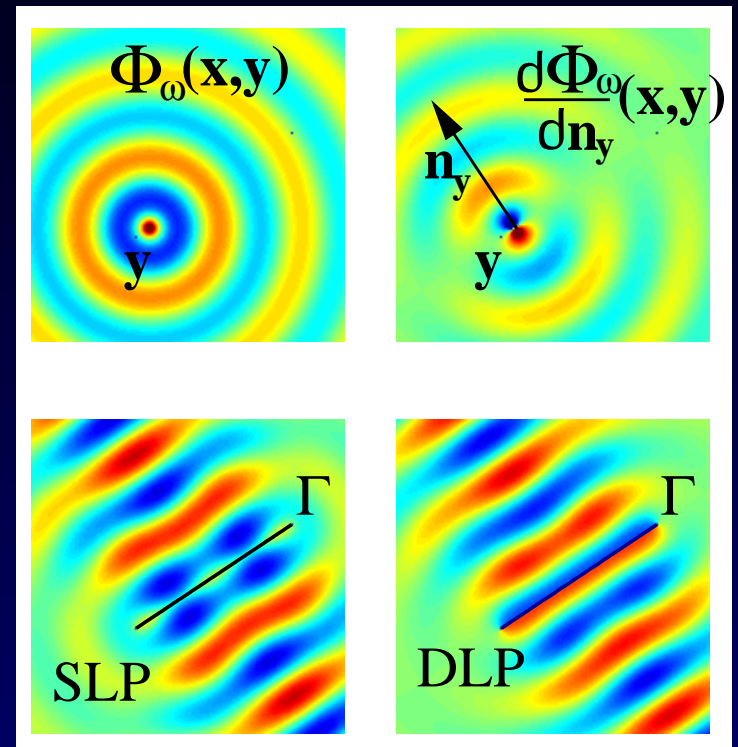
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Jump relations: limit as $\mathbf{x} \rightarrow \Gamma$ can depend on which side (\pm):

$$v^{\pm} = \mathcal{S}\sigma \quad \text{no jump}$$

$$u^{\pm} = \mathcal{D}\sigma \pm \frac{1}{2}\sigma \quad \text{jump}$$

\mathcal{S}, \mathcal{D} : bdry integral ops w/ above kernels,
smoothing, bounded $L_2(\Gamma) \rightarrow H^1(\Gamma)$

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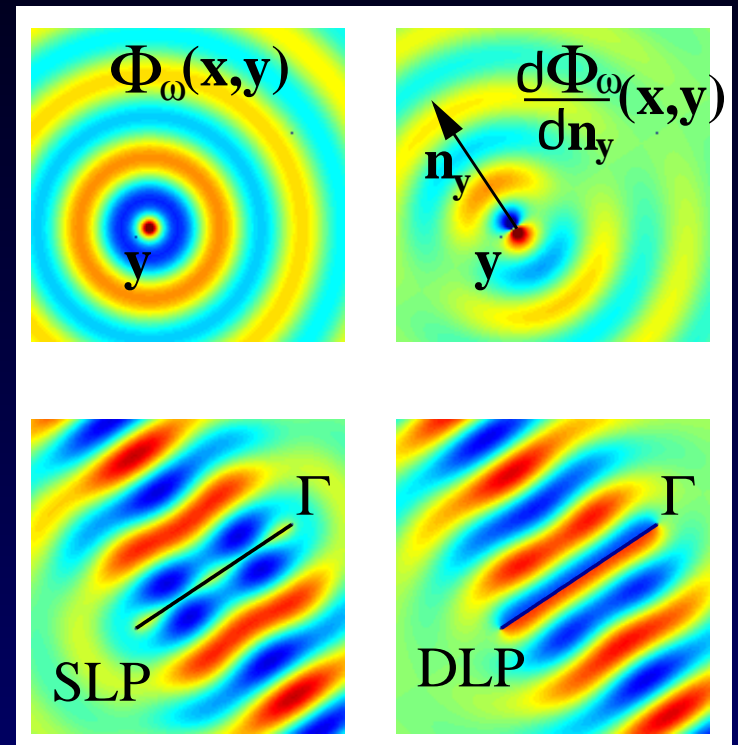
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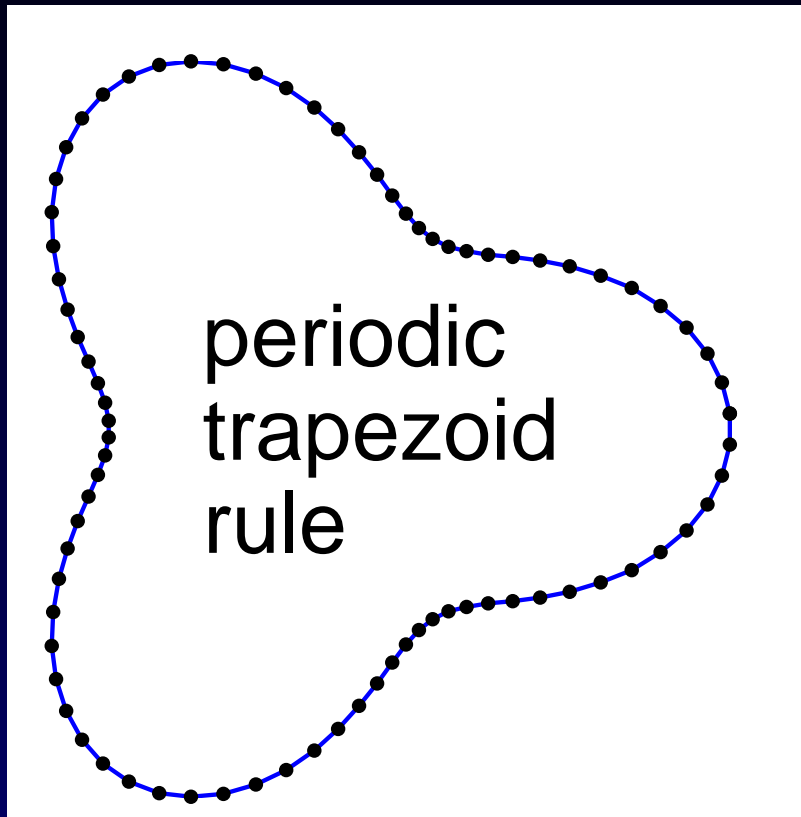
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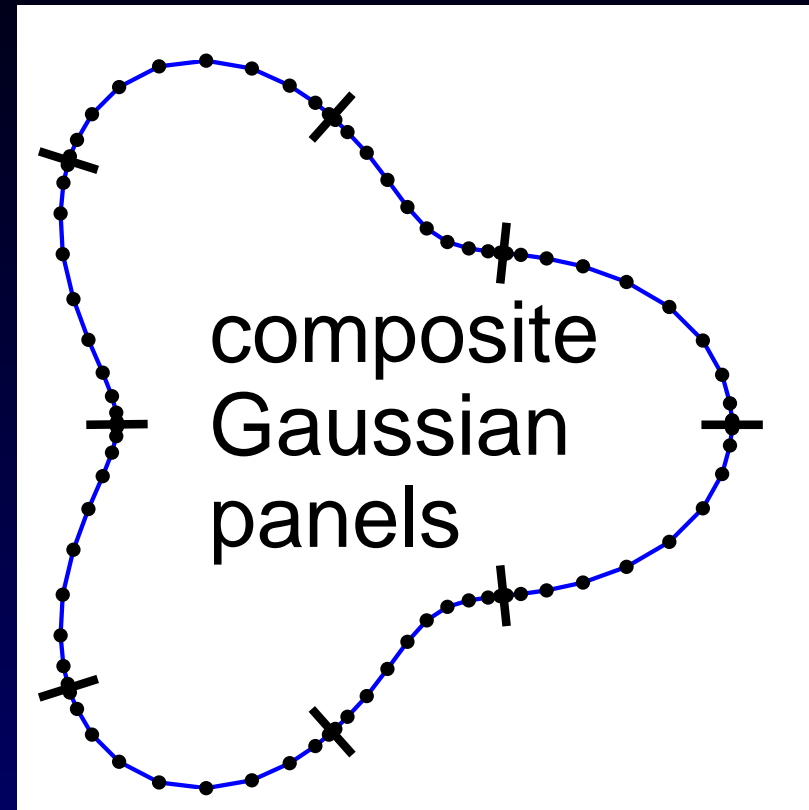
- From now fix $\Gamma = \partial\Omega$ i.e. densities live on obstacle boundary

Underlying quadrature schemes in 2D



err $O(e^{-\alpha N})$ if analytic f , $\partial\Omega$

vesicles, smooth bodies



err $O(N^{-2p})$ if $f, \partial\Omega \in C^{2p}$

adaptivity, corner refinement

Classification of log singular schemes in 2D

kernel:
$$K(s, t) = K_1(s, t) \log\left(4 \sin^2 \frac{s-t}{2}\right) + K_2(s, t)$$

| | split into K_1, K_2 explicit | split into K_1, K_2 unknown |
|--------------------------|--|---|
| global (PTR) | Kress '91: prod. quadr. but not FMM | Kapur–Rokhlin '97: corr. weights Alpert '99: aux. nodes QBX '12: local exp. for PDE |
| panel-based (Gauss–L) | Helsing '08: ℂ contour integr. | Gen. Gauss. Kolm–Rokhlin: sets of aux. nodes QBX '12 : local exp. for PDE |

- explicit split: more analytic info \Rightarrow gains efficiency
- unknown split: useful for new kernels (eg axisymmetric)

Potential evaluation close to boundary

2D interior Laplace ($k = 0$)

$\partial\Omega$ param by $Z(s)$, $s \in [0, 2\pi)$

say want eval. $u = \mathcal{D}\sigma$ $u = \operatorname{Re} v$, $v(z) = \frac{i}{2\pi} \int_{\partial\Omega} \frac{\sigma(y)}{z - y} dy$

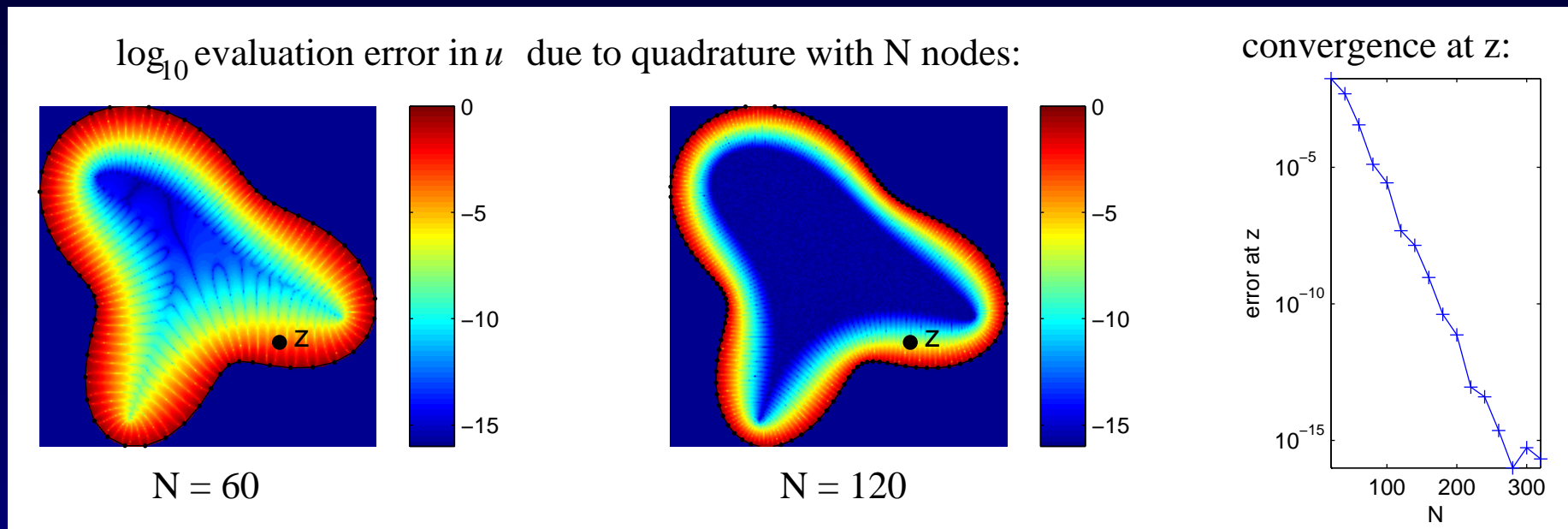
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Eg use PTR. “ $5h$ -rule”: target z must be $5h$ from $\partial\Omega$ to be accurate



- exponential convergence, but rate arbitrarily slow as $z \rightarrow \partial\Omega$

Thm (B '12): rate = dist. of $Z^{-1}(z)$ from real axis in **complex s plane**

Quadrature By eXpansion (QBX)

(B '11)

(Klöckner-B-Greengard-O'Neil '12)

$\sigma, v|_{\partial\Omega}$ analytic $\Rightarrow v$ extends analytically some dist. **outside** Ω

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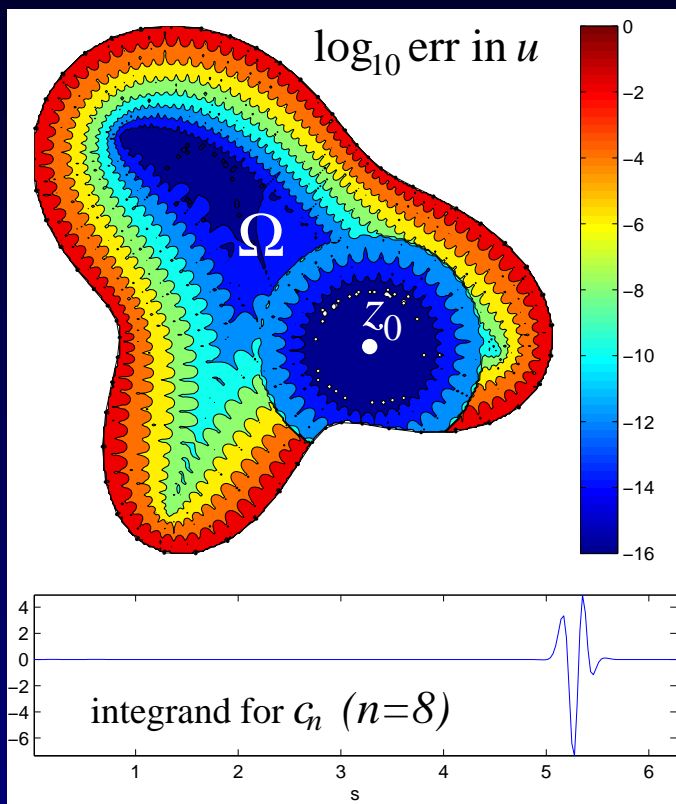
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Taylor exp. $v(z) = \sum_{n=0}^{\infty} c_n(z - z_0)$

rad. of conv. ρ takes you beyond $\partial\Omega$



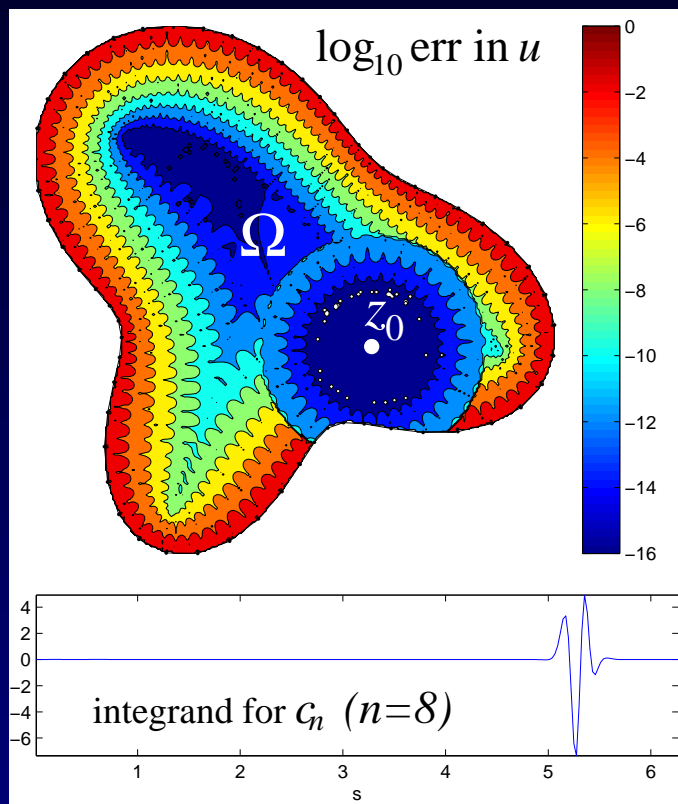
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- pick center z_0 about $2.5h$ from $\partial\Omega$
- eval. P (≈ 10) terms via Cauchy,

$$c_n = \frac{v^{(n)}(z_0)}{n!} = \frac{i}{2\pi} \int_{\partial\Omega} \frac{\sigma(y)}{(z - y)^{n+1}} dy$$

integrand more osc. \Rightarrow need βN nodes, $\beta \approx 4$
interpolate σ from original N

- eval. Taylor exp. in $|z - z_0| \leq R < \rho$
- repeat for z_0 's all around $\partial\Omega$

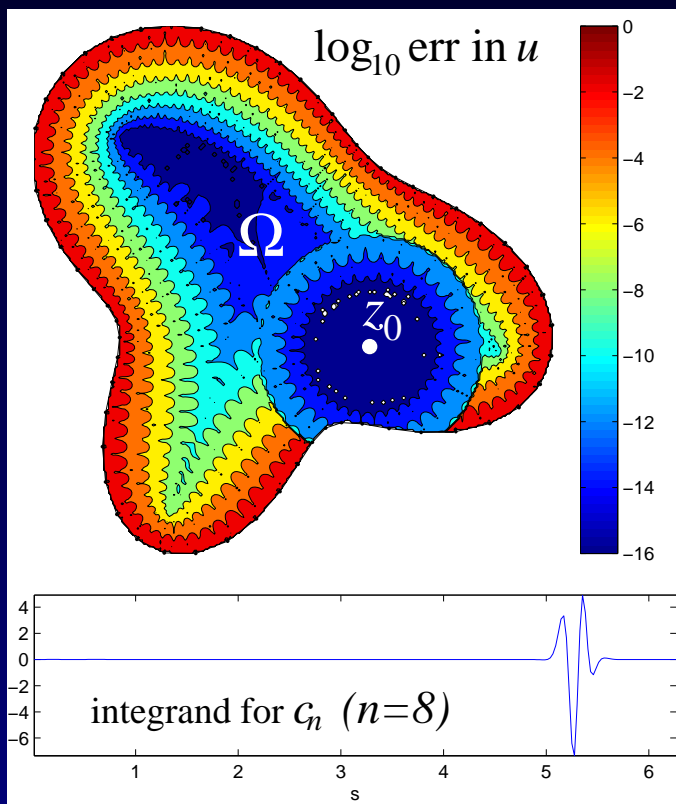
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Thm. (B '12) $\text{err} \leq C\left(\frac{R}{\rho}\right)^P + Cp\left(\frac{C\beta}{P}\right)^P e^{-C\beta}$ **asyp. exponential conv. in P, β**

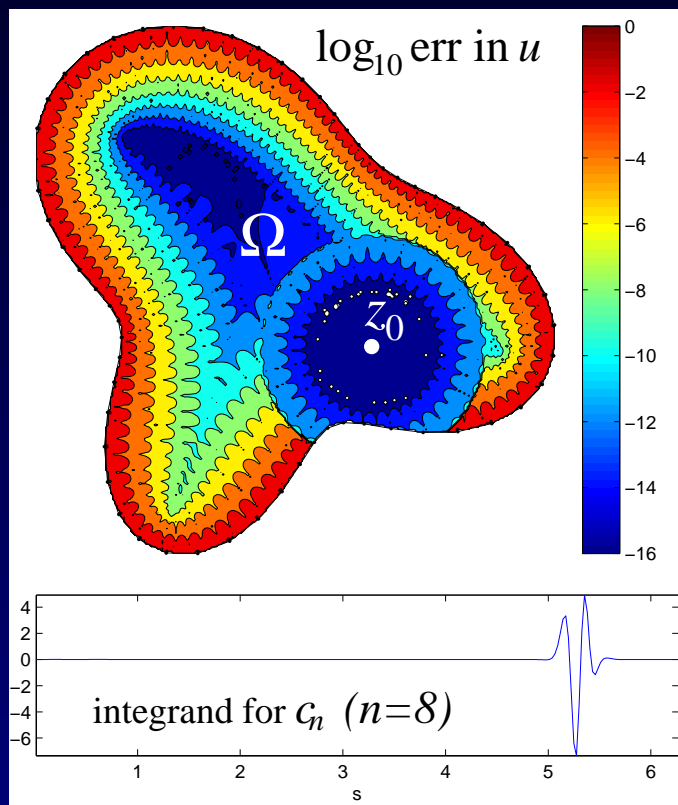
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Helmholtz ($k > 0$):

- Taylor \rightarrow **local expansion** $\sum_{|n| < P} c_n J_n(kr) e^{in\theta}$
- Cauchy \rightarrow Graf's addition theorem for Bessels

QBX, 2D, high- k close eval. for Helmholtz

100 λ diameter

700 λ perimeter

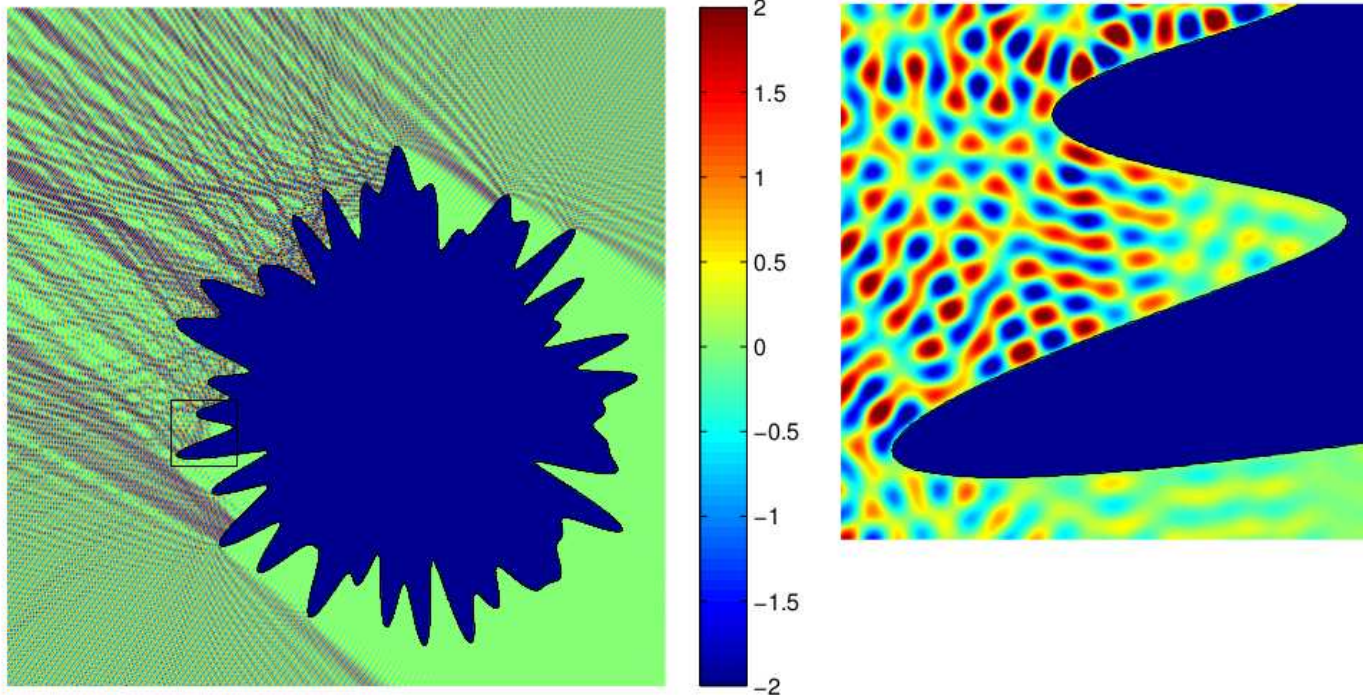
underlying Kress,
 $N=9000$ unknowns

fill + solve 90 sec

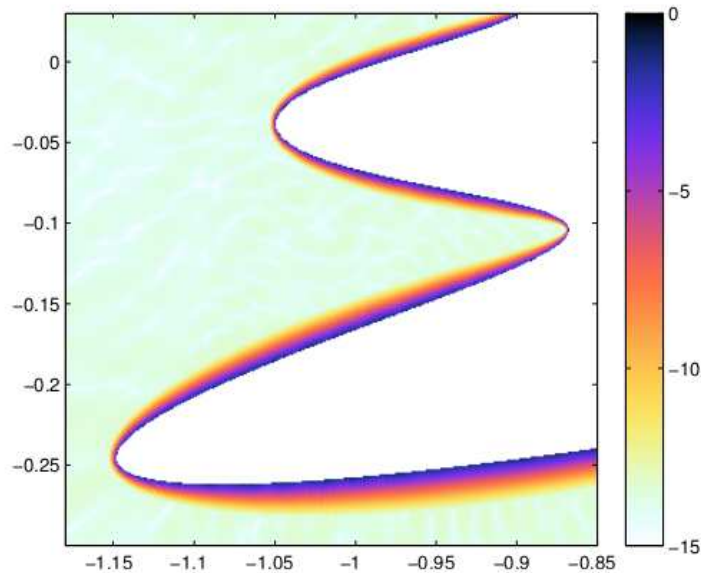
QBX eval in 30 sec
(2×10^5 pts)

rel. error $< 10^{-11}$

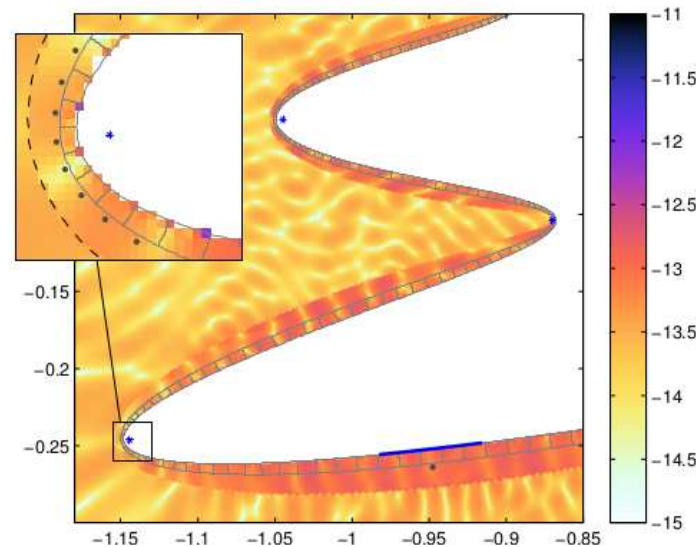
(B '12)



(c) $\log_{10} |u^{(N)} - u| / \|u_{\text{tot}}\|_{\infty}$



(d) $\log_{10} |\hat{u} - u| / \|u_{\text{tot}}\|_{\infty}$



Local vs global QBX; same scheme in 3D

- Local: use QBX to fill self and near panel matrix blocks, sparse $O(N)$
- far via plain rule; err $O(h^p + \epsilon)$ where ϵ fixed, controlled by p, P, β .
ie not formally convergent; needs P high to push to $\epsilon = O(\epsilon_{\text{mach}})$
- Global: use QBX with *all of* $\partial\Omega$ contrib to expansion at each center
- kills the ϵ , allows lower P (for engs. apps.), do all via FMM (FDS?)

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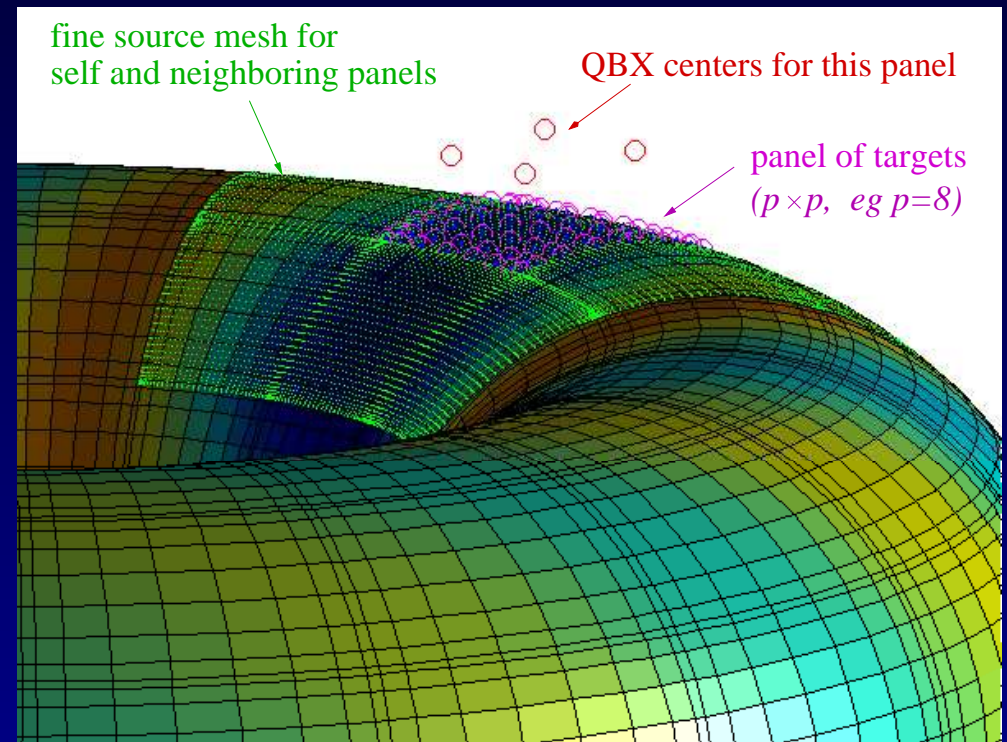
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3D: panels $p \times p$ Gauss nodes

Local expansion $u(r, \theta, \phi) =$

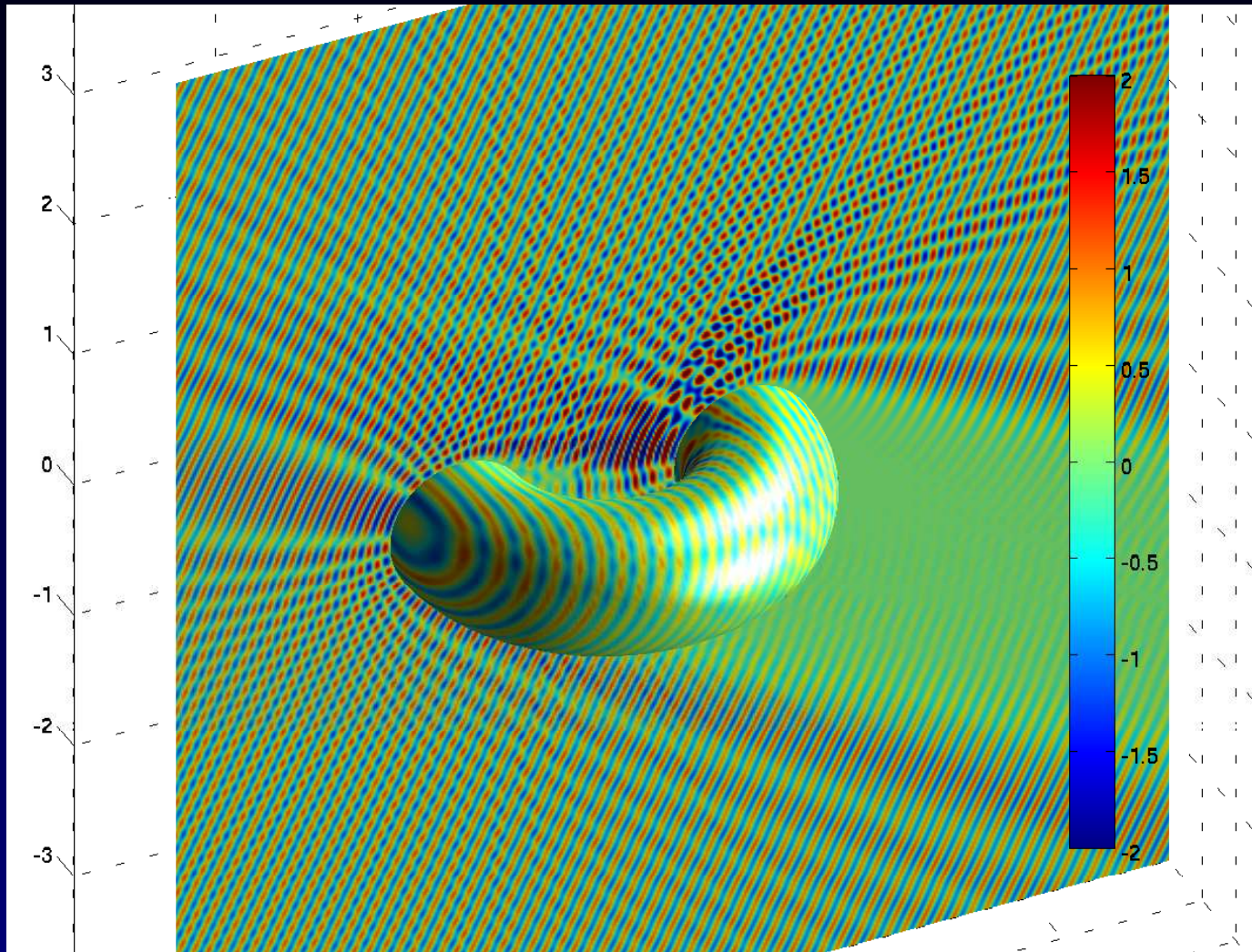
$$\sum_{|n| \leq P} \sum_{m=-n}^n c_{nm} j_n(kr) Y_n^m(\theta, \phi)$$

spherical harmonic addn thm



- $(P+1)$ th order proven for $\sigma \in W^{P+3+\epsilon, 2}$ (Epstein–Greengard–Klöckner '12)

QBX: 3D high-freq. torus scattering result



Dirichlet BC
(sound-soft acoustics)

30λ diameter

$N \approx 145000$

$q=8, p=10, \beta=4.5$

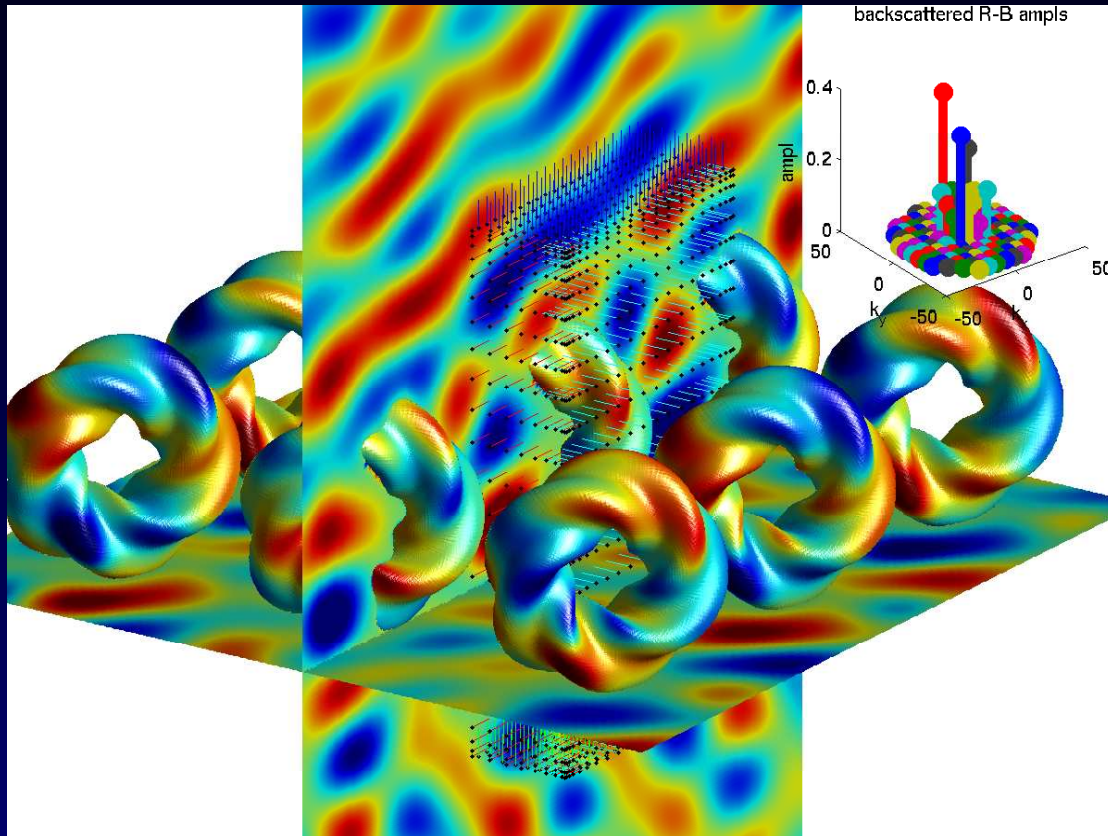
QBX quad 1.2 hr
GMRES+FMM 1 hr
laptop (4-core i7)

relative error 10^{-5}

- QBX in 3D still in primitive state (Barnett–Gimbutas–Greengard, in prep.)
- note FEM/FDTD at this high accuracy & freq. essentially prohibitive

QBX: 3D periodic scattering (prelim)

Doubly-periodic grating of sound-soft scatterers



Dirichlet obstacles

$$d = 2.4\lambda$$

$$N = 25200$$

(one obstacle)

$$p = 6.$$

QBX 4 min, laptop

$$p=6, P=8, \beta=4$$

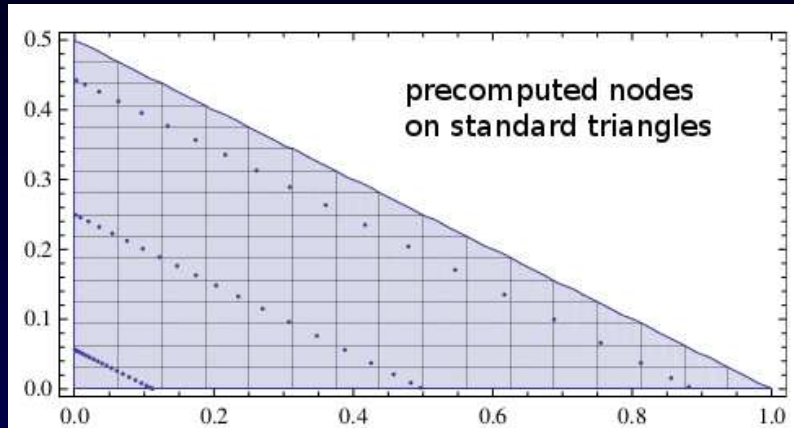
30 its 5 min

error 10^{-5}

- New periodizing scheme (Barnett–Gimbutas–Greengard, in prep.)

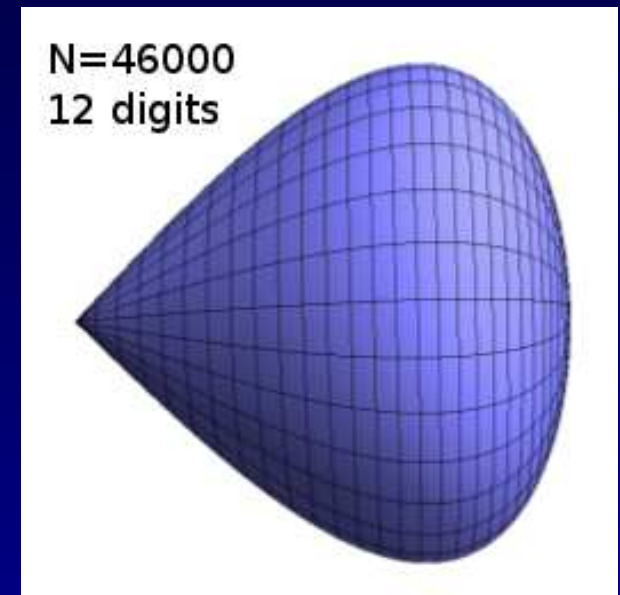
3D, Bremer–Gimbutas '12: triangle auxiliary nodes

Lots of precomputed nodes for various aspect triangles, kernels:



local correction (self & neighbors)
product grids in two parameters
polar coords removes $1/r$ singularity

Low-frequency Helmholtz Neumann BVP:



Research I: ongoing & what needs to be done

Complications (eg high-aspect ratio panels) in 3D, reducing constants

Edges and corners in 3D (Lintner–Bruno, Turc, Helsing, Bremer, ...)

– corner compression: turning 10^3 into 50 unknowns/corner

(Helsing, Bremer, Gillman–Martinsson, ...)

Other kernels: Stokes, elasticity, Maxwell, representations for topology

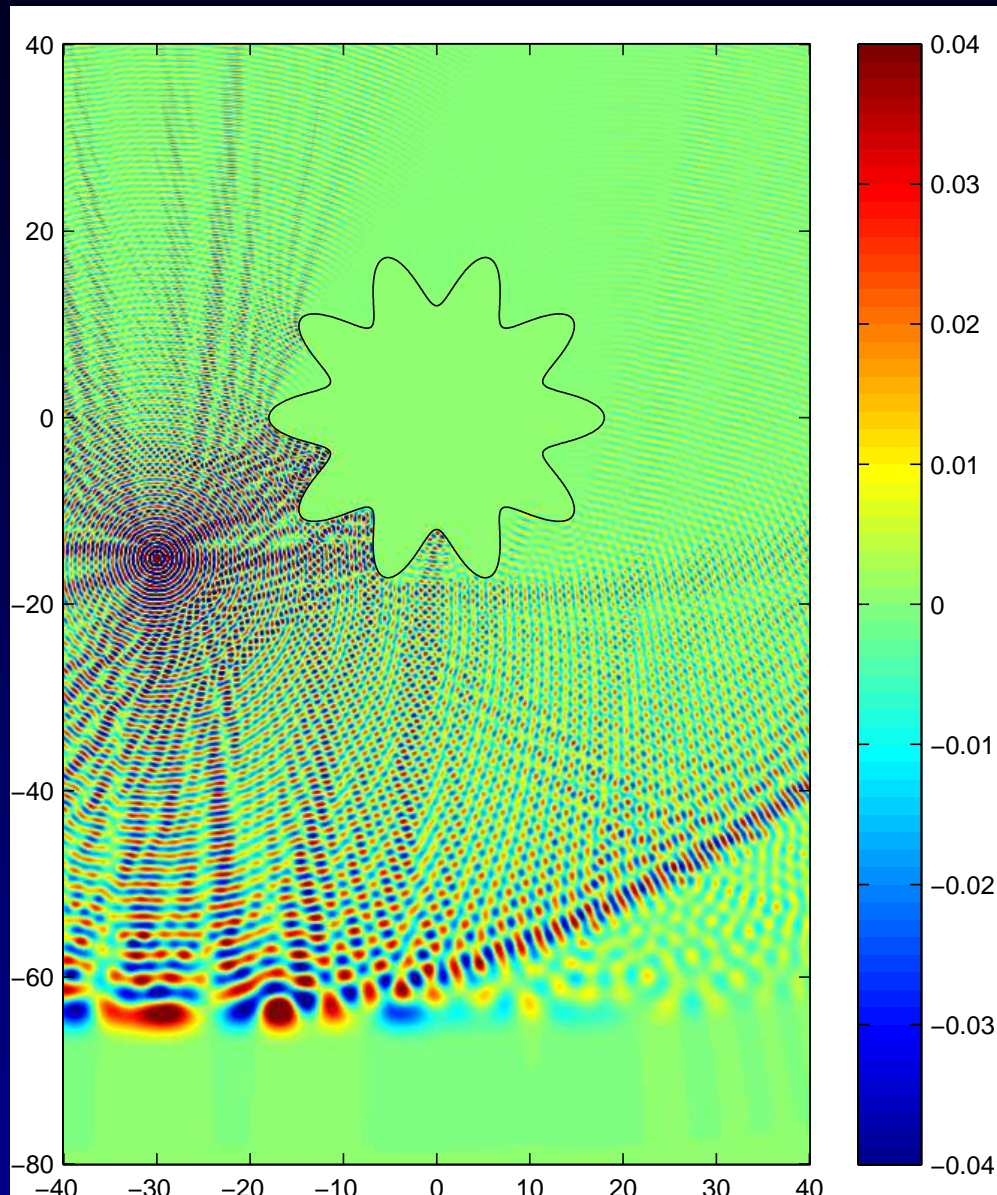
(Greengard+collabs, Veerapaneni, many ppl...)

Other BCs, hypersingular & Calderon precondition, time-domain (Sayas)

Software, 2D and 3D, quadrature and evaluation, documented!

Research II: variable-coeff PDEs

If you can evaluate the fundamental soln, you can do BIEs!



$$(\Delta + E + x_2)u(x_1, x_2) = 0$$

“gravity Helmholtz equation”

rays refract (bend) upwards

50λ diameter

$N = 1600$

PTR w/ 16th-order Alpert

err 10^{-12}

20 mins (fill)

w/ Brad Nelson '13



Research III: the local group



Lin Zhao
(grad student)

Nyström + Fredholm det for eigenvalue problems $-\Delta u = \lambda u$



Larry Liu
(grad student)

Axisymmetric bodies, Maxwell, periodic scattering



Adrianna Gillman
(Instructor)

Fast direct solvers, Poincaré-Steklov, corners, 3D, periodic, scattering



Min Hyung Cho
(Instructor)

Multi-layered media, Maxwell, volume integral equations

Say hello (& ask them research and local questions!)