Spectrally accurate direct solution of variable-media scattering problems via impedance maps

CIMS numerical analysis seminar 3/7/14

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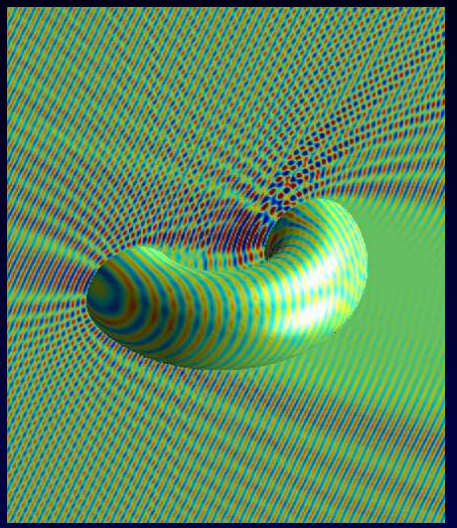
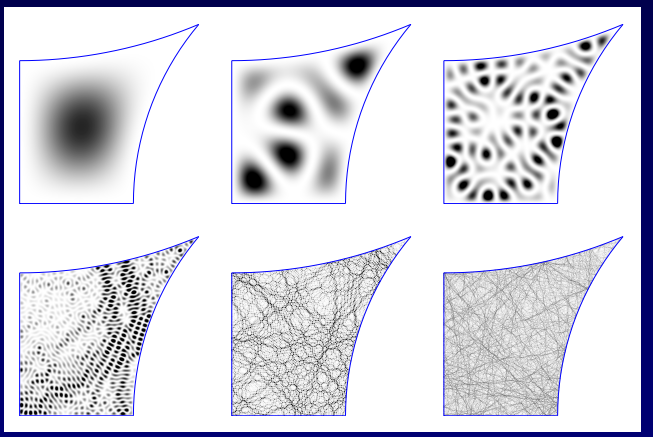
Collaborators: Adrianna Gillman (Dartmouth), Gunnar Martinsson (Boulder)

Barnett group research

- Numerical methods for scattering of waves
  - time-harmonic (frequency domain)
  - high-order accurate, “fast” algorithms
  - lattices, corners, variable media, 3D
  - now adapting methods for periodic Stokes

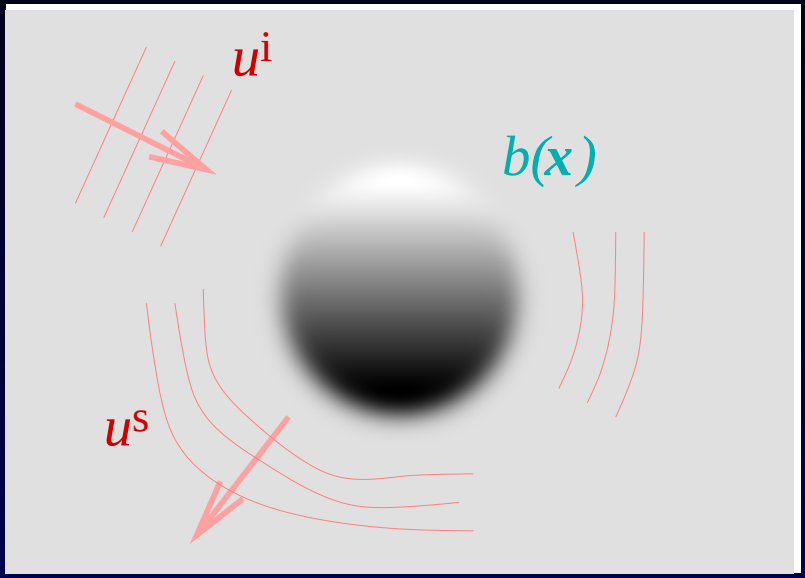


- Eigenvalue problems and quantum chaos
  - very high frequency methods
  - PDE & numerical analysis



- Other
  - neural signal processing, inverse problems
  - math of music, . . .

Variable-medium freq-domain scattering problem



incident wave u^{i}, frequency κ:

$$(\Delta + \kappa^2)u^{\mathrm{i}} = 0 \quad \text{in} \quad \mathbb{R}^2$$

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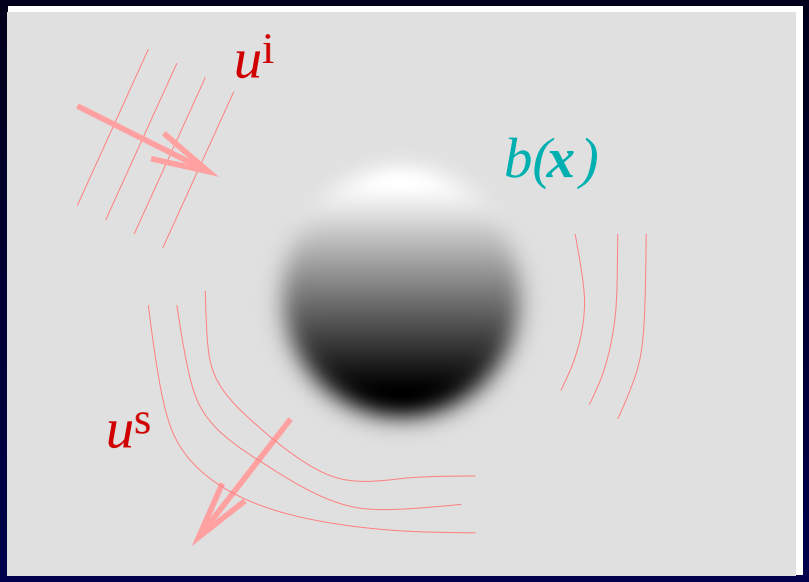

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total wave $u = u^{\mathrm{i}} + u^{\mathrm{s}}$ satisfies:

$$[\Delta + \kappa^2 (1 - b(\mathbf{x}))] u = 0 \quad \text{in} \quad \mathbb{R}^2$$

↖ scattering potential b

$\sqrt{1-b}$ 'slowness' (refractive index)

Scattered wave u^{s} radiative: $\frac{\partial u^{\mathrm{s}}}{\partial r} - i\kappa u^{\mathrm{s}} = o(r^{-1/2}), \quad r := |\mathbf{x}| \to \infty$

If $1 - b > 0$ everywhere, $\exists$ unique solution $\forall \kappa > 0$

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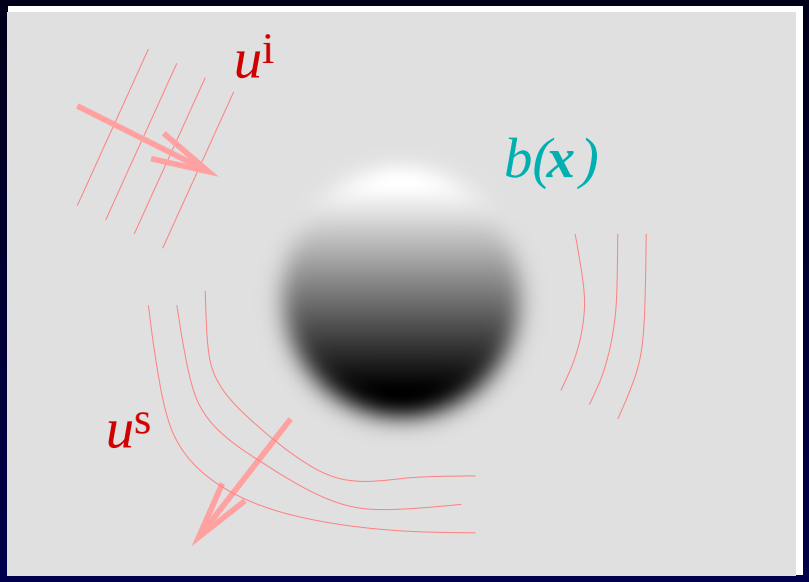

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- Applications: underwater acoustics, seismic imaging, ultrasound, quantum chemistry & physics, optics in graded index, metamaterials

Want: smooth b, high κ, multiple incident angles

Background

Fredholm integral equations:

given kernel $k(t,s)$, cont. for $s \neq t$, right-hand side cont. func. f,

solve for func. τ: $$c\tau(t) + \int_0^{2\pi} k(t,s)\tau(s)ds \;=\; f(t), \quad \forall t \in (0, 2\pi)$$

- if $c = 0$: 1st-kind, ill-posed. Discretize $\rightarrow$ ill-cond. as N grows
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nodes s_j, weights w_j s.t. $$\int_0^{2\pi} g(s)ds \;\approx\; \sum_{j=1}^{N} w_j g(s_j)$$

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- Solve 2nd-kind IE? Insert quadrature, then enforce solution at nodes $t = s_j$, $j = 1, \ldots, N$, get linear system $\boldsymbol{A\tau} = \boldsymbol{f}$ (Nyström '30)
- High order accurate schemes for k smooth easy; k singular harder

Background: potential theory

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

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

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

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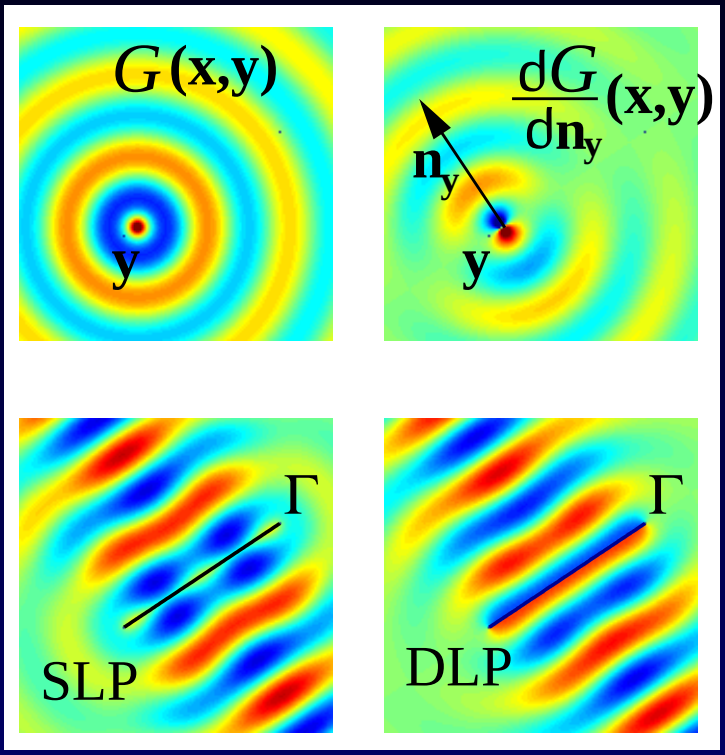
$$G(\mathbf{x},\mathbf{y}) := G(\mathbf{x}-\mathbf{y}) = \tfrac{i}{4}H_0^{(1)}(\kappa|\mathbf{x}-\mathbf{y}|)$$

kernel is Helmholtz fundamental soln

a.k.a. free space Greens func



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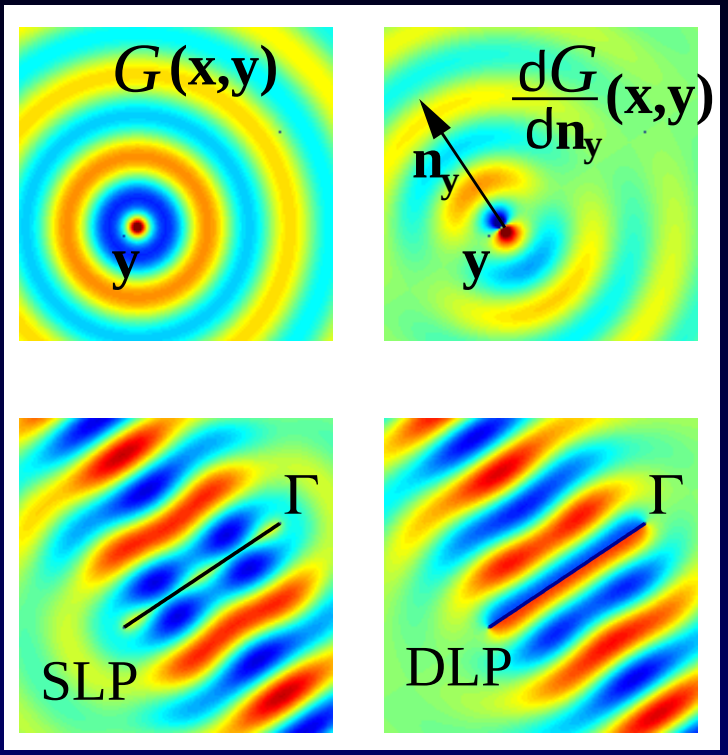

Jump relations: limit as $\mathbf{x} \to \Gamma$ can depend on which side ($\pm$):

$v^\pm = S\tau$ no jump

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

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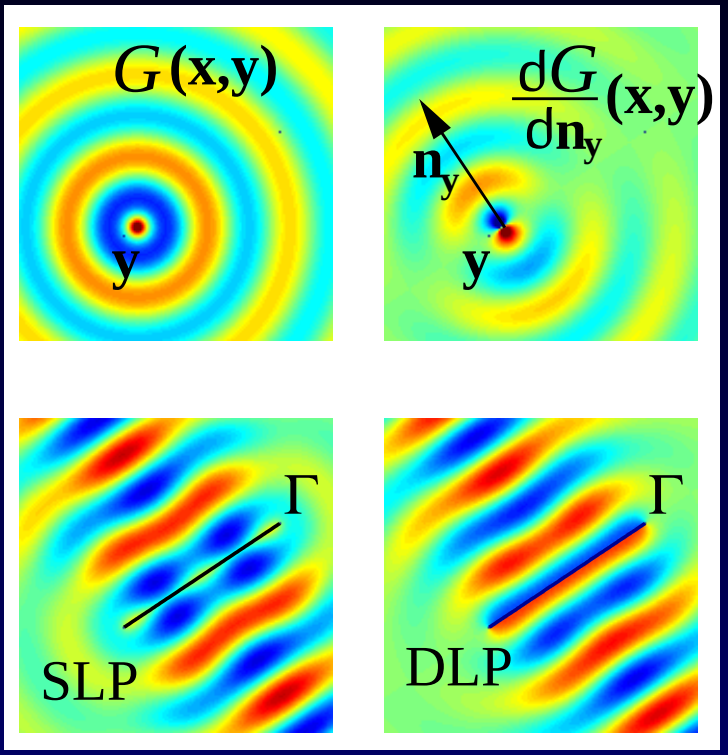

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Green's rep. outside a closed Γ, $u = \mathcal{D}u|_\Gamma - \mathcal{S}u_{n,\Gamma}$ u radiative Helm.

Coupling on enclosing box

Std: PDE for scatt. wave: $(\Delta + \kappa^2)u^{\mathrm{s}} - \kappa^2 b u^{\mathrm{s}} = \kappa^2 b u^{\mathrm{i}}$ ←inhomog.

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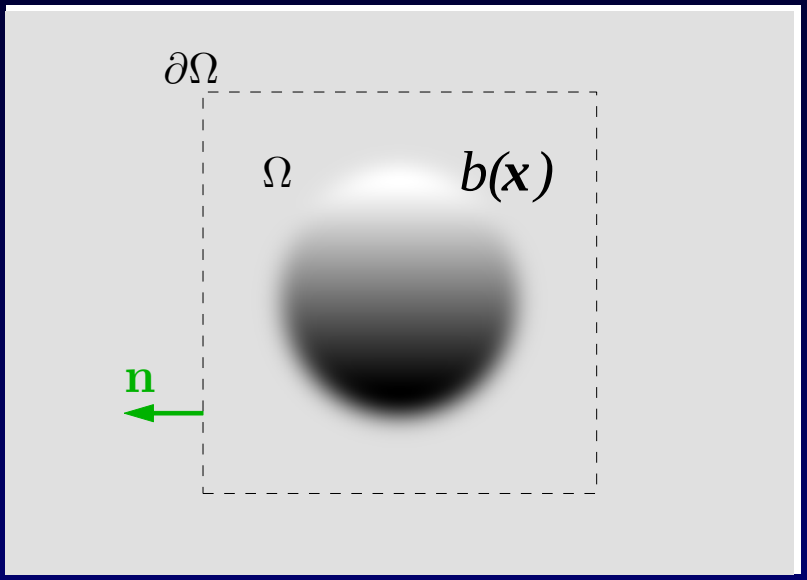

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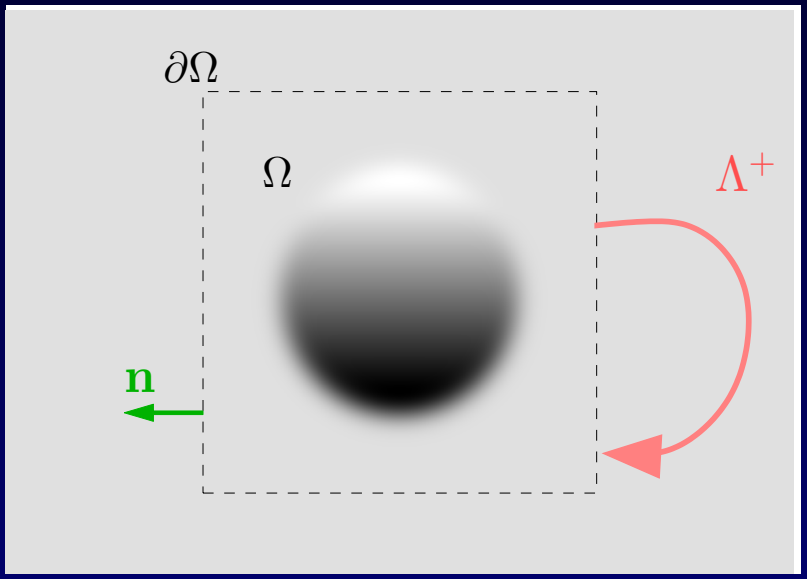

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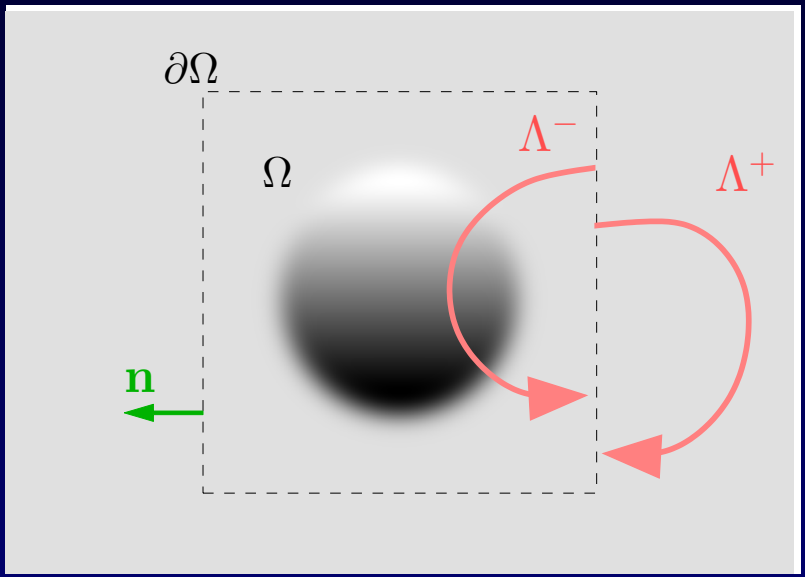

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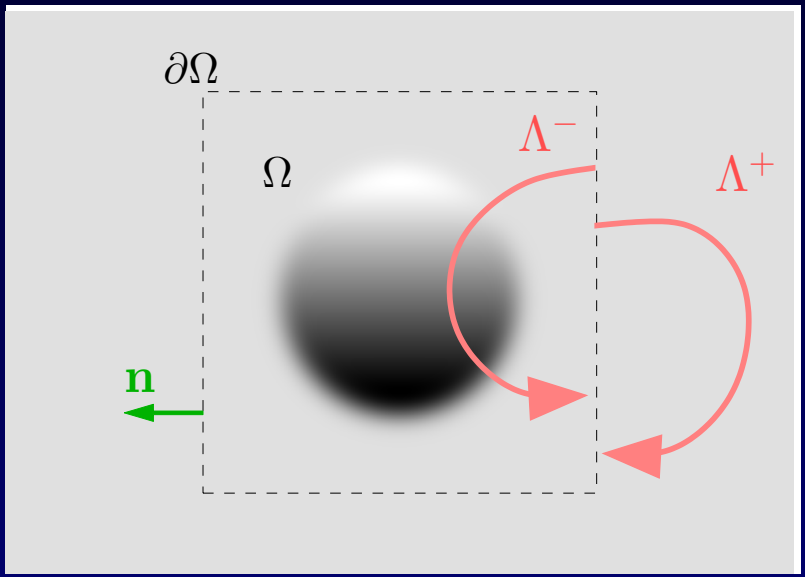

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(Kirsch–Monk '94, FEM coupling)

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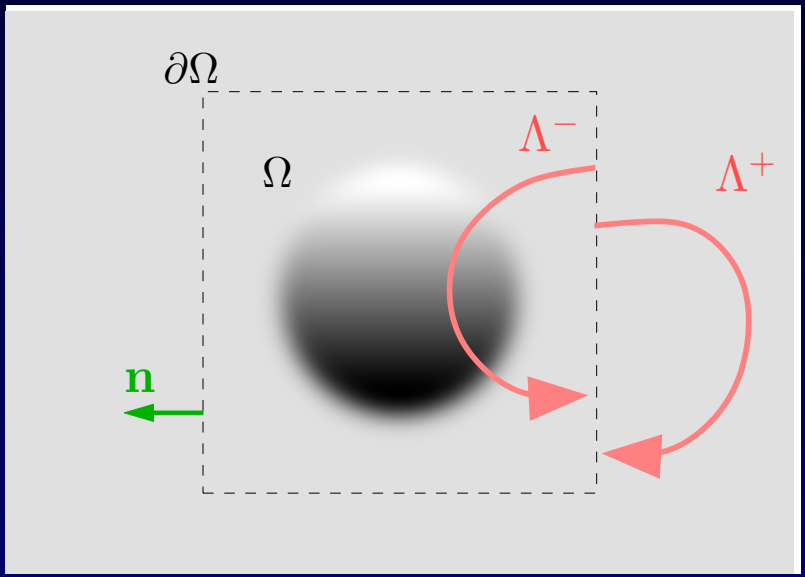

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↖ both order +1, signs *add* → ill-cond. → inversion would lose digits

2nd kind scattering formulation

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Left-regularize $(*)$ by S: $\qquad (\frac{1}{2} - D + S\Lambda^-)u^{\mathrm{s}}|_{\partial\Omega} \;=\; S(u^{\mathrm{i}}_n - \Lambda^- u^{\mathrm{i}}|_{\partial\Omega})$

Thm. Let $\partial\Omega$ be Lipschitz, $b(\mathbf{x})$ bnded, $0 < \kappa \neq \kappa_j$.

Then $A := \frac{1}{2} - D + S\Lambda^- = I +$ compact $\qquad$ above BIE is 2nd kind

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Pf. let $\mathcal{P} : L^2(\partial\Omega) \to L^2(\Omega)$ be interior solution operator: $u|_\Omega = \mathcal{P}u|_{\partial\Omega}$

$\mathcal{V} : L^2(\Omega) \to H^{1/2}(\partial\Omega)$ be volume potential $(\mathcal{V}\phi)(\mathbf{x}) = \int_\Omega \frac{i}{4} H_0^{(1)}(\kappa|\mathbf{x}-\mathbf{y}|)\phi(\mathbf{y})d\mathbf{y}$

$S\Lambda^- u|_{\partial\Omega} = Su_n = (\frac{1}{2} + D)u|_{\partial\Omega} + \kappa^2 \mathcal{V}(b \cdot \mathcal{P}u|_{\partial\Omega})$ G's 3rd id, $\forall u \in L^2(\partial\Omega)$

$\mathcal{V}b\mathcal{P}$ cpt by Sobolev imbedding $\nearrow$ (Lipschitz bdry: McLean '00) $\square$

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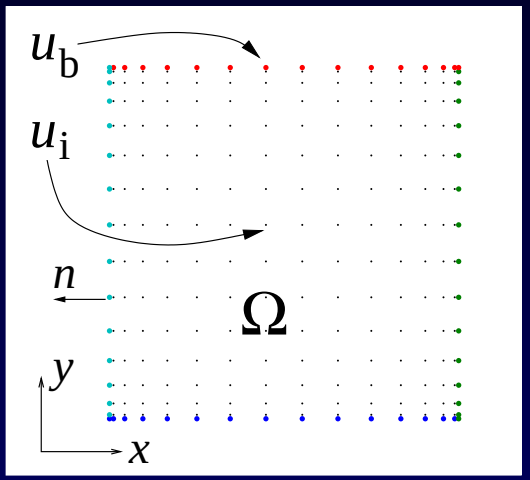
p^2 unknowns, vector $\boldsymbol{u} = \begin{bmatrix} u_\mathrm{b} \\ u_\mathrm{i} \end{bmatrix}$ ← boundary ← interior

$p^2 \times p^2$ spectral diff. matrices D_x, D_y act on $\boldsymbol{u}$

matrix $H = D_x^2 + D_y^2 + \kappa^2 \mathrm{diag}\{1 - b(\mathbf{x}_j)\}$

$H_{\mathrm{i},:}$ = rows of H imposing PDE at interior nodes



system $B\boldsymbol{u} := \left[\begin{array}{cc} I & 0 \\ \hline H_{\mathrm{i},:} \end{array}\right] \begin{bmatrix} u_\mathrm{b} \\ u_\mathrm{i} \end{bmatrix} = \begin{bmatrix} \boldsymbol{f} \\ 0 \end{bmatrix}$ ← Dirichlet BC (trivial) ← PDE at interior nodes

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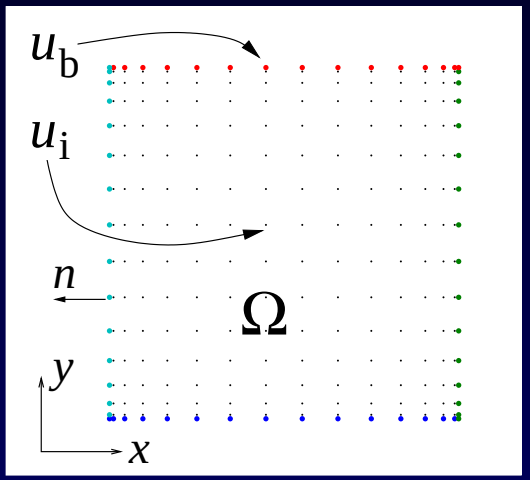

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solution matrix X, maps $\boldsymbol{f}$ to $\boldsymbol{u}$: solve $BX = \begin{bmatrix} I \\ 0 \end{bmatrix}$ dense, $O(p^6)$

Get approx. Λ^-: X left-mult. by rows of D_x, D_y to take normal deriv.

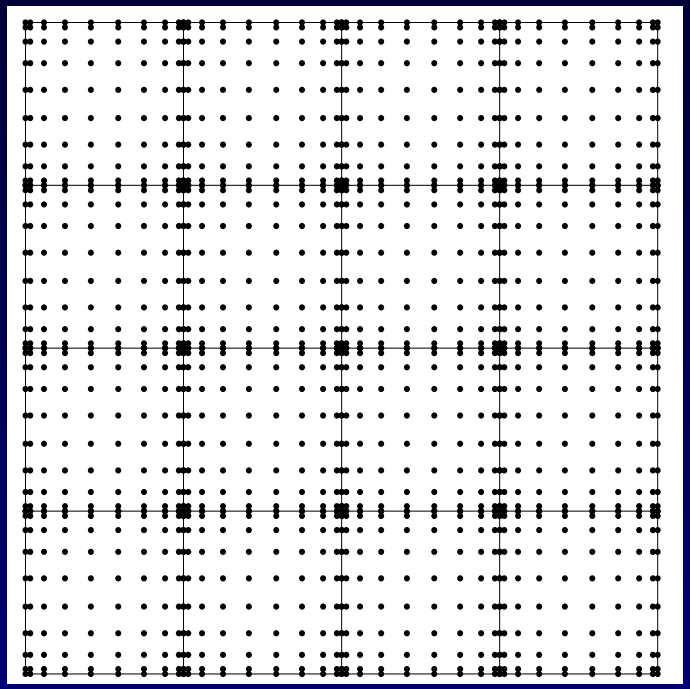
How build Λ^- for "large" scatterer?

One-box dense scheme was $O(p^6)$ terrible if need more resolution

Partition top-level box Ω into 2^L-by-2^L small square "leaf" boxes

Give each box p^2 spectral product nodes as before total unknowns $= N$

Here's $L = 2$:



How build Λ^- for "large" scatterer?

One-box dense scheme was $O(p^6)$ terrible if need more resolution

Partition top-level box Ω into 2^L-by-2^L small square "leaf" boxes

Give each box p^2 spectral product nodes as before total unknowns $= N$

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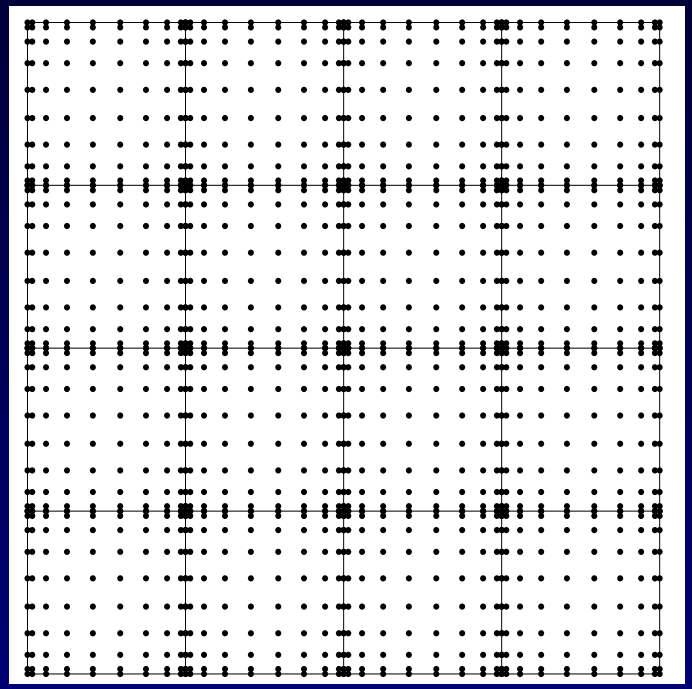
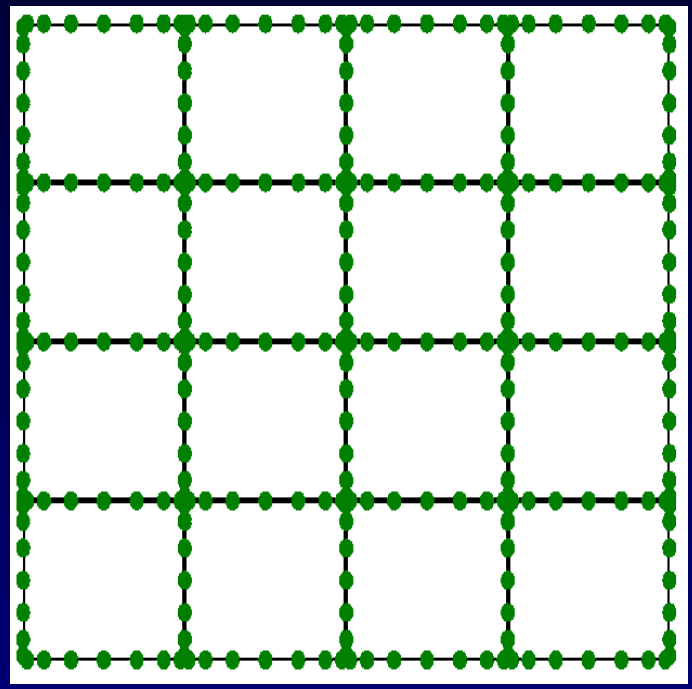


$\rightarrow$



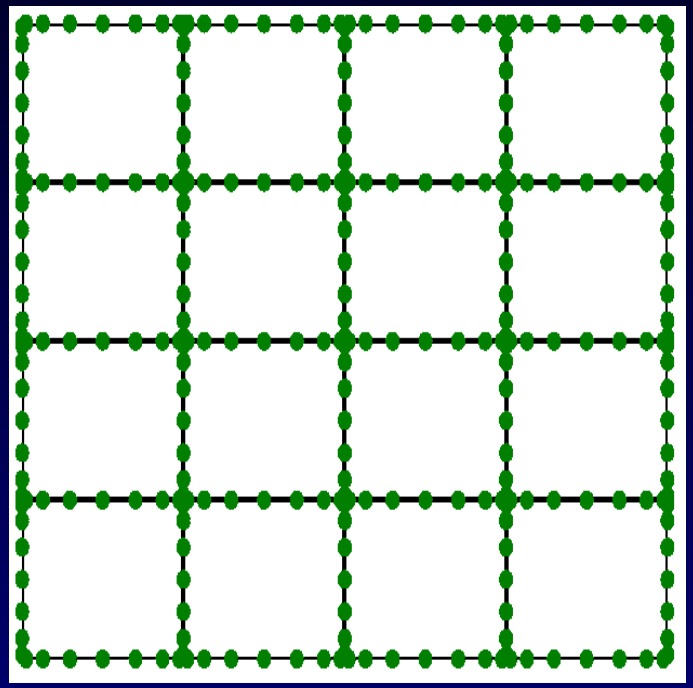
Step 1: build Λ^- for each box separately fix $p \approx 16$ effort $O(N)$

Merging leaf DtN operators

Can eliminate unknowns on common edge of two neighboring boxes

Creates Λ^- matrix for union of the boxes

dense inverse, $O(p^3)$



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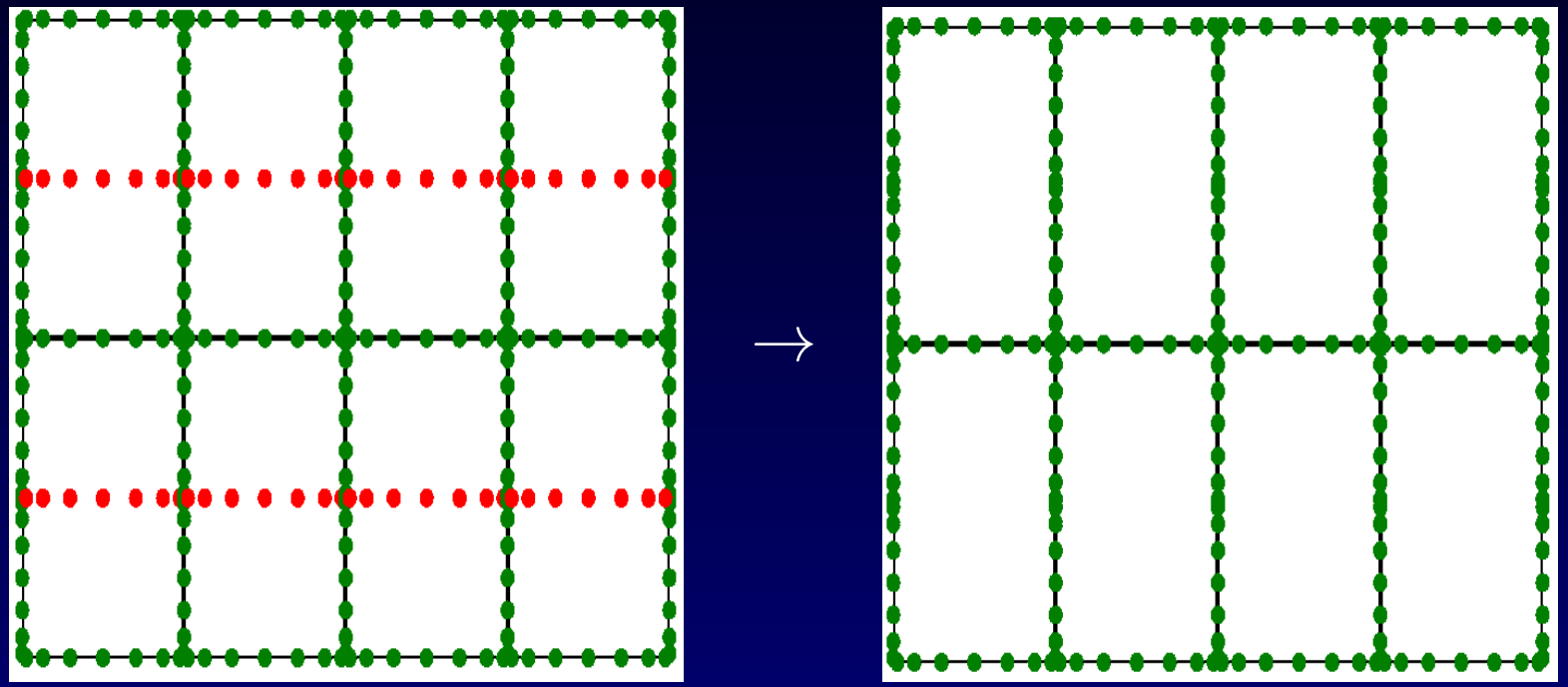

Now repeat: this is *upwards sweep* of the quad-tree...

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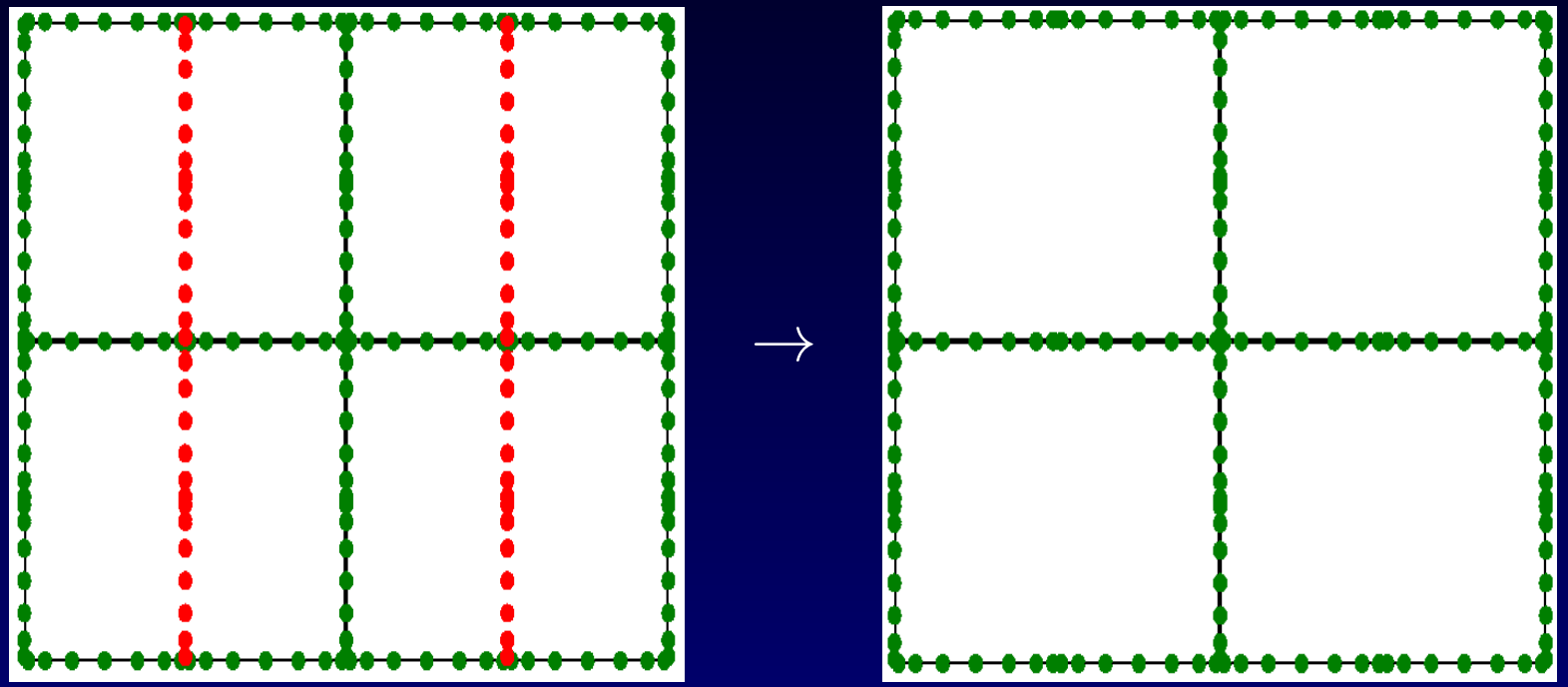

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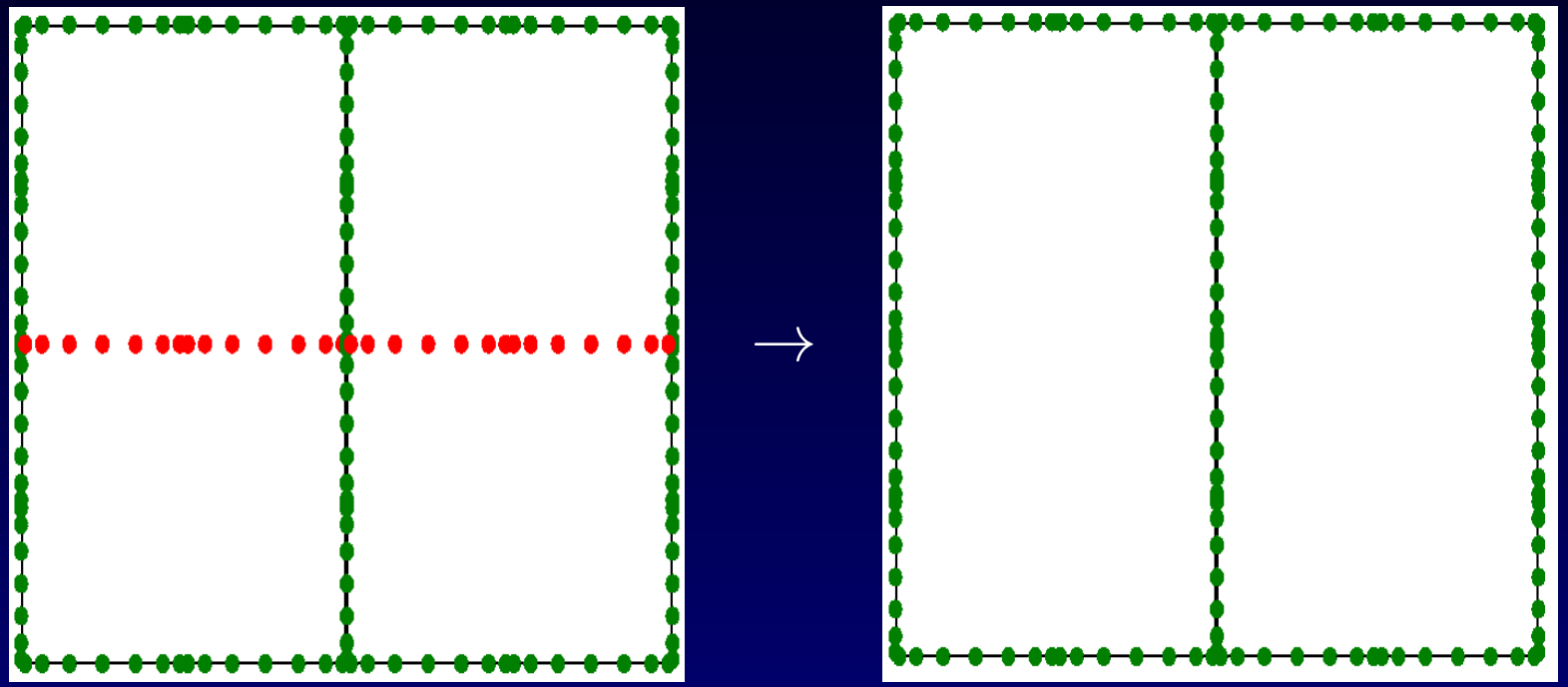

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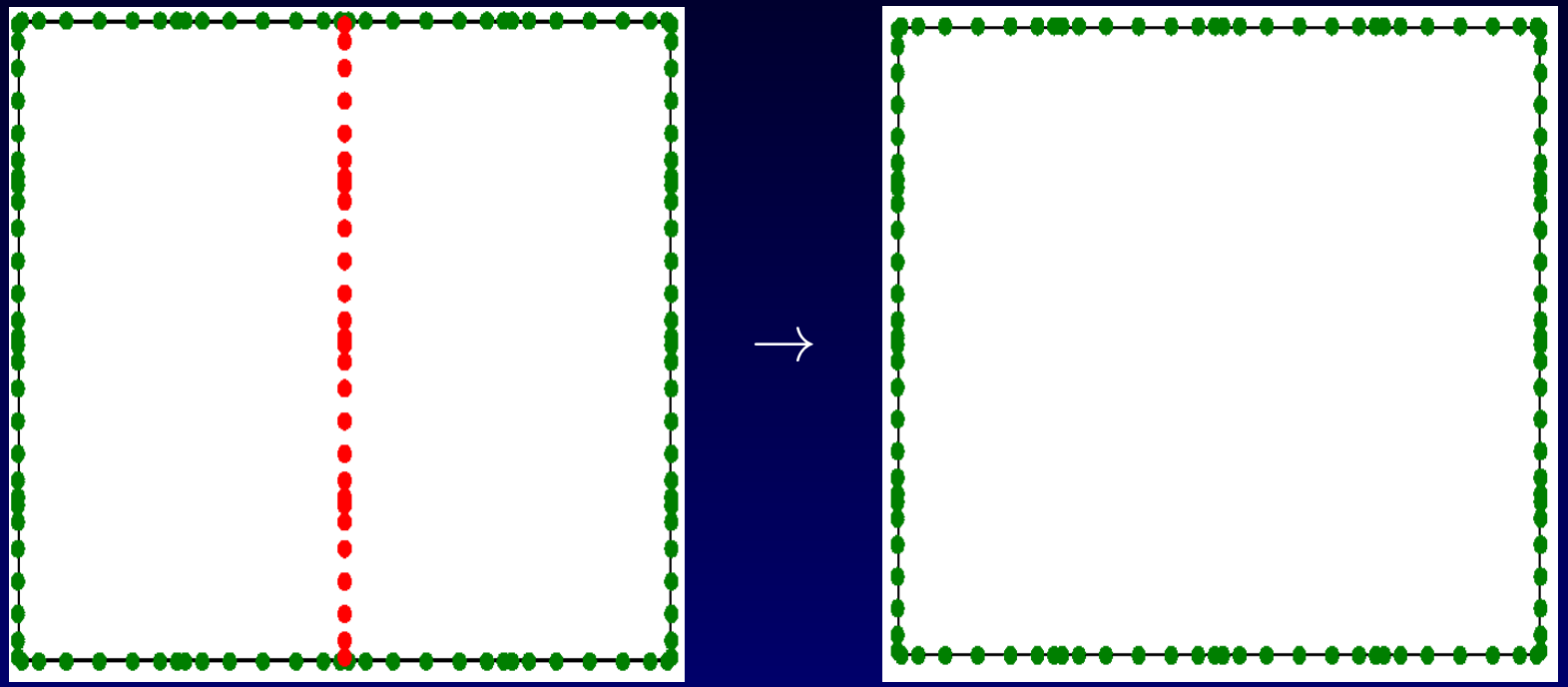

Top-level merge is $\frac{1}{2}$ total effort: $O(N^{1/2})$ dense inverse effort $O(N^{3/2})$

We now have matrix approx. to Λ^- on edge nodes of entire box

Details: actually we use Gauss–Legendre nodes; no corner refinement (soln. u smooth)

Problem: interior DtN resonances

Recall: DtN does not exist at discrete set of Dirichlet eigenfreqs. $\kappa = \kappa_j$

$\Rightarrow$ numerically not robust: DtN norm blows up near κ_j, lose digits

Every leaf *and merged box* has own (upredictable, b-dependent) eigenfreqs!

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Remedy, use $R : L^2(\partial\Omega) \to L^2(\partial\Omega)$ impedance-to-impedance map

fix η real, let $\begin{cases} f := u_n + i\eta u|_{\partial\Omega} & \text{“incoming”} \\ g := u_n - i\eta u|_{\partial\Omega} & \text{“outgoing”} \end{cases}$ then, $Rf = g$

classical facts: R exists for all κ. R is *unitary*.

Instead build ItI for all leaves upper block of B now: D_x, D_y rows + $[i\eta I \quad 0]$

Hierarchical ItI merge operations: max cond. # now 20 not 2×10^5

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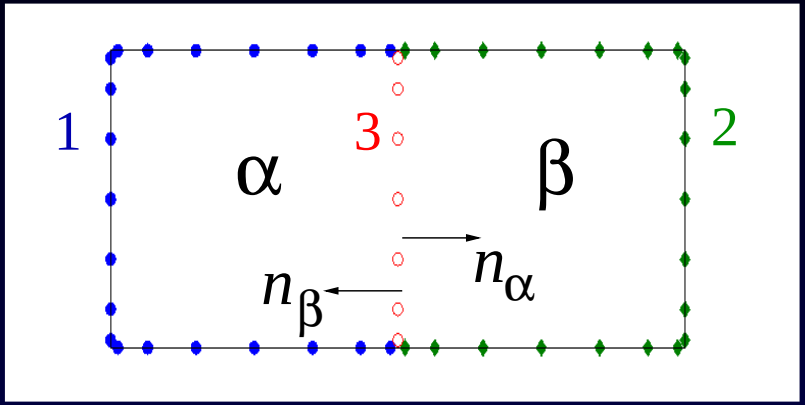
Then convert top-level ItI to DtN:

Cayley transform $\Lambda^- = -i\eta(R - I)^{-1}(R + I)$ $O(N^{3/2})$

ItI merge step for two boxes



1 = nodes only on α
2 = nodes only on β
3 = shared nodes

u, u_n match on edge 3

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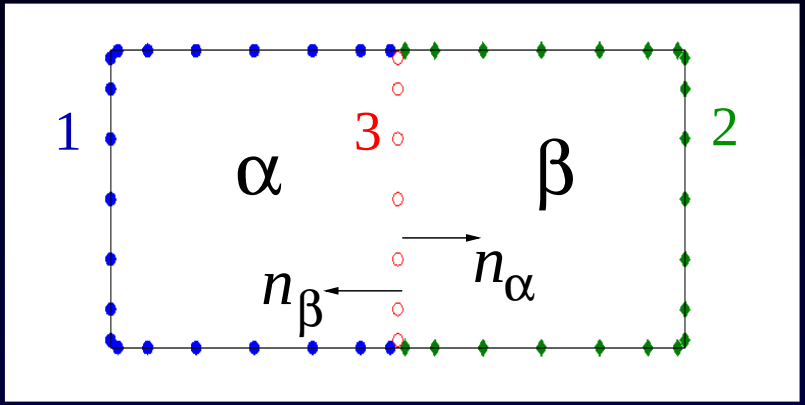

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Write edge 3 part of ItI relation $Rf = g$ in each box:

$$R^\alpha_{31} f_1 + R^\alpha_{33} f^\alpha_3 = g^\alpha_3 = -f^\beta_3 \qquad \text{by matching, normals opposed} \quad (2)$$
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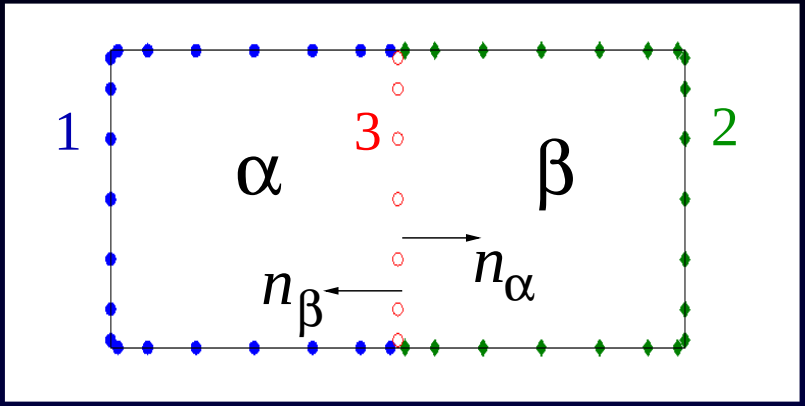

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Elim. f^α_3: $\quad f^\beta_3 = F^\beta \begin{bmatrix} f_1 \\ f_2 \end{bmatrix}, \quad F^\beta := (1 - R^\alpha_{33} R^\beta_{33})^{-1} [-R^\alpha_{31} \quad R^\alpha_{33} R^\beta_{32}]$

also $\quad F^\alpha := [0 \quad -R^\beta_{32}] - R^\beta_{33} F^\beta,$

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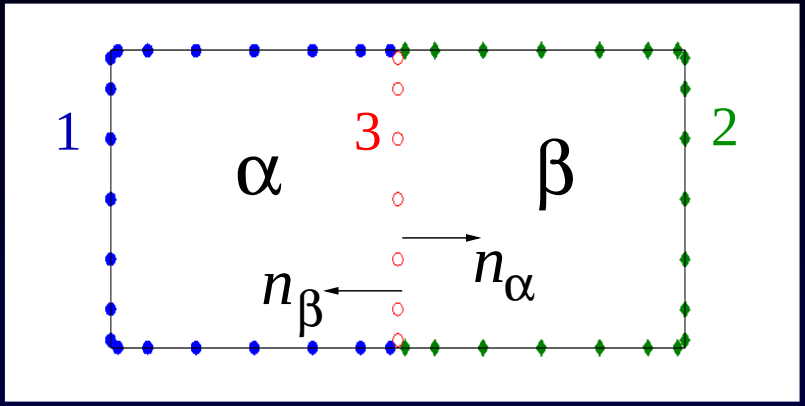

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also $\quad F^\alpha := [0 \;\; -R^\beta_{32}] - R^\beta_{33} F^\beta, \qquad$ then $\quad R = \begin{bmatrix} R^\alpha_{11} & 0 \\ 0 & R^\beta_{22} \end{bmatrix} + \begin{bmatrix} R^\alpha_{13} F^\alpha \\ R^\beta_{23} F^\beta \end{bmatrix}$

Summary of direct scattering solver

Pre-computation:

1) Nyström discretization of S, D at $n = O(N^{1/2})$ nodes on $\partial\Omega$

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6) eval. u inside Ω via reversing all merges, traverse down the tree

matvecs with soln. matrices F^α, etc, created during merges $O(N \log N)$

Relation to prior work

Existing methods for variable-medium scattering:

- time-domain (FDTD): low-order, dispersion errors, long settling time
- freq-domain: low κ or low accuracy, e.g. . .

  FEM-BIE coupling, low κ, precond. BIE, 3 digits (Kirsch–Monk '94)
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Our influences:

- multi-domain spectral collocation (Orszag, Patera, '80s; Hesthaven, Pfeiffer)
- direct solvers for block-sparse: nested dissection, multifrontal (George, Duff, '70s)
- $O(N)$ direct solvers (Martinsson–Rokhlin '05, Xia–Chandrasekaran–Gu–Li '09)
- $O(N^{3/2})$ direct solver using both u and u_n data (Chen '02, '13)
- DtN version (Martinsson '12); ItI makes robust for oscillatory PDE

Results: time and memory

8-core Xeon, MATLAB, not optim!

t_{pre} precomputation: build DtN, build A, dense A^{-1}

$t_{\text{new ext}}$ compute $u^{\text{s}}|_{\partial\Omega}$, u^{s}_n for new incident wave (ext. / far field)

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$L =$ # tree levels $N =$ # unknowns $n =$ # BIE unknowns

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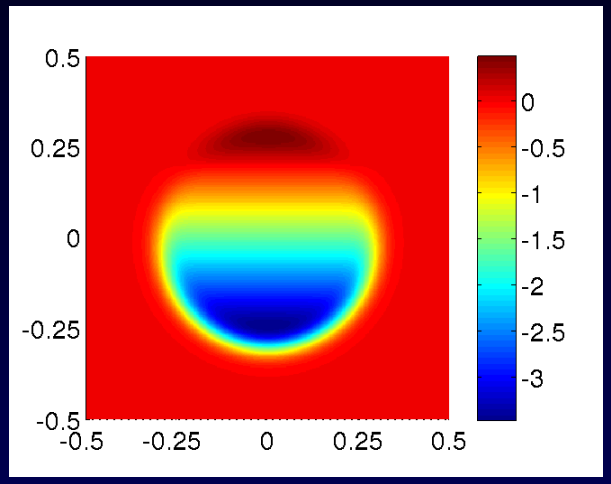
L	N	n	t_{pre}	$t_{\text{new ext}}$	$t_{\text{new int}}$	RAM
4	58081	1120	5 s	0.006 s	0.04 s	230 MB
5	231361	1760	17 s	0.013 s	0.16 s	1 GB
6	923521	3040	78 s	0.05 s	0.7 s	5 GB
7	3690241	5600	6 m	0.16 s	2.7 s	22 GB
8	14753281	10720	22 m	0.5 s	10 s	96 GB

- precomp. time close to $O(N)$, not yet reached $O(N^{3/2})$
- RAM is $O(N \log N)$ $\sim$ 400 complex doubles per unknown

Convergence: graded-index lens, high frequency

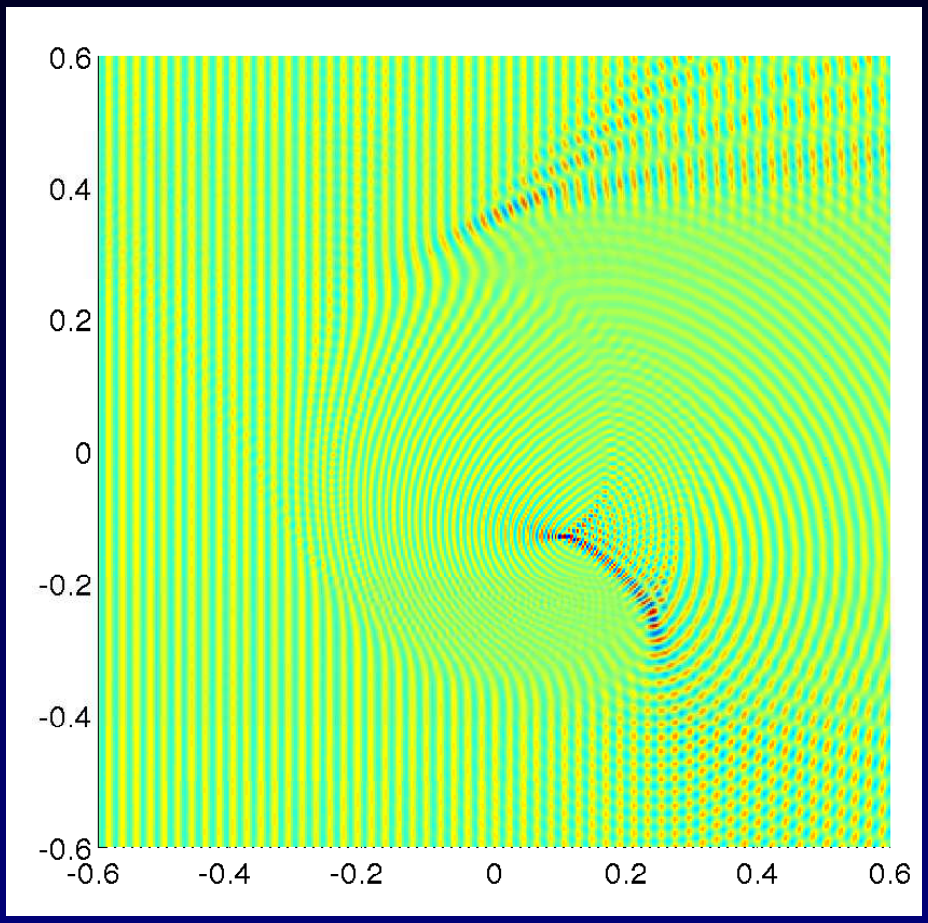
plane wave $u^{\mathrm{i}}(\mathbf{x}) = e^{i\kappa \boldsymbol{d}\cdot\mathbf{x}}$ $\quad \boldsymbol{d} = (\cos\theta, \sin\theta)$ $\quad \kappa = 300$ $\quad$ 100 shortest-λ's

$b(\mathbf{x})$:



N	ppw	error	t_{pre}
2.3e5	5	3e-3	17 s
9e5	10	2e-7	78 s
3.7e6	20	7e-10	6 m

high-order $\quad$ ptwise err rel. to N=1.4e7

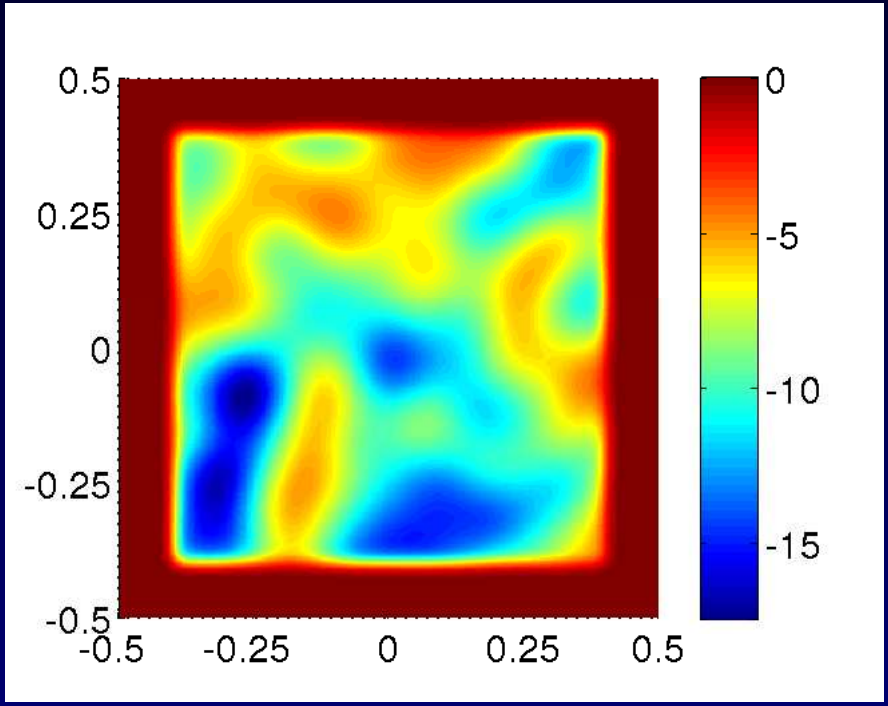


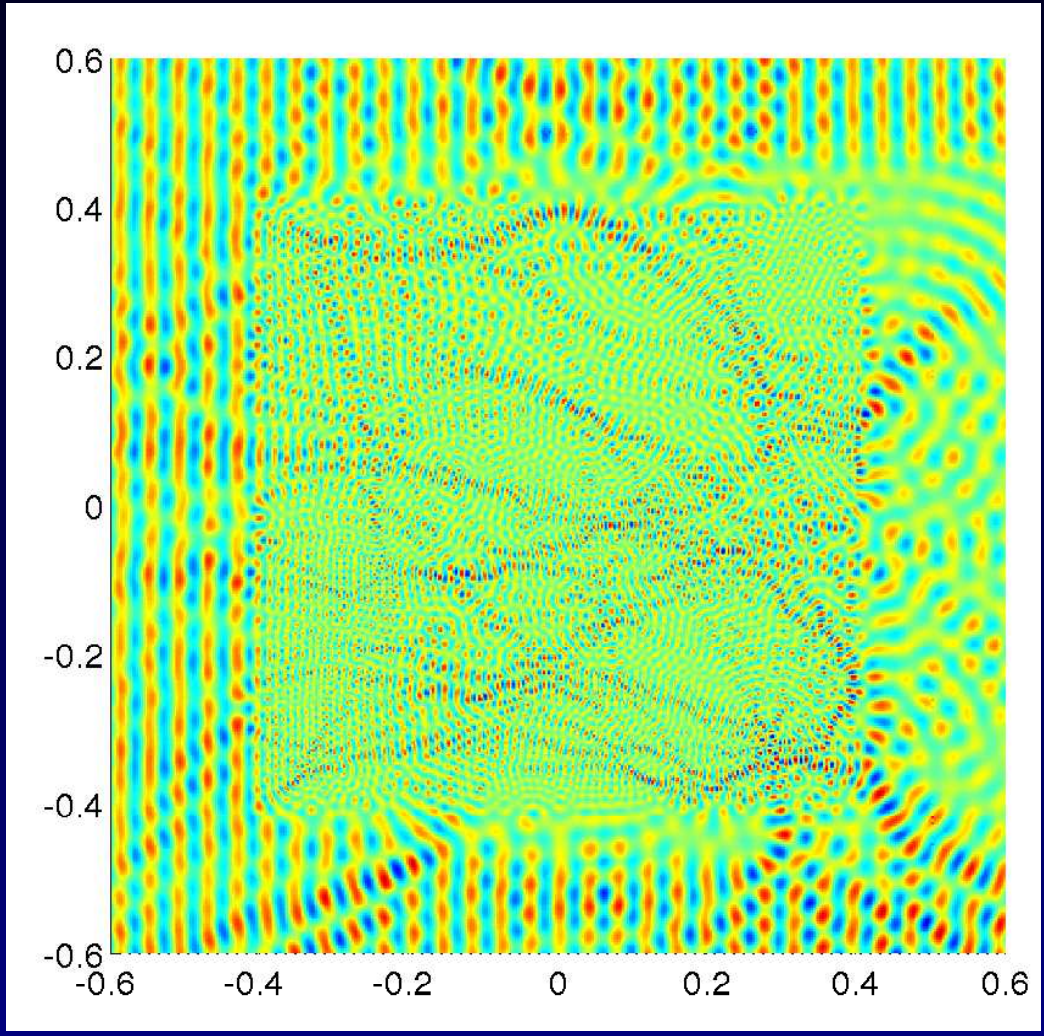
movie $\quad 10^3$ angles θ, $\quad$ 3 s each, $\quad$ incl. FMM to 240000 ext. targets

"Bathroom glass" at high frequency

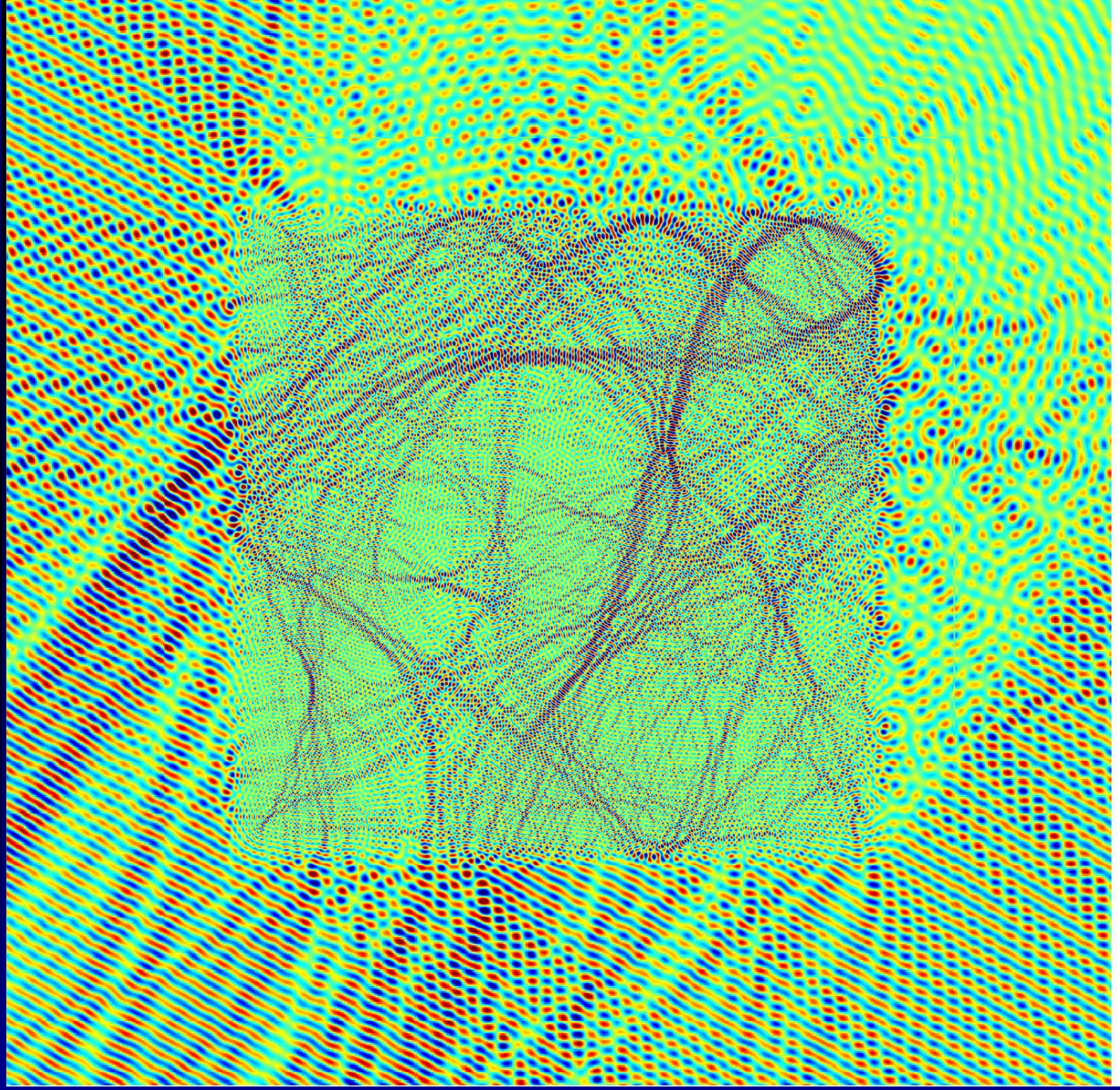
$b(\mathbf{x})$ = random smooth, rolled-off to zero

physics: "2D electron gas"





80λ on a side time & accuracy similar to before movie twinkling



$k = 320$

200λ across

9 digits (est.)

$N = 1.4\text{e}7$

$t_{\text{pre}} = 22$ min

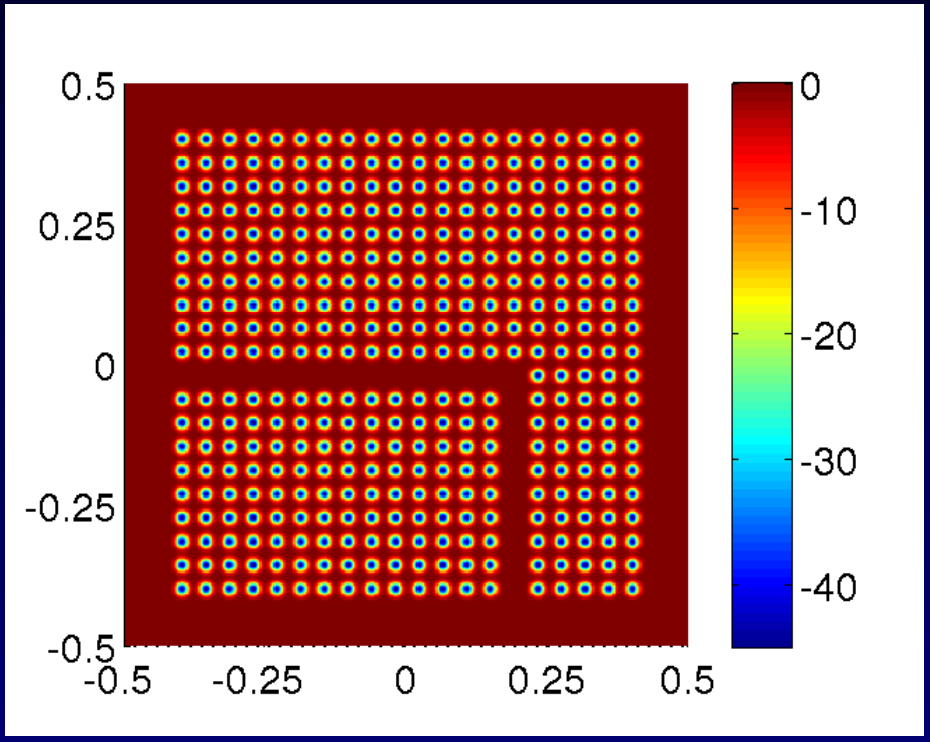
$t_{\text{new far}} = 0.5$ s

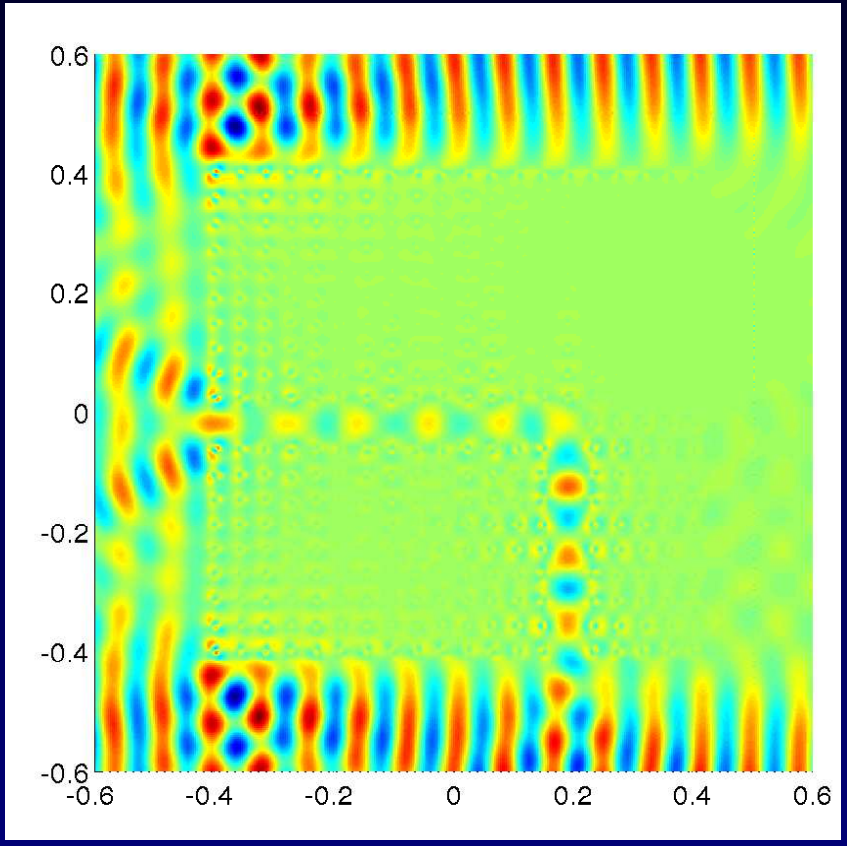
$t_{\text{new int}} = 10$ s

Photonic crystal waveguide

Until now largely propagating—what if resonances trap waves?

lattice of 400 bumps, each a resonator: choose κ in *bandgap* (can't prop.)





Again, 9 digits $N = 3.7\text{e}6$

- also test radially-symmetric $b(\mathbf{x})$ vs sep. of var. soln: stops at 10 digits

Conclusions

$O(N^{3/2})$ direct solver: multiple incident waves at same κ *very* fast

$N \sim 10^7$, 9 digits @ 200 λ, 100 GB, 20 mins, 0.5 s per u^{i}, close to $O(N)$

We made robust:
- new proven 2nd-kind BIE
- avoided all box resonances via ItI not DtN

Variants & improvements:

- adaptivity, 3D (Martinsson group); cut leaves, volume source?
- $O(N)$ low-κ DtN version: F^α's low rank, HBS (Gillman–Martinsson '13)
- $O(N)$ high-κ via butterfly compress F^α's, R's ?? $N > 10^8$ 1 TB RAM
- avoid top-level DtN? test a 2nd-kind ItI coupling

Gillman–B–Martinsson, *subm.* BIT '13

Preprints, talks, movies:

funding: NSF DMS-1216656

http://math.dartmouth.edu/∼ahb

2014 CBMS-NSF Conference:

Fast Direct Solvers for Elliptic PDEs

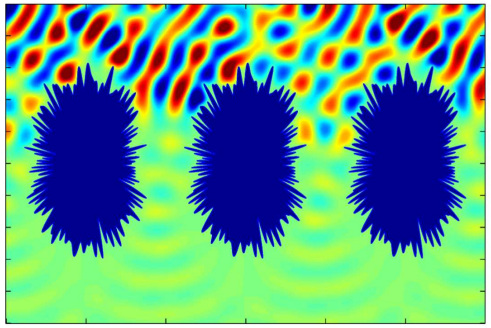
June 23 – 27, 2014, at Dartmouth College, Hanover, NH

Lecturer:

Per-Gunnar Martinsson (U. Colorado Boulder)

Speakers:

Alex Barnett (Dartmouth)
Adrianna Gillman (Dartmouth)
Leslie Greengard (Simons Foundation and NYU)
Vladimir Rokhlin (Yale)



Conference themes:

- Direct solvers with $O(N)$ complexity.
- Randomized methods for linear algebra.
- High-accuracy discretizations.
- Communication minimizing algorithms.
- Integral equation formulations.

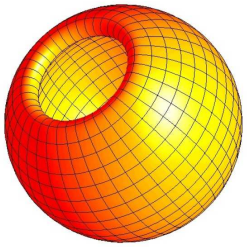
Application deadline: April 15th

Conference format: 10 lectures surveying the conference themes will be delivered by Per-Gunnar Martinsson of the University of Colorado. Participants will be given an opportunity to interact hands-on with the algorithms described through coding workshops using tutorial style software. Supplementary lectures on current research will be delivered by scientists in the field.

Workshop: The conference will be followed by a weekend workshop on the topic of fast analysis based methods for elliptic PDEs on June 28-29.

Support: Lodging, meals, and some travel expenses will be provided for up to 30 participants. Graduate students, junior researchers, and members of underrepresented groups are particularly encouraged to apply.

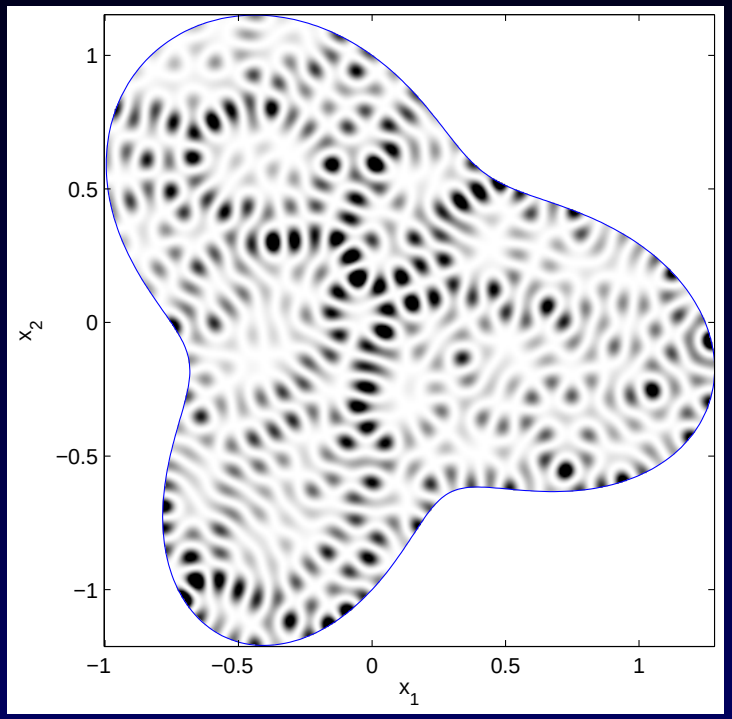
Website: http://www.math.dartmouth.edu/∼fastdirect



Teasers of other ongoing projects. . .

I. Bounds and methods for Neumann eigenvalues

(w/ A. Hassell)



$$-\Delta v_j = k_j^2 v_j \quad \text{in} \quad \Omega \subset \mathbb{R}^2 \quad \text{Helmholtz}$$

$$\partial v_j / \partial n = 0 \quad \text{on } \partial\Omega$$

$$||v_j||_{L^2(\Omega)} = 1$$

care about k_j large

- If v Helm. w/ freq. k, and $\partial v/\partial n$ "small", can we bound $k - k_j$?
- Use flow vs k of eigenvalues of DtN Λ^- to find eigenpairs?

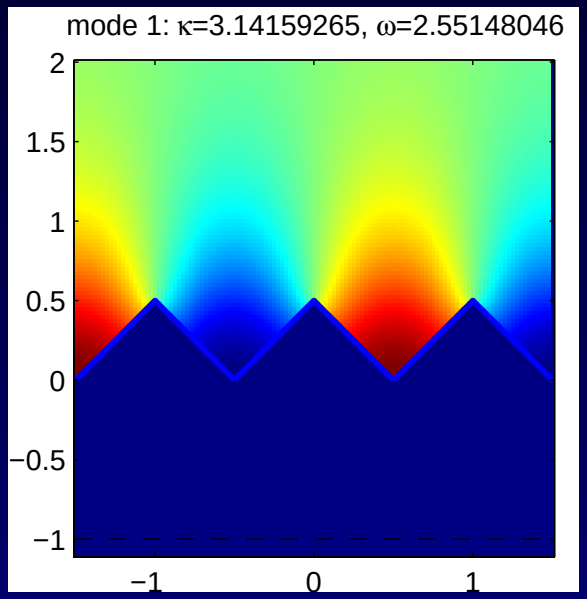
Harder than Dirichlet since $\|v_j\|_{L^2(\partial\Omega)} = O(k^{1/3})$; need study $\sqrt{k^2 - \Delta_{\partial\Omega}}v_j$

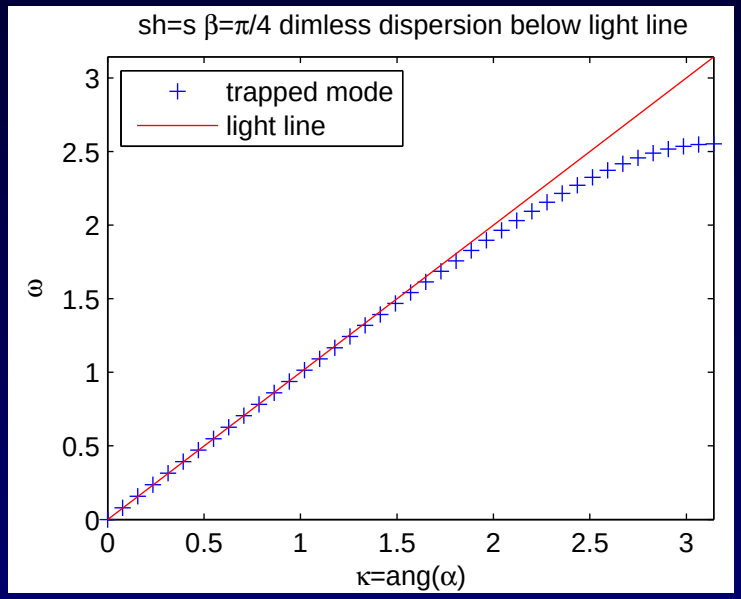
II. Acoustic surface modes of periodic structures

(w/ E. Heller)

Footsteps on staircases at Mayan pyramid sound like *raindrops*! Why?

- each freq. travels at own group velocity $\rightarrow$ impulse becomes *chirp*





- integral formulation, periodizing via least-squares collocation on a box
- dispersion curves to spectral accuracy, via Boyd's analytic rootfinding

III. Stokes 2D close-evaluation quadratures

(w/ S. Veerapaneni, B. Wu)

- global & panel-based schemes, built on Laplace potentials & gradients
- extend Laplace global (Helsing–Ojala '08) to single-layer case...

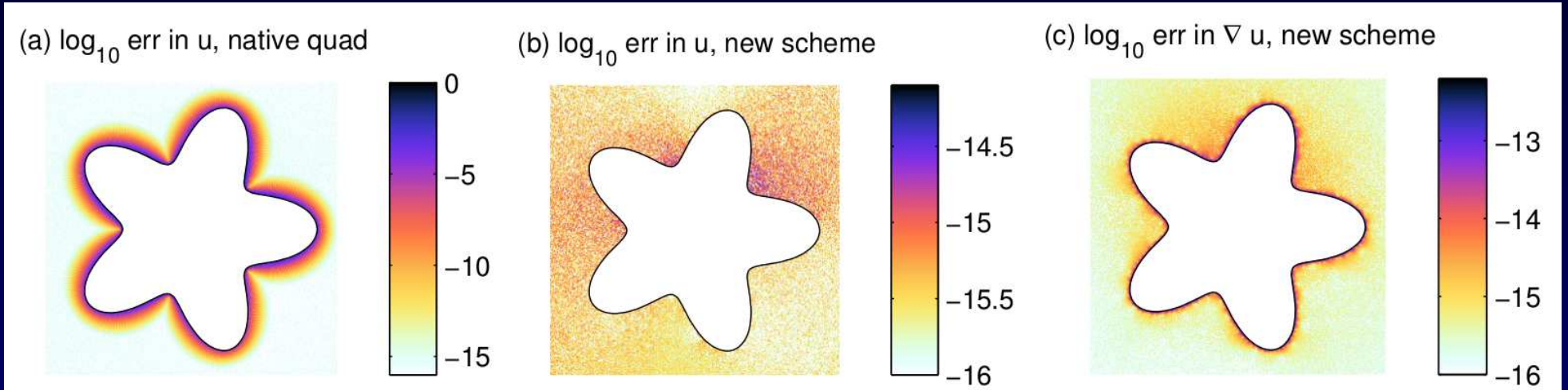


FIG. 4.1. *Evaluation error for the Laplace single-layer potential on a grid exterior to the closed curve* Γ

- Fix round-off instability in usual 1st derivative of barycentric form