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

Banff 12/10/13

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

First a teaser of projects that are *not* the topic of the talk…

I. 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...

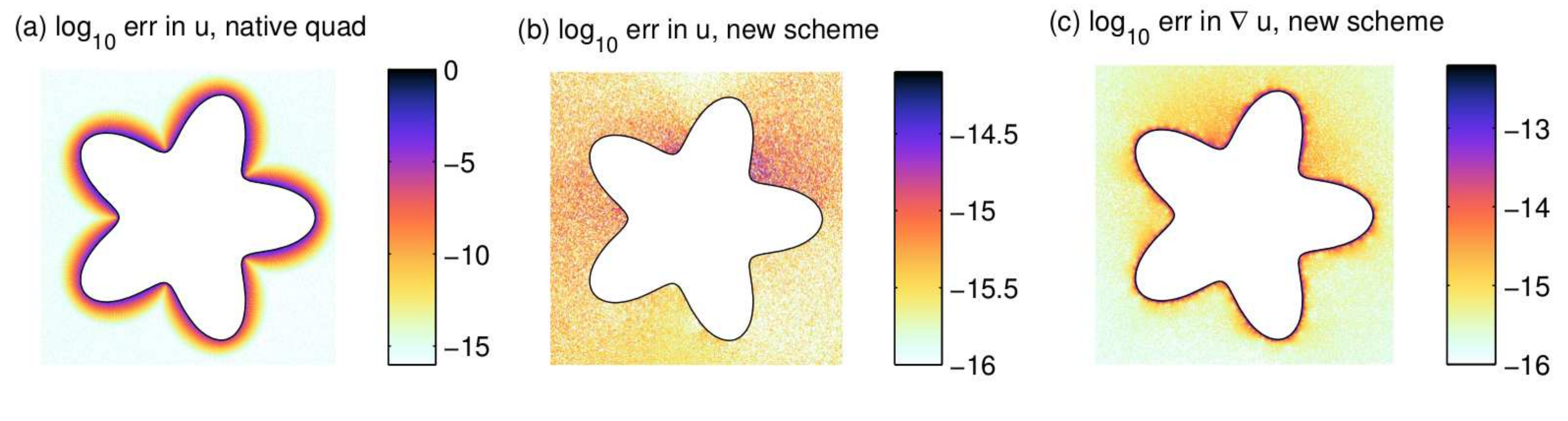


FIG. 4.1. *Evaluation error for the Laplace single-layer potential on a grid exterior to the closed curve* Γ

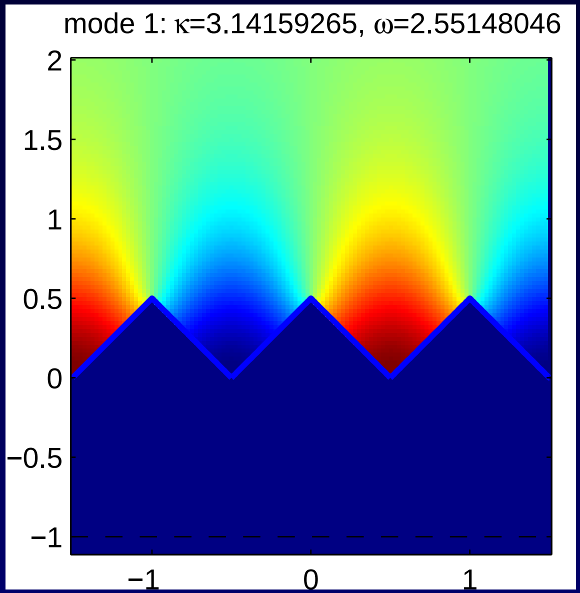
- Fix round-off instability in usual 1st derivative of barycentric form

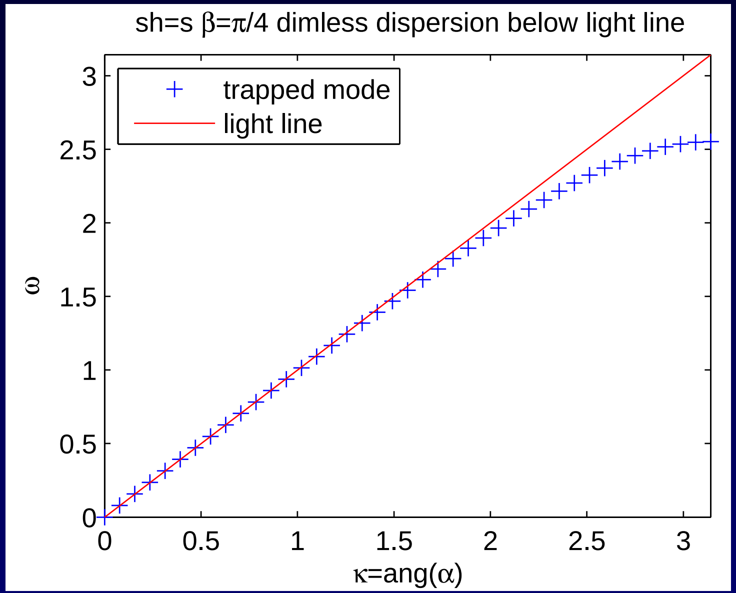
II. Acoustic surface modes of periodic structures

(w/ E. Heller)

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

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



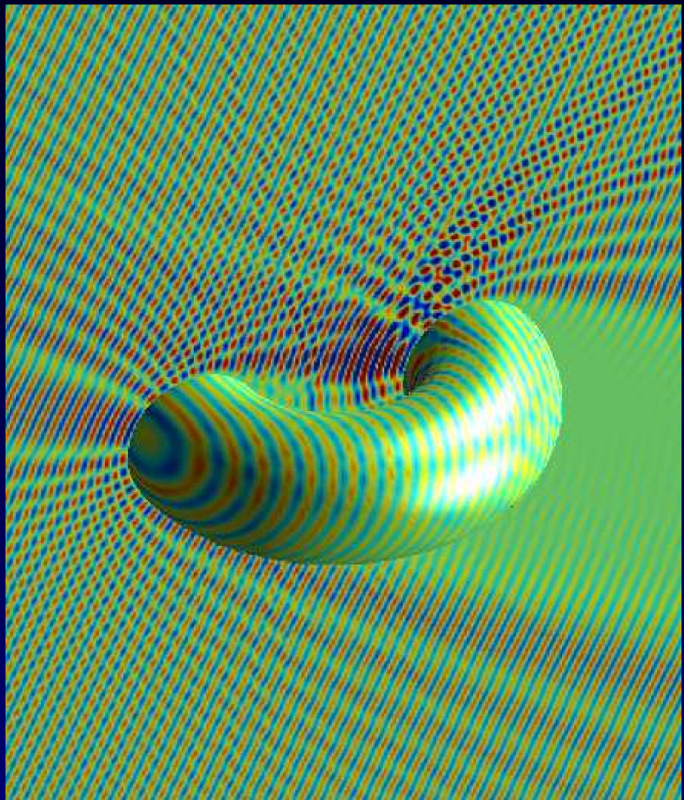


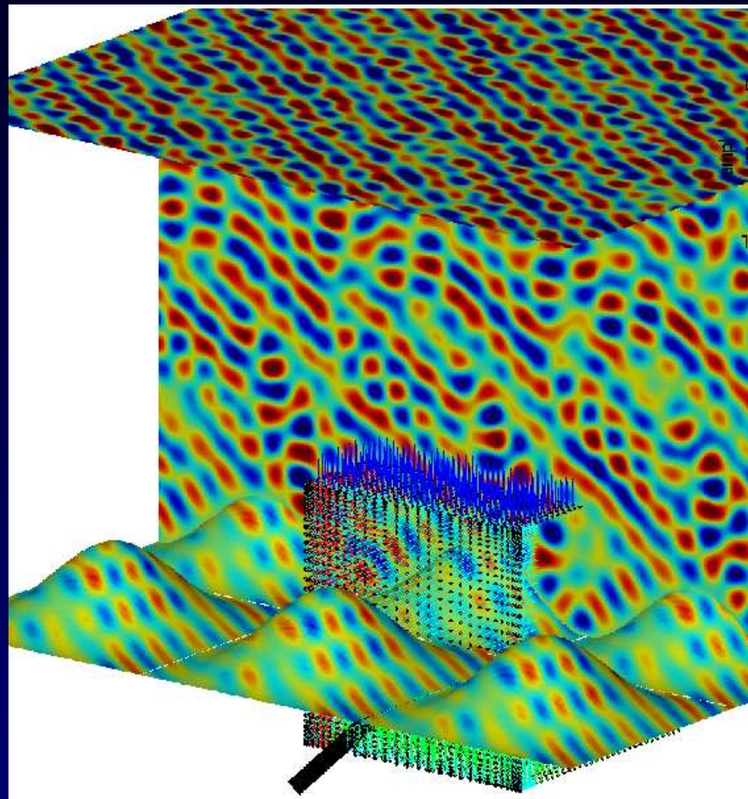
- integral formulation, periodizing via least-squares collocation on a box
- dispersion curves to spectral accuracy, via Boyd's analytic rootfinding

III. 3D Helmholtz QBX quadrature & periodizing

(w/ Z. Gimbutas and L. Greengard)

Sound-soft acoustic scatt: QBX setup $\approx$ 50 bare FMM GMRES iters.





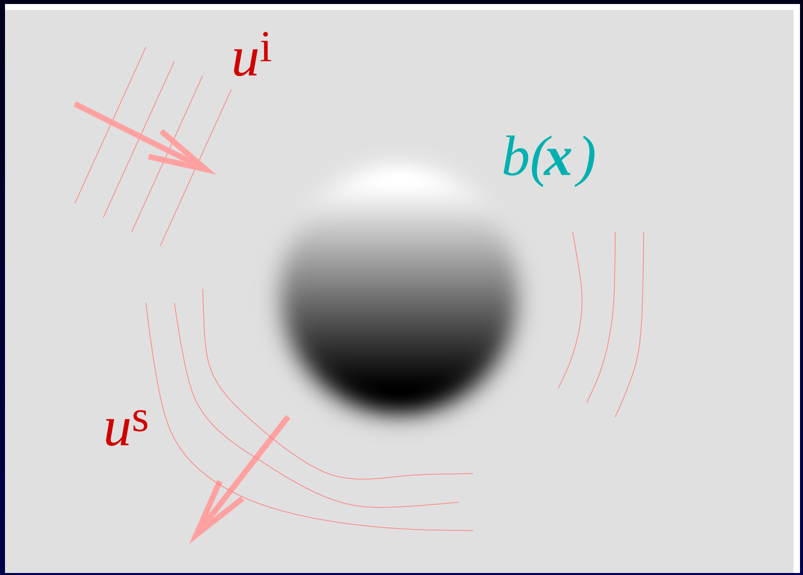
30λ across, 5 digits, 2 hrs

$8\lambda \times 8\lambda$ periodicity, 6 digits, 7 min

- periodizing via least-squares collocation, robust at Wood's anomalies

Please let's chat about them! Okay, now to the main talk. . .

Variable-medium freq-domain scattering problem



incident wave u^{i}, frequency κ:

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

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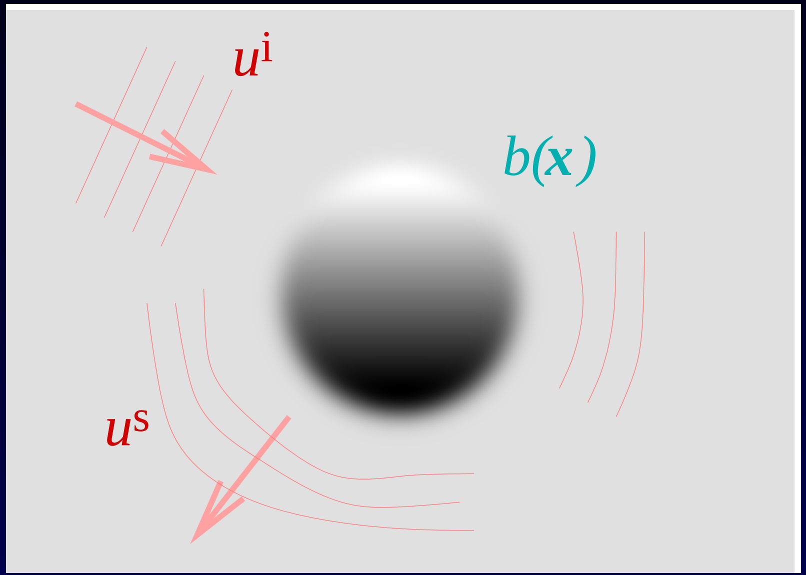

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total wave $u = u^{\mathrm{i}} + u^{\mathrm{s}}$ satisfies:

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

↖ 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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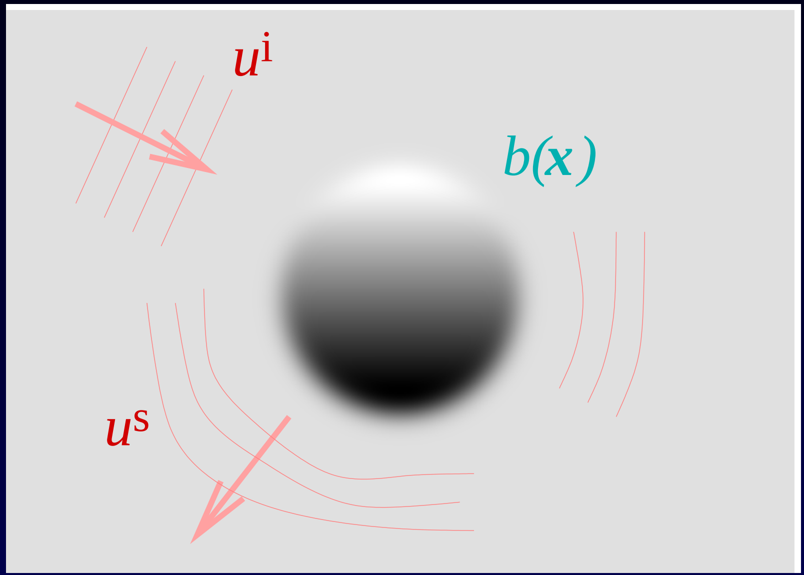

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- Applications: underwater acoustics, seismic imaging, ultrasound, quantum chemistry & physics, optics in graded index, metamaterials

Want: smooth b, high κ, multiple incident angles

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.

gives Lippmann-Schwinger volume IE. . .

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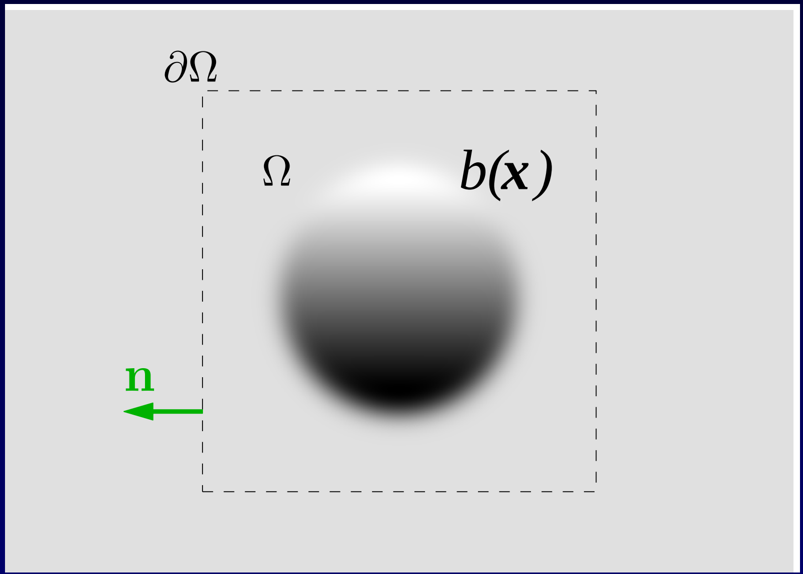
Instead: solve *full wave* u in square $\Omega \;\supset\;$ supp b, couple to u^s outside:



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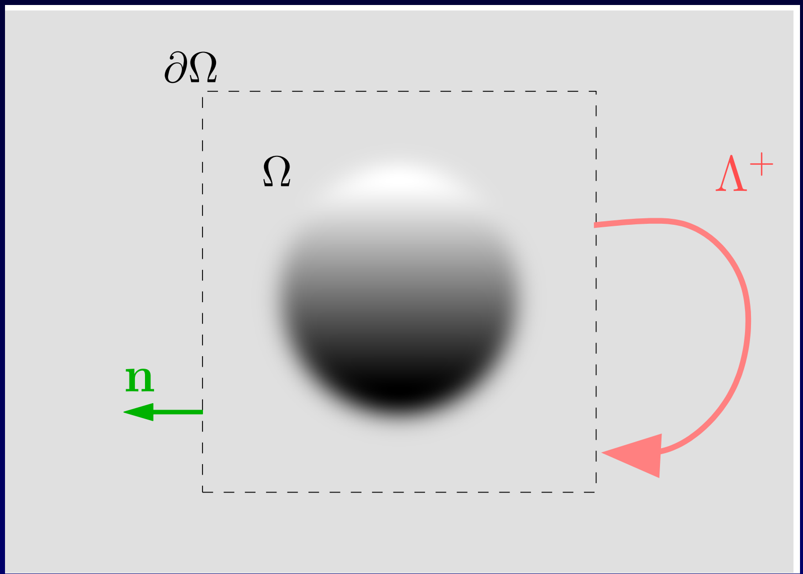

Λ^+: exterior Dirichlet-to-Neumann map

$$\Lambda^+ u^{\mathrm{s}}|_{\partial\Omega} = \frac{\partial u^{\mathrm{s}}}{\partial n} =: u^{\mathrm{s}}_n$$

u^{s} radiative, $(\Delta + \kappa^2)u^{\mathrm{s}} = 0$ in $\mathbb{R}^2 \backslash \overline{\Omega}$

operator exists $\forall \kappa > 0$

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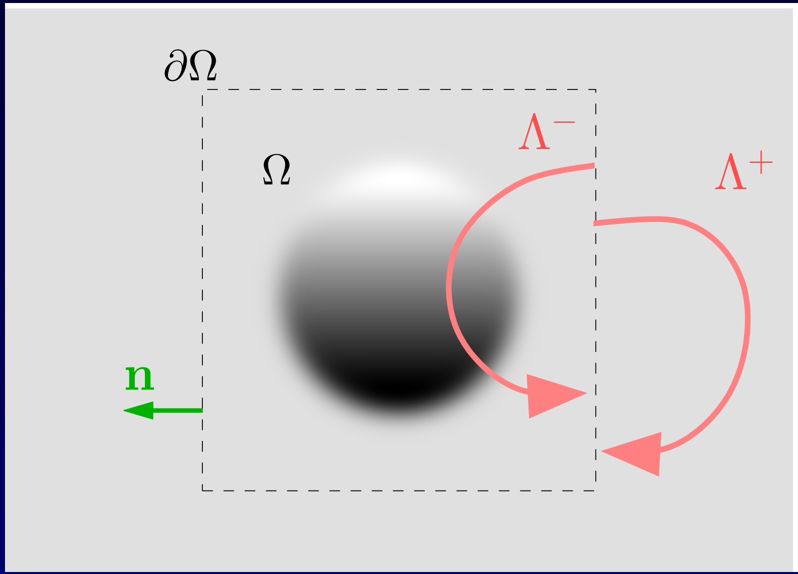

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exists for $\kappa \neq \kappa_j$, Dirichlet resonances of Ω

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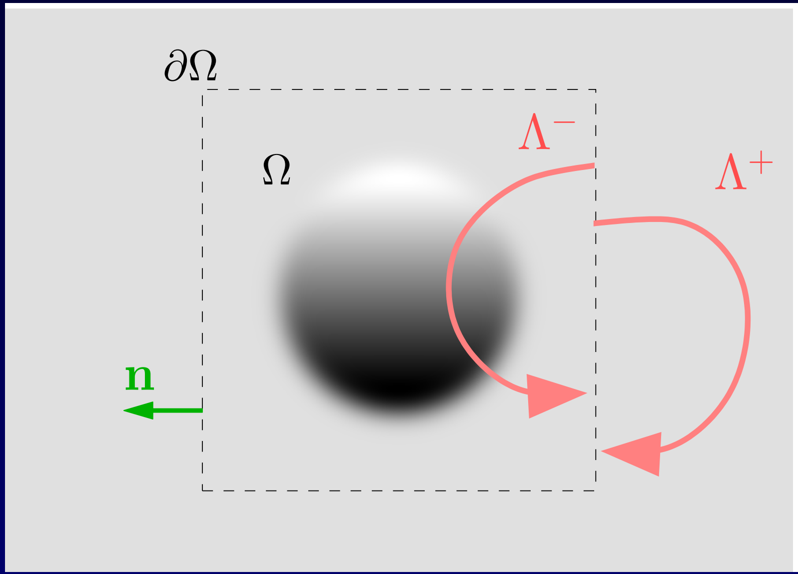

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$$\Rightarrow \quad (\Lambda^- - \Lambda^+)u^{\mathrm{s}}|_{\partial\Omega} \;=\; u^{\mathrm{i}}_n - \Lambda^+ u^{\mathrm{i}}|_{\partial\Omega}$$ (Kirsch–Monk ’94, FEM coupling)

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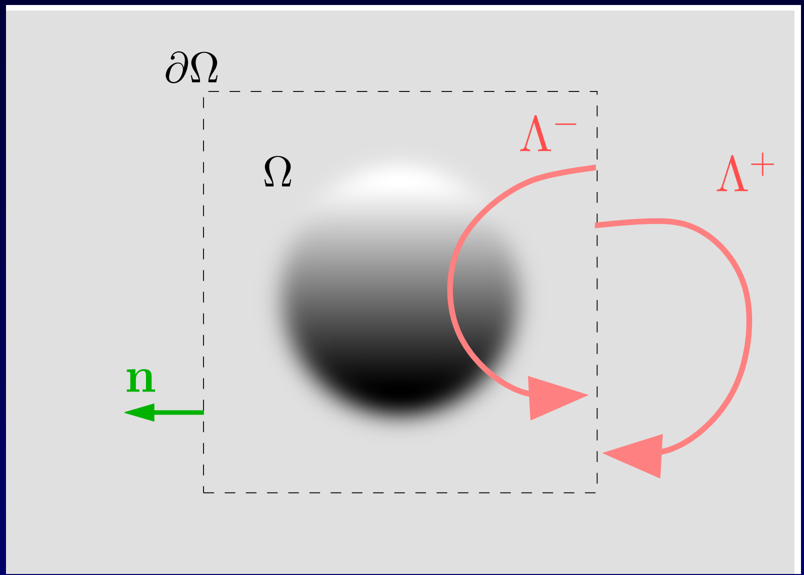

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$\nwarrow$ both order +1, signs *add* $\rightarrow$ ill-cond. $\rightarrow$ inversion would lose digits

2nd kind scattering formulation

$$(\Lambda^- - \Lambda^+)u^{\mathrm{s}}|_{\partial\Omega} \;=\; u_n^{\mathrm{i}} - \Lambda^+ u^{\mathrm{i}}|_{\partial\Omega} \qquad (*)$$

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Recall Helmholtz boundary integral operators on $\partial\Omega$:

single-layer $\quad (S\phi)(\mathbf{x}) := \int_{\partial\Omega} \frac{i}{4} H_0^{(1)}(\kappa|\mathbf{x}-\mathbf{y}|)\phi(\mathbf{y})ds_{\mathbf{y}}$

double-layer $\quad (D\phi)(\mathbf{x}) := \int_{\partial\Omega} \frac{i}{4} \frac{\partial}{\partial n_{\mathbf{y}}} H_0^{(1)}(\kappa|\mathbf{x}-\mathbf{y}|)\phi(\mathbf{y})ds_{\mathbf{y}}$

ext. Green's rep. $\quad u|_{\partial\Omega} = (D + \frac{1}{2})u|_{\partial\Omega} - Su_n, \quad$ so $\quad \Lambda^+ = S^{-1}(D - \frac{1}{2})$

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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 $(\mathcal{V}\phi)(\mathbf{x}) = \int_\Omega \frac{i}{4} H_0^{(1)}(\kappa|\mathbf{x}-\mathbf{y}|)\phi(\mathbf{y})d\mathbf{y}$

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

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

We need Λ^-: interior DtN map for box Ω

solve BVP: $\quad [\Delta + \kappa^2(1 - b(\mathbf{x}))]u = 0 \quad \text{in} \quad \Omega, \qquad u = f \quad \text{on} \quad \partial\Omega$

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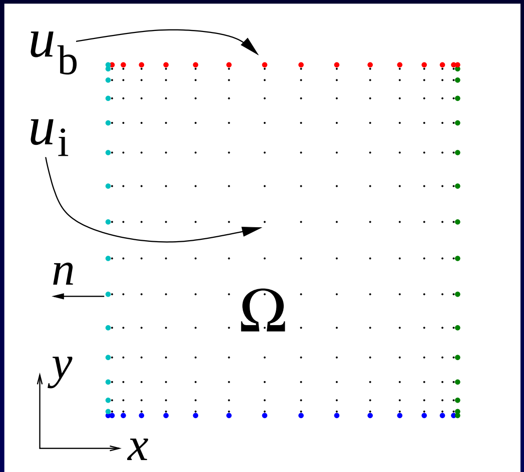
If small: spectral method, $p \times p$ product Chebyshev grid, nodes $\mathbf{x}_j$

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



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

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

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

system $\quad$ $$B\boldsymbol{u} := \left[\begin{array}{cc} I & 0 \\ \hline \multicolumn{2}{c}{H_{\mathrm{i},:}} \end{array}\right] \begin{bmatrix} u_\mathrm{b} \\ u_\mathrm{i} \end{bmatrix} = \begin{bmatrix} \boldsymbol{f} \\ 0 \end{bmatrix}$$

$\leftarrow$ Dirichlet BC (trivial)

$\leftarrow$ PDE at interior nodes

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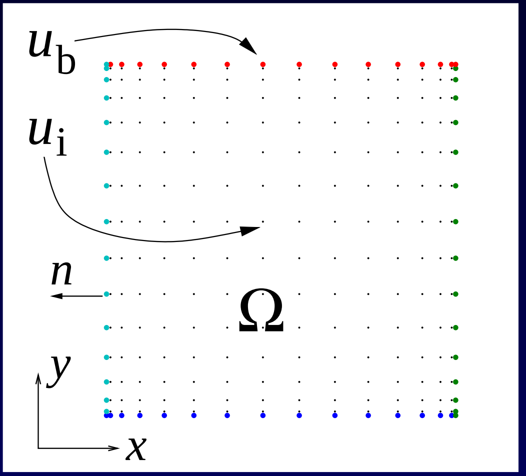

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solution matrix X, maps $\boldsymbol{f}$ to $\boldsymbol{u}$: solve $BX = \begin{bmatrix} I \\ 0 \end{bmatrix}$ dense, $O(p^6)$

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

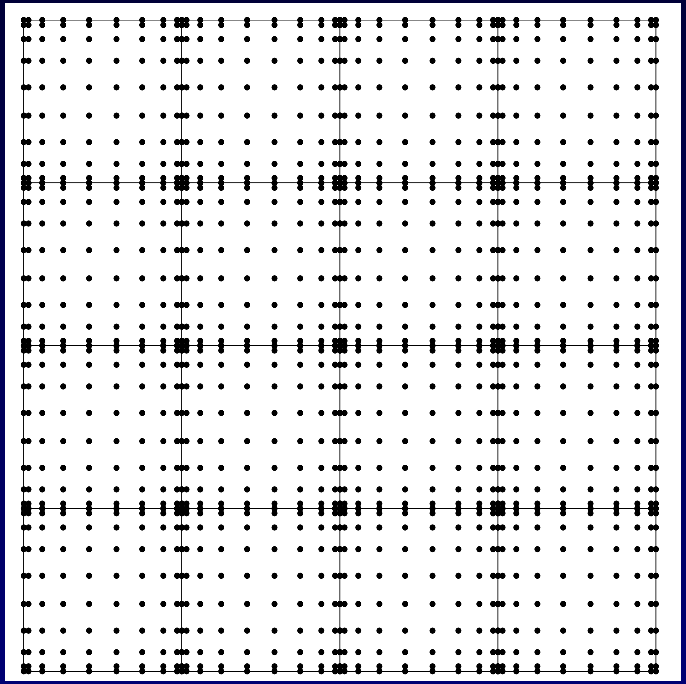
How build Λ^- for "large" scatterer?

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 $L = 2$:



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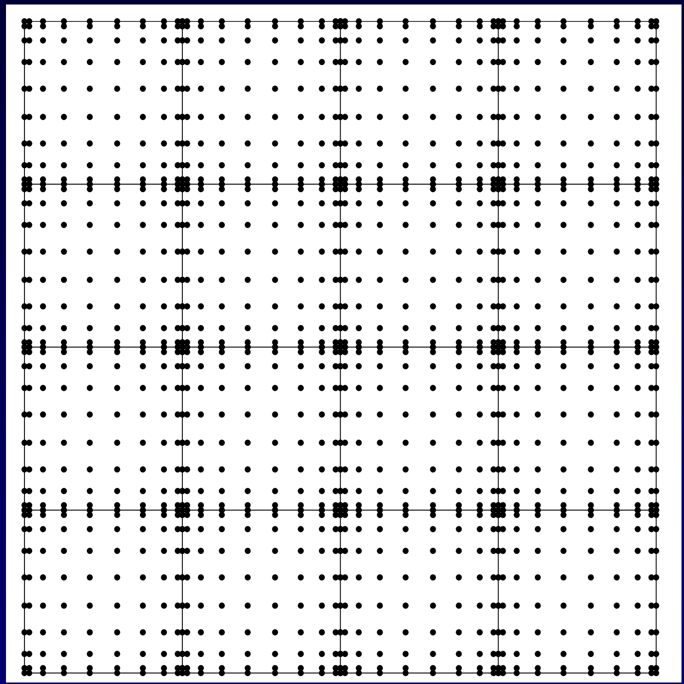

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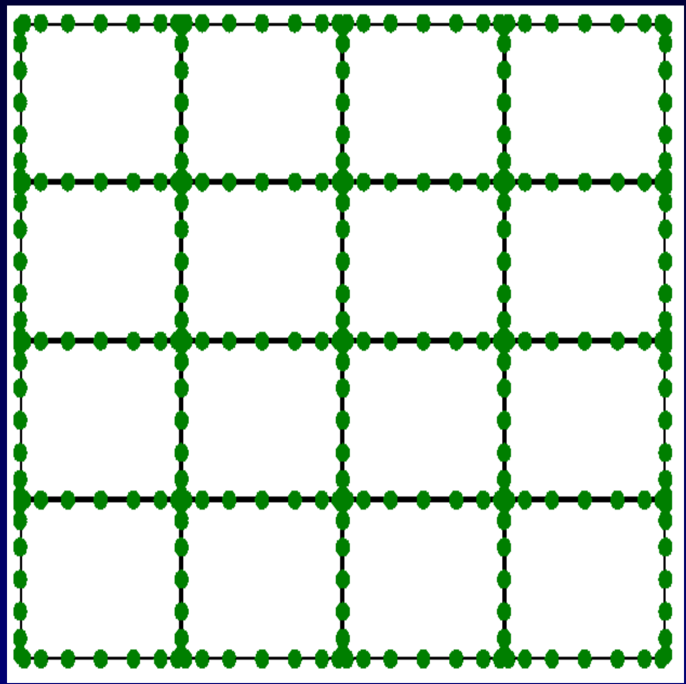


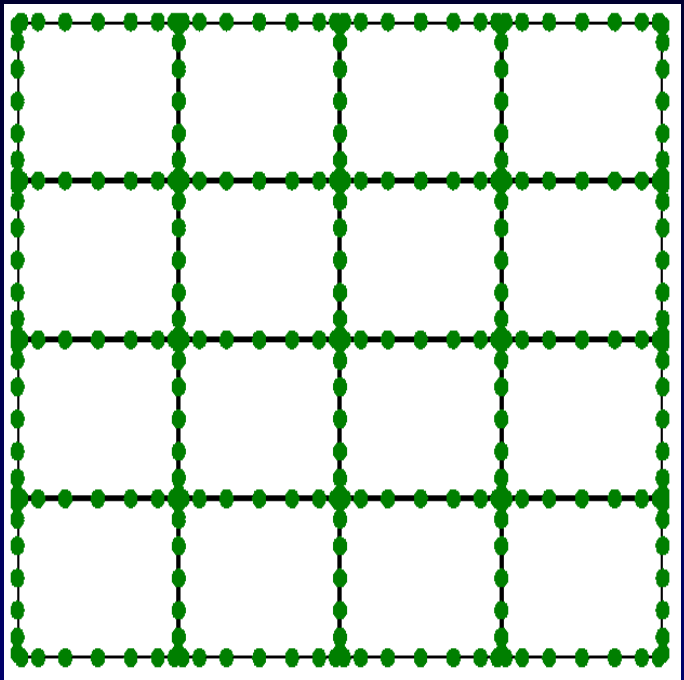
Step 1: build Λ^- for each box separately fix $p \approx 16$ effort $O(N)$

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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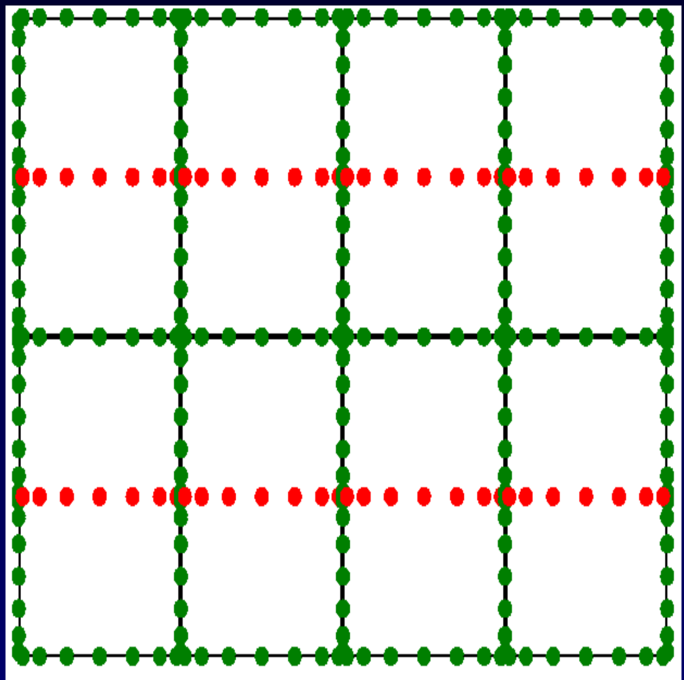

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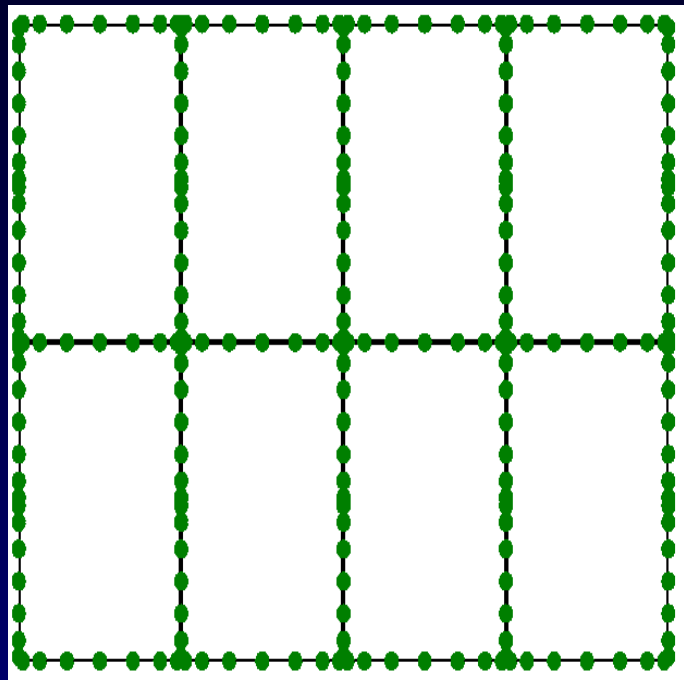

Now repeat: this is *upwards sweep* of the quad-tree…

Merging leaf DtN operators

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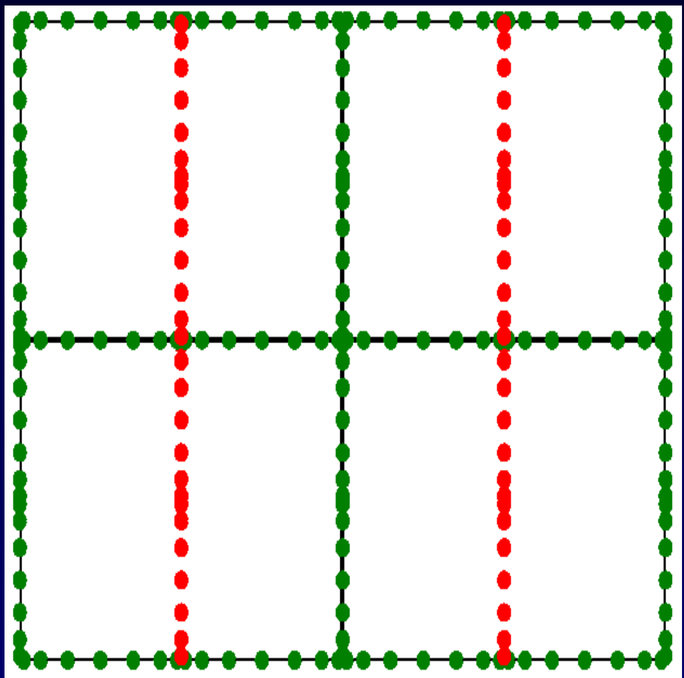
Creates Λ^- matrix for union of the boxes dense inverse, $O(p^3)$



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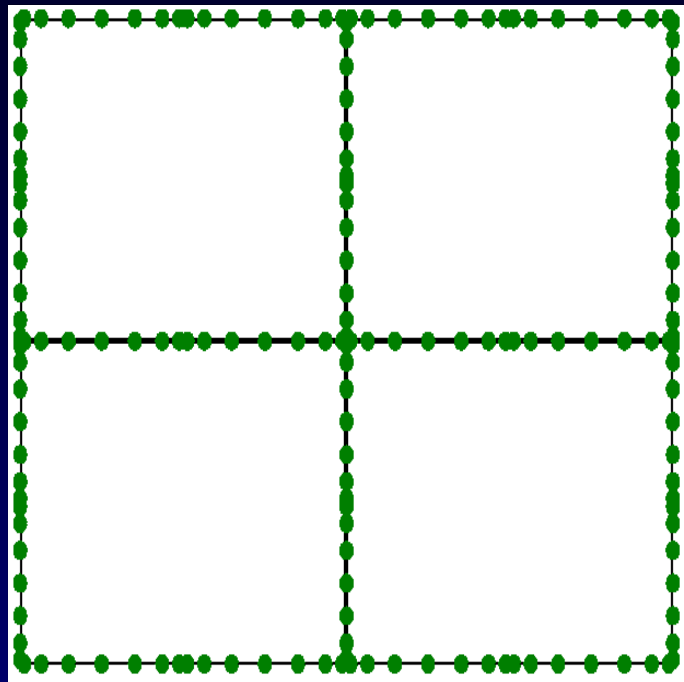

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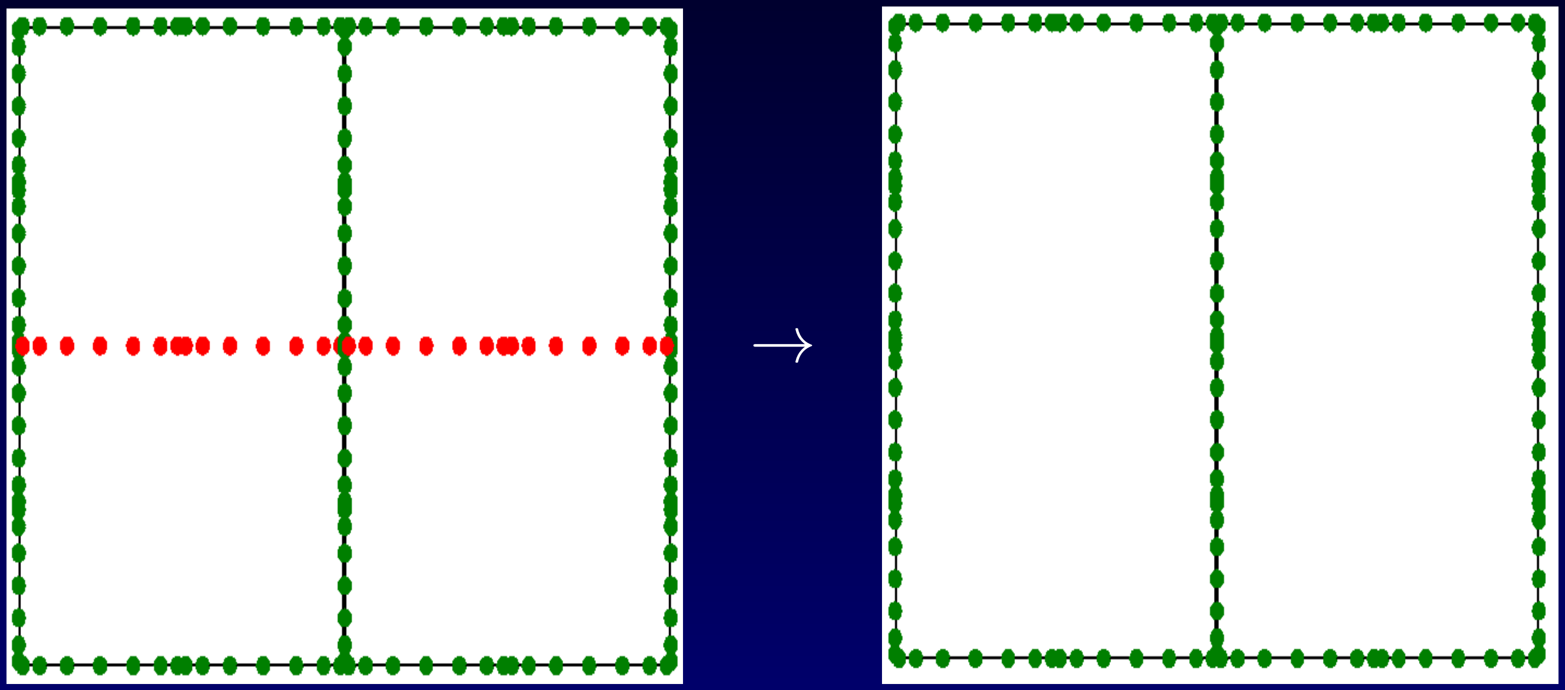

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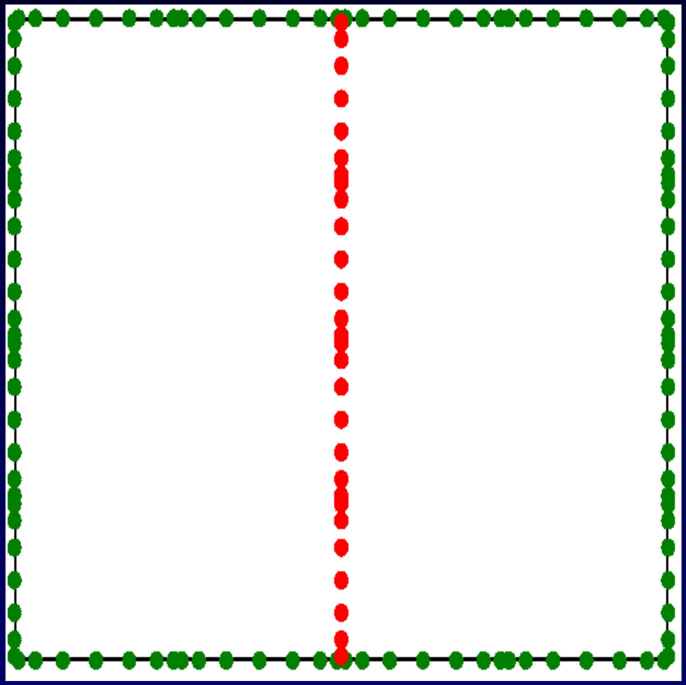

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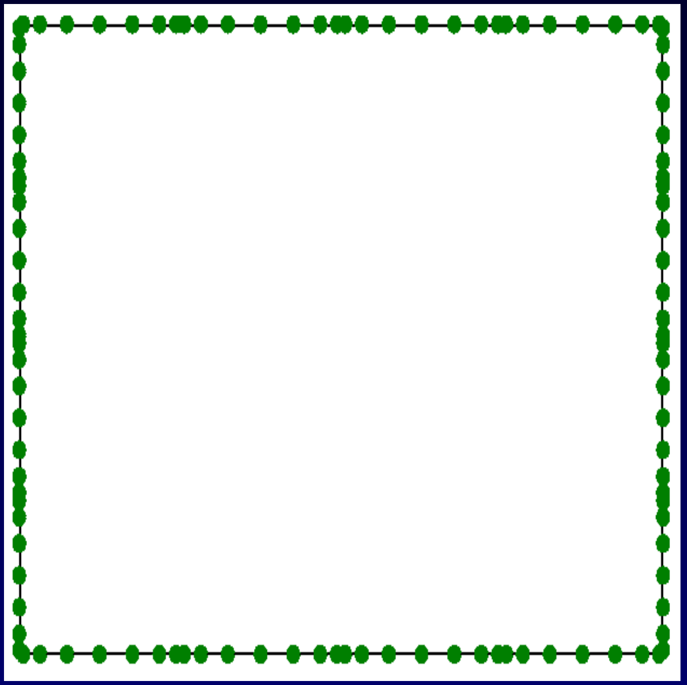

Top-level merge is $\frac{1}{2}$ total effort: $O(N^{1/2})$ dense inverse effort $O(N^{3/2})$

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

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

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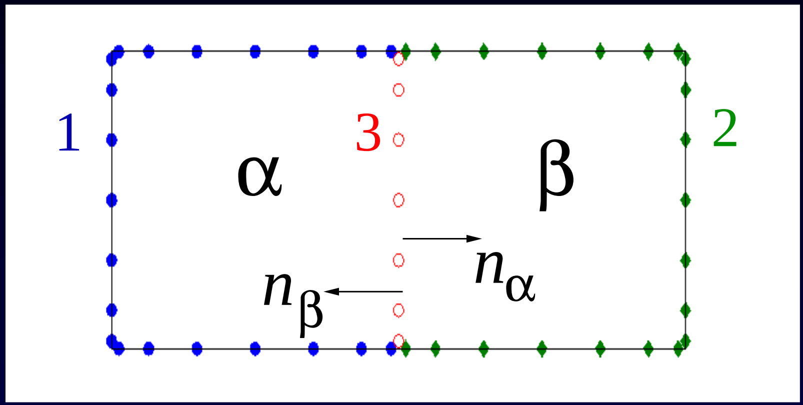
Then convert top-level ItI to DtN:

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

ItI merge step for two boxes



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2 = nodes only on β

3 = shared nodes

u, u_n match on edge 3

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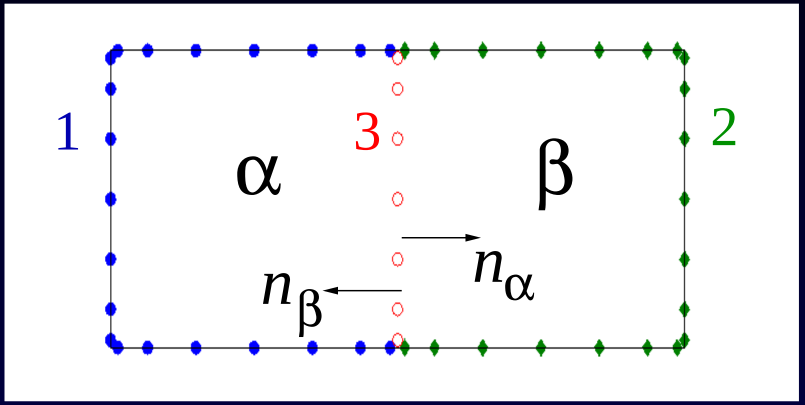

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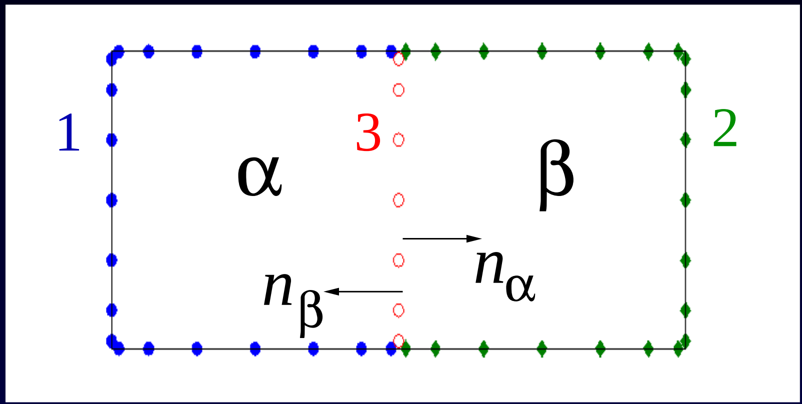

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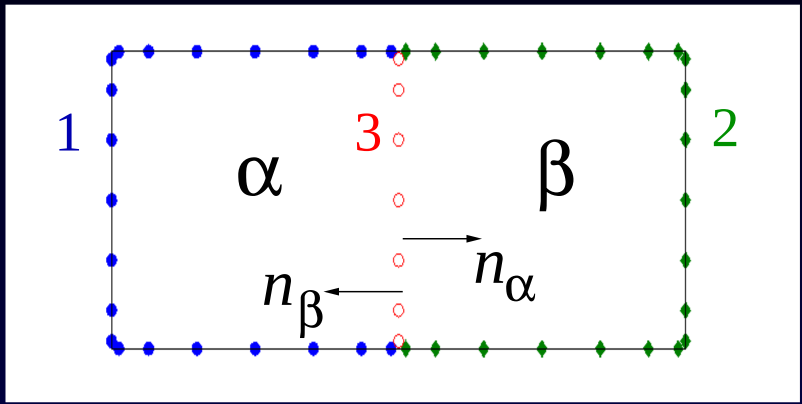

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Summary of direct scattering solver

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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 $O(N)$

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)
  4th-order FD + PML, UMFPACK, low κ (Britt–Tsynkov–Turkel '11)
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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

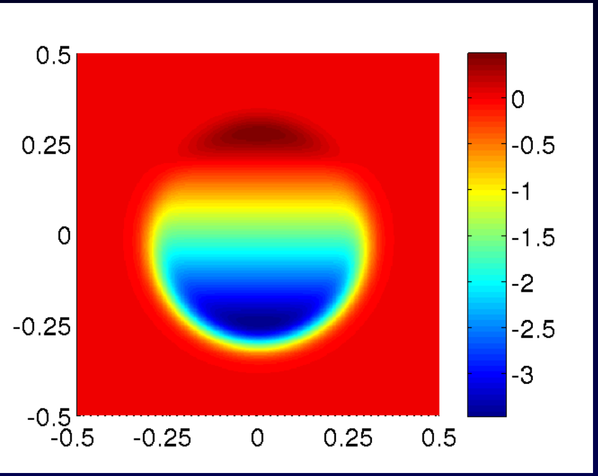
L	N	n	$t_{\rm pre}$	$t_{\rm new\ ext}$	$t_{\rm new\ int}$	RAM
4	58081	1120	5 s	0.006 s	0.04 s	230 MB
5	231361	1760	17 s	0.013 s	0.16 s	1 GB
6	923521	3040	78 s	0.05 s	0.7 s	5 GB
7	3690241	5600	6 m	0.16 s	2.7 s	22 GB
8	14753281	10720	22 m	0.5 s	10 s	96 GB

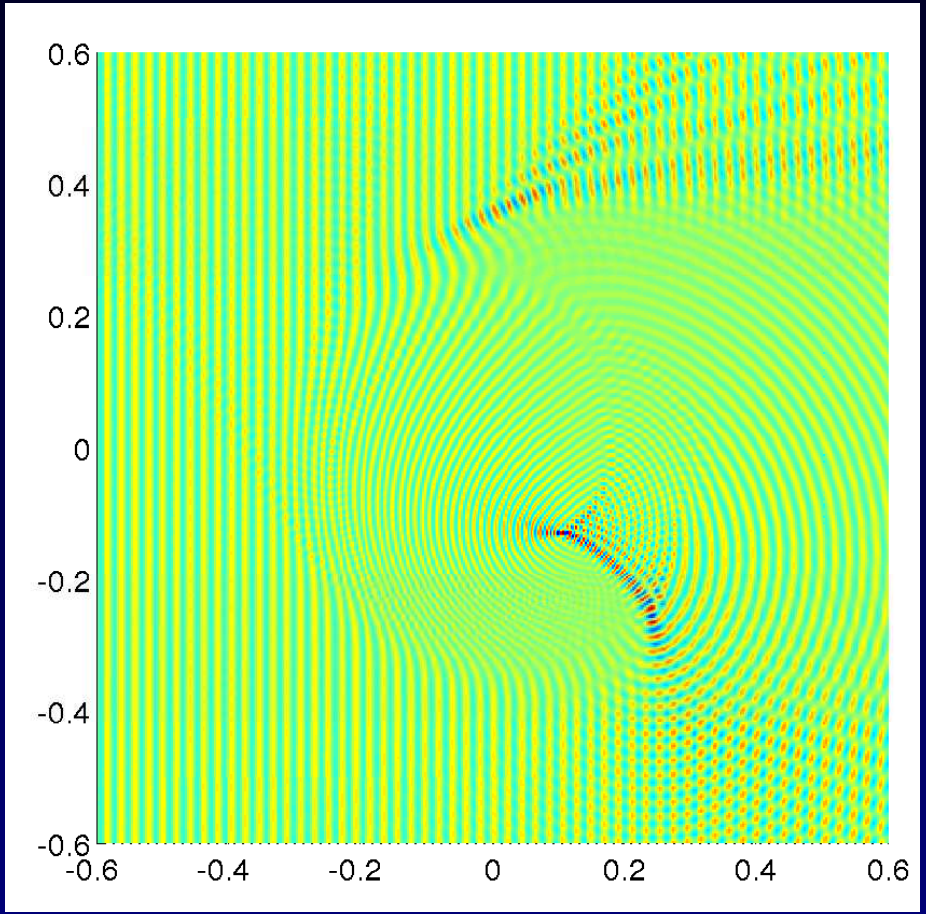
- precomp. time close to $O(N)$, not yet reached $O(N^{3/2})$
- RAM is $O(N \log N)$ $\sim$ 400 complex doubles per unknown

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

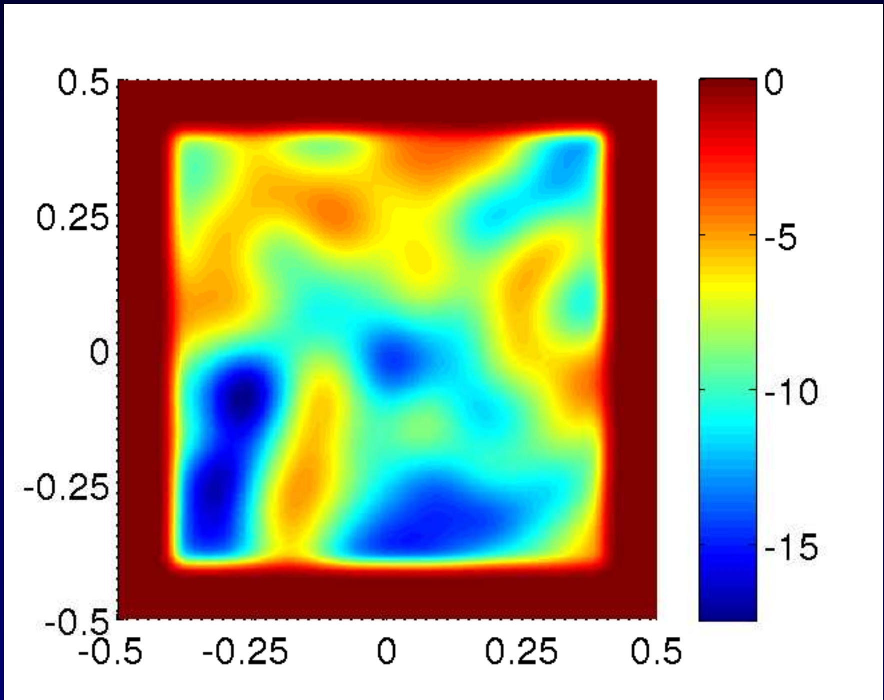
high-order $\quad$ ptwise err rel. to N=1.4e7

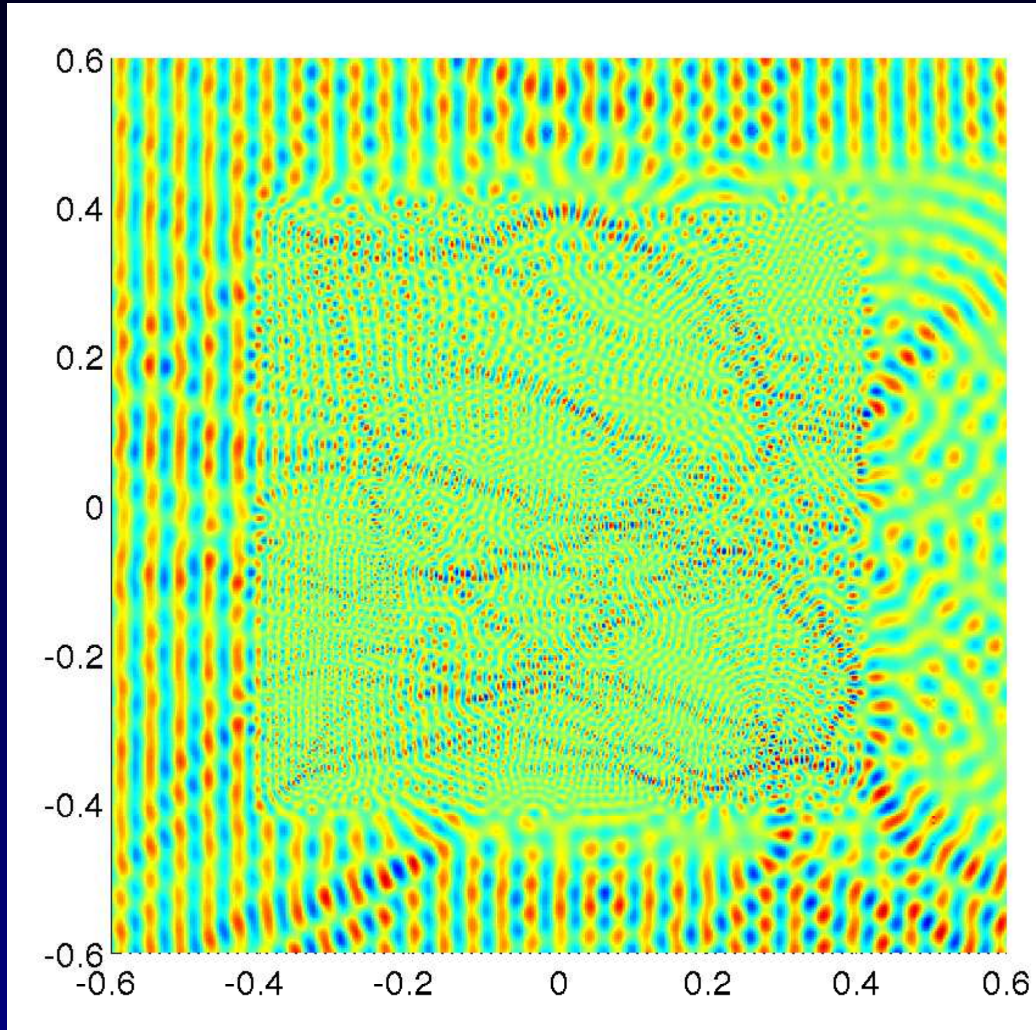
movie $\quad 10^3$ angles θ, 3 s each, incl. FMM to 240000 ext. targets

“Bathroom glass” at high frequency

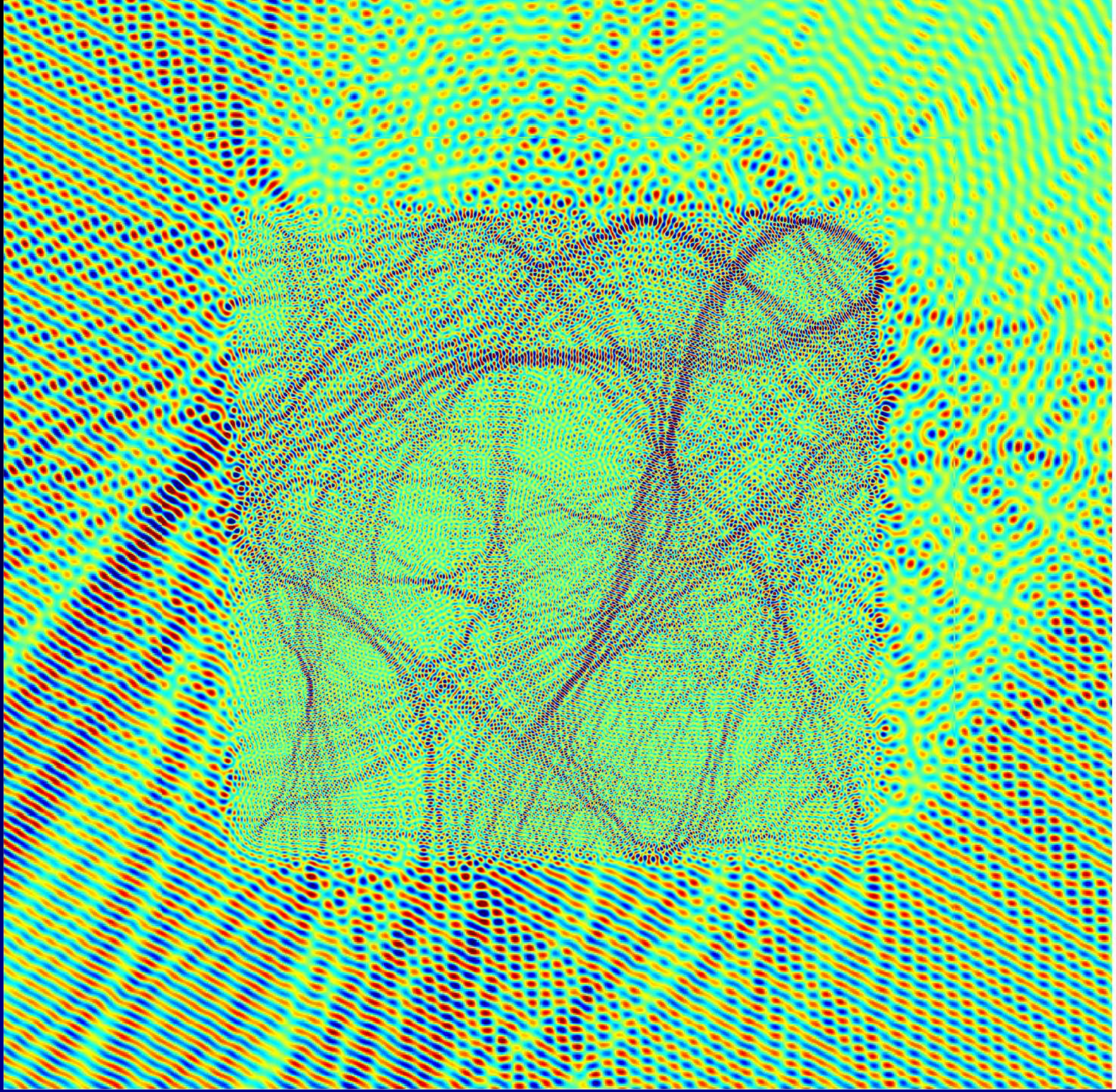
$b(\mathbf{x})$ = random smooth, rolled-off to zero

physics: “2D electron gas”





80λ on a side   time & accuracy similar to before $\boxed{\text{movie}}$ twinkling



$k = 320$

200λ across

9 digits (est.)

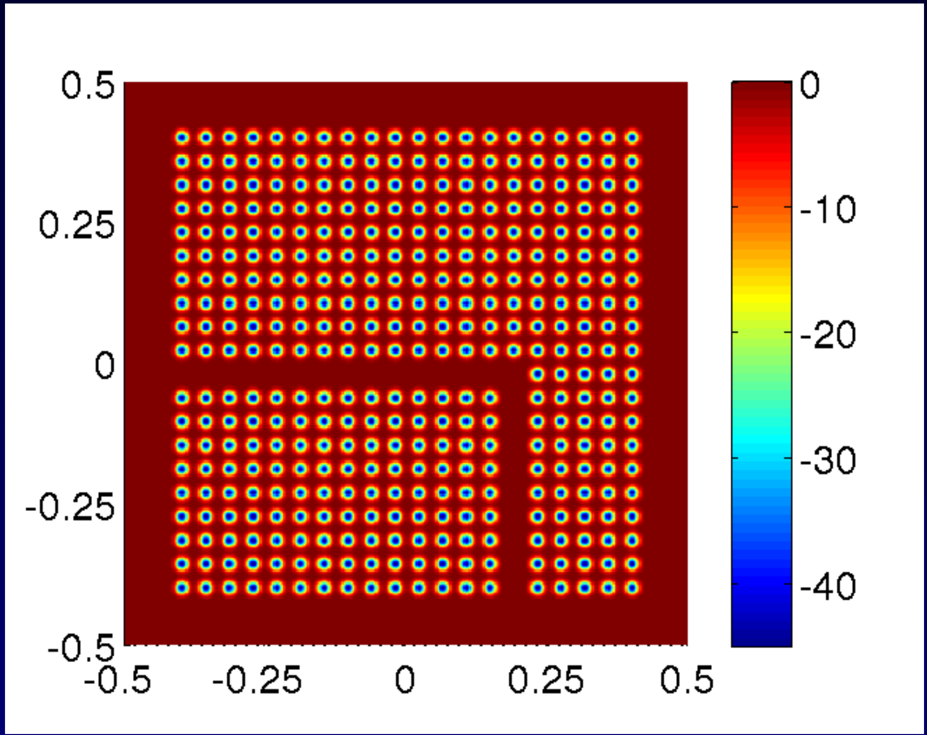
$N = 1.4\mathrm{e}7$

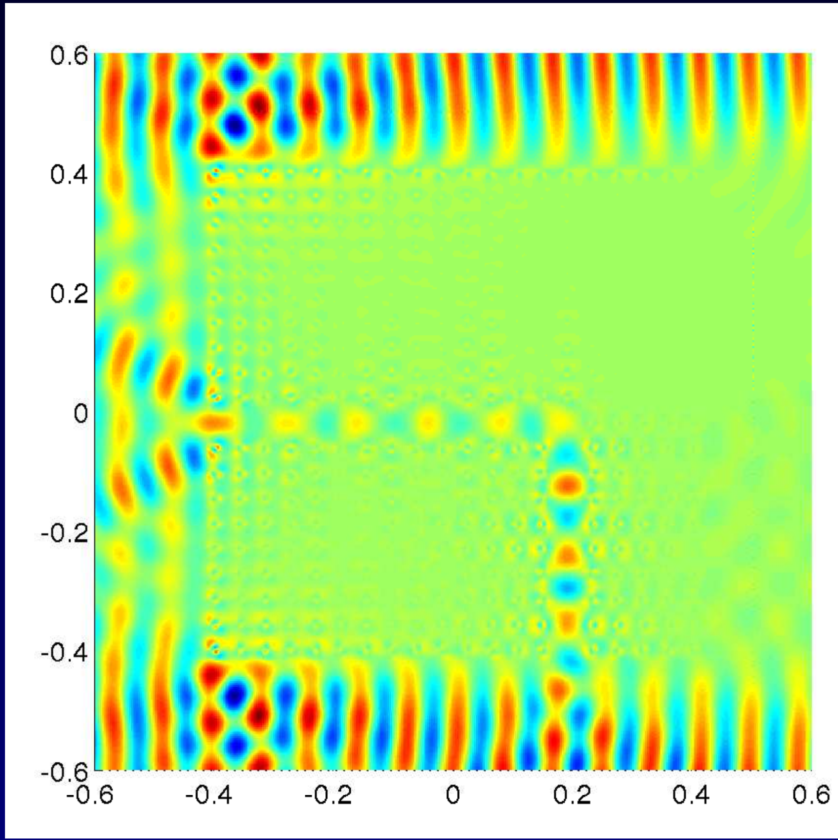
$t_{\mathrm{pre}} = 22$ min
$t_{\mathrm{new\,far}} = 0.5$ s
$t_{\mathrm{new\,int}} = 10$ s

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 $\quad N = 3.7\text{e}6$

- 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 my 2nd-kind ItI coupling

Gillman–B–Martinsson, *subm.* BIT '13

funding: NSF DMS-1216656

Preprints, talks, movies:

http://math.dartmouth.edu/∼ahb