Variable-medium freq-domain scattering problem

incident wave $u^i$, frequency $\kappa$:

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

total wave $u = u^i + u^s$ satisfies:

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

scattering potential $b$

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

Scattered wave $u^s$ radiative:

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

If $1 - b > 0$ everywhere, $\exists$ unique solution $\forall \kappa > 0$
Variable-medium freq-domain scattering problem

incident wave $u^i$, frequency $\kappa$:

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

total wave $u = u^i + u^s$ satisfies:

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

scattering potential $b$

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

Scattered wave $u^s$ radiative:

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

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

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

Want: smooth $b$, high $\kappa$, multiple incident angles
Coupling on enclosing box

Std: PDE for scatt. wave: \[(\Delta + \kappa^2)u^s - \kappa^2 bu^s = \kappa^2 bu^i\] ←inhomog.
gives Lippmann-Schwinger volume IE...
Coupling on enclosing box

Std: PDE for scatt. wave: \[(\Delta + \kappa^2)u^s - \kappa^2 bu^s = \kappa^2 bu^i\] ← inhomog.
gives Lippmann-Schwinger volume IE...

Instead: solve full wave \(u\) in square \(\Omega \supset \text{supp } b\), couple to \(u^s\) outside:
Coupling on enclosing box

Std: PDE for scatt. wave: \((\Delta + \kappa^2)u^s - \kappa^2 bu^s = \kappa^2 bu^i\) ← inhomog. gives Lippmann-Schwinger volume IE...

Instead: solve full wave \(u\) in square \(\Omega \supset \text{supp } b\), couple to \(u^s\) outside:

\[\Lambda^+: \text{exterior Dirichlet-to-Neumann map} \]

\[\Lambda^+ u^s|_{\partial \Omega} = \frac{\partial u^s}{\partial n} =: u^s_n\]

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

operator exists \(\forall \kappa > 0\)
Coupling on enclosing box

Std: PDE for scatt. wave: \[(\Delta + \kappa^2)u^s - \kappa^2 bu^s = \kappa^2 bu^i\] ← inhomog.
gives Lippmann-Schwinger volume IE...

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

\[\Lambda^+: \text{exterior Dirichlet-to-Neumann map}\]
\[\Lambda^+ u^s|_{\partial \Omega} = \frac{\partial u^s}{\partial n} =: u^s_n\]
$u^s$ radiative, \[(\Delta + \kappa^2)u^s = 0 \text{ in } \mathbb{R}^2 \setminus \overline{\Omega}\]
operator exists $\forall \kappa > 0$

\[\Lambda^-: \text{interior Dirichlet-to-Neumann map}\]
\[\Lambda^- u|_{\partial \Omega} = \frac{\partial u}{\partial n} =: u_n\]
where \[\left[\Delta + \kappa^2(1 - b(x))\right]u = 0 \text{ in } \Omega\]
exists for $\kappa \neq \kappa_j$, Dirichlet resonances of $\Omega$
Coupling on enclosing box

Std: PDE for scatt. wave: \( (\Delta + \kappa^2) u^s - \kappa^2 b u^s = \kappa^2 b u^i \) ← inhomog.
gives Lippmann-Schwinger volume IE...

Instead: solve full wave \( u \) in square \( \Omega \supset \text{supp } b \), couple to \( u^s \) outside:

\( \Lambda^+ : \) exterior Dirichlet-to-Neumann map

\[ \Lambda^+ u^s|_{\partial \Omega} = \frac{\partial u^s}{\partial n} =: u_n^s \]

\( u^s \) radiative, \( (\Delta + \kappa^2) u^s = 0 \) in \( \mathbb{R}^2 \setminus \overline{\Omega} \)
operator exists \( \forall \kappa > 0 \)

\( \Lambda^- : \) interior Dirichlet-to-Neumann map

\[ \Lambda^- u|_{\partial \Omega} = \frac{\partial u}{\partial n} =: u_n \]

where \[ [\Delta + \kappa^2 (1 - b(x))] u = 0 \] in \( \Omega \)
exists for \( \kappa \neq \kappa_j \), Dirichlet resonances of \( \Omega \)

\[ \Lambda^- (u^i + u^s)|_{\partial \Omega} = u_n^i + u_n^s = u_n^i + \Lambda^+ u^s|_{\partial \Omega} \]

\[ \Rightarrow \quad (\Lambda^- - \Lambda^+) u^s|_{\partial \Omega} = u_n^i - \Lambda^+ u^i|_{\partial \Omega} \quad \text{(Kirsch–Monk ’94, FEM coupling)} \]
Coupling on enclosing box

Std: PDE for scatt. wave: \[(\Delta + \kappa^2)u^s - \kappa^2 bu^s = \kappa^2 bu^i \leftarrow \text{inhomog.}\]
gives Lippmann-Schwinger volume IE...

Instead: solve full wave \(u\) in square \(\Omega \supset \text{supp } b\), couple to \(u^s\) outside:

\[\Lambda^+: \text{exterior Dirichlet-to-Neumann map}\]

\[\Lambda^+ u^s|_{\partial \Omega} = \frac{\partial u^s}{\partial n} =: u_n^s\]

\(u^s\) radiative, \((\Delta + \kappa^2)u^s = 0\) in \(\mathbb{R}^2 \setminus \overline{\Omega}\)
operator exists \(\forall \kappa > 0\)

\[\Lambda^-: \text{interior Dirichlet-to-Neumann map}\]

\[\Lambda^- u|_{\partial \Omega} = \frac{\partial u}{\partial n} =: u_n\]

where \([\Delta + \kappa^2(1 - b(x))]u = 0\) in \(\Omega\)
exists for \(\kappa \neq \kappa_j\), Dirichlet resonances of \(\Omega\)

\[\Lambda^- (u^i + u^s)|_{\partial \Omega} = u^i_n + u^s_n = u^i_n + \Lambda^+ u^s|_{\partial \Omega}\]

\[\Rightarrow (\Lambda^- - \Lambda^+)u^s|_{\partial \Omega} = u^i_n - \Lambda^+ u^i|_{\partial \Omega} \quad (\text{Kirsch–Monk '94, FEM coupling})\]

both order +1, signs \(add\) \(\rightarrow\) ill-cond. \(\rightarrow\) inversion would lose digits
2nd kind scattering formulation

\[(\Lambda^- - \Lambda^+) u^s|_{\partial\Omega} = u^i_n - \Lambda^+ u^i|_{\partial\Omega} \quad (*)\]
2nd kind scattering formulation

\[(\Lambda^- - \Lambda^+) u^s|_{\partial\Omega} = u^n_i - \Lambda^+ u^i|_{\partial\Omega} \quad (*)\]

Recall Helmholtz boundary integral operators on \(\partial\Omega\):

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

double-layer \((D\phi)(x) := \int_{\partial\Omega} \frac{i}{4} \frac{\partial}{\partial n_y} H_0^{(1)}(\kappa|x-y|)\phi(y)ds_y)\)

ext. Green’s rep. \(u|_{\partial\Omega} = (D + \frac{1}{2})u|_{\partial\Omega} - Su_n, \) so \(\Lambda^+ = S^{-1}(D - \frac{1}{2})\)
2nd kind scattering formulation

\[(\Lambda^- - \Lambda^+)u^s|_{\partial\Omega} = u^i_n - \Lambda^+u^i|_{\partial\Omega} \quad (\ast)\]

Recall Helmholtz boundary integral operators on \(\partial\Omega\):

- single-layer \((S\phi)(x) := \int_{\partial\Omega} \frac{i}{4} H_0^{(1)}(\kappa|x - y|)\phi(y) ds_y\)
- double-layer \((D\phi)(x) := \int_{\partial\Omega} \frac{i}{4} \frac{\partial}{\partial n_y} H_0^{(1)}(\kappa|x - y|)\phi(y) ds_y\)

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

Left-regularize \((\ast)\) by \(S\): \((\frac{1}{2} - D + S\Lambda^-)u^s|_{\partial\Omega} = S(u^i_n - \Lambda^-u^i|_{\partial\Omega})\)

**Thm.** Let \(\partial\Omega\) be Lipschitz, \(b(x)\) bnded, \(0 < \kappa \neq \kappa_j\).

Then \(A := \frac{1}{2} - D + S\Lambda^- = I + \text{compact}\) above BIE is 2nd kind
2nd kind scattering formulation

\[(\Lambda^- - \Lambda^+)u^s|_{\partial\Omega} = u^i_n - \Lambda^+u^i|_{\partial\Omega} \quad (\ast)\]

Recall Helmholtz boundary integral operators on \(\partial\Omega\):

- **single-layer** \((S\phi)(x) := \int_{\partial\Omega} i\frac{1}{4}H_0^{(1)}(\kappa|x-y|)\phi(y)ds_y\)
- **double-layer** \((D\phi)(x) := \int_{\partial\Omega} i\frac{1}{4}\frac{\partial}{\partial n_y}H_0^{(1)}(\kappa|x-y|)\phi(y)ds_y\)

ex. Green’s rep. \(u|_{\partial\Omega} = (D + \frac{1}{2})u|_{\partial\Omega} - Su_n\), so \(\Lambda^+ = S^{\ast -1}(D - \frac{1}{2})\)

Left-regularize \((\ast)\) by \(S\): \((\frac{1}{2} - D + S\Lambda^-)u^s|_{\partial\Omega} = S(u^i_n - \Lambda^-u^i|_{\partial\Omega})\)

**Thm.** Let \(\partial\Omega\) be Lipschitz, \(b(x)\) bnded, \(0 < \kappa \neq \kappa_j\).

Then \(A := \frac{1}{2} - D + S\Lambda^- = I + \text{compact} \quad \text{above BIE is 2nd kind}\)

**Pf.** let \(P : L^2(\partial\Omega) \rightarrow L^2(\Omega)\) be interior solution operator: \(u|_{\Omega} = Pu|_{\partial\Omega}\)

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

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

\(VbP\) cpt by Sobolev imbedding \(\uparrow\) \(\text{(Lipschitz bdry: McLean ’00)}\) 

\(\square\)
We need $\Lambda^-$: interior DtN map for box $\Omega$

solve BVP: $[\Delta + \kappa^2(1 - b(x))]u = 0$ in $\Omega$, $u = f$ on $\partial\Omega$
We need $\Lambda^-$: interior DtN map for box $\Omega$

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

If small: spectral method, $p \times p$ product Chebyshev grid, nodes $x_j$

$p^2$ unknowns, vector $u = \begin{bmatrix} u_b \\ u_i \end{bmatrix}$ ← boundary

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

matrix $H = D_x^2 + D_y^2 + \kappa^2 \text{diag}\{1 - b(x_j)\}$

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

system $Bu := \begin{bmatrix} I & 0 \\ H_{i,:} & \end{bmatrix} \begin{bmatrix} u_b \\ u_i \end{bmatrix} = \begin{bmatrix} f \\ 0 \end{bmatrix}$ ← Dirichlet BC (trivial)

← PDE at interior nodes
We need $\Lambda^{-}$: interior DtN map for box $\Omega$

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

If small: spectral method, $p \times p$ product Chebyshev grid, nodes $x_j$

$p^2$ unknowns, vector $u = \begin{bmatrix} u_b \\ u_i \end{bmatrix}$ ← boundary

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

matrix $H = D_x^2 + D_y^2 + \kappa^2 \text{diag}\{1 - b(x_j)\}$

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

system $Bu := \begin{bmatrix} I & 0 \\ \frac{H}{H_{i,:}} \end{bmatrix} \begin{bmatrix} u_b \\ u_i \end{bmatrix} = \begin{bmatrix} f \\ 0 \end{bmatrix}$ ← Dirichlet BC (trivial)

$H_{i,:} = \text{PDE at interior nodes}$

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

Get approx. $\Lambda^{-}$: $X$ left-mult. by rows of $D_x, D_y$ to take normal deriv.
How build $\Lambda^-$ for “large” scatterer?

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

Partition top-level box $\Omega$ 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 $\Lambda^-$ for “large” scatterer?

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

Partition top-level box $\Omega$ 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 $L = 2$:

Step 1: build $\Lambda^-$ 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 $\Lambda^-$ matrix for union of the boxes

dense inverse, $O(p^3)$
Merging leaf DtN operators

Can eliminate unknowns on common edge of two neighboring boxes

Creates $\Lambda^-$ matrix for union of the boxes

Now repeat: this is *upwards sweep* of the quad-tree...
Merging leaf DtN operators

Can eliminate unknowns on common edge of two neighboring boxes

Creates $\Lambda^-$ matrix for union of the boxes

dense inverse, $O(p^3)$
Merging leaf DtN operators

Can eliminate unknowns on common edge of two neighboring boxes

Creates $\Lambda^-$ matrix for union of the boxes

dense inverse, $O(p^3)$
Merging leaf DtN operators

Can eliminate unknowns on common edge of two neighboring boxes

Creates $\Lambda^-$ matrix for union of the boxes

$dense$ inverse, $O(p^3)$

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 $\Lambda^-$ 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 $\kappa_j$, lose digits

Every leaf and merged box has own (unpredictable, $b$-dependent) eigenfreqs!
Problem: interior DtN resonances

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

\[ \Rightarrow \text{numerically not robust: DtN norm blows up near } \kappa_j, \text{ lose digits} \]

Every leaf \textit{and merged box} has own (unpredictable, \( b \)-dependent) eigenfreqs!

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

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

classical facts: \( R \) exists for all \( \kappa \). \( R \) is unitary.

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

Hierarchical ItI merge operations: max cond. \# now 20 not \( 2 \times 10^5 \)
Problem: interior DtN resonances

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

\[ \Rightarrow \text{numerically not robust: DtN norm blows up near } \kappa_j, \text{ lose digits} \]

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

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

fix \( \eta \) real, let

\[
\begin{align*}
  f &= u_n + i\eta u|_{\partial\Omega} \quad \text{“incoming”} \\
  g &= u_n - i\eta u|_{\partial\Omega} \quad \text{“outgoing”}
\end{align*}
\]

classical facts: \( R \) exists for all \( \kappa \). \( R \) is unitary.

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

Hierarchical ItI merge operations: max cond. \# now 20 not \( 2 \times 10^5 \)

Then convert top-level ItI to DtN:

Cayley transform \( \Lambda^- = -i\eta(R - I)^{-1}(R + I) \quad O(N^{3/2}) \)
ItI merge step for two boxes

1 = nodes only on $\alpha$
2 = nodes only on $\beta$
3 = shared nodes

$u, u_n$ match on edge 3
ItI merge step for two boxes

1 = nodes only on $\alpha$
2 = nodes only on $\beta$
3 = shared nodes

$u, u_n$ match on edge 3

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

$$R_{31}^{\alpha} f_1 + R_{33}^{\alpha} f_3^\alpha = g_3^\alpha = -f_3^\beta$$

by matching, normals opposed (2)

$$R_{32}^{\beta} f_2 + R_{33}^{\beta} f_3^\beta = g_3^\beta = -f_3^\alpha$$
ItI merge step for two boxes

1 = nodes only on $\alpha$
2 = nodes only on $\beta$
3 = shared nodes

$u, u_n$ match on edge 3

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

$$R_3^{\alpha}f_1 + R_3^{\alpha}f_3^{\alpha} = g_3^{\alpha} = -f_3^{\beta} \quad \text{by matching, normals opposed (3)}$$

$$R_3^{\beta}f_2 + R_3^{\beta}f_3^{\beta} = g_3^{\beta} = -f_3^{\alpha}$$

Elim. $f_3^{\alpha}$: $f_3^{\beta} = F^{\beta} \begin{bmatrix} f_1 \\ f_2 \end{bmatrix}$, $F^{\beta} := (1 - R_3^{\alpha}R_3^{\beta})^{-1}[-R_3^{\alpha} \quad R_3^{\alpha}R_3^{\beta}]$

also $F^{\alpha} := [0 \quad -R_3^{\beta}] - R_3^{\beta}F^{\beta}$,
ItI merge step for two boxes

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

$$
R_3^\alpha f_1 + R_3^\alpha f_3^\alpha = g_3^\alpha = -f_3^\beta \text{ by matching, normals opposed (4)}
$$

$$
R_3^\beta f_2 + R_3^\beta f_3^\beta = g_3^\beta = -f_3^\alpha
$$

Elim. $f_3^\alpha$: $f_3^\beta = F^\beta \begin{bmatrix} f_1 \\ f_2 \end{bmatrix}$, $F^\beta := (1 - R_3^\alpha R_3^\beta)^{-1}[-R_3^\alpha \quad R_3^\alpha R_3^\beta]$

also $F^\alpha := [0 \quad -R_3^\beta] - R_3^\beta F^\beta$, then $R = \begin{bmatrix} R_{11}^\alpha & 0 \\ 0 & R_{22}^\beta \end{bmatrix} + \begin{bmatrix} R_{13}^\alpha F^\alpha \\ R_{23}^\beta F^\beta \end{bmatrix}$
Summary of direct scattering solver

Pre-computation:

1) Nyström discretization of $S$, $D$ at $n = O(N^{1/2})$ nodes on $\partial \Omega$
   e.g. generalized Gaussian quadrature, 6 levels dyadic corner-refinement
Summary of direct scattering solver

Pre-computation:

1) Nyström discretization of $S, D$ at $n = O(N^{1/2})$ nodes on $\partial \Omega$
   e.g. generalized Gaussian quadrature, 6 levels dyadic corner-refinement

2) Build interior DtN $\Lambda^-$ via merges up the tree, then Cayley $O(N^{3/2})$
Summary of direct scattering solver

Pre-computation:

1) Nyström discretization of $S$, $D$ at $n = O(N^{1/2})$ nodes on $\partial \Omega$
   e.g. generalized Gaussian quadrature, 6 levels dyadic corner-refinement

2) Build interior DtN $\Lambda^-$ via merges up the tree, then Cayley $O(N^{3/2})$

3) Fill $A = \frac{1}{2} - D + S\Lambda^-$, take $A^{-1}$ $O(N^{3/2})$

Per incident wave at this freq. $\kappa$, solution now very fast...
Summary of direct scattering solver

Pre-computation:

1) Nyström discretization of $S$, $D$ at $n = O(N^{1/2})$ nodes on $\partial \Omega$
   e.g. generalized Gaussian quadrature, 6 levels dyadic corner-refinement

2) Build interior DtN $\Lambda^-$ via merges up the tree, then Cayley $O(N^{3/2})$

3) Fill $A = \frac{1}{2} - D + S\Lambda^-$, take $A^{-1}$ $O(N^{3/2})$

Per incident wave at this freq. $\kappa$, solution now very fast...

4) fill RHS, apply $A^{-1}$ to get $u^s|_{\partial \Omega}$, $u^s_n = \Lambda^-(u^i|_{\partial \Omega} + u^s|_{\partial \Omega}) - u^i_n$ $O(N)$
Summary of direct scattering solver

Pre-computation:

1) Nyström discretization of $S, D$ at $n = O(N^{1/2})$ nodes on $\partial\Omega$
   e.g. generalized Gaussian quadrature, 6 levels dyadic corner-refinement

2) Build interior DtN $\Lambda^-$ via merges up the tree, then Cayley $O(N^{3/2})$

3) Fill $A = \frac{1}{2} - D + S\Lambda^-$, take $A^{-1}$ $O(N^{3/2})$

Per incident wave at this freq. $\kappa$, solution now very fast...

4) fill RHS, apply $A^{-1}$ to get $u^s|_{\partial\Omega}$, $u^s_n = \Lambda^-(u^i|_{\partial\Omega} + u^s|_{\partial\Omega}) - u^i_n$ $O(N)$

5) eval. outside $\Omega$ via Green’s rep. $u^s = Du^s|_{\partial\Omega} - Su^s_n$
Summary of direct scattering solver

Pre-computation:

1) Nyström discretization of $S, D$ at $n = O(N^{1/2})$ nodes on $\partial \Omega$
   e.g. generalized Gaussian quadrature, 6 levels dyadic corner-refinement

2) Build interior DtN $\Lambda^-$ via merges up the tree, then Cayley $O(N^{3/2})$

3) Fill $A = \frac{1}{2} - D + S \Lambda^-$, take $A^{-1}$ $O(N^{3/2})$

Per incident wave at this freq. $\kappa$, solution now very fast...

4) fill RHS, apply $A^{-1}$ to get $u^s|_{\partial \Omega}$, $u^s_n = \Lambda^-(u^i|_{\partial \Omega} + u^s|_{\partial \Omega}) - u^i_n$ $O(N)$

5) eval. outside $\Omega$ via Green’s rep. $u^s = \mathcal{D} u^s|_{\partial \Omega} - S u^s_n$

6) eval. $u$ inside $\Omega$ via reversing all merges, traverse down the tree
   matvecs with soln. matrices $F^\alpha$, 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 $\kappa$ or low accuracy, e.g.
  
  FEM-BIE coupling, low $\kappa$, precond. BIE, 3 digits \cite{KirschMonk1994}
  
  4th-order FD + PML, UMFPACK, low $\kappa$ \cite{BrittTsynkovTurkel2011}
  
  2nd-order FD + PML, cyclic, $O(N \log N)$, 3 digits \cite{Heikkola2010}
Relation to prior work

Existing methods for variable-medium scattering:

- time-domain (FDTD): low-order, dispersion errors, long settling time
- freq-domain: low $\kappa$ or low accuracy, e.g.
  
  FEM-BIE coupling, low $\kappa$, precond. BIE, 3 digits \cite{KirschMonk94}
  
  4th-order FD + PML, UMFPACK, low $\kappa$ \cite{BrittTsynkovTurkel11}
  
  2nd-order FD + PML, cyclic, $O(N \log N)$, 3 digits \cite{Heikkolaetal10}

Our influences:

- multi-domain spectral collocation \cite{OrszagPatera80s,HesthavenPfeiffer}
- direct solvers for block-sparse: nested dissection, multifrontal \cite{GeorgeDuff70s}
- $O(N)$ direct solvers \cite{MartinssonRokhlin05,XiaChandrasekaranGuLi09}
- $O(N^{3/2})$ direct solver using both $u$ and $u_n$ data \cite{Chen02,Chen13}
- DtN version \cite{Martinsson12}; ItI makes robust for oscillatory PDE
Results: time and memory

8-core Xeon, MATLAB, not optim!

\( t_{\text{pre}} \) \hspace{1em} \text{precomputation: build DtN, build } A, \text{ dense } A^{-1}

\( t_{\text{new ext}} \) \hspace{1em} \text{compute } u^s|_{\partial \Omega}, \ u^s_n \text{ for new incident wave (ext. / far field)}

\( t_{\text{new int}} \) \hspace{1em} \text{propagate } u \text{ from bdry down to all leaf interior nodes}

\( L = \# \text{ tree levels} \quad N = \# \text{ unknowns} \quad n = \# \text{ BIE unknowns} \)
Results: time and memory

8-core Xeon, MATLAB, not optim!

- $t_{\text{pre}}$: precomputation: build DtN, build $A$, dense $A^{-1}$
- $t_{\text{new ext}}$: compute $u^s|_{\partial\Omega}$, $u^s_n$ for new incident wave (ext. / far field)
- $t_{\text{new int}}$: propagate $u$ from bdry down to all leaf interior nodes

$L = \# \text{tree levels} \quad N = \# \text{unknowns} \quad n = \# \text{BIE unknowns}$

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

- 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 \( u^i(x) = e^{i\kappa d \cdot x} \)

\[ d = (\cos \theta, \sin \theta) \quad \kappa = 300 \quad 100 \text{ shortest-}\lambda\text{'s} \]

\( b(x) \):

<table>
<thead>
<tr>
<th>( N )</th>
<th>ppw</th>
<th>error</th>
<th>( t_{\text{pre}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.3e5</td>
<td>5</td>
<td>3e-3</td>
<td>17 s</td>
</tr>
<tr>
<td>9e5</td>
<td>10</td>
<td>2e-7</td>
<td>78 s</td>
</tr>
<tr>
<td>3.7e6</td>
<td>20</td>
<td>7e-10</td>
<td>6 m</td>
</tr>
</tbody>
</table>

high-order ptwise err rel. to \( N=1.4e7 \)

movie \( 10^3 \) angles \( \theta \), 3 s each, incl. FMM to 240000 ext. targets
“Bathroom glass” at high frequency

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

physics: “2D electron gas”

80\(\lambda\) on a side  
time & accuracy similar to before  

movie twinkling
$k = 320$

$200\lambda$ across

9 digits (est.)

$N = 1.4\times10^7$

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

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

$t_{\text{new int}} = 10\text{ s}$
Photonic crystal waveguide

Until now largely propagating—what if resonances trap waves?
lattice of 400 bumps, each a resonator: choose $\kappa$ in bandgap (can’t prop.)

Again, 9 digits $N = 3.7e6$

- also test radially-symmetric $b(x)$ vs sep. of var. soln: stops at 10 digits
**Conclusions**

\[ O(N^{3/2}) \] direct solver: multiple incident waves at same \( \kappa \) very fast

\( N \sim 10^7 \), 9 digits @ 200 \( \lambda \), 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-\( \kappa \) DtN version: \( F^{\alpha} \)'s low rank, HBS (Gillman–Martinsson ’13)
- \( O(N) \) high-\( \kappa \) via butterfly compress \( F^{\alpha} \)'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