FLATIRON INSTITUTE
Center for Computational Mathematics

Challenges in fast solvers for highly oscillatory problems

Alex H. Barnett[1]

5/26/22

[1]Center for Computational Mathematics, Flatiron Institute, Simons Foundation

∗ this is a collection of opinions, not a complete review (apologies if I omit an area)

Tasks: frequency-domain wave BVPs

Helmholtz $(\Delta + k(\mathbf{x})^2)u = g$ in $\Omega \subset \mathbb{R}^d$, $d = 1, 2, 3$ acoustic, quantum, 2D EM

usually radiation (or multilayer, or worse) outgoing conditions

non-scalar cases: Maxwell (3D EM), elastodynamics (seismic)

Tasks: frequency-domain wave BVPs

Helmholtz $(\Delta + k(\mathbf{x})^2)u = g$ in $\Omega \subset \mathbb{R}^d$, $d = 1, 2, 3$ acoustic, quantum, 2D EM

usually radiation (or multilayer, or worse) outgoing conditions

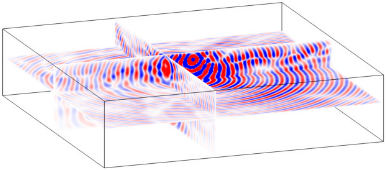
non-scalar cases: Maxwell (3D EM), elastodynamics (seismic)

Variable coeff $k(\mathbf{x})$:

shown: source g localized, in domain

Methods: FD, FFT, FEM, spec elem, HPS

Lippman–Schwinger (vol. IE), ...



(Zepeda-Nuñez + Demanet '15)

Tasks: frequency-domain wave BVPs

Helmholtz $(\Delta + k(\mathbf{x})^2)u = g$ in $\Omega \subset \mathbb{R}^d$, $d = 1, 2, 3$ acoustic, quantum, 2D EM

usually radiation (or multilayer, or worse) outgoing conditions

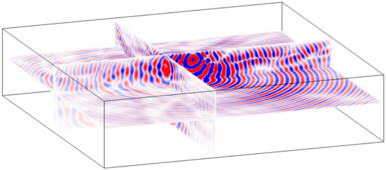
non-scalar cases: Maxwell (3D EM), elastodynamics (seismic)

Variable coeff $k(\mathbf{x})$:

shown: source g localized, in domain

Methods: FD, FFT, FEM, spec elem, HPS

Lippman–Schwinger (vol. IE), ...



(Zepeda-Nuñez + Demanet '15)

Piecewise-const $k(\mathbf{x})$:

eg $(\Delta + k^2)u = 0$ in $\mathbb{R}^d \backslash \overline{\Omega}$

$u = f$ on $\partial\Omega$ or $\partial u/\partial n$, Robin, etc

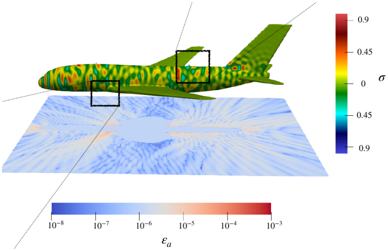
or transmission matching conditions

k_i in Ω_i, $i = 1, \ldots, n_{\text{media}}$

Scattering: f cancels incident wave

Methods: potential theory → Boundary IEs →

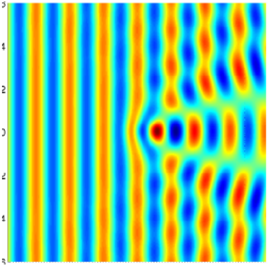
Nyström/Galerkin BEM; MPS, MFS



(Greengard, O'Neil, Rachh, Vico '21)

Three regimes

WEAK SCATTERING



$k(\mathbf{x}) \approx k_0, \quad u_{\text{scatt}} \ll u_{\text{inc}}$

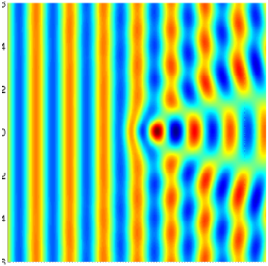
Born approx =
1st-ord. pert. th:

$u_{\text{scatt}} \approx G * (k^2 - k_0^2)$

optically "thin," microscopy,
Fourier imaging

Three regimes

WEAK SCATTERING



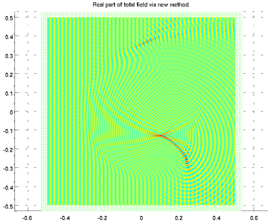
$k(\mathbf{x}) \approx k_0, \quad u_{\text{scatt}} \ll u_{\text{inc}}$

Born approx =
1st-ord. pert. th:

$u_{\text{scatt}} \approx G * (k^2 - k_0^2)$

optically "thin," microscopy, Fourier imaging

RAY-LIKE (EIKONAL)



bending ray/beam

refractive index $k(\mathbf{x})/k_{\text{inc}}$

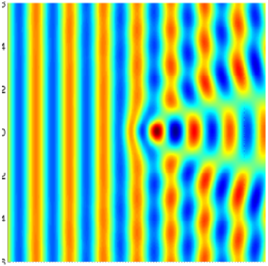
$u \approx$ locally 1 (or few)
plane-waves

no direct reflections
$\rightarrow$ no resonances

but: caustics!

Three regimes

WEAK SCATTERING



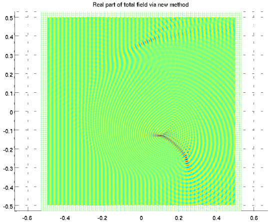
$k(\mathbf{x}) \approx k_0, \quad u_{\text{scatt}} \ll u_{\text{inc}}$

Born approx =
1st-ord. pert. th:

$u_{\text{scatt}} \approx G * (k^2 - k_0^2)$

optically "thin," microscopy,
Fourier imaging

RAY-LIKE (EIKONAL)



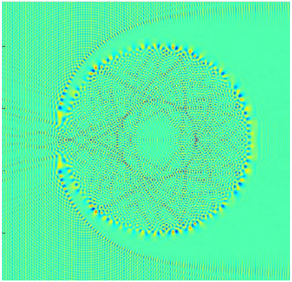
bending ray/beam

refractive index $k(\mathbf{x})/k_{\text{inc}}$

$u \approx$ locally 1 (or few)
plane-waves

no direct reflections
$\rightarrow$ no resonances
but: caustics!

STRONG SCATT. / RESONANT

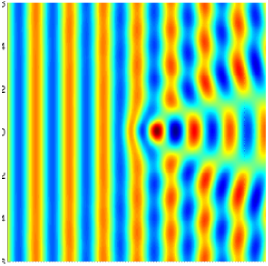


$k(\mathbf{x})$ big changes/jumps
multiple reflections
cavities, trapped rays
movie

resonances $\rightarrow$
rapid changes in u w.r.t. k_{inc}

Three regimes

WEAK SCATTERING



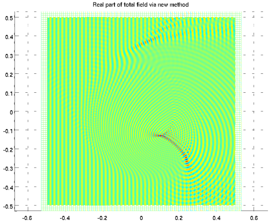
$k(\mathbf{x}) \approx k_0, \quad u_{\text{scatt}} \ll u_{\text{inc}}$

Born approx =
1st-ord. pert. th:

$u_{\text{scatt}} \approx G * (k^2 - k_0^2)$

optically "thin," microscopy,
Fourier imaging

RAY-LIKE (EIKONAL)



bending ray/beam

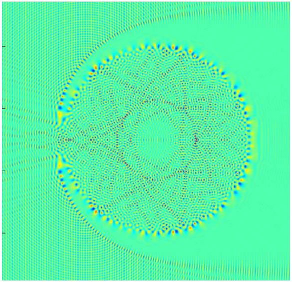
refractive index $k(\mathbf{x})/k_{\text{inc}}$

$u \approx$ locally 1 (or few)
plane-waves

no direct reflections
$\rightarrow$ no resonances

but: caustics!

STRONG SCATT. / RESONANT



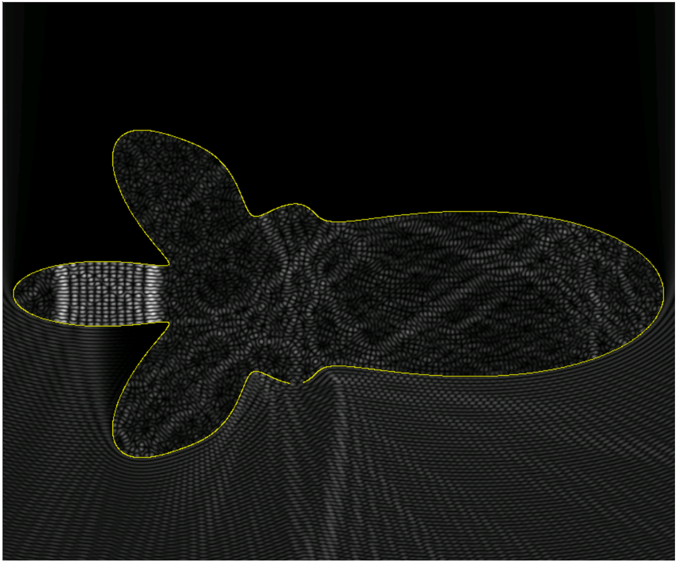
$k(\mathbf{x})$ big changes/jumps
multiple reflections
cavities, trapped rays

movie

resonances $\rightarrow$
rapid changes in u w.r.t. k_{inc}

Hard regime is $k \sim 10^2$ to 10^4; beyond this, geom. optics sometimes ok

Boundary conditions generally induce strong scattering: (unless convex)



cavity open arc Dirichlet Helmholtz 2D, k_{inc} hitting a resonance (Lintner–Bruno '12)

CHALLENGE 1: degrees of freedom (N)

usual discr. (even high order) needs $\geq$ few points per wavelength   Nyquist

- Vol discr: $N \sim k^d$ wavelength $\lambda = 2\pi/k$ eg 100λ in 3d: $N \sim 10^9$
- BIE discr: $N \sim k^{d-1}$ Kress (gold standard): > 4 ppw

CHALLENGE 1: degrees of freedom (N)

usual discr. (even high order) needs $\geq$ few points per wavelength Nyquist

- Vol discr: $N \sim k^d$ wavelength $\lambda = 2\pi/k$ eg 100λ in 3d: $N \sim 10^9$
- BIE discr: $N \sim k^{d-1}$ Kress (gold standard): > 4 ppw

IDEA i) For 1D $k(x)$ smooth (osc. 2nd-ord ODE): solve *phase function*

$u(x) = ae^{i\int \phi(x)dx} + be^{-i\int \phi(x)dx}$, only 2 directions! phase func $\phi(x)$ smooth

effort indep of k. Challenge: automate, adaptive/switching

(Bremer–Rokhlin; Agogs)

CHALLENGE 1: degrees of freedom (N)

usual discr. (even high order) needs $\geq$ few points per wavelength   Nyquist

- Vol discr: $N \sim k^d$ wavelength $\lambda = 2\pi/k$ eg 100λ in 3d: $N \sim 10^9$
- BIE discr: $N \sim k^{d-1}$ Kress (gold standard): > 4 ppw

IDEA i) For 1D $k(x)$ smooth (osc. 2nd-ord ODE): solve *phase function*

$u(x) = ae^{i\int \phi(x)dx} + be^{-i\int \phi(x)dx}$,   only 2 directions!   phase func $\phi(x)$ smooth

effort indep of k. Challenge: automate, adaptive/switching

(Bremer–Rokhlin; Agogs)

IDEA ii) For 2D/3D BIE & one convex obstacle   single scattering

bases inspired by geom. optics: then N grows v. weakly (eg $k^{1/9}$)

Challenge: scatt. from even 3 disks: exponential # rays (chaotic!)

FLATIRON INSTITUTE Center for Computational Mathematics

CHALLENGE 1: degrees of freedom (N)

usual discr. (even high order) needs $\geq$ few points per wavelength   Nyquist

- Vol discr: $N \sim k^d$ wavelength $\lambda = 2\pi/k$ eg 100λ in 3d: $N \sim 10^9$
- BIE discr: $N \sim k^{d-1}$ Kress (gold standard): > 4 ppw

IDEA i) For 1D $k(x)$ smooth (osc. 2nd-ord ODE): solve *phase function*

$u(x) = ae^{i\int \phi(x)dx} + be^{-i\int \phi(x)dx}$,   only 2 directions!   phase func $\phi(x)$ smooth

effort indep of k. Challenge: automate, adaptive/switching

(Bremer–Rokhlin; Agogs)

IDEA ii) For 2D/3D BIE & one convex obstacle   single scattering

bases inspired by geom. optics: then N grows v. weakly (eg $k^{1/9}$)

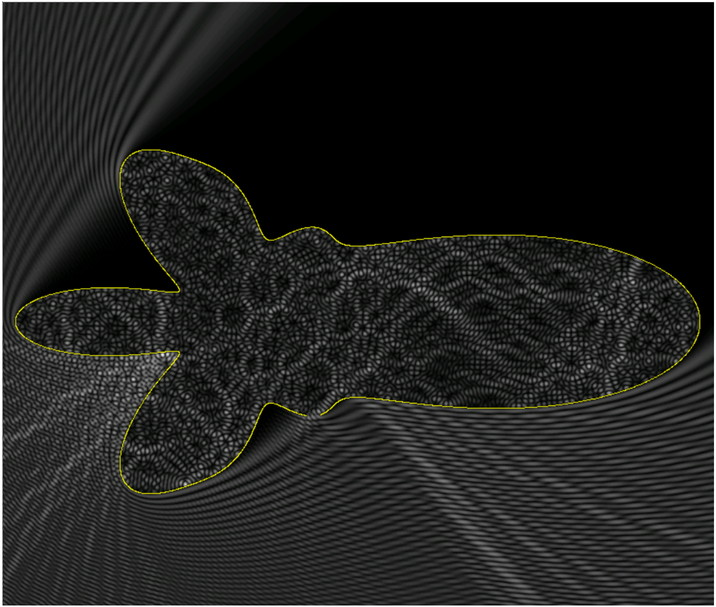
Challenge: scatt. from even 3 disks: exponential # rays (chaotic!)

IDEA iii) Soln. in Ω only $\sim k^{d-1}$ *effective* unknowns, scales like bdry $\partial\Omega$

eg, DtN map describes Ω response at freq k eg, exploited by HPS

Strong scatt $\rightarrow$ waves going in all directions $\rightarrow$ can't beat it (?)

Reminder that resonant cavity has waves traveling in all directions:



density on bdry contains all spatial freqs from 0 to k_{inc}, can't reduce N

CHALLENGE 2: Failure of iterative solvers

Vol. discr. (FD/FEM): multigrid precond fails for $k \gg 1$

Poission Greens kernel $k = 0$ was scale-invar/smoothing

- shifted Laplacian precond. has some claims   eg only $\mathcal{O}(k^{1/3})$ iter growth

IDEA: sweeping precond / one-way coupling of subdomains

- pretends that the half-space does not reflect $\rightarrow$ fails for strong scatt.
- how to use domain decomposition precond w/ resonant coupling?

CHALLENGE 2: Failure of iterative solvers

Vol. discr. (FD/FEM): multigrid precond fails for $k \gg 1$

Poission Greens kernel $k = 0$ was scale-invar/smoothing

- shifted Laplacian precond. has some claims   eg only $\mathcal{O}(k^{1/3})$ iter growth

IDEA: sweeping precond / one-way coupling of subdomains

- pretends that the half-space does not reflect $\to$ fails for strong scatt.
- how to use domain decomposition precond w/ resonant coupling?

BIE/BEM: resonant (eg, cavity): formally 2nd-kind but GMRES k^{d-1} iters

- BIE operator $\frac{1}{2} - D_k - i\eta S_k$ has eigenvalue density $\mathcal{O}(k^{d-1})$ at origin
- we will hear more about this today (analysis: Spence, Marchand...)

Challenge: new BIE precond. to remove (many?) resonances
Challenge: exploit/interpolate slow k-dep. of BIE op eigenvalues?

FLATIRON INSTITUTE
Center for Computational Mathematics

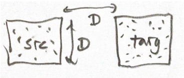
CHALLENGE 3: Low-rank separability of Green's kernel

BIE & VIE: fast algs (FMM, FDS) need kernel smoothing in far-field...

CHALLENGE 3: Low-rank separability of Green's kernel

BIE & VIE: fast algs (FMM, FDS) need kernel smoothing in far-field...

- Classical well-separated boxes — strong admissibility in HODLR, $\mathcal{H}$-mat, etc



$k \sim 1$: ε-rank $\mathcal{O}(\log^{d-1} \varepsilon^{-1})$ — basically $\mathcal{O}(1)$

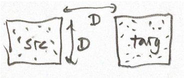
$k \gg 1$: ε-rank $\mathcal{O}((kD)^{d-1})$ — rank growth :(

...and for $k \gg 1$ FMM, $\exists$ diagonal translation ops

CHALLENGE 3: Low-rank separability of Green's kernel

BIE & VIE: fast algs (FMM, FDS) need kernel smoothing in far-field...

- Classical well-separated boxes strong admissibility in HODLR, $\mathcal{H}$-mat, etc

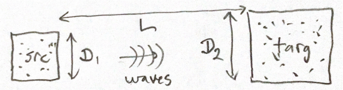


$k \sim 1$: ε-rank $\mathcal{O}(\log^{d-1} \varepsilon^{-1})$ basically $\mathcal{O}(1)$

$k \gg 1$: ε-rank $\mathcal{O}((kD)^{d-1})$ rank growth :(

...and for $k \gg 1$ FMM, $\exists$ diagonal translation ops

- But oscillatory kernel has "parabolic" separability $=$ Rayleigh diffraction limit



$k \gg 1$: rank $\mathcal{O}((kD_1D_2/L)^{d-1})$

low-rank if $(kD_1)(kD_2) < kL$

2D: similar to $D_1 \times D_2$ block of size-N DFT mat

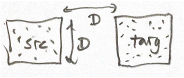
$\Rightarrow$ can "butterfly" compress BIE matrix

like FFT written as prod of $\log_2 N$ sparse mats

CHALLENGE 3: Low-rank separability of Green's kernel

BIE & VIE: fast algs (FMM, FDS) need kernel smoothing in far-field...

- Classical well-separated boxes   strong admissibility in HODLR, $\mathcal{H}$-mat, etc

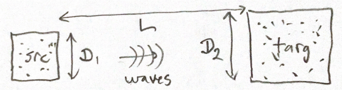


$k \sim 1$: ε-rank $\mathcal{O}(\log^{d-1} \varepsilon^{-1})$ basically $\mathcal{O}(1)$

$k \gg 1$: ε-rank $\mathcal{O}((kD)^{d-1})$ rank growth :(

...and for $k \gg 1$ FMM, $\exists$ diagonal translation ops

- But oscillatory kernel has "parabolic" separability   = Rayleigh diffraction limit



$k \gg 1$: rank $\mathcal{O}((kD_1D_2/L)^{d-1})$

low-rank if $(kD_1)(kD_2) < kL$

2D: similar to $D_1 \times D_2$ block of size-N DFT mat

$\Rightarrow$ can "butterfly" compress BIE matrix

like FFT written as prod of $\log_2 N$ sparse mats

Compression/inversion: solvers research phase (randomized lin alg, etc)
Challenge to interface to application users   (but see `butterflyPACK`, Liu)

Assorted CHALLENGES

4) Imposing Sommerfeld or "interesting media" radiation conditions

- for vol. discr: PMLs poor near corners, grazing rays; BIE op too big
- for BIE: half-space or multilayer media (Green's funcs/FMMs)
  photonic crystals ("half-space matching" method) (Fliss)

5) HPS: top-level merges $n \sim k^{d-1}$, dense inverse S_{glue}^{-1} takes $\mathcal{O}(n^3)$

- Idea: HPS merge at leaf (low) levels but iterate on high levels
  (Lucero-Lorca, Gillman)
- Challenge: can't use HODLR/HBS $\rightarrow$ butterfly compress S_{glue} ?

6) Ill-conditioning for $k \gg 1$ of Lippman–Schwinger VIE GMRES poor

FLATIRON INSTITUTE
Center for Computational Mathematics

CHALLENGE 7: Resonances and k-dependent information

Multiple reflections $\rightarrow$ resonances $\rightarrow$ rapid k-dependence of soln

$\ldots \rightarrow$ annoyingly fine k-sampling needed

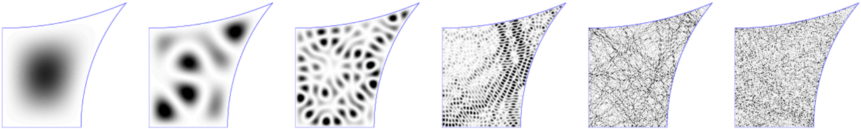
CHALLENGE 7: Resonances and *k*-dependent information

Multiple reflections $\to$ resonances $\to$ rapid k-dependence of soln

$\ldots \to$ annoyingly fine k-sampling needed

IDEA: more efficiency via solve together a *range* $k \in [k_1, k_2]$?

- exploit slow change of G_k, *rational* approx to inverses/soln?
- related to eigenvalue (closed cavity) BVP: $-\Delta\phi_j = \lambda_j \phi_j$



ϕ_j: $j = 1$ $\quad j = 10 \quad j = 100 \quad j = 10^3 \quad j = 10^4 \quad j = 10^5$

Sometimes $\mathcal{O}(N)$ speedup by linearize in k . . . apply to scattering?

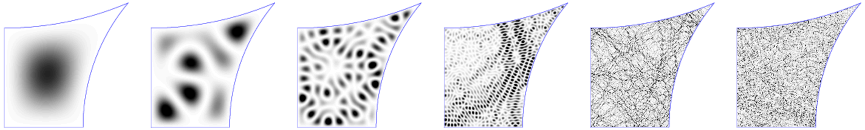
CHALLENGE 7: Resonances and k-dependent information

Multiple reflections $\to$ resonances $\to$ rapid k-dependence of soln

$\ldots \to$ annoyingly fine k-sampling needed

IDEA: more efficiency via solve together a *range* $k \in [k_1, k_2]$?

- exploit slow change of G_k, *rational* approx to inverses/soln?
- related to eigenvalue (closed cavity) BVP: $-\Delta\phi_j = \lambda_j \phi_j$



ϕ_j: $j = 1$ $\quad j = 10$ $\quad j = 100$ $\quad j = 10^3$ $\quad j = 10^4$ $\quad j = 10^5$

Sometimes $\mathcal{O}(N)$ speedup by linearize in k ... apply to scattering?

Conclusion: Highly-osc BVPs is a great place for numerics/software/analysis/applications to meet!