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IST program

Efficient methods for elliptic problems in heterogeneous media with applications

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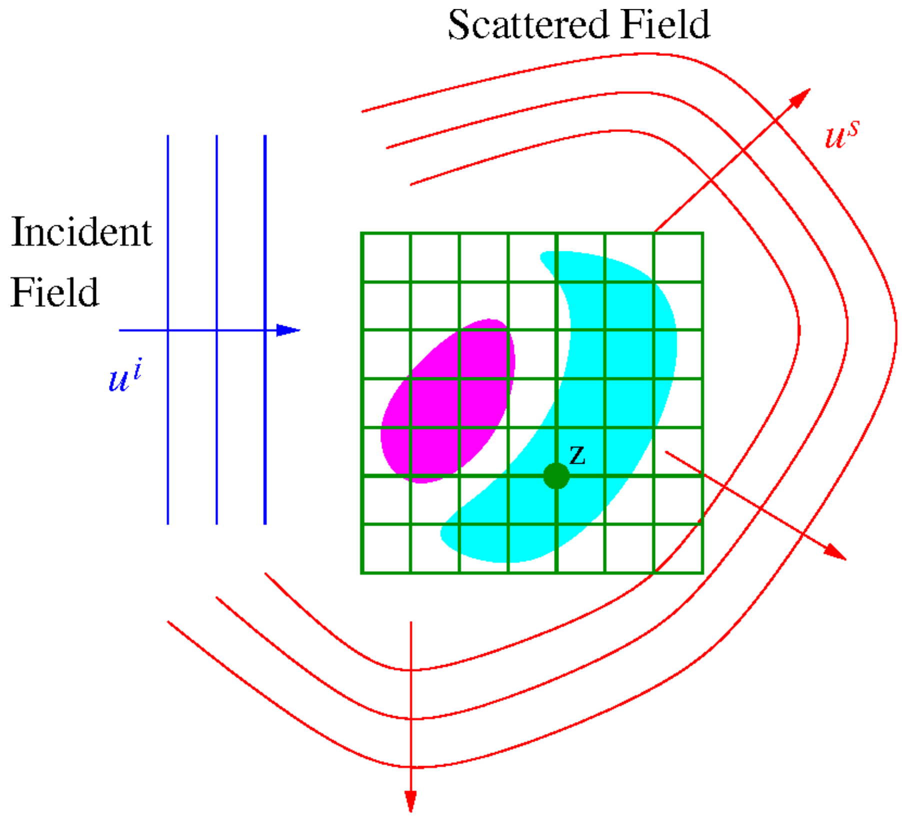
forward problem:

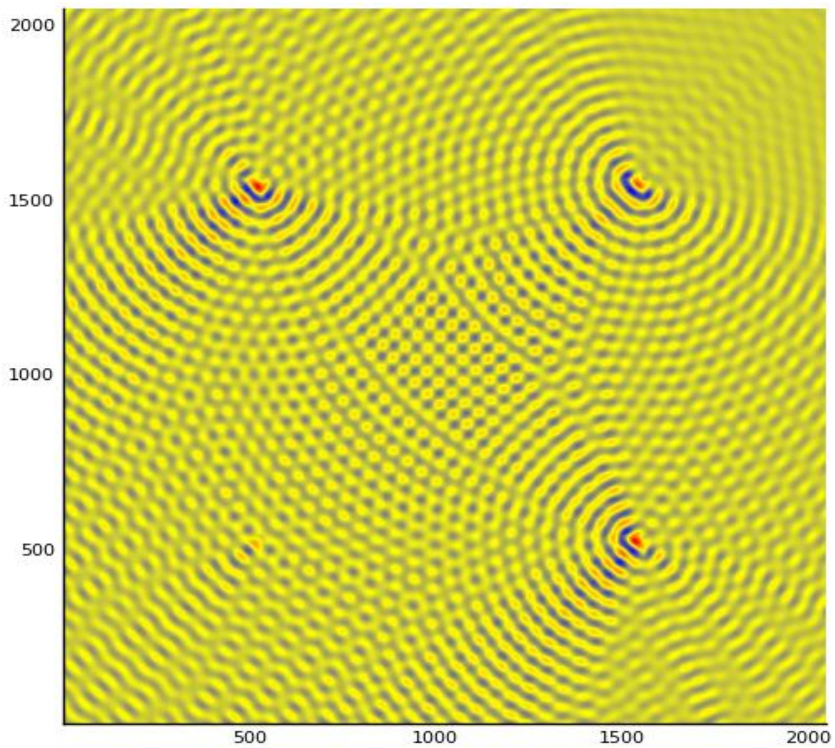
Scattering of acoustic waves by inhomogeneity

- **Incident field** u^i propagates through an inhomogeneous medium
- Determine: **Scattered field** u^s

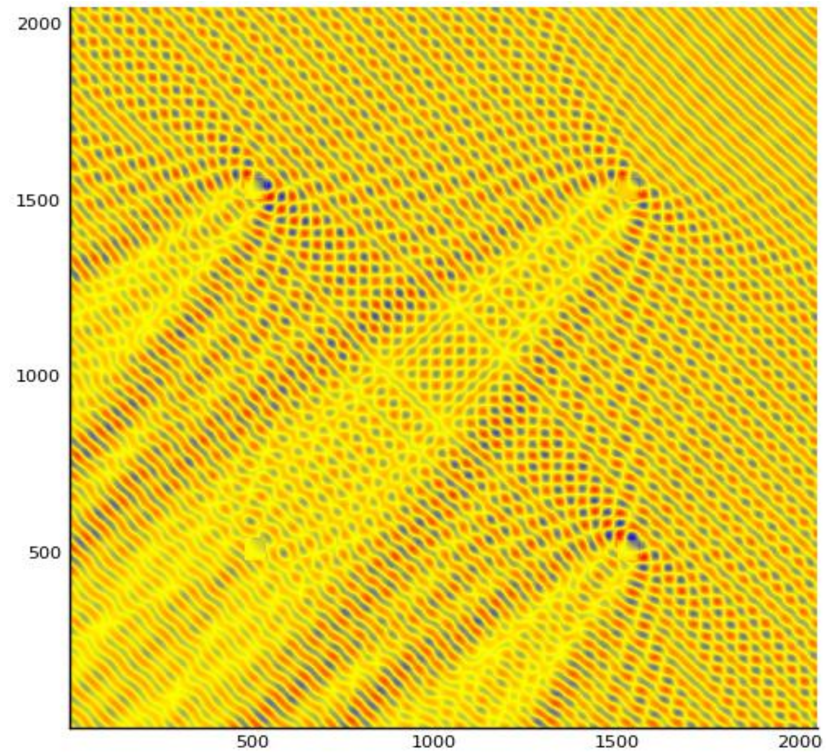


- External problem (infinite domain)
- Radiation conditions at infinity

Acoustics typically governed by the **Helmholtz** PDE



Scattered by inhomogeneity field



Full field

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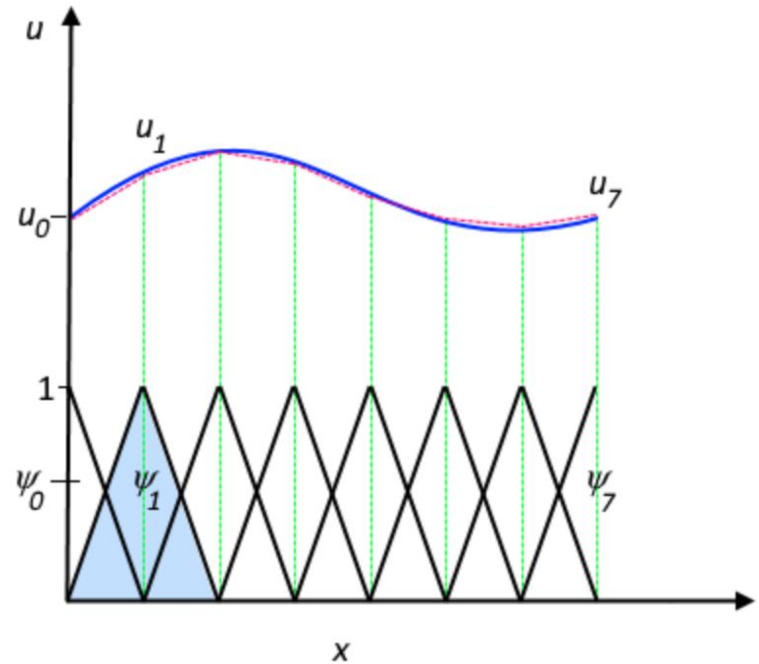
PDE form: the heterogeneous Helmholtz equation

$$\begin{cases} \Delta u(x) + k_0^2 n(x) u(x) = 0, \ \text{in } \mathbb{R}^3 \\ u(x) = u^{inc}(x) + u^s(x) \\ \Delta u^{inc} + k_0 u^{inc} = 0, \ \text{in } \mathbb{R}^3 \\ \lim_{r\to\infty} r\left(\frac{\partial u^s}{\partial r} - ik_0 u^s\right) = 0 \end{cases}$$

Numerical simulation: standard **local** methods

- Finite Element Method
- Finite Difference Method

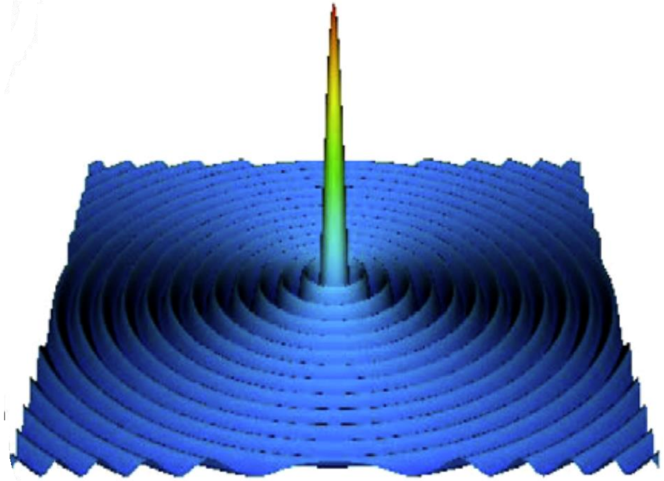
High frequency (short wavelength) regime: challenge remained unresolved for years



IE form: the Lippmann-Schwinger equation

$$u(x) = u^{inc}(x) + k_0^2 \int_{R^3} G(x,y)m(y)u(y)dy, \;\; x \in \mathbb{R}^3,$$

$$G(x,y) = \frac{1}{4\pi}\frac{e^{ik_0|x-y|}}{|x-y|}, \; x \neq y,$$ - fundamental solution (point source response)



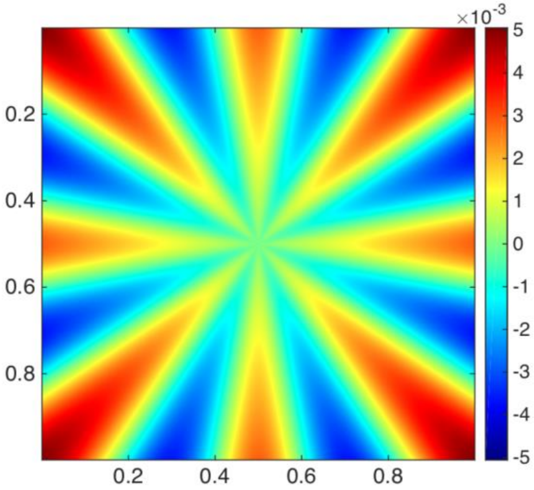
Main challenges for **local** methods:

Pollution Effect

- Discrete waves become **dispersive**
- Phase error **accumulates** with distance (see Figure)

$$\text{“}k^2 h \text{ is small”}$$

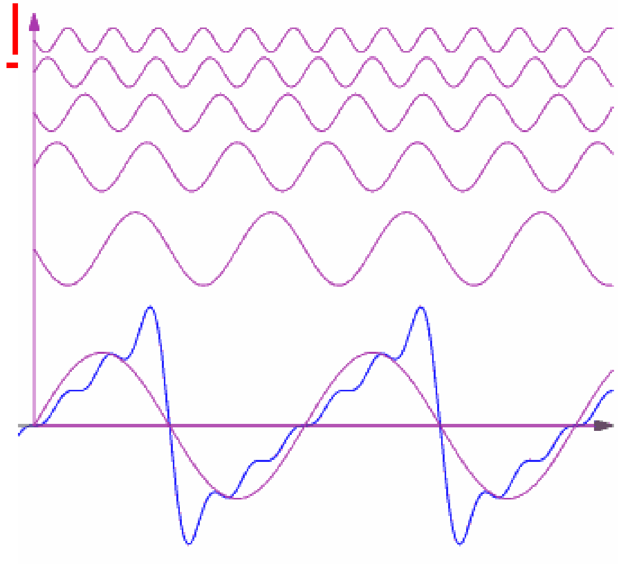
- The larger ***k*** the more points per minimal wavelength is required
- Overwhelmingly large systems
- The smaller ***h*** the worse **conditioning** of resulting system



How to eliminate the Pollution Effect?

Spectral Approximations

- Local methods: spatial derivatives are approximated with the second order of accuracy (with respect to ***h)***
- Global methods: approximate spatial derivatives



FEM/FDM require:

20 points per wavelength

(Pseudo-)Spectral methods require:

2 points per wavelength for homogeneous cases

4 points per wavelength for heterogeneous

IE vs PDE
Pollution Effect

Local methods:

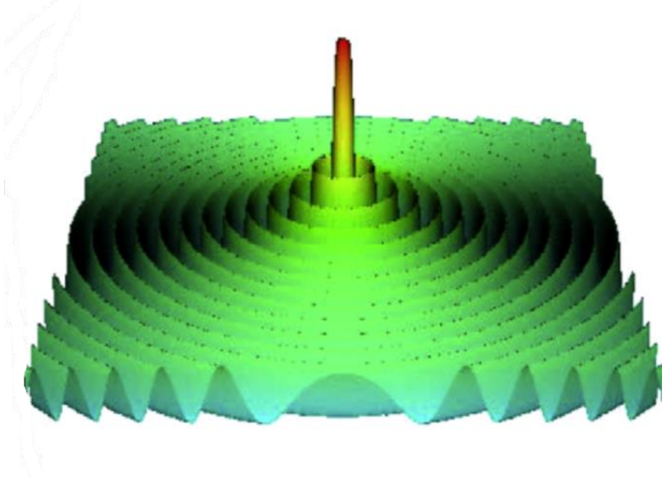
Field interactions are propagated from point A to point B

via a discrete numerical grid

Green's function is an exact propagator:

It propagates field interactions from point A to point B

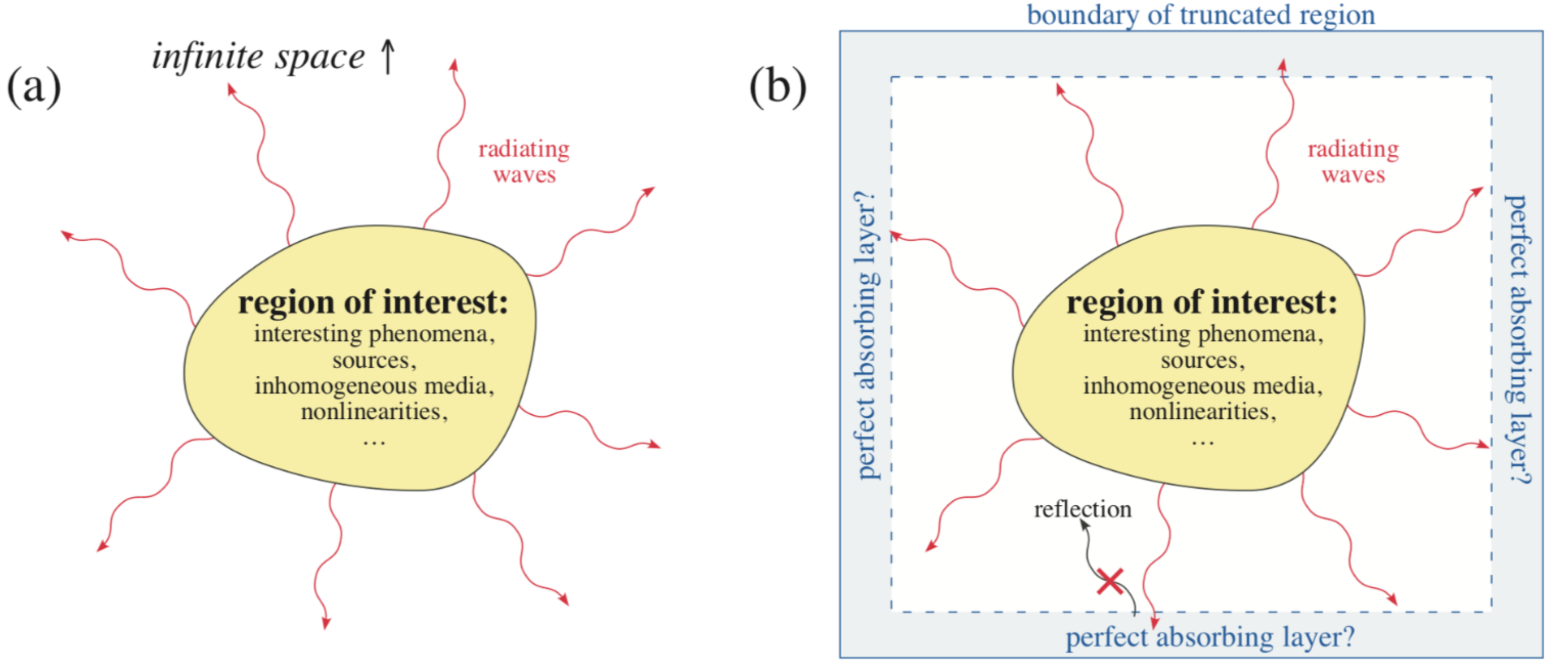
analytically



Hence IE methods are completely free from the Pollution Effect

Main challenges for **local** methods:

Radiation Conditions at infinity



Larger computational domain is required

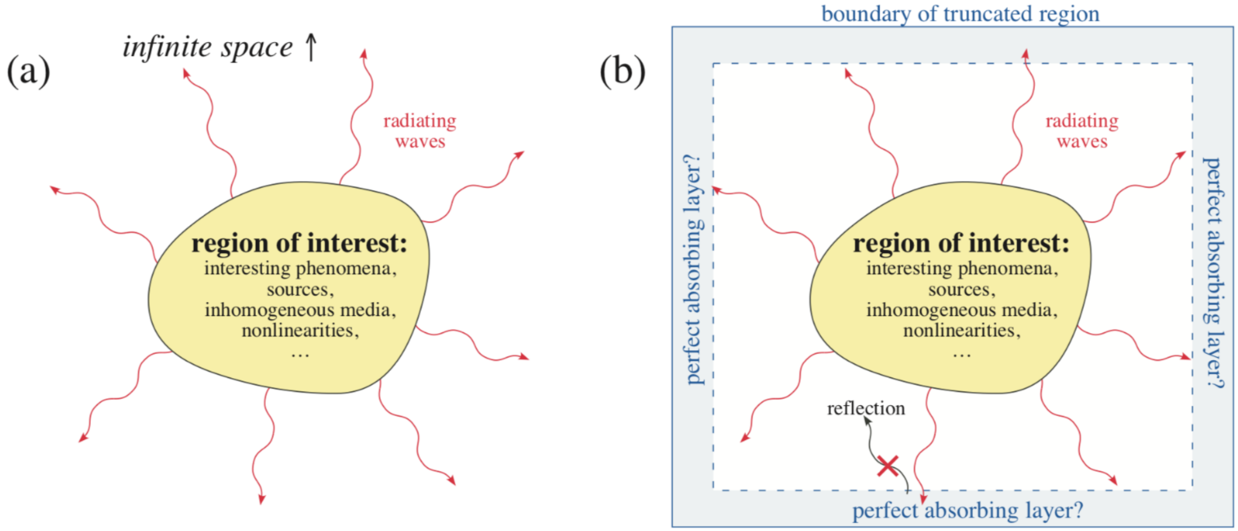
- Absorbing Boundary Conditions (ABC)
- Perfectly Matched Layer (PML)

IE vs PDE

Solutions of IEs automatically satisfy radiation conditions at infinity

No need for PML implementation:

- smaller computational domain, discretize only domain of interest
- PML is only an approximation, Green's function is exact



IE vs PDE

Resulting matrix when discretize IEs
is better conditioned
as opposed to PDEs

Condition number is crucial:

- Number of iterations before convergence (Krylov subspace methods)
- Numerical stability (w.r.t. machine precision)

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Pseudo-spectral Integral solver

Theory and methodology

$$u(x) = u^{inc}(x) + k_0^2 \int_{R^3} G(x,y)m(y)u(y)dy, \;\; x \in \mathbb{R}^3,$$

Underlying operator - volume potential:

$$\mathscr{A}[f](x) := k_0^2 \int_D G(x,y)f(y)dy, \;\; x \in \mathbb{R}^3.$$

Typically:

- Integration directly in physical domain
- Problem: weakly singular kernel, can be integrated in spherical coordinates
- Requires complex quadrature rules
- Piecewise constant basis functions ***limit accuracy to the first order***
- Tricky to implement

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u(x) = $\mathscr{A}[f](x) := k_0^2 \int_D G(x,y) f(y) dy, \;\; x \in \mathbb{R}^3.$

Moving to the Fourier domain (Convolution Theorem):

$$u(x) = \mathscr{F}^{-1}\left[\frac{\hat{f}(\mathbf{s})}{|\mathbf{s}|^2 - k_0^2}\right] = \left(\frac{1}{2\pi}\right)^d \int_{\mathbb{R}^d} e^{i\mathbf{s}\cdot x} \frac{\hat{f}(\mathbf{s})}{|\mathbf{s}|^2 - k_0^2} ds, \;\; x \in \mathbb{R}^d,$$

$\hat{f}(\mathbf{s}) = \mathscr{F}[f](\mathbf{s}) = \int_D e^{-i\mathbf{s}\cdot x} f(x) dx.$ - Fourier transform

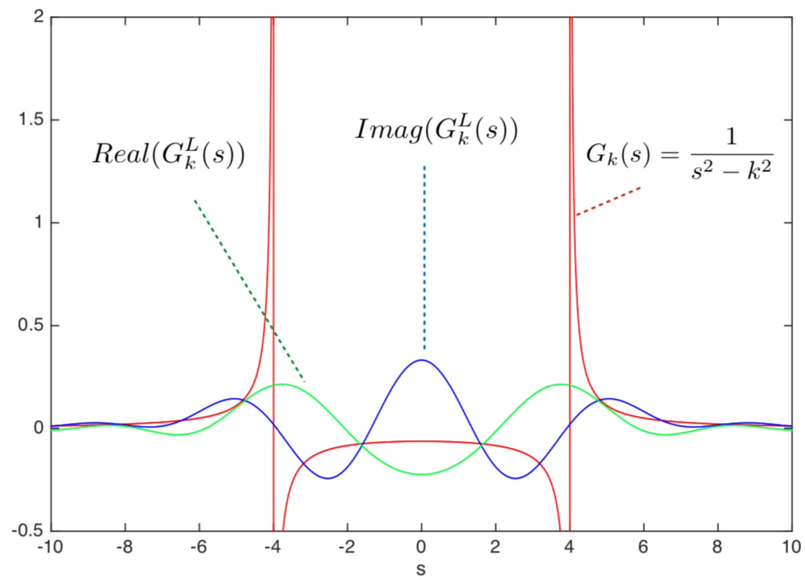
Principle difficulty - the kernel singularity: $\mathscr{F}[G](\mathbf{s}) = \frac{1}{|\mathbf{s}|^2 - k_0^2}, \;\; d = 1,2,3.$

- Can be integrated in spherical coordinates
- Require Non-uniform FFT (slow)
- Very tricky to implement

Pseudo-spectral Integral solver
Theory and methodology

Trick: truncate the Green's function to the domain of interest *

- Infinitely smooth Fourier transform
- Singularity is eliminated
- Analytical case–exponential accuracy
- Trapezoidal rule on a uniform grid
- Requires nothing more than FFT for implementation



* Vico, Greengard, Ferrando. "Fast convolution with free-space Green's functions", 2016

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Lippmann-Schwinger equation direct form:

$$u(x) = u^{inc}(x) + k_0^2 \mathscr{A}[mu](x), \quad x \in \mathbb{R}^3.$$

Lippmann-Schwinger equation potential form:

$$\psi(x) - k_0^2 m(x) \mathscr{A}[\psi](x) = f(x), \quad x \in \mathbb{R}^3,$$

Fourier series expansion

$$\psi(x) = \sum_{s=-\infty}^{\infty} \hat{\psi}_s e^{isx}, \quad f(x) = \sum_{s=-\infty}^{\infty} \hat{f}_s e^{isx}, \quad m(x) = \sum_{s=-\infty}^{\infty} \hat{m}_s e^{isx},$$

$$u^{inc}(x) = \sum_{s=-\infty}^{\infty} \hat{u}_s^{inc} e^{isx}, \quad u(x) = \sum_{s=-\infty}^{\infty} \hat{u}_s e^{isx},$$

Obtaining infinite systems:

$$\hat{U} + k_0^2 \hat{G}(\hat{M} * \hat{U}) = \hat{U}^{inc},$$

$$\hat{\Psi} - k_0^2 \hat{M} * (\hat{G}\hat{\Psi}) = \hat{F},$$

Pseudo-spectral Integral solver
conclusions

- Spectral accuracy:
  1. exponential convergence for analytical data
  2. second order convergence for general heterogeneous media
- No need for PML, No pollution effect

- The method of choice for wave scattering problems (using uniform grids)

- Superior efficiency for large-scale 3D problems

Domain size: $[120\lambda_0 \times 120\lambda_0 \times 120\lambda_0]$, λ_0 - minimal wavelength

Grid size: $[512 \times 512 \times 512]$ (requires approximately 500 Gb RAM)

Hardware used: 24 CPU cores Intel Xeon, 512Gb RAM

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Results

- Pseudo-spectral integral solver for the acoustic scattering problem was implemented and verified (2D/3D, Python and Julia)
- Deep theoretical and numerical study of the method was conducted
- Second order of convergence of the method for general heterogeneous scatterers was proven (1D)
- Superior efficiency of the method for large-scale wave phenomena was demonstrated
- A comparative study in the area was provided

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Thank you for your attention!

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