Fast High-Order Methods for Wave Scattering and Transformation Electromagnetics

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Outline

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   - Metamaterials, transformation electromagnetics and invisibility cloaks

2 Frequency-domain simulations
   - Seamless integration of Dirichlet-to-Neumann (DtN) BC with spectral elements
   - Wave-number explicit analysis of Helmholtz equations and time-harmonic Maxwell equations

3 Accurate simulation of perfect invisibility cloaks
   - Essential cloaking boundary conditions (CBCs)

4 Time-domain simulation
   - A semi-analytic approach for non-reflecting BCs
Typical setting of wave scattering

- Acoustic, electromagnetic, elastic or optical
- Incident wave, medium, scatterer, scattering wave
- Unbounded domain, high frequency, highly oscillatory, slow decay

- Many applications, e.g., the design of special media or material parameters to control and steer propagation of waves at will.
Electromagnetic metamaterials

• The material parameters: permittivity $\varepsilon$ and permeability $\mu$ characterize how electric and magnetic properties of materials affect and alter EM fields.

• Most materials are “double-positive”, and some are “single-negative”.

• No materials in nature are “double-negative”, which must be created artificially, and are referred to as metamaterials, negative index or left-handed materials.

• Zero-index materials: $\varepsilon = 0$ or $\mu = 0$. 
Motivations | Frequency domain | Invisibility Cloaks | Time-Domain Simulations
---|---|---|---

Transformation EM and invisibility cloaks

- **Pendry et al’06** and **Leonhardt’06** discovered steering EM and optical waves via coordinate transformations, which spawned the seminal field of Transformation EM and Optics (see, e.g., “Transformation Electromagnetics and Metamaterials”, Werner & Kwon, ed., Springer, 2014).

- A cloaking device can conceal and prevent waves from penetrating into a region so that the objects inside are “invisible” to observers outside (Figures adapted from Pendry et al, Science’06).

- Invisibility extends to thermodynamics, quantum mechanics (matter waves), and among others (cf. Wegener’13, Science; and Schittny et al.’14, Science).
**Zero-index materials with defects**

- **Goal**: Achieve total reflection and total transmission of an EM wave by tuning the geometrical and material parameters of certain "defects".

- Region 1: rectangular layer with width $d$ and zero-index medium $\varepsilon_1 = \mu_1 \approx 0$, and with some circular defects (normal materials).

- **Problems of interest**: (i) Find the material and geometrical parameters: $R$, $\varepsilon_2$, $\mu_2$ to achieve the goal. (ii) Verify the findings by simulation.
Time-harmonic acoustic scattering

Consider the Helmholtz equation:

$$\nabla \cdot (C(x) \nabla u(x)) + k^2 n(x) u(x) = f(x) \quad \text{in} \quad \mathbb{R}^d, \quad d = 2, 3,$$

where $k > 0$ is the wavenumber, $C \in \mathbb{R}^{d \times d}$ is symmetric positive definite, and $n > 0$ is piecewise. Assume that inhomogeneity of $C, n \subseteq \Omega_-$; $\text{supp}(f) \subseteq B_R$. Impose Sommerfeld radiation B.C on scattering field:

$$\partial_r u^s - i k u^s = o(r^{-(d-1)/2}) \quad \text{as} \quad r \to \infty.$$

- Unbounded domain
- Indefinite problem
- Solution ($k \gg 1$) oscillates highly and decays slowly
- Additional challenge: material parameters might be infinite at interior interfaces
Reduce unbounded domain by DtN B.C.

- Reduce the Helmholtz problem in unbounded domain to an equivalent BVP via exact Dirichlet-to-Neumann (DtN) B.C.

2D exact circular DtN B.C.:

\[ \partial_r u - \mathcal{T}_R u = \partial_r u^{\text{in}} - \mathcal{T}_R u^{\text{in}} := g, \]

where

\[ \mathcal{T}_R u := \sum_{|m|=0}^{\infty} \frac{kH_m^{(1)'}(kR)}{H_m^{(1)}(kR)} \left( \int_0^{2\pi} u(R, \theta)e^{-im\theta} d\theta \right) e^{im\theta}, \]

and \( H_m^{(1)} \) is the Hankel function.
Time-harmonic Maxwell equations

Consider

\[
\nabla \times (\mu^{-1} \nabla \times E) - k^2 \epsilon E = J \quad \text{in} \quad \mathbb{R}^3,
\]

where \( k = \sqrt{\epsilon_0 \mu_0 \omega} \), and the material parameters: \( \epsilon, \mu \in \mathbb{R}^{3 \times 3} \) are symmetric positive definite.

Assume that the background media are homogenous, and the support of \( J \) is confined in \( \Omega_- \).

Impose the Silver-Muller radiation B.C. upon scattering field:

\[
(\nabla \times E^s) \times n - i k E^s_T = o(r^{-1}) \quad \text{as} \quad r \rightarrow \infty.
\]
DtN for 3D Maxwell equations

Spherical DtN B.C. on the sphere $\Gamma_R$:

$$(\nabla \times E) \times n - ik\mathcal{T}_R[E_S] = G,$$

where $E_S$ is the tangential component of $E$, $\partial_z = d/dz + 1/r$, and

$$\mathcal{T}_R[E_S] = -i \sum_{l=1}^{\infty} \sum_{|m|=0}^{l} \left\{ - \frac{\hat{\partial}_z h_l^{(1)}(kR)}{h_l^{(1)}(kR)} \hat{E}_{1,l}^m(R) Y_l^m \times e_r + \frac{h_l^{(1)}(kR)}{\hat{\partial}_z h_l^{(1)}(kR)} \hat{\partial}_r E_{2,l}^m(R) \nabla S Y_l^m \right\}.$$

Here, $h_l^{(1)}$ is the spherical Hankel function, $\{Y_l^m\}$ are spherical harmonics and $\{Y_l^m e_r, \nabla S Y_l^m, \nabla S Y_l^m \times e_r\}$ are vector spherical harmonics (VSH). $\{\hat{E}_{1,l}^m, \hat{E}_{2,l}^m\}$ are VSH expansion coefficients of $E$ on $\Gamma_R$. 
Pros and Cons of DtN

Pros (compared with e.g., e.g., perfectly matched layers (PML) and lower-order absorbing BCs):

- Exact (transparent) BC can be placed as close as possible to the scatterers, and can impose the incident waves easily and naturally.
- It is compatible with high-order methods, e.g., spectral and spectral-element methods
- It is **local in frequency space**. Fast and robust (for $k \gg 1$) spectral solvera using Fourier/SH/VSH in angular directions, are available when the scatterer is a disk/ball (cf. Shen & W.’05,’07; Ma, Shen & W. 14).

Cons

- It is global in physical space due to Fourier/spherical harmonic/vector SH expansions in DtN B.C. Efficient technique is needed to integrate global DtN and with local spectral elements.
- It poses challenges in wave-number explicit analysis.
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Seamless integration of DtN with SEM

- For example, in 2D case, SEM involving DtN reads

\[
\langle T^e_R[u^e_N], v^e_N \rangle_{\Gamma_R} = \sum_{|m|=0}^{\infty} T_m \left( \int_0^{2\pi} u^e_N(R, \theta)e^{-im\theta} d\theta \right) \left( \int_0^{2\pi} v^e_N(R, \theta)e^{-im\theta} d\theta \right), \quad T_m = \frac{kH^{(1)'}(kR)}{H^{(1)}(kR)},
\]

where \( u^e_N, v^e_N \in V^e_N := \{ v \in C(B_R) : v(x)|_{\Omega_e} = v(\chi^e) \in P^2_N, \ 1 \leq e \leq E \} \) (piecewise \( C^0 \)-function).

- **Usual approach**: Interpolating between Fourier points and spectral element grids (with FFT) only has a convergence \( O(N^{-1}) \) as \( u^e_N \in C^0 \).
Seamless integration of DtN with SEM (cont’d)

- **Task:** Evaluate Fourier coefficient of a piecewise function on mapped LGL grids by Gordon-Hall mapping $\chi_e$ of curvilinear elements:

$$
\int_0^{2\pi} u^e_N|_{r=R} e^{-im\theta} d\theta = \sum_e \int_{\theta_e}^{\theta_{e+1}} u^e_N|_{r=R} e^{-im\theta} d\theta = \sum_e \int_{-1}^{1} \{ u^e_N e^{-im\theta(\chi_e)} J(\chi_e) \} \bigg|_{\eta=1} d\xi.
$$

- **Semi-analytic approach** (Yang, W., Wang’15): Using Gordon-Hall mapping with a new parameterisation of the arc $[\theta_e, \theta_{e+1}]$, we can analytically evaluate the Fourier coefficient via

$$
\int_{-1}^{1} P_n(\xi) \left\{ e^{-im\theta(\chi_e)} J(\chi_e) \right\} \bigg|_{\eta=1} d\xi = \frac{2\hat{\theta}_e R}{i^n} \sqrt{\frac{\pi}{2m\hat{\theta}_e}} J_{n+1/2}(m\hat{\theta}_e) e^{-im\beta_e},
$$

where $P_n$ is Legendre poly., $\hat{\theta}_e = (\theta_{e+1} - \theta_e)/2$, $\beta_e = (\theta_e + \theta_{e+1})/2$, and $J_{n+1/2}$ is the Bessel function.
**Task:** Given $u^e_N, E^e_N \in \text{SEM-solution-space}$, we need to evaluate the integral related spherical DtN or DtN for Maxwell equations

\[
\iint_{S^2} u^e_N|_{r=R} Y^m_l(\theta, \varphi) dS, \quad \iint_{S^2} E^e_N|_{r=R} \cdot \{ Y^m_l e_r, \nabla_S Y^m_l, \nabla_S Y^m_l \times e_r \} dS.
\]

**Approach:** Use Latitude ($\varphi \in [0, 2\pi]$)-Longitude ($\theta \in [0, \pi]$) partition of the sphere by e.g., $4 \times 3 = 12$ pieces. Then we can apply the exact formula in $\varphi$-direction as the previous Fourier case, which can be separated from $\theta$-direction.
**Accuracy of SH/VSH transformation on SEM grids**

Spherical harmonic expansion of $f(x) = \cos(k \cdot x): f \sim \mathcal{I}_N^k f \sim S_L(f) = \sum_{l=0}^{L} \sum_{|m|=0}^{l} \tilde{f}_l^m Y_l^m$.

| $k = (k_1, k_2, k_3)$ | N  | L  | $||f - \mathcal{I}_N(f)||_{\text{max}}$ | $||f - S_L(f)||_{\text{max}}$ |
|------------------------|----|----|--------------------------------------|--------------------------------|
| (10, 10, 10)          | 45 | 30 | 2.6931e-14                          | 3.4314e-6                     |
|                        | 45 | 35 | 2.6931e-14                          | 1.9054e-8                     |
|                        | 45 | 40 | 2.6931e-14                          | 3.1143e-12                    |
|                        | 45 | 45 | 2.6931e-14                          | 2.5868e-14                    |
| (20, 20, 20)          | 60 | 50 | 3.5749e-14                          | 8.8682e-6                     |
|                        | 60 | 55 | 3.5749e-14                          | 1.5096e-7                     |
|                        | 60 | 60 | 3.5749e-14                          | 1.7226e-10                    |
|                        | 60 | 65 | 3.5749e-14                          | 1.2649e-12                    |
|                        | 60 | 70 | 3.5749e-14                          | 4.2688e-14                    |

Vector spherical harmonic expansion of $A = (\cos(k \cdot x), \cos(k \cdot x), \cos(k \cdot x))^t$.

| $k = (k_1, k_2, k_3)$ | N  | L  | $||A - \mathcal{I}_N(A)||_{\text{max}}$ | $||A - V_L(A)||_{\text{max}}$ |
|------------------------|----|----|--------------------------------------|--------------------------------|
| (10, 10, 10)          | 45 | 30 | 2.3287e-14                          | 2.4310e-5                     |
|                        | 45 | 35 | 2.3287e-14                          | 3.4260e-8                     |
|                        | 45 | 40 | 2.3287e-14                          | 4.2913e-11                    |
|                        | 45 | 45 | 2.3287e-14                          | 8.1046e-14                    |
| (20, 20, 20)          | 60 | 50 | 3.5305e-14                          | 1.1981e-5                     |
|                        | 60 | 55 | 3.5749e-14                          | 2.0481e-7                     |
|                        | 60 | 65 | 3.5749e-14                          | 2.0477e-12                    |
|                        | 60 | 70 | 3.5749e-14                          | 8.0047e-14                    |

**Note:** The computation of e.g., $(L + 1)^2$-spherical harmonic coefficients with $L = 70$ is about 5 seconds. It is more accurate than Spherepack ($1e-10$), and allows for seamlessly integrating with 3D SEM (ongoing).
Wavenumber explicit analysis
Wave-number explicit analysis

**Wellposedness:** thanks to “\(\text{Im}(\mathcal{T}_R u, u)_{\Gamma_R} > 0\)” and “\(\text{Im}(\mathcal{T}_R [E_S], E_S)_{\Gamma_R} > 0\)” (cf. Harari & Hughes’92 and Nedelec’01).

**Indefiniteness** of Helmholtz equation:

\[
\left(\nabla u, \nabla v\right)_\Omega - k^2 (u, v)_\Omega + \langle \mathcal{T}_R u, u \rangle_{\Gamma_R} = (f, v)_\Omega + \langle g, v \rangle_{\Gamma_R}.
\]

**Wave-number explicit a prior estimates** are wanted:

\[
\|\nabla u\|_\Omega + k\|u\|_\Omega \lesssim k^\alpha \|f\|_\Omega + k^\beta \|g\|_{L^2(\Gamma_R)}.
\]

- 1D analysis based on (discrete) Green’s functions (cf. Douglas et.al’93, Babuška et.al’95, ’97, · · · ).
- Assume \(\Omega\) is a star-shape type domain (i.e., \((x - x_0) \cdot \mathbf{n}_{\partial\Omega} \geq C_{\Omega} > 0\)), and take \(v = u, \ (x - x_0) \cdot \nabla u\) (cf. Melenk’95, Cummings & Feng’06; Hetmaniuk’07 for \(\mathcal{T}_R u = iku\); Shen & W.’07; Chandler-Wilde & Monk’08 for exact DtN).
- Much recent interest in such analysis of FEM, DG-FEM, · · · · · ·
Wave-number explicit analysis (cont’d)

• **Hiptmair and Moiola’11** analysed Maxwell equations in a star-shaped domain with first-order approximate DtN BC:

\[(\nabla \times E) \times n - ik E_S = g,\]

by testing the equation with two test functions: \(E\) and \((x - x_0) \cdot \nabla \times E:\)

\[\|\nabla \times E\|_\Omega + k\|E\|_\Omega \leq C_1\|J\|_\Omega + C_2\|g\|_{\Gamma_R}.
\]

• Wave-number explicit stability analysis for exact DtN:

\[(\nabla \times E) \times n - ik \mathcal{T}_R[E_S] = G,\]

is not available so far and open, except for the spherical shell.

• The difficulty resides in estimating the explicit lower bound of

\[\text{Im}(\mathcal{T}_R[E_S], E_S)_{\Gamma_R} \geq C(k) =? > 0.\]
Wave-number explicit analysis (cont’d)

- Maxwell equations in a spherical shell using divergence-free VSH:

$$E = \sum_{l=1}^{\infty} \sum_{|m|=0}^{l} \left\{ E_{1,l}^m(r) \nabla S Y_l^m \times e_r + \nabla \times (E_{2,l}^m(r) \nabla S Y_l^m \times e_r) \right\},$$

which automatically satisfies $\text{div} \ E = 0$.

- Remarkably, both components satisfy the same Helmholtz equation but with different BC. at inside spherical surface $r = R_1$:

$$\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{du}{dr} \right) - \frac{l(l+1)}{r^2} u + k^2 u = 0, \quad u = E_{1,l}^m, E_{2,l}^m, \quad R_1 < r < R_2.$$

- Testing the equation with $u$ and $(r - R_1)u'$, we can obtain for exact DtN (Ma, Shen & W.’15):

$$\| \nabla \times E \|_\Omega + k \| E \|_\Omega \leq C_1 k^{4/3} \| J \|_\Omega + C_2 k^{1/3} \| g \|_{\Gamma_R},$$

where $C_1, C_2$ are independent of $k$. 
Invisibility cloaks

New cloaking boundary conditions (CBCs)
Form invariant of Maxwell equations

- **Form invariant** Consider

\[
\nabla_\tilde{x} \times \tilde{E} - i\omega\mu_0 \tilde{H} = 0, \quad \nabla_\tilde{x} \times \tilde{H} + i\omega\epsilon_0 \tilde{E} = 0 \quad \text{in} \quad \mathbb{R}^3.
\]

Given a coordinate transformation \( x = x(\tilde{x}) \) with Jacobian matrix \( J \), the Maxwell system in the new coordinates reads

\[
\nabla_x \times E - i\omega\mu_0 \mu H = 0, \quad \nabla_x \times H + i\omega\epsilon_0 \epsilon E = 0, \quad \mu = \epsilon = JJ^t / \det(J).
\]

This leads to new material parameter that can steer waves at will.

- **TE polarisation** Consider transverse-electric (TE) polarisation, where \( E = (0, 0, u(x, y))^t \) and \( H \) has only \( x, y \)-components. Then we have

\[
\nabla \cdot (C(x) \nabla u(x)) + k^2 n(x) u(x) = 0 \quad \text{in} \quad \Omega_-,
\]

where \( C = \frac{J_{cn} J_{cn}^t}{\det(J_{cn})} \), \( n = \frac{1}{\det(J_{cn})} \), \( J_{cn} := \begin{bmatrix} \partial_x x & \partial_y x \\ \partial_x y & \partial_y y \end{bmatrix} \).
Coordinate transformations

- **Spherical/cylindrical circular invisibility cloak**: Transformation blows up the origin $\tilde{r} = 0$ to a ball/disk $0 < r < R_1$ *(cf. Pendry et al’06)*:

  $$r = \frac{R_2 - R_1}{R_2} \tilde{r} + R_1, \quad \theta = \tilde{\theta}, \quad \varphi = \tilde{\varphi}.$$ 

- **Polygonal invisibility cloak** is based on a singular transformation that blows up the origin to a polygonal domain.

  $$r = (1 - \rho) \tilde{r} + R_1, \quad \theta = \tilde{\theta}, \quad \rho := OA_p/OA = OB_p/OB = \cdots.$$ 

![Coordinate transformations](image)
Circular cylindrical cloak

Governing equation in polar coordinates:

\[
\frac{1}{r - R_1} \frac{\partial}{\partial r} \left( (r - R_1) \frac{\partial u}{\partial r} \right) + \frac{1}{(r - R_1)^2} \frac{\partial^2 u}{\partial \theta^2} + k^2 b^2 u = 0, \quad R_1 < r < R_2;
\]

\[
\mathcal{L}[u] := \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial u}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 u}{\partial \theta^2} + k^2 u = 0, \quad r < R_1 \text{ or } r > R_2,
\]

where \( k = \omega \sqrt{\varepsilon_0 \mu_0} \), and \( b = R_2/(R_2 - R_1) \). Impose DtN BC at \( r = R_3 \):

\[
\partial_r u - \mathcal{T}_{R_3} u = \partial_r u_{\text{in}} - \mathcal{T}_{R_3} u_{\text{in}} := g, \quad \text{where as before the DtN operator}
\]

\[
\mathcal{T}_{R_3} u := \sum_{|m| = 0}^{\infty} \frac{kH_m^{(1)'}(kR_3)}{H_m^{(1)}(kR_3)} e^{im\theta} \times 
\]

\[
\int_0^{2\pi} u(R_3, \theta)e^{-im\theta} d\theta.
\]

Transmission condition at \( R_2 \):

\[
[u] = 0, \quad \partial_r u|_{R_2^-} = b \partial_r u|_{R_2^+}.
\]

Question: Clocking BC at \( R_1 \)?
Cloaking boundary conditions (CBCs)

- Singular material parameters:
  \[ [E]_{r=R_1} = J \neq 0 \] (1)
  
  induce electric surface currents (cf. Ruan et al’07, PRL & Zhang et al’07).

- **Critical issue**: How to impose cloaking BCs at \( R_1 \) to achieve perfect cloaking effects?

Some existing CBCs

- Perfect magnetic conductor (PMC): \( n \times H |_{r=R_1} = 0 \) in FEM simulations
  [PMC does not lead to an independent BC in polar coordinates]

- CBCs by Weder’08 for spherical cloaks from energy conservation
  [not applicable, as the condition \( (n \times E)|_{R_1} = 0 \) therein violates (1)]

- Non-local pseudo-differential CBCs by Lassas & Zhou’11’14
**Essential CBCs**

- **Viewpoint:** Well-behaved EM fields in the original coordinates should be still well-behaved after transformation. In other words, EM fields with finite energy should still have finite energy in new coordinates:

\[
\varepsilon_0 \iint_{\Omega} E^t \epsilon E^* d\Omega < \infty, \quad \mu_0 \iint_{\Omega} H^t \mu H^* d\Omega < \infty.
\]

- Recall that \( E = (0, 0, u)^t \) and

\[
H = (H_1, H_2, 0)^t = \frac{1}{i\omega\mu_0} \left( \frac{1}{r - R_1} \frac{\partial u}{\partial \theta}, -\frac{r - R_1}{r} \frac{\partial u}{\partial r}, 0 \right)^t.
\]

Letting \( r \to R_1^+ \) leads to

\[
\partial_\theta u(R_1^+, \theta) = 0.
\]

**Note:** This notion is related to essential “pole” conditions in polar coordinates (cf. Shen’97), applicable to general singular transformations, e.g., triangle-to-rectangle mapping (cf. Shen, W., Li’09)

- **Essential CBCs** = “(2)” + “[\( n \times H \)] r=R_1 = 0”. The 2nd condition is physical (cf. Ruan et al’07): leading to \( \partial_r u(R_1^-, \theta) = 0 \).
Decoupling of the inside and outside

Define the operators:

\[ \mathcal{L}_0[u] := \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial u}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 u}{\partial \theta^2} + k^2 u = 0, \]

\[ \mathcal{L}_1[u] := \frac{1}{r - R_1} \frac{\partial}{\partial r} \left( (r - R_1) \frac{\partial u}{\partial r} \right) + \frac{1}{(r - R_1)^2} \frac{\partial^2 u}{\partial \theta^2} + k^2 b^2 u. \]

Let \( \Omega_i = (R_{i-1}, R_i) \) and \( u^i = u|_{\Omega_i} \) with \( R_0 = 0 \) and \( i = 1, 2, 3 \). Then

\[ \mathcal{L}_0[u^0] = 0 \text{ in } \Omega_0; \quad \partial_\theta u^0(0, \theta) = \partial_r u^0(R_1, \theta) = 0; \]

\[ \mathcal{L}_1[u^1] = 0 \text{ in } \Omega_1; \quad \partial_\theta u^1(R_1, \theta) = 0; \]

\[ u^1 = u^2, \quad b^{-1} \partial_r u^1 = \partial_r u^2 \text{ at } r = R_2, \]

\[ \mathcal{L}_0[u^2] = 0 \text{ in } \Omega_2; \quad \partial_r u^2 - \mathcal{I}_{R_3} u^2 = g \text{ at } r = R_3. \]

**Note:** Under essential CBCs, \( u^0 \) is decoupled, and \( u^0 \equiv 0 \) (i.e., \( E = 0 \)) in the cloaked region. Thus, perfect cloaking effects can be achieved. It is also decoupled for an active compactly supported source: \( \mathcal{L}[u^0] = f. \)
Fourier & Legendre-spectral-element methods

Figure: Row 1: real (left) and imaginary (right) parts of the electric-field distributions. Row 2-3: profiles of the real and imaginary parts of the electric-field along $\theta = \pi/3$. Here, $k = 100$, and $(R_1, R_2, R_3) = (0.3, 0.9, 1.0)$. 
Fourier & Legendre-spectral-element methods

Place a point source in the outermost layer \( R_2 < r < R_3 \) that generates anti-plane wave.

**Figure:** Electric-field distributions with an external source compactly supported in the outmost shell. Left: real part; right: imaginary part. Here, \( k = 40 \) and \((R_1, R_2, R_3) = (0.2, 0.6, 1.0)\).
Elliptic cylindrical cloaks

- Elliptic coordinates:

\[ x = a \cosh \xi \cos \eta, \quad y = a \sinh \xi \sin \eta \]

where \( \xi \in [0, \infty), \eta \in [0, 2\pi) \) and \( \pm a \) are foci.

- \( \xi \) =constant gives confocal ellipses, and \( \eta \) =constant gives hyperbolae

- Mathieu functions: \( \text{ce}(\eta; q); \text{se}(\eta; q) \) are the counterparts of cosines and sines.

**Coordinate transformation** for elliptic cylindrical cloak: \((\zeta, \eta, z) \rightarrow (\xi, \eta, z)\) that blows up \( \zeta = 0 \) **to the ellipse** \( \xi = \xi_1 \):

\[
[0, \xi_2] \rightarrow [\xi_1, \xi_2]: \quad \xi = \zeta/d + \xi_1, \quad \eta = \eta, \quad z = z, \quad d = \xi_2/(\xi_2 - \xi_1).
\]

The elliptic domain \( 0 \leq \xi < \xi_1 \) forms the cloaked region to hide objects.
Elliptic CBCs and DtN BC

- Essential to decompose incident and total fields into elliptic-cosine and elliptic-sine components:

\[
v(\xi, \eta) = \sum_{m=0}^{\infty} \hat{v}_m^c(\xi) c_m(\eta; q) + \sum_{m=1}^{\infty} \hat{v}_m^s(\xi) s_m(\eta; q) = v_c + v_s.
\]

- **CBCs** must be imposed differently for two components (cf. Yang & W.’14), e.g., the essential “pole” conditions are

\[
\partial_\xi v_c(\xi_1^+, 0) = 0, \quad v_s(\xi_1^+, 0) = 0.
\]

- Elliptic DtN BC: \((\partial_\xi - \mathbb{T}_{\xi_3})v = \phi\) with

\[
\mathbb{T}_{\xi_3}v = \sum_{m=0}^{\infty} \frac{\partial_\xi \text{Mc}_m^{(3)}(\xi_3; q)}{\text{Mc}_m^{(3)}(\xi_3; q)} \hat{v}_m^c(\xi_3) c_m + \sum_{m=1}^{\infty} \frac{\partial_\xi \text{Ms}_m^{(3)}(\xi_3; q)}{\text{Ms}_m^{(3)}(\xi_3; q)} \hat{v}_m^s(\xi_3) s_m,
\]

where \(\text{Mc}_m^{(3)}, \text{Ms}_m^{(3)}\) are Hankel-Mathieu functions.
Mathieu & Legendre-spectral-element methods

Left: simulations from Ma et al’08 (Phys. Rev. A) by PMC+FEM+PML. Right: our simulation result with an incident angle $\theta_0 = \pi, \pi/4$. We also plot Poynting vector: $S = \text{Re} \{E \times H^*\}/2$, i.e., the energy flux density.
CBCs for polygonal invisibility cloaks

Use local coordinates $\tau, n$ to characterise the essential CBCs:

$$\nabla_{\tau}u^+ = 0 \text{ at } \Gamma^p_+; \quad \nabla_nu^- = 0 \text{ at } \Gamma^p_-,$$

where we recall the $E = (0, 0, u)$. This also allows for decoupling the equation inside and outside the cloaked region.

Note: Essential to build in $\partial_{\xi} u^+_{\text{sem}}(\xi, -1) = 0$ in SEM solution space to deal with the singular coefficients, e.g., $(1 + \eta)^{-1} \partial_{\xi} u^+_{\text{sem}}(\xi, -1)$. This can be done by using one nodal Lagrange basis $l_0(\eta)$ along $\eta = -1$. 
Spectral-element simulations of polygonal cloaks

Figure: Left: real part of the electric field distribution $k = 80$ and $\theta_0 = \pi/4$. Right: real part of the electric field distribution with a point source ($k = 40$).
Simulations of rotators and concentrators

EM rotators and concentrators are based on regular coordinate transformations.

(a) Rotator
(b) $k = 40$, $\theta_0 = 5\pi/4$
(c) Concentrator ($k = 40$)
Time-domain simulations

Non-reflecting boundary conditions

Fast temporal convolution algorithm
Time-domain acoustic scattering problem

The time-dependent wave equation exterior to a bounded obstacle:

\[ \partial_t^2 U = \nabla (C^2 \nabla U) + F \quad \text{in} \quad \Omega_\infty := \mathbb{R}^d \setminus \bar{D}, \quad t > 0, \quad d = 2, 3; \]
\[ U = G, \quad \text{on} \quad \Gamma_D, \quad t > 0; \]
\[ \partial_t U + c \partial_n U = o(|x|^{(1-d)/2}), \quad |x| \to \infty, \quad t > 0; \]
\[ U = U_0, \quad \partial_t U = U_1, \quad \text{in} \quad \Omega_\infty, \quad t = 0. \]

Here,

- \( D \) is a bounded scatterer with Lipschitz boundary \( \Gamma_D \).
- The inhomogeneity of the medium is confined in a finite region, and the given data \( F, U_0, U_1 \) are compactly supported.
- The radiation condition corresponds to the Sommerfeld radiation condition in the frequency domain.
Domain reduction by exact NRBCs

**Reduced wave equation:**

\[
\partial_t^2 U = \nabla \left( C^2 \nabla U \right) + F \quad \text{in} \quad \Omega := B \setminus \bar{D}; \\
U = G, \quad \text{on} \quad \Gamma_D, \quad t > 0; \\
(\partial_r U - T_b(U))|_{r=b} = 0, \quad t > 0, \quad \text{[NRBC]} \\
U = U_0, \quad \partial_t U = U_1, \quad \text{in} \quad \Omega, \quad t = 0,
\]

where \( T_b \) is the time-domain DtN map, and \( B \) is a disk/ball of radius \( b \).

**Note:** The NRBC can be obtained by solving the wave equation exterior to \( B \) via Laplace transform in time and separation of variables in space.
Formulation of time-domain DtN map

\[
\mathcal{T}_b(U) = \begin{cases} 
\left( -\frac{1}{c} \frac{\partial U}{\partial t} - \frac{U}{2r} \right)_{r=b} + \sum_{|n|=0}^{\infty} \sigma_n(t) \ast \hat{U}_n(b, t) e^{i n \phi}, & d = 2, \\
\left( -\frac{1}{c} \frac{\partial U}{\partial t} - \frac{U}{r} \right)_{r=b} + \sum_{n=0}^{\infty} \sum_{|m|=0}^{n} \sigma_{n+1/2}(t) \ast \hat{U}_{nm}(b, t) Y_n^m(\theta, \phi), & d = 3,
\end{cases}
\]

where for \( d = 2 \),

\[
\sigma_n(t) := \mathcal{L}^{-1} \left[ \frac{s}{c} + \frac{1}{2b} + \frac{s}{c} K'_n(sb/c) \right],
\]

and for \( d = 3 \),

\[
\sigma_{n+1/2}(t) := \mathcal{L}^{-1} \left[ \frac{s}{c} + \frac{1}{b} + \frac{s}{c} k'_n(sb/c) \right] = \mathcal{L}^{-1} \left[ \frac{s}{c} + \frac{1}{2b} + \frac{s}{c} K'_{n+1/2}(sb/c) \right].
\]

Here, \( K_\nu(z) \) is the modified Bessel function of the second kind, and \( \{Y_n^m\} \) are the spherical harmonic functions.
Well-posedness of reduced problem

It is essential to show that for any $t > 0$,

$$\text{Re} \int_0^t \int_{\{r=b\}} T_b(U) \overline{\partial_\tau U} d\gamma d\tau \leq 0.$$  

Then we have the energy conservation: $E'(t) = 0$ (if $G = F = 0$):

$$E(t) = \int_{\Omega} (|\partial_t U|^2 + c^2|\nabla U|^2) dx - 2c^2 \text{Re} \int_0^t \int_{\{r=b\}} T_b(U) \overline{\partial_\tau U} d\gamma d\tau.$$  

**Main tools** (Z. Chen'09, Z. Chen & Nedéléc'08, W., B. Wang and X. Zhao'13-14):

- Plancherel identity or Parseval’s identity for Laplace transform:

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} \mathcal{L}[f](s) \mathcal{L}[\tilde{g}](s) ds_2 = \int_0^\infty e^{-2s_1 t} f(t) \tilde{g}(t) dt, \quad \forall s = s_1 + is_2, \ s_1 > 0,$$

- Property: $\text{Re} \left( \frac{Z_n'(sb/c)}{Z_n(sb/c)} \right) \leq 0$ for $s_1 > 0$, where $Z_n = K_n, k_n$.  


Analytic formula for $\sigma_{\nu}(t)$

**Theorem** (Sofronov’98, W., Wang & Zhao’12). Let $\{z_{\nu}^j\}_{j=1}^{M_{\nu}}$ be zeros of $K_{\nu}(z)$. Then

$$\sigma_n(t) = \frac{c}{b^2} \left\{ \sum_{j=1}^{M_n} z_j^n e^{ctz_j^n/b} + (-1)^n \int_0^{\infty} \frac{e^{-crt/b}}{K_n^2(r) + \pi^2 I_n^2(r)} \, dr \right\}, \quad d = 2,$$

and

$$\sigma_{\nu}(t) = \frac{c}{b^2} \sum_{j=1}^{M_{\nu}} z_{\nu}^j e^{ctz_{\nu}^j/b}, \quad \nu = n + 1/2, \quad d = 3,$$

where $I_n(z)$ is the modified Bessel function of the first kind.
**Fast temporal convolution**

Temporal variable \( t \) only presents in exponentials, which allows for fast convolution. Defining

\[
f(t; r) := e^{-ctr/b} \ast g(t) = \int_0^t e^{-c(t-\tau)r/b} g(\tau) d\tau,
\]

we can evaluate the convolution \( f(t; r) \) recursively as follows:

\[
f(t + \Delta t; r) = e^{-c\Delta tr/b} f(t; r) + \int_t^{t+\Delta t} e^{-c(t+\Delta t-\tau)r/b} g(\tau) d\tau.
\]

For example, in the 2-D case,

\[
[\sigma_n \ast g](t) = \frac{c}{b^2} \sum_{j=1}^{M_n} z_j^n f(t; -z_j^n) + \frac{(-1)^n c}{b^2} \int_0^{+\infty} \frac{f(t; r)}{K_n^2(r) + \pi^2 I_n^2(r)} dr.
\]

Many zeros in the summation can be dropped for large \( n \) and \( t > t_0 \).
Accuracy of computing NRBCs

Examine the error:

\[ E_{N\phi}(t) = \max_{|n| \leq N_{\phi}} \left| \left( \frac{1}{c} \frac{\partial \hat{U}_n}{\partial t} + \frac{\partial \hat{U}_n}{\partial r} + \frac{\hat{U}_n}{2r} \right) \right| \bigg|_{r=b} - \sigma_n(t) \ast \hat{U}_n(b, t), \quad t > 0. \]

The numerical errors for \( N_{\phi} = 50 \) are tabulated below.

<table>
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<tr>
<th>( t )</th>
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<th>( \omega = 20\pi )</th>
<th>( \omega = 10\pi )</th>
<th>( \omega = 20\pi )</th>
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<td>9.0e-17</td>
<td>2.3e-16</td>
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Figure: Profiles of the “exact” solution with \( \omega = 10\pi \) and \( \omega = 20\pi \).
Domain truncation via exact NRBC:

\[
\begin{align*}
\frac{\partial^2}{\partial t^2} E + c^2 \nabla \times \nabla \times E &= F, \quad \text{in } \Omega := B \setminus \bar{D}, \quad t > 0, \\
E \times n &= g, \quad \text{at } \Gamma_D, \quad t > 0, \\
\partial_t E_T - c \hat{x} \times (\nabla \times E) &= \mathcal{T}_b[E], \quad \text{at } r = b, \quad t > 0 \quad \text{[NRBC],} \\
E|_{t=0} &= E_0, \quad \partial_t E|_{t=0} = E_1, \quad \text{in } \Omega,
\end{align*}
\]

where \( \mathcal{T}_b[E] \) is the electric-to-magnetic (EtM) operator, and \( c = 1/\sqrt{\varepsilon \mu} \).
Formulation of EtM operator

Let \( \{Y^m_l \hat{x}, \nabla_S Y^m_l, \nabla_S Y^m_l \times \hat{x}\} \) be the vector spherical harmonics (VSH), which forms an orthogonal basis of \([L^2(S)]^3\) (\(S\) is the unit spherical surface). Write

\[
E = \sum_{l=1}^{\infty} \sum_{m=-l}^{l} \left( E^{(1)}_{lm} Y^m_l \hat{x} + E^{(2)}_{lm} \nabla_S Y^m_l + E^{(3)}_{lm} \nabla_S Y^m_l \times \hat{x} \right) \quad \text{at} \quad r = b.
\]

Then we have

\[
\mathcal{T}_b[E] = \frac{c}{b} \sum_{l=1}^{\infty} \sum_{m=-l}^{l} \left( (\rho_l \ast E^{(1)}_{lm}) \nabla_S Y^m_l + (\sigma_l \ast E^{(2)}_{lm}) \nabla_S Y^m_l \times \hat{x} \right), \quad (6)
\]

where \(k_l(z) = \sqrt{2/(\pi z)}K_{l+1/2}(z), z = sb/c\), and convolution kernels are

\[
\rho_l(t) = \mathcal{L}^{-1} \left[ z \left( \frac{z k_l(z)}{k_l(z) + z k'_l(z)} + 1 \right) \right], \quad \sigma_l(t) = \mathcal{L}^{-1} \left[ 1 + z + z \frac{k'_l(z)}{k_l(z)} \right].
\]
Analytic formula for $\rho_l(t)$

**Theorem** (S. Jiang, W. & Zhao’14). Let $\{\tilde{z}_j^l\}_{j=1}^{l+1}$ be zeros of $\frac{1}{2} K_{l+1/2}(z) + z K'_{l+1/2}(z)$ with $l \geq 1$. Then we have

$$\rho_l(t) = \frac{c}{b} \sum_{j=1}^{l+1} \frac{(\tilde{z}_j^l)^3}{(\tilde{z}_j^l)^2 + l(l+1)} e^{ct \tilde{z}_j^l/b} + \delta(t) \sum_{j=1}^{l+1} \frac{(\tilde{z}_j^l)^2}{(\tilde{z}_j^l)^2 + l(l+1)},$$

where $\delta(t)$ is the Dirac delta function.

Distribution of zeros of $\frac{1}{2} K_{l+1/2}(z) + z K'_{l+1/2}(z)$, which has exactly $l + 1$ distinct zeros (see T. Tokita’72).
Regular scatterer: dimension reduction

Assume that the scatterer \( D \) is a disk/ball: \( r = a \). Expanding the solution and given data in Fourier/spherical harmonic series leads to the one-dimensional problem in space:

\[
\frac{\partial^2 u}{\partial t^2} - \frac{c^2}{r^{d-1}} \frac{\partial}{\partial r} \left( r^{d-1} \frac{\partial u}{\partial r} \right) + c^2 \beta_n \frac{u}{r^2} = f, \quad \text{in } a < r < b;
\]

\[
u|_{t=0} = u_0, \quad \partial_t u|_{t=0} = u_1, \quad a < r < b; \quad u|_{r=a} = 0, \quad t > 0; \quad (7)
\]

\[
\left( \frac{1}{c} \frac{\partial u}{\partial t} + \frac{\partial u}{\partial r} + \frac{d-1}{2r} u \right)|_{r=b} = \int_{0}^{t} \sigma_\nu(t-\tau)u(b,\tau)d\tau, \quad t > 0,
\]

where \( \beta_n = n^2, n(n + 1) \) and \( \nu = n, n + 1/2 \) for \( d = 2, 3 \), respectively.

- Efficient spectral-Galerkin method with optimal complexity in space
- Unconditionally stable (2nd-order) Newmark’s scheme in space, which can be upgraded to fourth or higher order by extrapolation.
Accuracy and order in time

(a) Exact vs. Numer.  (b) Exact vs. Numer.  (c) Exact vs. Numer.

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Table: Order of convergence in time with $N_r = 50$ and $N_\phi = 15$. 
Extrapolation in time

Table: Convergence of the Newmark scheme and Richardson extrapolation

\[ v_N(\cdot, \Delta t) = \frac{4}{3} w^R_N(\cdot, \Delta t/2) - \frac{1}{3} w_N(\cdot, \Delta t). \]

| \( t \) | \( \Delta t \) | \(|\text{Err (Newmark)}|\) | \( \text{order} \) | \(|\text{Err}^R \text{ (Richardson)}|\) | \( \text{order} \) |
|---|---|---|---|---|---|
| 0.5 | 5e-3 | 6.594800782692798e-003 | 3.065503258092415e-006 | 3.9926 |
|     | 2e-3 | 1.053652014017334e-003 | 7.900772787998441e-008 | 3.9986 |
|     | 1e-3 | 2.633585167623200e-004 | 4.942891832282835e-009 | 3.9986 |
| 1.0 | 5e-3 | 3.845725396096114e-003 | 2.744122628580332e-005 | 3.9959 |
|     | 2e-3 | 6.033468234830110e-004 | 7.051470841637524e-007 | 3.9992 |
|     | 1e-3 | 1.504099021627187e-004 | 4.409523163189837e-008 | 3.9992 |
| 1.5 | 5e-3 | 2.231571648061155e-003 | 3.281600598379895e-005 | 4.0044 |
|     | 2e-3 | 3.701429111082861e-004 | 8.367161254883683e-007 | 4.0009 |
|     | 1e-3 | 9.300845972330837e-005 | 5.226384927676982e-008 | 4.0009 |
| 2.0 | 5e-3 | 7.051912601612475e-003 | 2.099569683706111e-005 | 4.0201 |
|     | 2e-3 | 1.135256787194748e-003 | 5.277034056184911e-007 | 4.0039 |
|     | 1e-3 | 2.840528677428202e-004 | 3.289315904302148e-008 | 4.0039 |
Comparison with lower-order ABCs (3D)

Figure: Numerical solution at different time $t$ at the artificial surface $r = b$: (a)-(c): function plot on the outer spherical surface; (d): surf-plot on spherical coordinates. Contour of numerical solution at $t = 2$ sliced by $\theta = 15\pi/199$: (e)-(g): BT1, BT2, NRBC. (h): $L^2$-errors obtained by three boundary conditions and the full algorithm with $\Delta t = 10^{-4}, N_r = 30$ and $N_\phi = 100$. 
**Numerical results: Maxwell equations**

**Table:** The errors and order of convergence in time for the mode with $l = 1$.

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**Table:** The errors and order of convergence in time for the mode $l = 30$.

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Numerical results: Maxwell equations

Figure: $L^2$ errors with different time step sizes. Left: $l = 1$; Right: $l = 10$. This shows the stability of the discretization
Summary

• Imposing DtN reduces the unbounded problem to an equivalent BVP, and is very easy to add incident wave.

• Global DtN becomes local for circular/spherical scatterers, and can integrate with spectral-Galerkin solver seamlessly.

• For irregular (e.g., polygonal) scatterers, DtN can integrate SEM seamless based on new elemental mapping and analytic formulas.

• The ideas can be extended to time-domain simulations with analytic and fast approach for temporal convolution.
Acknowledgments

Collaborators

- **Zhiguo Yang** on simulation of invisibility cloaks
- **Bo Wang** & **Xiaodan Zhao** on time-domain simulations
- **Jie Shen** on high-order solvers and analysis for Helmholtz and Maxwell’s equations
- **Peijun Li** & **A. Wood** on EM Cavity problems
- **Shidong Jiang** on fast temporable convolution algorithms

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