Integral equation methods for scattering from multi-dielectric cylinders

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The Helmholtz transmission problem: \( N = 2 \) overview

Two regions \( \Omega_n \). Incident plane wave \( U^{\text{in}}(r), r = (x, y) \). Compute

\[
H(r, t) = \Re\left\{ U(r)e^{-it} \right\}, \quad E(r, t) = \Re\left\{ E(r)e^{-it} \right\},
\]

\[
H(r) = U(r)\hat{z}, \quad r \in \mathbb{R}^2,
\]

\[
E(r) = \begin{cases} 
    ik_1^{-1}\nabla_3 U(r) \times \hat{z}, & r \in \Omega_1, \\
    ik_1^{-1}\varepsilon^{-1}\nabla_3 U(r) \times \hat{z}, & r \in \Omega_2.
\end{cases}
\]
The Helmholtz transmission problem: $N > 2$, overview

$N$ regions $\Omega_n$, closed curves $C_n$, relative permittivities $\varepsilon_n$, wave-numbers $k_n$. $M$ subcurves $\Gamma_m$. Vacuum wavenumber $k_0$. Compute

$$H(r, t) = \Re \{ U(r) \hat{z} e^{-it} \} , \quad r \in \mathbb{R}^2,$$

$$E(r, t) = \Re \{ i k_0^{-1} \varepsilon_n^{-1} \nabla_3 U(r) \times \hat{z} e^{-it} \} , \quad r \in \Omega_n.$$
The Helmholtz transmission problem: \( N > 2 \), PDE

\[
U^{\text{in}}(r) = e^{ik_1(r \cdot d)},
\]
\[
k_n = \sqrt{\epsilon_n}k_0,
\]
\[
\Delta U(r) + k_n^2 U(r) = 0, \quad r \in \Omega_n.
\]
\[
U^R(r) = U^L(r), \quad r \in \Gamma_m,
\]
\[
(\epsilon^R_m)^{-1} \nu \cdot \nabla U^R(r) = (\epsilon^L_m)^{-1} \nu \cdot \nabla U^L(r), \quad r \in \Gamma_m.
\]
\[
U(r) = U^{\text{in}}(r) + U^{\text{sc}}(r), \quad r \in \Omega_1,
\]
\[
\lim_{|r| \to \infty} \sqrt{|r|} \left( \frac{\partial}{\partial |r|} - ik_1 \right) U^{\text{sc}}(r) = 0, \quad r \in \Omega_1.
\]

where L and R denote left/right limits.
Plasmonic conditions:

- $\Gamma$ has corners.
- $k_1$ is real and positive.
- $\varepsilon_2/\varepsilon_1$ approaches the negative real axis from above in the complex plane.

Now the Helmholtz transmission problem gets challenging:

- Existence and uniqueness of solutions.
- Function spaces.
- Resolution of oscillating $U(r)$ in corners.
- Resolution of surface plasmon waves along $\Gamma$ with wavenumbers $k_{sp} \gg k_1, k_2$. 
Convert the PDE (1-7) into a Fredholm second kind integral equation (SKIE) with compact operators.

A “global” representation for $U(r)$ is mandatory, but should we use “physical” or “abstract” surface layer densities?
Integral equation reformulation

Convert the PDE (1-7) into a Fredholm second kind integral equation (SKIE) with compact operators.

A “global” representation for $U(r)$ is mandatory, but should we use “physical” or “abstract” surface layer densities?

**TAKE HOME MESSAGE 1:**

- Physical and abstract layer densities can lead to similar systems of integral equations.
- When evaluating $H(r, t)$ and $E(r, t)$ close to $\Gamma$, physical densities offer great advantages over abstract densities.
\[ \Phi_k(r, r') = \frac{i}{2} H_0^{(1)}(k|r - r'|). \]

\[ S_k \sigma(r) = \int_{\Gamma} \Phi_k(r, r') \sigma(r') \, d\ell', \]

\[ K_k \sigma(r) = \int_{\Gamma} \frac{\partial \Phi_k}{\partial \nu'}(r, r') \sigma(r') \, d\ell', \]

\[ K_k^A \sigma(r) = \int_{\Gamma} \frac{\partial \Phi_k}{\partial \nu}(r, r') \sigma(r') \, d\ell', \]

\[ T_k \sigma(r) = \int_{\Gamma} \frac{\partial^2 \Phi_k}{\partial \nu \partial \nu'}(r, r') \sigma(r') \, d\ell', \]

\[ B_k \sigma(r) = \int_{\Gamma} \Phi_k(r, r') \tau(r') \sigma(r') \, d\ell', \]

\[ C_k \sigma(r) = \int_{\Gamma} \frac{\partial \Phi_k}{\partial \tau}(r, r') \sigma(r') \, d\ell'. \]
Integral representation; physical densities

Physical densities:

\[ \mu(r) = U(r), \quad r \in \Gamma, \]
\[ \rho(r) = (\varepsilon_m^R)^{-1} \nu \cdot \nabla U^R(r), \quad r \in \Gamma_m, \quad m = 1, \ldots, M. \]

Using Green’s theorem and the Ewald-Oseen extinction theorem (null-field equations), one can derive the integral representations...
Integral representation; physical densities

\[
U(r) = U^{\text{in}}(r) - \frac{1}{2} \sum_{n=1}^{N} (K_n \mu(r) - \varepsilon_n S_n \rho(r)) , \quad r \in \mathbb{R}^2.
\]

\[
E_x(r) = \frac{\varepsilon_1}{\varepsilon(r)} E^{\text{in}}_x(r) - \frac{i}{2k_0 \varepsilon(r)} \sum_{n=1}^{N} (\partial_y K_n \mu(r) - \varepsilon_n \partial_y S_n \rho(r)) , \quad r \in \mathbb{R}^2,
\]

\[
E_y(r) = \frac{\varepsilon_1}{\varepsilon(r)} E^{\text{in}}_y(r) + \frac{i}{2k_0 \varepsilon(r)} \sum_{n=1}^{N} (\partial_x K_n \mu(r) - \varepsilon_n \partial_x S_n \rho(r)) , \quad r \in \mathbb{R}^2.
\]

Here \(K_n\) and \(S_n\) are regional operators (sources on \(C_n\)).

Note: singularity cancellations in \(U\) and \(E\) for \(r\) close to \(\Gamma\).

Note: only one term in the sums is needed when \(r\) is away from \(\Gamma\).
Integral representation; physical densities

Formal definition of regional operators:

$$G_n \sigma(r) = \sum_{\text{ccw } \Gamma_m \in C_n} G^L_m \sigma(r) - \sum_{\text{cw } \Gamma_m \in C_n} G^R_m \sigma(r), \quad r \in \mathbb{R}^2,$$

where $G$ can represent $S$, $K$, $K^A$, $T$, $B$, and $C$. 
Using the same methods one can derive the SKIE system:

\[
\begin{bmatrix}
I + \alpha_m \sum_{n=1}^{N} \varepsilon_n^{-1} K_n & -\alpha_m \sum_{n=1}^{N} S_n \\
\beta_m \sum_{n=1}^{N} T_n & I - \beta_m \sum_{n=1}^{N} \varepsilon_n K_n^A 
\end{bmatrix}
\begin{bmatrix}
\mu(r) \\
\rho(r)
\end{bmatrix} = \begin{bmatrix}
f_{1m}(r) \\
f_{2m}(r)
\end{bmatrix}, \quad (8)
\]

where \( r \in \Gamma_m, \ m = 1, \ldots, M, \) and

\[
\alpha_m = \frac{\varepsilon^R_m \varepsilon^L_m}{\varepsilon^R_m + \varepsilon^L_m}, \quad \beta_m = \frac{1}{\varepsilon^R_m + \varepsilon^L_m},
\]

\[
f_{1m}(r) = 2\alpha_m \varepsilon_1^{-1} U_{\text{in}}(r), \quad f_{2m}(r) = 2\beta_m \nu \cdot \nabla U_{\text{in}}(r).
\]

Note: hypersingularities in \( T_n \) cancel.
In the special case of $N = 2$:

$$\begin{bmatrix}
I + \bar{\alpha}_1 \left( \varepsilon_1^{-1} K_1 + c \varepsilon_2^{-1} K_2 \right) & -\bar{\alpha}_1 \left( S_1 + c S_2 \right) \\
\beta_1 (T_1 + T_2) & I - \beta_1 \left( \varepsilon_1 K_1^A + \varepsilon_2 K_2^A \right)
\end{bmatrix}
\begin{bmatrix}
\mu(r) \\
\rho(r)
\end{bmatrix}
= \begin{bmatrix}
f_1(r) \\
f_2(r)
\end{bmatrix}.$$  

(9)

where

$$\bar{\alpha}_1 = \frac{\varepsilon_1 \varepsilon_2}{c \varepsilon_1 + \varepsilon_2}, \quad \beta_1 = \frac{1}{\varepsilon_1 + \varepsilon_2},$$

$$f_1(r) = 2\bar{\alpha}_1 \varepsilon_1^{-1} U^{\text{in}}(r), \quad f_2(r) = 2\beta_1 \nu \cdot \nabla U^{\text{in}}(r).$$

Note: the uniqueness parameter $c$. 
A solution to the PDE (1-7) with \( N = 2 \) and smooth \( \Gamma \) is unique if

\[
0 \leq \arg(k_1) < \pi, \quad |\varepsilon_2/\varepsilon_1| \neq \infty, \quad 0 \leq \arg(\varepsilon_2 k_1/\varepsilon_1) \leq \pi.
\] (10)

This covers plasmonic conditions [Kleinman & Martin 1988].

Kleinman & Martin also rewrote the PDE as a system of SKIEs. These “KM1 equations” use abstract densities, contain \( c \), and are uniquely solvable whenever (10) holds and \( c \) satisfies

\[
\arg(c) = \begin{cases} 
\arg(\varepsilon_2 k_2/\varepsilon_1) & \text{if } \Re\{k_1\} \geq 0, \\
\arg(\varepsilon_2 k_2/\varepsilon_1) - \pi & \text{if } \Re\{k_1\} < 0.
\end{cases}
\] (11)

Our system of SKIEs (9) is also uniquely solvable when \( c \) satisfies (11).

Note: our representations for \( U \) and \( E \) do not contain \( c \).
The importance of choosing the uniqueness parameter correctly:

Condition numbers of system matrices. $\Gamma$ is the unit circle, $\varepsilon_1 = 1$, $\varepsilon_2 = -1.1838$, and $k_0 \in [0, 10]$. 

Left: valid choice $c = -i \Rightarrow$ no false eigenvawenumber.
Right: invalid choice $c = 1 \Rightarrow$ nine false eigenvawenumerbs.
Numerical method

Key features:

- Nyström discretization of SKIEs.
- Kernel-split product integration for (nearly) singular integrals.
- Dyadic mesh refinement and lossless compression in tandem (RCIP).
- Full resolution. Execution in sub-linear time.
- Homotopy method for plasmonic conditions.
Numerical method

Key features:
- Nyström discretization of SKIEs.
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- Full resolution. Execution in sub-linear time.
- Homotopy method for plasmonic conditions.

TAKE HOME MESSAGE 2:
- Mix of off-the-shelf methods.
- Automated numerics $\Rightarrow$ no problem- or geometry-dependent analysis involved.
- System matrices are well-conditioned $\Rightarrow$ the Helmholtz transmission problem is “easy”.
For details on RCIP, see the web page:
http://www.maths.lth.se/na/staff/helsing/Tutor/
Contains useful demo programs and tutorial (revised 2018).
A first example; real and positive wavenumbers, $N = 3$

A split unit circle [Jerez-Hanckes & Pérez-Arancibia & Turc 2017]

Input data: $k_0 = 16$, $\varepsilon_1 = 1$, $\varepsilon_2 = 4$, $\varepsilon_3 = 16$, $d = (1, 0)$.

**Left:** the configuration.

**Right:** the field $H_z(r, 0)$ with colormap “hot” and a colorbar range restricted to $[-4, 4]$. 
The first example; real and positive wavenumbers, $N = 3$

Left: the field $H_z(r, 0)$ with colormap “jet” and an un-restricted colorbar range.
Right: $\log_{10}$ of estimated absolute field error in $H_z(r, 0)$. 
The first example; real and positive wavenumbers, $N = 3$

Left: the field $|\mathbf{E}(r, 0)|$.
Right: $\log_{10}$ of estimated absolute field error in $|\mathbf{E}(r, 0)|$. 
Nyström discretization

Nyström discretization is a popular method for solving SKIEs

\[ \sigma(r) + \int_{\Gamma} G(r, r') \sigma(r') \, d\ell' = f(r). \]

The integral is discretized using a quadrature rule with nodes and weights, \( r_j \) and \( w_j, j = 1, \ldots, n_{\text{pt}} \). The resulting semi-discrete equation for \( \sigma(r) \) is enforced at the nodes. Upon solving the linear system

\[ \sigma_a(r_j) + \sum_{k=1}^{n_{\text{pt}}} G(r_j, r_k) \sigma_a(r_k) w_k = f(r_j), \quad j = 1, \ldots, n_{\text{pt}}, \]

one obtains an approximation \( \sigma_a(r_j) \) to \( \sigma(r_j) \) whose convergence reflects that of the underlying quadrature.

This works well when \( G(r, r') \) and \( \sigma(r) \) are smooth. We use 16-point composite Gauss–Legendre quadrature.
Kernel-split-based product integration

Split of singular kernels:

\[ G(r, r') \, d\ell' = G_0(r, r') \, d\ell' + \log |r - r'| G_L(r, r') \, d\ell' \]

\[ + \Re \left\{ \frac{G_C(z, \tau) \, d\tau}{i(\tau - z)} \right\} + \Re \left\{ \frac{G_H(z, \tau) \, d\tau}{i(\tau - z)^2} \right\}, \]

where \( G_0(r, r') \), \( G_L(r, r') \), \( G_C(z, \tau) \), and \( G_H(z, \tau) \) are smooth functions. The scheme requires explicit formulas for \( G(r, r') \), \( G_L(r, r') \), \( G_C(z, \tau) \), and \( G_H(z, \tau) \), while \( G_0(r, r') \) needs only to be known if \( r \in \Gamma \) and then only in the limit \( r' \to r \).

Layer densities \( \sigma(r) \) are approximated by polynomials in \( \tau \) and integrated using semi-analytical methods. This works well when \( \sigma(r) \) is smooth.
A kernel written out explicitly:

\[
T_k(r, r') = \frac{i}{2} k |r - r'| H_1^{(1)}(k |r - r'|) \left( \frac{\nu \cdot \nu'}{|r - r'|^2} \right)
+ \frac{i}{2} (k |r - r'|)^2 H_2^{(1)}(k |r - r'|) D(r, r') D(r', r),
\]

where

\[
D(r, r') = -\frac{\nu \cdot (r - r')}{|r - r'|^2},
\]

\[
D(r', r) = \frac{\nu' \cdot (r - r')}{|r - r'|^2}.
\]
Example $G(r, r') = T_k(r, r')$:

\[
G_L(r, r') = -\frac{k}{\pi} J_1(k|r - r'|) \frac{(\nu \cdot \nu')}{|r - r'|} \\
- \frac{1}{\pi}(k|r - r'|)^2 J_2(k|r - r'|) D(r, r') D(r', r),
\]

\[
G_C(z, \tau) = -\frac{k^2}{2\pi} \Re \{ n_z(\bar{\tau} - \bar{z}) \},
\]

\[
G_H(z, \tau) = -\frac{n_z}{\pi},
\]

\[
\lim_{r' \to r} G_0(r, r') = \frac{i}{4} k^2 - \frac{1}{4\pi} k^2 (2 \log(k/2) - 2\psi(1) - 1).
\]

Note: the $k$-independence in $G_H$. 
The effect of corners; $N = 2$

The system (9), on $\Gamma$ with a corner of opening angle $\theta$, is a compact perturbation of the de-coupled system

$$\begin{bmatrix}
I + \lambda_1 K_2(k_2=0) & 0 \\
0 & I + \lambda_2 K^A_2(k_2=0)
\end{bmatrix}
\begin{bmatrix}
\mu(r) \\
\rho(r)
\end{bmatrix}
= \begin{bmatrix}
f_1(r) \\
f_2(r)
\end{bmatrix},$$

with

$$\lambda_1 = \frac{c\varepsilon_1 - \varepsilon_2}{c\varepsilon_1 + \varepsilon_2}, \quad \lambda_2 = \frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 + \varepsilon_2}, \quad c \approx -i.$$

The spectral properties of (12), including the essential spectrum of $K_{k=0}$ and $K^A_{k=0}$, have been analyzed by Perfekt & Putinar (2017). One can conclude that $\mu \in H^{1/2}(\Gamma)$, $\rho \in H^{-1/2}(\Gamma)$ and that there is essential spectrum for

$$\frac{|\pi - \theta| + \pi}{|\pi - \theta| - \pi} < \frac{\varepsilon_2}{\varepsilon_1} < \frac{|\pi - \theta| - \pi}{|\pi - \theta| + \pi}.$$
A second example; \( N = 2 \) and plasmonic conditions

An interface \( \Gamma \) with parameter \( 0 \leq s \leq 1 \):

\[
\begin{align*}
r(s) &= \sin(\pi s) (\cos((s - 0.5)\theta), \sin((s - 0.5)\theta)) .
\end{align*}
\]  

(13)

Input data: \( k_0 = 18, \epsilon_1 = 1, \epsilon_2 = -1.1838, d = (1, 1)/\sqrt{2}, \) and \( \theta = \pi/2 \). Left: the field \( H_z^+(r,0) \). Right: \( \log_{10} \) of estimated absolute error in \( H_z^+(r,0) \).
The second example; \( N = 2 \) and plasmonic conditions

Left: the diverging field \(|\nabla H_z^+(r, 0)|\). Colorbar range restricted to \([0, 133]\).
Right: \(\log_{10}\) of estimated absolute error in \(|\nabla H_z^+(r, 0)|\).
The second example; absorption cross section

**Left:** The absorption cross section $\sigma_{\text{abs}}^+$ as a function of $(\varepsilon_2 + \varepsilon_1)/(\varepsilon_2 - \varepsilon_1)$.

**Right:** $\sigma_{\text{abs}}^+$, $\epsilon_{\text{mach}}$ times the condition number $\kappa$, estimated absolute error in $\sigma_{\text{abs}}^+$, and the absolute difference of $\sigma_{\text{tot}}^+$ (computed in two ways) with logarithmic scale on the $y$-axis.
The second example; absorption cross section

Twenty times magnification.
A third example; \( N = 2 \), plasmonic conditions, zoom

A smaller opening angle, as in [Bonnet-Ben Dhia & Carvalho & Chesnel & Ciarlet 2016]

![Graphs showing field and log10 of estimated absolute error](image)

Same as second example, but smaller opening angle \( \theta = \pi/6 \), and \( d = (\cos(5\pi/12), \sin(5\pi/12)) \). **Left:** the field \( H_Z^+(r,0) \); **Right:** \( \log_{10} \) of estimated absolute error in \( H_Z^+(r,0) \).
Ten times magnification.
The third example; $N = 2$, plasmonic conditions, zoom

A 100 times magnification.
Even higher achievable accuracy in $\mathbf{E}$

Introduce the electric surface charge density

$$\rho_E(r) = \varepsilon_m^n \mathbf{v} \cdot \mathbf{E}^R(r).$$

Augment (9) with an electric charge integral equation

$$\rho_E(r) - \alpha_m \sum_{n=1}^N \left[ \varepsilon_n^{-1} K_n^A \rho_E(r) + i k_0^{-1} C_n \rho(r) + i k_0 \mathbf{v} \cdot \mathbf{B}_n \mu(r) \right]$$

$$= 2 \mathbf{v} \cdot \mathbf{E}^{\text{in}}(r), \quad r \in \Gamma_m,$$

to obtain a “charge current formulation”. The corresponding representation for $\mathbf{E}$:

$$\mathbf{E}(r) = \mathbf{E}^{\text{in}}(r) \delta_{n1} + \frac{1}{2} \varepsilon_n^{-1} \left( \hat{x} \partial_x S_n + \hat{y} \partial_y S_n \right) \rho_E(r)$$

$$+ \frac{1}{2} i k_0^{-1} \left( \hat{x} \partial_y S_n - \hat{y} \partial_x S_n \right) \rho(r) + \frac{1}{2} i k_0 \mathbf{B}_n \mu(r), \quad r \in \Omega_n.$$
A fourth example; $N = 4$, high contrast

Similar problem as in [Greengard & Lee 2012]

Input data: $k_0 = 10$, $\varepsilon_1 = 1$, $\varepsilon_2 = 100$, $\varepsilon_3 = \varepsilon_4 = 625$, $d = (1, 0)$.

**Left:** the field $H_z^+(r, 0)$.

**Right:** $\log_{10}$ of estimated absolute error in $H_z^+(r, 0)$. 
The fourth example; $N = 4$, high contrast

**Left:** the field $|\mathbf{E}(r, 0)|$.
**Right:** $\log_{10}$ of estimated absolute field error in $|\mathbf{E}(r, 0)|$. 
The fourth example; $N = 4$, high contrast, zoom

A 20 times magnification around the top left triple junction

Left: the field $|\mathbf{E}(r, 0)|$.
Right: $\log_{10}$ of estimated absolute field error in $|\mathbf{E}(r, 0)|$. 
The fourth example; \( N = 4 \), high contrast, convergence

**Left:** convergence of \( H_z(r,0) \) and \(|E(r,0)|\) as a function of the number of discretization points on the coarse mesh on \( \Gamma \).

**Right:** RCIP lends itself very well to automated asymptotic studies and the construction of bases. Here the behavior of \(|\rho_E(r)|\) close to the top left subcurve triple junction. \( \beta = -0.1125730127414 \).
Our schemes for high-contrast/plasmonic Helmholtz transmission problems in non-smooth domains allow for higher achievable accuracy in $\mathbf{H}$ and $\mathbf{E}$ than do other leading schemes. Also at a given computational cost, our schemes produce higher accuracy.

RCIP automatically constructs efficient 2D bases for surface densities in corners. These can be used in method-of-moment solvers and for problems involving sharp edges in 3D.

RCIP is easy to use. Ask Shidong. RCIP is geometry independent and problem independent. Feel free to download a demo code and modify a few lines for your specific needs!
References:


The slides of the talk are available at:
http://www.maths.lth.se/na/staff/helsing/talks.html