On a Helmholtz transmission problem in planar domains with corners

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The Helmholtz transmission problem: overview

Incident plane wave $U^{\text{in}}(r), \ r = (x, y) \in \mathbb{R}^2$. Compute

$$H(r, t) = \Re \{ U(r) e^{-it} \} ,$$

$$H(r) = U(r) \hat{z} ,$$

$$E(r) = \begin{cases} 
  i k_1^{-1} \nabla U(r) \times \hat{z} , & r \in \Omega_1 , \\
  i k_1^{-1} \varepsilon^{-1} \nabla U(r) \times \hat{z} , & r \in \Omega_2 . 
\end{cases}$$
The Helmholtz transmission problem: PDE

\[ U^{in}(r) = e^{i k_1 (r \cdot d)}, \quad (1) \]
\[ k_2 = \sqrt{\varepsilon} k_1, \quad (2) \]
\[ \Delta U(r) + k_1^2 U(r) = 0, \quad r \in \Omega_1, \quad (3) \]
\[ \Delta U(r) + k_2^2 U(r) = 0, \quad r \in \Omega_2, \quad (4) \]
\[ \lim_{\Omega_1 \ni r \to r^o} U(r) = \lim_{\Omega_2 \ni r \to r^o} U(r), \quad r^o \in \Gamma, \quad (5) \]
\[ \lim_{\Omega_1 \ni r \to r^o} \varepsilon \nu^o \cdot \nabla U(r) = \lim_{\Omega_2 \ni r \to r^o} \nu^o \cdot \nabla U(r), \quad r^o \in \Gamma, \quad (6) \]
\[ U(r) = U^{in}(r) + U^{sc}(r), \quad r \in \Omega_1, \quad (7) \]
\[ \lim_{|r| \to \infty} \sqrt{|r|} \left( \frac{\partial}{\partial |r|} - i k_1 \right) U^{sc}(r) = 0. \quad (8) \]
Cross sections:

\[ \sigma_{sc} = \Im \left\{ \frac{1}{k_1} \int_{\Gamma_C} (\nu \cdot \nabla U^{sc}(r)) \overline{U^{sc}}(r) \, d\ell \right\}, \]

\[ \sigma_{abs} = -\Im \left\{ \frac{1}{k_1} \int_{\Gamma_C} (\nu \cdot \nabla U(r)) \overline{U}(r) \, d\ell \right\}, \]

\[ \sigma_{tot} = \sigma_{sc} + \sigma_{abs} \]

or

\[ \sigma_{tot} = -\lim_{|r| \to \infty} \Im \left\{ \frac{4}{k_1} U^{sc}(|r|) \sqrt{\frac{\pi k_1 |r|}{2}} e^{-i(k_1 |r| - \pi/4)} \right\}. \]
We are interested in $\Gamma$ with an infinitely sharp corner of opening angle $\theta$, real and positive $k_1$, and $\varepsilon$ approaching the negative real axis from above in the complex plane: “plasmonics”.

Now the Helmholtz transmission problem gets challenging:

- Existence and uniqueness of solutions to the PDE (1-8) as a function of $k_1$, $\theta$, and $\varepsilon$? Function spaces?
- Numerical resolution of oscillating $U(r)$ for $r$ close to corner vertices?
- Occurrence and resolution of surface plasmon waves with wavenumbers $k_{sp} \gg k_1, k_2$ along $\Gamma$ when $\Re\{\varepsilon\} < -1$.
- Additional assumptions on $U(r)$ might be needed?
From a numerical point of view, it helps to convert the PDE (1-8) into a Fredholm second kind integral equation (SKIE).

In 1988, Kleinman & Martin showed that a solution to the PDE, for smooth \( \Gamma \), has a unique solution if

\[
0 \leq \arg(k_1) < \pi, \quad |\varepsilon| \neq \infty, \quad 0 \leq \arg(\varepsilon k_1) \leq \pi. \tag{9}
\]

This covers \( k_1 \) and \( \varepsilon \) in “plasmonics”.

Kleinman & Martin also converted the PDE into a system of SKIEs which is uniquely solvable whenever (9) holds. This SKIE system is relatively easy to solve. Almost full machine precision for \( U(r) \) can be obtained using off-the-shelf numerical tools.
A first example

An interface $\Gamma$ with parameter $0 \leq s \leq 1$:

$$r(s) = \sin(\pi s) (\cos((s - 0.5)\theta), \sin((s - 0.5)\theta)). \quad (10)$$

$H^+(r, 0)$ with $d = (\cos(\pi/4), \sin(\pi/4))$, $k_1 = 18$, $\varepsilon = -1.1838$, and $\theta = \pi/2$. Left: the field $H^+(r, 0)$. Right: $\log_{10}$ of estimated absolute error in $H^+(r, 0)$. 
Left: the diverging field $|\nabla H^+(r,0)|$ with colorbar range set to $[0, 133]$. Right: $\log_{10}$ of estimated absolute error in $|\nabla H^+(r,0)|$. 
The fundamental solution to the Helmholtz equation:

\[ \Phi_k(r, r') = \frac{i}{2} H_0^{(1)}(k| r - r'|). \]

A standard choice of operators:

\[ S_k \rho(r) = \int_{\Gamma} \Phi_k(r, r') \rho(r') \, d\ell', \]
\[ K_k \rho(r) = \int_{\Gamma} \frac{\partial \Phi_k}{\partial \nu'}(r, r') \rho(r') \, d\ell', \]
\[ K_k^A \rho(r) = \int_{\Gamma} \frac{\partial \Phi_k}{\partial \nu}(r, r') \rho(r') \, d\ell', \]
\[ T_k \rho(r) = \int_{\Gamma} \frac{\partial^2 \Phi_k}{\partial \nu \partial \nu'}(r, r') \rho(r') \, d\ell'. \]
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

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

\[ D(r', r) = \frac{\nu' \cdot (r - r')}{|r - r'|^2}. \]
The Kleinman–Martin representations and equations

The Kleinman–Martin field representation is:

\[ U(r) = U^{\text{in}}(r) + \frac{1}{2} K_{k_1} \mu(r) + \frac{1}{2} S_{k_1} \rho(r), \quad r \in \Omega_1, \quad (11) \]

\[ U(r) = \frac{\varepsilon}{2} K_{k_2} \mu(r) + \frac{c}{2} S_{k_2} \rho(r), \quad r \in \Omega_2, \quad (12) \]

\[ c = \varepsilon k_2 / |\varepsilon k_2|, \]

The corresponding system of integral equations on \( \Gamma \) is

\[
\begin{bmatrix}
I - \alpha_2 K_{k_2} + \alpha_1 K_{k_1} & -\alpha_1 (cS_{k_2} - S_{k_1}) \\
\alpha_4 (T_{k_2} - T_{k_1}) & I + c\alpha_3 K^A_{k_2} -\alpha_4 K^A_{k_1}
\end{bmatrix}
\begin{bmatrix}
\mu(r) \\ \rho(r)
\end{bmatrix} =
\begin{bmatrix}
f_1(r) \\ f_2(r)
\end{bmatrix},
\]

\[ f_1(r) = -2\alpha_1 U^{\text{in}}(r), \quad f_2(r) = 2\alpha_4 \frac{\partial U^{\text{in}}}{\partial \nu}(r), \]

\[ \alpha_1 = \frac{1}{1 + \varepsilon}, \quad \alpha_2 = \frac{\varepsilon}{1 + \varepsilon}, \quad \alpha_3 = \frac{1}{c + \varepsilon}, \quad \alpha_4 = \frac{\varepsilon}{c + \varepsilon}. \]
The operator differences $cS_{k_2} - S_{k_1}$ and $T_{k_2} - T_{k_1}$ in (13) are always compact, even though $T_k$ is a hypersingular operator.

The operator differences $\alpha_1 K_{k_1} - \alpha_2 K_{k_2}$ and $c\alpha_3 K_{k_2}^A - \alpha_4 K_{k_1}^A$ are compact only on smooth $\Gamma$. 
The effect of corners

The system (13), on $\Gamma$ with a corner, is a compact perturbation of the de-coupled system

$$\begin{bmatrix} I + \lambda_1 K_0 & 0 \\ 0 & I + \lambda_2 K_0^A \end{bmatrix} \begin{bmatrix} \mu(r) \\ \rho(r) \end{bmatrix} = \begin{bmatrix} f_1(r) \\ f_2(r) \end{bmatrix}, \quad (14)$$

with

$$\lambda_1 = \frac{1 - \varepsilon}{1 + \varepsilon}, \quad \lambda_2 = \frac{c - \varepsilon}{c + \varepsilon}, \quad c \approx -i.$$ 

The spectral properties of (14), including the essential spectrum of $K_0$ and $K_0^A$, have been analyzed by Perfekt and Putinar (2017). One can conclude that $\mu \in H^{1/2}(\Gamma)$ and that there is essential spectrum for

$$\frac{|\pi - \theta| + \pi}{|\pi - \theta| - \pi} < \varepsilon < \frac{|\pi - \theta| - \pi}{|\pi - \theta| + \pi}.$$
Numerical method for (11,12,13)

I) Nyström discretization of (13) with high-order quadrature on a dyadicaly refined mesh ⇒ huge linear system.

II) Kernel-split-based product integration for singular kernels in (11,12,13)

III) Lossless compression of the huge linear system based on low-rank properties of off-diagonal matrix blocks. (RCIP).

IV) Acceleration for compression in sub-linear time.

V) Homotopy method for $\Re\{\varepsilon\} < 0$, $\Im\{\varepsilon\} \to 0^+$. 
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Unique mix of standard methods? Just automated numerics – no physical reasoning or geometry-dependent analysis involved. System matrices are well-conditioned ⇒ the Helmholtz transmission problem is “easy”, if modeled and solved in our way.

For a detailed explanation, see:

When discussing numerical methods we consider a generic SKIE

\[ \rho(r) + \int_\Gamma G(r, r') \rho(r') \, d\ell' = f(r), \]

with kernel \( G(r, r') \), layer density \( \rho(r) \), and right hand side \( f(r) \).

The integral operator itself will be denoted \( K \), so we also have

\[ (I + K) \rho(r) = f(r). \]
Nyström discretization is a popular method for solving SKIEs

\[ \rho(r) + \int_{\Gamma} G(r, r') \rho(r') \, dl' = f(r). \]  

(15)

The integral in (15) is discretized using a quadrature rule with nodes and weights, \( r_j \) and \( w_j \), \( j = 1, \ldots, N \). The resulting semi-discrete equation for \( \rho(r) \) is enforced at the nodes. Upon solving the linear system

\[ \rho_a(r_j) + \sum_{k=1}^{N} G(r_j, r_k) \rho_a(r_k) w_k = f(r_j), \quad j = 1, \ldots, N, \]

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

This works well when \( G(r, r') \) and \( \rho(r) \) are smooth. We use 16-point composite Gauss–Legendre quadrature.
II) 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 \(\rho(r)\) are approximated by polynomials in \(\tau.\) This works well when \(\rho(r)\) is smooth.
Example $G(r, r') = T_k(r, r')$:

$$G_L(r, r') = -\frac{k}{\pi} J_1(k |r - r'|) \frac{(\nu \cdot \nu')}{|r - r'|}$$

$$- \frac{1}{\pi} (k |r - r'|)^2 J_2(k |r - r'|) D(r, r') D(r', r),$$

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

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

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

Note the $k$-dependence.
III) Lossless compression (RCIP)

1) Assume that $\Gamma$ has a corner and that $f(r)$ is piecewise smooth

$$
(I + K) \rho(r) = f(r), \quad r \in \Gamma.
$$

(16)

2) Split $K$ in a difficult and an easy part $K = K^* + K^\circ$ and do the local variable substitution

$$
\rho(r) = (I + K^*)^{-1} \tilde{\rho}(r).
$$

(17)

3) Substitute (17) into (16)

$$
(I + K^\circ(I + K^*)^{-1}) \tilde{\rho}(r) = f(r),
$$

Now $\tilde{\rho}(r)$ is a piecewise smooth function.

4) Discretize on a coarse mesh

$$
(I_{coa} + K_{coa}(I_{coa} + K_{coa}^*)^{-1}) \tilde{\rho}_{coa} = f_{coa}.
$$
III) Lossless compression (RCIP)

5) Discretize on a mesh, obtained from the coarse mesh by \( n_{\text{sub}} \) times refining it in the direction toward the corner vertex

\[
(I_{\text{fin}} + K_{\text{fin}}^\circ (I_{\text{fin}} + K_{\text{fin}}^*)^{-1}) \tilde{\rho}_{\text{fin}} = f_{\text{fin}}. \tag{18}
\]

6) Make a lossless compression of (18)

\[
(I_{\text{coa}} + K_{\text{coa}}^\circ R) \tilde{\rho}_{\text{coa}} = f_{\text{coa}}. \tag{19}
\]

Super-nice!, but

\[
R = P_W^T (I_{\text{fin}} + K_{\text{fin}}^*)^{-1} P,
\]

where \( P \) and \( P_W^T \) are interpolation matrices. The system to be inverted has a non-trivial block of size \( \approx 32n_{\text{sub}} \times 32n_{\text{sub}} \). The computational cost is \( O(n_{\text{sub}}^3) \).
III) Lossless compression (RCIP)

Sparsity patterns. **Left:** $K^\circ_{\text{coa}}$. **Right:** $R$. 
7) Fortunately, the non-trivial block of $\mathbf{R}$ can be computed as the matrix $\mathbf{R}_{n_{\text{sub}}}$ obtained via the recursion

$$
\mathbf{R}_i = \mathbf{P}_W^{T} \left( \mathbf{F}\{\mathbf{R}_{(i-1)}^{-1}\} + \mathbf{I}_b + \mathbf{K}_{ib}^o \right)^{-1} \mathbf{P}_{bc}, \quad i = 1, \ldots, n_{\text{sub}},
$$

where $\mathbf{K}_{ib}^o$ are $96 \times 96$ matrices corresponding to the discretization of $K$ on level $i$ in a hierarchy of small local meshes around the corner vertex. The computational cost is only $O(n_{\text{sub}})$.

8) Now solve (19) for $\tilde{\rho}_{\text{coa}}$ and, if necessary, reconstruct $\rho_{\text{fin}}$ from $\tilde{\rho}_{\text{coa}}$ and the $\mathbf{R}_i$. 
III) Lossless compression (RCIP)

\[ R_i = P_{Wbc}^T \left( \mathcal{F}\left\{ R_{(i-1)}^{-1} \right\} + I_b^o + K_b^o \right)^{-1} P_{bc}, \quad i = 1, \ldots, n_{\text{sub}}. \]

Figure: Recursion on a refined mesh surrounding a corner.
III) Lossless compression (RCIP)

A MATLAB code

```matlab
starL=[17:80];
R=eye(64);
for level=1:nsub
    Kmat=Kdisc(nodes,weights,level,96);
    MAT=eye(96)+Kmat;
    MAT(starL,starL)=inv(R);
    R=Pwbc'*inv(MAT)*Pbc;
end
```
IV) Acceleration

The layer densities in the Kleinman–Martin system (13) may behave so badly close to the corner vertex that $n_{\text{sub}} \approx 10^5$ is needed. Fortunately, several speedups of the recursion

$$R_i = P^T_{Wbc} \left( \mathcal{F}\{R^{-1}{(i-1)}\} + I^\circ_b + K^\circ_{ib} \right)^{-1} P_{bc}, \quad i = 1, \ldots, n_{\text{sub}},$$

are possible when $K$ is a double-layer type operator.

Most importantly, for $n_{\text{sub}} - i \gg 1$, the matrix $K^\circ_{ib}$ is independent of level $i$ and the recursion becomes a fixed-point iteration

$$R_i = P^T_{Wbc} \left( \mathcal{F}\{R^{-1}{(i-1)}\} + I^\circ_b + K^\circ_b \right)^{-1} P_{bc}, \quad i = 1, \ldots.$$

The fixed-point matrix $R_\star$ can be obtained by Newton’s method and replace most $R_i$ with $n_{\text{sub}} - i \gg 1$. Typically, around fifty $R_i$ are distinct in double precision arithmetic.
IV) Acceleration

From the “tutorial”: Fixed-point iteration for the matrix $R_*$ without and with Newton acceleration.
V) Homotopy

The recursion for $\mathbf{R}$ with $K$ from (13) fails when $\varepsilon$ is such that there is discrete spectrum.

The recursion for $\mathbf{R}$ with $K$ from (13) also runs into trouble when $\varepsilon$ is close to the interval where there is essential spectrum. Then, start with $\Im \{\varepsilon\} = 1$, say, and let $\Im \{\varepsilon\}$ slowly approach $0^+$ while running the Newton-accelerated fixed-point iteration

$$\mathbf{R}_i = \mathbf{P}_{\mathcal{W}_{bc}}^T \left( \mathcal{F}\{\mathbf{R}_{(i-1)}^{-1}\} + \mathbf{I}_b + K_b^o \right)^{-1} \mathbf{P}_{bc}, \quad i = 1, \ldots .$$

The convergence of $\mathbf{R}_i$ is then excellent and one can, eventually, let $\Im \{\varepsilon\} = 0.$
$H^+(r,0)$ with $\Gamma$ as in (10), $k_1 = 18$, $\varepsilon = -1.1838$, $\theta = \pi/6$, and $d = (\cos(5\pi/12), \sin(5\pi/12))$. **Left:** the field $H^+(r,0)$; **Right:** $\log_{10}$ of estimated absolute error in $H^+(r,0)$. 

Ten times magnification.
A second example

A hundred times magnification.
Left: The absorption cross section $\sigma_{\text{abs}}^+$ with $\Gamma$ as in (10), $\theta = \pi/2$, $d = (\cos(\pi/4), \sin(\pi/4))$, $k_1 = 18$, and $\varepsilon < 0$. 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.
Twenty times magnification.
Actual proofs for several parts of the numerical scheme.

The scheme, for $U(r)$, converges pointwise with mesh refinement and saturates at almost machine precision.

The scheme reproduces (semi-)analytic results when available.

The scheme accurately predicts essential spectrum, values of $\varepsilon$ for which surface plasmon waves can exist, the wavenumber $k_{sp}$, and gives consistent results for the total cross section.
Conclusions

- Planar time-harmonic scattering problems can be solved with the same ease, with the same numerical methods, and to the same accuracy as static problems in “plasmonics”.
- Limits of absorption cross section reminiscent of densities of the spectral measure for polarizability.
- What is the next step for numerics?


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