Solving integral equations on boundaries with corners, edges, and nearly singular points

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A transmission problem for Laplace. The electro-quasi-static inclusion problem:

\[
\lim_{r \to \infty} \nabla U(r) = e \\
\Delta U(r) = 0 \\
\varepsilon_1 \frac{\partial}{\partial \nu_r} U^{\text{ext}}(r) = \varepsilon_2 \frac{\partial}{\partial \nu_r} U^{\text{int}}(r) \\
\Gamma \quad \Delta U(r) = 0
\]
The ansatz

\[ U(r) = e \cdot r + \int_{\Gamma} G(r, r') \rho(r') \, ds' \]

gives the SKIE [Greengard & Moura 1994]

\[ (z - K) \rho(r) = 2(e \cdot \nu_r), \quad r \in \Gamma, \quad (1) \]

where

\[ G(r, r') = -\log |r - r'|/2\pi, \]
\[ z = -(\varepsilon_2 + \varepsilon_1)/(\varepsilon_2 - \varepsilon_1), \]
\[ K \rho(r) = 2 \int_{\Gamma} \frac{\partial G}{\partial \nu_r}(r, r') \rho(r') \, ds'. \]

Equation (1) has a unique solution as long as \( z \notin [-1, 1] \).

An interesting quantity is the dipole moment

\[ \alpha(z) = -\frac{1}{V} \int_{\Gamma} \rho(r)(e \cdot r) \, ds. \]
If $\Gamma$ is smooth, there is only a discrete set of $z \in [-1, 1]$, accumulating at $z = 0$, where $z - K$ is not invertible (discrete spectrum). If $\Gamma$ has corners, then there may also be subintervals of $z \in [-1, 1]$ where $z - K$ is not invertible (continuous spectrum).

For $z = x + iy$ approaching the continuous spectrum from above/below in the complex plane, there are pointwise converging unique solutions $\rho^{\pm}(r)$ to (1). The function space for $\rho$ is $H^{-1/2} \approx L^1$.

Finding $\rho^+(r)$ and computing $\alpha^+(x)$, $x \in [-1, 1]$, for $\Gamma$ with corners is of great interest in pure(r) mathematics and plasmonics. Preferably in 3D. $\Im \{\alpha^+(x)\}$ shows where $K$ has spectrum.

Finding $\rho^+(r)$ is the mother of many other non-smooth problems (MoMoNSP) in computational electromagnetics.
The RCIP method was designed to solve the MoMoNSP using Nyström discretization. Thanks to its generality, RCIP applies to any Fredholm second kind boundary integral equation

\[(I + K) \rho(r) = g(r), \quad r \in \Gamma,\]

with compact operators \(K\), involving singularities in \(\rho(r)\) at individual points \(r\) in a broad sense.

The only restriction is that \(g(r)\) be piecewise smooth.
The RCIP method

Key features of RCIP:

- computational cost similar to that with smooth $\Gamma$
- geometry independent
- problem independent
- refinement and compression in tandem
- faster and faster the more you refine $\Rightarrow$ always full resolution
- everything on the fly
- lossless compression $\Rightarrow$ full reconstruction
- automated asymptotic analysis
- automated construction of basis functions for $\rho$ on 3D edges
- singular boundary points are treated independently
- output well suited for near-boundary field evaluations
The RCIP method

Input:
- $\Gamma$, $K$, and $g$
- coarse mesh on $\Gamma$
- Gauss–Legendre quadrature nodes and weights $s_j$ and $w_j$

Output:
- $\hat{\rho}_{\text{coa}}$
- $\rho_{\text{fin}}$ and $\rho_{\text{coa}}$
- discrete bases for $\rho$
- quadrature weights for bases
- singularity exponents

\[
\int_{\Gamma} \rho(\mathbf{r}) f(\mathbf{r}) \, d\ell \approx \sum_j \rho_{\text{fin}} j \zeta_{\text{fin}} j w_{\text{fin}} j = \sum_j \hat{\rho}_{\text{coa}} j \zeta_{\text{coa}} j w_{\text{coa}} j ,
\]
\[
\zeta_j = f(r(s_j))|\dot{r}(s_j)|.
\]
To understand RCIP is not difficult. Comparable to understanding basic versions of the FMM. The proofs may be more non-standard, but the implementation is simpler.

You do not need to understand everything to use RCIP. There are plenty of demo-codes that can be mildly modified.
1) Assume that $\Gamma$ has a corner and that $f(r)$ is piecewise smooth

\[ (I + K) \rho(r) = g(r), \quad r \in \Gamma. \]  \hspace{1cm} (2)

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

\[ \rho(r) = (I + K^*)^{-1} \tilde{\rho}(r). \]  \hspace{1cm} (3)

3) Substitute (3) into (2)

\[ (I + K^\circ (I + K^*)^{-1}) \tilde{\rho}(r) = g(r), \]

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

4) Discretize on a coarse mesh

\[ (I_{\text{coa}} + K^\circ_{\text{coa}} (I_{\text{coa}} + K^*_{\text{coa}})^{-1}) \tilde{\rho}_{\text{coa}} = g_{\text{coa}}. \]
5) Discretize on a mesh, obtained from the coarse mesh by $n_{\text{sub}}$ times refining it in the direction toward the corner vertex

$$\left( I_{\text{fin}} + K_{\text{fin}}^o (I_{\text{fin}} + K_{\text{fin}}^*)^{-1} \right) \tilde{\rho}_{\text{fin}} = g_{\text{fin}} . \quad (4)$$

6) Make a super-fast lossless compression of (4)

$$\left( I_{\text{coa}} + K_{\text{coa}}^o R \right) \tilde{\rho}_{\text{coa}} = g_{\text{coa}} . \quad (5)$$

where the compressed inverse is

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

and $P$ and $P_W^T$ are interpolation matrices.

In practice, refinement and compression are done in tandem \( \Rightarrow \) no large matrices.
Sparsity patterns. **Left:** $K_{\text{coa}}^o$. **Right:** $R$. 
The RCIP forward recursion for $R$

$$
R_i = P_{Wbc}^T \left( \mathbb{F}\{R_{(i-1)}^{-1}\} + I_b^o + K_{ib}^o \right)^{-1} P_{bc}, \quad i = 1, \ldots, n_{sub} .
$$

Figure: Recursion on a refined mesh surrounding a corner.
If the forward recursion is initialized with the initializer

$$\mathcal{F}\{R_0^{-1}\} = I_b^* + \lambda K_{1b}^*,$$

then each forward recursion step corresponds to one level of dyadic refinement.

There are much more efficient initializers, whose use bound the number of recursion steps needed for full resolution in $\mathbf{R}$.

If an efficient initializer is used, the fine mesh can be viewed as infinitely refined. The dyadic-refinement analogy is gone.
There is also a backward recursion for the lossless reconstruction of $\rho_{\text{fin}}$ from $\tilde{\rho}_{\text{coa}}$ and $R_i$:

$$\tilde{\rho}_{\text{coa},i} = \left[ I_b - \lambda K_{ib}^o \left( \mathbb{F}\{ R_{i-1}^{-1} \} + I_b^o + \lambda K_{ib}^o \right)^{-1} \right] P_{bc} \tilde{\rho}_{\text{coa},i} ,$$

$$i = n_{\text{sub}}, \ldots, 1.$$
The RCIP backward recursion for $\rho_{\text{fin}}$

There is also a backward recursion for the lossless reconstruction of $\rho_{\text{fin}}$ from $\tilde{\rho}_{\text{coa}}$ and $R_i$:

$$
\tilde{\rho}_{\text{coa},i} = \left[ I_b - \lambda K_{ib}^o \left( F \{ R_{i-1}^{-1} \} + I_b^o + \lambda K_{ib}^o \right)^{-1} \right] P_{bc} \tilde{\rho}_{\text{coa},i}, \\
i = n_{\text{sub}}, \ldots, 1.
$$

Here $\tilde{\rho}_{\text{coa},i}$ is a column vector with 64 elements. In particular, $\tilde{\rho}_{\text{coa},n_{\text{sub}}}$ is the restriction of $\tilde{\rho}_{\text{coa}}$ to $\Gamma^*$, while $\tilde{\rho}_{\text{coa},i}$ are taken as elements $\{17:80\}$ of $\tilde{\rho}_{\text{coa},i+1}$ for $i < n_{\text{sub}}$. The elements $\{1:16\}$ and $\{81:96\}$ of $\tilde{\rho}_{\text{coa},i}$ are the reconstructed values of $\rho_{\text{fin}}$ on the outermost panels of a type b mesh on $\Gamma^*_i$. Outside of $\Gamma^*$, $\rho_{\text{fin}}$ coincides with $\tilde{\rho}_{\text{coa}}$. 
Polarizability: the square

RCIP gives $\alpha^+(x)$ to essentially machine precision for a square:

Note: is there no discrete spectrum for $K$?
Polarizability: the unit circular cylinder

The same for the unit circular cylinder (soda can), [unpublished]

Note: how do we know that this is correct?
Polarizability: the unit cube

The same for the unit cube, where 2D bases for $\rho$ are used along edges and 3D RCIP is used in corners.
The leading singularity exponent, $\rho^+(s) \propto s^\beta$, in the direction toward a cube corner vertex.
The snow cone

\[ r_3 \]

\[ r_1 \]

\[ r_2 \]

\[ r \]

\[ \nu \]

\[ \gamma \]

\[ \Gamma \]

\[ 2\alpha \]
A snow cone with small opening angle:

\[ \omega_{33}(x) \equiv \alpha^+(-x) \text{ in the axial direction.} \]
Polarizability: the snow cone

A snow cone with large opening angle:

\[ \omega_{33}(x) \equiv \alpha^+(-x) \text{ in the axial direction.} \]
A 176-ply branched crack with 178 endpoints, three of which are A, B, and C.
**Left:** a nine-unit-cell cutout from a square array of disks with conductivities \( \sigma_2 \). The background medium has \( \sigma_1 = 1 \).

**Right:** the estimated relative error in \( \sigma_{\text{eff}} \) for three setups with different \( \sigma_2 \) and separation distances \( d = 1/(c^2 + c\sqrt{c^2 - 1}) \).
RCIP: singular boundary points in a broader sense

A mixed Steklov eigenvalue problem

Right: Flow of system matrix eigenvalues as a function of the Steklov parameter $\varsigma$. The Steklov eigenvalues are those values $\varsigma$ for which the smallest system matrix eigenvalue is zero.
The one cell elliptic cavity

Note: curved shape, entrant and re-entrant edges.
Eigenvalue problem for the time harmonic Maxwell equations

PDE1: \[ \Delta E(r) + k^2 E(r) = 0, \quad r \in V, \]
PDE2: \[ \nabla \cdot E(r) = 0, \quad r \in V, \]
BC: \[ \nu \times E(r) = 0, \quad r \in \Gamma^+. \]

Fourier methods will be used in the azimuthal direction.
The electric eigenfield for the elliptic cavity and with $k_{0,662} = 31.65910852052012$.

**Left:** the field map of $\Im \{E_{z0}(r)\}$ in the $xz$-plane.

**Right:** $\log_{10}$ of estimated pointwise absolute error in $E_{z0}$. 

RCIP for Maxwell: One cell elliptic cavity
RCIP for Maxwell: One cell elliptic cavity

Eigenfield $E_z$ at $k=31.65910852052012$

Log$_{10}$ of estimated absolute error in $E_z$

Edge zoom $\times 10$. 
RCIP for Maxwell: One cell elliptic cavity

Eigenfield $E_{z0}$ at $k = 31.65910852052012$

Log$_{10}$ of estimated absolute error in $E_{z0}$

Edge zoom $\times 100$. 
The electric eigenfield for the elliptic cavity with $k_{1.9928} = 120.2309391499240$.

Left: field maps in the $xz$-plane of $\Im \{ E_{z1}(r)e^{i\theta} \}$.
Right: $\log_{10}$ of estimated pointwise absolute error.
Convergence and divergence

Left: convergence of $E_{\rho 1}(r)$, $E_{\theta 1}(r)$, and $E_{z 1}(r)$ at eigenwave-number $k_{1,9928} = 120.2309391499240$. The average pointwise absolute error in $A$ has converged to less than $10^{-12}$ at 16 discretization points per wavelength along $\gamma$.

Right: (diverging) behavior of $\varrho_{s 1}(r)$, $J_{\tau 1}(r)$, and $J_{\theta 1}(r)$ at $\gamma_2$. 

Behavior of layer densities close to $\gamma_2$
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.
RCIP for Helmholtz: scattering of TM-waves

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

$$r(s) = \sin(\pi s) \left( \cos((s - 0.5)\theta), \sin((s - 0.5)\theta) \right).$$  \hspace{1cm} (6)

Input data: $k_0 = 18$, $\varepsilon_1 = 1$, $\varepsilon_2 = -1.1838$, $d = (1, 1)/\sqrt{2}$, and $\theta = \pi/2$. Left: the field $H_2^+(r, 0)$. Right: $\log_{10}$ of estimated absolute error in $H_2^+(r, 0)$. 
Left: the diverging field $|\nabla H_z^+(r,0)|$. Colorbar range restricted to $[0, 133]$.

Right: $\log_{10}$ of estimated absolute error in $|\nabla H_z^+(r,0)|$. 
Left: The absorption cross section $\sigma^+_{abs}$ as a function of $(\varepsilon_2 + \varepsilon_1)/(\varepsilon_2 - \varepsilon_1)$.

Right: $\sigma^+_{abs}$, $\epsilon_{mach}$ times the condition number $\kappa$, estimated absolute error in $\sigma^+_{abs}$, and the absolute difference of $\sigma^+_{tot}$ (computed in two ways) with logarithmic scale on the $y$-axis.
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 $H_z^+(r, 0)$. 
Left: the field $|E(r, 0)|$.
Right: $\log_{10}$ of estimated absolute field error in $|E(r, 0)|$. 
RCIP for Helmholtz: scattering of TM-waves

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 $|\mathbf{E}(r, 0)|$. 
Conclusions and outlook

RCIP accelerated Nyström schemes offer advantages over other leading schemes for solving SKIEs in the presence of boundary singularities in 2D. Both in terms of achievable accuracy and in terms of overall computational efficiency.

“Corner-problems” come with widely varying degrees of difficulty. The harder the problem, the greater the advantage with RCIP.

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!

I find the discretization of SKIEs on general curved smooth surfaces in 3D difficult. What kind of input (basis functions) do you need for your solvers in the presence of sharp edges?