Accurate solvers for boundary value problems in 2D domains

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What problems could be of interest as Chebfun is moving up to 2D, given the philosophy of the software system?
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I suggest: linear, elliptic, boundary value problems (BVPs) with piecewise-constant coefficients, solved using Fredholm second kind integral equation techniques.

In particular:

- Laplace’s equation: electrostatic problems
- The biharmonic equation: elasticity, Stokes flow
- Helmholtz equation: scattering problems

All similar, at least for small-scale problems. If you can solve one, you can solve all. Loosely speaking, it is known how to solve most such problems. Thousands of contributors.
Problem details

The Devil is in the details.

**Problems types**: exterior and interior problems; Dirichlet-, Neumann-, Robin-, mixed-, periodic boundary conditions, etc; range of material parameters. All rather similar.

**Topologies**: closed contours; open arcs; simply/multiply connected domains. Somewhat similar. Integral equations available.

**Boundary characteristics**: smooth, well-separated boundaries; almost touching boundaries, corners, multiple-junctions. Not similar, but can be treated within a uniform framework*.

**Output**: “field plot” or “functional of the solution”? Dirichlet-to-Neumann map; scattering cross section; effective material property; stress intensity/concentration factor; resultant torque and force. Hard to tell what sells.

For small-scale problems, all this can be done in a few seconds and with optimal accuracy.
What is optimal accuracy?

Optimal accuracy should be $\kappa \epsilon_{\text{mach}}$, where

$$\kappa = \frac{\text{relative change in output}}{\text{relative change in input}}.$$

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Well, it depends on various things, including geometric description. At the bottom line: most small-scale BVPs can be modeled in a well-conditioned manner and 15 digits are realistic.
Possibly open 2D problems

Issues in 2D that may not be completely resolved:

- Fast direct solvers for all problem setups?
- Apriori error estimates/adaptive mesh generation?
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Issues in 2D that may not be completely resolved:

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- Apriori error estimates/adaptive mesh generation?

Perhaps not crucial for small-scale 2D problems? GMRES, experience and progressively increased resolution takes you far?
1) Start with an elliptic linear BPV for a field $U(r)$ as a PDE with BC at the boundary $\Gamma$ and, perhaps, at infinity.

2) Make an ansatz which solves the PDE and takes care of BC at infinity:

$$U(r) = e \cdot r + \int_{\Gamma} G(r, r') \rho(r') \, d\ell_{r'},$$

(1)

where $\rho(r)$, living on $\Gamma$, is a layer density representing $U(r)$. The kernel $G(r, r')$ is known analytically. Therefore, in 2D, $\rho(r)$ is a 1D numerical representation of the 2D field $U(r)$.

3) Insertion of $U(r)$ in BC at $\Gamma$:

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

(2)

4) Discretize and solve (2) for $\rho(r)$ and evaluate $U(r)$ via (1).
Our method RCIP (for non-smooth domains)

4a) Split $K$ in a difficult and an easy part $K = K^* + K^\circ$ and do the variable substitution

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

(3)

Use (3) as a right inverse preconditioner in (2)

$$\left(I + K^\circ (I + K^*)^{-1}\right) \tilde{\rho}(r) = g(r), \quad r \in \Gamma.$$  

(4)

4b) Discretize and evaluate $(I + K^*)^{-1}$ on a highly refined mesh. Compress without the loss of precision to a coarse mesh. Use a recursion to avoid large matrices. Can be done in sub-linear time.

4c) Solve (4) for $\tilde{\rho}(r)$ on a coarse mesh and evaluate $U(r)$ via (3) and (1). → Recursively Compressed Inverse Preconditioning.
Algorithmic building blocks

- A Fredholm second kind integral equation.
- A coarse mesh of quadrature panels.
- Composite 16-point Gauss-Legendre quadrature.
- High-order accurate analytic product rules.
- Intermediate discretizations of $K^*$ on small nested meshes.
- Prolongation operators.
- Low-threshold stagnation avoiding GMRES.
- Forward- and backward recursions (compress/reconstruct).
- Barycentric interpolation and Newton’s method (optional).

\[ \Gamma_3^* = \Gamma^* \]
\[ \Gamma_2^* \]
\[ \Gamma_1^* \]

Figure: Small nested meshes close to a corner vertex.
The fast forward recursion

\[ R_i = P_{Wbc}^T \left( \mathbb{R}\{R^{-1}_{(i-1)}\} + I_b^\circ + K_b^\circ \right)^{-1} P_{bc}, \quad i = 1, \ldots, n. \]

**Figure:** Recursion on a refined mesh surrounding a corner.
Kmat=Kinit(zloc,wloc,nzloc,96);
MAT=eye(96)+Kmat;
starL=[17:80];
R=inv(MAT(starL,starL));
myerr=1;
while myerr>eps
    Rold=R;
    MAT(starL,starL)=inv(R);
    R=Pwbc'*inv(MAT)*Pbc;
    myerr=norm(R-Rold,'fro')/norm(R,'fro');
end
Helmholtz – scattering

Scattering of H-waves: a Helmholtz Neumann problem exterior to a closed contour. Corners are important in scattering applications.

PDE: \[ \nabla^2 U_s(r) + k^2 U_s(r) = 0, \ r \in E \]

BC1: \[ \frac{\partial U_s(r)}{\partial \nu_r} = -\frac{\partial e^{iky}}{\partial \nu_r}, \ r \in \Gamma^- \]

BC2: \[ \lim_{|r| \to \infty} \left( \frac{\partial}{\partial |r|} - ik \right) U_s(r) = 0. \]
Helmholtz – scattering

A regularized combined field integral equation

$$(l + K_1 + K_2 K_3 + K_4 K_5) \rho(r) = 2 \frac{\partial e^{iky}}{\partial \nu_r}$$

and for wavenumber $k = 10$, RCIP gives the field plot

Left: $U(r) = \Re \{e^{iky} + U_s(r)\}$. Right: absolute error in $U(r)$. 
Helmholtz – scattering

Field plot zoomed. Wavenumber higher.

Left: $U(r) = \Re \{ e^{iky} + U_s(r) \}$. Right: absolute error in $U(r)$. One digit is lost for $k = 100$ compared to $k = 10$. 
Suitable Chebfun 2D problems  The RCIP method  Simple numerical examples  Challenging RCIP examples

Helmholtz – scattering

Field plot zoomed again. Wavenumber even higher.

Left: \( U(r) = \Re \{ e^{iky} + U_s(r) \} \). Right: absolute error in \( U(r) \). One and a half digit is lost for \( k = 1000 \) compared to \( k = 100 \).
Helmholtz – scattering

The scattering cross-section $\sigma_{\text{scat}}$ is a functional of the solution

$$\sigma_{\text{scat}} = - \lim_{y \to \infty} \Re \left\{ \frac{4}{k} U_s(0, y) \sqrt{\frac{\pi ky}{2}} e^{-i(ky - \pi/4)} \right\}.$$ 

**Figure:** Left: cross-section with wavenumber. Right: relative error. Good candidate for Chebfun2D? Functionals of the solution generally allow for somewhat higher achievable accuracy than field plots.
Stress around a zigzag-shaped crack: a biharmonic Neumann problem exterior to an open arc.

\[ \sigma_{yy}^\infty \]

A reduced Fredholm second kind integral equation with a compact composition of operators

\[(I + K_1 K_2) \rho(r) = g(r)\]

and RCIP gives for the so-called stress intensity factor ...
the biharmonic – elasticity

Convergence of stress intensity factor

GMRES iterations for full convergence

Figure: Stress intensity factors (a functional of the solution) for a varying numbers $q$ of corners. A direct solver would not pay off.
Laplace – electrostatics

The electrostatic problem: a harmonic interior/exterior Neumann problem with possible resonances.

\[ \lim_{r \to \infty} \nabla U(r) = e \]

\[ U(r) \text{ continuous} \]

\[ \epsilon_2 \frac{\partial}{\partial \nu_r} U^{\text{int}}(r) = \epsilon_1 \frac{\partial}{\partial \nu_r} U^{\text{ext}}(r) \]

\[ \Delta U(r) = 0 \]

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Laplace – electrostatics

A functional of the solution, called polarizability, is given by

\[ \alpha = \frac{\epsilon_2 - \epsilon_1}{\epsilon_1 V} \int_V (e \cdot \nabla U(r)) \, dr . \]

RCIP can give \( \alpha^+ \left( \frac{\epsilon_1 + \epsilon_2}{\epsilon_1 - \epsilon_2} \right) \) to essentially machine precision
Laplace – periodic boundary conditions

Staggered array of square cylinders at $p_1 = 0.49999999995$

Figure: Effective permittivity and error estimates, $\sigma = \varepsilon / \varepsilon_0$. 
The Dirichlet-to-Neumann map for an exterior harmonic problem.
No RCIP needed. Other algorithmic improvement.

Left: The contour $\Gamma$. Right: performance of various schemes.
Laplace – DtN

Adaptive mesh generation and primitive *a priori* error estimates give promising results

**Figure:** A desired tolerance is given as input. The number of points $N$ on the grid and the solution are determined via an adaptive algorithm.
Laplace – challenging problems

Let us apply RCIP to two more ambitious problems

Left: a partially refined mesh on the unit cube.
Right: a conducting random checkerboard with $10^4$ squares.
Suitable Chebfun 2D problems  The RCIP method  Simple numerical examples  Challenging RCIP examples

The cube: convergence

Figure: Convergence of $\alpha^+(x)$ and the capacitance $C$ of a unit cube. The values of $x$ correspond to: cube with infinite permittivity ($x = -1$), resonance in corners ($x = -0.6$), resonance along edges ($x = 0.25$), and cube with zero permittivity ($x = 1$).
### Table: Numerical progress for the capacitance of the unit cube.

<table>
<thead>
<tr>
<th>value</th>
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<tr>
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<td>1957</td>
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Figure: A random checkerboard with a million squares in the unit cell. The permittivity ratio is $\epsilon_2/\epsilon_1 = 10^6$. The effective permittivity is obtained with a relative error of $10^{-9}$. 
J. Helsing and A. Karlsson “An accurate solver for boundary value problems applied to the scattering of electromagnetic waves from two-dimensional objects with corners” (in progress).


Conclusions