

2D boundary integral equations and the Nyström method

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Computational Tools 2024 BIE workshop. Day 1, 6/10/24

¹Center for Computational Mathematics, Flatiron Institute, Simons Foundation

Source/codes: <https://github.com/flatironinstitute/comptools24>

Integral equations on 1D interval

Given: i) function $\sigma(t)$ defined on interval $[0, 2\pi)$, periodic: $\sigma(2\pi) = \sigma(0)$, etc
ii) “kernel” function $k(t, s)$ defined on square $[0, 2\pi)^2$,

Integral *operator* K acts on σ to give another function $K\sigma$:

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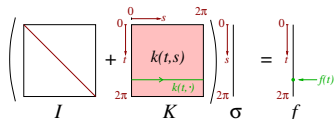
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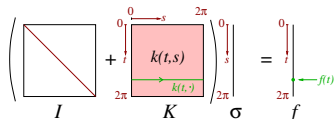
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If kernel continuous, or “weakly” singular (integrable), K is **compact**:

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 unless some $\lambda_k = -1$, 2nd kind IE has at most one soln: $\text{Nul}(I + K) = \{0\}$
- $\text{Nul}(I + K) = \{0\} \Rightarrow$ existence of solution for any f Fredholm Alternative
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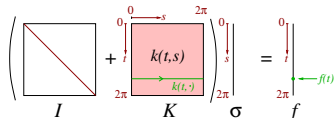
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Contrast 1st kind IE $K\sigma = f$ is ill-posed problem (unstable)!

Nyström discretization of 2nd kind IE on interval

Simplest quadrature for periodic funcs: periodic trapezoid rule (PTR)

$$\int_0^{2\pi} f(t) dt \approx \sum_{j=1}^N \frac{2\pi}{N} f\left(\frac{2\pi j}{N}\right) = \sum_{j=1}^N w_j f(t_j) \quad w_j = \text{weights}, \quad t_j = \text{nodes}$$

For f smooth, superalgebraically convergent ("spectral"): error = $\mathcal{O}(N^{-p})$ for any p

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Write as: $A\sigma = f$ $N \times N$ lin sys, entries $a_{ij} = \delta_{ij} + k(t_i, t_j) w_j$, and $f_j := f(t_j)$

solve? dense direct $\mathcal{O}(N^3)$; dense iter. $\mathcal{O}(N^2)$; fast iter. $\approx \mathcal{O}(N)$; fast direct $\approx \mathcal{O}(N^{(d+1)/2})$

Why want 2nd kind? eigs(A) accumulate only at $+1 \Rightarrow$ iterative converges fast

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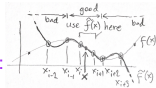
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Sometimes for BIE (eg, far-field eval), node values $\{\sigma_j\}_{j=1}^N$ suffice.

If not, interpolate from them to any $t \in [0, 2\pi)$. Two approaches:

- either: rearrange $(*)$ to give $\tilde{\sigma}(t) = \dots$, called "Nyström interpolant" (rare)
- or (common): use local high-order Lagrange (or global spectral) interpolation:

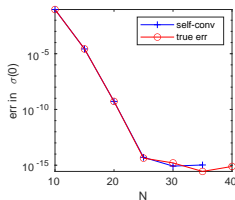
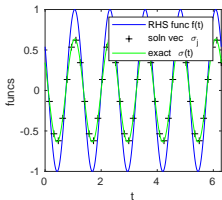
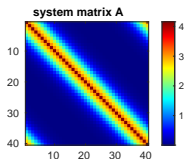


Demo Nyström on interval (1D)

day1/code/nyst1d_demos.m

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kfun = @(t,s) exp(3*cos(t-s));  
ffun = @(t) cos(5*t+1);  
N = 30;  
t = 2*pi/N*(1:N); w = 2*pi/N*ones(1,N);  
A = eye(N) + bsxfun(kfun,t',t)*diag(w);  
rhs = ffun(t');  
sigmaj = A\rhs;
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% smooth convolutional kernel, periodic domain $[0,2\pi)$
% smooth data (RHS) func
% number of unknowns: should study convergence as N grows...
% PTR nodes and weights, row vecs
% identity plus fill $k(t_i, t_j)w_j$ for $i, j=1..N$
% col vec
% dense direct square solve (pivoted LU), gives col vec



“self-convergence”:
use $N=40$ as “true”

f and k smooth

$\Rightarrow \sigma$ smooth

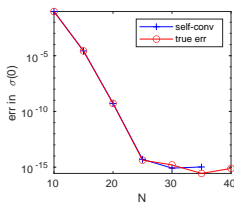
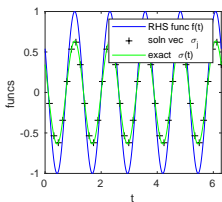
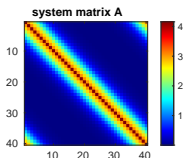
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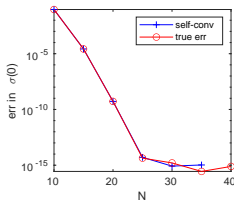
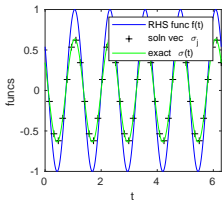
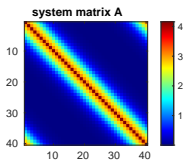
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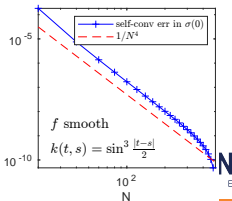
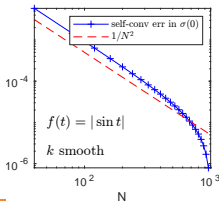
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- Then, f or k nonsmooth?
worse (here *algebraic*) convergence using plain PTR rule:

Qu: why does order appear to improve at end?



Laplace fundamental solution in \mathbb{R}^2

Eg PDE: Poisson eqn $\Delta u = g$

$\Delta := (\partial/\partial x_1)^2 + (\partial/\partial x_2)^2$ Laplacian

notation: $\mathbf{x} := (x_1, x_2) \in \mathbb{R}^2$ is a point. This frees up $\mathbf{y} \in \mathbb{R}^2$ as another point (not y-coord!)

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A well-posed* BVP:

$$\Delta u = 0 \text{ in } \Omega$$

PDE (u harmonic)

$$u = f \text{ on } \Gamma$$

Dirichlet BC

*exists, unique,
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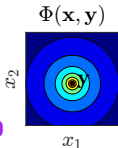
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obeys $-\Delta_{\mathbf{x}} \Phi = -\Delta_{\mathbf{y}} \Phi = \delta_{\mathbf{x}}$ Φ harmonic except unit point-mass at $\mathbf{0}$

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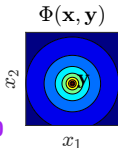
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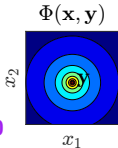
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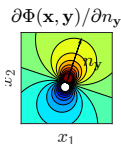
Now some fun: fix "target" $\mathbf{x} \in \Omega$, let $v = \Phi(\mathbf{x}, \cdot)$, G2I gives:

Green's representation formula:

$$\int_{\Gamma} \Phi(\mathbf{x}, \mathbf{y}) u_n(\mathbf{y}) - \frac{\partial \Phi(\mathbf{x}, \mathbf{y})}{\partial n_{\mathbf{y}}} u(\mathbf{y}) \, ds_{\mathbf{y}} = u(\mathbf{x}) \quad \text{for } \mathbf{x} \in \Omega$$

recovers soln from "Cauchy data" $(u, u_n)|_{\Gamma}$

also versions for Helmholtz, Stokes, Maxwell,...

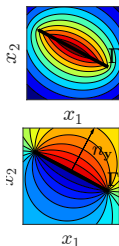


Layer potentials and their jump relations

Representations of harmonic functions off a curve Γ : “density” σ

Single-layer potential $(\mathcal{S}\sigma)(\mathbf{x}) := \int_{\Gamma} \Phi(\mathbf{x}, \mathbf{y}) \sigma(\mathbf{y}) d\mathbf{s}_{\mathbf{y}}$ charge sheet

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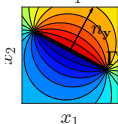
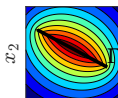
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interior (-) / exterior (+) limits:

$$u^{\pm}(\mathbf{x}) := \lim_{h \rightarrow 0^+} u(\mathbf{x} \pm h \mathbf{n}_{\mathbf{x}})$$

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Jump relations:

$(\mathcal{S}\sigma)^{\pm} = S\sigma$ S (Roman font) means *restriction* of \mathcal{S} to Γ : a bdry int. op.

$(\mathcal{D}\sigma)^{\pm} = (D \pm I/2)\sigma$ jump in potential equal to σ ; D restriction to Γ in P.V. sense

$(\mathcal{S}\sigma)_n^{\pm} = (D^T \mp I/2)\sigma$ jump in normal derivative; D^T kernel $\partial \Phi(\mathbf{x}, \mathbf{y}) / \partial \mathbf{n}_{\mathbf{x}}$

$(\mathcal{D}\sigma)_n^{\pm} = T\sigma$ T hypersingular, kernel $\partial^2 \Phi(\mathbf{x}, \mathbf{y}) / \partial \mathbf{n}_{\mathbf{x}} \partial \mathbf{n}_{\mathbf{y}} \sim 1/r^2$

- D smooth kernel on smooth Γ , while S always log (weakly) singular

Layer potentials and their jump relations

Representations of harmonic functions off a curve Γ : “density” σ

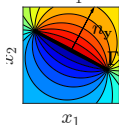
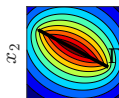
Single-layer potential $(\mathcal{S}\sigma)(\mathbf{x}) := \int_{\Gamma} \Phi(\mathbf{x}, \mathbf{y})\sigma(\mathbf{y})d\mathbf{s}_{\mathbf{y}}$ charge sheet

Double-layer potential $(\mathcal{D}\sigma)(\mathbf{x}) := \int_{\Gamma} \frac{\partial\Phi(\mathbf{x}, \mathbf{y})}{\partial\mathbf{n}_{\mathbf{y}}} \sigma(\mathbf{y})d\mathbf{s}_{\mathbf{y}}$ dipole sheet

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Recap GRF in LP notation: u harmonic in $\Omega \Rightarrow \mathcal{S}u_n^- - \mathcal{D}u^- = u$ in Ω

Converting BVP to BIE and solving

Say wish to solve interior

Dirichlet Laplace BVP:

$$\Delta u = 0 \text{ in } \Omega \quad \text{PDE}$$

$$u^- = f \text{ on } \Gamma \quad \text{BC}$$



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This shows: let σ solve BIE, then $u = \mathcal{D}\sigma$ solves BVP (i.e., no spurious solns)

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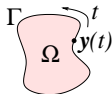
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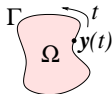
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familiar form $(I + K)\sigma = -2f$, with kernel $k(s, t) = \frac{-2}{2\pi} \frac{\mathbf{n}_{\mathbf{y}(s)} \cdot (\mathbf{y}(t) - \mathbf{y}(s))}{\|\mathbf{y}(t) - \mathbf{y}(s)\|^2} \|\mathbf{y}'(s)\|$

formula on diagonal: $k(t, t) = \lim_{s \rightarrow t} k(t, s) = \kappa(t)/2\pi$, κ curvature of Γ (check!)

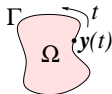
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Now Nyström discretize with PTR, solve lin. sys. for $\boldsymbol{\sigma} := \{\sigma_j\}_{j=1}^N$

Finally evaluate soln: $u(\mathbf{x}) = (\mathcal{D}\sigma)(\mathbf{x}) \stackrel{\text{PTR}}{\approx} \sum_{j=1}^N \frac{\mathbf{n}_{\mathbf{y}(t_j)} \cdot (\mathbf{x} - \mathbf{y}(t_j))}{2\pi \|\mathbf{x} - \mathbf{y}(t_j)\|^2} \|\mathbf{y}'(t_j)\| w_j \sigma_j$

Interior Laplace Dirichlet BVP solve demo

demo_lapintdir.m

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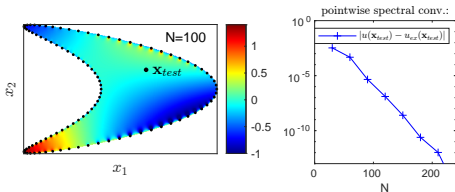
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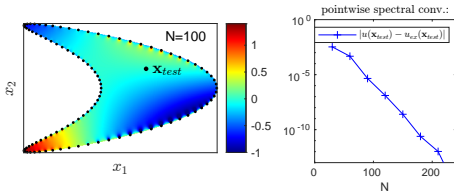
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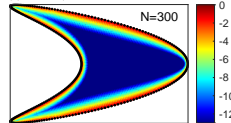
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$\log_{10} |u - u_{ex}|$: naive PTR quadr. eval.



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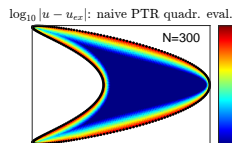
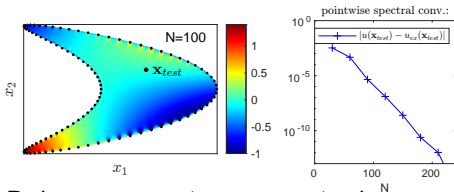
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Debug: $\sigma \equiv -1 \Rightarrow u \equiv 1$, then test data from (generic!) soln u , and...

- ① check/plot n , κ . First test unit circle!
- ② check Nyström matrix smooth at diag (before add I)

Indirect vs direct formulations

using Laplace interior Dirichlet BVP

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Indirect BIE	Direct BIE
unknown density (unphysical)	unknown is physical
RHS is plain data	RHS needs BIO apply to data
eval the representation (may be simpler)	eval the GRF

- indirect: more flexibility, but need math to prove equivalence to BVP
- accuracy differences for domains with corners (Hoskins–Rachh...)

Indirect 2nd-kind BIE for Neumann, exterior

recap: Laplace int. Dir.

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uniqueness, existence $\forall f$

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$$\Delta u = 0 \text{ in } \mathbb{R}^2 \setminus \overline{\Omega}$$

$$u^+ = f \text{ on } \Gamma$$

$$u_{\infty} := \lim_{\|x\| \rightarrow \infty} u(x) \text{ exists}$$

uniqueness, existence $\forall f$

- $u = \mathcal{D}\sigma + \int_{\Gamma} \sigma ds$ modified rep.
 $(D + I/2 + 11^T)\sigma = f$ well-cond.

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③ Exterior: don't test with $u = \log r$ why not? BVPs enforce zero net charge

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$$(\Delta + \omega^2)u = 0$$

time-harmonic scalar waves

comes from scalar wave equation $\Delta u - u_{tt} = 0$ when $u(\mathbf{x}, t) = u(\mathbf{x})e^{-i\omega t}$

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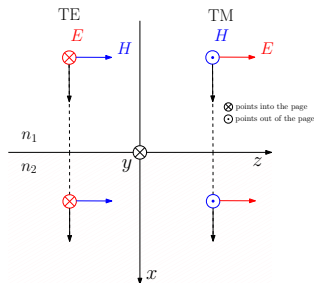
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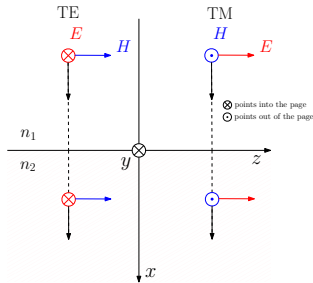
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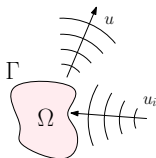
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Dirichlet BC in TE formalism = PEC perfect electric conductor; $\mathbf{E} \perp$ to surface

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Split physical potential into incident (known) and scattered (unknown) parts: $u_{\text{tot}} = u_i + u$



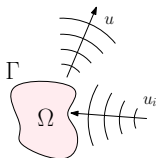
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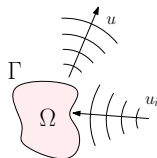
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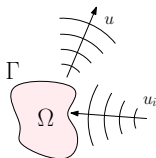
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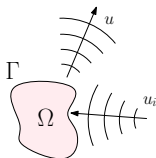
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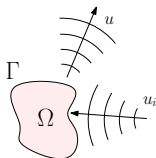
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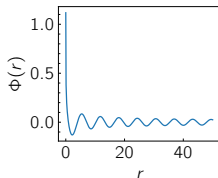
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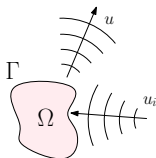
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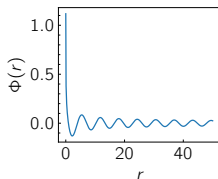
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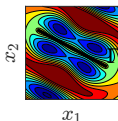
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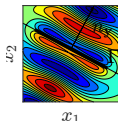
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Layer potentials



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DLP

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Fix: $u = (\mathcal{D} - i\eta\mathcal{S})\sigma$ combined field integral eq (CFIE), same # unknowns, new kernel

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We made use of the **complementary BVP** (int Neu), this is an “internal resonance”.

Fix: $u = (\mathcal{D} - i\eta S)\sigma$ combined field integral eq (CFIE), same # unknowns, new kernel
ext Dir BIE becomes $(I + 2D - 2i\eta S)\sigma = -2u_i$ on Γ

Proof: Let τ solve $(I/2 + D - i\eta S)\tau = 0$, wish to show $\tau = 0$.

From τ construct potential $v := (\mathcal{D} - i\eta S)\tau$, then $v^+ = 0$ by construction.

Then $v = 0$ in $\mathbb{R}^2 \setminus \overline{\Omega}$ by uniqueness of the complementary BVP (ext Dir)

Then v_n^+ on Γ , and by JRs and Green's 1st thm (exercise for the reader ☺), $\tau = 0$.

Helmholtz — Dirichlet demo

`demo_helmextdir.m`

Solve the Helmholtz ext Dir BVP with the $u = \mathcal{D}\sigma$ repr, u_j plane wave

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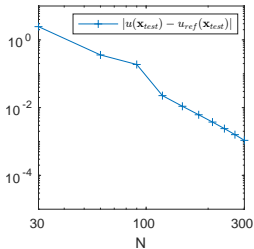
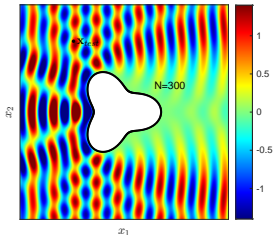
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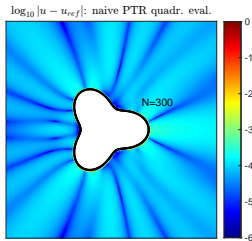
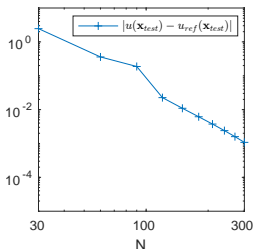
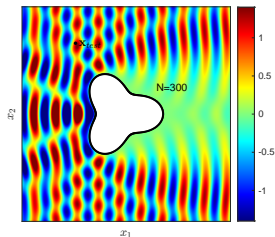
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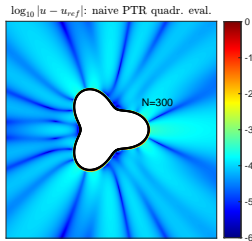
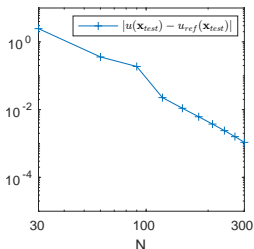
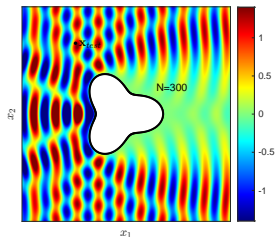
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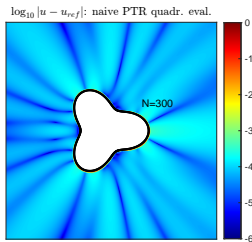
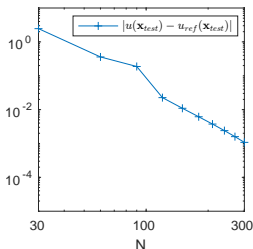
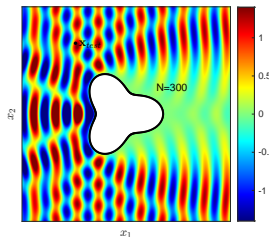


- ④ Debug BVP with known data from a radiative soln sources inside Ω

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- 4 Debug BVP with known data from a radiative soln sources inside Ω
- 5 Without analytic soln: test both via self-convergence and conserved physical qty e.g. optical theorem, or no net QM flux over closed curve C containing no sources or sinks, $0 = \text{Im}(\int_C \bar{u} u_n ds)$ (eg, Agocs–Barnett '23)

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usual splitting $u^{\text{tot}} = u^{\text{inc}} + u$

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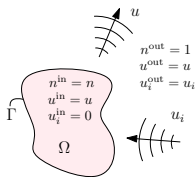
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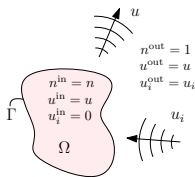
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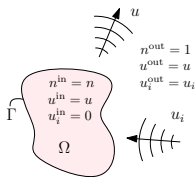
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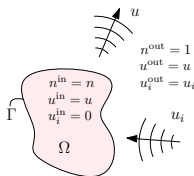
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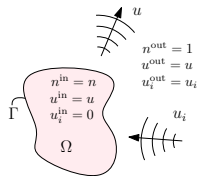


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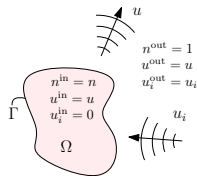
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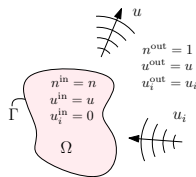
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...but $\mathcal{T}(\omega) - \mathcal{T}(n\omega)$ is at most log-singular! ☺ (Show via asymptotics of $H_n^{(1)}$)

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Spectral accuracy Nyström for log-singular kernels: possible, but beyond today

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See also libraries: chunkie, BIE2D, etc.

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- Well-posed Laplace & Helmholtz BVPs exterior need condition as $\|x\| \rightarrow \infty$
- Choosing representation to get 2nd kind BIE if poss., equivalent to BVP if poss.
Can switch interior/exterior, Laplace/Helmholtz/etc, via simple code changes
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Useful 2D tools we did not yet cover: Hai's talk; in libraries, eg chunkIE, BIE2D

- panel (composite) quadratures essential for adaptivity
- high-order quadratures for log-singular kernel SLP, Helmholtz, etc
- special quadratures for evaluation close to the curve
some need interpolation of $\sigma(t)$ off the nodes t_j , some not
- corners, open arcs, slits, multi-material junctions

Resources

Many numerical analysis (mathematics heavy). Somewhat accessible:

- *Linear Integral Equations*, R. Kress, (1999, Springer). Ch. 6 & 12.
- *The Numerical Solution of Integral Equations of the Second Kind*, K. E. Atkinson, (1997, CUP).

Fewer on the practical/tutorial side, few with last 15 years of progress:

- “High-order accurate methods for Nyström discretization of integral equations on smooth curves in the plane”, S Hao, AH Barnett, PG Martinsson, P Young. *Adv. Comput. Math.* **40**, 245–272 (2014).

various quadratures for logarithmic singularities, for, eg, SLP, Helmholtz

- <https://users.flatironinstitute.org/~ahb/BIE/>
- <https://github.com/ahbarnett/BIEbook> (private for now)