2D boundary integral equations and the Nyström method

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

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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 $K\sigma$:

$$(K\sigma)(t) := \int_0^{2\pi} k(t, s)\sigma(s)ds, \quad t \in [0, 2\pi)$$

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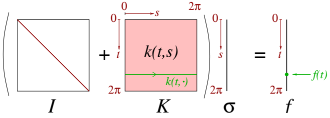

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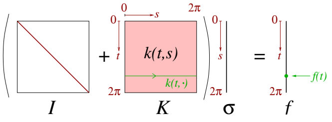

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- eigenvalues ($K\phi_k = \lambda_k\phi_k$) discrete, with $\lim_{k\to\infty} \lambda_k = 0$

  unless some $\lambda_k = -1$, 2nd kind IE has at most one soln: Nul $(I + K) = \{0\}$
- Nul $(I + K) = \{0\} \;\Rightarrow\;$ *existence* of solution for *any* f Fredholm Alternative

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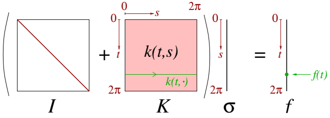

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Contrast 1st kind IE $K\sigma = f$ is ill-posed problem (unstable)!

Nyström discretization of 2nd kind IE on interval

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

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

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Write as: $A\boldsymbol{\sigma} = \boldsymbol{f}$ $N \times N$ 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 $\approx \mathcal{O}(N^{(d+1)/2})$

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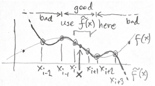
Sometimes for BIE (eg, far-field eval), node values $\{\sigma_j\}_{j=1}^{N}$ suffice.
If not, interpolate from them to any $t \in [0, 2\pi)$. Two approaches:

- either: rearrange (*) to give $\tilde{\sigma}(t) = \ldots$, 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

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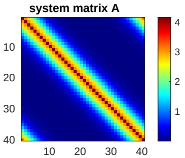

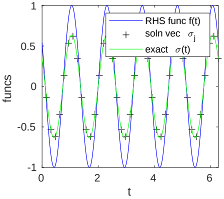

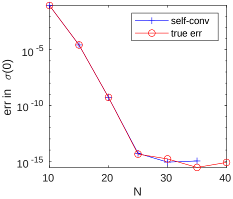

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f and k smooth

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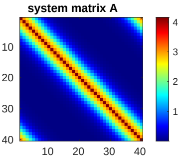

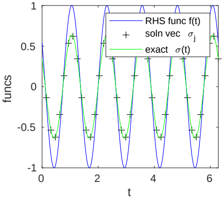

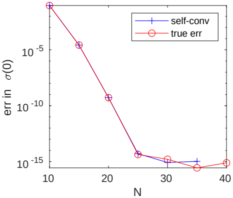

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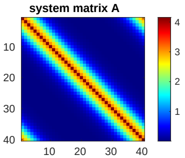

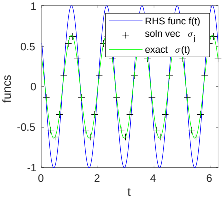

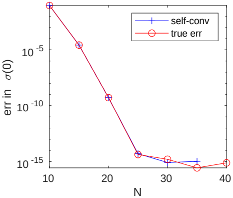

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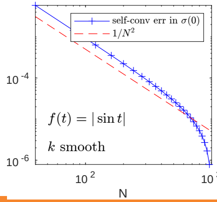
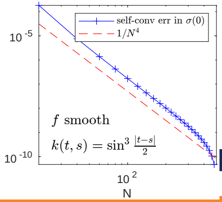
- Then, f or k nonsmooth?

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

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

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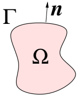

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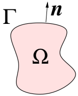

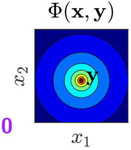

Laplace fundamental soln: $\Phi(\boldsymbol{x}, \boldsymbol{y}) = \frac{1}{2\pi} \log \frac{1}{r}$ where $r := \|\boldsymbol{x} - \boldsymbol{y}\|$

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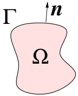

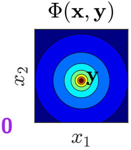

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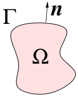

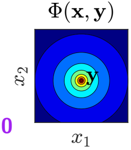

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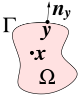
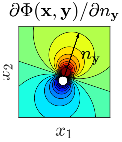
Now some fun: fix "target" $\boldsymbol{x} \in \Omega$, let $v = \Phi(\boldsymbol{x}, \cdot)$, G2I gives:

Green's representation formula:

$$\int_\Gamma \Phi(\boldsymbol{x}, \boldsymbol{y}) u_n(\boldsymbol{y}) - \frac{\partial \Phi(\boldsymbol{x}, \boldsymbol{y})}{\partial \boldsymbol{n}_{\boldsymbol{y}}} u(\boldsymbol{y}) \, ds_{\boldsymbol{y}} = u(\boldsymbol{x}) \qquad \text{for } \boldsymbol{x} \in \Omega$$



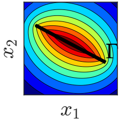


recovers soln from "Cauchy data" $(u, u_n)|_\Gamma$

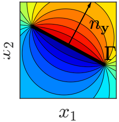
also versions for Helmholtz, Stokes, Maxwell,...

Layer potentials and their jump relations

Representations of harmonic functions off a curve Γ: "density" σ



Single-layer potential $(\mathcal{S}\sigma)(\boldsymbol{x}) := \int_\Gamma \Phi(\boldsymbol{x}, \boldsymbol{y})\sigma(\boldsymbol{y}) ds_{\boldsymbol{y}}$ charge sheet



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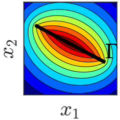

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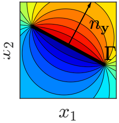

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interior (-) / exterior (+) limits:

$$u^\pm(\boldsymbol{x}) := \lim_{h\to 0^+} u(\boldsymbol{x} \pm h\boldsymbol{n_x})$$

$$u_n^\pm(\boldsymbol{x}) := \lim_{h\to 0^+} \boldsymbol{n_x}\cdot\nabla u(\boldsymbol{x} \pm h\boldsymbol{n_x})$$

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 $\partial\Phi(\boldsymbol{x},\boldsymbol{y})/\partial\boldsymbol{n_x}$

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

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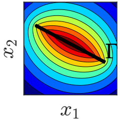

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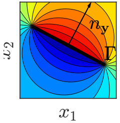

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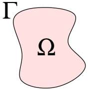
Recap GRF in LP notation: u harmonic in Ω $\Rightarrow$ $\mathcal{S}u_n^- - \mathcal{D}u^- = u$ in Ω

Converting BVP to BIE and solving

Say wish to solve interior Dirichlet Laplace BVP:

$$\Delta u = 0 \text{ in } \Omega \qquad \text{PDE}$$
$$u^- = f \text{ on } \Gamma \qquad \text{BC}$$



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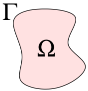

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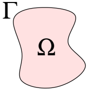

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This shows: let σ solve BIE, then $u = \mathcal{D}\sigma$ solves BVP (i.e., no spurious solns)

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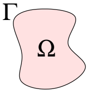

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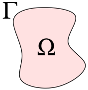

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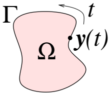

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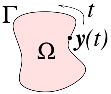

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familiar form $(I + K)\sigma = -2f$, with kernel $k(s,t) = \frac{-2}{2\pi} \frac{\boldsymbol{n}_{\boldsymbol{y}(s)} \cdot (\boldsymbol{y}(t) - \boldsymbol{y}(s))}{\|\boldsymbol{y}(t) - \boldsymbol{y}(s)\|^2} \|\boldsymbol{y}'(s)\|$

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

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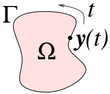

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Now Nyström discretize with PTR, solve lin. sys. for $\boldsymbol{\sigma} := \{\sigma_j\}_{j=1}^N$

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

Interior Laplace Dirichlet BVP solve demo

demo_lapintdir.m

```
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N = 100;
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y = Y(t);                                                       % bdry nodes, 2-by-N
n = [0 1;-1 0]*Yp(t); speed = sqrt(sum(n.^2,1)); n = n./speed;  % bdry normals
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uex = @(x) ([1 0]*x) .* ([0 1]*x-0.3);                          % test u(x) = x_1(x_2-0.3), not symmetric!
f = @(t) uex(Y(t));                                             % read off its Dirichlet data
rhs = -2*f(t)';
sigma = A\rhs;                                                  % solve. Leave u = D.sigma eval to reader
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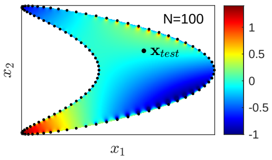

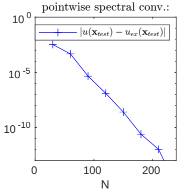

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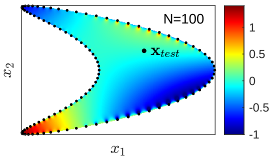

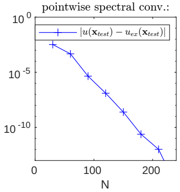

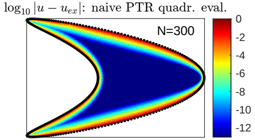

error: "5h" rule.

Note: special quadratures can fix near Γ (Helsing, QBX...)

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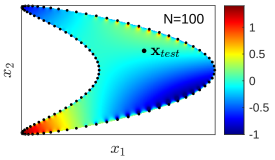
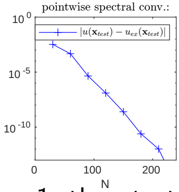
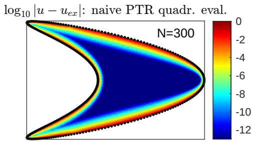
A = eye(N) + A*diag(speed.*w);                                   % note Id gets no "speed weights"
uex = @(x) ([1 0]*x) .* ([0 1]*x-0.3);                          % test u(x) = x_1(x_2-0.3), not symmetric!
f = @(t) uex(Y(t));                                              % read off its Dirichlet data
rhs = -2*f(t)';
sigma = A\rhs;                                                   % solve. Leave u = D.sigma eval to reader
```







error: "5h" rule.

Note: special quadratures can fix near Γ (Helsing, QBX...)

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

1. check/plot $\boldsymbol{n}$, κ. First test unit circle!
2. check Nyström matrix smooth at diag (*before* add I)

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Indirect vs direct formulations

using Laplace interior Dirichlet BVP

So far "indirect" BIE: pick representation (eg $u = \mathcal{D}\sigma$), get BIE from JRs

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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.	Laplace int. Neu.
$\Delta u = 0$ in Ω	$\Delta u = 0$ in Ω
$u^- = f$ on Γ	$u_n^- = g$ on Γ
uniqueness, existence $\forall f$	require $\int_\Gamma g ds = 0$
	unique only up to a const.
• $u = \mathcal{D}\sigma$ rep.	• $u = \mathcal{S}\sigma$ kernel≡1, kills nullspace
$(D - I/2)\sigma = f$ BIE: well-cond.	$(D^T + I/2 + 11^T)\sigma = g$ 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 $u(\boldsymbol{x}, t) = u(\boldsymbol{x})e^{-i\omega t}$

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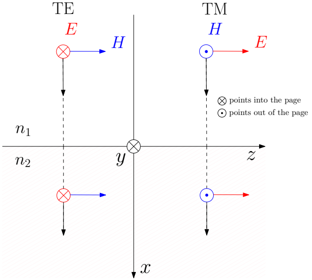

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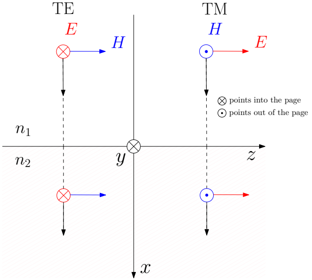
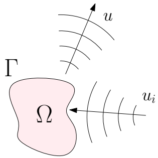


Dirichlet BC in TE formalism = PEC perfect electric conductor; $\mathbf{E} \perp$ to surface

Helmholtz — scattering formalism



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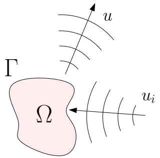

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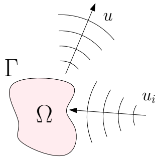

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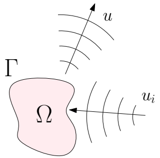

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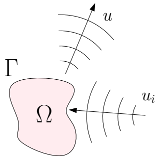

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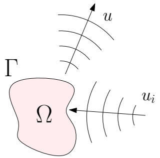

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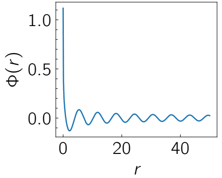

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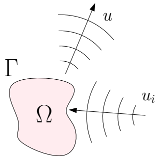

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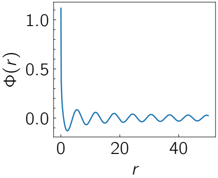
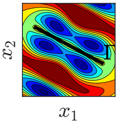
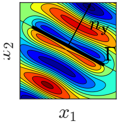


Layer potentials



SLP



DLP

Helmholtz — interior resonances and how to avoid them

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Why? Suppose $\phi \not\equiv 0$ s.t. $\begin{cases} (\Delta + \omega^2)\phi = 0 & \text{in } \Omega \\ \phi_n = 0 & \text{on } \Gamma \end{cases}$ ϕ is interior Neumann eigenfunction with eigenvalue ω^2

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ext Dir BIE becomes $(I + 2D - 2i\eta S)\sigma = -2u_i \quad$ on Γ

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

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

Then $v = 0$ in $\mathbb{R}^2 \backslash \overline{\Omega}$ 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 ☺), $\tau = 0$.

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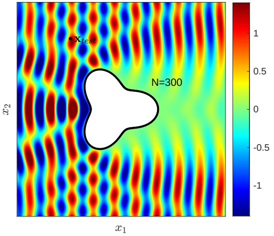

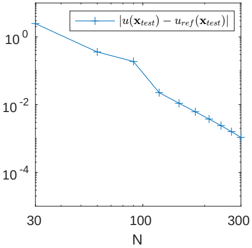

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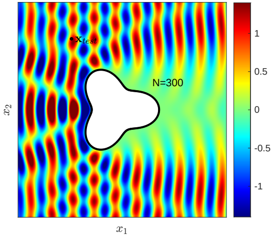

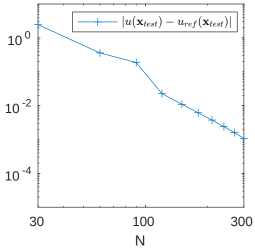

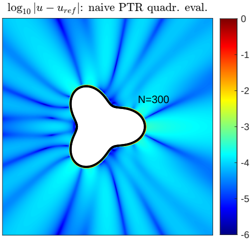

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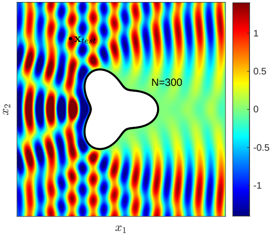

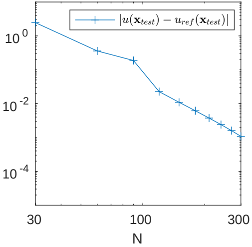

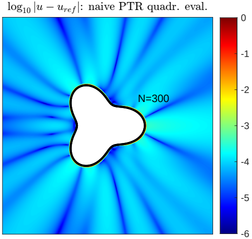

4. Debug BVP with known data from a radiative soln sources inside Ω

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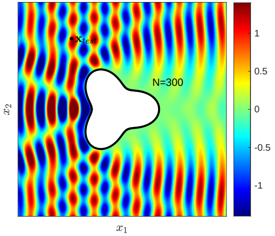

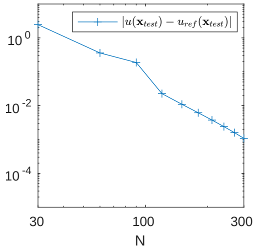

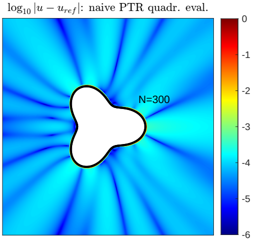

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5. Without analytic soln: test both via self-convergence and conserved physical qty e.g. optical theorem, or no net QM flux over closed curve C containing no sources or sinks, $0 = \mathrm{Im}\left(\int_C \bar{u} u_n ds\right)$ (eg, Agocs–Barnett '23)

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If different refractive index n in Ω than outside, use usual splitting $u^{\text{tot}} = u^{\text{inc}} + u$

can always scale such that one is $n = 1$

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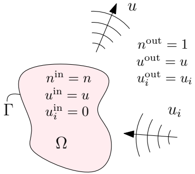

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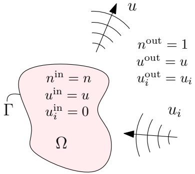

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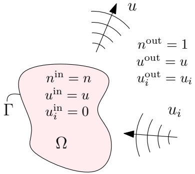

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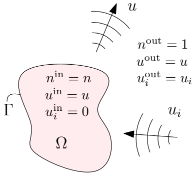

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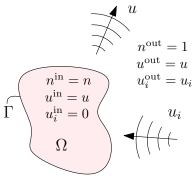

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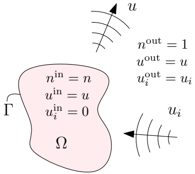

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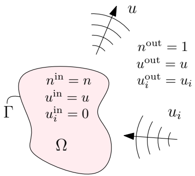

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...but $T^{(\omega)} - T^{(n\omega)}$ is at most log-singular! ☺ (Show via asymptotics of $H_n^{(1)}$)

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Divide bdry into panels instead of global set of nodes, adaptive panel sizes & quadrature rules

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Kernel-split: decompose kernel $G(\boldsymbol{x}, \boldsymbol{y}) = \underbrace{G^S(\boldsymbol{x}, \boldsymbol{y})}_{\text{smooth}} + \underbrace{G^L(\boldsymbol{x}, \boldsymbol{y}) \log |\boldsymbol{y} - \boldsymbol{x}|}_{\text{log singularity}} + \underbrace{G^C(\boldsymbol{x}, \boldsymbol{y}) \frac{(\boldsymbol{y} - \boldsymbol{x}) \cdot \mathbf{n}}{|\boldsymbol{y} - \boldsymbol{x}|^2}}_{\text{Cauchy singularity}}$

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Kernel-split: decompose kernel $G(\boldsymbol{x}, \boldsymbol{y}) = \underbrace{G^S(\boldsymbol{x}, \boldsymbol{y})}_{\text{smooth}} + \underbrace{G^L(\boldsymbol{x}, \boldsymbol{y}) \log |\boldsymbol{y} - \boldsymbol{x}|}_{\text{log singularity}} + \underbrace{G^C(\boldsymbol{x}, \boldsymbol{y}) \frac{(\boldsymbol{y} - \boldsymbol{x}) \cdot \mathbf{n}}{|\boldsymbol{y} - \boldsymbol{x}|^2}}_{\text{Cauchy singularity}}$

Product integration: target-specific quadrature rules, e.g.

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Helmholtz – high-order accuracy

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See also libraries: chunkie, BIE2D, etc.

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Covered BIE basics for smooth curves with global quadrature:

- Well-posed Laplace & Helmholtz BVPs   exterior need condition as $\|\boldsymbol{x}\| \to \infty$
- 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
- Nyström discretization   high-order/spectral convergence, if poss.
- Build/debug codes via well-chosen sequence of test cases   also for libraries

practise! write out theory yourself + try HW exer. in repo + run demos

`https://github.com/flatironinstitute/comptools24`

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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

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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` in progress...