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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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 $K\sigma$:

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

continuous analog of matrix-vector prod. $A\boldsymbol{x}$

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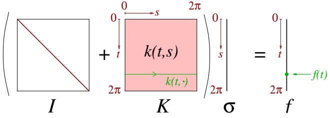

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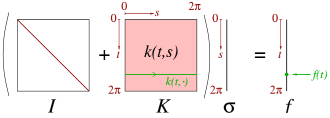

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- eigenvalues ($K\phi_k = \lambda_k\phi_k$) discrete, with $\lim_{k\to\infty} \lambda_k = 0$

  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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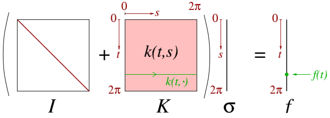

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Contrast 1st kind IE $K\sigma = f$ is ill-posed problem (unstable)!

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

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

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Apply quadr. to integral in 2nd kind IE: $\quad$ call the resulting approx soln $\tilde{\sigma}$

$$\tilde{\sigma}(t) + \sum_{j=1}^N k(t, t_j) w_j \tilde{\sigma}(t_j) = f(t), \quad t \in [0, 2\pi) \qquad (*)$$

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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 $\approx \mathcal{O}(N^{(d+1)/2})$

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

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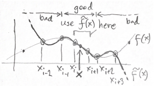
Sometimes for BIE (eg, far-field eval), node values $\{\sigma_j\}_{j=1}^N$ suffice.
If not, interpolate from them to any $t \in [0, 2\pi)$. Two approaches:

- 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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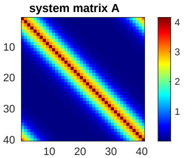

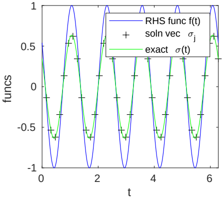

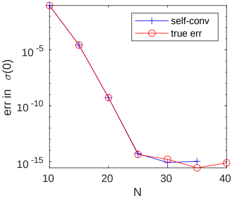

"self-convergence": use N=40 as "true"

f and k smooth

$\Rightarrow$ σ smooth

$\Rightarrow$ spectral conv?

Thm. (Anselone, Kress,...): error at node values (and Nyström interpolant) same order as that of quadrature rule applied to integrand $k(t,\cdot)\sigma$.

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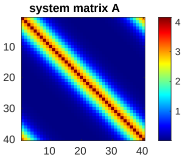

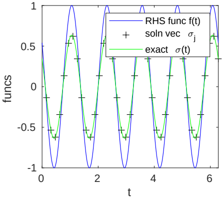

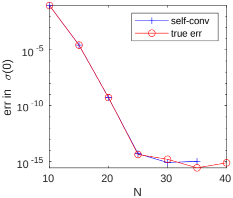

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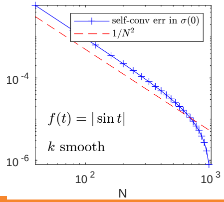
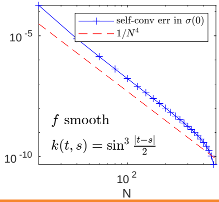
- Then, f or k nonsmooth?

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

not well-posed unless add BC! BIEs are good for *homogeneous* PDEs (driving $g \equiv 0$)

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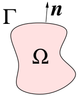

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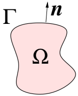

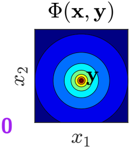

Laplace fundamental soln: $\Phi(\boldsymbol{x},\boldsymbol{y}) = \frac{1}{2\pi}\log\frac{1}{r}$ where $r := \|\boldsymbol{x}-\boldsymbol{y}\|$

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

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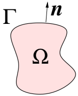

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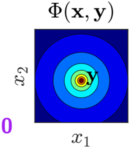

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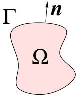

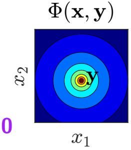

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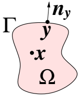
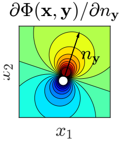
Now some fun: fix "target" $\boldsymbol{x} \in \Omega$, let $v = \Phi(\boldsymbol{x}, \cdot)$, G2I gives:

Green's representation formula:

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





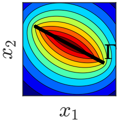
recovers soln from "Cauchy data" $(u, u_n)|_\Gamma$

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

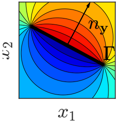
Layer potentials and their jump relations

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



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



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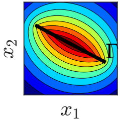
Representations of harmonic functions off a curve Γ: "density" σ

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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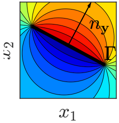

interior (-) / exterior (+) limits:

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

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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

$(\mathcal{D}\sigma)_n^\pm = T\sigma$ — T hypersingular, kernel $\partial^2\Phi(\boldsymbol{x},\boldsymbol{y})/\partial\boldsymbol{n_x}\partial\boldsymbol{n_y} \sim 1/r^2$

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

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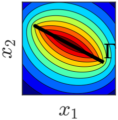

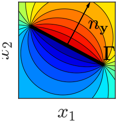

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Recap GRF in LP notation: u harmonic in Ω $\Rightarrow$ $\mathcal{S}u_n^- - \mathcal{D}u^- = u$ in Ω

Converting BVP to BIE and solving

Say wish to solve interior Dirichlet Laplace BVP:

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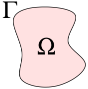

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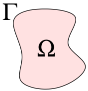

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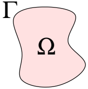

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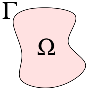

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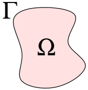

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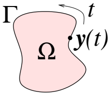

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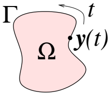

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familiar form $(I + K)\sigma = -2f$, with kernel $k(s,t) = \frac{-2}{2\pi} \frac{\mathbf{n}_{\mathbf{y}(s)} \cdot (\mathbf{y}(t) - \mathbf{y}(s))}{\|\mathbf{y}(t) - \mathbf{y}(s)\|^2} \|\mathbf{y}'(s)\|$

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

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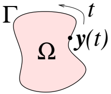

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Now Nyström discretize with PTR, solve lin. sys. for $\boldsymbol{\sigma} := \{\sigma_j\}_{j=1}^N$

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

Interior Laplace Dirichlet BVP solve demo

demo_lapintdir.m

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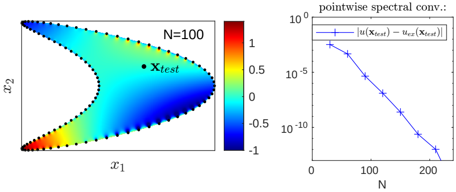

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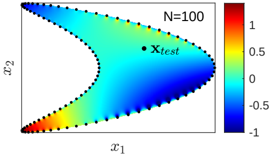

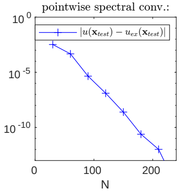

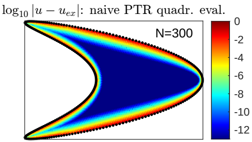

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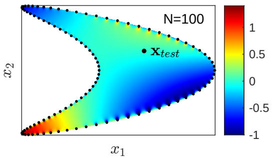

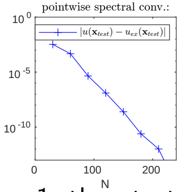

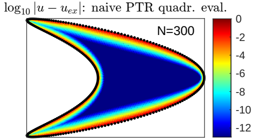

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Debug: $\sigma \equiv -1 \;\Rightarrow\; u \equiv 1$, then test data from (generic!) soln u, and...

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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Alternative is "direct": take limit of GRF on Γ, rearrange to get BIE:

GRF $u = \mathcal{S}u^- - \mathcal{D}u_n^- \quad \xrightarrow{\text{JRs}} \quad u_n^- = (D^T + I/2)u_n^- - Tu^- \quad \xrightarrow{\text{BC}} \quad (D^T - I/2)u_n^- = Tf$

Needs hypersingular apply ☹. Then solve BIE for u_n^-, eval u via GRF (needs two LP evals)

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Alternative is "direct": take limit of GRF on Γ, rearrange to get BIE:

GRF $u = \mathcal{S}u^- - \mathcal{D}u_n^- \xrightarrow{\text{JRs}} u_n^- = (D^T + I/2)u_n^- - Tu^- \xrightarrow{\text{BC}} (D^T - I/2)u_n^- = Tf$

Needs hypersingular apply ☹. Then solve BIE for u_n^-, eval u via GRF (needs two LP evals)

Notice BIO $(D^T - I/2)$ **adjoint** of that for indirect $(D - I/2)$

generally true. So, spectra the same, thus iterative convergence rates too

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

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complementary BVPs

complementary BVPs

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

Helmholtz — introduction and connection to Maxwell

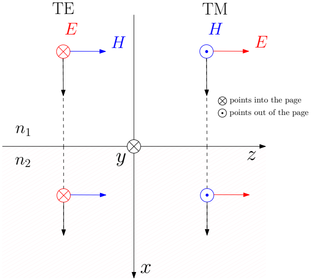
$(\Delta + \omega^2)u = 0$ time-harmonic scalar waves

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

ω is the wavenumber spatial frequency, related to wavelength via $\lambda = 2\pi/\omega$

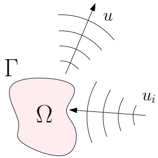
Also used for Maxwell's equations in cylindrical symm (z-invariance):

1. Assume $\mathbf{E}, \mathbf{H}(x, y, z) = \mathbf{E}, \mathbf{H}(x, y)$
2. Write Maxwell's eqs: $\nabla \times \mathbf{E} = i\omega\mu\mathbf{H}$, $\nabla \times \mathbf{H} = -i\omega\varepsilon\mathbf{E}$,
3. Notice only E_z, H_z are indep $\to$ 2 polarizations, TE or TM: $E_z = 0$, $H_z = 0$ resp.
4. Choose TE and let $u := H_z$, then: $\mathbf{H} = (0, 0, u)$, $\mathbf{E} = \frac{1}{i\omega\varepsilon}(\partial_x u, -\partial_y u, 0)$, and $(\Delta + n^2\omega^2)u = 0$ with $n^2 = \varepsilon\mu$



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

Helmholtz — scattering formalism



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

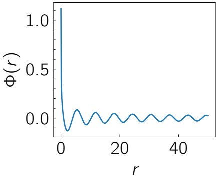
BVP for u:

$(\Delta + \omega^2)u = 0 \quad \text{in } \mathbb{R}^d \backslash \overline{\Omega}$ PDE

$u = -u_i \quad \text{on } \Gamma$ Dirichlet BC, or $u_n = -(u_i)_n$ for Neumann

$\lim_{r\to\infty} \left(\frac{\partial u}{\partial r} - i\omega u\right) = 0$ $r := |\boldsymbol{x} - \boldsymbol{y}|$, Sommerfeld radiation condition for uniqueness

Fundamental solution $\Phi(\boldsymbol{x}, \boldsymbol{y}) = \frac{i}{4} H_0^{(1)}(\omega|\boldsymbol{x} - \boldsymbol{y}|)$

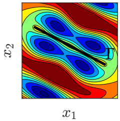


Asymptotics: $\lim_{r\to 0} \Phi(r) = \frac{1}{2\pi} \log \frac{1}{r} + \mathcal{O}(1)$

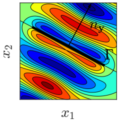
$\lim_{r\to\infty} \Phi(r) = \sqrt{\frac{2}{\pi r}} e^{i(r - \nu\pi/2 - \pi/4)} + \mathcal{O}(r^{-1})$

Same singularity as Laplace → same JRs!

Layer potentials



SLP



DLP

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Helmholtz — interior resonances and how to avoid them

Try the ext Dir BVP with $u = \mathcal{D}\sigma$ $(\Delta+\omega)^2 u = 0$ in $\mathbb{R}^2\backslash\overline{\Omega}$, $u = -u_i$ on Γ, SRC for u

Observe that for some ω, condition # of BIE blows up, not always solvable

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

Then by (interior) GRF (same as for Laplace), $\mathcal{S}\cancel{\phi_n|_\Gamma} - \mathcal{D}\phi|_\Gamma = u$ in Ω.

Take $\mathbf{x} \to \Gamma^-$ and use JR: $(-D - I/2)\phi|_\Gamma = \phi_\Gamma$, i.e. $(I+2D)\phi|_\Gamma = 0$.

Since $\phi|_\Gamma$ was nontrivial (otherwise $\phi = 0$ by GRF), nullity of $I + 2D > 0$, i.e. singular, by FA not solvable $\forall f$ (u_i).

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

Fix: $u = (\mathcal{D} - i\eta\mathcal{S})\sigma$ 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 $v := (\mathcal{D} - i\eta\mathcal{S})\tau$, 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 ☺), $\tau = 0$.

Helmholtz — Dirichlet demo

`demo_helmextdir.m`

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

Diagonal limit for Nyström matrix $k(t,t)$ same as Laplace

PTR with N nodes, test via self-convergence What's the conv. rate? Why N^{-3}?

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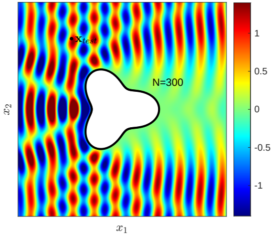

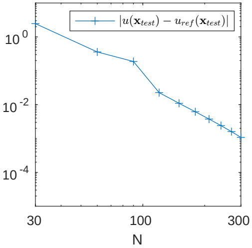

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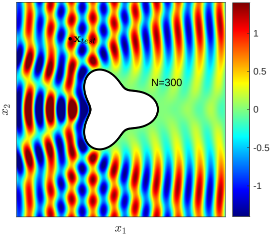

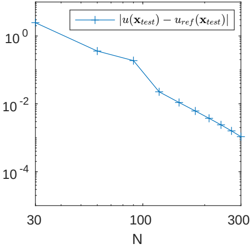

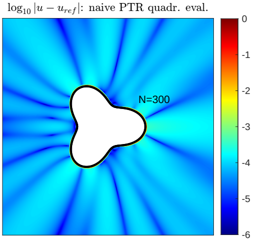

4. Debug BVP with known data from a radiative soln sources inside Ω
5. Without analytic soln: test both via self-convergence and conserved physical qty e.g. optical theorem, or no net QM flux over closed curve C containing no sources or sinks, $0 = \mathrm{Im}\left(\int_C \bar{u} u_n ds\right)$ (eg,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

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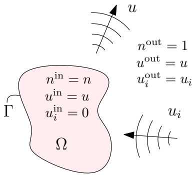
Helmholtz – transmission BVP

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 $n = 1$

inc wave only on outside, e.g. $u_i = \begin{cases} 0 & \text{in } \Omega \\ e^{i\mathbf{k}\cdot x} & \text{in } \mathbb{R}^2\backslash\overline{\Omega} \end{cases}$, $\mathbf{k} = \begin{bmatrix} \omega\cos\theta \\ \omega\sin\theta \end{bmatrix}$

BVP for u:

$(\Delta + \omega^2)u = 0 \quad \text{in } \mathbb{R}^d\backslash\overline{\Omega}$ PDE outside

$(\Delta + n^2\omega^2)u = 0 \quad \text{in } \overline{\Omega}$ PDE inside

$[u] = -u_i \quad \text{on } \Gamma$ $[u] := u^+ - u^-$, continuity of u^{tot}

$[u_n] = -(u_i)_n \quad \text{on } \Gamma$ continuity of u_n^{tot}

$\lim_{r\to\infty}\left(\frac{\partial u}{\partial r} - i\omega u\right) = 0$ SRC outside

Formulate as sys of integral eqs Rokhlin–Müller scheme, (Müller '69, Rokhlin '83)

$$u = \begin{cases} \mathcal{S}^{(n\omega)}\sigma + \mathcal{D}^{(n\omega)}\tau & \text{in } \Omega \\ \mathcal{S}^{(\omega)}\sigma + \mathcal{D}^{(\omega)}\tau & \text{in } \mathbb{R}^2\backslash\Omega \end{cases}$$

$\begin{bmatrix} [u] \\ [u_n] \end{bmatrix} = \left(\begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix} + \begin{bmatrix} D^{(\omega)} - D^{(n\omega)} & S^{(n\omega)} - S^{(\omega)} \\ T^{(\omega)} - T^{(n\omega)} & D^{(n\omega)*} - D^{(\omega)*} \end{bmatrix} \right) \begin{bmatrix} \tau \\ -\sigma \end{bmatrix}$ T is hypersingular operator

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

Helmholtz – high-order accuracy

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

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

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.

$\int_\Gamma f(\boldsymbol{x},\boldsymbol{y})\log|\boldsymbol{x}-\boldsymbol{y}|ds_y \approx \sum_{j=1}^N f(\boldsymbol{x},\boldsymbol{y}_j)w_j^L(\boldsymbol{x})$ (Helsing, Holst, '15), (Kress), ...

Generalized Gaussian quadrature (Bremer)

Close evaluation: target close to bdry

Kernel-split approach

QBX: quadrature by expansion (Kloeckner, Barnett, Greengard, O'Neil '13), (Epstein, Greengard, Kloeckner '13)

See also libraries: chunkie, BIE2D, etc.

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Summary

Covered BIE basics for smooth curves with global quadrature:

- Well-posed Laplace & Helmholtz BVPs — exterior need condition as $\|\mathbf{x}\| \to \infty$
- 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

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Useful 2D tools we did not yet cover: — 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 modern devels:

- "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).

focuses on quadrature for logarithmic singularities, eg SLP, Helmholtz

- `https://users.flatironinstitute.org/~ahb/BIE/`
- `https://github.com/ahbarnett/BIEbook` in progress...