Overview of Nyström (and not-so-Nyström) high-order surface quadratures for fast solvers

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SIAM CSE, Spokane, minisymposium MS355, 3/1/19

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Setting: solving linear BVPs

$Lu = 0$ in Ω, $\Omega \subset \mathbb{R}^d$, interior or exterior domain in $d = 2, 3$ dims

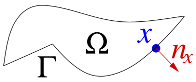
$u = f$, or $\partial u/\partial n = f$, or mix on boundary $\Gamma := \partial\Omega$ (& decay conds)

$L = 2^{nd}$-order elliptic diff. op. whose fundamental soln G known

L usually constant-coeff. but need not be! (B–Nelson–Mahoney '15)

Apps: electrostatics, waves (EM/acoustic), fluids & vesicles, t-step heat

- u scalar: Laplace, Helmholtz (& mod.), biharmonic (& mod.)
- u vector: Stokes, Maxwell, Beltrami
- data f: e.g. cancels incident field, or effect of volume potential



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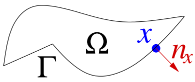

- Convert to IE: e.g. "indirect", interior Dirichlet Lap. 2D, unknown "density" τ on Γ

$u(x) = (\mathcal{D}\tau)(x) := \int_\Gamma \frac{\partial G(x,y)}{\partial n_y} \tau(y) ds_y$ $\quad G(x,y) = \log(1/r)/2\pi, \quad r = \|x - y\|$

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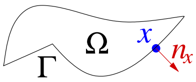

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jump relation: $u^-(x) := \lim_{h\to 0+} u(x - hn_x) = \left((D - \tfrac{1}{2})\tau\right)(x) = f(x) \quad x \in \Gamma$

(Also $\exists$ "direct" formulation: adjoint BIE, physical unknown, RHS more painful)

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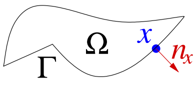

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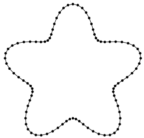
Fredholm 2^{nd}-kind BIE on Γ: $\boxed{(I + K)\tau = f}$ $\leftarrow$ task: approx. this by lin. sys.

$K(x,y)$ is as smooth as Γ, plus weak (i.e. integrable) singularity at $x = y$:

If Γ smooth: $\log r$ or $r^2 \log r$ in $d = 2$; r^{-1} in $d = 3$

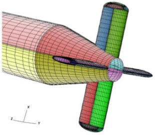
Two routes to represent density τ

(G) global   spectral accuracy, convergence via degree $p \to \infty$,   err $\sim c^{-p}$, $N \sim p^{d-1}$



peri. trap. rule

sph. harms.
(Rahimian et al)



macro Cheby. patches
(Bruno, Turc et al.)

obstacles simple, smooth

some adaptivity poss. (Kress corners)

(sinh-bunching, B et al. '16)

underlying basis: Fourier / sph. harm.

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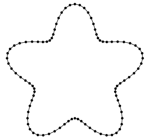

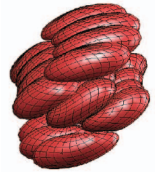

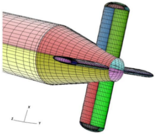

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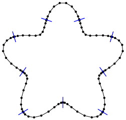
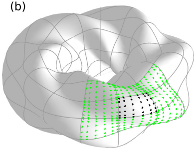
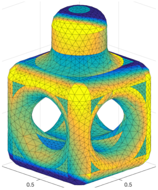
(L) local   fixed panel order p, conv. via $h \to 0$,   err $\mathcal{O}(h^p)$. $N \sim h^{1-d}$

adaptivity and/or CAD geoms.





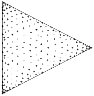


can split any panel indep. of others

$h \to 0$ with a CAD mesh? we wish

recent tri nodes:

Vioreanu–Rokhlin



G–L panels   G–L quads (B et al. '19)   4th-ord tri's (O'Neil '17)

Well-cond $p^{d-1} \times p^{d-1}$ matrices map values at nodes $\leftrightarrow$ basis coeffs

Two religions of discretizing the IE $(I+K)\tau = f$

- Nyström, impose IE at nodes $\{x_i\}_{i=1}^N$: $\tau_i + (K\tau)(x_i) = f_i \quad i = 1,\dots,N$

N $(d-1)$-dim singular ints, using τ interp from $\{\tau_j\} := \{\tau(x_j)\}$ ↗

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(G) global 3D: smoothly deformed sphere, cost $\mathcal{O}(p^5)$ (Graham–Sloan '02)

Stokes: vesicles, red blood cells (Rahimian, Veerapaneni, Biros,...)

smooth bodies, Helmholtz, Maxwell (Ganesh, Hawkins,...)

(L) tri/quad panels: many 4D quadrature rules (Sauter–Schwab, Ch. 5)

software, $p = 0, 1$ & Maxwell RWG: `BEM++` (Betcke, Smigaj et al '15)

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Which use? At same order, accuracy basically same (Kress '99, etc)

Galerkin: nastier numerical integrals, slower set-up (Canino '98)

Galerkin more mature convergence theory, industrial codes

Thus, the rest of this review is about Nyström...

Quadrature task & categories

Recall Nyström: $\tau_i + (K\tau)(x_i) = f_i$, surface nodes $i = 1, \ldots, N$

Task: given vector $\boldsymbol{\tau} := \{\tau_j\}_{j=1}^N$, eval. $(K\tau)(x_i)$ at all N targets x_i

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Apart from (G) vs (L) for density τ rep, other axes to categorize...

- FMM/FDS-compatible? only $\mathcal{O}(N)$ els. differ from native $A_{ij} = K(x_i, x_j) w_j$
- Precomputation (store A; good for rigid body) vs on-the-fly? (moving geoms.)
- Solely Nyström (on-surf.) task, vs also bonus off-surf. target evals.?
- Needs only on-surf. geom, vs also needs off-surf. pts?
- Ease of switching to new kernels? e.g. toroidal ...

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2D: product quadratures, exact for freqs. up to $\pm N/2$ (Kress '91)

split $K(t,s) = \psi(t,s)\log\left(4\sin^2 \frac{1}{2}|t-s|\right) + \phi(t,s)$, for some $\psi, \phi \in C^\infty([0,2\pi)^2)$

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(Ioakimidis '91; DLP Helsing '08, SLP B–Veerapaneni–Wu '14)

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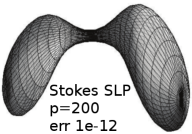
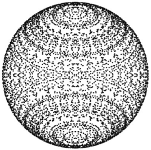
3D: diffeo. of sphere: $\mathcal{O}(N^2 \log N)$ recall $N = p^2$ (Gimbutas–Veerapaneni '14)





grid vals $\leftrightarrow$ sph harms fast

(azimuthal 1D FFT)

eval sph harms at p^4 rot grid pts

(elevational 1D NUFFT)

A.(G) on-surf. global [cont.]

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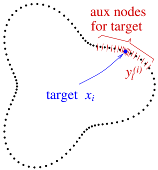

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via $\approx 2p$ off-grid aux. nodes (Alpert '99)

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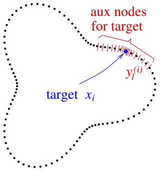

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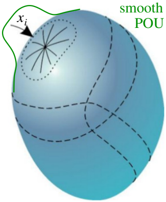

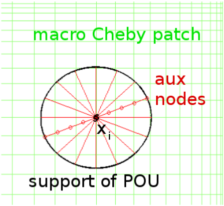

polar idea:

$1/r$ cancelled by metric $r dr d\theta$

note $\lim_{r\to 0} rK(x_i, y(r,\theta))$ varies with θ!

partition of unity, polar aux grid

(Bruno–Kunyansky '01)

(Malhotra '19)

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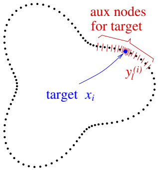

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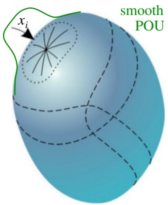

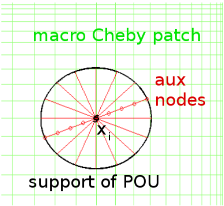

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partition of unity, polar aux grid

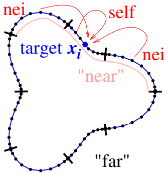
(Bruno–Kunyansky '01)

(Malhotra '19)

How get τ at aux nodes? local p-order Lagrange interp.

Thus: (near-diag blk of A) $\approx$ (kernel eval at aux nodes) $\times$ (interp matrix)

A.(L) on-surf. for local panel density



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- special rules for near (self+nei) panels
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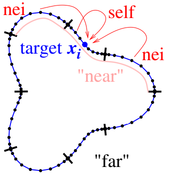

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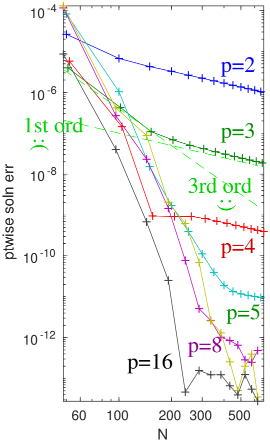
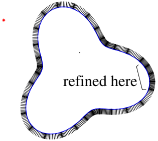
Bizarre, little-known $h \to 0$ convergence! :





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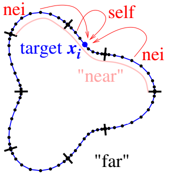
freq $k = 2$, std level-restricted splits

Why bottom out at 1st-order?

A.(L) on-surf. for local panel density



Common idea in $d = 2, 3$ for pth order scheme:

- special rules for near (self+nei) panels
- native rule $A_{ij} = K(x_i, x_j)w_j$ for far

FMM-compat.

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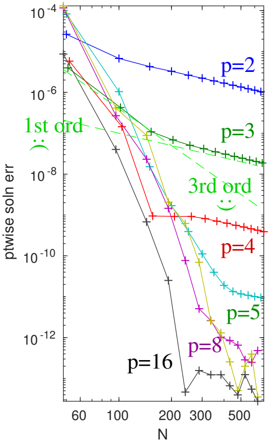

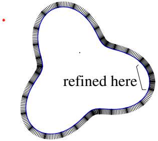

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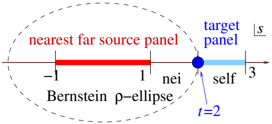
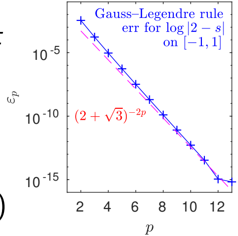
Why bottom out at 1st-order?

"nearest far panel" (NFP) controls *native* err:

G–L $\varepsilon_p \sim \rho^{-2p}$, $\quad \frac{\rho+\rho^{-1}}{2} = t$





scheme formally $\mathcal{O}(h^p + \varepsilon_p h)$

Thus my rule of thumb: pick $p \approx$ # digits you seek

With that caveat . . . on-surf. panel schemes: two types

A.(L).i: analytic

2D: complex Cauchy integral ψ, ϕ formulae avail. (Helsing–Ojala '08)

Ideas: monomial rep. $\tau(z) = \sum_{n=0}^{p-1} c_n z^n, \quad z \in \mathbb{C}$ (prefer $\tau(s)$: af Klinteberg)

2-term recurrence for $\int_{-1}^{1} \frac{y^n}{x-y} dy$, then e.g. DLP $(D\tau)(x) = \mathrm{Re} \frac{1}{2\pi i} \int_\Gamma \frac{\tau(y)}{x-y} dy$

Bonus: great for close off-surf. eval. code: `demo*.m` (Helsing)

3D: singularity subtraction? in infancy, hard (Helsing note `arXiv:1301.7276`)

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A.(L).ii: aux-node based   analytic split not needed

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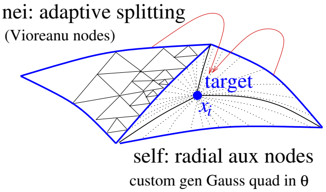

reach 10^{-12}, even v. high aspect ratio

∃ `Fortran` (Gimbutas, Rachh in prep.)

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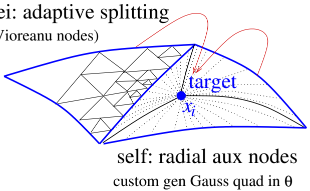

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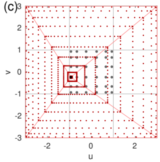
Structured quads easier

radial aux scheme for 3×3 near patch:

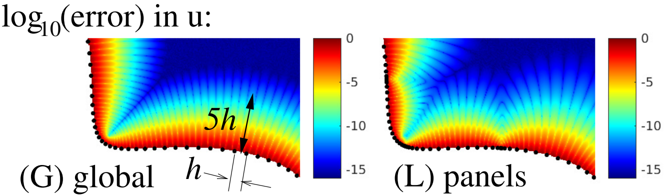


not versatile yet: torus diffeo's only

(wave eqn: B–Hagstrom–Greengard '19)

Interlude: close evaluation task

Recall native rule, off-surf. eval. $u(x) \approx \sum_{j=1}^{N} K(x, x_j) w_j \tau_j$ $\quad x \in \Omega$



How accurate is it? Exponential in N, but rate depends on target x:

Thm: (B '14) For global peri. trap. rule, analytic curve,
rate = Im (preimage of x under complexification of Γ param.)

- Similar estimates for panels (af Klinteberg–Tornberg '17)

2D summary: err $\approx \mathcal{O}\left(e^{-2\pi d/h}\right)$ $\quad d$ = dist to surf, h = local node spacing

"5h rule": $d \geq 5h$ gets you 10^{-14}, closer and lose digits linearly

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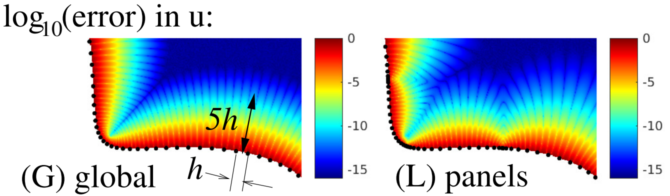

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Idea: native eval to points *near* Γ, then extrapolate *back* to target on Γ

(Yes, sounds crazy. Bonus: also does close-eval task!)

Let's call idea CATEGORY B: off-surface methods

Method B.1: "Hedgehog" quadrature

Originally scheme for eval at *close* target x: (Ying–Biros–Zorin '06; Quaife...)

i) pick line ("spine") through x hitting Γ at x_0, near

ii) upsample τ by factor $\beta > 1$ in each dim, e.g. $\beta = 2$–4

iii) eval at few pts dist $\geq 5h/\beta$ via upsampled native rule

iv) interpolate to x, from these pts *plus known* $u(x_0) = f(x_0)$

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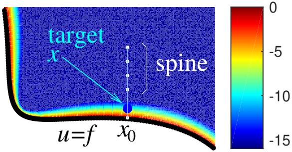
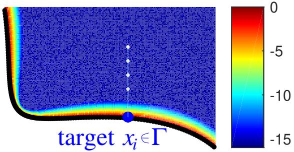
Interpolate for close eval:



Can also extrapolate for Nyström surf quadr:



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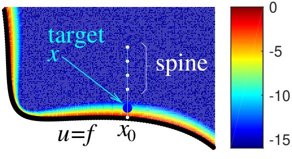

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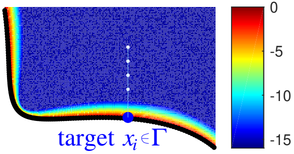


Adv: PDE-indep, dim-indep, τ-rep-indep, FMM’able. . . but params to adjust

movie: 10^4 vesicles + quad panels: $N = 6 \times 10^6$ (Morse–Lu–Rahimian–Zorin, in prep)

- Note: all category B methods eval $(I + A)\boldsymbol{\tau}$, not $A\boldsymbol{\tau}$

  $\rightarrow$ need 2-sided average, explicit I, to avoid GMRES stagnation

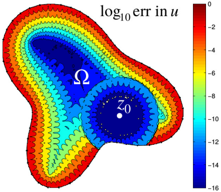
B.2: QBX (quadrature by expansion)

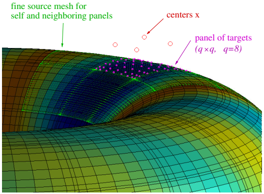
Finally (!) use the fact: u satisfies the PDE $Lu = 0$

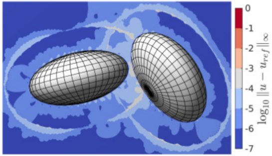
Idea: eval. "local exp." $u(z) = \text{Re} \sum_{n=0}^{p} a_n (z - z_0)^n$ here 2D Lap. case

- center $z_0 \in \Omega$, pick e.g. $3h$ from Γ
- each a_n given by a surf int (addition thm): use β-upsampled native rule

"Global" all of Γ, vs "local" just near panels (Klöckner–B–O'Neil–Greengard, '13; B '14)







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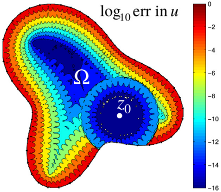

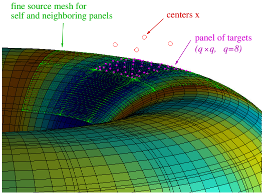

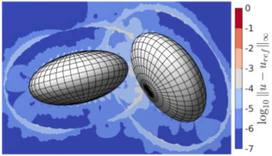

(b) Error using QBX.

Recent variants:

- AQBX: automated target-wise choice of p, β (af Klinteberg–Tornberg '17)
- QBKIX: PDE-indep, via proxy sources (Rahimian–B–Zorin '17)
- 3D Line QBX: p not p^2 terms, closer to hedgehog (Siegel–Tornberg '18)
- GIGAQBX: integrate w/ FMM: `pytential` (Wala–Klöckner, '17, '18)

Promise: prescribed-tolerance black-box A apply or A_{ij} fill not yet

Omitted topics

- corners and edges   either geometric refinement, or make custom quadr, or both
  (Chandler–Graham) (Helsing) (Serkh–Rokhlin) (Lintner–Bruno)
- various special methods   (Slevinsky–Olver '15) (Carvalho–Khatri–Kim, '18)
- analysis
- transmission BVPs, diel. contrast, D-N junctions
- bodies of revolution   curves w/ toroidal kernels
- line integrals in 3D   (Tornberg–Shelley '04; af Klinteberg–B in prep.)
- fundamental solutions (MFS) as alternative to SKIE+Nyström ...

State of the art & community to do list

2D: use Alpert/Kress if global, Helsing if panels; speed faster than FMM
corners: RCIP (Helsing), or (Serkh, Hoskins–Rachh) if analysis avail, N/corner ≈ 40
`Code?` partial, not adaptive, not much ready to non-experts to use

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Lots of fun challenges:

- 3D speed   currently 10^2–10^3 targs/sec/core err 10^{-6}: ≥ 10x slower than 3D FMM
- automatic apply of high-order Nyström to CAD/industrial meshes
- 3D corners, cones, and (generic curving) edges, to high order
- related: high aspect ratio / skew panels
- fair error/speed comparisions on 3D test probs (2D basically benchmarked)
  we're starting to address: needs uniform code interface (O'Neil–Rachh–B)
- 2D/3D documented code for non-experts w/ sensible/adaptive params

Review references

R. Kress, *Linear Integral Equations*, '99

Colton–Kress, *Inverse Acoustic & Electromagnetic Scattering Theory*, '89

I. Sloan, Acta Num. '91

J. Helsing, RCIP tutorial, `arXiv:1207.6737` '18

K. E. Atkinson book, '97

Hao–B–Martinsson–Young, Adv. Comput. Math. '14

`http://math.dartmouth.edu/~fastdirect/notes/quadr.pdf`