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Quadrature by fundamental solutions: kernel-independent layer potential evaluation for large collections of simple objects

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MS27, ICOSAHOM, planet Earth, 7/12/21
"Fast and high order solution techniques for boundary integral equations"

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Motivations and goal

Many simulations using boundary integral equations (BIE) involve large number of simple bodies (inclusions, vesicles, swimmers ...)

"simple": N unknowns per body s.t. $\mathcal{O}(N^3)$ dense lin. alg. ok... $N \lesssim 10^3$ in 2D, 10^4 in 3D

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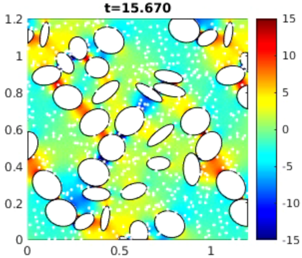
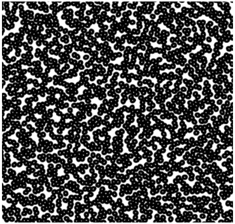


sheared rigid suspensions

(Wang–Nazockdast–B '21)



10^4 active-fluid deformable drops

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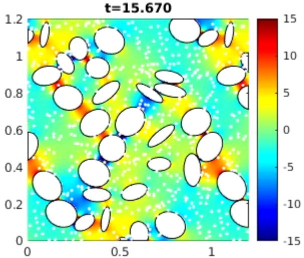

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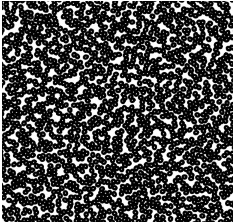

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- other apps: multiple scattering (acoustic/EM), electrohydrodynamics
- dense / non-Newtonian / bdry layers: *many/most* targets near bdry!
- accurate evaluation near bdry often slow, complex, PDE-specific

Goal: new BIE quadrature/evaluator tool, simply FMM-able, PDE-indep.

Setup: solving linear BVPs (exterior Dirichlet case)

BVP: $Lu = 0$ in $\mathbb{R}^d \backslash \overline{\Omega}$ — Ω = one or many bodies

$u = f$ on $\partial\Omega$

decay/radiation condition on $u(\mathbf{x})$ as $r := \|\mathbf{x}\| \to \infty$

Laplace $L = \Delta$ Helmholtz $L = \Delta + k^2$ Stokes system for $(\mathbf{u}, p)$, vel. data $\mathbf{u}$

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Represent $u = (\alpha \mathcal{S} + \beta \mathcal{D})\tau$ in $\mathbb{R}^d \backslash \overline{\Omega}$ $\quad (*)$ $\quad$ desired LP to eval

τ "density" $\quad$ α, β mixing params, chosen for unique soln of indirect BIE

Eg "completed" for Lap, Stokes $\alpha = \beta = 1$; CFIE for Helm $\alpha = ik$, $\beta = 1$.

where $(\mathcal{S}\tau)(\mathbf{x}) := \int_{\partial\Omega} G(\mathbf{x}, \mathbf{y})\tau(\mathbf{y}) ds_{\mathbf{y}}$ $\quad$ G = fundamental soln for L

$G(\mathbf{x}, \mathbf{y})$ convolutional for const-coeff. But: axisymm, layered media, etc, not so

$(\mathcal{D}\tau)(\mathbf{x}) := \int_{\partial\Omega} \frac{\partial G(\mathbf{x},\mathbf{y})}{\partial \mathbf{n}_{\mathbf{y}}} \tau(\mathbf{y}) ds_{\mathbf{y}}$ scalar only; not so for Stokes

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Take $\mathbf{x} \to \partial\Omega^+$ (ie exterior) and use *jump relations*, get BIE for τ:

$\frac{\beta}{2}\tau + (\alpha S + \beta D)\tau = f$ Id + cpt if $\partial\Omega$ smooth $\Rightarrow$ Fredholm 2nd kind

By quadrature + Nyström on $\partial\Omega$, approx BIE by: $A\boldsymbol{\tau} = \boldsymbol{f}$

Tasks: $f_j = f(\mathbf{x}_j)$, $\mathbf{x}_j$ nodes on $\partial\Omega$

A) Fill A matrix: equiv to on-surface LP evaluation

B) Eval $(*)$ off-surf, given soln vec $\boldsymbol{\tau} := \{\tau_j\}_{j=1}^N$

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Prior work on high-order Nyström quadratures

- task A) fill A: needs high-order weakly-singular quadr (except Lap 2D)
- task B) eval LP $(*)$ for $\mathbf{x}$ arbitrarily close to $\partial\Omega$ ("close eval")

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Incomplete history: (also see my CSE19 review slides)	task B?	PDE-indep?
2D global product-quadr. analytic split (Kress '91)	N	N
2D panel analytic split, Lap+Helm (Helsing '08–'15)	Y	N
2D gen-Gauss. aux nodes (Rokhlin–Duan, Alpert, '99)	N	Y
3D radial interp, $r\,dr$ (Bruno–Kunyansky '01; Malhotra)	N	Y
3D global spherical harmonics (Ganesh, Corona...)	N	N
QBX+ (Klöckner–O'Neil–B–Greengard '12; Rachh, Wala, af K)	Y	if proxy
2D barycentric (Ioakimidis, Helsing, Wu–B–Veerapaneni '14)	Y	N
3D radial triangle-split gen-Gauss. (Bremer, Gimbutas)	N	Y
3D adaptive off-surf panels (Rachh, Greengard, O'Neil)	Y	Y
Density interpolation (2D,3D) (Perez-A., Turc, Faria '18)	Y	if proxy
off-surf radial + cancellation (Carvalho–Khatri–Kim '18)	Y	N
3D "hedgehog" extrapolation (Morse–Zorin '20)	Y	Y
zeta functions for global (2D,3D) (Wu–Martinsson '20)	N	N
Lap 3D quaternion line-integral (Zhu–Veerapaneni '21)	Y	N

Our contribution

Many methods/pubs [academia], few usable codes we try to fix at Flatiron

All "close-evaluation" (task B) methods listed have an issue:

- need split targs into "near" (special method) vs far (plain Nyström)
- to couple to fast alg need: 1) apply FMM to all targs, 2) subtract near wrong parts, 3) add correct near
- issues: cancellations, per-target bookkeeping, slow

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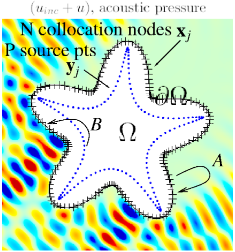
Beautiful idea: for exterior of $\partial\Omega$=sphere, project LPs into (vector) spherical harmonics, eval those when close to $\partial\Omega$

(Corona–Veerapaneni, Yan, Shelley, etc)

Our plan: a global rep for general shape Ω, using point sources only, so plugs in to point FMM without per-target FMM bookkeepping?

- show 2D only, find useful for large # simple bodies
- we stick to global quadr each body — separations $\gtrsim h^2$; ie not locally adapt.

Simplest QFS idea for $(*)$ eval: 2D, one body, exterior



Here user supplies:

- desired tolerance ϵ
- on-surface rule: $\mathbf{x}_j$ nodes, w_j weights, s.t.
  $\int_{\partial\Omega} g(\mathbf{y}) ds_y - \sum_{j=1}^{N} w_j g(\mathbf{x}_j) = \mathcal{O}(\epsilon)$ quadr. error
  for "relevant" smooth funcs g (eg τ, $\mathbf{n}$, geom. . .)
- A (Nyström mat incl. $I/2$ jump term) for now :)

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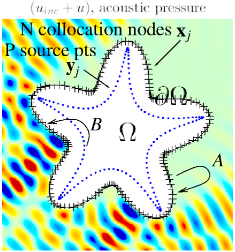

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Pick $P \approx N$ sources $\mathbf{y}_j \in \Omega$ near $\partial\Omega$ use ϵ to control dist

Simplest QFS rep. is: $\tilde{u}(\mathbf{x}) = \sum_{j=1}^{P} G(\mathbf{x}, \mathbf{y}_j)\sigma_j$ σ_j = unknown charges

Fill $B \in \mathbb{C}^{N\times P}$ via $B_{ij} := G(\mathbf{x}_i, \mathbf{y}_j)$

When user gives us new density vec $\boldsymbol{\tau}$:

i) solve $B\boldsymbol{\sigma} = A\boldsymbol{\tau}$ ill-cond. $\kappa(B) \approx \epsilon^{-1/2} \leq 10^8$, need bkw. stab, $\mathcal{O}(N^3)$

meaning: match potentials on $\partial\Omega^+$, so by BVP uniqueness $\tilde{u} \approx u$ in $\mathbb{R}^2\backslash\overline{\Omega}$

ii) eval. QFS rep at targets *everywhere* in $\mathbb{R}^2\backslash\Omega$ via point FMM

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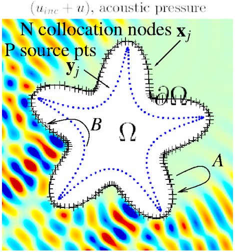

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Better: precompute $B = U\Sigma V^*$, then store $Y = V\Sigma^{-1}$ and $Z = U^*A$

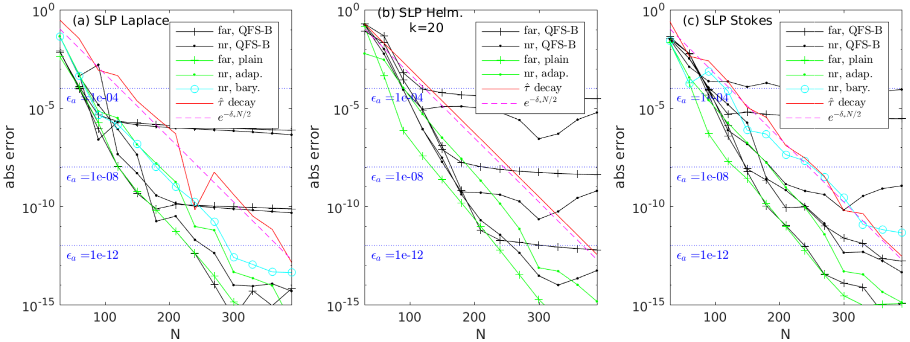
- when user inputs $\boldsymbol{\tau}$, two matvecs gives $\boldsymbol{\sigma} = Y(Z\boldsymbol{\tau})$ — bkw stab order!

Error convergence for SLP eval in 2D, three PDEs

Given $\boldsymbol{\tau} \in \mathbb{R}^N$ sampling a density τ: QFS (black) vs gold-std (green):

gold-standards: "far" target = plain Nyström rule for $(*)$

"near" (dist 10^{-4}) = adaptive Gauss on trig poly interp of $\boldsymbol{\tau}$



Results: QFS similar to gold, then flattens at around ϵ; DLP sim.

- exp. conv. *rate* $\approx$ decay of Nyquist Fourier coeff $\hat{\tau}_{N/2}$ (red)

Raises qu's! Why stable? How choose $\mathbf{y}_j$?

Wouldn't it be nice not to have to supply A?

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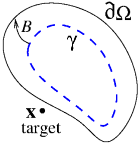
QFS Theory: continuous limit I

Recall: we approx $u = (\alpha\mathcal{S} + \beta\mathcal{D})\tau$ $(*)$ in ext. by $\tilde{u} = \mathcal{S}_\gamma\sigma$

QFS lin sys $B\boldsymbol{\sigma} = \mathbf{u}^+$ is discretization of 1st-kind IE

For *analytic* data, it is not crazy to demand it works...



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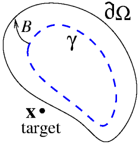

Thm. Let u be harmonic in $\mathbb{R}^d \backslash \overline{\Omega}$ with $u(\mathbf{x}) = C \log r + o(1)$ in $d = 2$ or $o(1)$ in $d = 3$, and continue as regular PDE soln in the closed annulus (shell) btw $\partial\Omega$ and γ. Then 1st-kind IE

$$\int_\gamma G(\mathbf{x}, \mathbf{y})\sigma(\mathbf{y}) ds_{\mathbf{y}} = u(\mathbf{x}) \ , \qquad \mathbf{x} \in \partial\Omega \qquad (\dagger)$$

has a solution. If $d = 3$ or *logarithmic capacity* $C_\Omega \neq 1$, it's unique, and $(\dagger)$ recovers u throughout $\mathbb{R}^d \backslash \overline{\Omega}$.

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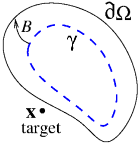

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Pf: Let v solve the int Lap Dir BVP for $v = u$ on γ
Green's rep. formula exterior to γ: $u = -\mathcal{S}_\gamma u_\mathbf{n} + \mathcal{D}_\gamma u$ by const $u_\infty = 0$
GRF (extinction) exterior to γ: $0 = \mathcal{S}_\gamma v_\mathbf{n} - \mathcal{D}_\gamma v$
Add them: $u = \mathcal{S}_\gamma(v_\mathbf{n} - u_\mathbf{n})$ outside γ, in particular on $\partial\Omega$ $\Rightarrow$ soln
Uniqueness: jump relations & unique cont. from Cauchy data... $\square$

QFS Theory: continuous limit II

Summary: continuous QFS robust to evaluate $(*)$ for analytic data if...

i) Source curve (surf) γ "close enough" to $\partial\Omega$

τ analytic $\Rightarrow$ u cont. as PDE soln in some annulus (anal. theory of PDE, eg Colton; B'14)

ii) Range of QFS rep $\tilde{u} = \mathcal{S}_\gamma \sigma$ same as desired $(*)$

Lap 2D range of LPs: $C \log r + u_\infty + o(1)$, with const term $u_\infty = 0$

iii) Data type on $\partial\Omega$ must lead to unique ext BVP *in this range*

Here Dirichlet data u^+. 2D subtelty: $C_\Omega = 1 \;\Rightarrow\; C$ undetermined by u^+

easy: also fix tot charge $\int_\gamma \sigma = \alpha \int_{\partial\Omega} \tau$, extra row of QFS lin sys

- Similar robustness thms for Stokes $\mathcal{S}_\gamma$; Helm $(\mathcal{D} + ik\mathcal{S})_\gamma$ (CFIE)

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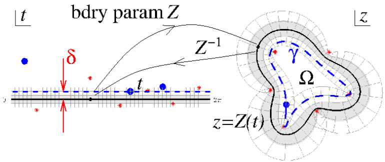
How choose curve γ (2D)?



$\partial\Omega$ param by $Z(t) \in \mathbb{C} \simeq \mathbb{R}^2$

$t \in [0, 2\pi)$ periodic, anal. in a strip

$\mathbf{x}_j = Z(2\pi j/N)$ periodic trap. rule (PTR)

User promised us N such that PTR achieves err ϵ for their τ

Thm (Davis '59): If $\tau(t)$ anal. in $|\mathrm{Im}\, t| \le \delta$, PTR error rate $\mathcal{O}(e^{-\delta N})$

Equate Davis to ϵ gives: $\delta \approx N^{-1} \log \epsilon^{-1}$ our rule for "close"

Then choose $\gamma = \{Z(t + i\delta) : t \in [0, 2\pi)\}$ "imaginary translation" of $\partial\Omega$

Choice of source (proxy) points $\mathbf{y}_j$ in 2D

Recipe: set imag. dist. param $\delta = N^{-1} \log \epsilon^{-1}$, and $P = N$, then

$$\mathbf{y}_j := \mathbf{x}(t_j) - \delta \, \|\mathbf{x}'(t_j)\| \, \mathbf{n}(t_j) + \delta^2 \mathbf{x}''(t_j) \qquad t_j = \frac{2\pi j}{P}, \quad j = 1, \ldots, P$$

nearly imag. transl. (2nd-order Taylor approx) $\quad \epsilon = 10^{-14}$ gives dist. $\approx 5h$ (see B'14)

Details: if γ self-intersects, reduce δ until doesn't, then grow P to match

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Method of Fundamental Solns (Kupradze '67, Bogomolny, Golberg–Chen, Eremin)

a.k.a. method of aux. sources, charge simulation method, ...

related to (not same as!) proxy points (Martinsson, Rokhlin, Gillman; Chow '19)

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Thm (Katsurada '96 Laplace; Kangro '10 Helmholtz): Let $Z(t)$ and Dirichlet data $f(t)$ be analytic in a suff. wide strip. Choose N sources $\mathbf{y}_j = Z(2\pi j/N + i\delta)$. Then MFS err in solving the BVP for data f is, in exact arithmetic, up to algebraic factors, $\mathcal{O}(e^{-\delta N})$.

this is the smooth-data, annular conformal map case of various MFS thms

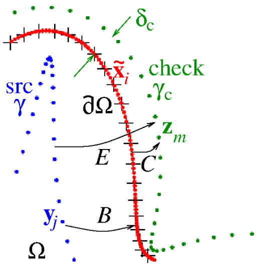
MFS analysis incomplete, technical: exp.-weighted Sobolev

- Note: MFS exponential rate matches our δ rule

Desingularized QFS: goodbye singular quadrature

Goal: also fill Nyström A (task A) recall until now user had to supply A :(

Idea: match data u not on $\partial\Omega$, but on new exterior "check" curve γ_c



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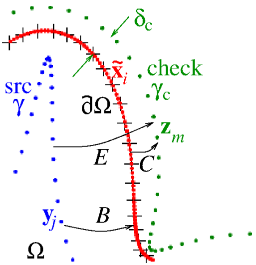

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fill $E_{mj} = G(\mathbf{z}_m, \mathbf{y}_j)$

upsample $\partial\Omega$ by factor ρ to get nodes $\tilde{\mathbf{x}}_i$

fill $\tilde{C}_{mi} = \alpha G(\mathbf{z}_m, \tilde{\mathbf{x}}_i) + \beta \frac{\partial G}{\partial \mathbf{n}_{\tilde{\mathbf{x}}_i}}(\mathbf{z}_m, \tilde{\mathbf{x}}_i)$

chk-eval. mat. $C = \tilde{C} L_{\rho N \times N}$ L = spectral upsampling

Solve $E\boldsymbol{\sigma} = C\boldsymbol{\tau}$ for $\boldsymbol{\sigma}$: as before   take $E = U\Sigma V^*$

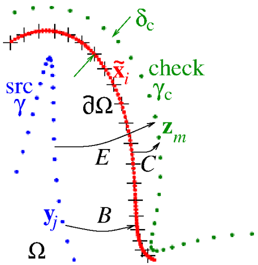
$Y = V\Sigma^{-1}$, $Z = U^* C$, then $\boldsymbol{\sigma} = Y(Z\boldsymbol{\tau})$

Task B done, all off-surf!   Finally $A \approx \tilde{A} = (BY)Z$ gives 1-sided lim

Desingularized QFS: goodbye singular quadrature

Goal: also fill Nyström A (task A) recall until now user had to supply A :(

Idea: match data u not on $\partial\Omega$, but on new exterior "check" curve γ_c



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- pick ρ upsampling (as in QBX, hedgehog) so C has err ϵ_{mach} at γ_c, via:
  Thm (B'14): At target $\mathbf{x}$, LP eval via N-node plain PTR has err $\mathcal{O}(e^{-|\operatorname{Im} Z^{-1}(\mathbf{x})|N})$. rate is imag dist of preimage, so set $e^{-\delta_c \rho N} = \epsilon_{\text{mach}}$

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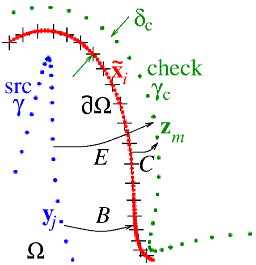

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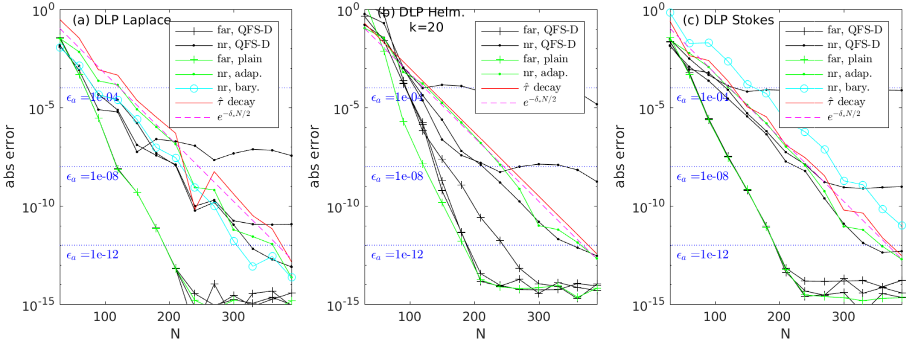
- upper bnd on chk dist: $\frac{\delta}{\delta+\delta_c} \geq \frac{\log \epsilon}{\log \epsilon_{\text{mach}}}$ — err growth of mode $M/2$, heuristic

in practice: $\epsilon = 10^{-8}$: $\delta_c \approx \delta$, $\rho \approx 2$ $\qquad$ $\epsilon = 10^{-12}$: $\delta_c \approx \delta/3$, $\rho \approx 4$

Error convergence for desingularized QFS, three PDEs

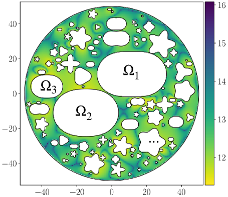
Again we compare QFS (black) vs gold-standard LP eval (green):



Results: QFS-D v. similar to gold, flattening around ϵ as expected

- Stokes: slight upsampling $P \approx 1.3N$, $M \approx 1.2P$, to get good spec$(\tilde{A})$.
- unlike QBX or hedgehog, no 2-sided averaging needed
- no SVD truncation needed since $\kappa(E) = \mathcal{O}(\epsilon_{\text{mach}}^{-1/2})$ only

Fast solver for multi-body applications



Recall exterior BVP gives BIE $\quad A\tau = f$

$A =$ Nyström mat $\quad$ eg Lap. "completed" $A = \frac{I}{2} + D + S$

For $K > 1$ bodies, A has $K \times K$ block structure

- QFS-D fills dense diag blocks $A^{(k,k)}$ self-int, task A

- Apply all off-diag $A^{(j,k)}$, $j \neq k$, by a point FMM: QFS srcs $\{\mathbf{y}_j\} \to$ bdry $\{\mathbf{x}_j\}$
  task B: bundle close & far targets together, no bookkeepping/corrections
  each body's strength vector from its own QFS-D $\boldsymbol{\sigma} = Y(Z\boldsymbol{\tau})$

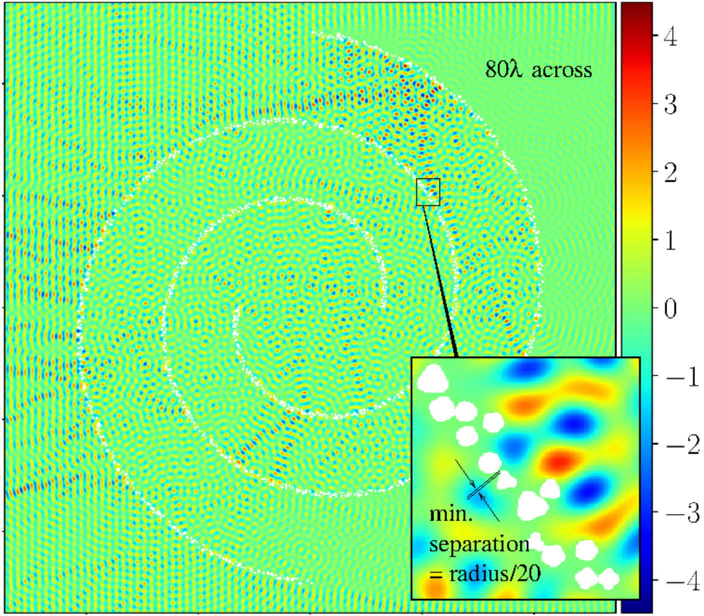
- To reduce iter count, block-diag right-precondition, so GMRES sees:

$$\begin{bmatrix} I & A^{(1,2)}(A^{(2,2)})^{-1} & \cdots \\ A^{(2,1)}(A^{(1,1)})^{-1} & I & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} \tilde{\tau}^{(1)} \\ \tilde{\tau}^{(2)} \\ \vdots \end{bmatrix} = \begin{bmatrix} f^{(1)} \\ f^{(2)} \\ \vdots \end{bmatrix}$$

Once solved, recover actual densities $\boldsymbol{\tau}^{(k)} = (A^{(k,k)})^{-1}\tilde{\boldsymbol{\tau}}^{(k)}$

- Eval solution u everywhere: again QFS-D task B

Application: multibody scattering (2D Helmholtz)



$K = 10^3$ bodies

$N \approx 190000$

7e-10 est max err
(2000^2 grid)

1e-11 diff vs Kress
+ upsampling

need 1237 iters
QFS, Kress same

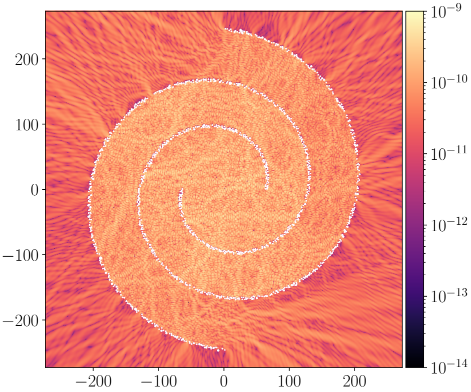
Solve: 13 min
(AMD server)

QFS setup:
0.14 core-hr

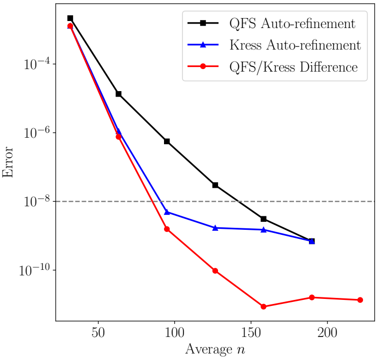
FMM: 9 core-hr

FMM effort: 80%

Error for multibody scattering (2D Helmholtz)



Max err convergence vs $n := \frac{N}{K}$



- QFS similar convergence rate to Kress
- resonant (errors 1 digit worse inside "leaky cavity")

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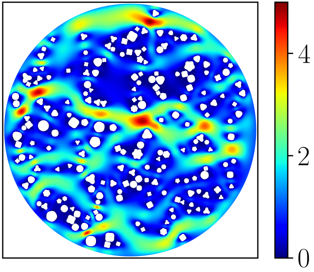
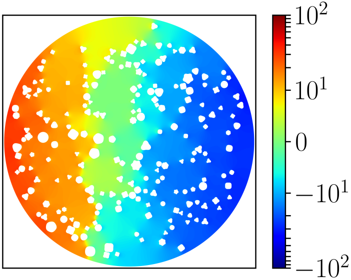
Application: multibody Stokes

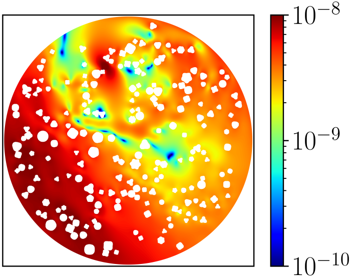
$|\mathbf{u}|$ solution (fluid speed):

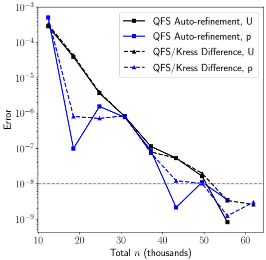


p solution (fluid pressure):



Estim pointwise error:





K = 200 bodies
min. sep. = rad/20
$N \approx 56000$ ($2N$ unkn.)
451 iters to 1e-8

7 min (AMD server)

$\geq 90\%$ FMM effort

Conclusions

QFS is a useful BIE quadrature tool when (many) "simple" bodies:

- *one* simple representation covers on-surface, near-surface, far-field
- fast & trivial to apply by point FMM, kills near-vs-far bookkeepping
- stably fills 1-body Nyström matrices w/o singular quadrature
- kernel-independent   current: Laplace, Helmholtz, modified Helmholtz, Stokes
- as accurate (spectral) as slower gold-standard schemes   Kress + adaptive

...PS: bkw. stab. apply of pseudoinv. needs *two* matvecs: $\boldsymbol{\sigma} = Y(Z\boldsymbol{\tau})$

2D Py code/demos: `https://github.com/dbstein/qfs`

Future:

- dim-indep: works in 3D; smooth multi-body tests ongoing
- corners? Yes (MFS), but not full acc. (Hochman '07, Liu–B '16, Gopal–Tref.'20)
- more analysis for MFS/QFS (Stokes, disk, analytic domains, ...)