Fast direct solvers for elliptic partial differential equations on locally-perturbed geometries

Yabin Zhang

RICE

(Joint work with **Adrianna Gillman**)

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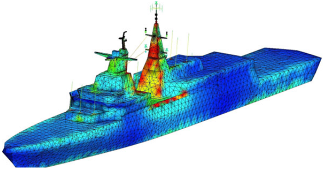
For a direct solver to be fast, the cost of constructing $\boldsymbol{T}$ and applying $\boldsymbol{T}$ to a vector needs to be low.

Motivation



https://altairhyperworks.com/product/FEKO/Applications-Antenna-Placement

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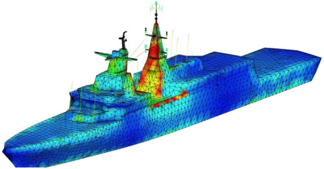

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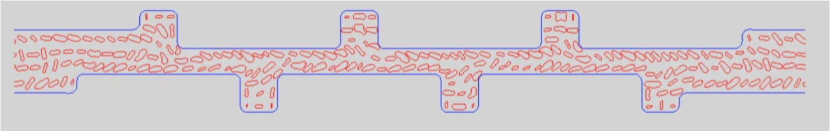
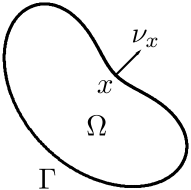


G Marple, A. Barnett, A. Gillman, and A. Veerapaneni, *A Fast Algorithm for Simulating Multiphase Flows Through Periodic Geometries of Arbitrary Shape.*

Model problem

Consider the Laplace BVP

$$
\begin{aligned}
-\Delta u(x) &= 0 && \text{for } x \in \Omega, \\
u(x) &= f(x) && \text{for } x \in \Gamma = \partial\Omega.
\end{aligned}
$$



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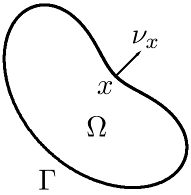

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The solution to the BVP can be represented as a double-layer potential

$$u(x) = \int_\Gamma \frac{\partial G(x,y)}{\partial \nu_y} \sigma(y) dl(y),\ x \in \Omega$$

where $\sigma(x)$ is an unknown boundary charge density and $G(x,y) = -\frac{1}{2\pi} \log\left(\frac{1}{|x-y|}\right)$ is the Green's function.

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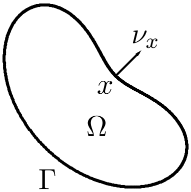

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Enforcing the boundary condition yields the **boundary integral equation** (BIE)

$$-\frac{1}{2}\sigma(x) + \int_\Gamma \frac{\partial G(x,y)}{\partial \nu_y}\sigma(y)dl(y) = f(x), \text{ for } x \in \Gamma.$$

The discretized linear system

Let $\vec{\sigma} = (\sigma(x_1), \ldots, \sigma(x_n))^T$, $\vec{f} = (f(x_1), \ldots, f(x_n))^T$, $\boldsymbol{I}$ be the identity matrix, and $\boldsymbol{D}$ be a matrix with entries $\boldsymbol{D}_{ij} = \frac{\partial G(x_i, x_j)}{\partial \nu_{x_j}} w_j$, then the discretized BIE can be written as

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Properties of the coefficient matrix $\boldsymbol{A}$:

- $\boldsymbol{A}$ is a dense matrix.
- The size of $\boldsymbol{A}$ depends on the number of discretization points N on the boundary Γ.
- $\boldsymbol{A}$ is data-sparse.
    - Particularly, the off-diagonal blocks of $\boldsymbol{A}$ are low-rank.

Data-sparse property of the coefficient matrix

Definition: A matrix $\boldsymbol{S} \in \mathbb{R}^{m \times n}$ is ϵ-rank if it has exactly $k = k(\epsilon)$ singular values that are greater than ϵ. $\boldsymbol{S}$ is called a low-rank matrix if $k << m$.

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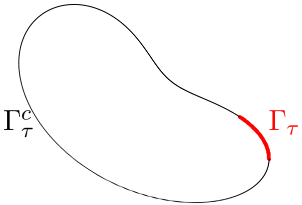

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Matrix block: $\boldsymbol{A}(\Gamma_\tau, \Gamma_\tau^c) \in \mathbb{R}^{100 \times 900}$

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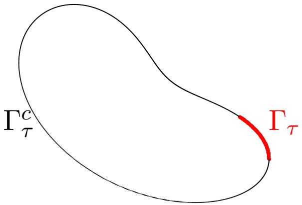

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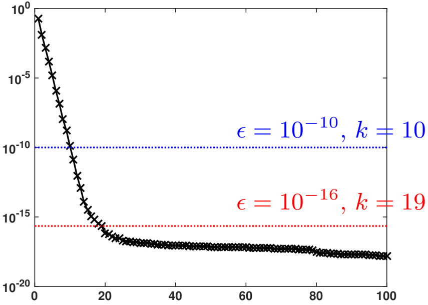


The singular values of $\boldsymbol{A}(\Gamma_\tau, \Gamma_\tau^c)$

Block-separable matrix

A matrix $\boldsymbol{A}$ of dimension $(np) \times (np)$ is *block-separable* if it consists $p \times p$ blocks each of size $n \times n$: e.g. for $p = 4$,

$$\boldsymbol{A} = \begin{bmatrix} \boldsymbol{D}_{11} & \boldsymbol{A}_{12} & \boldsymbol{A}_{13} & \boldsymbol{A}_{14} \\ \boldsymbol{A}_{21} & \boldsymbol{D}_{22} & \boldsymbol{A}_{23} & \boldsymbol{A}_{24} \\ \boldsymbol{A}_{31} & \boldsymbol{A}_{32} & \boldsymbol{D}_{33} & \boldsymbol{A}_{34} \\ \boldsymbol{A}_{41} & \boldsymbol{A}_{42} & \boldsymbol{A}_{43} & \boldsymbol{D}_{44} \end{bmatrix}.$$

And each of the off-diagonal block admits the factorization

$$\begin{array}{ccccc} \boldsymbol{A}_{ij} & = & \boldsymbol{U}_i & \tilde{\boldsymbol{A}}_{ij} & \boldsymbol{V}_j^* \\ n \times n & & n \times k & k \times k & k \times n \end{array}$$

where the rank k is significantly smaller than the block size n.

A. Gillman, P. Young, and P.G. Martinsson, *A direct solver with O(N) complexity for integral equations on one-dimensional domains*

Then we have $\boldsymbol{A} = \begin{bmatrix} \boldsymbol{D}_{11} & \boldsymbol{U}_1\tilde{\boldsymbol{A}}_{12}\boldsymbol{V}_2^* & \boldsymbol{U}_1\tilde{\boldsymbol{A}}_{13}\boldsymbol{V}_3^* & \boldsymbol{U}_1\tilde{\boldsymbol{A}}_{14}\boldsymbol{V}_4^* \\ \boldsymbol{U}_2\tilde{\boldsymbol{A}}_{21}\boldsymbol{V}_1^* & \boldsymbol{D}_{22} & \boldsymbol{U}_2\tilde{\boldsymbol{A}}_{23}\boldsymbol{V}_3^* & \boldsymbol{U}_2\tilde{\boldsymbol{A}}_{24}\boldsymbol{V}_4^* \\ \boldsymbol{U}_3\tilde{\boldsymbol{A}}_{31}\boldsymbol{V}_1^* & \boldsymbol{U}_3\tilde{\boldsymbol{A}}_{32}\boldsymbol{V}_2^* & \boldsymbol{D}_{33} & \boldsymbol{U}_3\tilde{\boldsymbol{A}}_{34}\boldsymbol{V}_4^* \\ \boldsymbol{U}_4\tilde{\boldsymbol{A}}_{41}\boldsymbol{V}_1^* & \boldsymbol{U}_4\tilde{\boldsymbol{A}}_{42}\boldsymbol{V}_2^* & \boldsymbol{U}_4\tilde{\boldsymbol{A}}_{43}\boldsymbol{V}_3^* & \boldsymbol{D}_{44} \end{bmatrix}$,

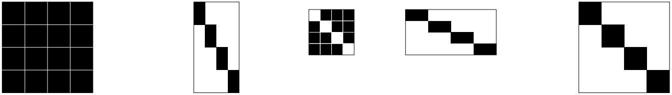
and it can be factored as

$$\boldsymbol{A} = \underbrace{\begin{bmatrix} \boldsymbol{U}_1 & & & \\ & \boldsymbol{U}_2 & & \\ & & \boldsymbol{U}_3 & \\ & & & \boldsymbol{U}_4 \end{bmatrix}}_{=\boldsymbol{U}} \underbrace{\begin{bmatrix} \boldsymbol{0} & \tilde{\boldsymbol{A}}_{12} & \tilde{\boldsymbol{A}}_{13} & \tilde{\boldsymbol{A}}_{14} \\ \tilde{\boldsymbol{A}}_{21} & \boldsymbol{0} & \tilde{\boldsymbol{A}}_{23} & \tilde{\boldsymbol{A}}_{24} \\ \tilde{\boldsymbol{A}}_{31} & \tilde{\boldsymbol{A}}_{32} & \boldsymbol{0} & \tilde{\boldsymbol{A}}_{34} \\ \tilde{\boldsymbol{A}}_{41} & \tilde{\boldsymbol{A}}_{42} & \tilde{\boldsymbol{A}}_{43} & \boldsymbol{0} \end{bmatrix}}_{=\tilde{\boldsymbol{A}}} \underbrace{\begin{bmatrix} \boldsymbol{V}_1^* & & & \\ & \boldsymbol{V}_2^* & & \\ & & \boldsymbol{V}_3^* & \\ & & & \boldsymbol{V}_4^* \end{bmatrix}}_{=\boldsymbol{V}^*} + \underbrace{\begin{bmatrix} \boldsymbol{D}_{11} & & & \\ & \boldsymbol{D}_{22} & & \\ & & \boldsymbol{D}_{33} & \\ & & & \boldsymbol{D}_{44} \end{bmatrix}}_{=\boldsymbol{D}},$$

Block separable matrix and its inversion

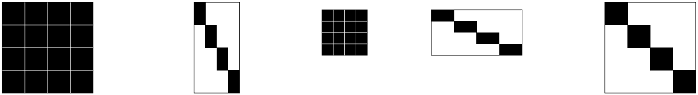
$\boldsymbol{A}$ admits the factorization:

$$\underset{pn \times pn}{\boldsymbol{A}} = \underset{pn \times pk}{\boldsymbol{U}} \quad \underset{pk \times pk}{\tilde{\boldsymbol{A}}} \quad \underset{pk \times pn}{\boldsymbol{V}^*} + \underset{pn \times pn}{\boldsymbol{D}},$$



Lemma (Variation of Woodbury) If $\boldsymbol{A}$ admits the factorization above, the inverse can be evaluated as

$$\underset{pn \times pn}{\boldsymbol{A}^{-1}} = \underset{pn \times pk}{\boldsymbol{E}} \quad \underset{pk \times pk}{(\tilde{\boldsymbol{A}} + \hat{\boldsymbol{D}})^{-1}} \quad \underset{pk \times pn}{\boldsymbol{F}^*} + \underset{pn \times pn}{\boldsymbol{G}},$$



where (provided all intermediate matrices are invertible)
$\hat{\boldsymbol{D}} = \left(\boldsymbol{V}^* \boldsymbol{D}^{-1} \boldsymbol{U}\right)^{-1}$, $\boldsymbol{E} = \boldsymbol{D}^{-1} \boldsymbol{U} \hat{\boldsymbol{D}}$, $\boldsymbol{F} = (\hat{\boldsymbol{D}} \boldsymbol{V}^* \boldsymbol{D}^{-1})^*$, and
$\boldsymbol{G} = \boldsymbol{D}^{-1} - \boldsymbol{D}^{-1} \boldsymbol{U} \hat{\boldsymbol{D}} \boldsymbol{V}^* \boldsymbol{D}^{-1}$.

Hierarchically block separable(HBS) matrix

The lemma reduces the cost of inversion from $(pn)^3$ to $(pk)^3$!

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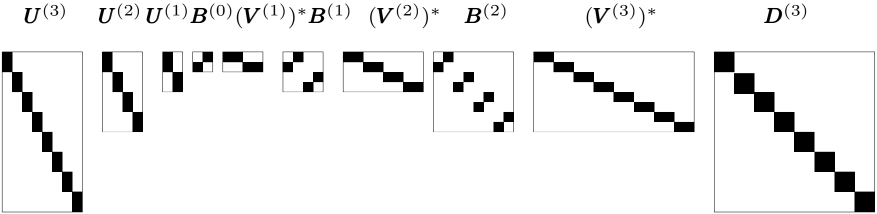
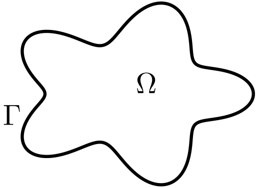
For example, a "3-level" telescoping factorization of $\boldsymbol{A}$ will be

$$\boldsymbol{A} = \boldsymbol{U}^{(3)}\big(\boldsymbol{U}^{(2)}\big(\boldsymbol{U}^{(1)}\,\boldsymbol{B}^{(0)}\,(\boldsymbol{V}^{(1)})^*\big) + \boldsymbol{B}^{(1)}\big)(\boldsymbol{V}^{(2)})^* + \boldsymbol{B}^{(2)}\big)(\boldsymbol{V}^{(3)})^* + \boldsymbol{D}^{(3)}.$$

And the block structure will look like:



Numerical examples



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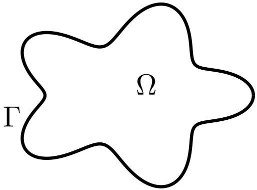

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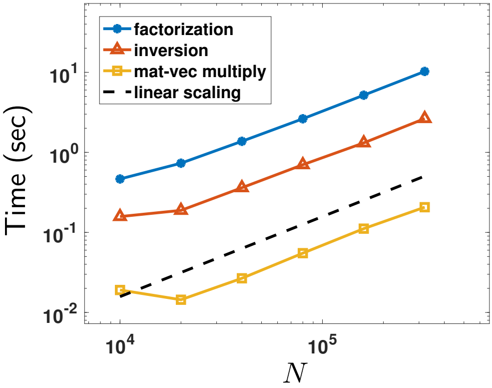
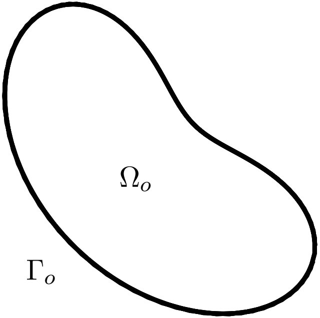


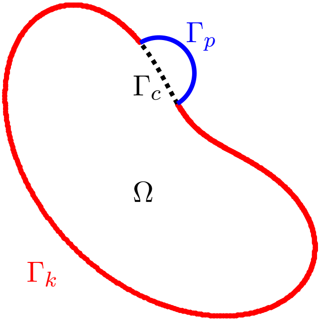
Problem with locally perturbed geometry

Consider a BIE defined on Γ_o.
We can solve this by building a direct solver.



Problem with locally perturbed geometry

Now, suppose we already have a direct solver for $\Gamma_o = \Gamma_k \cup \Gamma_c$.
We want to solve the BIE defined on $\Gamma := \Gamma_k \cup \Gamma_p$



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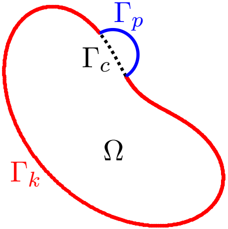

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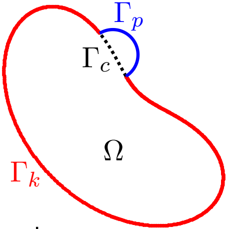

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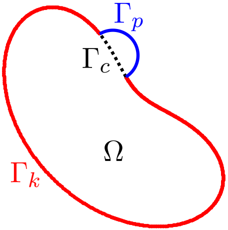
The discretized integral equation on Γ can be expressed as

$$\left(\underbrace{\begin{bmatrix} \boldsymbol{A}_{oo} & 0 \\ 0 & \boldsymbol{A}_{pp} \end{bmatrix}}_{\boldsymbol{A}} + \underbrace{\begin{bmatrix} 0 & \begin{pmatrix} -\boldsymbol{A}_{kc} \\ -\boldsymbol{B}_{cc} \end{pmatrix} & \boldsymbol{A}_{op} \\ \boldsymbol{A}_{pk} & 0 & 0 \end{bmatrix}}_{\boldsymbol{M}} \right) \begin{pmatrix} \boldsymbol{\sigma}_k \\ \boldsymbol{\sigma}_c \\ \boldsymbol{\sigma}_p \end{pmatrix} = \begin{pmatrix} \boldsymbol{f}_k \\ 0 \\ \boldsymbol{f}_p \end{pmatrix}$$

where $\boldsymbol{B}_{cc}$ equals to $\boldsymbol{A}_{cc}$ with diagonal entries set to zero, $\boldsymbol{A}_{oo}$ denotes the interaction matrix on Γ_o, $\boldsymbol{A}_{kc}$ denotes the interaction between Γ_k and Γ_c, and the rest follows the same notation.

L. Greengard, D. Gueyffier, P.G. Martinsson, V. Rokhlin, *Fast direct solvers for integral equations in complex three-dimensional domains*

A closer look at the update matrix $\boldsymbol{M}$



$\boldsymbol{M}$ has three low-rank sub-blocks:

$\boldsymbol{A}_{pk} \approx \boldsymbol{L}_{pk}\boldsymbol{R}_{pk}, \quad \boldsymbol{A}_{kc} \approx \boldsymbol{L}_{kc}\boldsymbol{R}_{kc},$

and $\boldsymbol{A}_{op} \approx \boldsymbol{L}_{op}\boldsymbol{R}_{op}$.

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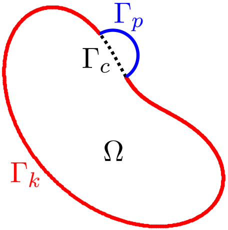

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and $\boldsymbol{A}_{op} \approx \boldsymbol{L}_{op}\boldsymbol{R}_{op}$.

Combining the three factorizations, we obtain a low-rank factorization of the update matrix:

$$\boldsymbol{M} \approx \underbrace{\begin{bmatrix} 0 & \begin{pmatrix} -\boldsymbol{L}_{kc} & 0 \\ 0 & -\boldsymbol{B}_{cc} \end{pmatrix} & \boldsymbol{L}_{op} \\ \boldsymbol{L}_{pk} & 0 & 0 \end{bmatrix}}_{\boldsymbol{L}} \underbrace{\begin{bmatrix} \boldsymbol{R}_{pk} & 0 & 0 \\ 0 & \begin{pmatrix} \boldsymbol{R}_{kc} \\ \boldsymbol{I} \end{pmatrix} & 0 \\ 0 & 0 & \boldsymbol{R}_{op} \end{bmatrix}}_{\boldsymbol{R}}$$

Why building a low-rank factorization of $\boldsymbol{M}$?

The inverse of $(\boldsymbol{A}+\boldsymbol{M})$ can be approximated as

$$\underbrace{(\boldsymbol{A}+\boldsymbol{L}\boldsymbol{R})^{-1}}_{N\times N} \quad = \quad \boldsymbol{A}^{-1} \quad + \quad \boldsymbol{A}^{-1}\boldsymbol{L} \quad \underbrace{(\boldsymbol{I}+\boldsymbol{R}\boldsymbol{A}^{-1}\boldsymbol{L})^{-1}}_{K\times K} \quad \boldsymbol{R}\boldsymbol{A}^{-1}$$

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The solution to the extended system can be approximated as

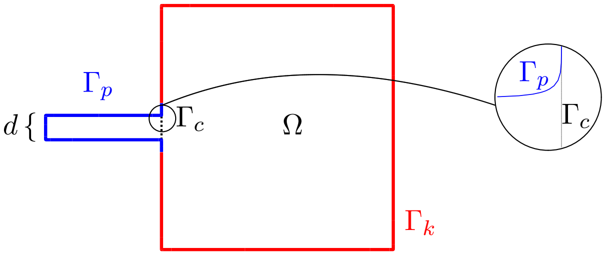
$$(\boldsymbol{A}+\boldsymbol{M})^{-1}\boldsymbol{f} \approx \boldsymbol{A}^{-1}\boldsymbol{f} + \boldsymbol{A}^{-1}\boldsymbol{L}(\boldsymbol{I}+\boldsymbol{R}\boldsymbol{A}^{-1}\boldsymbol{L})^{-1}\boldsymbol{R}\boldsymbol{A}^{-1}\boldsymbol{f}.$$

The existing direct solver for the BIE on Γ_o can be reused to calculate the repeated terms

$$\boldsymbol{A}^{-1}\boldsymbol{f} = \begin{bmatrix} \boldsymbol{A}_{oo}^{-1} & 0 \\ 0 & \boldsymbol{A}_{pp}^{-1} \end{bmatrix} \begin{pmatrix} \boldsymbol{f}_k \\ 0 \\ \boldsymbol{f}_p \end{pmatrix} \text{ and } \boldsymbol{A}^{-1}\boldsymbol{L} = \begin{bmatrix} \boldsymbol{A}_{oo}^{-1} & 0 \\ 0 & \boldsymbol{A}_{pp}^{-1} \end{bmatrix} \boldsymbol{L}.$$

Numerical tests

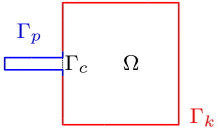
Consider the Laplace BVP defined on the "square with thinning nose geometry":

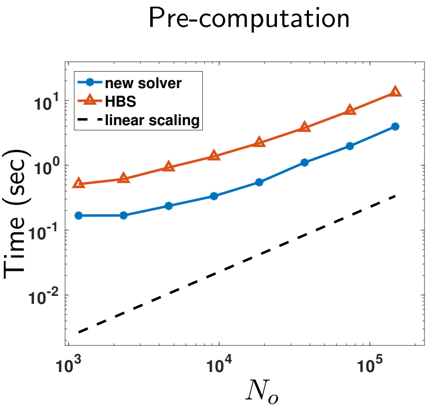


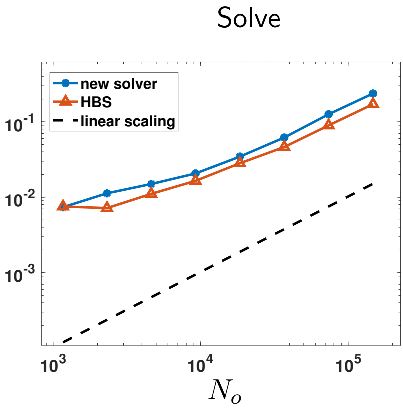
- d decreases as N_o increases so that $N_c = 16$ remains a constant.

Corners are smoothed by the method in C. Eptein and M. O'Neil, *Smoothed corners and scattered waves*.

Laplace on a square with thinning nose







($N_c = 16$, and $N_p \in [700, 900]$.)

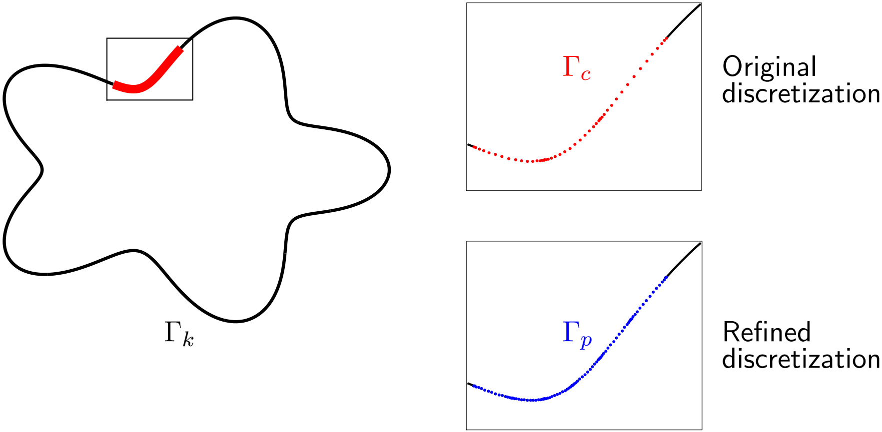
Laplace on a square with thinning nose

N_o	$T_{new,p}$	$T_{hbs,p}$	$\frac{T_{new,p}}{T_{hbs,p}}$	$T_{new,s}$	$T_{hbs,s}$	$\frac{T_{new,s}}{T_{hbs,s}}$
4624	0.24	0.92	0.26	1.5e-02	1.1e-02	1.4
9232	0.33	1.37	0.24	2.0e-02	1.6e-02	1.3
18448	0.55	2.20	0.25	3.5e-02	2.8e-02	1.2
36880	1.10	3.76	0.29	6.2e-02	4.6e-02	1.3
73744	1.98	6.88	0.29	0.13	9.0e-02	1.4
147472	4.00	13.2	0.30	0.24	0.17	1.4

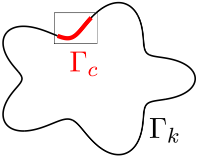
- With $\epsilon = 1 \times 10^{-10}$, the relative error is around 1×10^{-9}.
- New solver scales linearly w.r.t. N_o.
- In terms of total cost, it would take 100 to 260 solves to make the new solver slower than building a new HBS solver from scratch.

Numerical tests

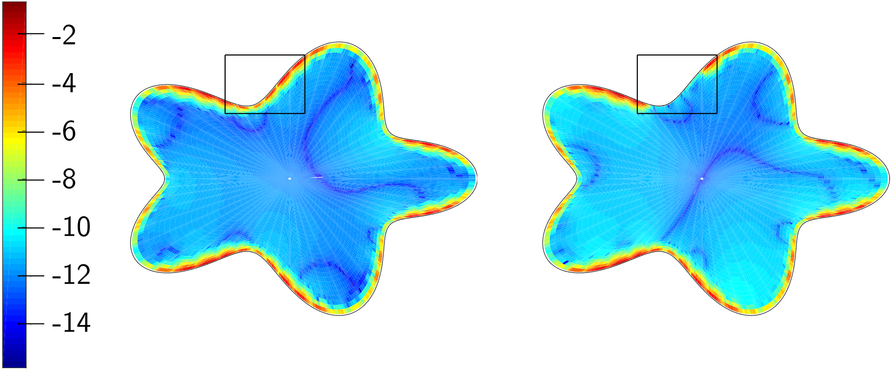
Consider the Laplace BVP defined on the smooth star with the boxed segment locally refined:



Star with locally refined discretization

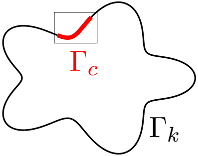


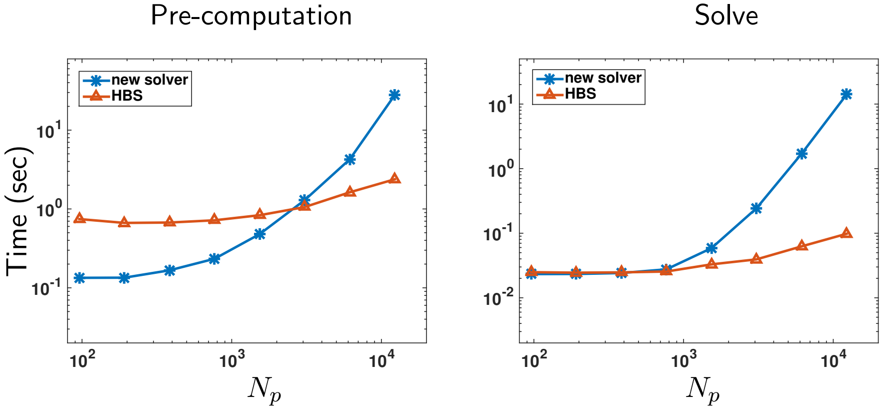
Relative error on a log10 scale:



Original discretization Refined discretization

Star with locally refined discretization





$(N_k = 592, N_c = 48$ remain constant.)

Star with locally refined discretization

N_p	$T_{new,p}$	$T_{hbs,p}$	$\frac{T_{new,p}}{T_{hbs,p}}$	$T_{new,s}$	$T_{hbs,s}$	$\frac{T_{new,s}}{T_{hbs,s}}$
96	4.2e-02	0.20	0.21	4.3e-03	5.7e-03	0.75
192	4.9e-02	0.191	0.25	3.5e-03	3.5e-03	1.00
384	7.0e-02	0.20	0.34	4.5e-03	4.1e-03	1.11
768	0.13	0.24	0.55	8.3e-03	5.4e-03	1.54
1536	0.34	0.32	1.07	3.5e-02	9.8e-03	3.60

- The new solver can be incorporated into an adaptive discretization technique for BIEs if the local refinement only adds a reasonable number of new points.
- For N_p large, the new solver is much more expensive than HBS. Cost is dominated by $\boldsymbol{A}_{pp}^{-1}$.

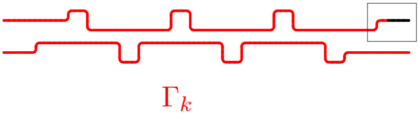
Application in modeling objects in Stokes flow

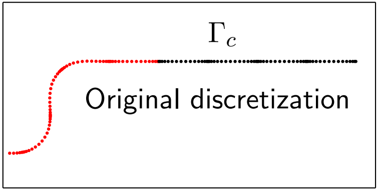
(click for video)

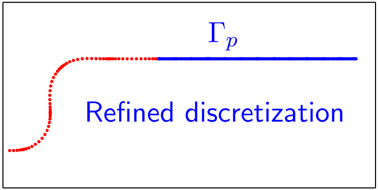
Example is from G. Marple, A. Barnett, A. Gillman, and S. Veerapaneni, *A fast algorithm for simulating multiphase flows through periodic geometries of arbitrary shape.*

Stokes on locally refined periodic pipes

Consider the periodic Stokes problem defined on the following pipe geometry. (The boundary wall consists infinite copies of the shown piece.)







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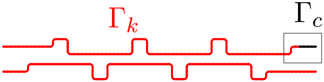

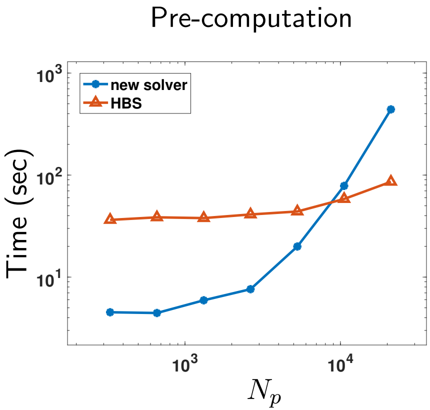

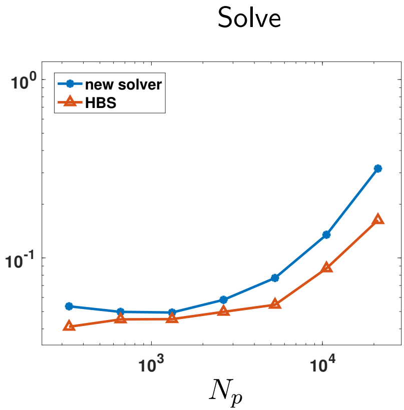

($N_k = 6290$ and $Nc = 110$ remain constant.)

Stokes on locally refined periodic pipes

N_p	$T_{new,p}$	$T_{hbs,p}$	$\frac{T_{new,p}}{T_{hbs,p}}$	$T_{new,s}$	$T_{hbs,s}$	$\frac{T_{new,s}}{T_{hbs,s}}$
330	4.5e+00	3.6e+01	0.12	5.4e-02	4.1e-02	1.3
660	4.4e+00	3.9e+01	0.12	5.0e-02	4.5e-02	1.1
1320	5.9e+00	3.8e+01	0.16	4.9e-02	4.5e-02	1.1
2640	7.6e+00	4.1e+01	0.19	5.8e-02	5.0e-02	1.2
5280	2.0e+01	4.4e+01	0.45	7.7e-02	5.5e-02	1.4

- With tolerance for (matrix) low-rank approximation $\epsilon = 1 \times 10^{-12}$, the relative error is about 3×10^{-8}.

Conclusion

Summary

- A brief introduction to fast direct solvers for BIEs and particularly the Hierarchically block-sparable (HBS) solver.
  - Linear scaling 2D
  - Great for problems with multipole right-hand-sides
- A new fast direct solver for problems defined on locally-perturbed geometries
  - Reuses the inverse approximation previously constructed for the original geometry
  - Outperforms HBS from scratch when the size of changes is small.
  - Very efficient in handling local refinement in discretization

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Future directions

- Continue on building an adaptive discretization technique for Stokes and a fast direct solver that works with it.
- 3D problems.