A QBX-based Direct Solver

CS598APK: Fast Algorithms and Integral Equations

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Equations

- **Laplace** equation with **Dirichlet** boundary conditions:

$$\begin{cases} \Delta u = 0, & \mathbf{x} \in \Omega \subset \mathbb{R}^2, \\ u(\mathbf{x}) = g(\mathbf{x}), & \mathbf{x} \in \Gamma \equiv \partial\Omega. \end{cases}$$

- Single and/or **double layer** representation:

$$u(\mathbf{x}) = \mathcal{S}\sigma(\mathbf{x}) = \int_\Gamma G(\mathbf{x}, \mathbf{y})\sigma(\mathbf{y})\,\mathrm{d}\mathbf{y},$$

$$u(\mathbf{x}) = \mathcal{D}\sigma(\mathbf{x}) = \int_\Gamma \frac{\partial}{\partial \mathbf{n}} G(\mathbf{x}, \mathbf{y})\sigma(\mathbf{y})\,\mathrm{d}\mathbf{y},$$

- **Integral equation**:

$$\frac{1}{2}\sigma \pm \int_\Gamma \frac{\partial}{\partial \mathbf{n}} G(\mathbf{x}, \mathbf{y})\sigma(\mathbf{y})\,\mathrm{d}\mathbf{y} = g(\mathbf{x})$$

Quadrature by Expansion

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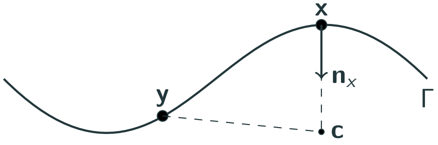


- **Potential** at $\mathbf{x} \in \Gamma$:

$$\phi(\mathbf{x}) = \int_\Gamma K(\mathbf{x}, \mathbf{y})\sigma(\mathbf{y})\,\mathrm{d}\mathbf{y}.$$

- Off-surface **local** expansion:

$$\phi(\mathbf{x}) \approx \sum_{|\mathbf{p}|\le p} \int_\Gamma \frac{(\mathbf{x}-\mathbf{c})^{\mathbf{p}}}{\mathbf{p}!} \left.\frac{\partial^{\mathbf{p}}}{\partial \mathbf{x}^{\mathbf{p}}} K(\mathbf{x}, \mathbf{y})\right|_{\mathbf{x}=\mathbf{c}} \sigma(\mathbf{y})\,\mathrm{d}\mathbf{y}.$$

Quadrature by Expansion: Interpretation

- **Regularized** kernel:

$$\phi(\mathbf{x}) \approx \int_\Gamma \tilde{K}_\pm(\mathbf{x}, \mathbf{y}) \sigma(\mathbf{y}) \, \mathrm{d}\mathbf{y},$$

  where:

$$\tilde{K}_\pm(\mathbf{x}, \mathbf{y}) = \sum_{|\mathbf{p}| < p} \frac{(\mathbf{x} - \mathbf{c})^\mathbf{p}}{\mathbf{p}!} \left. \frac{\partial^\mathbf{p}}{\partial \mathbf{x}^\mathbf{p}} K(\mathbf{x}, \mathbf{y}) \right|_{\mathbf{x} = \mathbf{c}}$$

- Local **expansion**:

$$\phi(\mathbf{x}) \approx \sum_{|\mathbf{p}| < p} Q_\mathbf{p} (\mathbf{x} - \mathbf{c})^\mathbf{p},$$

  where:

$$Q_\mathbf{p} = \int_\Gamma \frac{\sigma(\mathbf{y})}{\mathbf{p}!} \left. \frac{\partial^\mathbf{p}}{\partial \mathbf{x}^\mathbf{p}} K(\mathbf{x}, \mathbf{y}) \right|_{\mathbf{x} = \mathbf{c}} \, \mathrm{d}\mathbf{y}.$$

Quadrature by Expansion: Discrete

- Discretize $\Gamma = \cup\Gamma_m$ into M **panels** of arclength h_m.
- On each panel put q **Gauss-Legendre quadrature** nodes $\mathbf{y}_{m,k}$ and weights $\omega_{m,k}$.

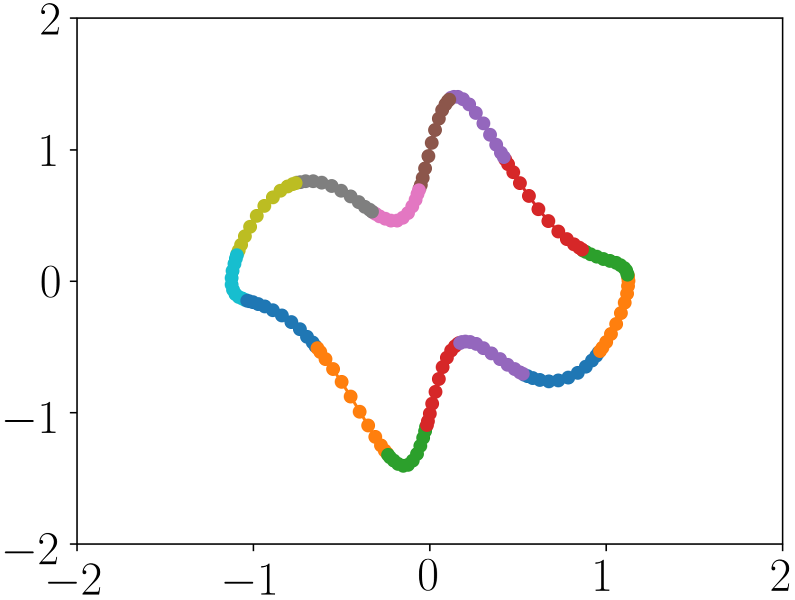
$$\begin{aligned}\phi(\mathbf{x}_i) &= \sum_{m=1}^{M}\sum_{k=1}^{q} \tilde{K}_{\pm}(\mathbf{x}_i, \mathbf{y}_{m,k})\sigma(\mathbf{y}_{m,k})\omega_{m,k} \\ &= \sum_{j=1}^{N} \tilde{K}_{\pm}(\mathbf{x}_i, \mathbf{y}_j)\sigma_j\omega_j\end{aligned}$$

- **Accuracy**?

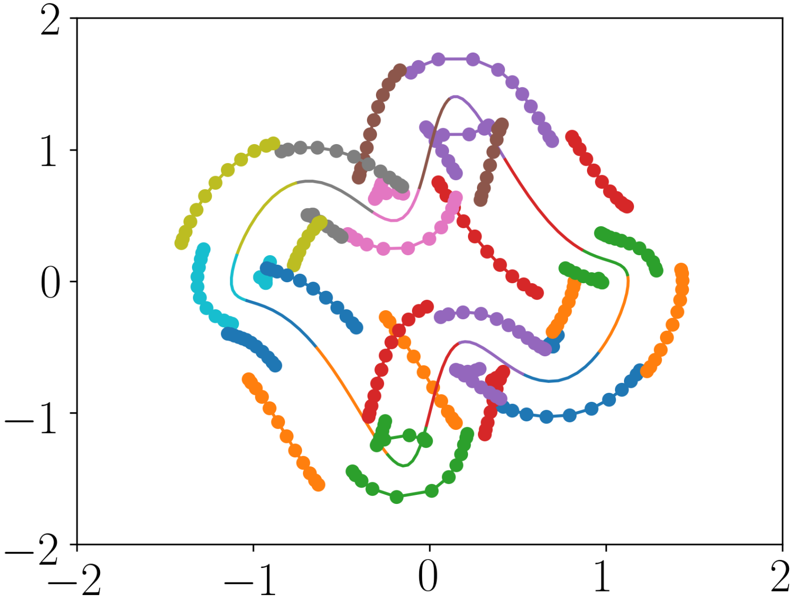
$$\epsilon \approx C_1 r^{p+1} + C_2\left(\frac{h}{4r}\right)^{2q}.$$

[1] M. Rachh, A. Klöckner, M. O'Neil, *Quadrature by Expansion: A New Method for the Evaluation of Layer Potentials*, JCP, 2013.

Quadrature by Expansion: Uniform Panels



Quadrature by Expansion: Uniform Panels



Quadrature by Expansion: Adapting Geometry

Condition I No intersections:

$$\mathrm{d}(\mathbf{c}_{m,k}, \Gamma_{m'}) \geq \frac{h_m}{2}.$$

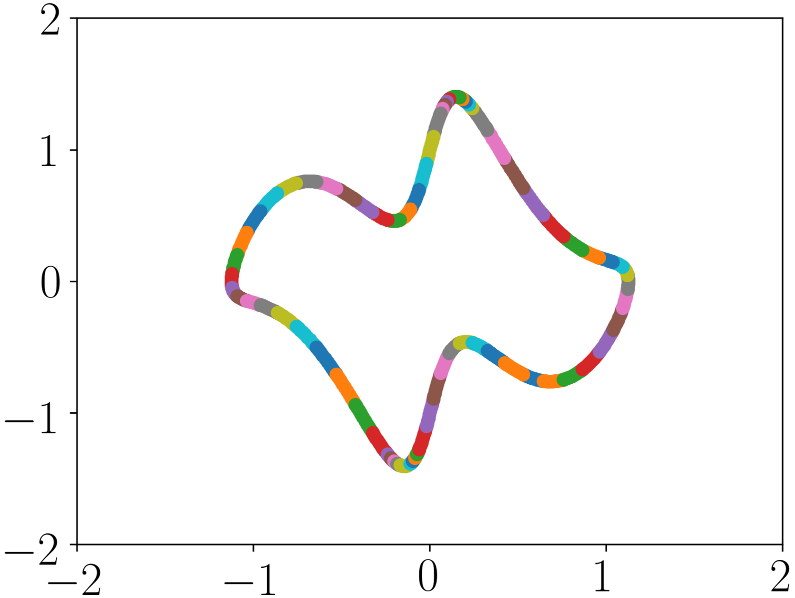
Condition II Sufficient resolution:

$$\mathrm{d}(\mathbf{c}_{m,k}, \Gamma_{m'}) \geq \frac{h_{m'}}{2}.$$

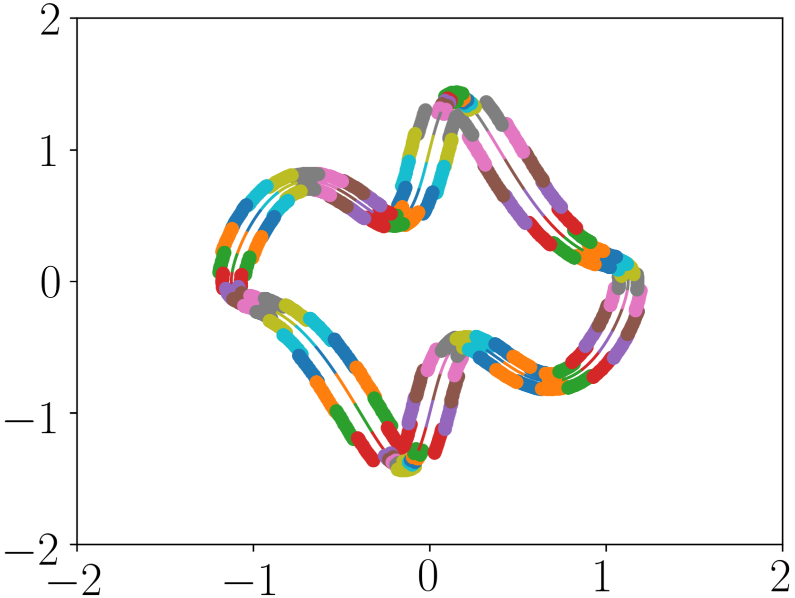
Condition III Neighbor balance:

$$\frac{h_{m'}}{h_m} \in [0.5, 2].$$

Quadrature by Expansion: Adapted Geometry



Quadrature by Expansion: Adapted Geometry



Quadrature by Expansion: Double Layer

- QBX gives us interior / exterior limits for $\mathbf{x} \in \Gamma$:

$$\lim_{r \to 0^+} \mathcal{D}\sigma(\mathbf{x} \pm r\mathbf{n}) = \frac{1}{2}\sigma(\mathbf{x}) \pm \mathcal{D}\sigma(\mathbf{x})$$

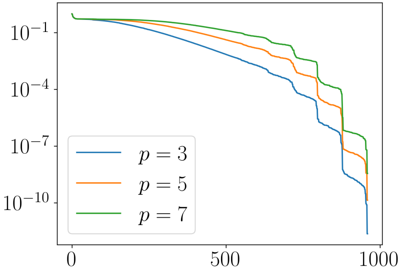
- For an **interior problem**, we can set:

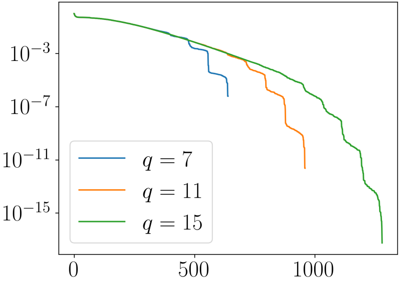
$$a_{ij} = \tilde{K}_{-}(\mathbf{x}_i, \mathbf{y}_j)\omega_j.$$

- Or the **average**:

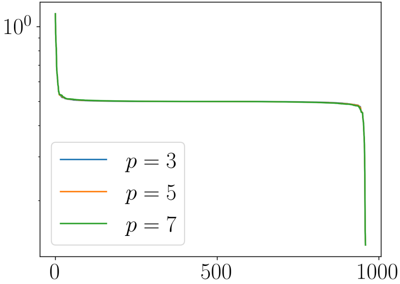
$$a_{ij} = \frac{1}{2}\delta_{ij} - \frac{1}{2}\left(\tilde{K}_{-}(\mathbf{x}_i, \mathbf{y}_j) + \tilde{K}_{+}(\mathbf{x}_i, \mathbf{y}_j)\right)\omega_j.$$

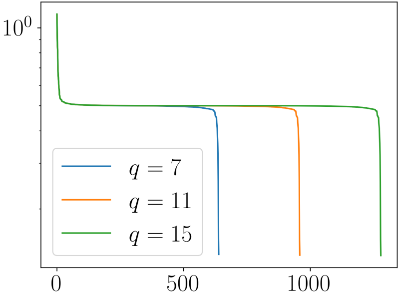
Quadrature by Expansion: Interior Eigenvalues





Quadrature by Expansion: Average Eigenvalues



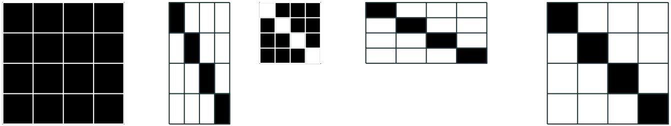


Direct Solver

Direct Solver: Single Level Decomposition

- Given a system $A\mathbf{x} = \mathbf{b}$.
- A is **block-separable**, i.e. low-rank off-diagonal.
- Construct **decomposition**.

$$A = L \quad S \quad R + D$$



Direct Solver: Single Level Solve

- Equivalent system:

$$\begin{bmatrix} D & LS \\ -R & I \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ \mathbf{0} \end{bmatrix}.$$

multiply first row by RD^{-1} and add to second row:

$$\begin{bmatrix} R & RD^{-1}LS \\ 0 & I + RD^{-1}LS \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} = \begin{bmatrix} RD^{-1}\mathbf{b} \\ RD^{-1}\mathbf{b} \end{bmatrix}.$$

- Solve **compressed system** with $\Lambda = (RD^{-1}L)^{-1}$:

$$(\Lambda + S)\mathbf{y} = \Lambda RD^{-1}\mathbf{b}.$$

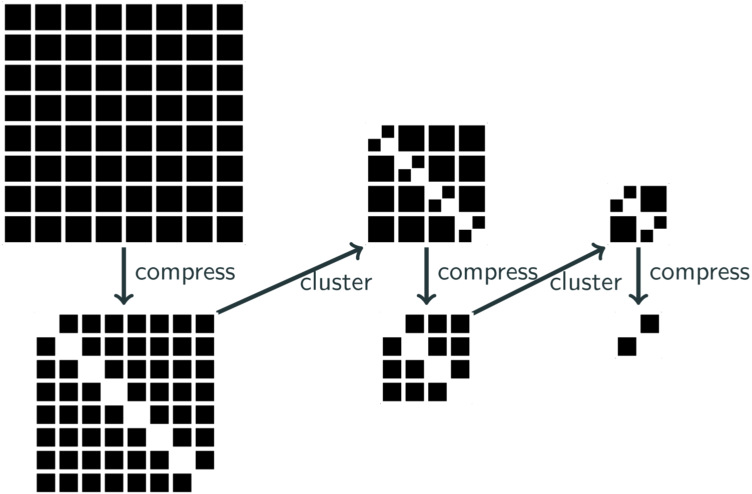
- **Back substitute**:

$$\mathbf{x} = D^{-1}\mathbf{b} - D^{-1}L\Lambda RD^{-1}\mathbf{b} + D^{-1}L\Lambda\mathbf{y}.$$

Direct Solver: Multilevel Decomposition

- Start with decomposing the reduced S and repeat.

$$A = L^{(1)} \left[L^{(2)} \left(\cdots L^{(l)} S R^{(l)} + D^{(l)} \cdots \right) R^{(2)} + D^{(2)} \right] R^{(1)} + D^{(1)}$$



Direct Solver: Multilevel Solve

Algorithm 1: Recursive direct solver.

Data: Right-hand side $\mathbf{b}^{(l)}$ at level l.

Compute $\mathbf{b}^{(l+1)} = \Lambda^{(l)} R^{(l)} (D^{(l)})^{-1} b^{(l)}$;

if root level then

  Directly solve $(\Lambda^{(l+1)} + S)\mathbf{y}^{(l+1)} = \mathbf{b}^{(l+1)}$;

else

  Solve on next level with $\mathbf{b}^{(l+1)}$ to obtain $\mathbf{y}^{(l+1)}$;

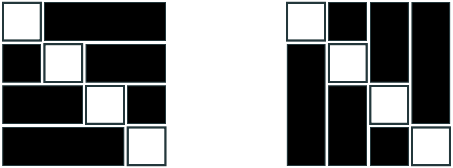
end

Back substitute and return $\mathbf{x}^{(l)}$:

$$\mathbf{x}^{(l)} = (D^{(l)})^{-1}\mathbf{b} - (D^{(l)})^{-1} L^{(l)} (\mathbf{b}^{(l+1)} - \Lambda^{(l)} \mathbf{y}^{(l+1)}).$$

Direct Solver: Interpolative Decomposition

- ID full off-diagonal blocks:



- Step by step:

Direct Solver: Skeletonization

- Add a set of **proxy** source / target points:

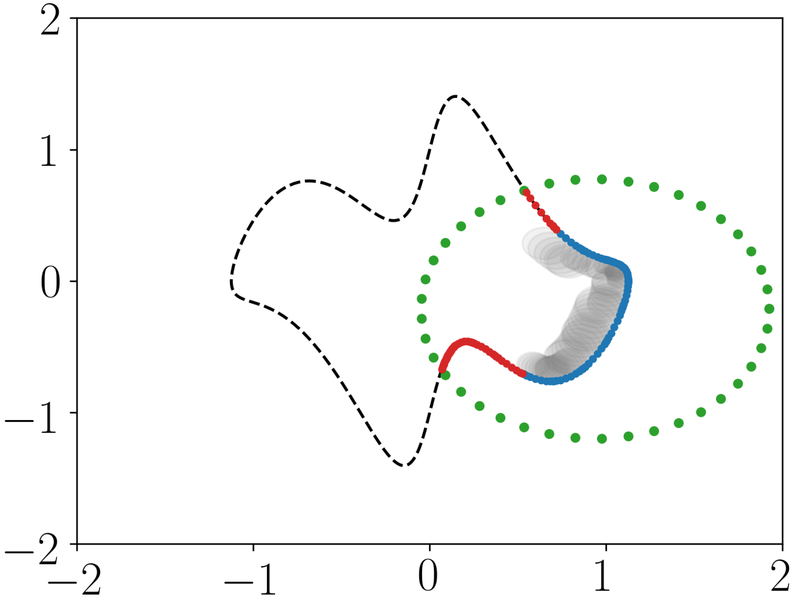
$$\mathbf{x} = \begin{pmatrix} r\cos\theta \\ r\sin\theta \end{pmatrix}.$$

- What's a **safe distance**?
- Shouldn't intersect any **expansion centers**.

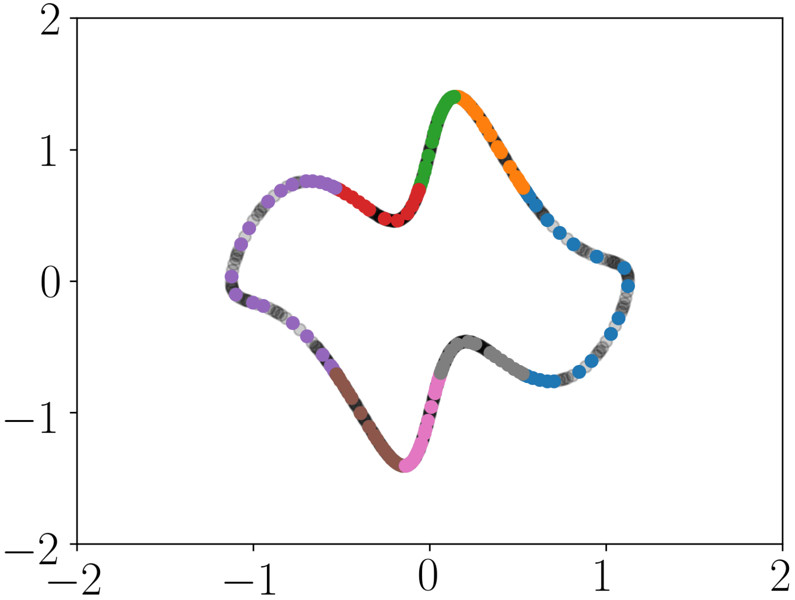
$$r = (1 + \epsilon) \max_i (\|\mathbf{m}_b - \mathbf{c}_i\| + r_i),$$

where $\mathbf{m}_b$ is the center of mass of the block.

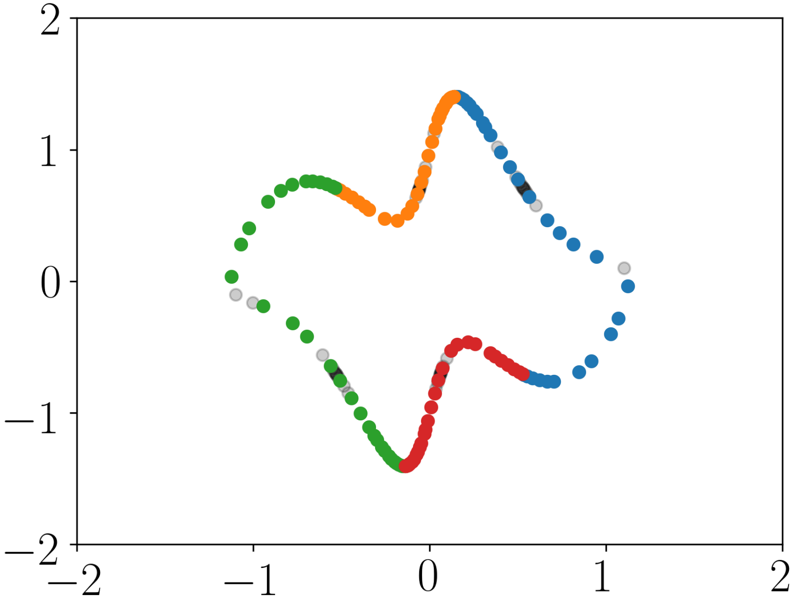
Direct Solver: QBX Skeletons



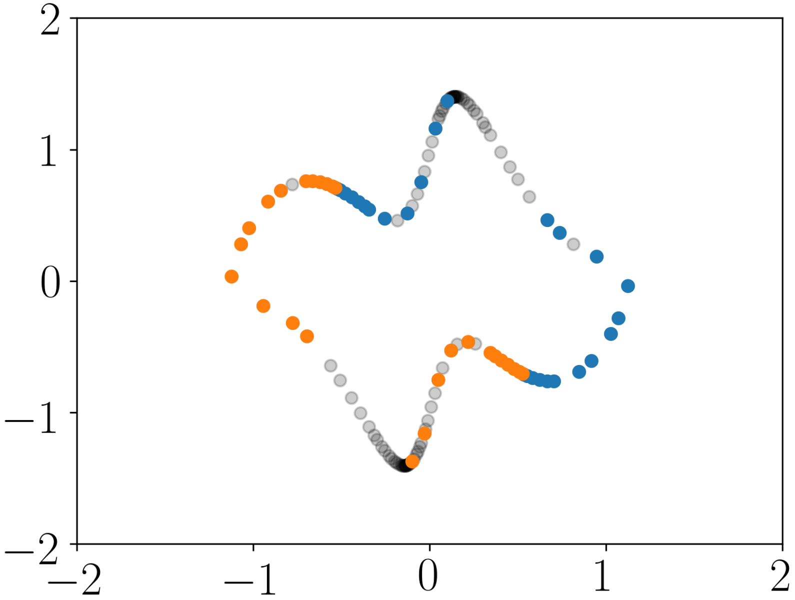
Direct Solver: Level 1 Skeletons



Direct Solver: Level 2 Skeletons



Direct Solver: Level 3 Skeletons



Numerical Results

Test: Randomized Exact Solution

Parameters:

- **Double layer** representation.
- QBX order $\mathbf{p = 3}$.
- Quadrature points $\mathbf{q = 8}$.
- Number of panels **npanels** $\mathbf{= 128}$.
- Number of blocks **nblocks** $\mathbf{= 16}$.
- ID tolerance **epsilon** $\mathbf{= 1.0e\text{-}10}$.
- Number of proxies **nproxies** $\mathbf{= 50}$.
- Proxy radius added **repsilon** $\mathbf{= 0.2}$.

Errors:

- Relative error:

$$\frac{\|\hat{\mathbf{x}} - \mathbf{x}\|_2}{\|\mathbf{x}\|_2}.$$

- Relative residual:

$$\frac{\|A\hat{\mathbf{x}} - \mathbf{b}\|_2}{\|\mathbf{b}\|_2}.$$

Test: Single Level Relative Errors

Full ID

p \ q	4	8	16
3	9.12872e-09	2.76578e-08	5.01436e-09
5	1.39169e-09	4.96305e-09	1.90317e-09
7	2.39623e-10	5.33001e-10	3.38780e-10

Skeleton ID

p \ q	4	8	16
3	2.54206e-08	6.51848e-08	3.66725e-08
5	4.11533e-09	8.23051e-09	4.38584e-09
7	7.07775e-10	5.75930e-10	9.00992e-10

Test: Multilevel Relative Errors

Full ID

blocks \ level	2	3	4
16	2.31175e-09	2.26341e-09	1.80893e-09
32	7.19358e-09	6.56725e-09	6.68821e-09
64	7.96960e-09	8.86560e-09	8.83224e-09

Skeleton ID

blocks \ level	2	3	4
16	5.18507e-09	8.49552e-09	4.44692e-09
32	7.67471e-09	1.01932e-08	1.27750e-08
64	6.31291e-09	8.10852e-09	1.03811e-08

Test: Proxy Points

Relative Error

proxy \ radius	-0.2	0.5	1.2
30	2.17671e-04	5.64100e-08	1.07313e-08
50	1.33253e-04	2.63332e-08	1.36580e-08
70	6.94320e-05	1.98028e-08	1.04501e-08

Relative Residual

proxy \ radius	-0.2	0.5	1.2
30	1.18686e-04	2.96544e-08	5.85785e-09
50	7.37563e-05	1.45011e-08	7.39889e-09
70	3.86785e-05	1.06562e-08	5.78254e-09

Test: Decomposition Scaling

Full ID

level / panel	numpy	1	2	4
128	0.223459	0.087522	0.125639	0.149225
256	1.743877	0.216969	0.257622	0.284817
512	15.761304	0.868573	0.931527	0.985756
1024	134.603205	4.315787	4.293598	4.349963
Order	3.08	1.93	1.77	1.70

Skeleton ID

level / panel	numpy	1	2	4
128	0.223459	0.054367	0.062884	0.091416
256	1.743877	0.067689	0.098431	0.135409
512	15.761304	0.194028	0.238213	0.322106
1024	134.603205	0.805866	0.874878	0.957627
Order	3.08	1.40	1.27	1.18

Test: Solve Scaling

Full ID

panel \ level	numpy	1	2	4
128	0.001124	0.093797	0.031990	0.008003
256	0.003797	0.131069	0.041528	0.012495
512	0.015309	0.188231	0.061076	0.025766
1024	0.056273	0.262167	0.102924	0.064412
Order	1.88	0.49	0.55	1.0

Skeleton ID

panel \ level	numpy	1	2	4
128	0.001124	0.118155	0.039818	0.012252
256	0.003797	0.195297	0.058118	0.020289
512	0.015309	0.310070	0.088699	0.040509
1024	0.056273	0.450505	0.148544	0.093247
Order	1.88	0.65	0.62	0.98

Questions?