ADAPTIVE MESHES AND EMBEDDED BOUNDARY INTEGRAL METHODS

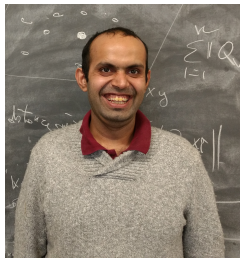
Travis Askham (University of Washington)

March 15, 2018. ICERM workshop on “Fast Algorithms for Static and Dynamically Changing Point Configurations”

EMBEDDED BOUNDARY INTEGRAL METHODS

Collaborators:

Leslie Greengard



Manas Rachh

Ludvig af Klinteberg

Antoine Cerfon

Mary Catherine Kropinski

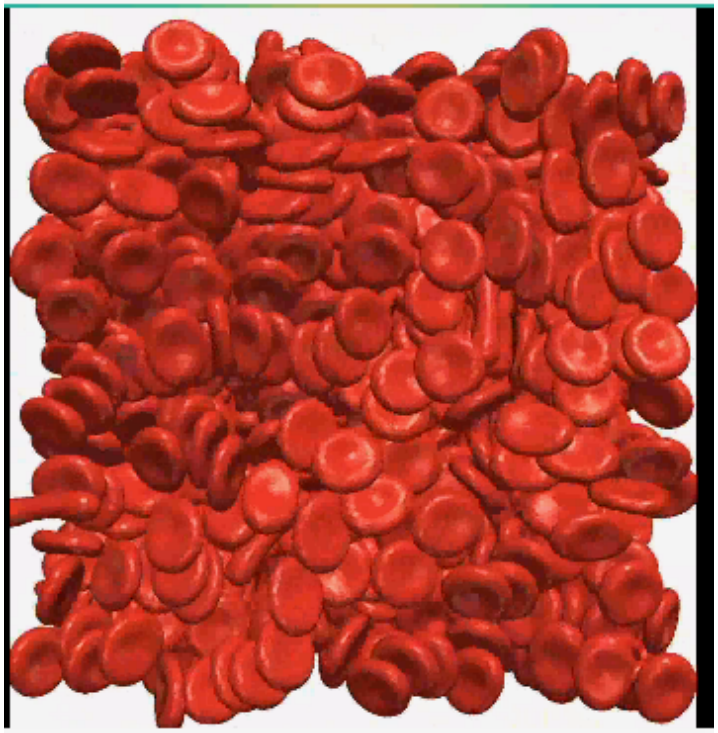
Bryan Quaife

Funding from the Air Force Office of Scientific Research (FA9550-10-1-0180 and FA9550-15-1-0385).

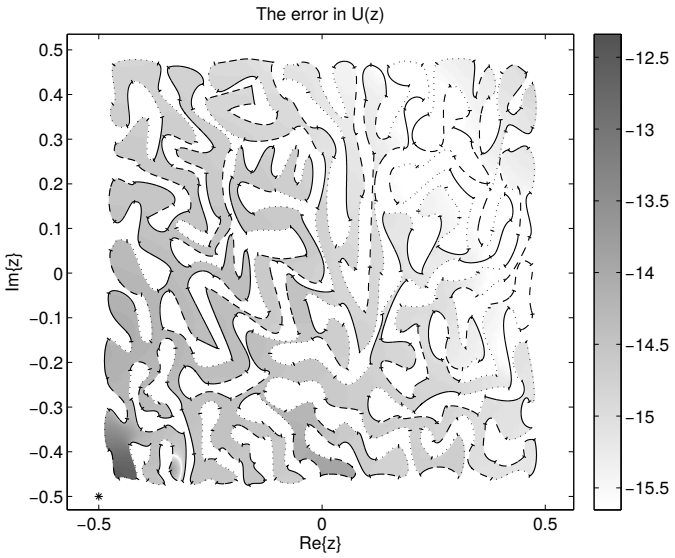
INTEGRAL EQUATION METHODS FOR FLUIDS

Why integral equation methods?

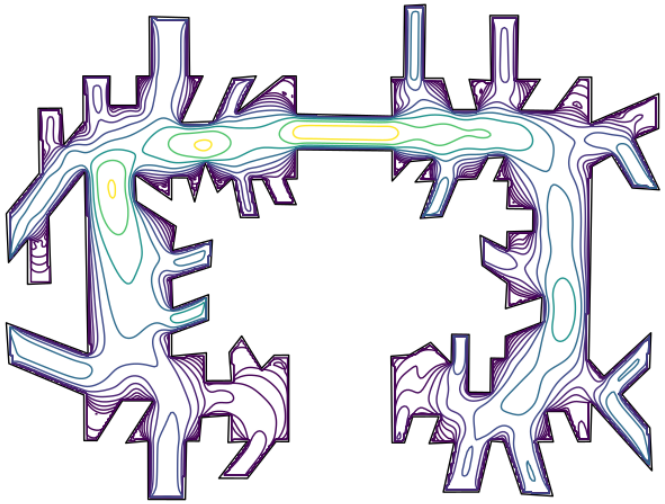
- Geometric flexibility
- Well-conditioned formulations
- Existence of fast algorithms (FMM)



[Malhotra et al., 2017]



[Ojala, 2012]



Hoskins, Rachh, Serkh

NAVIER-STOKES TO MODIFIED STOKES

Navier-Stokes

$$
\begin{aligned}
\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} &= -\nabla p + \frac{1}{\mathrm{Re}} \Delta \mathbf{u}, && \mathbf{x} \in \Omega \\
\nabla \cdot \mathbf{u} &= 0, && \mathbf{x} \in \Omega\ , \\
\mathbf{u} &= \mathbf{f}, && \mathbf{x} \in \partial\Omega.
\end{aligned}
$$

NAVIER-STOKES TO MODIFIED STOKES

Navier-Stokes

$$
\begin{aligned}
\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} &= -\nabla p + \frac{1}{\mathrm{Re}} \Delta \mathbf{u}, && \mathbf{x} \in \Omega \\
\nabla \cdot \mathbf{u} &= 0, && \mathbf{x} \in \Omega\ , \\
\mathbf{u} &= \mathbf{f}, && \mathbf{x} \in \partial\Omega.
\end{aligned}
$$

IMEX (Euler) Discretization

$$
\begin{aligned}
\frac{\mathbf{u}^{N+1} - \mathbf{u}^{N}}{\delta t} - \frac{1}{\mathrm{Re}} \Delta \mathbf{u}^{N+1} + \nabla p^{N+1} &= \mathbf{F}, && \mathbf{x} \in \Omega, \\
\nabla \cdot \mathbf{u}^{N+1} &= 0, && \mathbf{x} \in \Omega, \\
\mathbf{u}^{N+1} &= \mathbf{f}, && \mathbf{x} \in \partial\Omega.
\end{aligned}
$$

NAVIER-STOKES TO MODIFIED STOKES (CONT.)

Let $\mathbf{u}^{N+1} = \mathbf{v} + \mathbf{u}_H$.

Particular Solution (v)

$$\begin{aligned} \mathbf{v} - \frac{\delta t}{\mathrm{Re}} \Delta \mathbf{v} + \delta t \nabla p_V &= \delta t \mathbf{F} + \mathbf{u}^N, & \mathbf{x} \in \Omega\,, \\ \nabla \cdot \mathbf{v} &= 0, & \mathbf{x} \in \Omega\,. \end{aligned}$$

NAVIER-STOKES TO MODIFIED STOKES (CONT.)

Let $\mathbf{u}^{N+1} = \mathbf{v} + \mathbf{u}_H$.

Particular Solution (v)

$$\begin{aligned} \mathbf{v} - \frac{\delta t}{\mathrm{Re}}\Delta\mathbf{v} + \delta t \nabla p_V &= \delta t \mathbf{F} + \mathbf{u}^N, && \mathbf{x} \in \Omega\,, \\ \nabla \cdot \mathbf{v} &= 0, && \mathbf{x} \in \Omega\,. \end{aligned}$$

Boundary Correction ($\mathbf{u}_H$) — Modified Stokes Equation

$$\begin{aligned} \mathbf{u}_H - \frac{\delta t}{\mathrm{Re}}\Delta\mathbf{u}_H + \nabla p_H &= 0, && \mathbf{x} \in \Omega\,, \\ \nabla \cdot \mathbf{u}_H &= 0, && \mathbf{x} \in \Omega\,, \\ \mathbf{u}_H &= \mathbf{f} - \mathbf{v}, && \mathbf{x} \in \partial\Omega\,. \end{aligned}$$

THE MODIFIED STOKESLET

Let $\lambda = \sqrt{\mathrm{Re}/\delta t}$. The fundamental solution of the modified Stokes equations is the

Modified Stokeslet

$$\mathbf{G}(\mathbf{x}, \mathbf{y}) = (-\nabla^{\perp} \otimes \nabla^{\perp})\mathcal{G}(\mathbf{x}, \mathbf{y}),$$

where

Modified Biharmonic Green's Function

$$\mathcal{G}(\mathbf{x}, \mathbf{y}) = -\frac{1}{2\pi\lambda^2}\left(\log\|\mathbf{x}-\mathbf{y}\| + K_0(\lambda\|\mathbf{x}-\mathbf{y}\|)\right) .$$

THE MODIFIED STOKESLET

Let $\lambda = \sqrt{\mathrm{Re}/\delta t}$. The fundamental solution of the modified Stokes equations is the

Modified Stokeslet

$$\mathbf{G}(\mathbf{x}, \mathbf{y}) = (-\nabla^{\perp} \otimes \nabla^{\perp})\mathcal{G}(\mathbf{x}, \mathbf{y}),$$

where

Modified Biharmonic Green's Function

$$\mathcal{G}(\mathbf{x}, \mathbf{y}) = -\frac{1}{2\pi\lambda^2}\left(\log\|\mathbf{x}-\mathbf{y}\| + K_0(\lambda\|\mathbf{x}-\mathbf{y}\|)\right) .$$

Particular Solution

$$\mathbf{v}(\mathbf{x}) = \int_{\Omega} \mathbf{G}(\mathbf{x}, \mathbf{y})(\delta t \mathbf{F}(\mathbf{y}) + \mathbf{u}^N(\mathbf{y}))\, dV(\mathbf{y})$$

is a particular solution.

DOUBLE LAYER POTENTIAL

We represent the boundary correction $\mathbf{u}_H$ as a

Double Layer Potential

$$\mathbf{u}_H(\mathbf{x}) = \int_{\partial\Omega} \mathbf{D}(\mathbf{x},\mathbf{y})\boldsymbol{\sigma}(\mathbf{y})\, ds(\mathbf{y}) \ ,$$

where

$$\mathbf{D}(\mathbf{x},\mathbf{y}) = \nabla G_L(\mathbf{x},\mathbf{y}) \otimes \nu + \nabla^\perp \otimes \nabla^\perp (\partial_\nu \mathcal{G}(\mathbf{x},\mathbf{y})) + \nabla^\perp \otimes \nabla (\partial_\tau \mathcal{G}(\mathbf{x},\mathbf{y})) \ .$$

Get a second kind integral equation (SKIE) for $\boldsymbol{\sigma}$. This is a good thing!

EVALUATING THE BOUNDARY CORRECTION

BOUNDARY INTEGRAL EQUATIONS

For good performance, need:

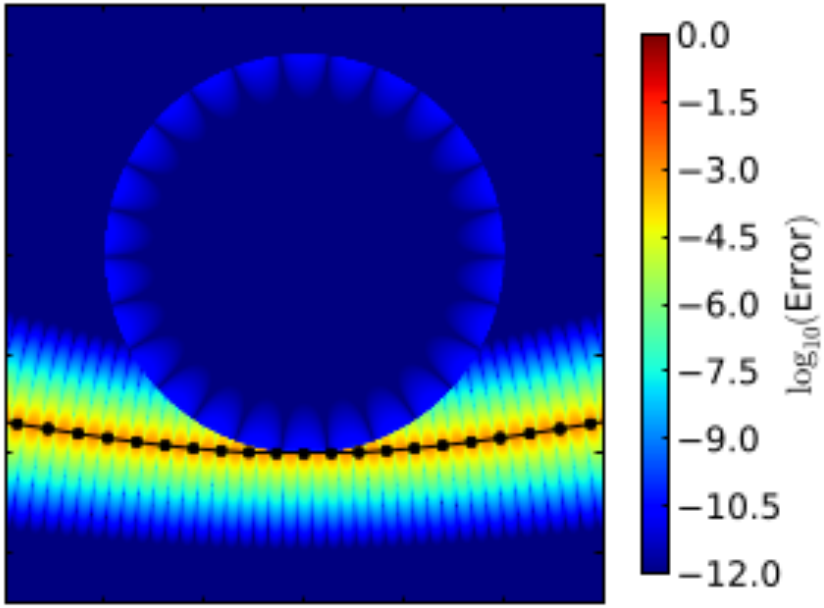


Figure: Visualization of QBX idea. Taken from *Klöckner, et al. 2012*.

BOUNDARY INTEGRAL EQUATIONS

For good performance, need:

- High-order accurate quadrature for singular integrals (e.g. generalized Gaussian quadrature)

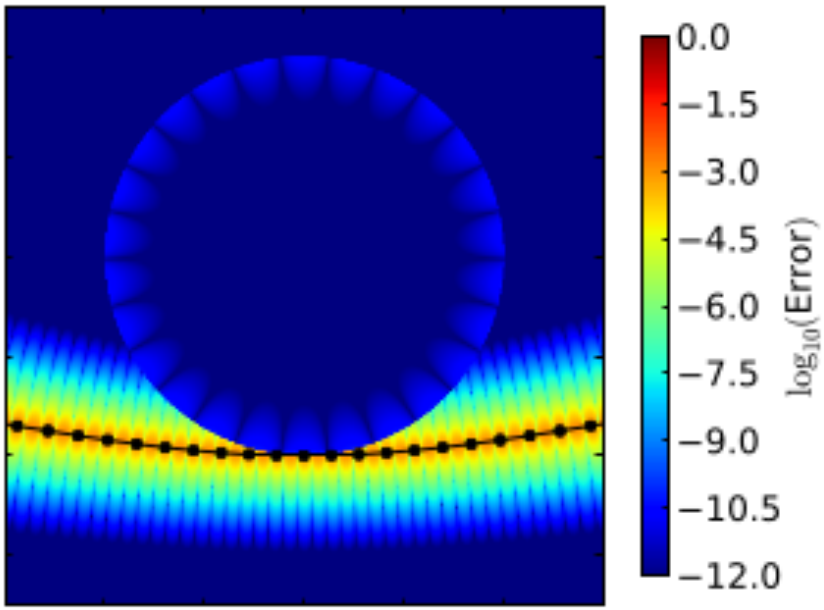


Figure: Visualization of QBX idea. Taken from *Klöckner, et al. 2012*.

BOUNDARY INTEGRAL EQUATIONS

For good performance, need:

- High-order accurate quadrature for singular integrals (e.g. generalized Gaussian quadrature)
- Fast solution methods for structured, dense linear systems (e.g. HSS, HODLR, GMRES)

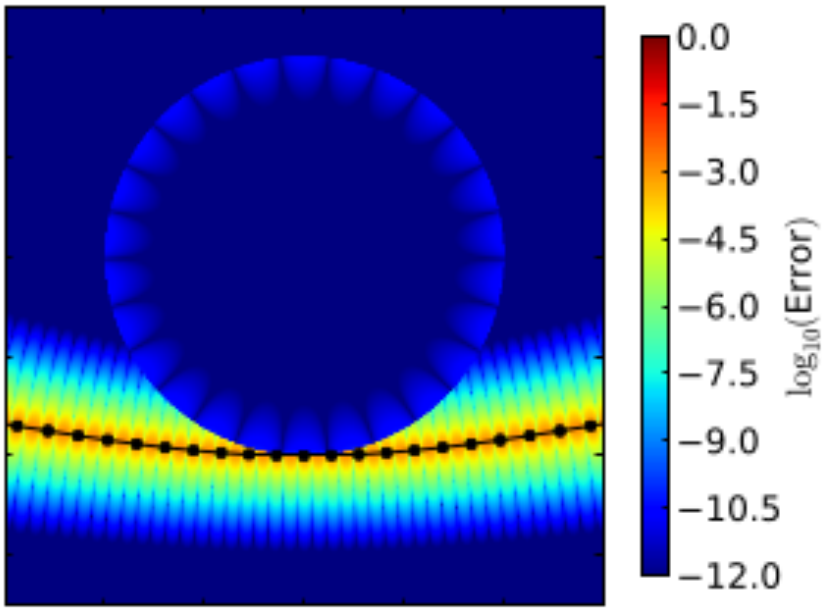


Figure: Visualization of QBX idea. Taken from *Klöckner, et al. 2012*.

BOUNDARY INTEGRAL EQUATIONS

For good performance, need:

- High-order accurate quadrature for singular integrals (e.g. generalized Gaussian quadrature)
- Fast solution methods for structured, dense linear systems (e.g. HSS, HODLR, GMRES)
- Fast, accurate layer potential evaluation, including near-singular points (e.g. quadrature by expansion)

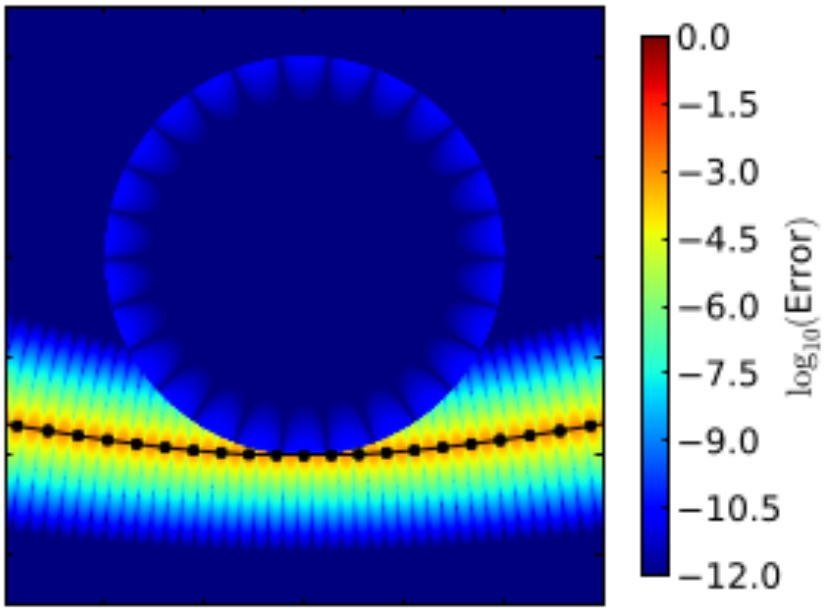


Figure: Visualization of QBX idea. Taken from *Klöckner, et al. 2012*.

FAST, STABLE SUMS

To implement an integral equation method (both fast solvers and fast QBX), we need to be able to compute sums of the form

$$u(\mathbf{x}_i) = \sum_{j=1}^{n} q_j \partial_{v_j w_j} \mathcal{G}(\mathbf{x}_i, \mathbf{s}_j)$$

quickly and stably (and its derivatives)

FAST, STABLE SUMS

To implement an integral equation method (both fast solvers and fast QBX), we need to be able to compute sums of the form

$$u(\mathbf{x}_i) = \sum_{j=1}^{n} q_j \partial_{v_j w_j} \mathcal{G}(\mathbf{x}_i, \mathbf{s}_j)$$

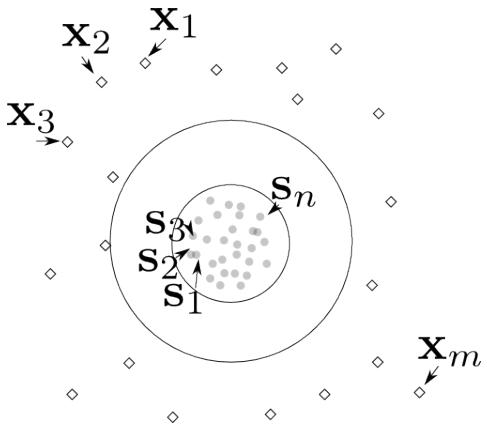
quickly and stably (and its derivatives)

Let

$$A = \begin{pmatrix} \partial_{v_1 w_1} \mathcal{G}(\mathbf{x}_1, \mathbf{s}_1) & \partial_{v_2 w_2} \mathcal{G}(\mathbf{x}_1, \mathbf{s}_2) & \cdots & \partial_{v_n w_n} \mathcal{G}(\mathbf{x}_1, \mathbf{s}_n) \\ \partial_{v_1 w_1} \mathcal{G}(\mathbf{x}_2, \mathbf{s}_1) & \partial_{v_2 w_2} \mathcal{G}(\mathbf{x}_2, \mathbf{s}_2) & \cdots & \partial_{v_n w_n} \mathcal{G}(\mathbf{x}_2, \mathbf{s}_n) \\ \vdots & \vdots & & \vdots \\ \partial_{v_1 w_1} \mathcal{G}(\mathbf{x}_m, \mathbf{s}_1) & \partial_{v_2 w_2} \mathcal{G}(\mathbf{x}_m, \mathbf{s}_2) & \cdots & \partial_{v_n w_n} \mathcal{G}(\mathbf{x}_m, \mathbf{s}_n) \end{pmatrix}$$

LOW-RANK INTERACTIONS

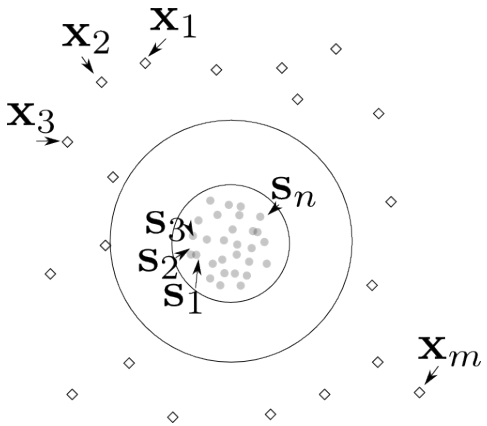
$$A = \begin{pmatrix} \partial_{v_1 w_1} \mathcal{G}(\mathbf{x}_1, \mathbf{s}_1) & \partial_{v_2 w_2} \mathcal{G}(\mathbf{x}_1, \mathbf{s}_2) & \cdots & \partial_{v_n w_n} \mathcal{G}(\mathbf{x}_1, \mathbf{s}_n) \\ \partial_{v_1 w_1} \mathcal{G}(\mathbf{x}_2, \mathbf{s}_1) & \partial_{v_2 w_2} \mathcal{G}(\mathbf{x}_2, \mathbf{s}_2) & \cdots & \partial_{v_n w_n} \mathcal{G}(\mathbf{x}_2, \mathbf{s}_n) \\ \vdots & \vdots & & \vdots \\ \partial_{v_1 w_1} \mathcal{G}(\mathbf{x}_m, \mathbf{s}_1) & \partial_{v_2 w_2} \mathcal{G}(\mathbf{x}_m, \mathbf{s}_2) & \cdots & \partial_{v_n w_n} \mathcal{G}(\mathbf{x}_m, \mathbf{s}_n) \end{pmatrix}$$



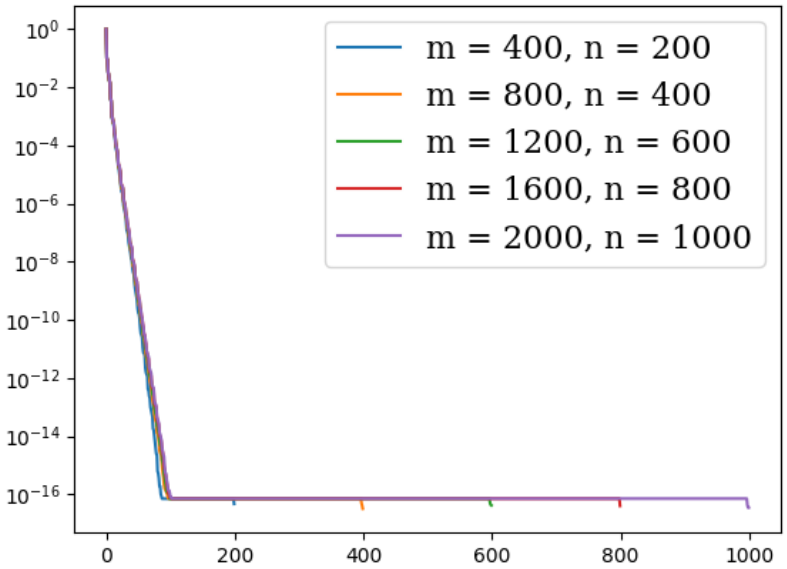
Well-separated points

LOW-RANK INTERACTIONS

$$A = \begin{pmatrix} \partial_{v_1 w_1} \mathcal{G}(\mathbf{x}_1, \mathbf{s}_1) & \partial_{v_2 w_2} \mathcal{G}(\mathbf{x}_1, \mathbf{s}_2) & \cdots & \partial_{v_n w_n} \mathcal{G}(\mathbf{x}_1, \mathbf{s}_n) \\ \partial_{v_1 w_1} \mathcal{G}(\mathbf{x}_2, \mathbf{s}_1) & \partial_{v_2 w_2} \mathcal{G}(\mathbf{x}_2, \mathbf{s}_2) & \cdots & \partial_{v_n w_n} \mathcal{G}(\mathbf{x}_2, \mathbf{s}_n) \\ \vdots & \vdots & & \vdots \\ \partial_{v_1 w_1} \mathcal{G}(\mathbf{x}_m, \mathbf{s}_1) & \partial_{v_2 w_2} \mathcal{G}(\mathbf{x}_m, \mathbf{s}_2) & \cdots & \partial_{v_n w_n} \mathcal{G}(\mathbf{x}_m, \mathbf{s}_n) \end{pmatrix}$$



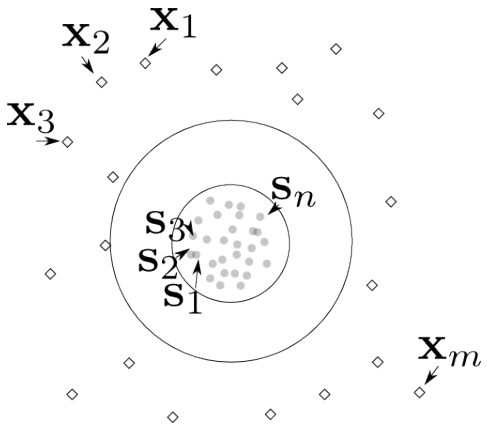
Well-separated points



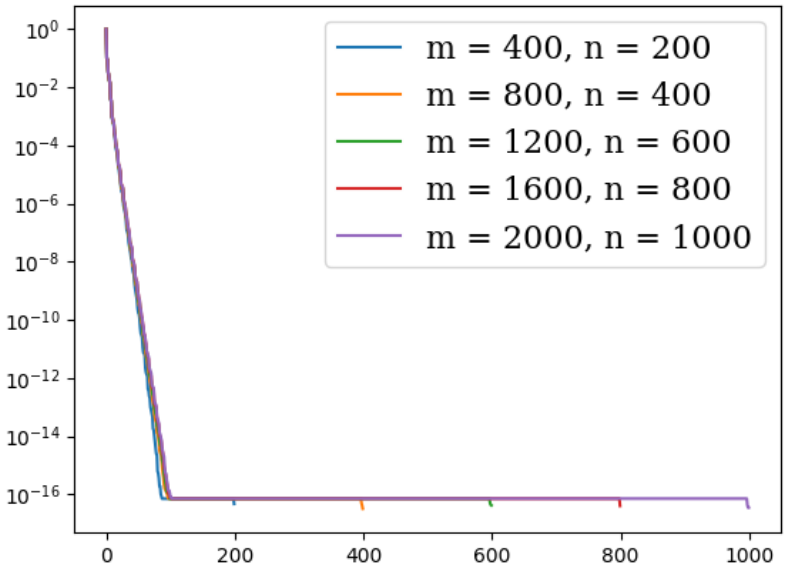
singular values of A for various values of m and n

LOW-RANK INTERACTIONS

$$A = \begin{pmatrix} \partial_{v_1 w_1} \mathcal{G}(\mathbf{x}_1, \mathbf{s}_1) & \partial_{v_2 w_2} \mathcal{G}(\mathbf{x}_1, \mathbf{s}_2) & \cdots & \partial_{v_n w_n} \mathcal{G}(\mathbf{x}_1, \mathbf{s}_n) \\ \partial_{v_1 w_1} \mathcal{G}(\mathbf{x}_2, \mathbf{s}_1) & \partial_{v_2 w_2} \mathcal{G}(\mathbf{x}_2, \mathbf{s}_2) & \cdots & \partial_{v_n w_n} \mathcal{G}(\mathbf{x}_2, \mathbf{s}_n) \\ \vdots & \vdots & & \vdots \\ \partial_{v_1 w_1} \mathcal{G}(\mathbf{x}_m, \mathbf{s}_1) & \partial_{v_2 w_2} \mathcal{G}(\mathbf{x}_m, \mathbf{s}_2) & \cdots & \partial_{v_n w_n} \mathcal{G}(\mathbf{x}_m, \mathbf{s}_n) \end{pmatrix}$$



Well-separated points

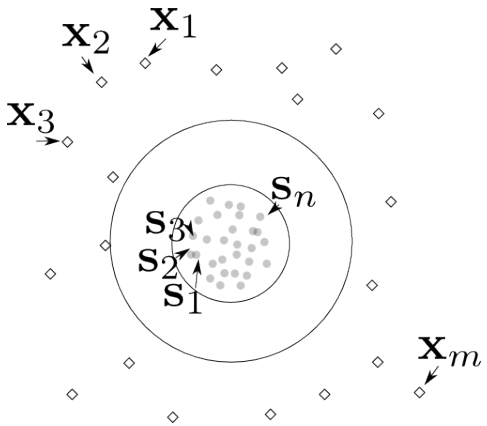


singular values of A for various values of m and n

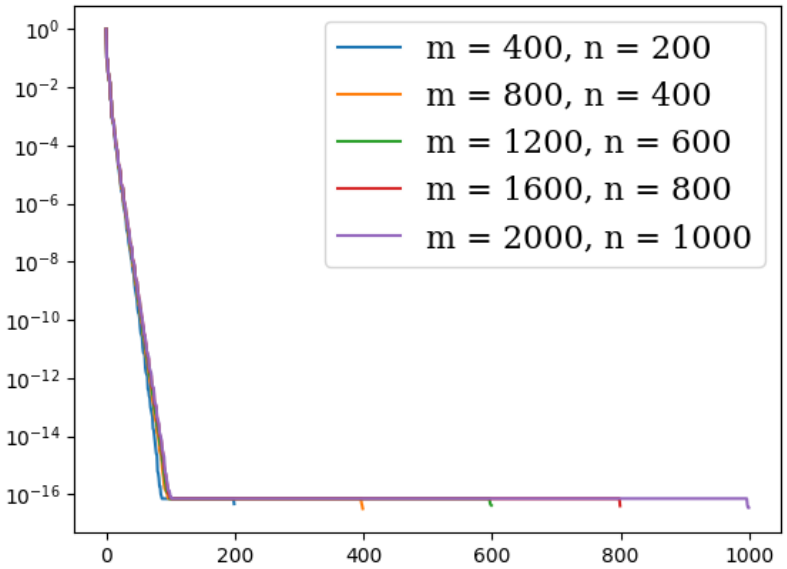
- The rank is low, independent of number of sources and targets

LOW-RANK INTERACTIONS

$$A = \begin{pmatrix} \partial_{v_1 w_1} \mathcal{G}(\mathbf{x}_1, \mathbf{s}_1) & \partial_{v_2 w_2} \mathcal{G}(\mathbf{x}_1, \mathbf{s}_2) & \cdots & \partial_{v_n w_n} \mathcal{G}(\mathbf{x}_1, \mathbf{s}_n) \\ \partial_{v_1 w_1} \mathcal{G}(\mathbf{x}_2, \mathbf{s}_1) & \partial_{v_2 w_2} \mathcal{G}(\mathbf{x}_2, \mathbf{s}_2) & \cdots & \partial_{v_n w_n} \mathcal{G}(\mathbf{x}_2, \mathbf{s}_n) \\ \vdots & \vdots & & \vdots \\ \partial_{v_1 w_1} \mathcal{G}(\mathbf{x}_m, \mathbf{s}_1) & \partial_{v_2 w_2} \mathcal{G}(\mathbf{x}_m, \mathbf{s}_2) & \cdots & \partial_{v_n w_n} \mathcal{G}(\mathbf{x}_m, \mathbf{s}_n) \end{pmatrix}$$



Well-separated points



singular values of A for various values of m and n

- The rank is low, independent of number of sources and targets
- For certain kernels, low-rank decompositions are known analytically

NUMERICAL INSTABILITY

$$\mathcal{G}(\mathbf{x}, \mathbf{y}) = -\frac{1}{2\pi\lambda^2} \left(\log \|\mathbf{x} - \mathbf{y}\| + K_0(\lambda \|\mathbf{x} - \mathbf{y}\|) \right) \ .$$

Why not use existing tech for log and K_0 and add together?

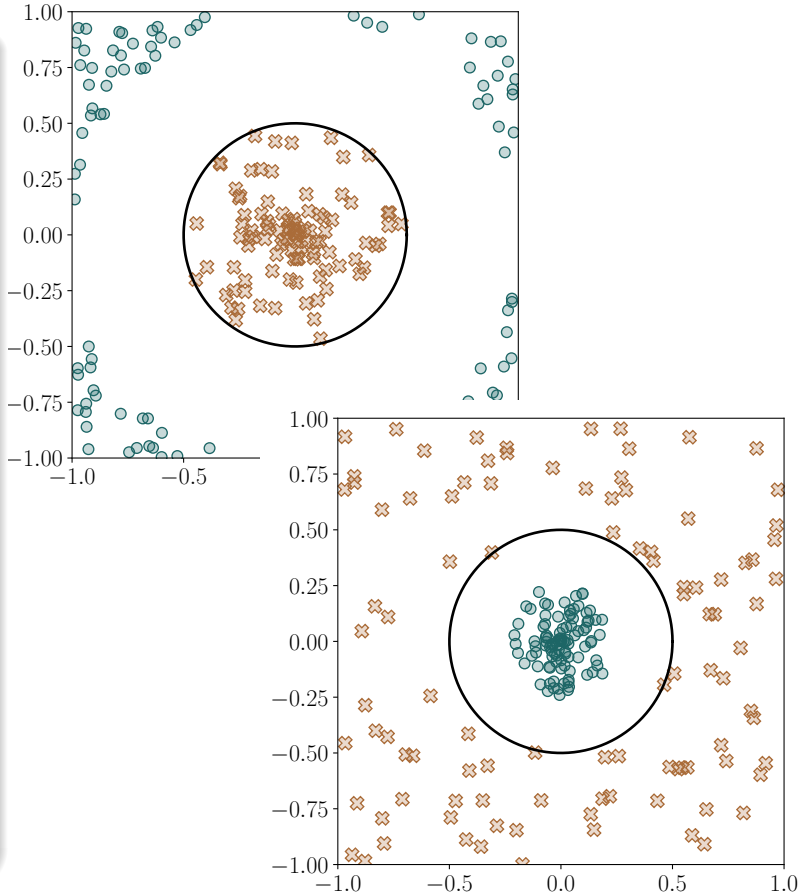
NUMERICAL INSTABILITY

$$\mathcal{G}(\mathbf{x},\mathbf{y}) = -\frac{1}{2\pi\lambda^2}\left(\log\|\mathbf{x}-\mathbf{y}\| + K_0(\lambda\|\mathbf{x}-\mathbf{y}\|)\right) \ .$$

Why not use existing tech for log and K_0 and add together?

Numerical Experiment

$$u(\mathbf{x};\lambda) = \sum_{j=1}^{n_s} q_j \partial_{v_j w_j}\mathcal{G}(\mathbf{x},\mathbf{s}_j)\,,$$



NUMERICAL INSTABILITY

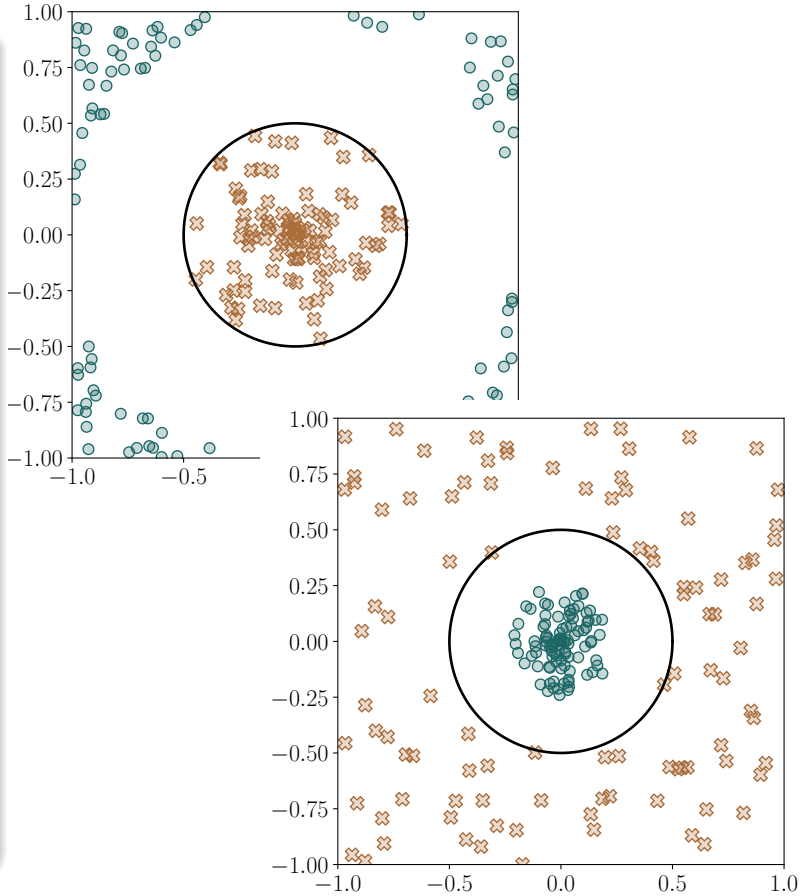
$$\mathcal{G}(\mathbf{x},\mathbf{y}) = -\frac{1}{2\pi\lambda^2}\left(\log\|\mathbf{x}-\mathbf{y}\| + K_0(\lambda\|\mathbf{x}-\mathbf{y}\|)\right) \ .$$

Why not use existing tech for log and K_0 and add together?

Numerical Experiment

$$u(\mathbf{x};\lambda) = \sum_{j=1}^{n_s} q_j \partial_{v_j w_j} \mathcal{G}(\mathbf{x},\mathbf{s}_j)\,,$$

$$u_L(\mathbf{x};\lambda) = -\frac{1}{2\pi\lambda^2}\sum_{j=1}^{n_s} q_j \partial_{v_j w_j} \log\|\mathbf{x}-\mathbf{s}_j\|\,,$$



NUMERICAL INSTABILITY

$$\mathcal{G}(\mathbf{x},\mathbf{y}) = -\frac{1}{2\pi\lambda^2}\left(\log\|\mathbf{x}-\mathbf{y}\| + K_0(\lambda\|\mathbf{x}-\mathbf{y}\|)\right) \ .$$

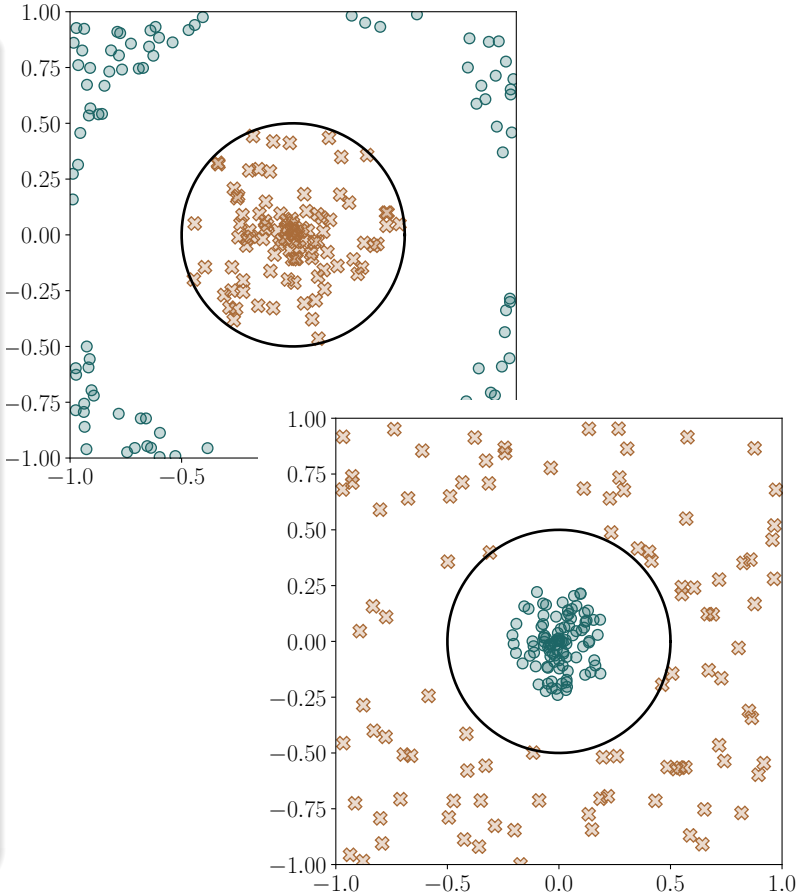
Why not use existing tech for log and K_0 and add together?

Numerical Experiment

$$u(\mathbf{x};\lambda) = \sum_{j=1}^{n_s} q_j \partial_{v_j w_j} \mathcal{G}(\mathbf{x},\mathbf{s}_j)\,,$$

$$u_L(\mathbf{x};\lambda) = -\frac{1}{2\pi\lambda^2}\sum_{j=1}^{n_s} q_j \partial_{v_j w_j} \log\|\mathbf{x}-\mathbf{s}_j\|\,,$$

$$u_K(\mathbf{x};\lambda) = \frac{1}{2\pi\lambda^2}\sum_{j=1}^{n_s} q_j \partial_{v_j w_j} K_0(\lambda\|\mathbf{x}-\mathbf{s}_j\|)\,.$$



NUMERICAL INSTABILITY

$$\mathcal{G}(\mathbf{x},\mathbf{y}) = -\frac{1}{2\pi\lambda^2}\left(\log\|\mathbf{x}-\mathbf{y}\| + K_0(\lambda\|\mathbf{x}-\mathbf{y}\|)\right) \ .$$

Why not use existing tech for log and K_0 and add together?

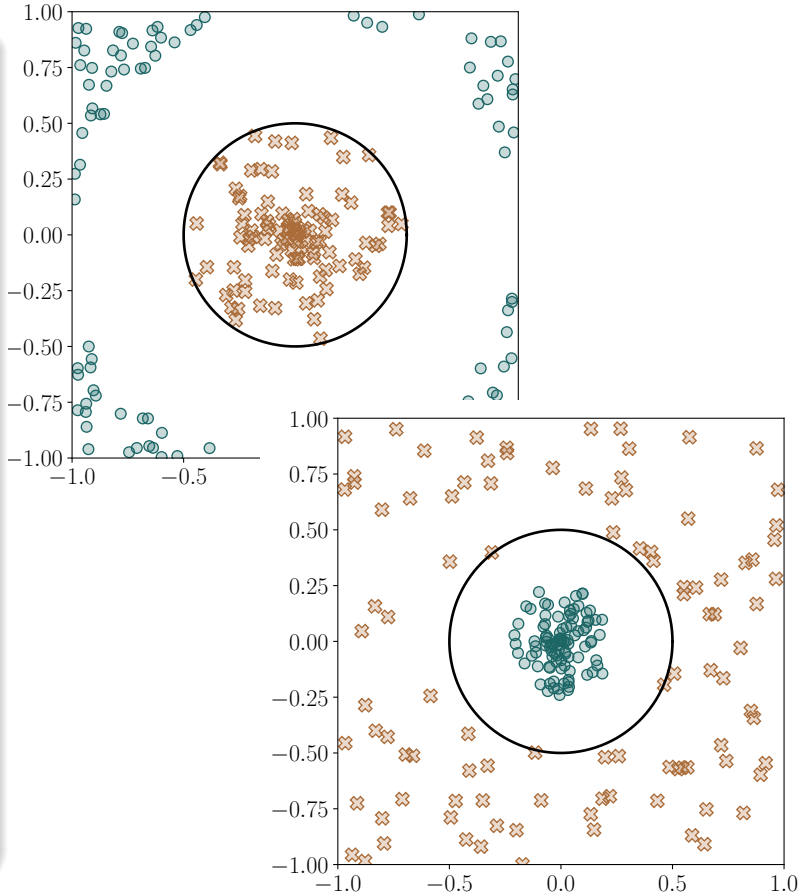
Numerical Experiment

$$u(\mathbf{x};\lambda) = \sum_{j=1}^{n_s} q_j \partial_{v_j w_j} \mathcal{G}(\mathbf{x},\mathbf{s}_j)\,,$$

$$u_L(\mathbf{x};\lambda) = -\frac{1}{2\pi\lambda^2}\sum_{j=1}^{n_s} q_j \partial_{v_j w_j} \log\|\mathbf{x}-\mathbf{s}_j\|\,,$$

$$u_K(\mathbf{x};\lambda) = \frac{1}{2\pi\lambda^2}\sum_{j=1}^{n_s} q_j \partial_{v_j w_j} K_0(\lambda\|\mathbf{x}-\mathbf{s}_j\|)\,.$$

What is the error (in floating point) in evaluating u as $u = u_L - u_K$?

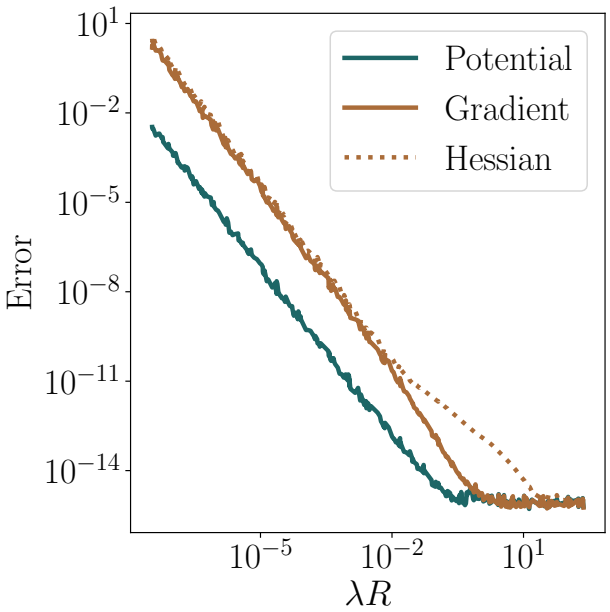


NUMERICAL INSTABILITY (CONT.)

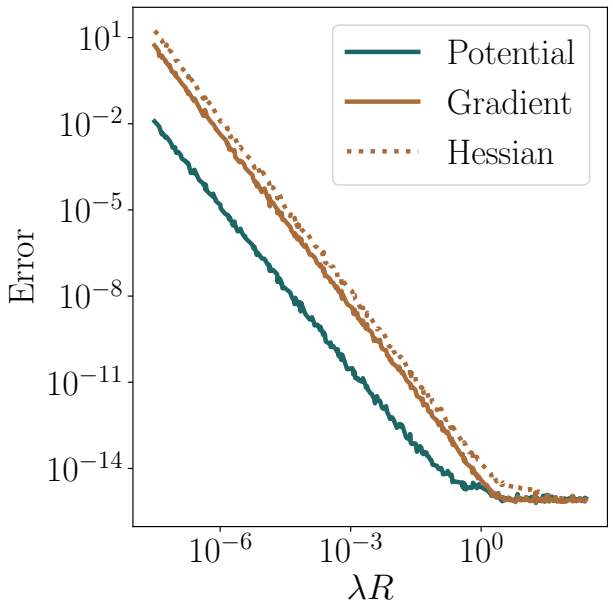
$$\mathcal{G}(\mathbf{x}, \mathbf{y}) = -\frac{1}{2\pi\lambda^2}\left(\log\|\mathbf{x}-\mathbf{y}\| + K_0(\lambda\|\mathbf{x}-\mathbf{y}\|)\right) .$$

Why not use existing tech for log and K_0 and add together?

(a) Interior problem



(b) Exterior problem



The error increases as the product of $\lambda = \sqrt{\mathrm{Re}/\delta t}$ and the radius of the disc R goes to zero.

THE MEANING OF λR

Note that $\lambda = \sqrt{\mathrm{Re}/\delta t}$

THE MEANING OF λR

Note that $\lambda = \sqrt{\mathrm{Re}/\delta t}$

The value of λR is small if

THE MEANING OF λR

Note that $\lambda = \sqrt{\mathrm{Re}/\delta t}$

The value of λR is small if

- The Reynolds number is small (viscous fluids)

THE MEANING OF λR

Note that $\lambda = \sqrt{\mathrm{Re}/\delta t}$

The value of λR is small if

- The Reynolds number is small (viscous fluids)
- The grid is fine

THE MEANING OF λR

Note that $\lambda = \sqrt{\mathrm{Re}/\delta t}$

The value of λR is small if

- The Reynolds number is small (viscous fluids)
- The grid is fine
- Time steps are relatively long

THE MEANING OF λR

Note that $\lambda = \sqrt{\mathrm{Re}/\delta t}$

The value of λR is small if

- The Reynolds number is small (viscous fluids)
- The grid is fine
- Time steps are relatively long

Note that $\lambda R < 1$ when $\delta t > \mathrm{Re} R^2$, i.e. when the CFL condition is violated. This regime is important for implicit methods for viscous fluids.

OUR GOAL

Our goal: analytical formulas for the low rank interaction between well separated points which are stable for any λR.

OUR GOAL

Our goal: analytical formulas for the low rank interaction between well separated points which are stable for any λR.

Go back to basics: look that the separation of variables problem for the modified biharmonic equation

SEPARATION OF VARIABLES

Let Ω be the interior or exterior of a disc of radius R and consider the modified biharmonic equation:

$$\Delta(\Delta - \lambda^2)u = 0 \ , \ \mathbf{x} \in \Omega \ ,$$
$$u = f \ , \partial_n u = g \ , \ \mathbf{x} \in \partial\Omega \ .$$

SEPARATION OF VARIABLES

Let Ω be the interior or exterior of a disc of radius R and consider the modified biharmonic equation:

$$\Delta(\Delta - \lambda^2)u = 0 \ , \ \mathbf{x} \in \Omega \ ,$$
$$u = f \ , \partial_n u = g \ , \ \mathbf{x} \in \partial\Omega \ .$$

Separation of Variables Representation

$$u(r,\theta) = \sum_{n=-\infty}^{\infty} u_n(r) e^{in\theta} \ .$$

SEPARATION OF VARIABLES

Let Ω be the interior or exterior of a disc of radius R and consider the modified biharmonic equation:

$$\Delta(\Delta - \lambda^2)u = 0 \ , \ \mathbf{x} \in \Omega \ ,$$
$$u = f \ , \partial_n u = g \ , \ \mathbf{x} \in \partial\Omega \ .$$

Separation of Variables Representation

$$u(r,\theta) = \sum_{n=-\infty}^{\infty} u_n(r) e^{in\theta} \ .$$

ODE for $u_n(r)$

$$\left(\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} - \frac{n^2}{r^2}\right)\left(\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} - \frac{n^2}{r^2} - \lambda^2\right) u_n(r) = 0 \ .$$

SEPARATION OF VARIABLES (CONT.)

ODE for $u_n(r)$

$$\left(\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} - \frac{n^2}{r^2}\right)\left(\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} - \frac{n^2}{r^2} - \lambda^2\right) u_n(r) = 0 \ .$$

Four linearly independent solutions: $r^{|n|}$, $I_n(\lambda r)$, $r^{-|n|}$, and $K_n(\lambda r)$.

SEPARATION OF VARIABLES (CONT.)

ODE for $u_n(r)$

$$\left(\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} - \frac{n^2}{r^2}\right)\left(\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} - \frac{n^2}{r^2} - \lambda^2\right) u_n(r) = 0 \ .$$

Four linearly independent solutions: $r^{|n|}$, $I_n(\lambda r)$, $r^{-|n|}$, and $K_n(\lambda r)$.

Interior Problem

By imposing continuity at $r = 0$, the functions $r^{|n|}$ and $I_n(\lambda r)$ are a basis for the interior problem.

SEPARATION OF VARIABLES (CONT.)

ODE for $u_n(r)$

$$\left(\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} - \frac{n^2}{r^2}\right)\left(\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} - \frac{n^2}{r^2} - \lambda^2\right) u_n(r) = 0 \ .$$

Four linearly independent solutions: $r^{|n|}$, $I_n(\lambda r)$, $r^{-|n|}$, and $K_n(\lambda r)$.

Interior Problem

By imposing continuity at $r = 0$, the functions $r^{|n|}$ and $I_n(\lambda r)$ are a basis for the interior problem.

Exterior Problem

By imposing decay conditions $r = \infty$, the functions $r^{-|n|}$ and $K_n(\lambda r)$ are a basis for the exterior problem.

A BAD BASIS (EXT.)

For the exterior problem, we have $u_n(r) = \alpha_n r^{-|n|} + \beta_n K_n(\lambda r)$.

A BAD BASIS (EXT.)

For the exterior problem, we have $u_n(r) = \alpha_n r^{-|n|} + \beta_n K_n(\lambda r)$.

Coefficient Recovery Problem

$$\begin{pmatrix} R^{-|n|} & K_n(\lambda R) \\ -|n|R^{-|n|-1} & -\frac{\lambda}{2}\left(K_{n-1}(\lambda R) + K_{n+1}(\lambda R)\right) \end{pmatrix} \begin{pmatrix} \alpha_n \\ \beta_n \end{pmatrix} = \begin{pmatrix} f_n \\ g_n \end{pmatrix} .$$

This problem is ill-conditioned for small λR. Intuitively, this is because $K_n(\lambda r)$ and $r^{-|n|}$ are similar functions for small r.

A BAD BASIS (EXT.)

For the exterior problem, we have $u_n(r) = \alpha_n r^{-|n|} + \beta_n K_n(\lambda r)$.

Coefficient Recovery Problem

$$\begin{pmatrix} R^{-|n|} & K_n(\lambda R) \\ -|n|R^{-|n|-1} & -\frac{\lambda}{2}\left(K_{n-1}(\lambda R) + K_{n+1}(\lambda R)\right) \end{pmatrix} \begin{pmatrix} \alpha_n \\ \beta_n \end{pmatrix} = \begin{pmatrix} f_n \\ g_n \end{pmatrix} .$$

This problem is ill-conditioned for small λR. Intuitively, this is because $K_n(\lambda r)$ and $r^{-|n|}$ are similar functions for small r.

Asymptotic Expansion for $K_n(\lambda r)$

$$K_n(\lambda r) = \tfrac{1}{2}(\tfrac{1}{2}\lambda r)^{-|n|} \sum_{k=0}^{|n|-1} \frac{(|n|-k-1)!}{k!}(-\tfrac{1}{4}\lambda r^2)^k + (-1)^{|n|+1} \ln\left(\tfrac{1}{2}\lambda r\right) I_n(\lambda r)$$
$$+ (-1)^{|n|}\tfrac{1}{2}(\tfrac{1}{2}\lambda r)^{|n|} \sum_{k=0}^{\infty} \left(\psi(k+1) + \psi(|n|+k+1)\right) \frac{(\frac{1}{4}\lambda r^2)^k}{k!(|n|+k)!} .$$

A BETTER BASIS (EXT.)

We can define a new basis function for the exterior problem which is *not* asymptotically similar to $r^{-|n|}$ and K_n.

A BETTER BASIS (EXT.)

We can define a new basis function for the exterior problem which is *not* asymptotically similar to $r^{-|n|}$ and K_n.

Definition of Q_n

$$Q_n(r) = K_n(\lambda r) - \frac{2^{|n|-1}\,(|n|-1)!}{\lambda^{|n|} r^{|n|}}\,.$$

A BETTER BASIS (EXT.)

We can define a new basis function for the exterior problem which is *not* asymptotically similar to $r^{-|n|}$ and K_n.

Definition of Q_n

$$Q_n(r) = K_n(\lambda r) - \frac{2^{|n|-1}\,(|n|-1)!}{\lambda^{|n|} r^{|n|}}\,.$$

- Q_n has a different leading order term for small λ and R.

A BETTER BASIS (EXT.)

We can define a new basis function for the exterior problem which is *not* asymptotically similar to $r^{-|n|}$ and K_n.

Definition of Q_n

$$Q_n(r) = K_n(\lambda r) - \frac{2^{|n|-1}\,(|n|-1)!}{\lambda^{|n|} r^{|n|}}\,.$$

- Q_n has a different leading order term for small λ and R.
- The pair (Q_n, K_n) is a better conditioned basis than $(r^{-|n|}, K_n)$ in the small λR regime.

A BETTER BASIS (EXT.)

We can define a new basis function for the exterior problem which is *not* asymptotically similar to $r^{-|n|}$ and K_n.

Definition of Q_n

$$Q_n(r) = K_n(\lambda r) - \frac{2^{|n|-1}\,(|n|-1)!}{\lambda^{|n|} r^{|n|}}\,.$$

- Q_n has a different leading order term for small λ and R.
- The pair (Q_n, K_n) is a better conditioned basis than $(r^{-|n|}, K_n)$ in the small λR regime.
- Q_n is still a solution of the ODE for u_n because it's a linear combo of $r^{-|n|}$ and K_n.

A BETTER BASIS (EXT.)

We can define a new basis function for the exterior problem which is *not* asymptotically similar to $r^{-|n|}$ and K_n.

Definition of Q_n

$$Q_n(r) = K_n(\lambda r) - \frac{2^{|n|-1}\,(|n|-1)!}{\lambda^{|n|} r^{|n|}}\,.$$

- Q_n has a different leading order term for small λ and R.
- The pair (Q_n, K_n) is a better conditioned basis than $(r^{-|n|}, K_n)$ in the small λR regime.
- Q_n is still a solution of the ODE for u_n because it's a linear combo of $r^{-|n|}$ and K_n.
- It is simple to evaluate Q_n with tweaks to existing software.

A BAD BASIS (INT.)

For the interior problem, we have that $u_n(r) = \alpha_n r^{|n|} + \beta_n I_n(\lambda r)$.

A BAD BASIS (INT.)

For the interior problem, we have that $u_n(r) = \alpha_n r^{|n|} + \beta_n I_n(\lambda r)$.

Coefficient Recovery Problem

$$\begin{pmatrix} R^{|n|} & I_n(\lambda R) \\ |n| R^{|n|-1} & \frac{\lambda}{2}\left(I_{n-1}(\lambda R) + I_{n+1}(\lambda R)\right) \end{pmatrix} \begin{pmatrix} \alpha_n \\ \beta_n \end{pmatrix} = \begin{pmatrix} f_n \\ g_n \end{pmatrix} .$$

This problem is again ill-conditioned for small λR.

A BAD BASIS (INT.)

For the interior problem, we have that $u_n(r) = \alpha_n r^{|n|} + \beta_n I_n(\lambda r)$.

Coefficient Recovery Problem

$$\begin{pmatrix} R^{|n|} & I_n(\lambda R) \\ |n| R^{|n|-1} & \frac{\lambda}{2}\left(I_{n-1}(\lambda R) + I_{n+1}(\lambda R)\right) \end{pmatrix} \begin{pmatrix} \alpha_n \\ \beta_n \end{pmatrix} = \begin{pmatrix} f_n \\ g_n \end{pmatrix} .$$

This problem is again ill-conditioned for small λR.

Asymptotic Expansion for $I_n(\lambda r)$

$$I_n(\lambda r) = \sum_{k=0}^{\infty} \frac{\left(\frac{\lambda r}{2}\right)^{2k+|n|}}{k!(k+|n|)!} = \frac{1}{2^{|n|}|n|!}(\lambda r)^{|n|} + \frac{1}{2^{|n|+2}(|n|+1)!}(\lambda r)^{|n|+2} + \cdots$$

A BETTER BASIS (INT.)

Again, we can define a new basis function for the interior problem which is *not* asymptotically similar to $r^{|n|}$ and I_n.

A BETTER BASIS (INT.)

Again, we can define a new basis function for the interior problem which is *not* asymptotically similar to $r^{|n|}$ and I_n.

Definition of P_n

$$P_n(r) = I_n(\lambda r) - \left(\frac{\lambda r}{2}\right)^{|n|} \frac{1}{|n|!} \, .$$

A BETTER BASIS (INT.)

Again, we can define a new basis function for the interior problem which is *not* asymptotically similar to $r^{|n|}$ and I_n.

Definition of P_n

$$P_n(r) = I_n(\lambda r) - \left(\frac{\lambda r}{2}\right)^{|n|} \frac{1}{|n|!} \, .$$

- P_n has a different leading order term for small λ and R.

A BETTER BASIS (INT.)

Again, we can define a new basis function for the interior problem which is *not* asymptotically similar to $r^{|n|}$ and I_n.

Definition of P_n

$$P_n(r) = I_n(\lambda r) - \left(\frac{\lambda r}{2}\right)^{|n|} \frac{1}{|n|!} \, .$$

- P_n has a different leading order term for small λ and R.
- The pair $(r^{|n|}, P_n)$ is a better conditioned basis than $(r^{|n|}, I_n)$ in the small λR regime.

A BETTER BASIS (INT.)

Again, we can define a new basis function for the interior problem which is *not* asymptotically similar to $r^{|n|}$ and I_n.

Definition of P_n

$$P_n(r) = I_n(\lambda r) - \left(\frac{\lambda r}{2}\right)^{|n|} \frac{1}{|n|!} \, .$$

- P_n has a different leading order term for small λ and R.
- The pair $(r^{|n|}, P_n)$ is a better conditioned basis than $(r^{|n|}, I_n)$ in the small λR regime.
- P_n is still a solution of the ODE for u_n because it's a linear combo of $r^{|n|}$ and I_n.

A BETTER BASIS (INT.)

Again, we can define a new basis function for the interior problem which is *not* asymptotically similar to $r^{|n|}$ and I_n.

Definition of P_n

$$P_n(r) = I_n(\lambda r) - \left(\frac{\lambda r}{2}\right)^{|n|} \frac{1}{|n|!} \, .$$

- P_n has a different leading order term for small λ and R.
- The pair $(r^{|n|}, P_n)$ is a better conditioned basis than $(r^{|n|}, I_n)$ in the small λR regime.
- P_n is still a solution of the ODE for u_n because it's a linear combo of $r^{|n|}$ and I_n.
- It is simple to evaluate P_n with tweaks to existing software.

NUMERICAL RESULTS (CONT.)

Question

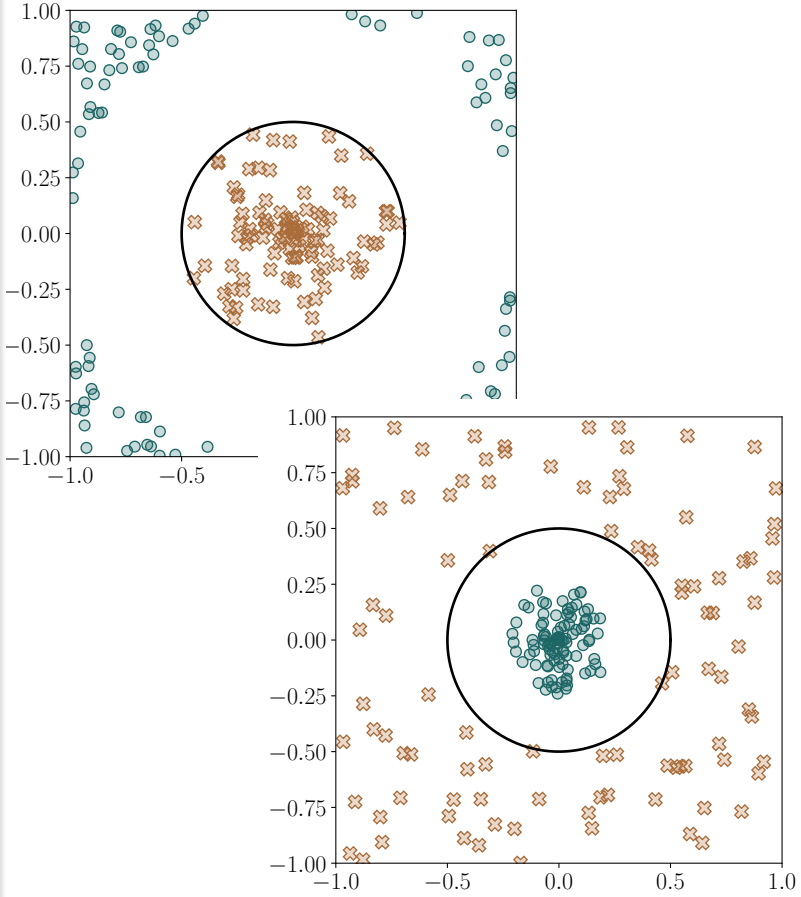
What is the practical effect of the condition number of the coefficient recovery problem on the accuracy of the solution?

NUMERICAL RESULTS (CONT.)

Numerical Experiment

$$u(\mathbf{x};\lambda) = \sum_{j=1}^{n_s} \lambda^2 c_j \mathcal{G}(\mathbf{x},\mathbf{s}_j) + \lambda d_j \partial_{v_{j,1}} \mathcal{G}(\mathbf{x},\mathbf{s}_j) + q_j \partial_{v_{j,2} v_{j,3}} \mathcal{G}(\mathbf{x},\mathbf{s}_j)\,.$$

For several values of λ and R:



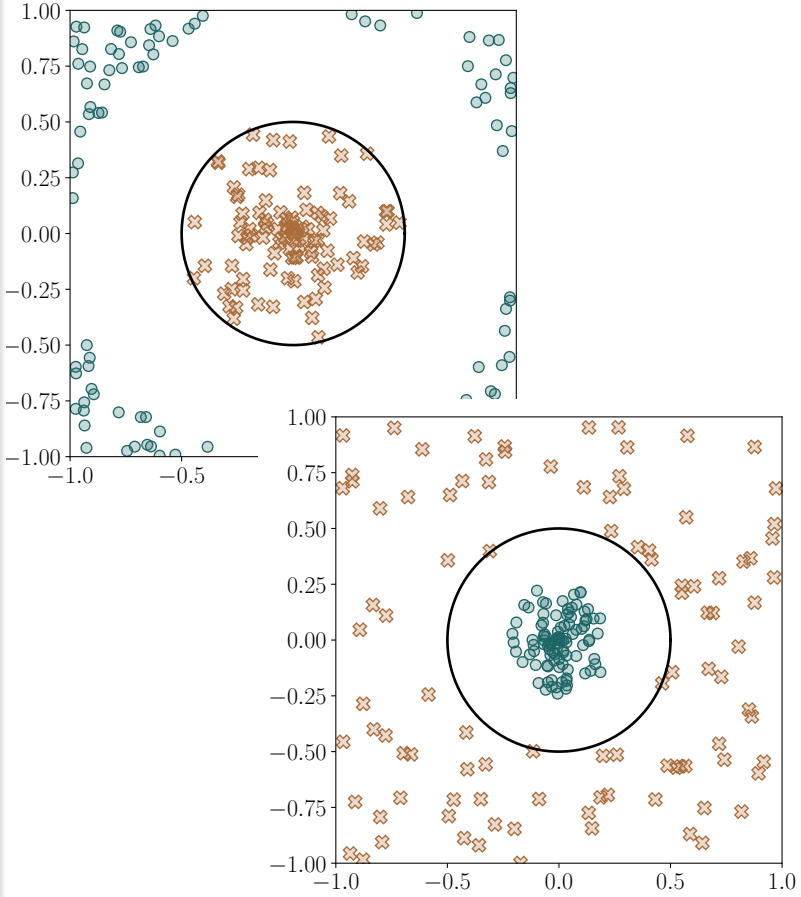
NUMERICAL RESULTS (CONT.)

Numerical Experiment

$$u(\mathbf{x};\lambda) = \sum_{j=1}^{n_s} \lambda^2 c_j \mathcal{G}(\mathbf{x},\mathbf{s}_j) + \lambda d_j \partial_{v_{j,1}} \mathcal{G}(\mathbf{x},\mathbf{s}_j) + q_j \partial_{v_{j,2} v_{j,3}} \mathcal{G}(\mathbf{x},\mathbf{s}_j)\,.$$

For several values of λ and R:

- Evaluate u and $\partial_n u$ on $\partial\Omega$



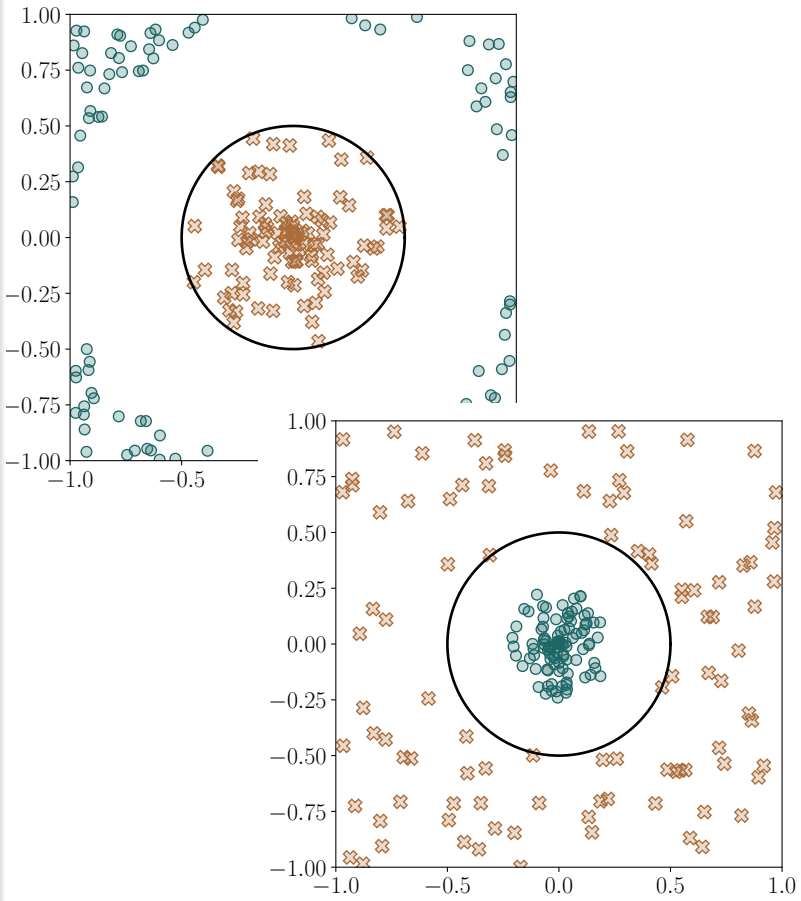
NUMERICAL RESULTS (CONT.)

Numerical Experiment

$$u(\mathbf{x};\lambda) = \sum_{j=1}^{n_s} \lambda^2 c_j \mathcal{G}(\mathbf{x},\mathbf{s}_j) + \lambda d_j \partial_{v_{j,1}} \mathcal{G}(\mathbf{x},\mathbf{s}_j) + q_j \partial_{v_{j,2} v_{j,3}} \mathcal{G}(\mathbf{x},\mathbf{s}_j)\,.$$

For several values of λ and R:

- Evaluate u and $\partial_n u$ on $\partial\Omega$
- Solve corresponding separation of variables problem (order $N = 50$, using 100 points on $\partial\Omega$) with new and old basis functions



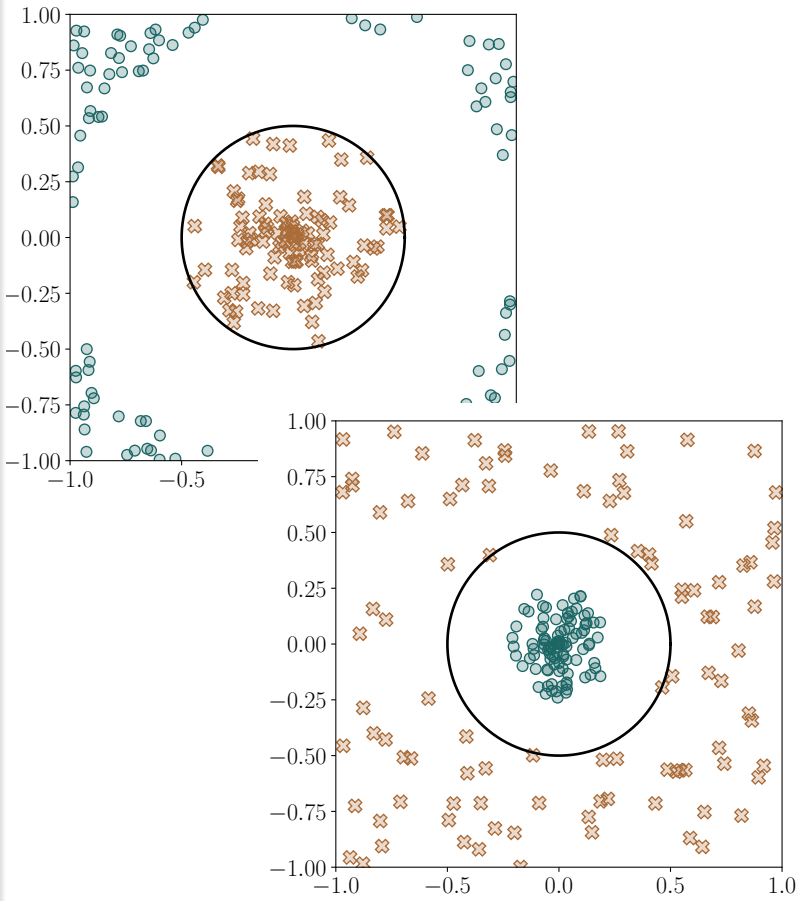
NUMERICAL RESULTS (CONT.)

Numerical Experiment

$$u(\mathbf{x};\lambda) = \sum_{j=1}^{n_s} \lambda^2 c_j \mathcal{G}(\mathbf{x},\mathbf{s}_j) + \lambda d_j \partial_{v_{j,1}} \mathcal{G}(\mathbf{x},\mathbf{s}_j) + q_j \partial_{v_{j,2} v_{j,3}} \mathcal{G}(\mathbf{x},\mathbf{s}_j)\,.$$

For several values of λ and R:

- Evaluate u and $\partial_n u$ on $\partial\Omega$
- Solve corresponding separation of variables problem (order $N = 50$, using 100 points on $\partial\Omega$) with new and old basis functions
- Evaluate error in potential, gradient, and Hessian



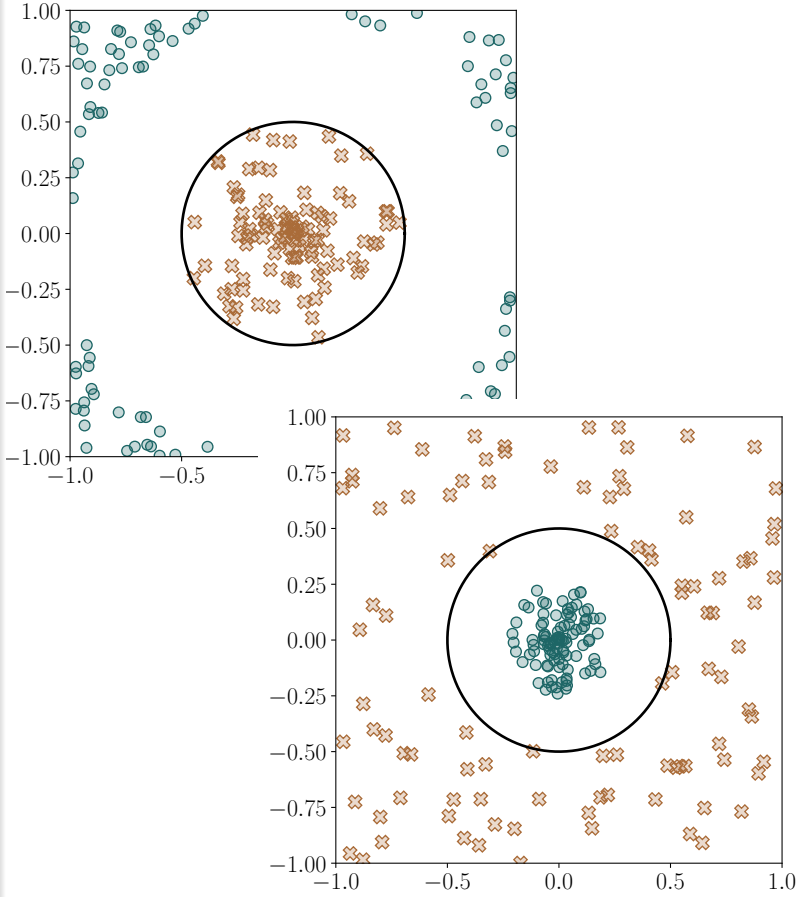
NUMERICAL RESULTS (CONT.)

Numerical Experiment

$$u(\mathbf{x};\lambda) = \sum_{j=1}^{n_s} \lambda^2 c_j \mathcal{G}(\mathbf{x},\mathbf{s}_j) + \lambda d_j \partial_{v_{j,1}} \mathcal{G}(\mathbf{x},\mathbf{s}_j) + q_j \partial_{v_{j,2} v_{j,3}} \mathcal{G}(\mathbf{x},\mathbf{s}_j)\,.$$

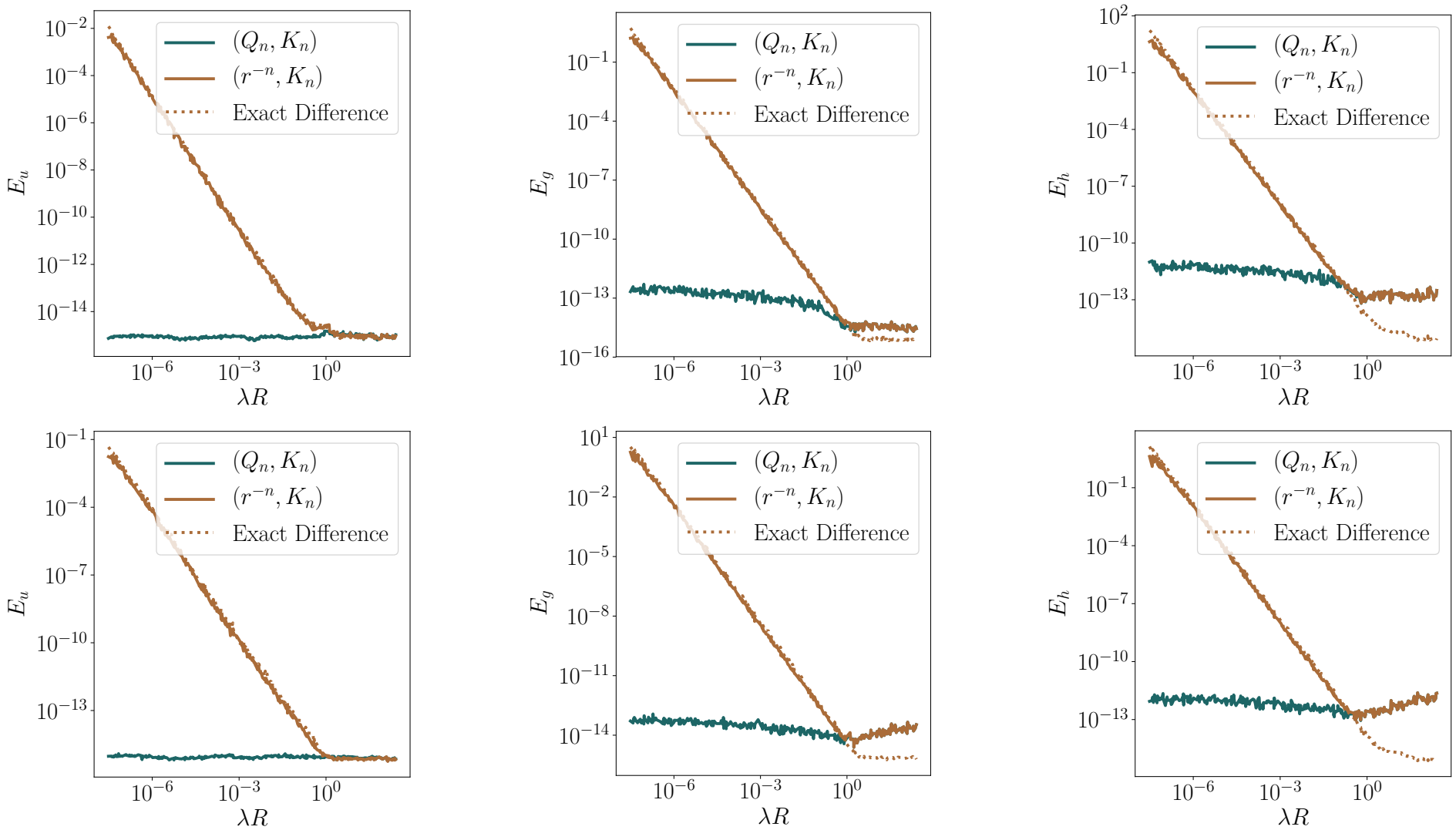
For several values of λ and R:

- Evaluate u and $\partial_n u$ on $\partial\Omega$
- Solve corresponding separation of variables problem (order $N = 50$, using 100 points on $\partial\Omega$) with new and old basis functions
- Evaluate error in potential, gradient, and Hessian
- Should be good to about machine precision, with some precision loss in the derivatives



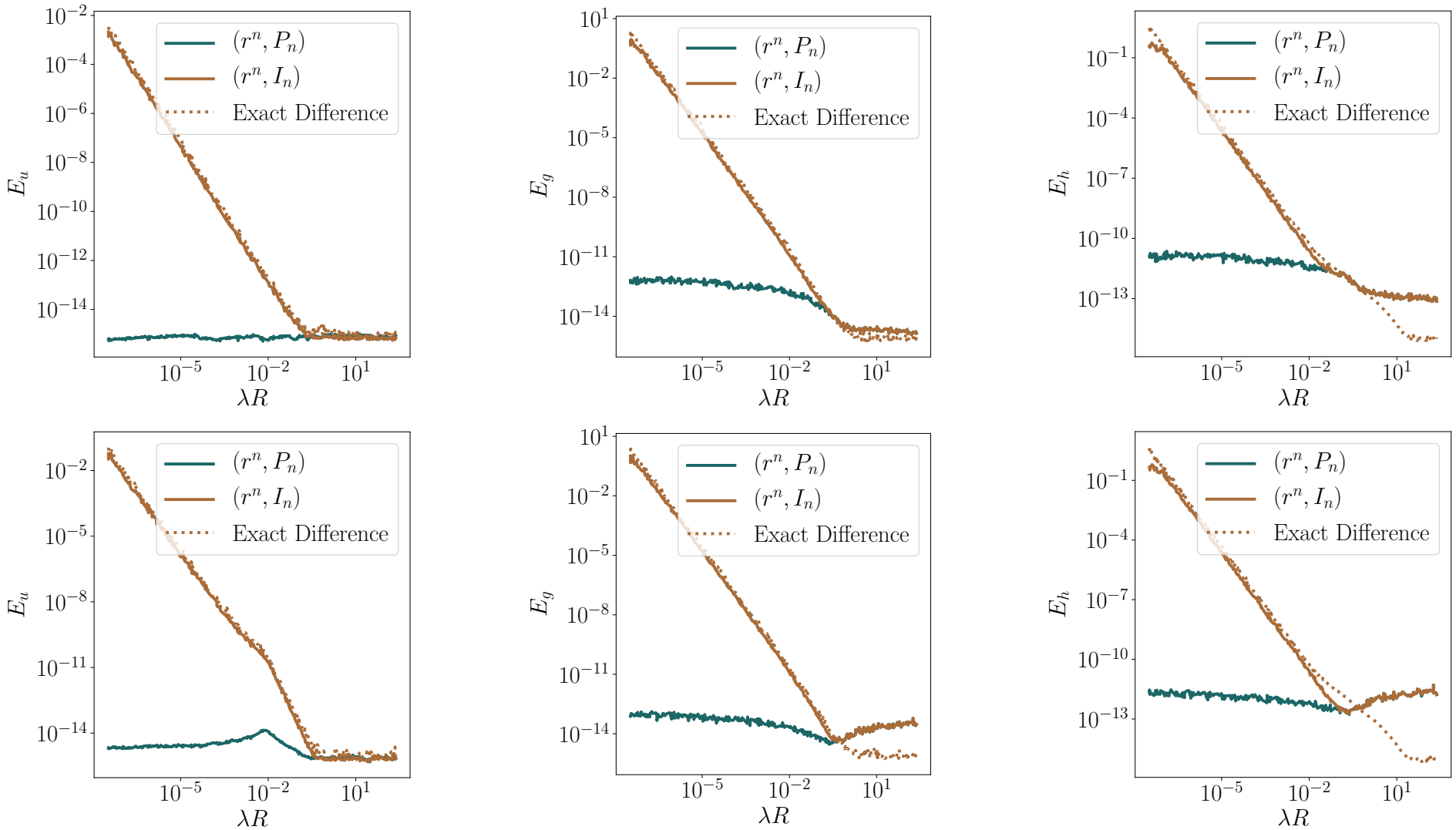
NUMERICAL RESULTS (CONT.)

Errors for the exterior problem: $(r^{-|n|}, K_n)$ vs (Q_n, K_n). Top row: $\lambda \to 0$. Bottom row: $R \to 0$.



NUMERICAL RESULTS (CONT.)

Errors for the interior problem: $(r^{|n|}, I_n)$ vs $(r^{|n|}, P_n)$. Top row: $\lambda \to 0$. Bottom row: $R \to 0$.



REALITY CHECK

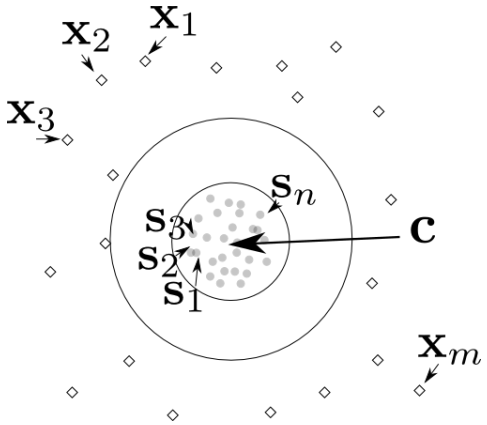
How is this a decomposition?

REALITY CHECK

How is this a decomposition? Recall

$$u(\mathbf{x}_i) = \sum_{j=1}^{n} q_j \partial_{v_j w_j} \mathcal{G}(\mathbf{x}_i, \mathbf{s}_j)$$

$$A = \begin{pmatrix} \partial_{v_1 w_1} \mathcal{G}(\mathbf{x}_1, \mathbf{s}_1) & \partial_{v_2 w_2} \mathcal{G}(\mathbf{x}_1, \mathbf{s}_2) & \cdots & \partial_{v_n w_n} \mathcal{G}(\mathbf{x}_1, \mathbf{s}_n) \\ \partial_{v_1 w_1} \mathcal{G}(\mathbf{x}_2, \mathbf{s}_1) & \partial_{v_2 w_2} \mathcal{G}(\mathbf{x}_2, \mathbf{s}_2) & \cdots & \partial_{v_n w_n} \mathcal{G}(\mathbf{x}_2, \mathbf{s}_n) \\ \vdots & \vdots & & \vdots \\ \partial_{v_1 w_1} \mathcal{G}(\mathbf{x}_m, \mathbf{s}_1) & \partial_{v_2 w_2} \mathcal{G}(\mathbf{x}_m, \mathbf{s}_2) & \cdots & \partial_{v_n w_n} \mathcal{G}(\mathbf{x}_m, \mathbf{s}_n) \end{pmatrix}$$



Well-separated points

ANALYTICAL DECOMPOSITION

$$A = LR^{\mathsf{T}}.$$

ANALYTICAL DECOMPOSITION

$A = LR^{\mathsf{T}}$. The form of L is straightforward

$$L = \begin{pmatrix} Q_0(|\mathbf{x}_1 - \mathbf{c}|) & K_0(\lambda|\mathbf{x}_1 - \mathbf{c}|) & \cdots & Q_p(|\mathbf{x}_1 - \mathbf{c}|)e^{ip\theta_1} & K_p(\lambda|\mathbf{x}_1 - \mathbf{c}|)e^{ip\theta_1} \\ Q_0(|\mathbf{x}_2 - \mathbf{c}|) & K_0(\lambda|\mathbf{x}_2 - \mathbf{c}|) & \cdots & Q_p(|\mathbf{x}_2 - \mathbf{c}|)e^{ip\theta_2} & K_p(\lambda|\mathbf{x}_2 - \mathbf{c}|)e^{ip\theta_2} \\ \vdots & \vdots & & \vdots & \vdots \\ Q_0(|\mathbf{x}_m - \mathbf{c}|) & K_0(\lambda|\mathbf{x}_m - \mathbf{c}|) & \cdots & Q_p(|\mathbf{x}_m - \mathbf{c}|)e^{ip\theta_m} & K_p(\lambda|\mathbf{x}_m - \mathbf{c}|)e^{ip\theta_m} \end{pmatrix}$$

ANALYTICAL DECOMPOSITION

$A = LR^{\mathsf{T}}$. The form of L is straightforward

$$L = \begin{pmatrix} Q_0(|\mathbf{x}_1 - \mathbf{c}|) & K_0(\lambda|\mathbf{x}_1 - \mathbf{c}|) & \cdots & Q_p(|\mathbf{x}_1 - \mathbf{c}|)e^{ip\theta_1} & K_p(\lambda|\mathbf{x}_1 - \mathbf{c}|)e^{ip\theta_1} \\ Q_0(|\mathbf{x}_2 - \mathbf{c}|) & K_0(\lambda|\mathbf{x}_2 - \mathbf{c}|) & \cdots & Q_p(|\mathbf{x}_2 - \mathbf{c}|)e^{ip\theta_2} & K_p(\lambda|\mathbf{x}_2 - \mathbf{c}|)e^{ip\theta_2} \\ \vdots & \vdots & & \vdots & \vdots \\ Q_0(|\mathbf{x}_m - \mathbf{c}|) & K_0(\lambda|\mathbf{x}_m - \mathbf{c}|) & \cdots & Q_p(|\mathbf{x}_m - \mathbf{c}|)e^{ip\theta_m} & K_p(\lambda|\mathbf{x}_m - \mathbf{c}|)e^{ip\theta_m} \end{pmatrix}$$

What is R^{T}?

ANALYTICAL DECOMPOSITION

$A = LR^{\mathsf{T}}$. The form of L is straightforward

$$L = \begin{pmatrix} Q_0(|\mathbf{x}_1 - \mathbf{c}|) & K_0(\lambda|\mathbf{x}_1 - \mathbf{c}|) & \cdots & Q_p(|\mathbf{x}_1 - \mathbf{c}|)e^{ip\theta_1} & K_p(\lambda|\mathbf{x}_1 - \mathbf{c}|)e^{ip\theta_1} \\ Q_0(|\mathbf{x}_2 - \mathbf{c}|) & K_0(\lambda|\mathbf{x}_2 - \mathbf{c}|) & \cdots & Q_p(|\mathbf{x}_2 - \mathbf{c}|)e^{ip\theta_2} & K_p(\lambda|\mathbf{x}_2 - \mathbf{c}|)e^{ip\theta_2} \\ \vdots & \vdots & & \vdots & \vdots \\ Q_0(|\mathbf{x}_m - \mathbf{c}|) & K_0(\lambda|\mathbf{x}_m - \mathbf{c}|) & \cdots & Q_p(|\mathbf{x}_m - \mathbf{c}|)e^{ip\theta_m} & K_p(\lambda|\mathbf{x}_m - \mathbf{c}|)e^{ip\theta_m} \end{pmatrix}$$

What is R^{T}? It is the map from the sources to the coefficients

$R^{\mathsf{T}} =$

each mode solve 2×2 for coeffs	separate modes with FFT	evaluate both u and $\partial_n u$ on disc boundary

Note that there is an analytical formula for R^{T} [Askham, 2017].

WHAT OF EFFICIENCY?

Because the formulas for L and $R^\intercal$ are known, forming these matrices is $\mathcal{O}((m+n)p)$.

WHAT OF EFFICIENCY?

Because the formulas for L and $R^\intercal$ are known, forming these matrices is $\mathcal{O}((m+n)p)$. The SVD, on the other hand is $\mathcal{O}(mn^2)$.

WHAT OF EFFICIENCY?

Because the formulas for L and $R^\intercal$ are known, forming these matrices is $\mathcal{O}((m+n)p)$. The SVD, on the other hand is $\mathcal{O}(mn^2)$. Even randomized methods for the SVD are $\mathcal{O}(mnp)$.

WHAT OF EFFICIENCY?

Because the formulas for L and $R^\intercal$ are known, forming these matrices is $\mathcal{O}((m+n)p)$. The SVD, on the other hand is $\mathcal{O}(mn^2)$. Even randomized methods for the SVD are $\mathcal{O}(mnp)$.

It is not always the case that sources are well-separated from targets. Can we make a stable FMM with the above?

AN FMM

The preceding provides a stable fast multipole method

A fast multipole method is based on:

AN FMM

The preceding provides a stable fast multipole method

A fast multipole method is based on:

1. a formula for representing the sum due to a localized subset of the points (a multipole expansion). (Q_n, K_n)

AN FMM

The preceding provides a stable fast multipole method

A fast multipole method is based on:

1. a formula for representing the sum due to a localized subset of the points (a multipole expansion). (Q_n, K_n)
2. a formula for representing the sum due to points outside of a disc (a local expansion). $(r^{|n|}, P_n)$

AN FMM

The preceding provides a stable fast multipole method

A fast multipole method is based on:

1. a formula for representing the sum due to a localized subset of the points (a multipole expansion). (Q_n, K_n)
2. a formula for representing the sum due to points outside of a disc (a local expansion). $(r^{|n|}, P_n)$
3. formulas for translating between these representations (translation operators). see the preprint!

AN FMM

The preceding provides a stable fast multipole method

A fast multipole method is based on:

1. a formula for representing the sum due to a localized subset of the points (a multipole expansion). (Q_n, K_n)
2. a formula for representing the sum due to points outside of a disc (a local expansion). $(r^{|n|}, P_n)$
3. formulas for translating between these representations (translation operators). see the preprint!
4. a hierarchical organization of source and target points in space

COMPUTING THE PARTICULAR SOLUTION

EVALUATING THE PARTICULAR SOLUTION

To compute the particular solution, we need to evaluate integrals of the form

$$v(\mathbf{x}) = Vf(\mathbf{x}) := \int_{\Omega} \mathcal{K}(\mathbf{x}, \mathbf{y}) f(\mathbf{y})\, dy \quad ,$$

where $\mathcal{K}(\mathbf{x}, \mathbf{y}) = \log |\mathbf{x} - \mathbf{y}|$ or $\mathcal{K}(\mathbf{x}, \mathbf{y}) = K_0(\lambda |\mathbf{x} - \mathbf{y}|)$.

EVALUATING THE PARTICULAR SOLUTION

To compute the particular solution, we need to evaluate integrals of the form

$$v(\mathbf{x}) = Vf(\mathbf{x}) := \int_{\Omega} \mathcal{K}(\mathbf{x}, \mathbf{y}) f(\mathbf{y})\, dy \quad ,$$

where $\mathcal{K}(\mathbf{x}, \mathbf{y}) = \log |\mathbf{x} - \mathbf{y}|$ or $\mathcal{K}(\mathbf{x}, \mathbf{y}) = K_0(\lambda |\mathbf{x} - \mathbf{y}|)$.

- No solve, just apply

EVALUATING THE PARTICULAR SOLUTION

To compute the particular solution, we need to evaluate integrals of the form

$$v(\mathbf{x}) = Vf(\mathbf{x}) := \int_{\Omega} \mathcal{K}(\mathbf{x}, \mathbf{y}) f(\mathbf{y})\, dy \quad ,$$

where $\mathcal{K}(\mathbf{x}, \mathbf{y}) = \log |\mathbf{x} - \mathbf{y}|$ or $\mathcal{K}(\mathbf{x}, \mathbf{y}) = K_0(\lambda |\mathbf{x} - \mathbf{y}|)$.

- No solve, just apply
- Weakly singular integrand

EVALUATING THE PARTICULAR SOLUTION

To compute the particular solution, we need to evaluate integrals of the form

$$v(\mathbf{x}) = Vf(\mathbf{x}) := \int_\Omega \mathcal{K}(\mathbf{x}, \mathbf{y}) f(\mathbf{y})\, dy \quad ,$$

where $\mathcal{K}(\mathbf{x}, \mathbf{y}) = \log|\mathbf{x} - \mathbf{y}|$ or $\mathcal{K}(\mathbf{x}, \mathbf{y}) = K_0(\lambda|\mathbf{x} - \mathbf{y}|)$.

- No solve, just apply
- Weakly singular integrand
- Expensive on an unstructured discretization (adpative quadrature, etc.)

EVALUATING THE PARTICULAR SOLUTION

To compute the particular solution, we need to evaluate integrals of the form

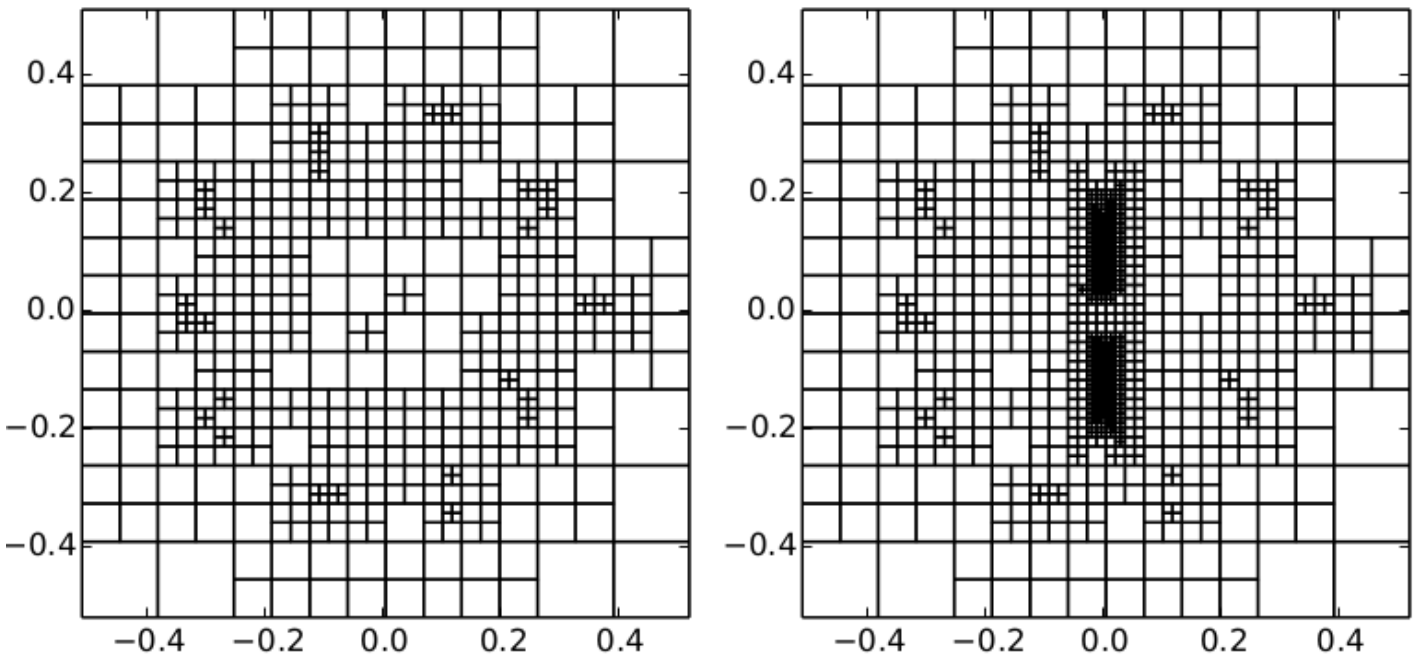
$$v(\mathbf{x}) = Vf(\mathbf{x}) := \int_\Omega \mathcal{K}(\mathbf{x}, \mathbf{y}) f(\mathbf{y})\, dy \quad ,$$

where $\mathcal{K}(\mathbf{x}, \mathbf{y}) = \log|\mathbf{x} - \mathbf{y}|$ or $\mathcal{K}(\mathbf{x}, \mathbf{y}) = K_0(\lambda|\mathbf{x} - \mathbf{y}|)$.

- No solve, just apply
- Weakly singular integrand
- Expensive on an unstructured discretization (adpative quadrature, etc.)
- Fast methods for regular domains
  - Disc solvers
  - "Box codes" (Ethridge and Greengard, Cheng et al., Langston and Zorin)

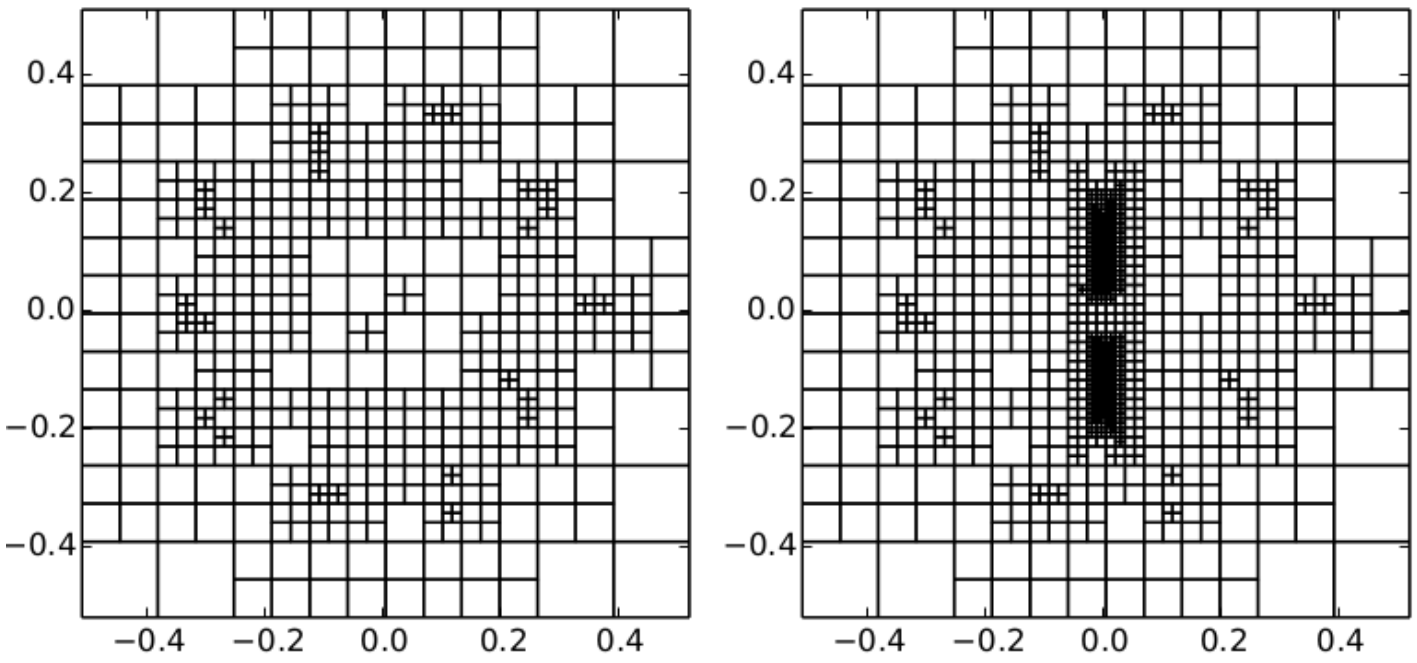
BOX CODES, IN BRIEF

Box codes (typically) work on level-restricted trees and are very efficient (density f defined on leaves):



BOX CODES, IN BRIEF

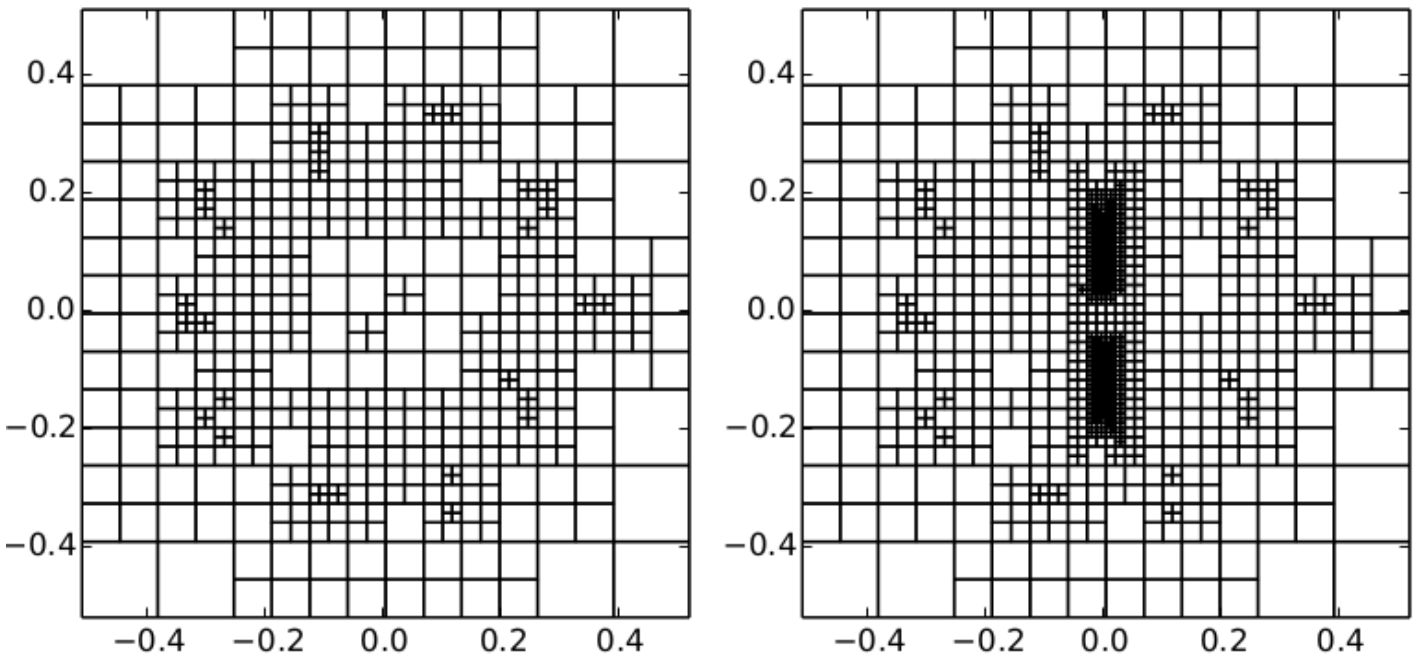
Box codes (typically) work on level-restricted trees and are very efficient (density f defined on leaves):



- Limited number of possible local interactions (precomputation of integrals to near machine precision)

BOX CODES, IN BRIEF

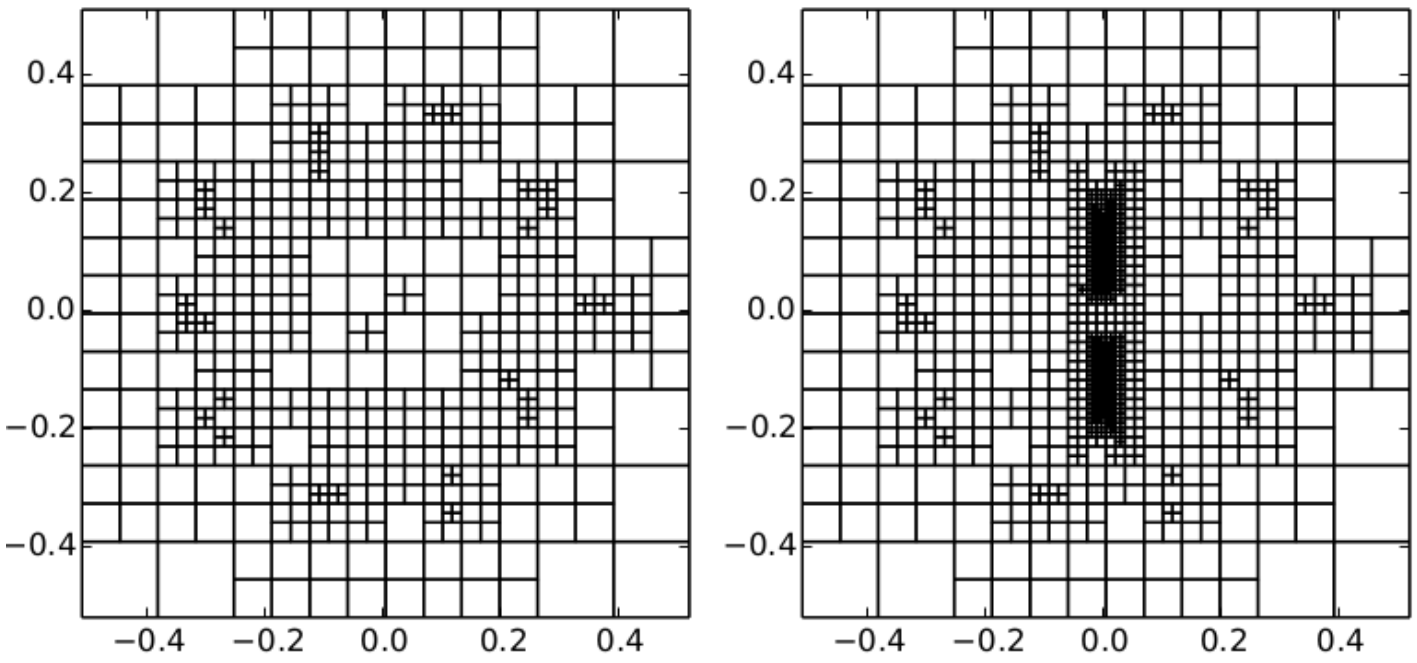
Box codes (typically) work on level-restricted trees and are very efficient (density f defined on leaves):



- Limited number of possible local interactions (precomputation of integrals to near machine precision)
- (plane wave) FMM for far-field

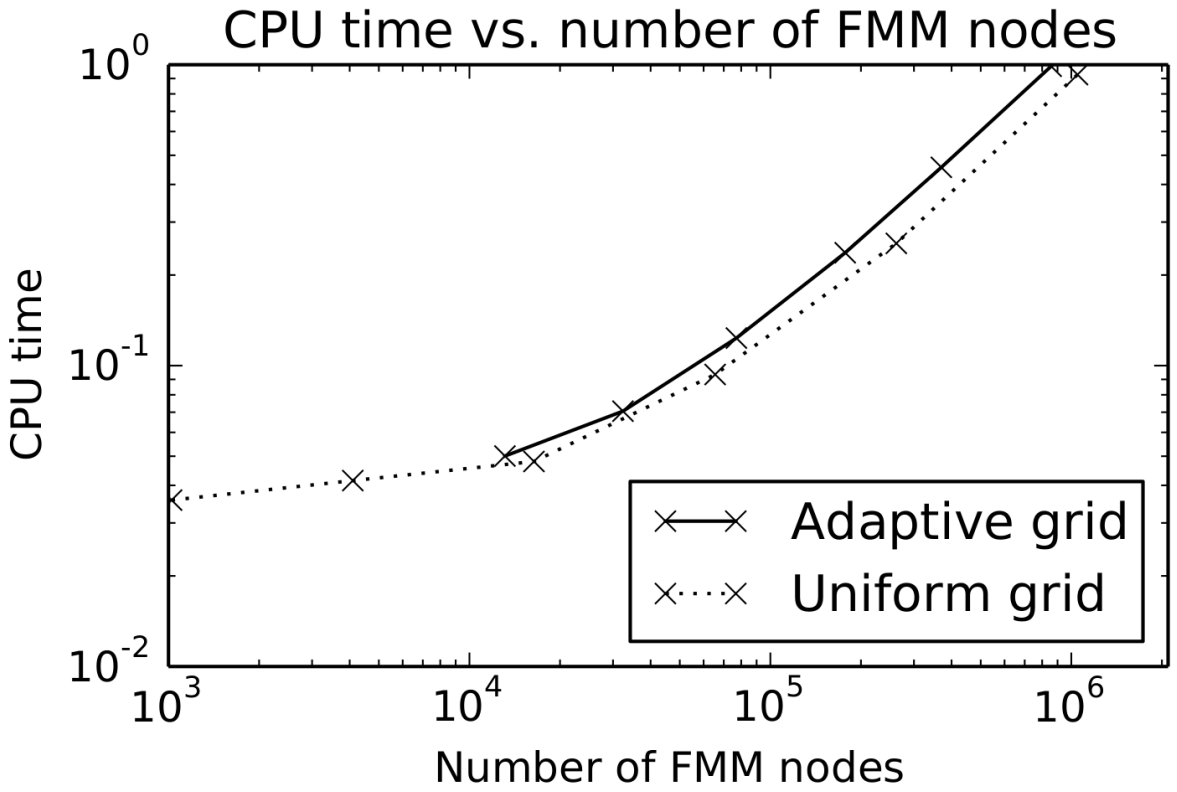
BOX CODES, IN BRIEF

Box codes (typically) work on level-restricted trees and are very efficient (density f defined on leaves):



- Limited number of possible local interactions (precomputation of integrals to near machine precision)
- (plane wave) FMM for far-field
- Very fast, even on adaptive grids

BOX CODE SPEED



BOX CODE ERROR ESTIMATE

The application of a bounded operator is easy to analyze

BOX CODE ERROR ESTIMATE

The application of a bounded operator is easy to analyze

The box code computes the volume integral at **collocation nodes** to a specified precision.

BOX CODE ERROR ESTIMATE

The application of a bounded operator is easy to analyze

The box code computes the volume integral at **collocation nodes** to a specified precision.

Notation:

- $\tilde{f}$: approximation to f by polynomials on each leaf
- $\tilde{V}\tilde{f}(\mathbf{x})$: value of $V\tilde{f}(\mathbf{x})$ computed using box code
- ϵ: precision of FMM

BOX CODE ERROR ESTIMATE

The application of a bounded operator is easy to analyze

The box code computes the volume integral at **collocation nodes** to a specified precision.

Notation:

- $\tilde{f}$: approximation to f by polynomials on each leaf
- $\tilde{V}\tilde{f}(\mathbf{x})$: value of $V\tilde{f}(\mathbf{x})$ computed using box code
- ϵ: precision of FMM

From multipole estimates:

$$|\tilde{V}\tilde{f}(\mathbf{x}) - V\tilde{f}(\mathbf{x})| \leq \epsilon \|\tilde{f}\|_1 \ ,$$

BOX CODE ERROR ESTIMATE

The application of a bounded operator is easy to analyze

The box code computes the volume integral at **collocation nodes** to a specified precision.

Notation:

- $\tilde{f}$: approximation to f by polynomials on each leaf
- $\tilde{V}\tilde{f}(\mathbf{x})$: value of $V\tilde{f}(\mathbf{x})$ computed using box code
- ϵ: precision of FMM

From multipole estimates:

$$|\tilde{V}\tilde{f}(\mathbf{x}) - V\tilde{f}(\mathbf{x})| \leq \epsilon \|\tilde{f}\|_1 \ ,$$

From triangle inequality and boundedness of V:

$$\frac{|\tilde{V}\tilde{f}(\mathbf{x}) - Vf(\mathbf{x})|}{\|\tilde{f}\|_\infty} \leq \epsilon|\Omega| + C(\Omega)\frac{\|f - \tilde{f}\|_\infty}{\|\tilde{f}\|_\infty} \ .$$

BOX CODE ERROR ESTIMATE

The application of a bounded operator is easy to analyze

The box code computes the volume integral at **collocation nodes** to a specified precision.

Notation:

- $\tilde{f}$: approximation to f by polynomials on each leaf
- $\tilde{V}\tilde{f}(\mathbf{x})$: value of $V\tilde{f}(\mathbf{x})$ computed using box code
- ϵ: precision of FMM

From multipole estimates:

$$|\tilde{V}\tilde{f}(\mathbf{x}) - V\tilde{f}(\mathbf{x})| \leq \epsilon \|\tilde{f}\|_1 \ ,$$

From triangle inequality and boundedness of V:

$$\frac{|\tilde{V}\tilde{f}(\mathbf{x}) - Vf(\mathbf{x})|}{\|\tilde{f}\|_\infty} \leq \epsilon|\Omega| + C(\Omega)\frac{\|f - \tilde{f}\|_\infty}{\|\tilde{f}\|_\infty} \ .$$

Gives an a priori error estimate (similar for ∇V).

EMBEDDING IN A BOX

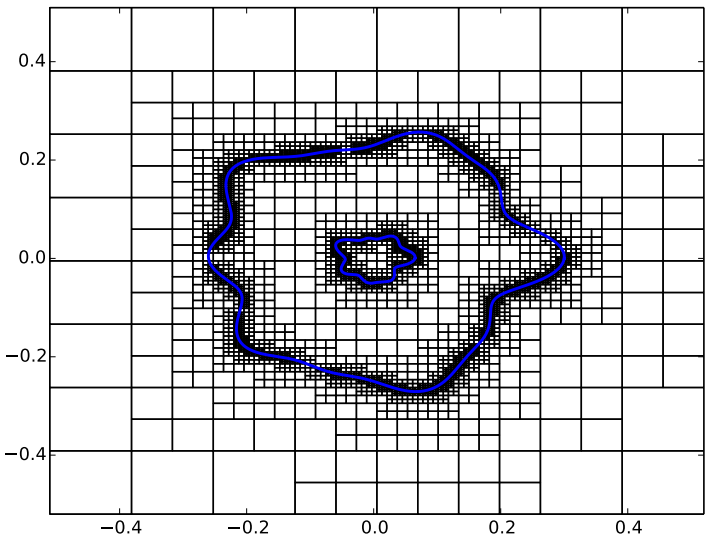


Figure: The domain Ω with an adaptive tree structure overlaying it.

Let Ω be contained in a box Ω_B and let $f_e|_\Omega = f$ be defined on all of Ω_B. Then

$$Vf_e(\mathbf{x}) = \int_{\Omega_B} G_L(\mathbf{x}, \mathbf{y}) f_e(\mathbf{y})\, dy$$

is another particular solution and Vf_e can be computed using a box code.

FUNCTION EXTENSION

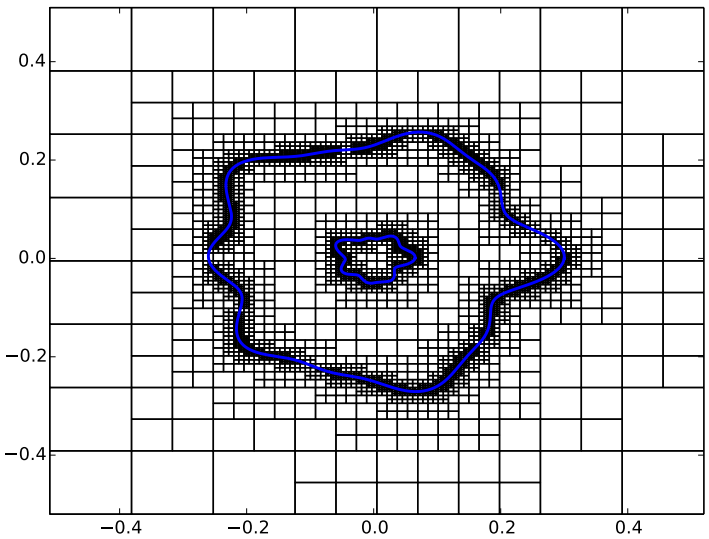


Figure: The domain Ω with an adaptive tree structure overlaying it.

What if a smooth extension f_e is not readily available?

It must be computed in some way.

COMPUTING THE EXTENDED FUNCTION

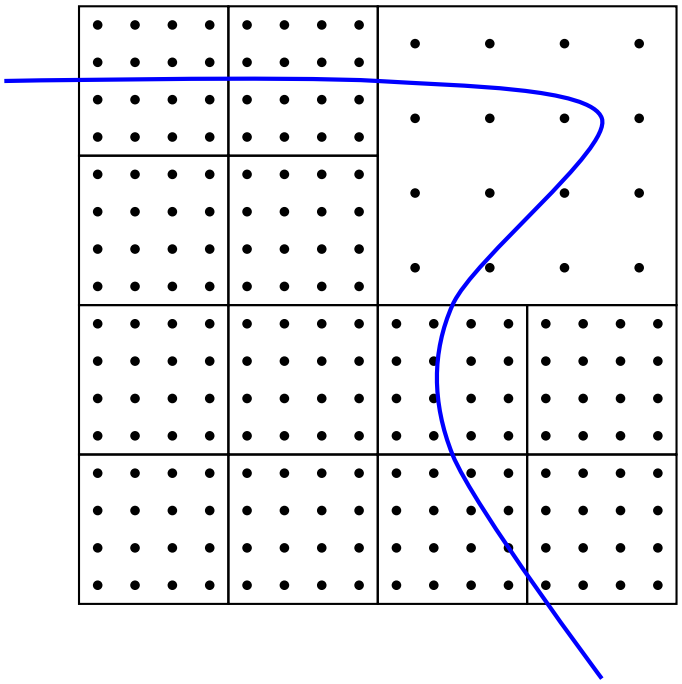


Figure: Example of a "cut-cell".

COMPUTING THE EXTENDED FUNCTION

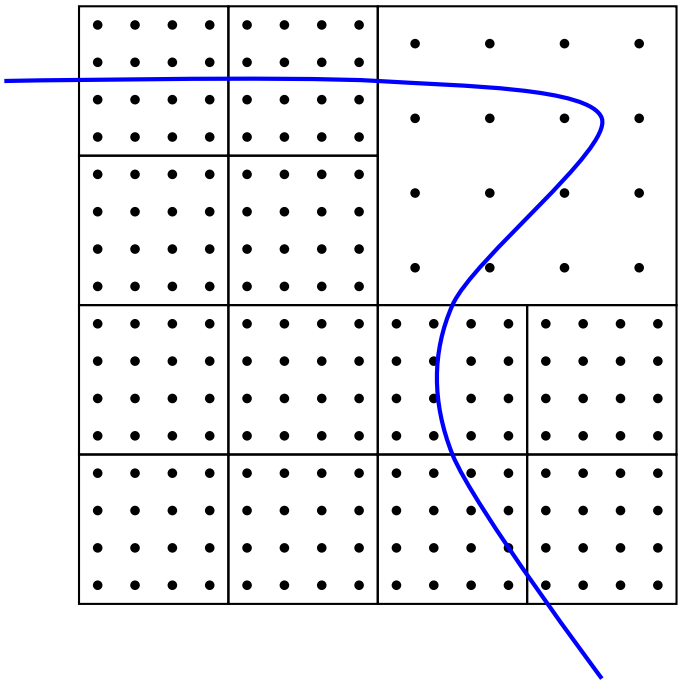


Figure: Example of a "cut-cell".

- Extend by zero
  [Ethridge and Greengard, 2001]

COMPUTING THE EXTENDED FUNCTION

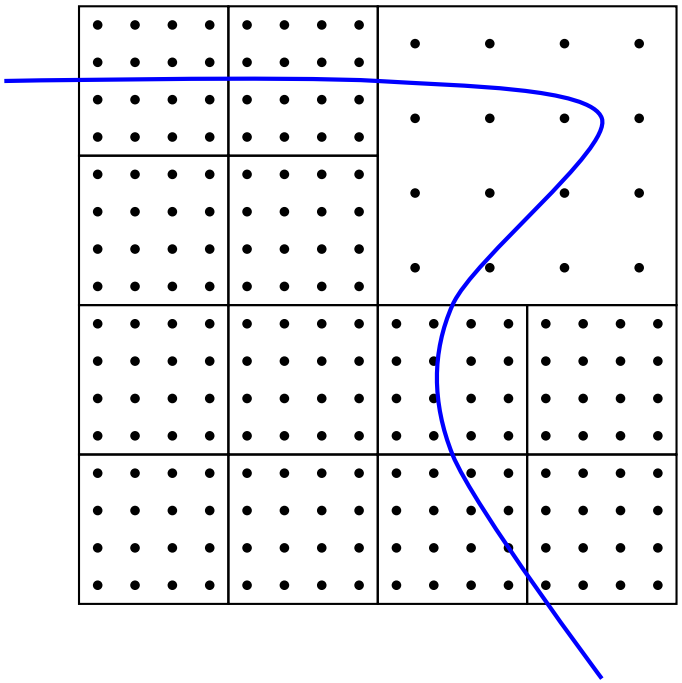


Figure: Example of a "cut-cell".

- Extend by zero
  [Ethridge and Greengard, 2001]
- Local function extension
  [Ethridge, 2000, Langston, 2012]

COMPUTING THE EXTENDED FUNCTION

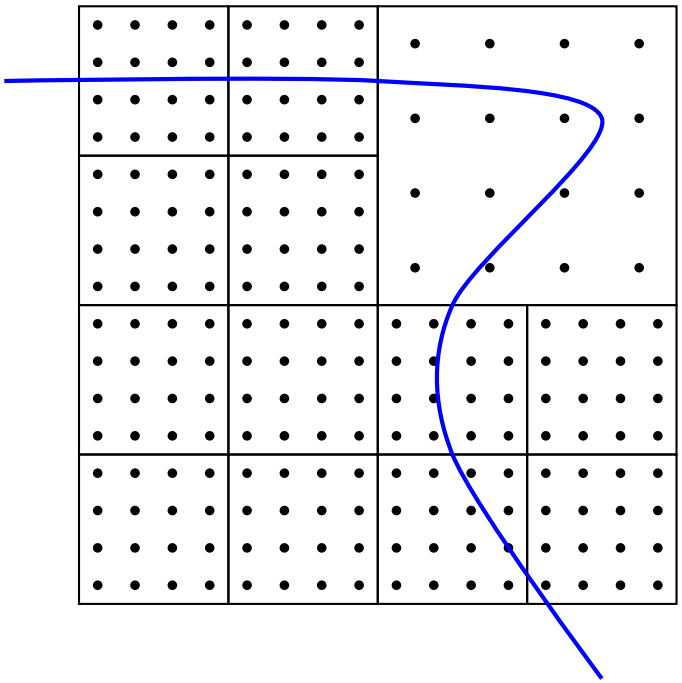


Figure: Example of a "cut-cell".

- Extend by zero
  [Ethridge and Greengard, 2001]
- Local function extension
  [Ethridge, 2000, Langston, 2012]
- Global extension by layer potential
  [Askham, 2016] (C^0) and
  [Rachh and Askham, 2017] (C^1)

COMPUTING THE EXTENDED FUNCTION

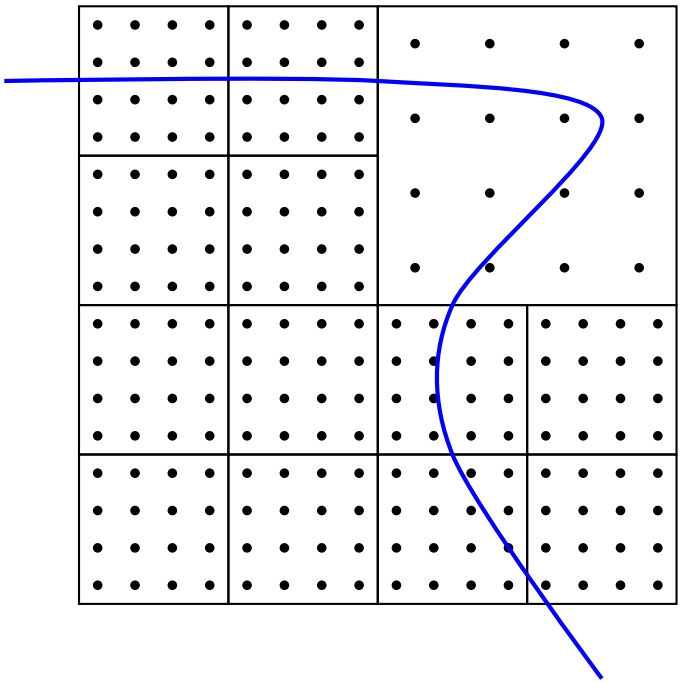


Figure: Example of a "cut-cell".

- Extend by zero
  [Ethridge and Greengard, 2001]
- Local function extension
  [Ethridge, 2000, Langston, 2012]
- Global extension by layer potential
  [Askham, 2016] (C^0) and
  [Rachh and Askham, 2017] (C^1)
- Globalized local extension
  [Fryklund et al., 2017] (PUX)

EXTENSION WITH LAYER POTENTIALS

Let f be defined on Ω with boundary Γ. Then, define a function w on $\mathbb{R}^2 \setminus \Omega$ as the solution of

$$\begin{aligned} \Delta w &= 0 \quad \text{in } \mathbb{R}^2 \setminus \Omega \,, \\ w &= f|_\Gamma \quad \text{on } \Gamma \,. \end{aligned}$$

Then $f_e = f$ on Ω and $f_e = w$ outside is a globally continuous extension of f.

EXTENSION WITH LAYER POTENTIALS

Let f be defined on Ω with boundary Γ. Then, define a function w on $\mathbb{R}^2 \setminus \Omega$ as the solution of

$$\begin{aligned} \Delta w &= 0 \quad \text{in } \mathbb{R}^2 \setminus \Omega \,, \\ w &= f|_\Gamma \quad \text{on } \Gamma \,. \end{aligned}$$

Then $f_e = f$ on Ω and $f_e = w$ outside is a globally continuous extension of f.

- w can be computed using the same numerical tools as for u_h (generalized Gaussian quads, fast solvers, QBX)

EXTENSION WITH LAYER POTENTIALS

Let f be defined on Ω with boundary Γ. Then, define a function w on $\mathbb{R}^2 \setminus \Omega$ as the solution of

$$\begin{aligned} \Delta w &= 0 \quad \text{in } \mathbb{R}^2 \setminus \Omega \,, \\ w &= f|_\Gamma \quad \text{on } \Gamma \,. \end{aligned}$$

Then $f_e = f$ on Ω and $f_e = w$ outside is a globally continuous extension of f.

- w can be computed using the same numerical tools as for u_h (generalized Gaussian quads, fast solvers, QBX)
- smoother extensions can be obtained as solutions of polyharmonic problems.

ERROR ESTIMATE FOR NON-SMOOTH f_e

Recall the a priori error bound

$$\frac{|\tilde{V}\tilde{f}_e(\mathbf{x}) - Vf_e(\mathbf{x})|}{\|\tilde{f}_e\|_\infty} \leq \epsilon|\Omega| + C(\Omega)\frac{\|f_e - \tilde{f}_e\|_\infty}{\|\tilde{f}_e\|_\infty}$$

ERROR ESTIMATE FOR NON-SMOOTH f_e

Recall the a priori error bound

$$\frac{|\tilde{V}\tilde{f}_e(\mathbf{x}) - Vf_e(\mathbf{x})|}{\|\tilde{f}_e\|_\infty} \leq \epsilon|\Omega| + C(\Omega)\frac{\|f_e - \tilde{f}_e\|_\infty}{\|\tilde{f}_e\|_\infty}$$

Implied convergence rate

	Conv. Order Vf	Conv. Order ∇Vf
zero extension	0	0
C^0 extension	1	1
C^1 extension	2	2

ERROR ESTIMATE FOR NON-SMOOTH f_e

Recall the a priori error bound

$$\frac{|\tilde{V}\tilde{f}_e(\mathbf{x}) - Vf_e(\mathbf{x})|}{\|\tilde{f}_e\|_\infty} \leq \epsilon|\Omega| + C(\Omega)\frac{\|f_e - \tilde{f}_e\|_\infty}{\|\tilde{f}_e\|_\infty}$$

Implied convergence rate

	Conv. Order Vf	Conv. Order ∇Vf
zero extension	0	0
C^0 extension	1	1
C^1 extension	2	2

These aren't amazing. What rate do we observe?

POISSON EQUATION EXAMPLES

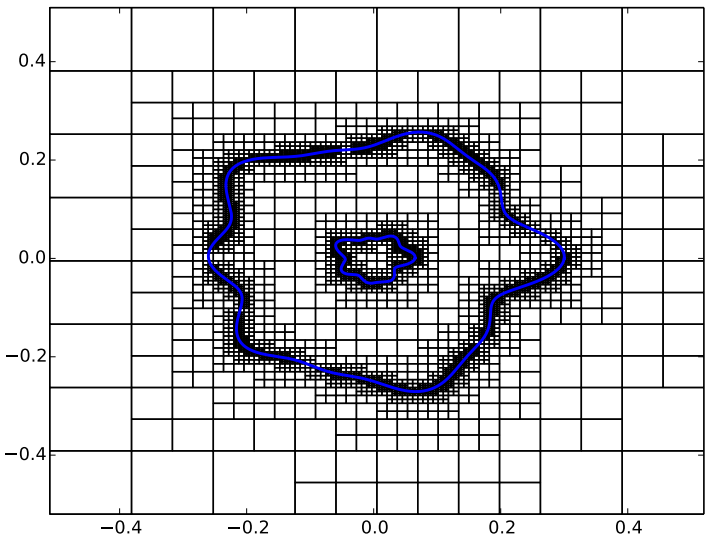


Figure: The domain Ω with an adaptive tree structure overlaying it.

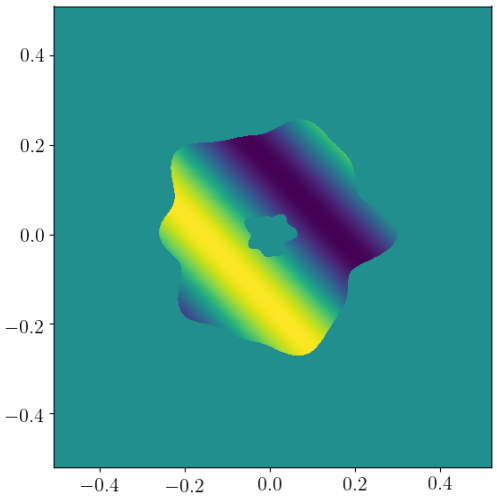
$$\begin{aligned} \Delta u &= f \quad \text{in } \Omega \,, \\ u &= u_b \quad \text{on } \Gamma \,. \end{aligned}$$

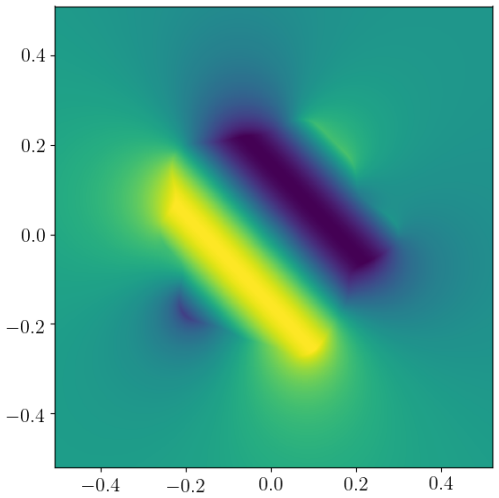
We set f and u_b so that the solution u is given by

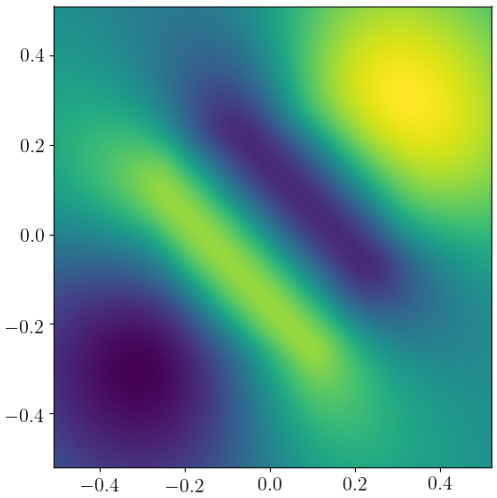
$$u(\mathbf{x}) = \sin(10(x_1+x_2))+x_1^2-3x_2+8 \,.$$

EXTENDED f

We extend f using the method and tools described above.

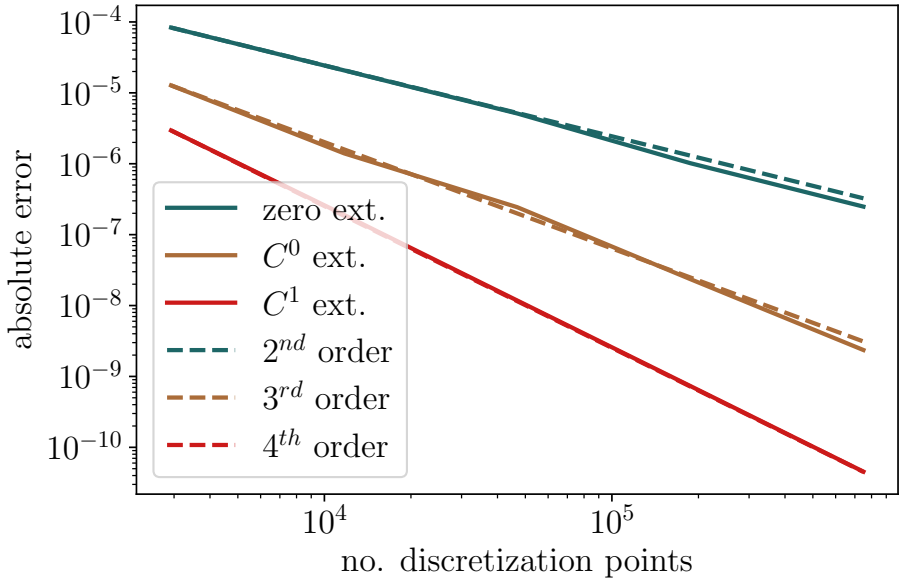




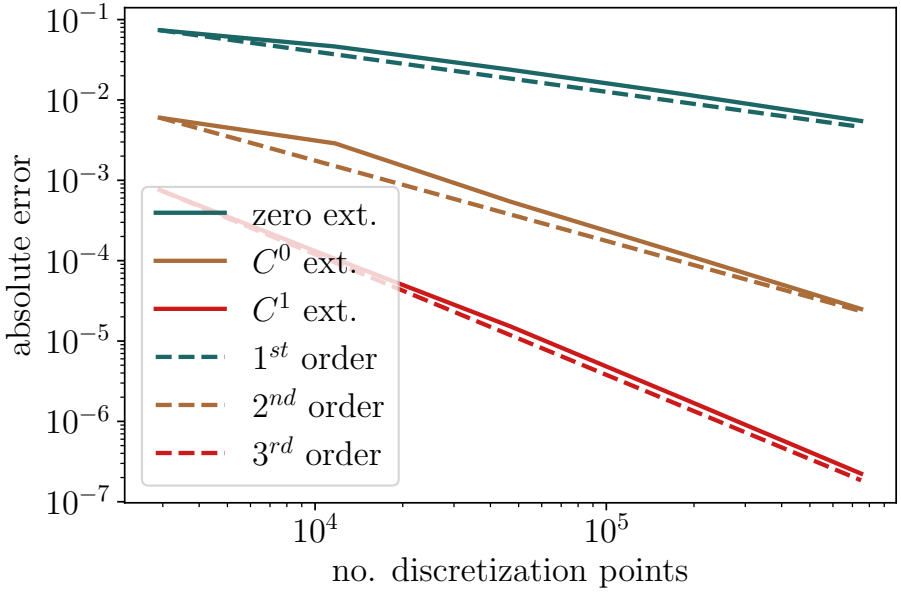


CONVERGENCE RATE (UNIFORM GRID)

Error in potential

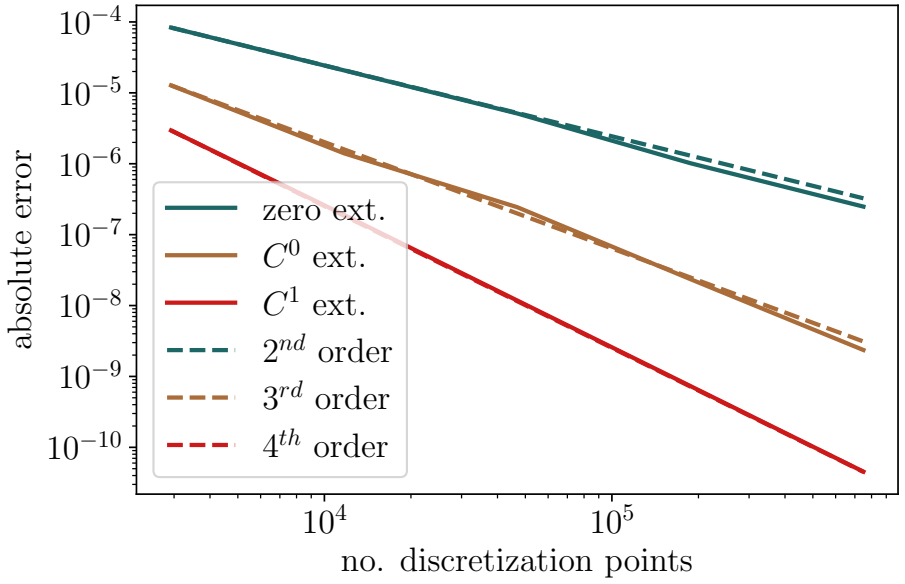


Error in gradient

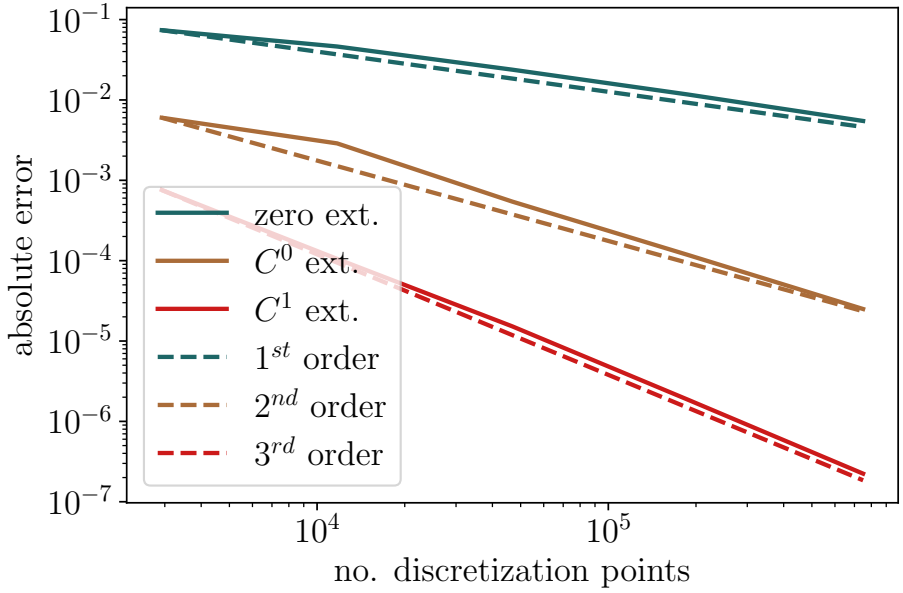


CONVERGENCE RATE (UNIFORM GRID)

Error in potential



Error in gradient

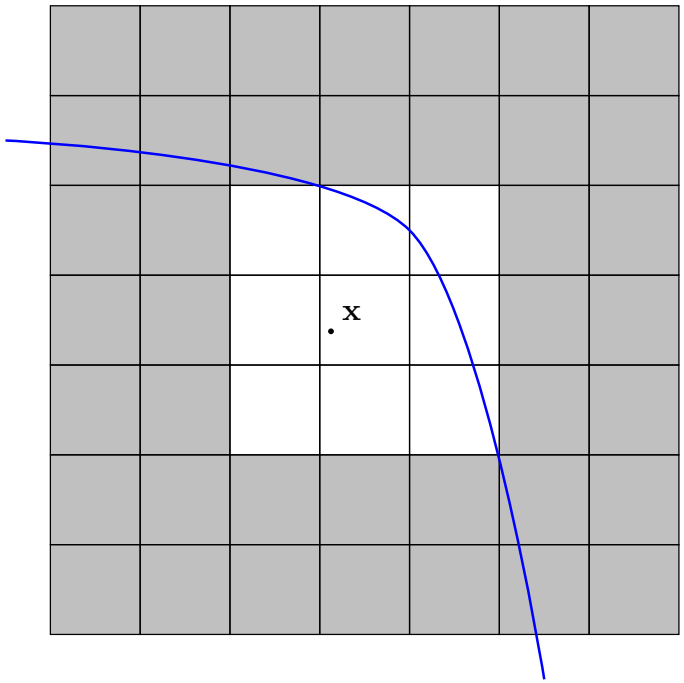


	Conv. Order u		Conv. Order ∇u	
	predicted	observed	predicted	observed
zero extension	0	2	0	1
C^0 extension	1	3	1	2
C^1 extension	2	4	2	3

OBSERVED CONVERGENCE RATE

To see that you gain 1 order:

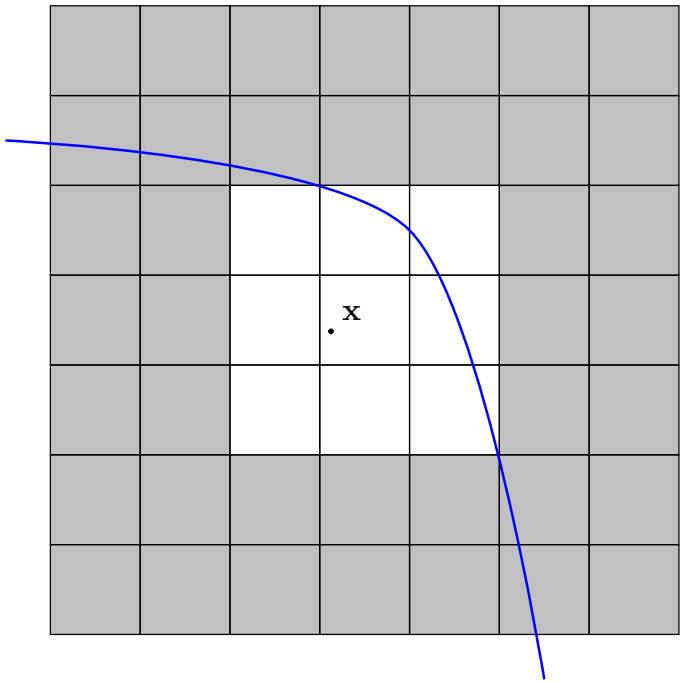
$$v(\mathbf{x}) = -\frac{1}{2\pi}\int \log\|\mathbf{x}-\mathbf{y}\| f(\mathbf{y})\,dy\,,\ \nabla v(\mathbf{x}) = -\frac{1}{2\pi}\int \frac{\mathbf{x}-\mathbf{y}}{\|\mathbf{x}-\mathbf{y}\|^2} f(\mathbf{y})\,dy$$



OBSERVED CONVERGENCE RATE

To see that you gain 1 order:

$$v(\mathbf{x}) = -\frac{1}{2\pi}\int \log\|\mathbf{x}-\mathbf{y}\| f(\mathbf{y})\,dy\,,\ \nabla v(\mathbf{x}) = -\frac{1}{2\pi}\int \frac{\mathbf{x}-\mathbf{y}}{\|\mathbf{x}-\mathbf{y}\|^2} f(\mathbf{y})\,dy$$

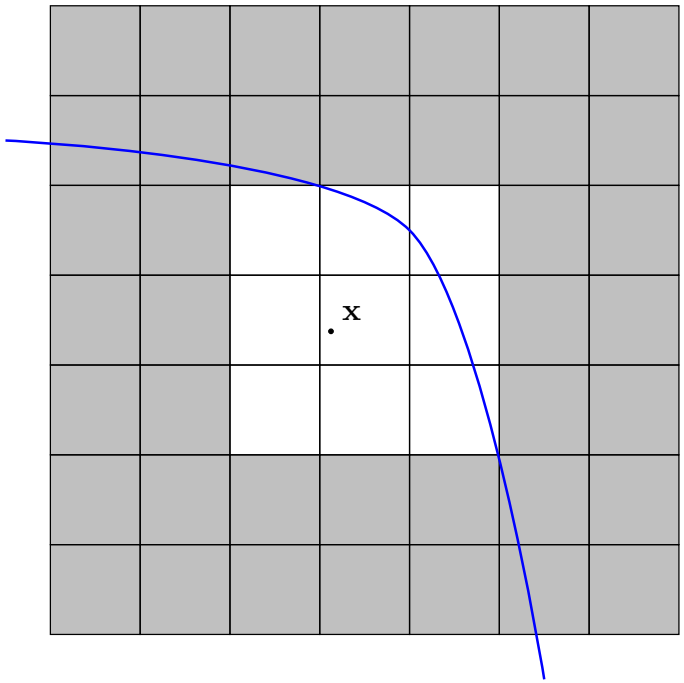


- Local contribution gets weighted by area of a cell (gain h^2 for $\log r$ and h for $1/r$)

OBSERVED CONVERGENCE RATE

To see that you gain 1 order:

$$v(\mathbf{x}) = -\frac{1}{2\pi}\int \log\|\mathbf{x}-\mathbf{y}\| f(\mathbf{y})\,dy\,,\ \nabla v(\mathbf{x}) = -\frac{1}{2\pi}\int \frac{\mathbf{x}-\mathbf{y}}{\|\mathbf{x}-\mathbf{y}\|^2} f(\mathbf{y})\,dy$$

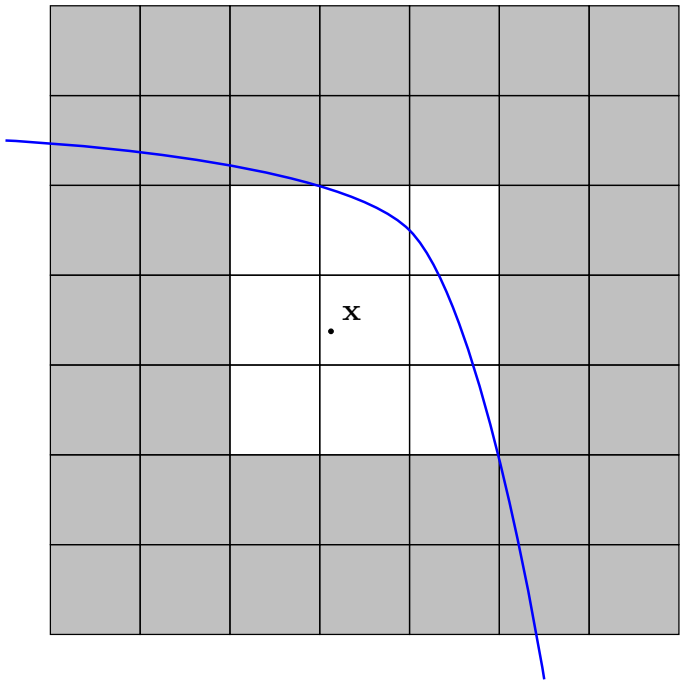


- Local contribution gets weighted by area of a cell (gain h^2 for $\log r$ and h for $1/r$)
- For the far-field, only $O(1/h)$ of the boxes are irregular (have to add up carefully for gradient) and each is area h^2

OBSERVED CONVERGENCE RATE

To see that you gain 1 order:

$$v(\mathbf{x}) = -\frac{1}{2\pi}\int \log\|\mathbf{x}-\mathbf{y}\| f(\mathbf{y})\,dy\,,\ \nabla v(\mathbf{x}) = -\frac{1}{2\pi}\int \frac{\mathbf{x}-\mathbf{y}}{\|\mathbf{x}-\mathbf{y}\|^2} f(\mathbf{y})\,dy$$



- Local contribution gets weighted by area of a cell (gain h^2 for $\log r$ and h for $1/r$)
- For the far-field, only $O(1/h)$ of the boxes are irregular (have to add up carefully for gradient) and each is area h^2

The gain of 2 orders for u is somewhat mysterious!

ADAPTIVE GRIDDING STRATEGIES

What are good (a priori) strategies for adaptive grids? Recall that $\tilde{f}_e$ is the local polynomial interpolant on each box.

ADAPTIVE GRIDDING STRATEGIES

What are good (a priori) strategies for adaptive grids? Recall that $\tilde{f}_e$ is the local polynomial interpolant on each box.

1. Enforce that $\|f_e - \tilde{f}_e\| \leq \text{tol}$ on each leaf

ADAPTIVE GRIDDING STRATEGIES

What are good (a priori) strategies for adaptive grids? Recall that $\tilde{f}_e$ is the local polynomial interpolant on each box.

1. Enforce that $\|f_e - \tilde{f}_e\| \leq \text{tol}$ on each leaf
2. Enforce that $h^2\|f_e - \tilde{f}_e\| \leq \text{tol}$ on each leaf

ADAPTIVE GRIDDING STRATEGIES

What are good (a priori) strategies for adaptive grids? Recall that $\tilde{f}_e$ is the local polynomial interpolant on each box.

1. Enforce that $\|f_e - \tilde{f}_e\| \leq \text{tol}$ on each leaf
2. Enforce that $h^2\|f_e - \tilde{f}_e\| \leq \text{tol}$ on each leaf
3. Enforce that $h\|f_e - \tilde{f}_e\| \leq \text{tol}$ on each leaf

ADAPTIVE GRIDDING STRATEGIES

What are good (a priori) strategies for adaptive grids? Recall that $\tilde{f}_e$ is the local polynomial interpolant on each box.

1. Enforce that $\|f_e - \tilde{f}_e\| \leq \text{tol}$ on each leaf
2. Enforce that $h^2\|f_e - \tilde{f}_e\| \leq \text{tol}$ on each leaf
3. Enforce that $h\|f_e - \tilde{f}_e\| \leq \text{tol}$ on each leaf
4. Hybrid: enforce one criterion on irregular boxes and another on regular boxes (these perform best)

ADAPTIVE GRIDDING STRATEGIES

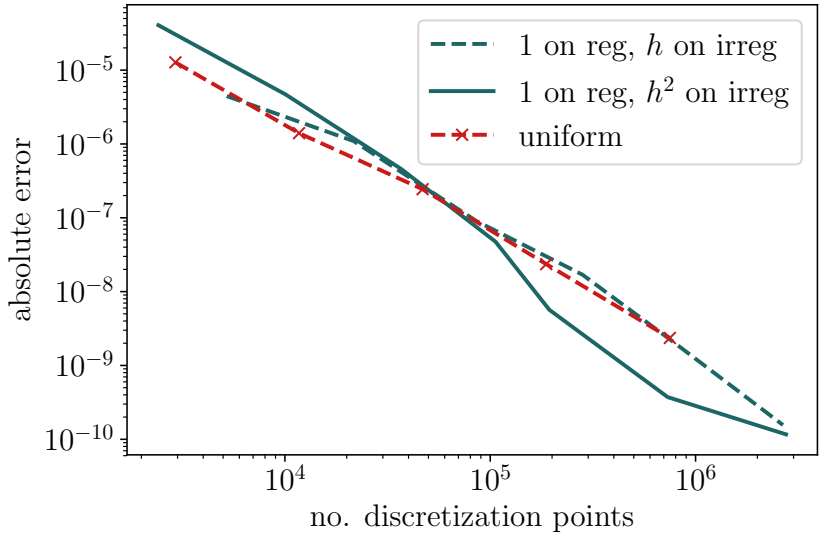
What are good (a priori) strategies for adaptive grids? Recall that $\tilde{f}_e$ is the local polynomial interpolant on each box.

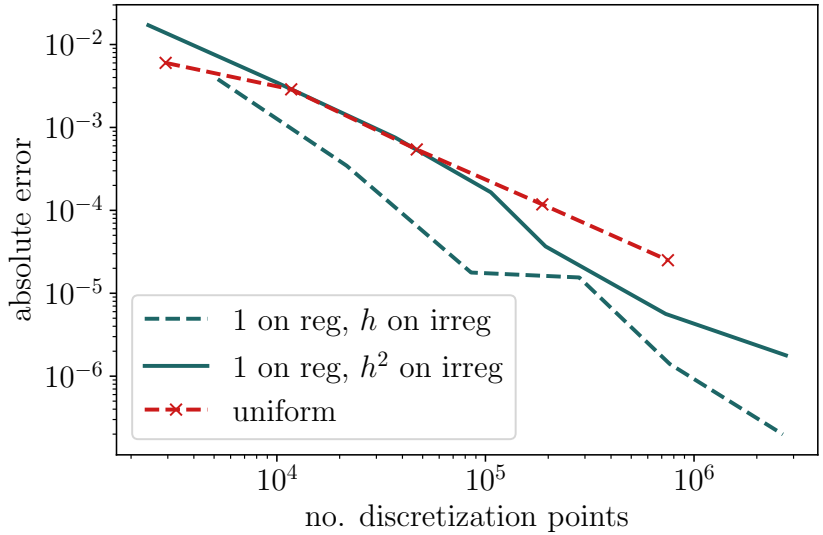
1. Enforce that $\|f_e - \tilde{f}_e\| \leq \text{tol}$ on each leaf
2. Enforce that $h^2\|f_e - \tilde{f}_e\| \leq \text{tol}$ on each leaf
3. Enforce that $h\|f_e - \tilde{f}_e\| \leq \text{tol}$ on each leaf
4. Hybrid: enforce one criterion on irregular boxes and another on regular boxes (these perform best)

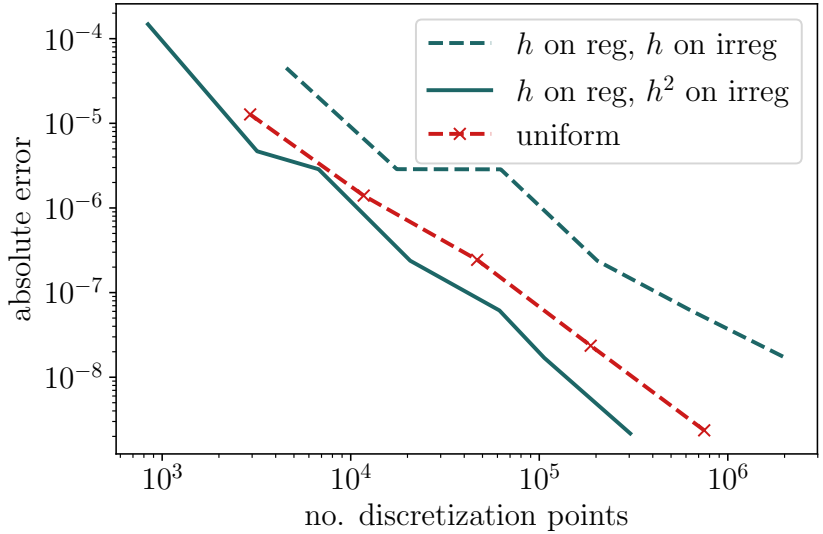
Note that by storing local expansions and QBX expansions from a QBX FMM, the QBX method gives you an oracle for f_e

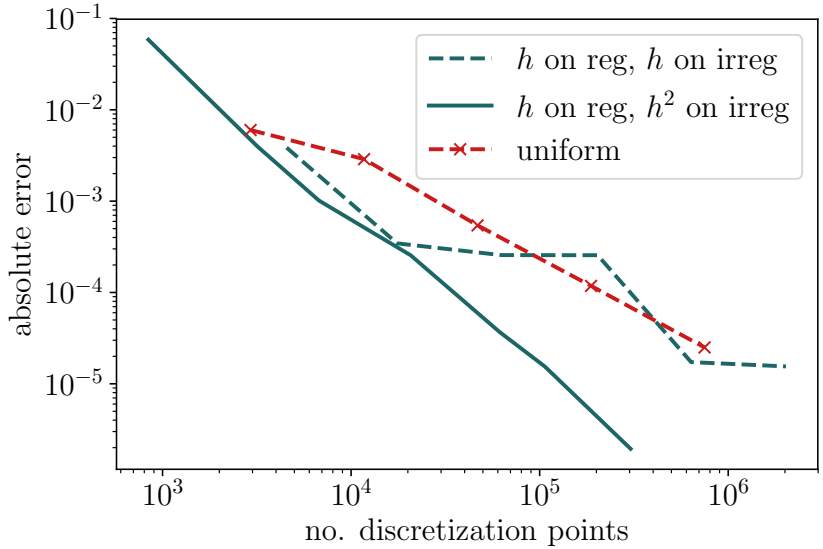
ADAPTIVE PERFORMANCE

Results for hybrid schemes









MORE DIFFICULT PROBLEM

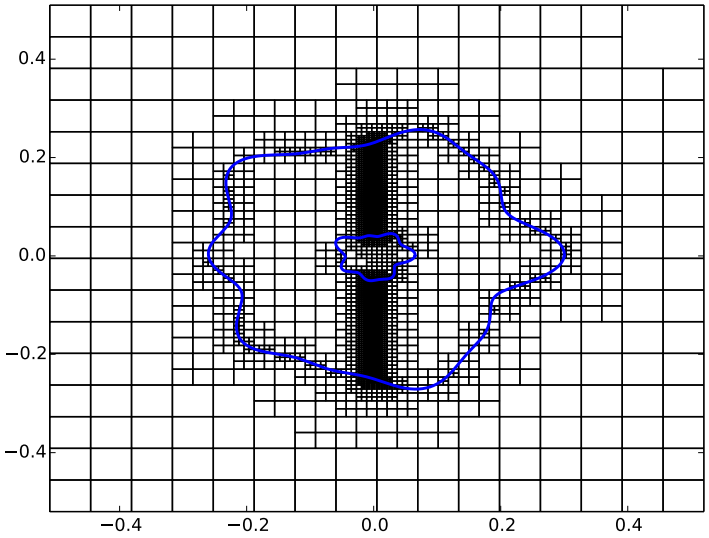


Figure: Adaptive box structure.

$$\begin{aligned} \Delta u &= f \quad \text{in } \Omega \,, \\ u &= u_b \quad \text{on } \Gamma \,. \end{aligned}$$

We set f and u_b so that the solution u is given by

$$\begin{aligned} u(\mathbf{x}) &= \sin(10(x_1 + x_2)) + x_1^2 \\ &\quad -3x_2 + 8 + e^{-(500x_1)^2} \,, \end{aligned}$$

which requires lots of refinement near the x_2 axis.

ERROR (ADAPTIVE PERFORMANCE)

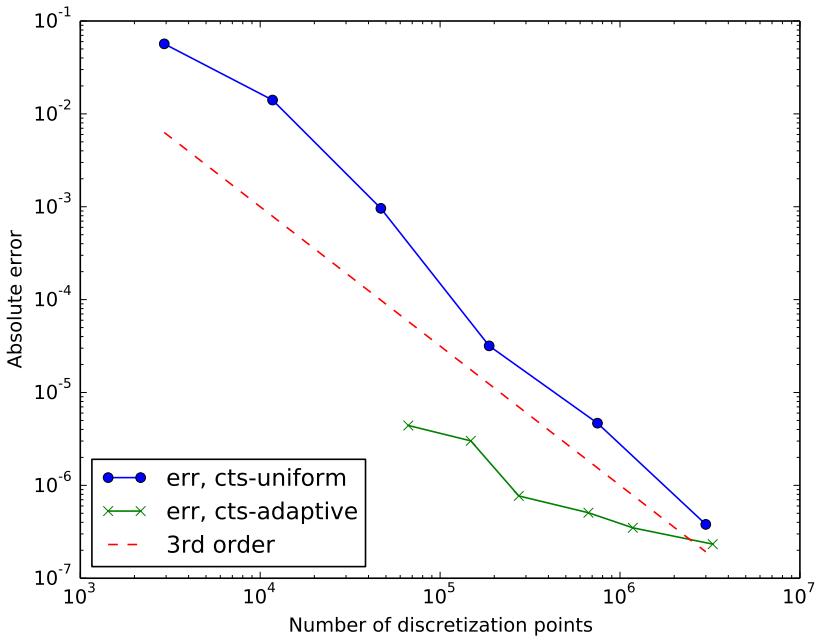


Figure: Error in potential vs. number of discretization nodes

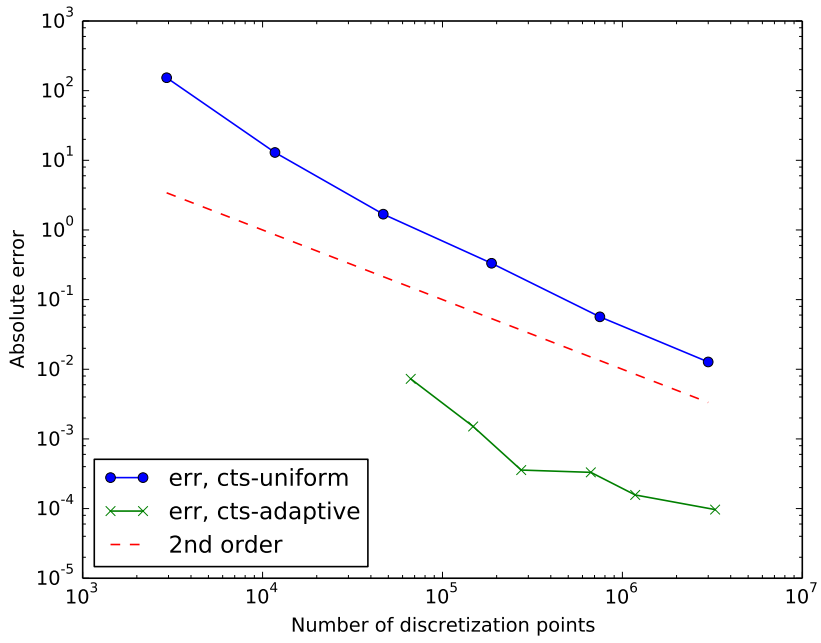


Figure: Error in gradient vs. number of discretization nodes

FUTURE WORK

Some plans

- Apply modified biharmonic FMM to Navier-Stokes integral equation methods
- Release wrapped solver with latest and greatest QBX implementation
- Implement adaptive-friendly version of biharmonic code

THANK YOU

Thank you.

BIBLIOGRAPHY I

[Askham, 2016] Askham, T. (2016).
Integral-equation methods for inhomogeneous elliptic partial differential equations in complex geometry.
PhD thesis, New York University.

[Askham, 2017] Askham, T. (2017).
A stabilized separation of variables method for the modified biharmonic equation.
arXiv preprint arXiv:1710.05408.

[Askham and Cerfon, 2017] Askham, T. and Cerfon, A. J. (2017).
An adaptive fast multipole accelerated poisson solver for complex geometries.
Journal of Computational Physics, 344:1–22.

[Biros et al., 2002] Biros, G., Ying, L., and Zorin, D. (2002).
The embedded boundary integral method for the incompressible navier-stokes equations.
In *Proceedings of the International Association for Boundary Element Methods 2002 Symposium*.

[Cheng et al., 2006] Cheng, H., Huang, J., and Leiterman, T. J. (2006).
An adaptive fast solver for the modified helmholtz equation in two dimensions.
Journal of Computational Physics, 211(2):616–637.

[Ethridge and Greengard, 2001] Ethridge, F. and Greengard, L. (2001).
A new fast-multipole accelerated poisson solver in two dimensions.
SIAM Journal on Scientific Computing, 23(3):741–760.

[Ethridge, 2000] Ethridge, J. F. (2000).
Fast algorithms for volume integrals in potential theory.
PhD thesis, New York University.

[Fryklund et al., 2017] Fryklund, F., Lehto, E., and Tornberg, A.-K. (2017).
Partition of unity extension of functions on complex domains.
arXiv preprint arXiv:1712.08461.

BIBLIOGRAPHY II

[Greengard and Rokhlin, 1987] Greengard, L. and Rokhlin, V. (1987).
A fast algorithm for particle simulations.
Journal of computational physics, 73(2):325–348.

[Langston, 2012] Langston, M. H. (2012).
An Adaptive Fast Multipole Method-Based PDE Solver in Three Dimensions.
PhD thesis, New York University.

[Malhotra et al., 2017] Malhotra, D., Rahimian, A., Zorin, D., and Biros, G. (2017).
A parallel algorithm for long-timescale simulation of concentrated vesicle suspensions in three dimensions.
preprint.

[Mayo, 1984] Mayo, A. (1984).
The fast solution of poisson's and the biharmonic equations on irregular regions.
SIAM Journal on Numerical Analysis, 21(2):285–299.

[McKenney et al., 1995] McKenney, A., Greengard, L., and Mayo, A. (1995).
A fast poisson solver for complex geometries.
Journal of Computational Physics, 118(2):348–355.

[Ojala, 2012] Ojala, R. (2012).
A robust and accurate solver of laplace's equation with general boundary conditions on general domains in the plane.
Journal of Computational Mathematics, 30(4):433–448.

[Rachh and Askham, 2017] Rachh, M. and Askham, T. (2017).
Integral equation formulation of the biharmonic dirichlet problem.
Journal of Scientific Computing, pages 1–20.