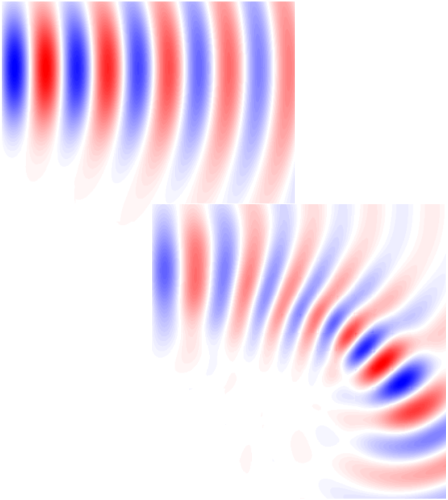

Fast Multipole Methods for Continuous Charge Densities

Travis Askham — New Jersey Institute of Technology
SIAM Conference on Image Science 2020 (IS20), via Zoom.




Joint work with

- Libin Lu (Flatiron Institute)
- Manas Rachh (Flatiron Institute)
- Alex Townsend (Cornell)
- Leslie Greengard (NYU)

This work was supported by the Flatiron Institute.

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`askham@njit.edu`

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Outline

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- Example: scattering in variable media

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    - On-demand quadrature generation scheme

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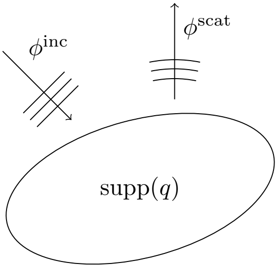
  - Fast multipole method overview
  - On-demand quadrature generation scheme
- Future work

Scattering in variable media

$$(\Delta + k^2(1+q(\mathbf{x})))\phi = 0$$



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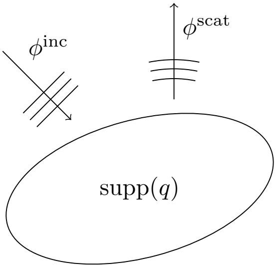


$$(\Delta + k^2(1 + q(\mathbf{x})))\phi = 0$$

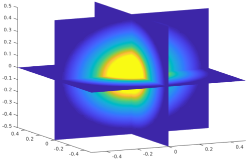
Setting $\phi = \phi^{\mathrm{inc}} + \phi^{\mathrm{scat}}$,

$$(\Delta+k^2(1+q(\mathbf{x})))\phi^{\mathrm{scat}} = -k^2 q(\mathbf{x})\phi^{\mathrm{inc}} \ .$$

- ϕ^{inc} is an *incident* wave which satisfies the constant coefficient Helmholtz equation (e.g. a plane wave)
- ϕ^{scat} is the *scattered* wave which satisfies an outgoing condition at infinity.

Scattering example[1]

- Let $q(\mathbf{x})$ correspond to an "Eaton" lens, which bends light through an angle

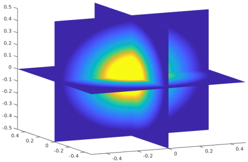


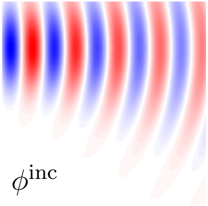
[1] Vico, Greengard, and Ferrando 2016; Danner and Leonhardt 2009.

Scattering example[1]

- Let $q(\mathbf{x})$ correspond to an "Eaton" lens, which bends light through an angle
- Let ϕ^{inc} be a Gaussian beam

$$\phi^{\text{inc}}(\mathbf{x}) = G_k(\mathbf{x}, \mathbf{z}) e^{-k/2} \;,$$
$$\mathbf{z} = (x_0 + i/2, y_0, z_0)$$





ϕ^{inc}

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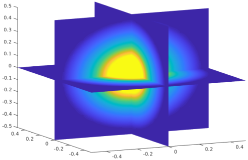
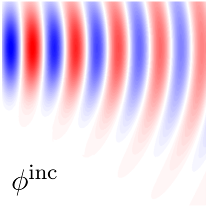
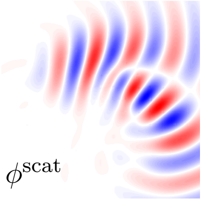
- Solve for scattered field







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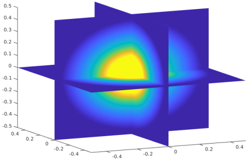
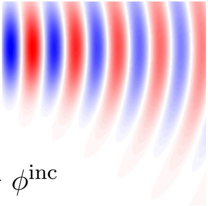
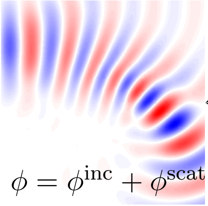
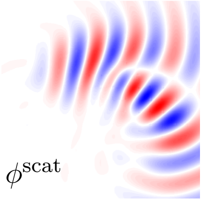




ϕ^{inc}



$\phi = \phi^{\mathrm{inc}} + \phi^{\mathrm{scat}}$



ϕ^{scat}

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Integral equation formulation

$$(\Delta + k^2(1 + q(\mathbf{x})))\phi^{\mathrm{scat}} = -k^2 q(\mathbf{x})\phi^{\mathrm{inc}}$$

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Represent ϕ^{scat} as a *volume integral*, i.e.

$$\phi^{\text{scat}}(\mathbf{x}) = V[\sigma](\mathbf{x}) = \int_\Omega G_k(\mathbf{x},\mathbf{y})\sigma(\mathbf{y})\,dv\ , \ \ G_k(\mathbf{x},\mathbf{y}) = \begin{cases} \frac{e^{ik|\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|} \\ \\ \frac{iH_0^{(1)}(k|\mathbf{x}-\mathbf{y}|)}{4} \end{cases}$$

where $\operatorname{supp}(q) \subset \Omega$.

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where $\mathrm{supp}(q) \subset \Omega$. Then

$$\sigma(\mathbf{x}) + k^2 q(\mathbf{x}) V[\sigma](\mathbf{x}) = -k^2 q(\mathbf{x})\phi^{\mathrm{inc}}\ ,$$

which is a second-kind integral equation on $L^2(\Omega)$.

The need for speed

Solving

$$\sigma(\mathbf{x}) + k^2 q(\mathbf{x}) V[\sigma](\mathbf{x}) = -k^2 q(\mathbf{x}) \phi^{\mathrm{inc}}$$

- Apply quadrature to discretize the integral $V[\sigma]$. Resolving σ requires at least $O(k^d)$ nodes in $\mathbb{R}^d$.

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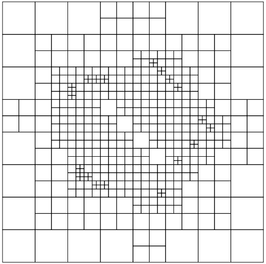
- Apply quadrature to discretize the integral $V[\sigma]$. Resolving σ requires at least $O(k^d)$ nodes in $\mathbb{R}^d$.
- Solve iteratively (e.g. GMRES or BICGstab)
- Need a fast method for $V[\sigma]$, which is a dense operator.

Box codes[2]

$$V[\sigma](\mathbf{x}_i) = \int_\Omega G_k(\mathbf{x}_i, \mathbf{y})\sigma(\mathbf{y})\, dv$$

$\Omega = [-L/2, L/2]^d$



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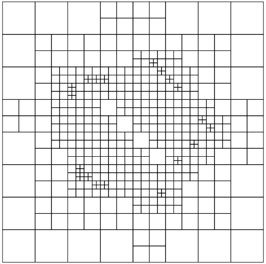

$$V[\sigma](\mathbf{x}_i) = \int_\Omega G_k(\mathbf{x}_i, \mathbf{y})\sigma(\mathbf{y})\, dv \;\approx\; \sum_{j=1}^{N_b} \int_{B_j} G_k(\mathbf{x}_i, \mathbf{y}) p_j(2(\mathbf{y} - \mathbf{y}_j)/L_j)\, dv$$

- N_b boxes, B_j, are leaves of a (balanced) quadtree/octree, which can be adaptively refined to capture small features

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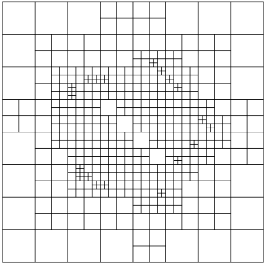

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- $\sigma|_{B_j}(\mathbf{y}) \approx p_j(2(\mathbf{y} - \mathbf{y}_j)/L_j)$ with coefficients in

$$\mathcal{L}_M^{(d)} = \{P_{p_1}(y_1)P_{p_2}(y_2)\cdots P_{p_d}(y_d) \text{ s.t. } p_1{+}p_2{+}\cdots{+}p_d < M\}$$

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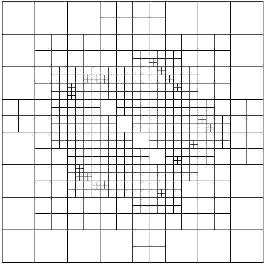

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- $\mathbf{x}_i$ are M^d scaled, tensor-product Legendre nodes on each leaf.

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$$\sum_{j=1}^{N_b} \int_{B_j} G_k(\mathbf{x}_i, \mathbf{y}) p_j(\mathbf{y})\, dv$$

Naïve evaluation at all targets $\mathbf{x}_i$ costs $O(N_b^2)$.

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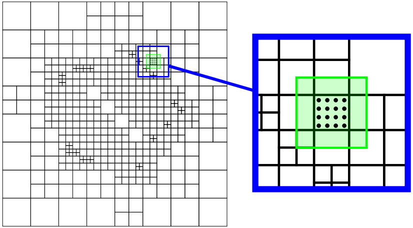

Outside of green box — smooth quadrature sufficient

$$\int_B G_k(\mathbf{x}, \mathbf{y}) \sigma(\mathbf{y})\, dv \approx$$

$$\underbrace{\sum_{l=1}^{N_p} G_k(\mathbf{x}, \mathbf{y}_l(B)) p[\sigma; B](\mathbf{y}_l(B)) w_l(B)}_{\text{“equivalent charges”}}$$

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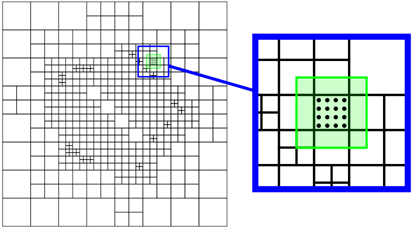

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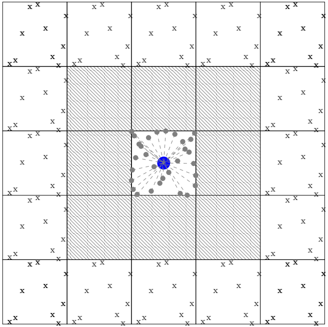
The FMM can compute the separated interactions for equivalent charges in $O(N_b \log(1/\epsilon))$.

FMM basics (far field)

Multipole expansions for well-separated targets



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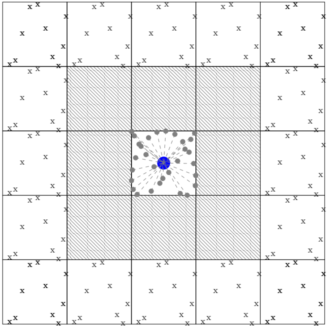
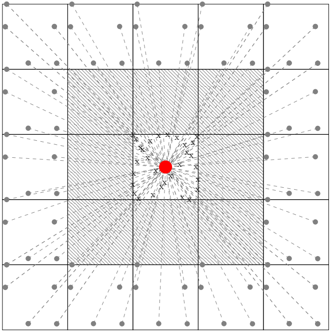
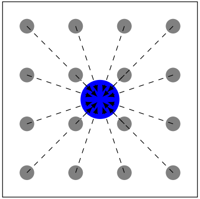


Local expansions for well-separated sources



FMM basics (far field)

Form multipoles (leaves)



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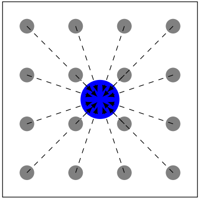
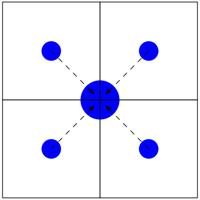


Merge multipoles
(upward pass)



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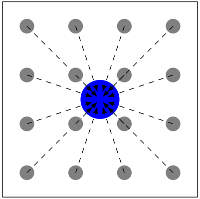

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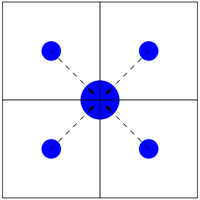
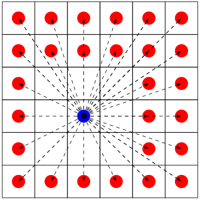


Multipole to local



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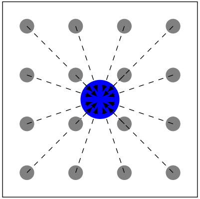

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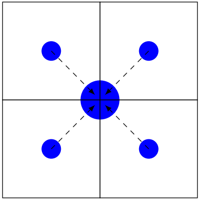

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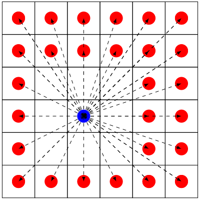
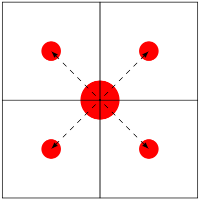


Local to local (downward pass)



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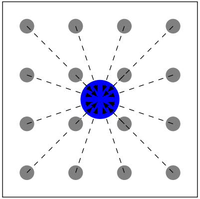

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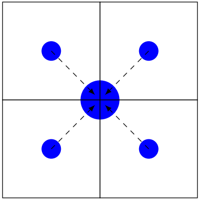

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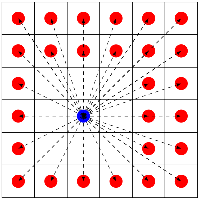

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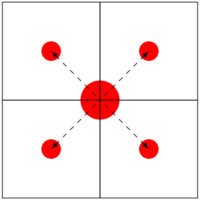
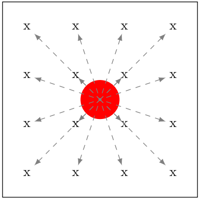


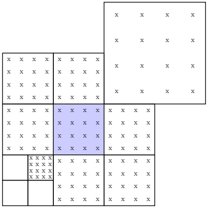
Evaluate local (leaves)



Local work in a box code

$$\int_{B_j} G_k(\mathbf{x},\mathbf{y}) p_j(2(\mathbf{y}-\mathbf{y}_j)/L_j)\, dv$$

These integrals on self and neighbors are weakly singular/ near singular and require special quadrature.



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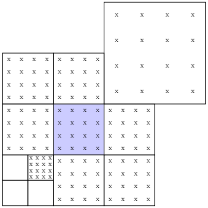
Simplifications



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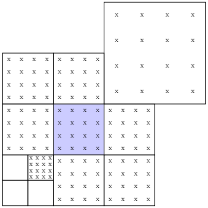

Simplifications

- Linearity: compute for basis and recombine

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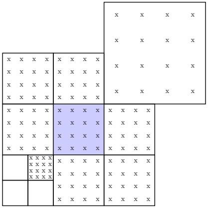


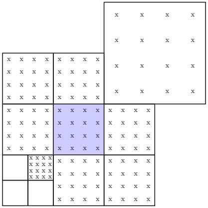
Simplifications

- Linearity: compute for basis and recombine
- Translation invariance and tree balance: relative target positions come from a small(ish), fixed set.

Local work in a box code

$$\int_{B_j} G_k(\mathbf{x}, \mathbf{y}) p_j(2(\mathbf{y} - \mathbf{y}_j)/L_j)\, dv$$

These integrals on self and neighbors are weakly singular/ near singular and require special quadrature.



Simplifications

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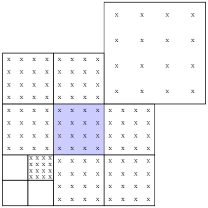

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Plan: precompute all possible interactions, reducing direct interaction calculations to mat-vecs

Box code vs point FMM

In a box code, can precompute and use mat-vecs for work that depends on source/target locations

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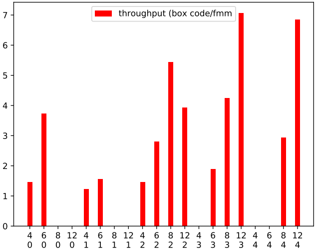
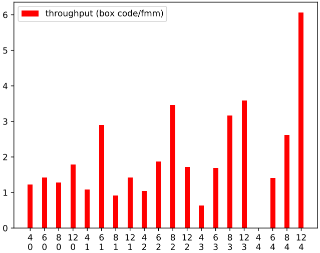
Less adaptive tree



Highly adaptive tree



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- Can still store table on a per-problem basis

Quadrature generation

$$\int_{(-1,1)^d} G_{k'}(\mathbf{x},\mathbf{y}) p_{\mathbf{p}}(\mathbf{y})\, dv\ , \quad p_{\mathbf{p}}(\mathbf{y}) = P_{p_1}(y_1)\cdots P_{p_d}(y_d)$$

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Idea[3]: Green's identity. If $\psi_{\mathbf{p}}$ is an "anti-Helmholtzian", i.e.

$$(\Delta + k'^2)\psi_{\mathbf{p}} = p_{\mathbf{p}}$$

then

$$\int_B G_{k'}(\mathbf{x},\mathbf{y}) p_{\mathbf{p}}(\mathbf{y})\, dv = \chi_B(\mathbf{x})\psi_{\mathbf{p}}(\mathbf{x}) + \underbrace{\int_{\partial B} G_{k'}(\mathbf{x},\mathbf{y})\partial_n \psi_{\mathbf{p}}(\mathbf{y}) - \partial_n G_{k'}(\mathbf{x},\mathbf{y})\psi_{\mathbf{p}}(\mathbf{y})\, da}_{\text{problem reduced to a surface integral}^4}\,.$$

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Anti-Helmholtzians

Goal: compute $\psi_{\mathbf{p}}$ satisfying

$$\max_{\mathbf{x}\in[-1,1]^d} |(\Delta + k'^2)\psi_{\mathbf{p}}(\mathbf{x}) - p_{\mathbf{p}}(\mathbf{x})| < \epsilon$$

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- Stable and efficient formula for $\psi_{\mathbf{p}}$

Differentiation and integration on polynomials

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Smooths, but embiggens the set

Anti-Laplacian[5]

Let $p(\mathbf{y}) = P_{n_1}(y_1)P_{n_2}(y_2)\cdots P_{n_d}(y_d)$. Let $n_1 \geq n_2, \ldots, n_d$ and $m = n_2 + \cdots + n_d$. Set $\tilde{\Delta} = (\partial^2_{y_2} + \cdots + \partial^2_{y_d})$.

Observe

$$\tilde{\Delta} : \mathcal{P}_M^{(d-1)} \to \mathcal{P}_{M-2}^{(d-1)}$$

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\Delta\psi^{(2)} &= p - [\mathcal{I}^4 P_{n_1}](y_1)\tilde{\Delta}^2(P_{n_2}(y_2)\cdots P_{n_d}(y_d))
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\Delta\psi^{(2)} &= p - [\mathcal{I}^4 P_{n_1}](y_1)\tilde{\Delta}^2(P_{n_2}(y_2)\cdots P_{n_d}(y_d)) \\
&\vdots \\
\Delta^{-1}p &:= \sum_{j=0}^{\lfloor m/2 \rfloor} (-1)^j [\mathcal{I}^{2j+2} P_{n_1}](y_1)\tilde{\Delta}^{2j}(P_{n_2}(y_2)\cdots P_{n_d}(y_d)) \in \mathcal{P}_{M+2}^{(d)}
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Sum converges in $L^\infty[-1,1]$ for any p. Formula only good when $|k'|$ small.

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Formula only good when $|k'|$ large.

Have two anti-Helmholtzians:

$$\psi^{(1)} = \frac{1}{k'^2} \sum_{j=0}^{\lfloor M/2 \rfloor} (-1)^j \frac{\Delta^j p}{k'^{2j}} \,, \quad \psi^{(2)} = \Delta^{-1} \sum_{j=0}^{\infty} (-1)^j k'^{2j} \Delta^{-j} p$$

Are they good enough for all values $|k'|$?

Stability

- Test k' with $|k'| = 1, 3, 5.5$.
- Set cut-off for sum for $\psi^{(2)}$ very high.
- Plot error $\max|(\Delta + k'^2)\psi - p|$ (double precision)

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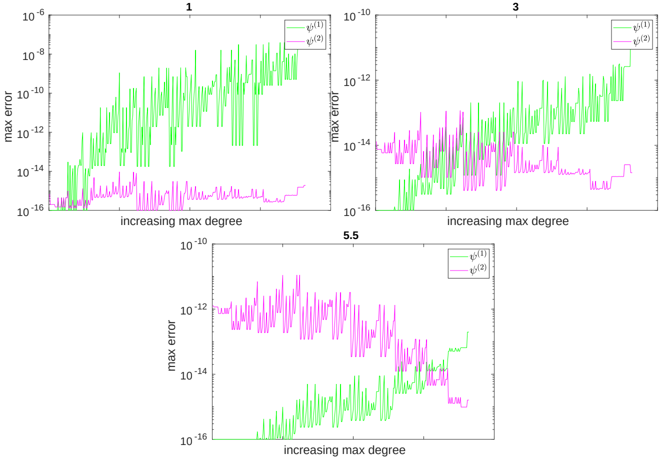

Stability

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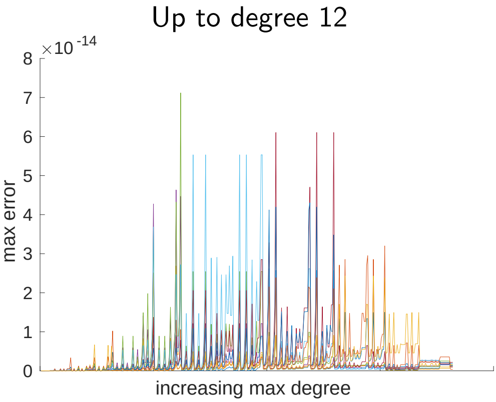

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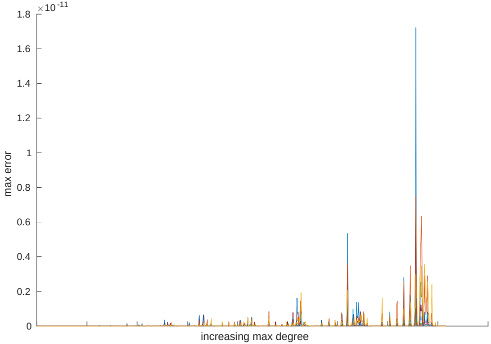
Up to degree 16



Efficiency

- Test k' with $|k'| = 1, 1.5, \ldots, 5.5$.
- Set cut-off for sum for $\psi^{(2)}$ at 16 terms.
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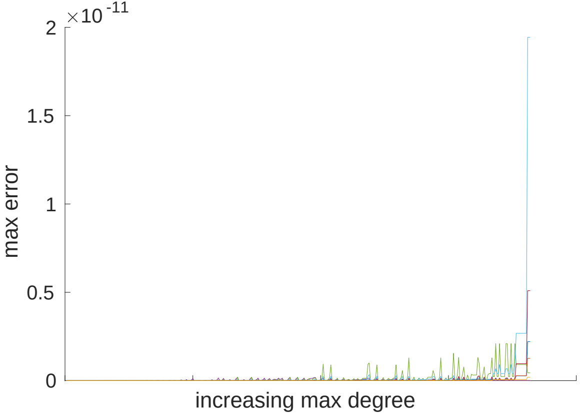
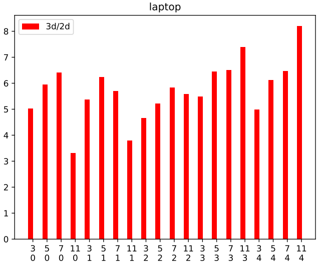
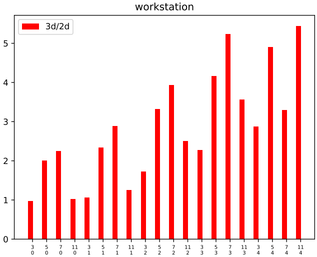
Up to degree 12

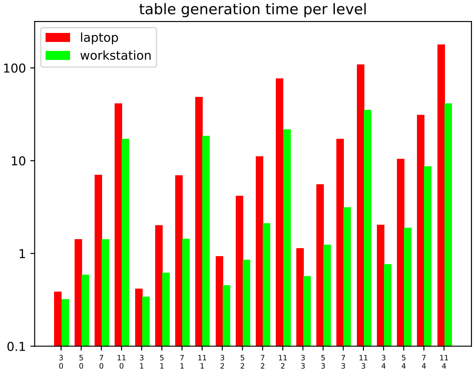


Compare to 3D adaptive integration





What does this do for us?



Future work

- Iteration count appears to be $O(k^2)$ for solving

$$\sigma + k^2 q V[\sigma] = -k^2 q \phi^{\mathrm{inc}}$$

  Overall that's $O(k^5)$. Yikes! Experiment with preconditioning/domain decomposition strategies.

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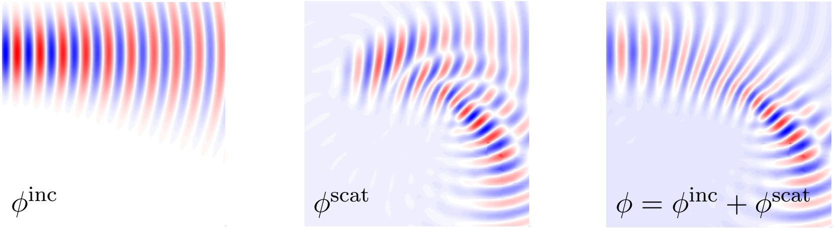
- A posteriori adaptive refinement



Thank you.

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