Fast Directional Matrix-Vector Multiplications

Analysis and Numerical Experiments

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Institute of Applied Mathematics

AANMPDE12, July 1-5 2019

FWF
Der Wissenschaftsfonds.

Outline

1. Motivation
2. Fast Directional Matrix-Vector Multiplications
3. Numerical Examples - Parameter Study
4. Conclusion

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Helmholtz equation

For $\kappa > 0$ consider the boundary value problem

$$\begin{aligned} \Delta u + \kappa^2 u &= 0, && \text{in } \Omega^{\text{ext}} \subset \mathbb{R}^3, \\ u &= g, && \text{on } \Gamma := \partial\Omega, \\ &+ \text{radiation condition}, \end{aligned}$$

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Consider the single layer potential $\tilde{V}t$ of a function t on Γ:

$$\tilde{V}t(x) = \int_\Gamma f(x,y)t(y)dy, \qquad f(x,y) := \frac{\exp(i\kappa|x-y|)}{4\pi|x-y|}.$$

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If $Vt := \gamma_0^{\text{ext}} \tilde{V}t = g$ we have a solution.

Problem Formulation and Discretization

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for piecewise constant test and trial functions ($t_h, \tau_h \in S_h^0(\Gamma)$).

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Equivalent system of linear equations: $V_h \underline{t} = \underline{g}$,

$$V_h[j,k] = \langle V\varphi_k, \varphi_j \rangle = \int_{\Gamma_j} \int_{\Gamma_k} f(x,y) \, \mathrm{d}s_y \, \mathrm{d}s_x,$$

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Remedy: directional approximation methods

The model problem

Instead of V_h consider $A \in \mathbb{C}^{N \times N}$,

$$A[j,k] = \begin{cases} f(x_j, x_k) = \frac{\exp(i\kappa|x_j - x_k|)}{4\pi|x_j - x_k|}, & j \neq k, \\ 0, & j = k, \end{cases}$$

for points $\{x_j\}_{j=1}^{N} \subset \mathbb{R}^3$.

Goal: Derive fast matrix-vector multiplications for matrix A.

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Fundamental idea:
Smoothing of Helmholtz kernel by plane wave term:

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where $c \in \mathbb{R}^3$ with $|c| = 1$.

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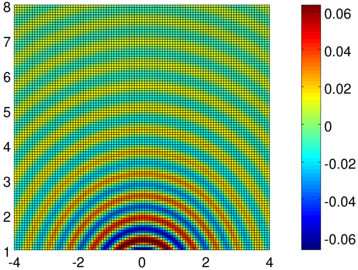
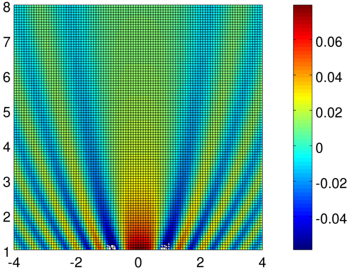
where $c \in \mathbb{R}^3$ with $|c| = 1$.

[Brandt, 1991, Engquist and Ying, 2007, Messner et al., 2012, Bebendorf et al., 2015, Börm and Melenk, 2017]

Comparison of f and f_c



$\Re[f(0,y)]$



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Parameters: $\kappa = 10$, $c = (0, -1, 0)$; $y = (y_1, y_2, 0)$

Directional approximation of the kernel

Let $x \in X$ and $y \in Y$ for two axis-parallel boxes $X, Y \subset \mathbb{R}^3$.
Substitute f_c with its interpolant:

$$f(x, y) = f_c(x, y) \exp\left(i\kappa\langle c, x - y\rangle\right)$$

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$$f(x,y) \approx \sum_{\substack{\|\alpha\|_\infty \le m \\ \|\beta\|_\infty \le m}} f_c(\xi_{X,\alpha}, \xi_{Y,\beta})(L_{X,\alpha}(x)e^{i\kappa\langle c,x\rangle})(L_{Y,\beta}(y)e^{-i\kappa\langle c,y\rangle}),$$

with interpolation degree m, Lagrange polynomials $L_{X,\alpha}$, $L_{Y,\beta}$.

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Reminder:

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Approximate subblocks of A corresponding to points in $X \times Y$ by

$$A_{X,Y} \approx L_{X,c} A_{c,X,Y} L_{Y,c}^*,$$

$$L_{X,c}[j,k] = L_{X,\alpha_k}(x)e^{i\kappa\langle c,x_j\rangle}, \qquad A_{c,X,Y}[j,k] = f_c(\xi_{X,\alpha_j}, \xi_{Y,\beta_k}).$$

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Admissibility criteria

Sufficient criteria ensuring a good approximation quality:
[Messner et al., 2012, Bebendorf et al., 2015,
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Admissibility criteria controlling box distances

$$\max\{\operatorname{diam}(X), \operatorname{diam}(Y)\} \leq \eta_2 \operatorname{dist}(X, Y), \quad \text{(A1)}$$

$$\kappa(\max\{\operatorname{diam}(X), \operatorname{diam}(Y)\})^2 \leq \eta_2 \operatorname{dist}(X, Y). \quad \text{(A2)}$$

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Admissibility criterion controlling the direction c

$$\kappa \left| \frac{m_X - m_Y}{|m_X - m_Y|} - c \right| \leq \frac{\eta_1}{\max\{\operatorname{diam}(X), \operatorname{diam}(Y)\}}, \qquad \text{(A3)}$$

where m_X and m_Y are the midpoints of the boxes X and Y.

Uniform clustering

Find admissible subblocks of A with uniform clustering strategy.

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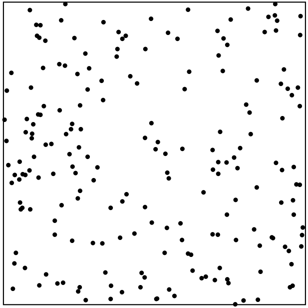
Level 0

Initial box X^0 s.t. $\{x_j\}_{j=1}^N \subset X^0$



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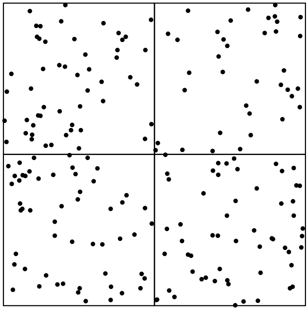
Find admissible subblocks of A with uniform clustering strategy.

Level 1

Uniformly subdivide X^0 into 8 boxes (4 boxes in 2D).



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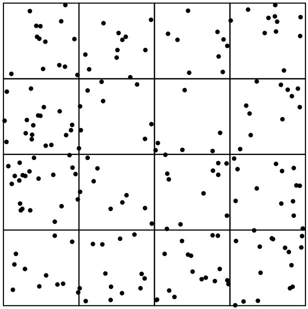
Level 2

Subdivide resulting boxes further ...



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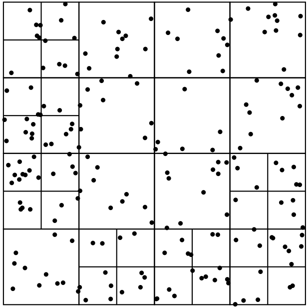
Level 3

Continue with subdivision ...

Stop if box contains few points.



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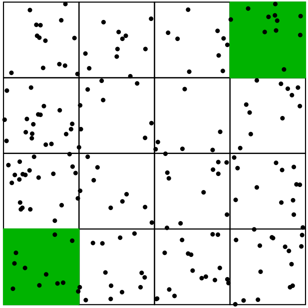

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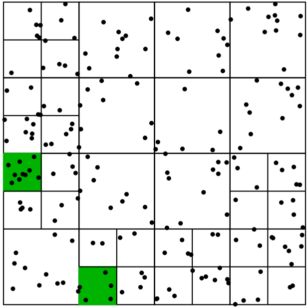

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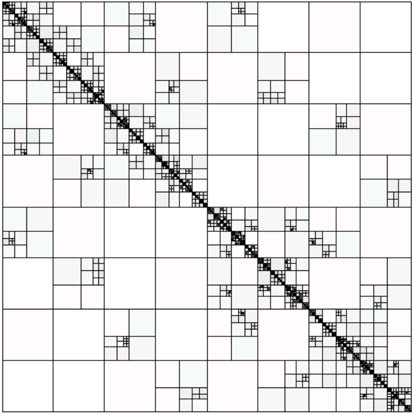

[Rjasanow and Steinbach, 2007]

Choice of directions

Let X^ℓ and Y^ℓ satisfy (A1) and (A2)
Find direction c such that

$$\left| \frac{m_{X^\ell} - m_{Y^\ell}}{|m_{X^\ell} - m_{Y^\ell}|} - c \right| \leq \frac{\eta_1}{\kappa \max\{\operatorname{diam}(X^\ell), \operatorname{diam}(Y^\ell)\}}. \tag{A3}$$

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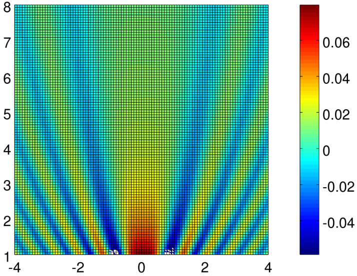

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Here: Construction combining the approaches of [Engquist and Ying, 2007, Messner, 2012], such that (A3) holds.

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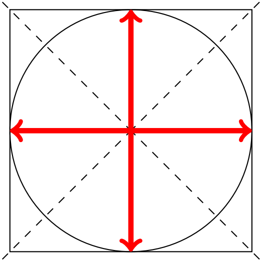

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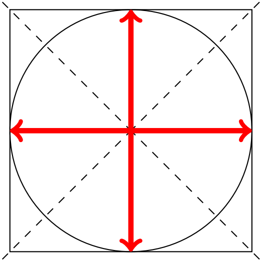

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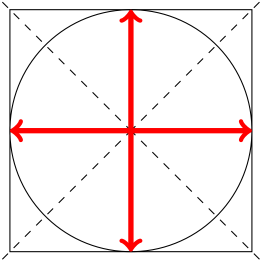

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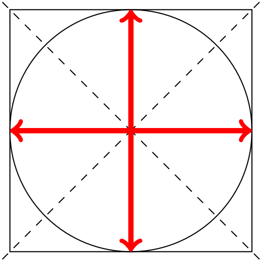

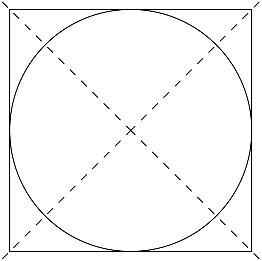

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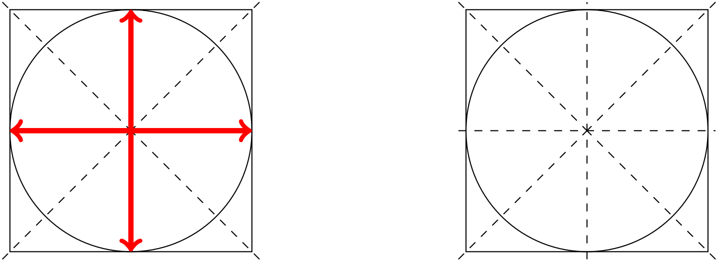

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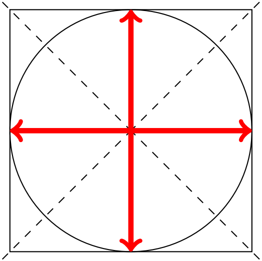

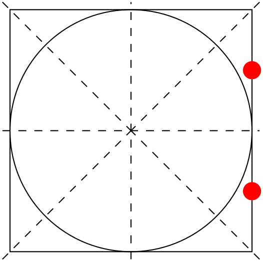

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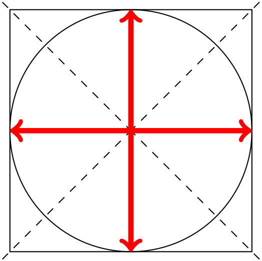

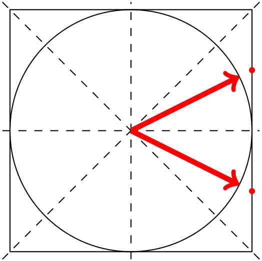

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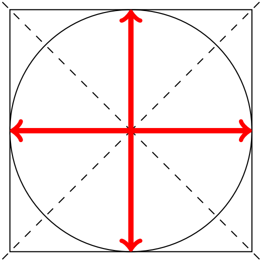

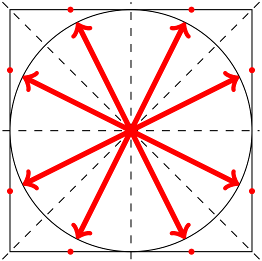

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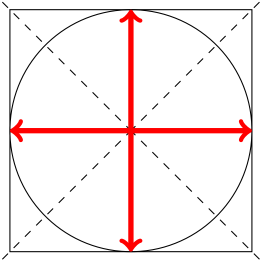

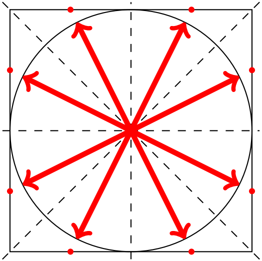

(A3) holds for η_1 depending linearly on $\kappa q_{\ell_{\mathrm{hf}}}$
Here: $q_{\ell_{\mathrm{hf}}}$ diameter of boxes at level ℓ_{hf}.

Fast directional matrix-vector multiplication

Basic idea:
Matrix partitioning (via clustering of the domain)
Approximation of admissible subblocks ($A_{XY} \approx L_{X,c} A_{c,X,Y} L^*_{Y,c}$)

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Complexity of order $N \log(N)$ under reasonable assumptions on the set of points $\{x_j\}_{j=1}^N$ and the wavenumber κ.
[Messner et al., 2012, Börm, 2017]

Outline

Choice of parameters

Effective runtime and accuracy depend on the choice of η_2

Admissibility criteria controlling box distances

$$\max\{\operatorname{diam}(X), \operatorname{diam}(Y)\} \leq \eta_2 \operatorname{dist}(X, Y), \qquad \text{(A1)}$$

$$\kappa(\max\{\operatorname{diam}(X), \operatorname{diam}(Y)\})^2 \leq \eta_2 \operatorname{dist}(X, Y). \qquad \text{(A2)}$$

Choice of parameters

Effective runtime and accuracy depend on the choice of η_2 and ℓ_{hf} (first high frequency level).

Admissibility criterion controlling the box direction

$$\kappa \left| \frac{m_X - m_Y}{|m_X - m_Y|} - c \right| \leq \frac{\eta_1}{\max\{\mathrm{diam}\,(X), \mathrm{diam}\,(Y)\}}, \tag{A3}$$

where η_1 depends on $\kappa q_{\ell_{\mathrm{hf}}}$

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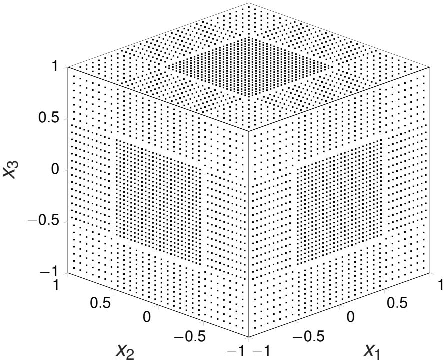
Suitable choice of parameters is determined in parameter study

Test setting

Place $N = 829176$ points $\{x_j\}_{j=1}^{N}$ on surface of cube $[-1, 1]^3$.



Test setting

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For $\kappa = 25.12$ consider the matrix

$$A[j,k] = \begin{cases} \frac{\exp(i\kappa|x_j - x_k|)}{4\pi|x_j - x_k|}, & j \neq k, \\ 0, & j = k, \end{cases}$$

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Choose vector $v \in \mathbb{C}^N$ (randomly) and compute $g = Av$:

- directly (g_{exct})
- approximately (g_{aprx}) with the fast directional matrix-vector multiplication.

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The Choice of η_2

Execution times for varying η_2
(first high frequency level $\ell_{\mathrm{hf}} = 4$, interpolation degree $m = 3$)

η_2	1	4	5	10
total time [s]	1487.33	262.37	110.38	104.86
nearfield evaluation [s]	1426.76	244.22	95.72	95.54
farfield evaluation [s]	23.38	6.80	5.49	3.14

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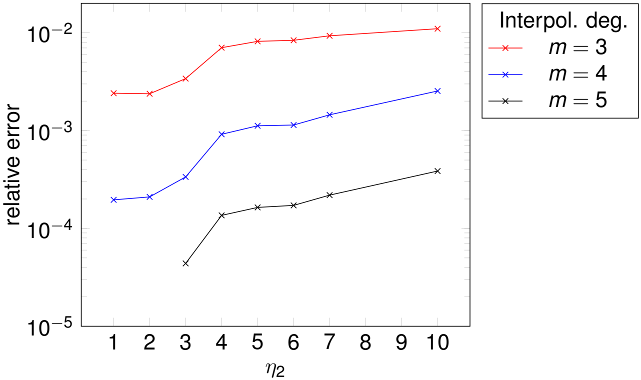
Minimizing the nearfield evaluations crucial.

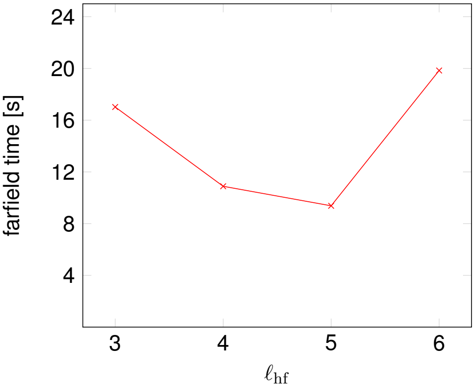
The choice $\eta_2 \geq \sqrt{3}\max\{1, \kappa q_{\ell_{\mathrm{hf}}+1}\}$ minimizes the nearfield evaluations for levels $> \ell_{\mathrm{hf}}$.
($q_{\ell_{\mathrm{hf}}+1}$ diameter of boxes at level $\ell_{\mathrm{hf}} + 1$)

The choice of η_2



Relative errors $\|g_{\mathrm{aprx}} - g_{\mathrm{exct}}\|_2 / \|g_{\mathrm{exct}}\|_2$ for varying η_2 ($\ell_{\mathrm{hf}} = 4$)

The choice of the first high frequency level ℓ_{hf}



(ℓ_{hf}, m)	rel. error
$(3,5)$	$1.01 \cdot 10^{-3}$
$(4,4)$	$1.12 \cdot 10^{-3}$
$(5,3)$	$2.74 \cdot 10^{-3}$
$(6,3)$	$1.87 \cdot 10^{-3}$

Farfield computation times and relative errors for varying ℓ_{hf}, $\eta_2 = 5$ and appropriate interpolation degrees m

The choice of the first high frequency level ℓ_{hf}

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The choice $C = 1.36$ was determined in the parameter study.

Outline

1. Motivation
2. Fast Directional Matrix-Vector Multiplications
3. Numerical Examples - Parameter Study
4. Conclusion

Conclusion and outlook

Presented Results:

- Overview (and analysis) of a fast directional matrix-vector multiplication
- Parameter study for the choice of parameters η_2 and ℓ_{hf}
  $\Rightarrow$ Parameter selection strategy

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Outlook:

- Further validation of the parameter selection strategy is required

[W (2019), A directional approximation of the Helmholtz kernel and its application to fast matrix-vector multiplications. MA thesis. TU Graz.]

Thank you for your attention!

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