Hierarchical interpolative factorization

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Joint work with Lexing Ying

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Introduction

Elliptic PDEs in differential or integral form:

$$-\nabla \cdot (a(x)\nabla u(x)) + v(x)u(x) = f(x)$$
$$a(x)u(x) + \int_{\Omega} K(x,y)u(y)\, d\Omega(y) = f(x)$$

- Fundamental to physics and engineering
- Interested in 2D/3D, complex geometry
- Discretize $\rightarrow$ structured linear system $Ax = b$

Goal: fast and accurate algorithms for the discrete operators

- Fast matrix-vector multiplication
- Fast solver, good preconditioner
- Linear or nearly linear complexity, high practical efficiency

Previous work

Fast matrix-vector multiplication

- Trivial for differential operators (sparse)
- Achieved for integral operators by FMM, treecode, $\mathcal{H}$-matrices, etc.

However, fast solvers have been much harder to come by

- Iterative methods
  - Number of iterations can be large
  - Inefficient for multiple right-hand sides
- Nested dissection/multifrontal, HSS matrices/recursive skeletonization
  - Small constants, optimal in quasi-1D
  - Rank growth in higher dimensions yields superlinear cost
- $\mathcal{H}$-matrices
  - Optimal complexity but large prefactor
- MF/RS with structured matrix algebra
  - Improved prefactor, complex geometry can be difficult

Many contributors; apologies for not listing names

Hierarchical interpolative factorization

- MF/RS + recursive dimensional reduction
- Same idea as with using structured algebra but in a new matrix framework
- Explicit sparsification, generalized LU decomposition
- Extends to 3D, complex geometry, etc.

Tools: Schur complement, interpolative decomposition, skeletonization

Schur complement

Let

$$A = \begin{bmatrix} A_{pp} & A_{pq} & \\ A_{qp} & A_{qq} & A_{qr} \\ & A_{rq} & A_{rr} \end{bmatrix}.$$

(Think of A as a sparse matrix.) If A_{pp} is nonsingular, define

$$R_p^* = \begin{bmatrix} I & & \\ -A_{qp}A_{pp}^{-1} & I & \\ & & I \end{bmatrix}, \quad S_p = \begin{bmatrix} I & -A_{pp}^{-1}A_{pq} & \\ & I & \\ & & I \end{bmatrix}$$

so that

$$R_p^* A S_p = \begin{bmatrix} A_{pp} & & \\ & * & A_{qr} \\ & A_{rq} & A_{rr} \end{bmatrix}.$$

- DOFs p have been eliminated
- Interactions involving r are unchanged

Interpolative decomposition

If $A_{:,q}$ is numerically low-rank, then there exist

- redundant ($\check{q}$) and skeleton ($\hat{q}$) columns partitioning $q = \check{q} \cup \hat{q}$
- an interpolation matrix T_q with $\| T_q \|$ small

such that

$$A_{:,\check{q}} \approx A_{:,\hat{q}} T_q.$$

- Essentially an RRQR written slightly differently
- Can be computed adaptively to any specified precision
- Fast randomized algorithms are available

Interactions between separated regions are low-rank.

Skeletonization

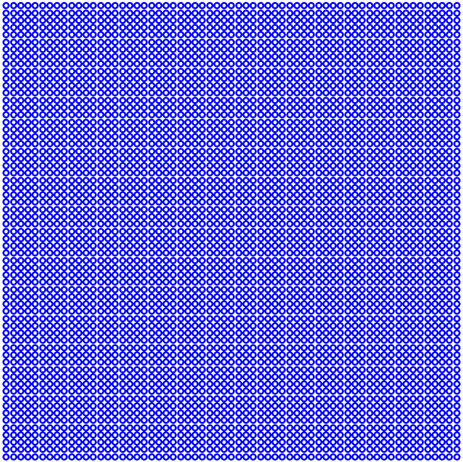
- Use ID + Schur complement to eliminate redundant DOFs
- Let $A = \begin{bmatrix} A_{pp} & A_{pq} \\ A_{qp} & A_{qq} \end{bmatrix}$ with A_{pq} and A_{qp} low-rank
- Apply ID to $\begin{bmatrix} A_{qp} \\ A_{pq}^* \end{bmatrix}$: $\begin{bmatrix} A_{q\check{p}} \\ A_{\check{p}q}^* \end{bmatrix} \approx \begin{bmatrix} A_{q\hat{p}} \\ A_{\hat{p}q}^* \end{bmatrix} T_p \implies \begin{array}{c} A_{q\check{p}} \approx A_{q\hat{p}} T_p \\ A_{\check{p}q} \approx T_p^* A_{\hat{p}q} \end{array}$
- Reorder $A = \begin{bmatrix} A_{\check{p}\check{p}} & A_{\check{p}\hat{p}} & A_{\check{p}q} \\ A_{\hat{p}\check{p}} & A_{\hat{p}\hat{p}} & A_{\hat{p}q} \\ A_{q\check{p}} & A_{q\hat{p}} & A_{qq} \end{bmatrix}$, define $Q_p = \begin{bmatrix} I & & \\ -T_p & I & \\ & & I \end{bmatrix}$
- Sparsify via ID: $Q_p^* A Q_p \approx \begin{bmatrix} * & * & \\ * & A_{\hat{p}\hat{p}} & A_{\hat{p}q} \\ & A_{q\hat{p}} & A_{qq} \end{bmatrix}$
- Schur complement: $R_p^* Q_p^* A Q_p S_p \approx \begin{bmatrix} * & & \\ & * & A_{\hat{p}q} \\ & A_{q\hat{p}} & A_{qq} \end{bmatrix}$

Differential equations

Algorithm: multifrontal

Build quadtree/octree.
for each level $\ell = 0, 1, 2, \ldots, L$ from finest to coarsest **do**
    Let C_ℓ be the set of all cells on level ℓ.
    for each cell $c \in C_\ell$ **do**
        Schur complement remaining interior DOFs in c.
    end for
end for

MF in 2D: level 0



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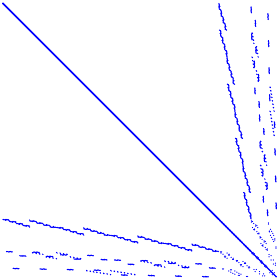
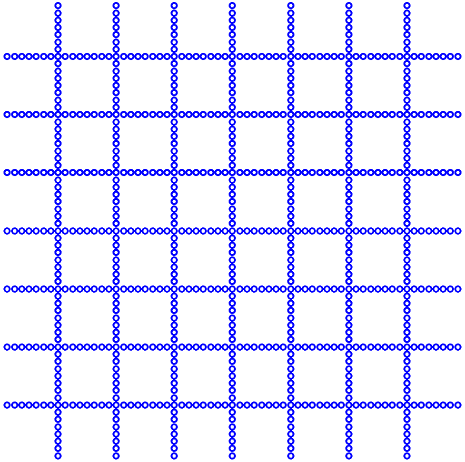


matrix

MF in 2D: level 1



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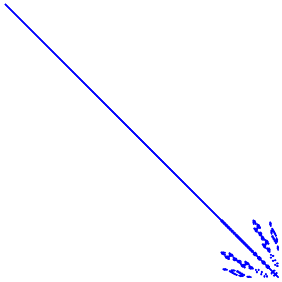
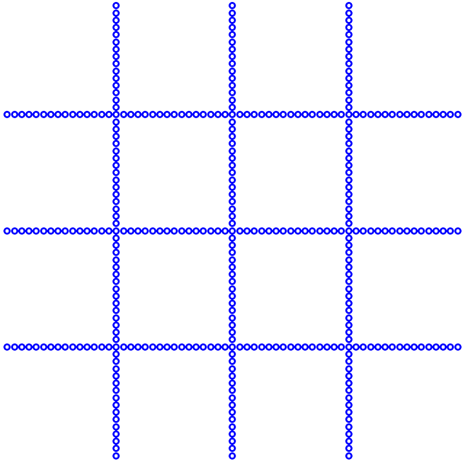


matrix

MF in 2D: level 2



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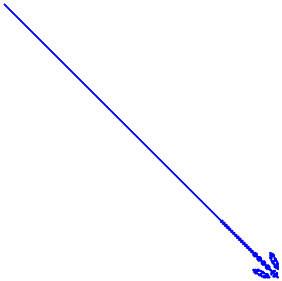
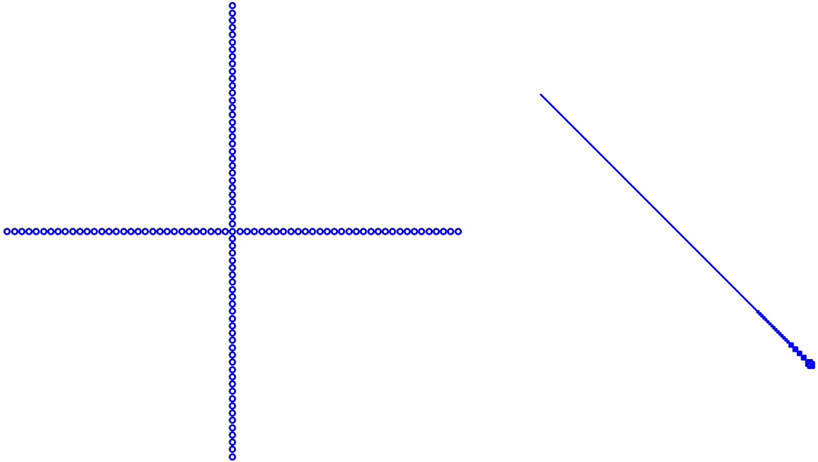


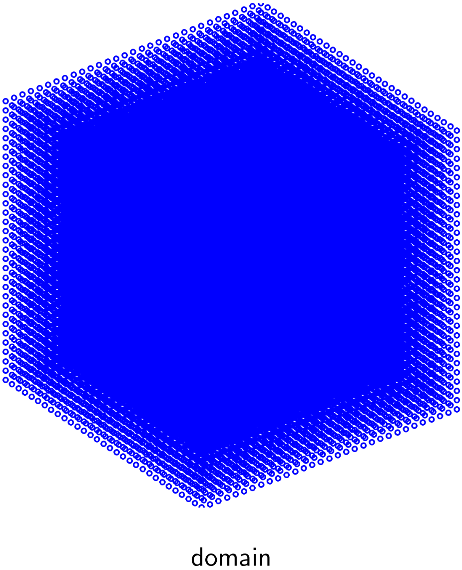
matrix

MF in 2D: level 3

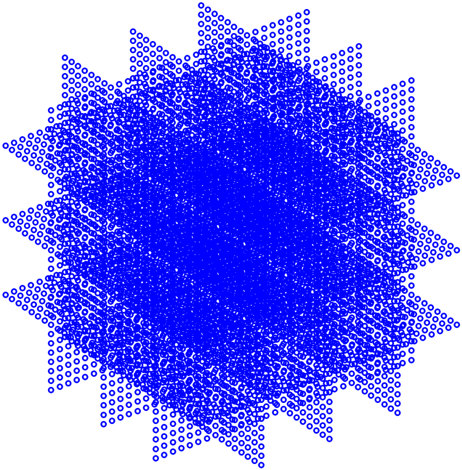


domain matrix

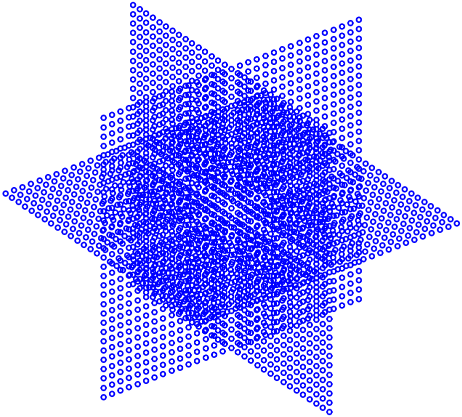
MF in 3D: level 0



MF in 3D: level 1



MF in 3D: level 2



domain

MF analysis

- Schur complement operator (assume SPD):

$$W_\ell = \prod_{c \in C_\ell} S_c$$

- Block diagonalization:

$$D \approx W_{L-1}^* \cdots W_0^* A W_0 \cdots W_{L-1}$$

- LU decomposition:

$$A \approx W_0^{-*} \cdots W_{L-1}^{-*} D W_{L-1}^{-1} \cdots W_0^{-1}$$
$$A^{-1} \approx W_0 \cdots W_{L-1} D^{-1} W_L^* \cdots W_0^*$$

- Numerically exact: fast direct solver

MF analysis

The cost is determined by the separator/front size.

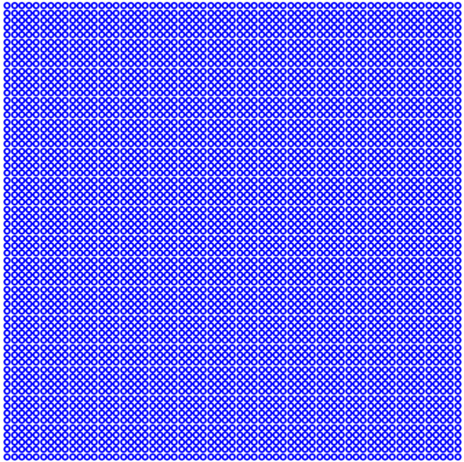
	1D	2D	3D
Front size	$\mathcal{O}(1)$	$\mathcal{O}(N^{1/2})$	$\mathcal{O}(N^{2/3})$
Factorization cost	$\mathcal{O}(N)$	$\mathcal{O}(N^{3/2})$	$\mathcal{O}(N^2)$
Solve cost	$\mathcal{O}(N)$	$\mathcal{O}(N \log N)$	$\mathcal{O}(N^{4/3})$

Question: How to reduce the front size in 2D and 3D?

- Frontal matrices are dense but rank-structured
- Exploit separator geometry by skeletonizing along edges
- Dimensional reduction

Build quadtree.
for each level $\ell = 0, 1, 2, \ldots, L$ from finest to coarsest **do**
  Let C_ℓ be the set of all cells on level ℓ.
  for each cell $c \in C_\ell$ **do**
    Schur complement remaining interior DOFs in c.
  end for
  Let $C_{\ell+1/2}$ be the set of all edges on level ℓ.
  for each cell $c \in C_{\ell+1/2}$ **do**
    Skeletonize remaining interior DOFs in c.
  end for
end for

HIF-DE in 2D: level 0



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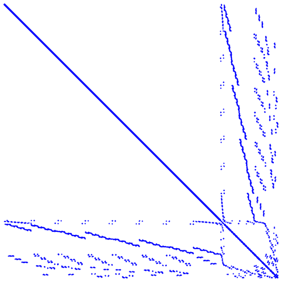
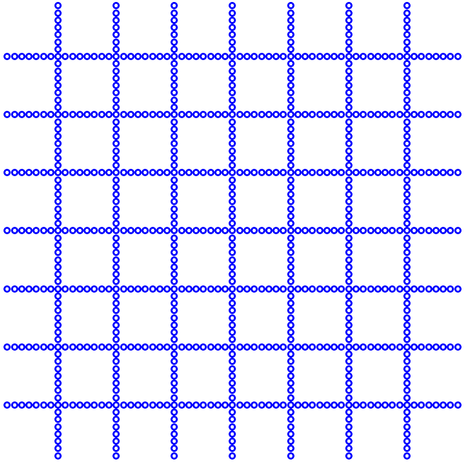


matrix

HIF-DE in 2D: level 1/2



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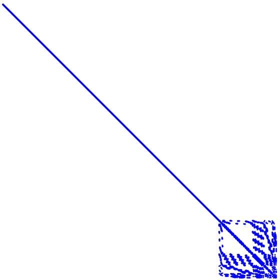
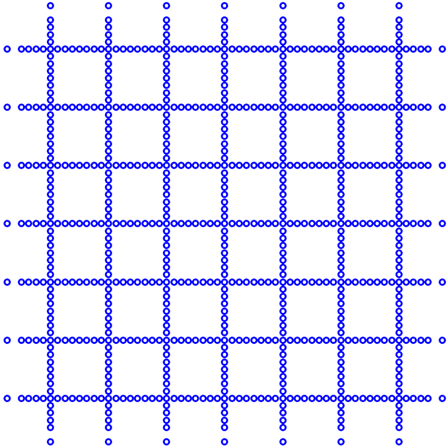


matrix

HIF-DE in 2D: level 1



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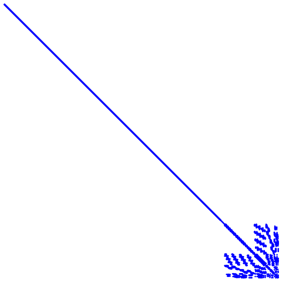
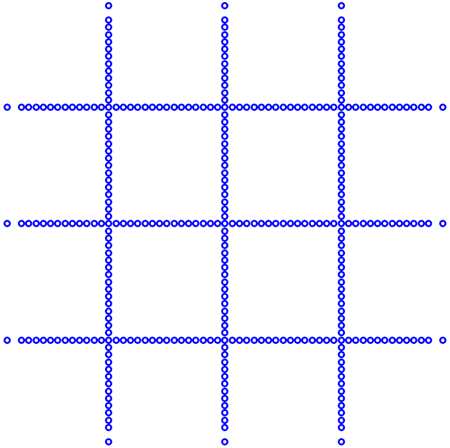


matrix

HIF-DE in 2D: level 3/2



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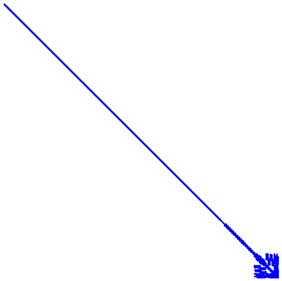
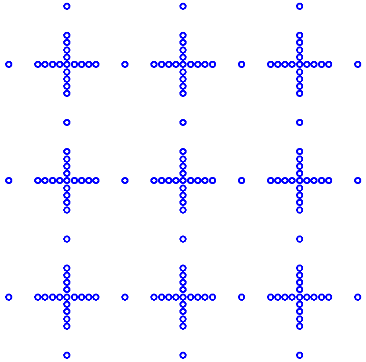


matrix

HIF-DE in 2D: level 2



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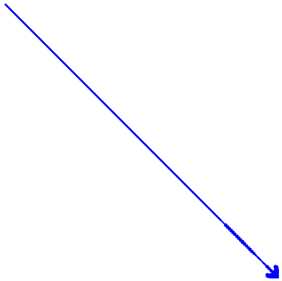
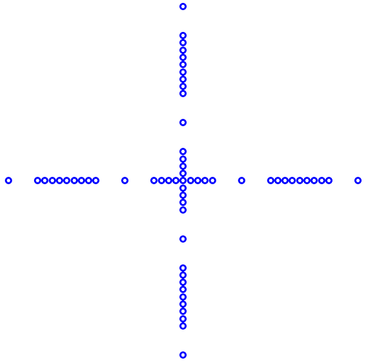


matrix

HIF-DE in 2D: level 5/2



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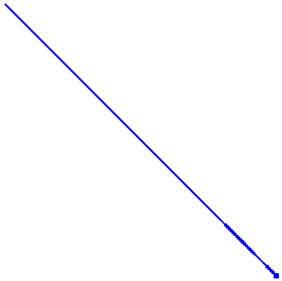
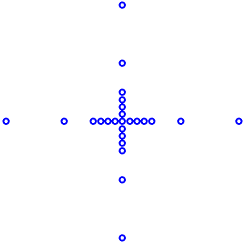


matrix

HIF-DE in 2D: level 3



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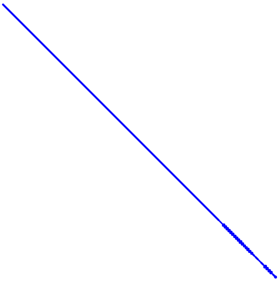
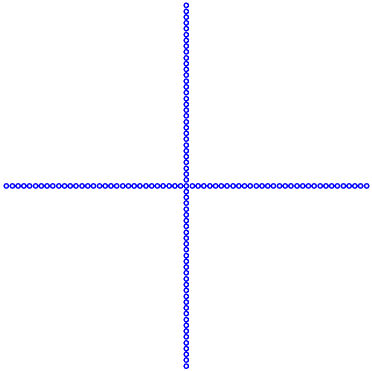
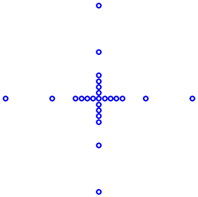


matrix

MF vs. HIF-DE in 2D

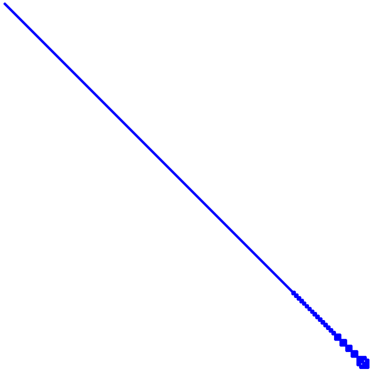


MF

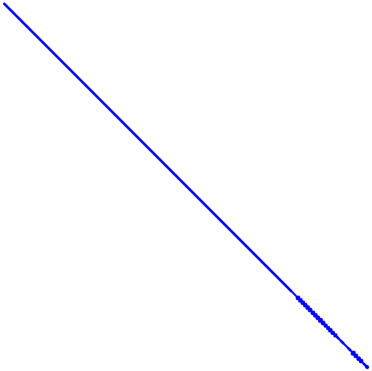


HIF-DE

MF vs. HIF-DE in 2D



MF



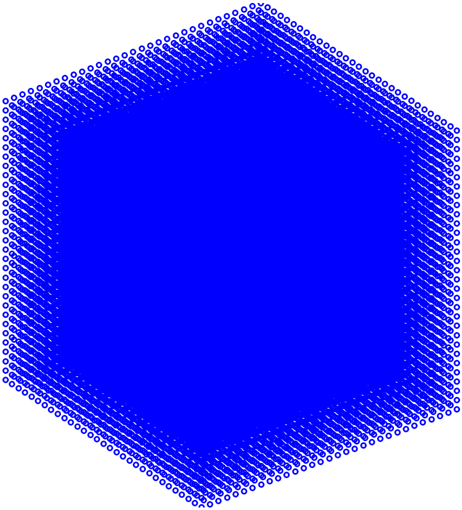
HIF-DE

Algorithm: hierarchical interpolative factorization in 3D

Build octree.
for each level $\ell = 0, 1, 2, \ldots, L$ from finest to coarsest **do**
    Let C_ℓ be the set of all cells on level ℓ.
    for each cell $c \in C_\ell$ **do**
        Schur complement remaining interior DOFs in c.
    end for
    Let $C_{\ell+1/2}$ be the set of all faces on level ℓ.
    for each cell $c \in C_{\ell+1/2}$ **do**
        Skeletonize remaining interior DOFs in c.
    end for
end for

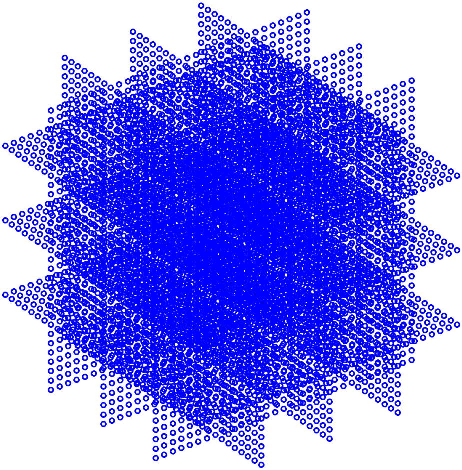
- Can also do additional skeletonization along edges for true linear complexity
- This algorithm is sufficient for $\mathcal{O}(N \log N)$ and better exploits sparsity

HIF-DE in 3D: level 0



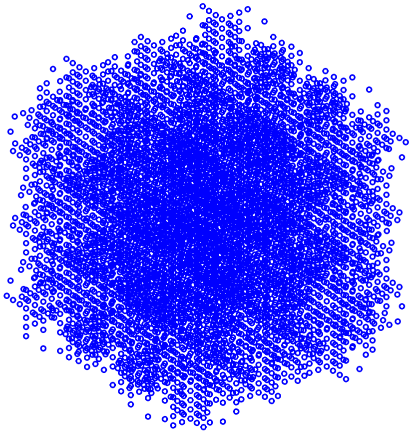
domain

HIF-DE in 3D: level 1/2



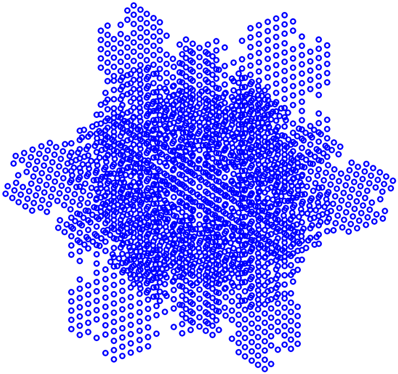
domain

HIF-DE in 3D: level 1



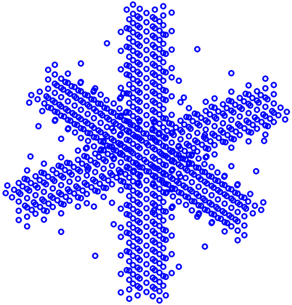
domain

HIF-DE in 3D: level 3/2



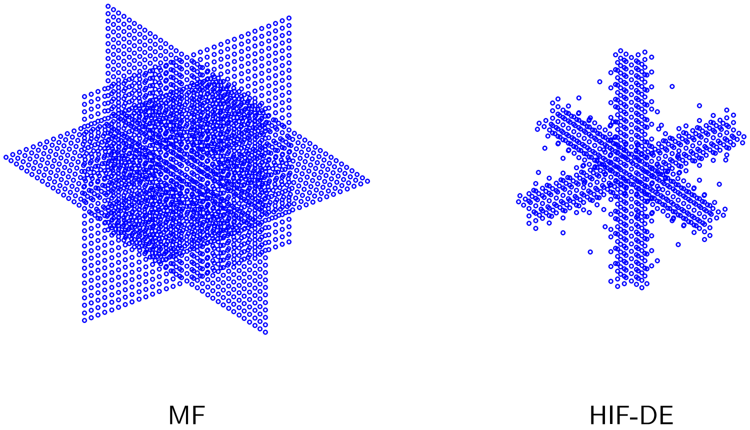
domain

HIF-DE in 3D: level 2



domain

MF vs. HIF-DE in 3D



HIF-DE analysis

- Skeletonization operator (assume SPD):

$$U_\ell = \prod_{c \in C_\ell} Q_c S_c$$

- Generalized LU decomposition:

$$A \approx W_0^{-*} U_{1/2}^{-*} \cdots W_{L-1}^{-*} U_{L-1/2}^{-*} D U_{L-1/2}^{-1} W_{L-1}^{-1} \cdots U_{1/2}^{-1} W_0^{-1}$$
$$A^{-1} \approx W_0 U_{1/2} \cdots W_{L-1} U_{L-1/2} D^{-1} U_{L-1/2}^{*} W_L^{*} \cdots U_{1/2}^{*} W_0^{*}$$

- No longer exact, fast direct solver or preconditioner depending on accuracy

	2D	3D
Skeleton size	$\mathcal{O}(\log N)$	$\mathcal{O}(N^{1/3})$
Factorization cost	$\mathcal{O}(N)$	$\mathcal{O}(N \log N)$
Solve cost	$\mathcal{O}(N)$	$\mathcal{O}(N)$

Numerical results in 2D

Finite difference discretization on a square with

$$a(x) = \prod_{\ell=0}^{L} \left(\frac{3}{8} \sin(2\pi 2^{\ell} x_1) \sin(2\pi 2^{\ell} x_2) + \frac{5}{8} \right), \quad v(x) \equiv 0$$

ϵ	N	$\lvert\hat{c}\rvert$	m_f (GB)	t_f (s)	$t_{a/s}$ (s)	e_a	e_s	n_i
10^{-6}	255^2	20	1.4e−1	3.6e+0	1.6e−1	2.3e−08	3.2e−06	3
	511^2	22	5.8e−1	1.7e+1	6.5e−1	2.2e−08	1.1e−05	3
	1023^2	23	2.4e+0	8.1e+1	2.4e+0	2.3e−08	1.8e−05	3
10^{-9}	255^2	31	1.5e−1	3.8e+0	2.1e−1	9.9e−12	1.1e−09	2
	511^2	35	6.0e−1	1.9e+1	6.3e−1	1.5e−11	2.7e−09	2
	1023^2	38	2.4e+0	8.1e+1	2.3e+0	1.6e−11	2.5e−08	2
10^{-12}	255^2	38	1.5e−1	3.5e+0	1.4e−1	1.4e−14	9.9e−13	1
	511^2	44	6.0e−1	1.8e+1	6.2e−1	1.5e−14	6.7e−12	2
	1023^2	50	2.5e+0	9.2e+1	2.6e+0	1.7e−14	7.4e−12	2

Numerical results in 3D

Finite difference discretization on a cube with

$$a(x) = \prod_{\ell=0}^{L} \left(\frac{3}{8} \sin(2\pi 2^\ell x_1) \sin(2\pi 2^\ell x_2) \sin(2\pi 2^\ell x_3) + \frac{5}{8} \right), \quad v(x) \equiv 0$$

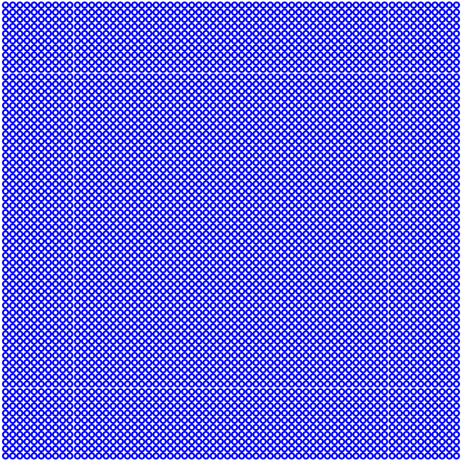
ϵ	N	$\lvert\hat{c}\rvert$	m_f (GB)	t_f (s)	$t_{a/s}$ (s)	e_a	e_s	n_i
10^{-3}	31^3	83	1.9e−1	6.5e+0	7.4e−2	4.4e−05	5.8e−04	6
	63^3	189	2.1e+0	1.3e+2	8.3e−1	5.1e−05	1.1e−03	7
	127^3	388	2.2e+1	2.0e+3	8.7e+0	6.4e−05	3.2e−03	11
10^{-6}	31^3	152	2.4e−1	8.1e+0	8.5e−2	2.5e−08	1.3e−07	2
	63^3	367	3.1e+0	2.0e+2	1.1e+0	3.1e−08	3.2e−07	3
	127^3	802	3.6e+1	4.1e+3	1.1e+1	4.2e−08	1.3e−06	3
10^{-9}	31^3	197	2.7e−1	8.8e+0	7.9e−2	1.9e−11	6.6e−11	2
	63^3	531	3.7e+0	2.4e+2	1.0e+0	1.8e−11	1.2e−10	2
	127^3	1225	4.6e+1	6.2e+3	1.3e+1	2.7e−11	4.6e−10	2

Integral equations

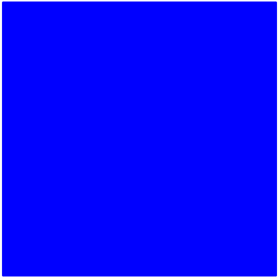
Algorithm: recursive skeletonization

Build quadtree/octree.
for each level $\ell = 0, 1, 2, \dots, L$ from finest to coarsest **do**
    Let C_ℓ be the set of all cells on level ℓ.
    for each cell $c \in C_\ell$ **do**
        Skeletonize remaining DOFs in c.
    end for
end for

RS in 2D: level 0

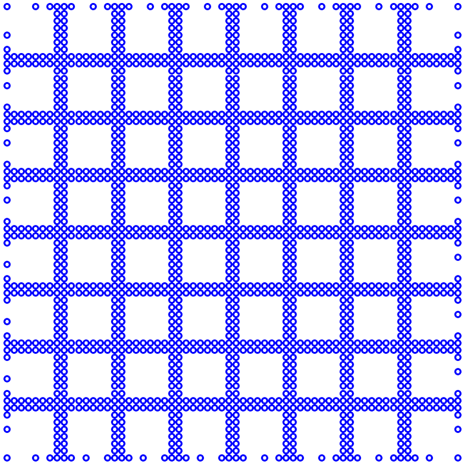


domain



matrix

RS in 2D: level 1



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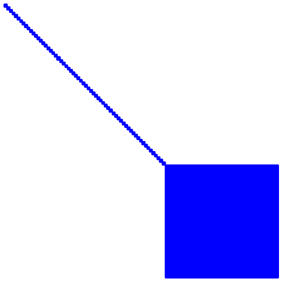

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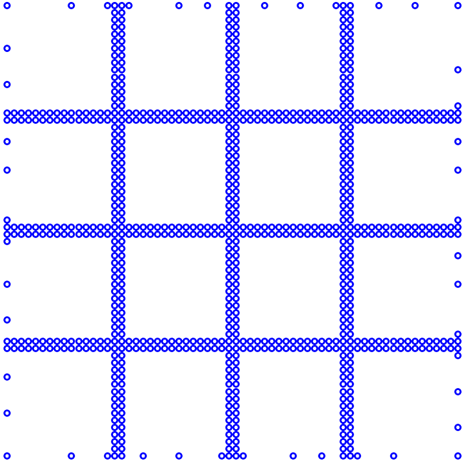
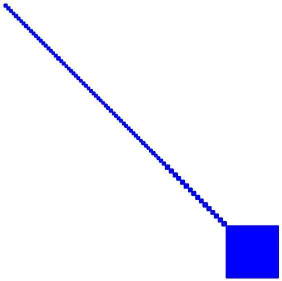
RS in 2D: level 2

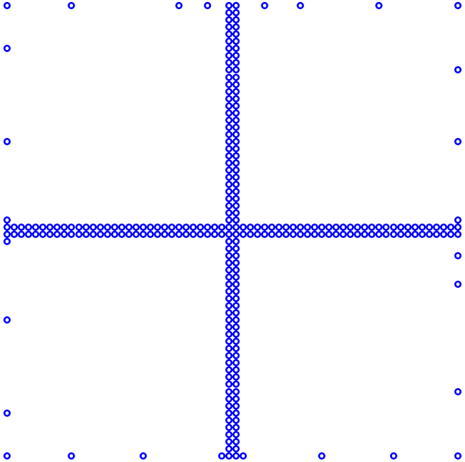


domain

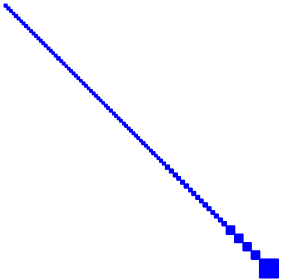


matrix

RS in 2D: level 3

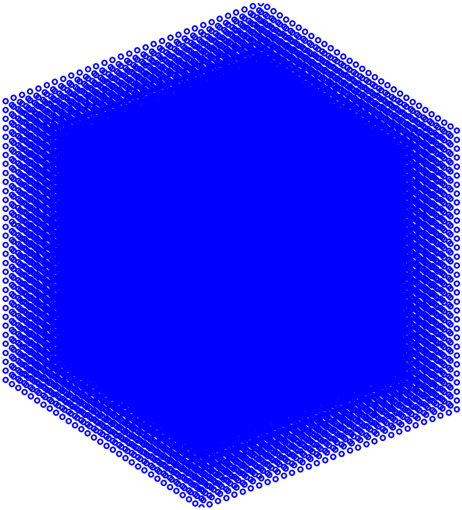


domain



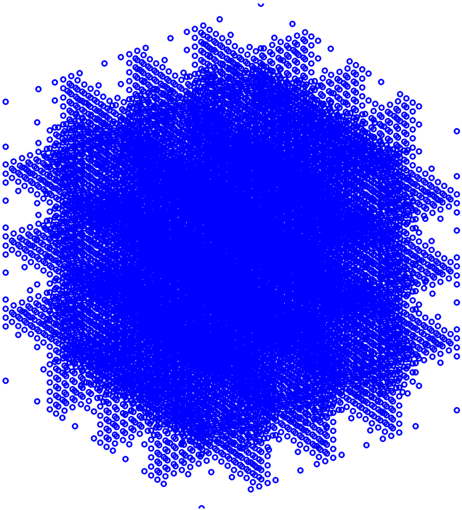
matrix

RS in 3D: level 0



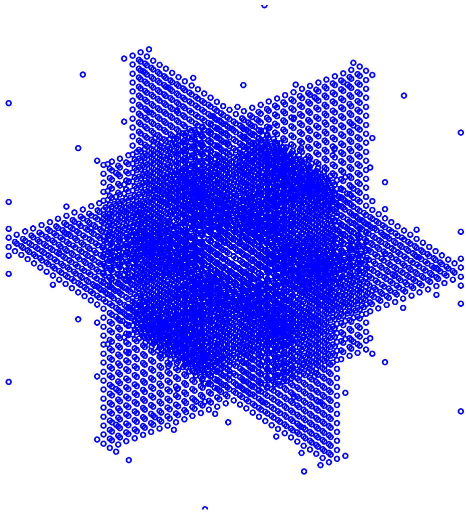
domain

RS in 3D: level 1



domain

RS in 3D: level 2



domain

RS analysis

- Skeletonization operators:

$$U_\ell = \prod_{c \in C_\ell} Q_c R_c, \quad V_\ell = \prod_{c \in C_\ell} Q_c S_c$$

- Block diagonalization:

$$D \approx U_{L-1}^* \cdots U_0^* A V_0 \cdots V_{L-1}$$

- Generalized LU decomposition:

$$A \approx U_0^{-*} \cdots U_{L-1}^{-*} D V_{L-1}^{-1} \cdots V_0^{-1}$$
$$A^{-1} \approx V_0 \cdots V_{L-1} D^{-1} U_L^* \cdots U_0^*$$

- Fast direct solver or preconditioner

The cost is determined by the skeleton size.

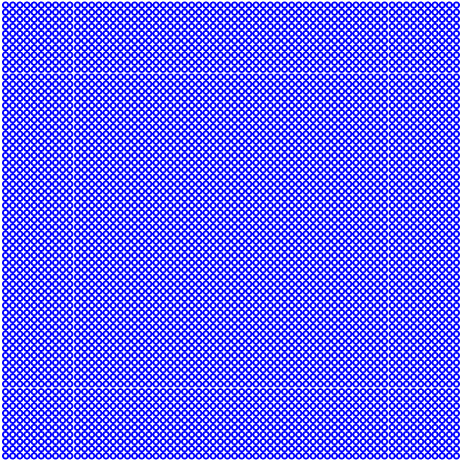
	1D	2D	3D
Skeleton size	$\mathcal{O}(\log N)$	$\mathcal{O}(N^{1/2})$	$\mathcal{O}(N^{2/3})$
Factorization cost	$\mathcal{O}(N)$	$\mathcal{O}(N^{3/2})$	$\mathcal{O}(N^2)$
Solve cost	$\mathcal{O}(N)$	$\mathcal{O}(N \log N)$	$\mathcal{O}(N^{4/3})$

Question: How to reduce the skeleton size in 2D and 3D?

- Skeletons cluster near cell interfaces
- Exploit skeleton geometry by skeletonizing along interfaces
- Dimensional reduction

Build quadtree.
for each level $\ell = 0, 1, 2, \ldots, L$ from finest to coarsest **do**
    Let C_ℓ be the set of all cells on level ℓ.
    for each cell $c \in C_\ell$ **do**
        Skeletonize remaining DOFs in c.
    end for
    Let $C_{\ell+1/2}$ be the set of all edges on level ℓ.
    for each cell $c \in C_{\ell+1/2}$ **do**
        Skeletonize remaining DOFs in c.
    end for
end for

HIF-IE in 2D: level 0



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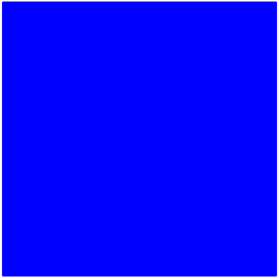
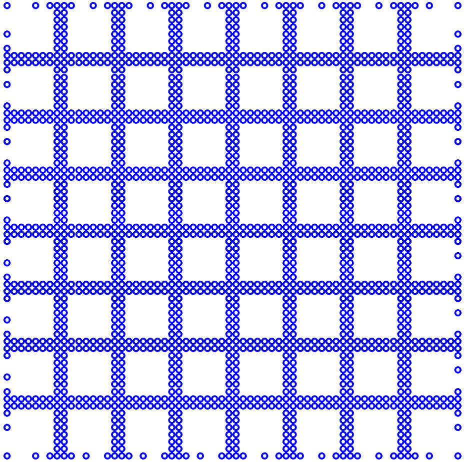


matrix

HIF-IE in 2D: level 1/2



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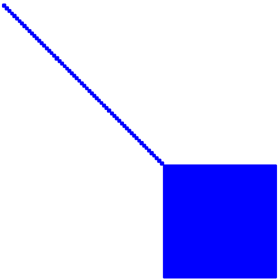
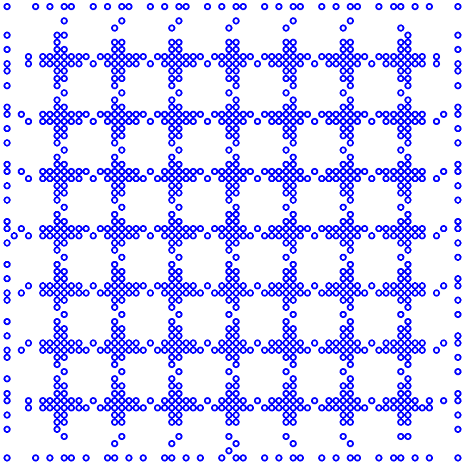


matrix

HIF-IE in 2D: level 1



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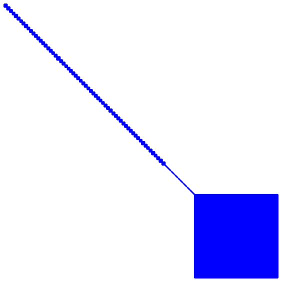
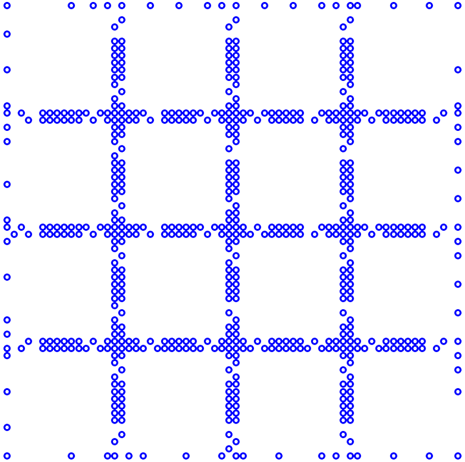
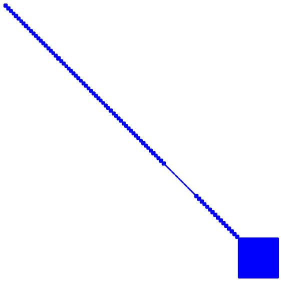


matrix

HIF-IE in 2D: level 3/2

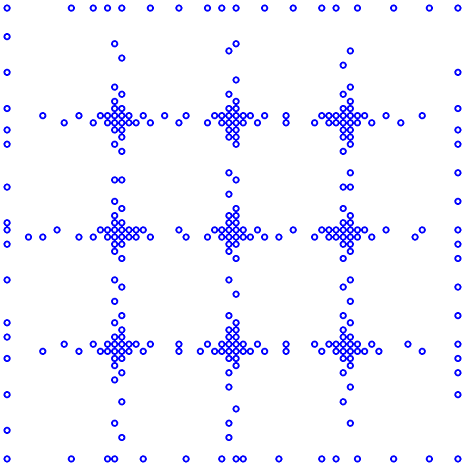


domain

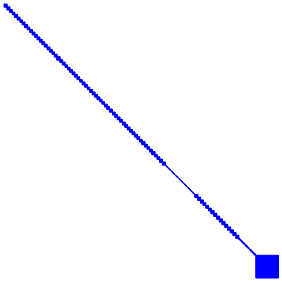


matrix

HIF-IE in 2D: level 2

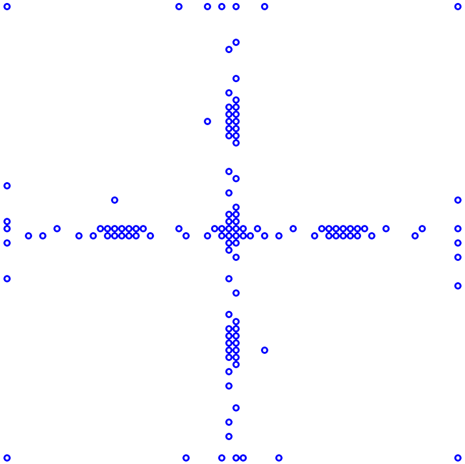


domain

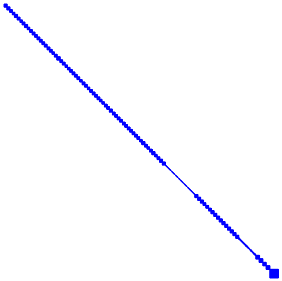


matrix

HIF-IE in 2D: level 5/2

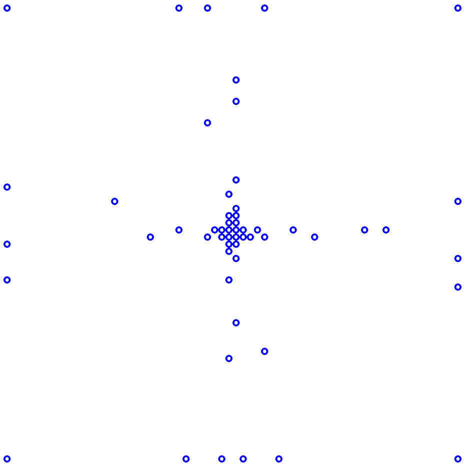


domain

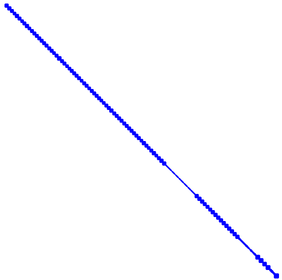


matrix

HIF-IE in 2D: level 3

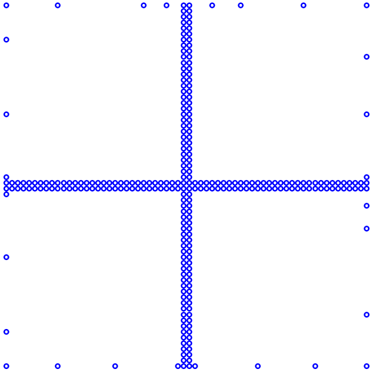


domain

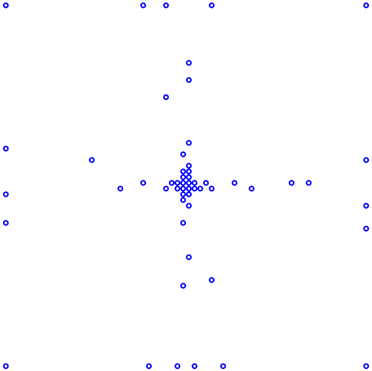


matrix

RS vs. HIF-IE in 2D

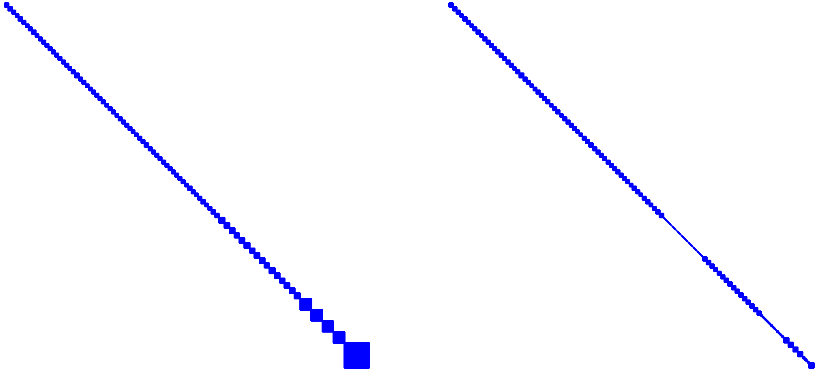


RS



HIF-IE

RS vs. HIF-IE in 2D

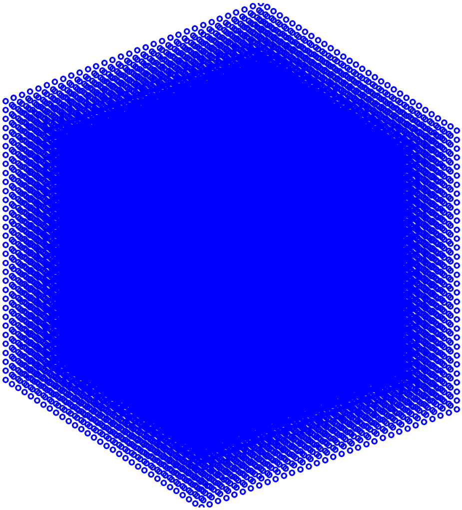


RS HIF-IE

Algorithm: hierarchical interpolative factorization in 3D

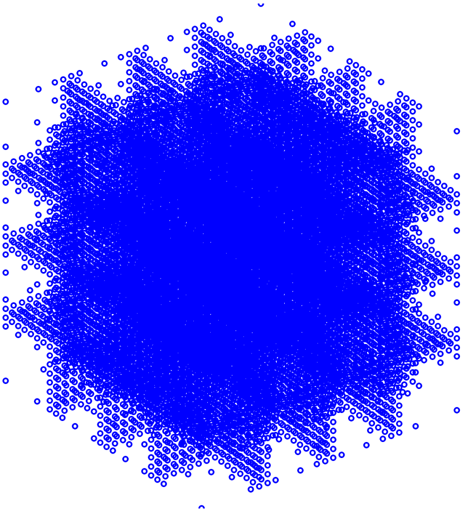
Build octree.
for each level $\ell = 0, 1, 2, \ldots, L$ from finest to coarsest **do**
    Let C_ℓ be the set of all cells on level ℓ.
    for each cell $c \in C_\ell$ **do**
        Skeletonize remaining DOFs in c.
    end for
    Let $C_{\ell+1/3}$ be the set of all faces on level ℓ.
    for each cell $c \in C_{\ell+1/3}$ **do**
        Skeletonize remaining DOFs in c.
    end for
    Let $C_{\ell+2/3}$ be the set of all edges on level ℓ.
    for each cell $c \in C_{\ell+2/3}$ **do**
        Skeletonize remaining DOFs in c.
    end for
end for

HIF-IE in 3D: level 0



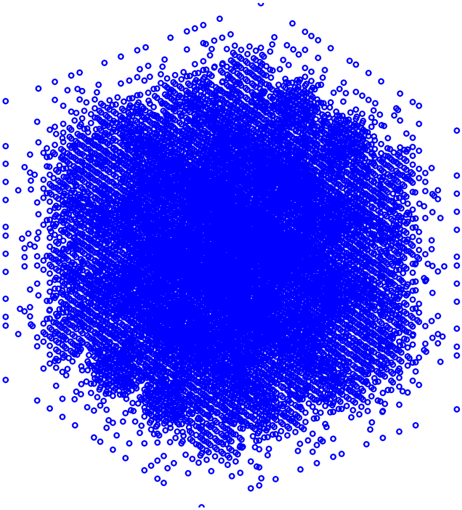
domain

HIF-IE in 3D: level 1/3



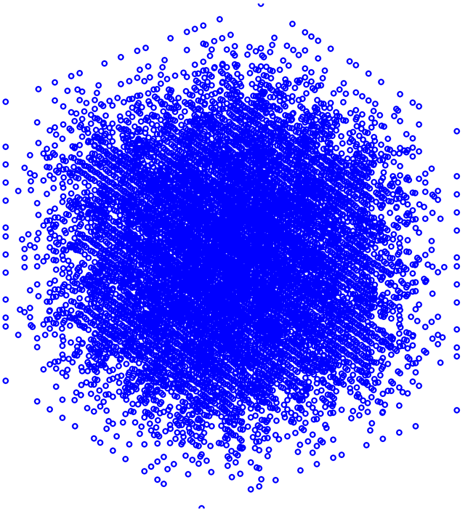
domain

HIF-IE in 3D: level 2/3



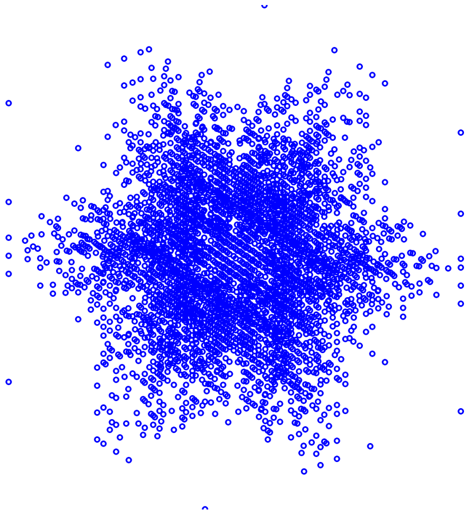
domain

HIF-IE in 3D: level 1



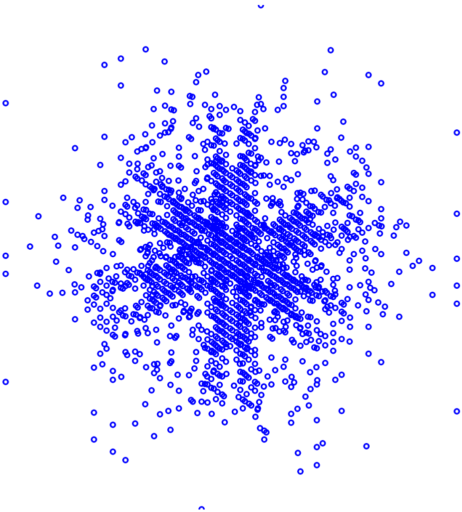
domain

HIF-IE in 3D: level 4/3



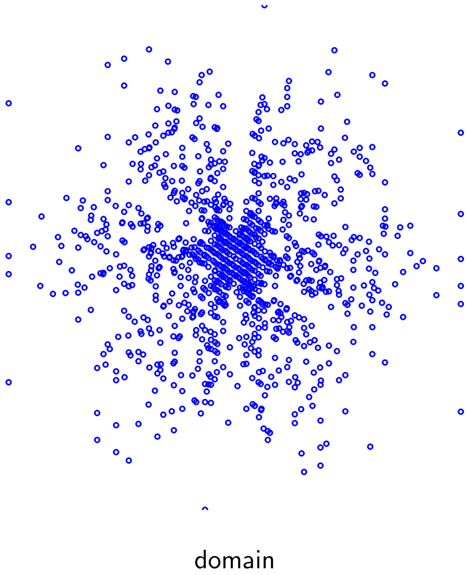
domain

HIF-IE in 3D: level 5/3

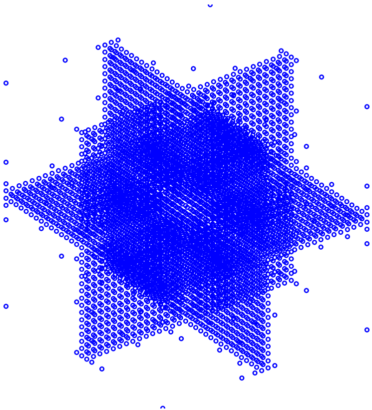


domain

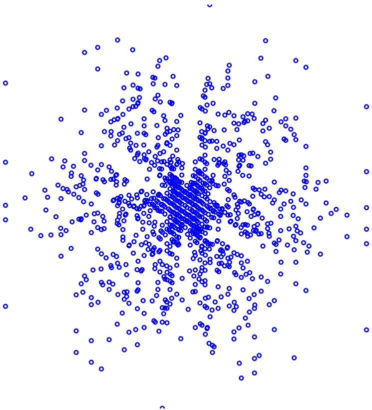
HIF-IE in 3D: level 2



RS vs. HIF-IE in 3D



RS



HIF-IE

HIF-IE analysis

- 2D:

$$A \approx U_0^{-*} U_{1/2}^{-*} \cdots U_{L-1/2}^{-*} D V_{L-1/2}^{-1} \cdots V_{1/2}^{-1} V_0^{-1}$$
$$A^{-1} \approx V_0 V_{1/2} \cdots V_{L-1/2} D^{-1} U_{L-1/2}^{*} \cdots U_{1/2}^{*} U_0^{*}$$

- 3D:

$$A \approx U_0^{-*} U_{1/3}^{-*} U_{2/3}^{-*} \cdots U_{L-1/3}^{-*} D V_{L-1/3}^{-1} \cdots V_{2/3}^{-1} V_{1/3}^{-1} V_0^{-1}$$
$$A^{-1} \approx V_0 V_{1/3} V_{2/3} \cdots V_{L-1/3} D^{-1} U_{L-1/3}^{*} \cdots U_{2/3}^{*} U_{1/3}^{*} U_0^{*}$$

Skeleton size:	$\mathcal{O}(\log N)$
Factorization cost:	$\mathcal{O}(N)$
Solve cost:	$\mathcal{O}(N)$

Numerical results in 2D

First-kind volume integral equation on a square with

$$a(x) \equiv 0, \quad K(x,y) = -\frac{1}{2\pi}\log\|x-y\|.$$

ϵ	N	$\lvert\hat{c}\rvert$	m_f (GB)	t_f (s)	$t_{a/s}$ (s)	e_a	e_s	n_i
10^{-3}	256^2	19	9.8e−2	1.0e+1	1.6e−1	1.8e−04	1.1e−2	8
	512^2	20	3.8e−1	4.3e+1	6.3e−1	1.6e−04	1.6e−2	8
	1024^2	20	1.5e+0	1.8e+2	2.6e+0	2.1e−04	1.4e−2	9
	2048^2	21	6.1e+0	7.5e+2	1.1e+1	2.2e−04	3.4e−2	9
10^{-6}	256^2	85	3.0e−1	2.7e+1	1.2e−1	2.0e−07	1.6e−5	3
	512^2	99	1.3e+0	1.3e+2	5.0e−1	1.3e−07	2.3e−5	3
	1024^2	115	5.4e+0	5.9e+2	2.1e+0	2.5e−07	3.4e−5	3
10^{-9}	256^2	132	4.4e−1	4.5e+1	1.2e−1	7.8e−11	1.3e−8	2
	512^2	155	1.8e+0	2.1e+2	4.9e−1	1.1e−10	1.6e−8	2
	1024^2	181	7.5e+0	9.7e+2	2.0e+0	1.8e−10	3.1e−8	2

Numerical results in 3D

Second-kind boundary integral equation on a sphere with

$$a(x) \equiv 1, \quad K(x,y) = \frac{1}{4\pi\|x-y\|}.$$

ϵ	N	$\lvert\hat{c}\rvert$	m_f (GB)	t_f (s)	$t_{a/s}$ (s)	e_a	e_s
10^{-3}	20480	201	1.4e−1	9.8e+0	3.8e−2	7.2e−4	7.1e−4
	81920	307	5.6e−1	5.0e+1	1.8e−1	1.8e−3	1.8e−3
	327680	373	2.1e+0	2.2e+2	7.5e−1	3.8e−3	3.7e−3
	1310720	440	8.1e+0	8.9e+2	3.2e+0	9.7e−3	9.5e−3
10^{-6}	20480	497	5.2e−1	6.3e+1	5.3e−2	1.1e−7	1.1e−7
	81920	841	2.1e+0	4.1e+2	2.4e−1	2.3e−7	2.3e−7
	327680	1236	8.2e+0	2.3e+3	1.0e+0	1.2e−6	1.2e−6

Numerical results in 3D

First-kind volume integral equation on a cube with

$$a(x) \equiv 0, \quad K(x,y) = \frac{1}{4\pi\|x-y\|}.$$

ϵ	N	$\lvert\hat{c}\rvert$	m_f	t_f	$t_{a/s}$	e_a	e_s	n_i
10^{-2}	16^3	39	1.5e−2	1.5e+0	1.5e−2	6.0e−3	2.8e−2	10
	32^3	51	1.7e−1	2.1e+1	1.5e−1	9.0e−3	5.7e−2	14
	64^3	65	1.7e+0	2.8e+2	1.4e+0	1.3e−2	1.3e−1	17
10^{-3}	16^3	92	4.3e−2	2.7e+0	9.6e−3	2.2e−4	1.0e−3	6
	32^3	171	4.1e−1	4.8e+1	5.9e−2	4.0e−4	2.0e−3	8
	64^3	364	4.2e+0	8.8e+2	5.7e−1	7.1e−4	2.4e−3	8
10^{-4}	16^3	182	6.1e−2	3.1e+0	7.2e−3	1.2e−5	1.2e−4	4
	32^3	360	7.7e−1	1.5e+2	8.6e−2	2.8e−5	2.3e−4	5
	64^3	793	9.1e+0	3.5e+3	9.1e−1	5.7e−5	3.6e−4	5

Conclusions

- Linear-time algorithm for structured operators in 2D and 3D
  - Fast matrix-vector multiplication
  - Fast direct solver at high accuracy, preconditioner otherwise
- Main novelties:
  - Dimensional reduction by alternating between cells, faces, and edges
  - Matrix factorization via new linear algebraic formulation
- Explicit elimination of DOFs, no nested hierarchical operations
- Can be viewed as adaptive numerical upscaling
- **Extensions**: $A^{1/2}$, $\log \det A$, $\operatorname{diag} A^{-1}$
- High accuracy for IEs in 3D still challenging, may require new ideas

- **Perspective**: structured dense matrices can be sparsified very efficiently
- Can borrow directly from sparse algorithms, e.g., RS = MF
- What other features of sparse matrices can be exploited?