Scalable and Robust Hierarchical Matrix Factorizations via Randomization

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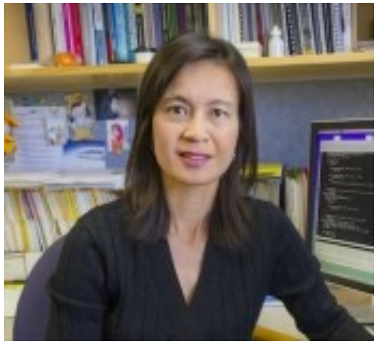
People

Sherry Li



Lisa Claus

Pieter Ghysels

Yang Liu

Past members:

- Gustavo Chavez, Machinify
- Chris Gorman, UC Santa Barbara
- Liza Rebrova, Princeton
- Francois-Henry Rouet, LSTC

Acknowledgement

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Fast direct solvers, preconditioners using ideas from structured matrices

Two types of structured matrices (for the purpose of this talk …)

- "Dense" → data-sparse

  e.g., low-rank, butterfly representation

- "Sparse" → structurally-sparse

  becomes sparser when combining with data-sparse

Software

- ButterflyPACK https://github.com/liuyangzhuan/ButterflyPACK
  (**Yang Liu** et al.)
  - Distributed-memory, OpenMP, Fortran2008
  - Support H, HODLR with LR and Butterfly
  - Dense
- STRUMPACK https://portal.nersc.gov/project/sparse/strumpack/
  (**Pieter Ghysels** et al.)
  - Distributed-memory, OpenMP, C++
  - Support HSS, BLR with LR, interface with most ButterflyPACK functionalities
  - Dense and sparse (multifrontal + data-sparse fronts)

	H (LR/BF)	HODLR (LR/BF)	HSS	BLR	H^2
ButterflyPACK	☺	☺			
STRUMPACK		☺	☺	☺	*WIP*

Outline

- Adaptive random sketching, error estimate, stopping criteria

  C. Gorman, G. Chavez, P. Ghysels, T. Mary, F.-H. Rouet, X.S. Li, “Robust and Accurate Stopping Criteria for Adaptive Randomized Sampling in Matrix-free Hierarchically Semiseparable Construction", SIAM J. Sci. Comput., 2019

- Butterfly compression for high frequency wave equations

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- Sparse direct solver enhanced with data-sparse

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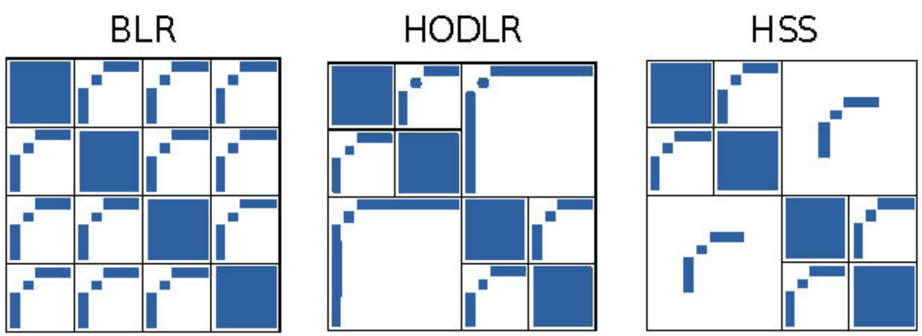
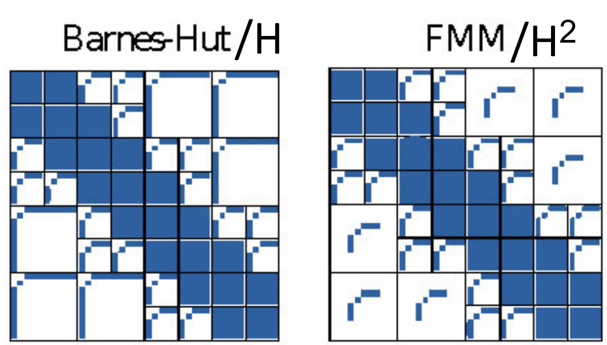
Classes of LR structured matrices

Lower complexity usually requires multilevel / hierarchical approach

	Strong admissibility	Weak admissibility
Independent bases	H matrix	(Hierarchically off-diagonal low-rank) HODLR matrix
Nested bases	H^2 matrix Inverse FMM	HSS matrix Recursive Skeletonization HIF



Weak admissibility



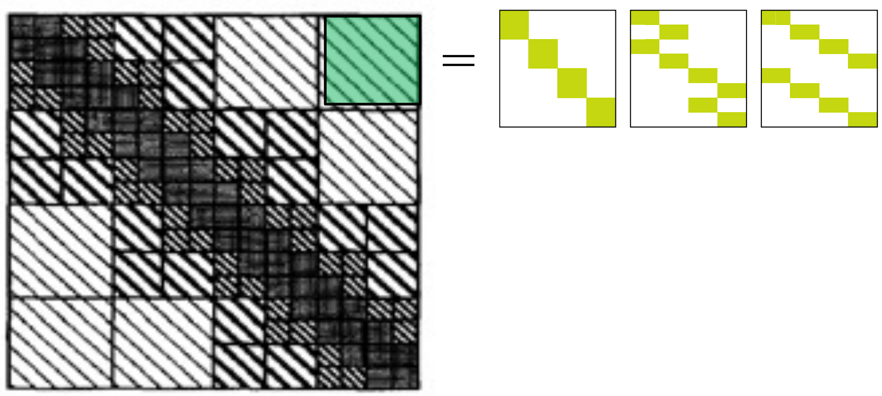
Strong admissibility

Butterfly structured matrices

- Butterfly factorization: generalized FFT

  Michielssen/Boag (1996), Li, Liu, Poulson, Yang, Ying, …

	Strong admissibility	Weak admissibility
Independent bases	H-BF	HOD-BF
Nested bases	Directional H^2 ?	HSS-BF



Stages of operations

- **Data clustering, matrix reordering**
  - minimize off-diag ranks

- **Compression** – usually dominating cost
  complexity depends on two situations:
  1. only black-box matvec K*g and K'*g are available
  2. only black-box entry evaluation K(i,j) is available

  Goal: $O(N \log^{\alpha} N)$

- **Matrix operations with compressed format**
  - Matrix-vector multiplication
  - Factorization / solve, inversion, …

Sweeping through **"trees"** upward / downward:

- HSS tree, butterfly tree
- Principal tools for parallelization

LR compression mechanisms

- SVD
- RRQR

- Randomized projection (sampling, sketching) : $O(n^2r)$

- ACA, block ACA → hierarchical blocked ACA : $O(nr^2)$
  (Liu, Sid-Lakhdar, Rebrova, Ghysels, Li, 2020)
- Interpolative Decomposition (ID) (skeletonization)

$B \approx B(:,J)\,X$, $B(:,J)$ has k columns, X is called interpolation matrix

- Nearest neighbors: relies on geometry

Compression via randomized sketching (RS)

… more flexible and faster than traditional rank-revealing QR

Approximate range of A:

1. Pick random matrix $\Omega_{nx(k+p)}$, k target rank, p small, e.g. 10
2. Sample matrix $S = A\,\Omega$ (tall-skinny)
3. Compute Q = ON-basis(S) via rank-revealing QR

   Can show: $\|(I - QQ^*)A\|$ is small with high probability

$$\mathrm{E}[\| A - QQ^* A \|] = \left(1 + \frac{4\sqrt{k+p}}{p-1}\sqrt{\min\{m,n\}}\right)\sigma_{k+1}$$

(Halko, Martinsson, Tropp, SIAM Rev. 2011)

Benefits:

- Matrix-free, only need matvec
- When embedded in sparse frontal solver, simplifies “extend-add”

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Practical issue: do not know target rank!

Earlier adaptive strategy

- Sample based posterior error estimation
  (Halko, Martinsson, Tropp, SIAM Rev. 2011)

LEMMA 4.1. *Let* $\boldsymbol{B}$ *be a real* $m \times n$ *matrix. Fix a positive integer* r *and a real number* $\alpha > 1$. *Draw an independent family* $\{\boldsymbol{\omega}^{(i)} : i = 1, 2, \ldots, r\}$ *of standard Gaussian vectors. Then*

$$\|\boldsymbol{B}\| \le \alpha \sqrt{\frac{2}{\pi}} \max_{i=1,\ldots,r} \|\boldsymbol{B}\boldsymbol{\omega}^{(i)}\|$$

except with probability α^{-r}.

- Drawback:
  - Only provide absolute bound, not relative
    (relative is particularly desirable when B are submatrices in hierarchical matrices)

New: Incremental RS for robustness and performance

Increase sample size d, build Q incrementally (block Gram-Schmidt)
S = [S_1 , S_2 , S_3 , …]

- Projection:

$$\hat{S} = (I - QQ^*)S_{i+1} \quad \text{(one step block Gram−Schmidt)}$$

$$\hat{S} = (I - QQ^*)^2 S_{i+1} \quad \text{(in practice, “twice” to ensure orthogonality)}$$

- $\hat{S}$ is used to expand Q, only need internal orthogonalizing $\hat{S}$

$$[\bar{Q}, \mathrm{R}] = \mathrm{QR}(\hat{S}), \quad \text{augment } Q \leftarrow [Q \ \ \overline{Q}]$$

Need good error estimation to bound error for A: ||(I – QQ$^{*)}$A||

- only have S (only matvec available)
- want relative error estimate

Stochastic norm estimation

Let $A \in \Re^{mxn}$, and $x \in \Re^{n}$ with $x_i \sim N(0,1)$. Consider SVD:

$$A = U\Sigma V^* = [U_1 \;\; U_2]\begin{bmatrix} \Sigma_r & 0 \\ 0 & 0 \end{bmatrix}\begin{bmatrix} V_1^* \\ V_2^* \end{bmatrix}$$

Define $\zeta = V^* x$, ζ is also a Gaussian random vector.

$$\|Ax\|_2^2 = \|\Sigma\zeta\|_2^2 = \zeta_1^2\sigma_1^2 + \cdots + \zeta_r^2\sigma_r^2$$

here, $\sigma_1 \geq \sigma_2 \cdots \geq \sigma_r > 0$ are positive singular values. Then:

$$\mathrm{E}\left[\|Ax\|_2^2\right] = \sigma_1^2 + \cdots + \sigma_r^2 = \|A\|_F^2$$

For d sample vectors: $\mathrm{E}\left[\|S\|_F^2\right] = d\,\|A\|_F^2$

Probabilistic tail bounds: Gorman et al., SISC 2019

Adaptive sampling: stopping criteria

Let $[S_1 \ \ S_2] = A\,[R_1 \ R_2\,]$, $Q = QR(S_1)$, block size d

Absolute stopping criterion:

$$\|(I \ - QQ^*)A\|_F \approx \frac{1}{\sqrt{d}} \|(I \ - QQ^*)S_2\|_F \leq \varepsilon_a$$

Relative stopping criterion:

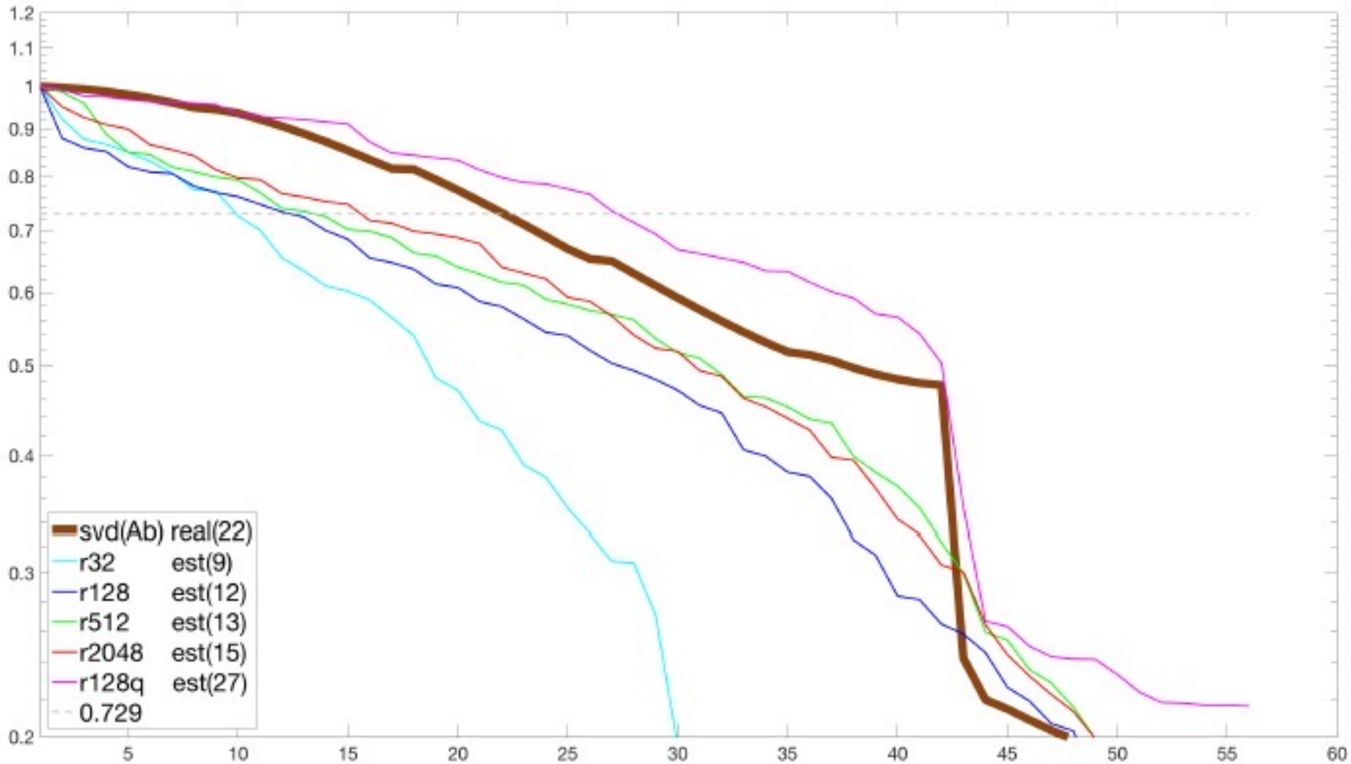
$$\frac{\|(I - QQ^*)A\|_F}{\|A\|_F} \approx \frac{\|(I - QQ^*)S_2\|}{\|S_2\|} \leq \varepsilon_r$$

- Cost: one reduction to compute norms of the sample vectors
- Give enough samples (robustness), but not too many (performance)

Example from HSS compression

- One internal rectangular Hankel block decay (56x3544) (from the 3600x3600 dense Poisson front)

- Older strategy stops at rank 15. New strategy stops at 27 (real 22)



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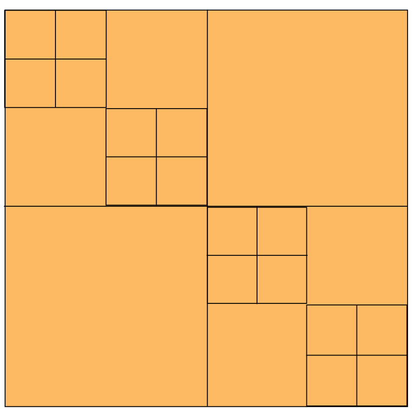
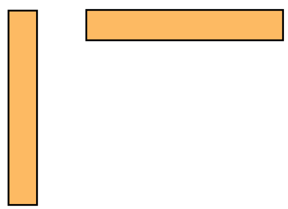
What about wave equations ?

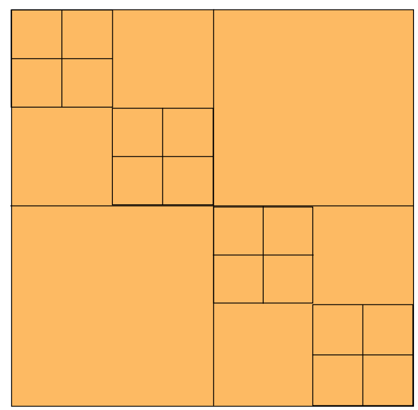
- Low/medium frequency: inversion cost $O(N \log^{\alpha} N)$
- High frequency: LR is not effective, inversion cost $O(N^3)$
- Remedies:
  - High-frequency FMM (Rokhlin 1993)
  - L-Sweeps (Taus), approximate-inverse (Ying), Xi, Vuik, etc.
  - Butterfly factorization (this talk)

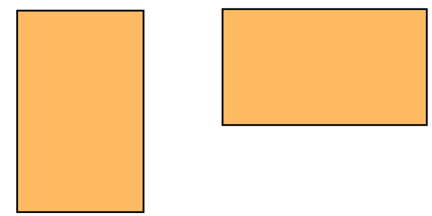




Z_{12} rank const
Memory $O(N)$

Z: low-freq

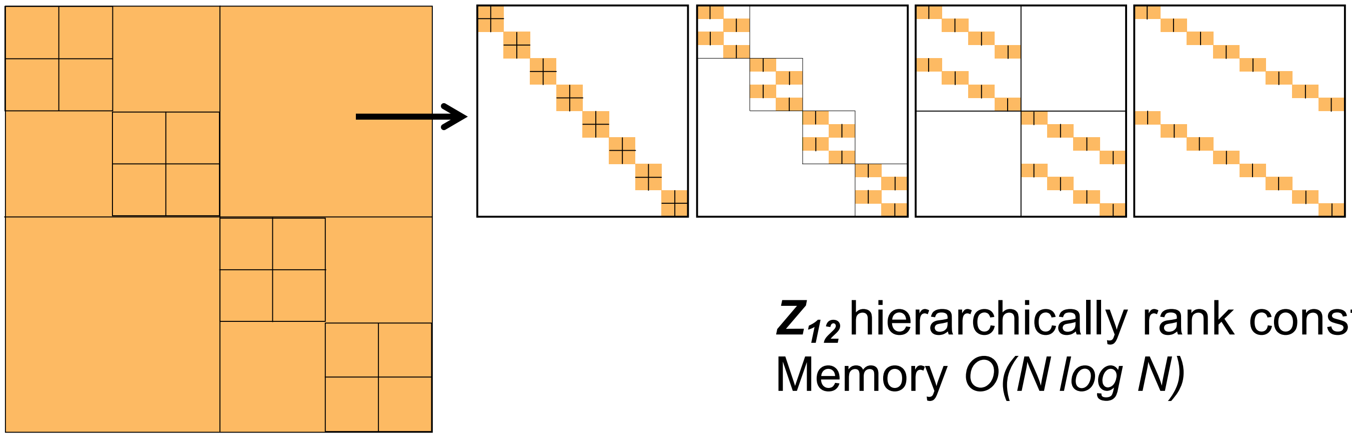




Z_{12} rank $O(N)$
Memory $O(N^2)$

Z: high-freq

Butterfly factorization



$\boldsymbol{Z}$: high-freq

$\boldsymbol{Z_{12}}$ hierarchically rank const
Memory $O(N \log N)$

- Butterfly is a FFT-inspired compression tool for highly oscillatory kernels
- Applications
  - Special function transforms (Radon, Fourier, spherical harmonic)
  - Fast direct and iterative integral (IE) equation solvers for high-frequency Helmholtz
  - Fast direct differential equation solvers for high-frequency Helmholtz
  - Scalable machine learning algorithms

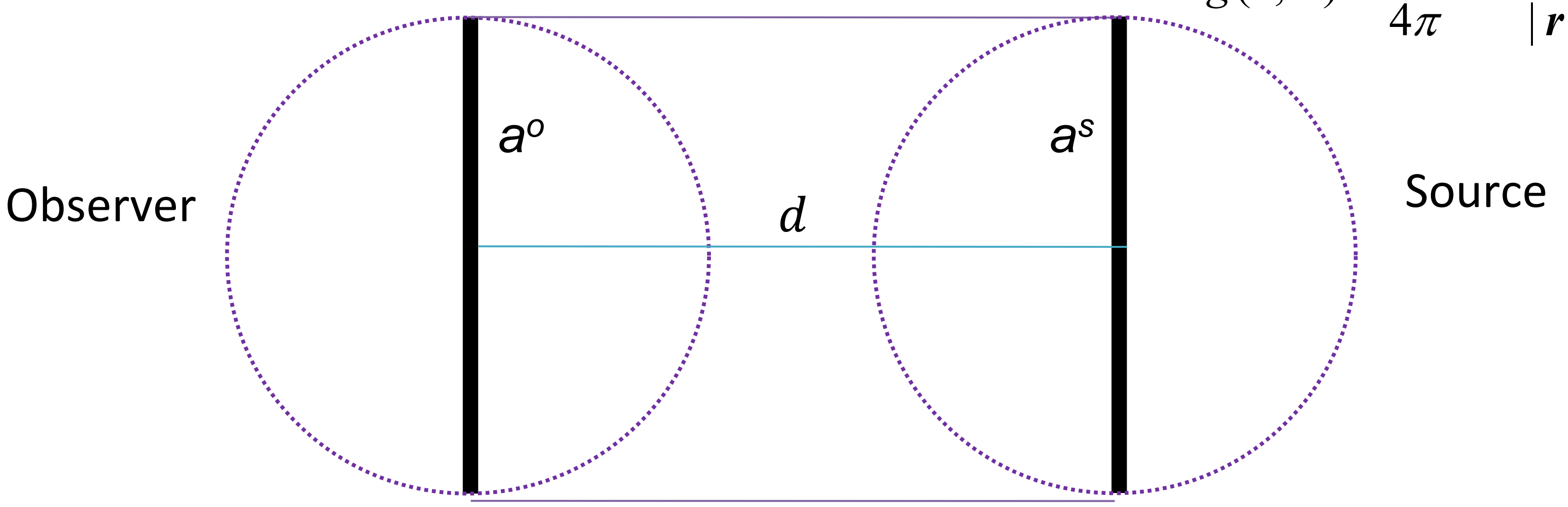
Physical interpretation of Butterfly

Degree of freedom (interaction rank): 2D $\sim \dfrac{k\,a^s a^o}{d}$, $\quad 3D \sim \left(\dfrac{k\,a^s a^o}{d}\right)^2$

a^o : diameter of sub-observer. a^s : diameter of sub-source.

d : distance between source observer centers. k : wave number.

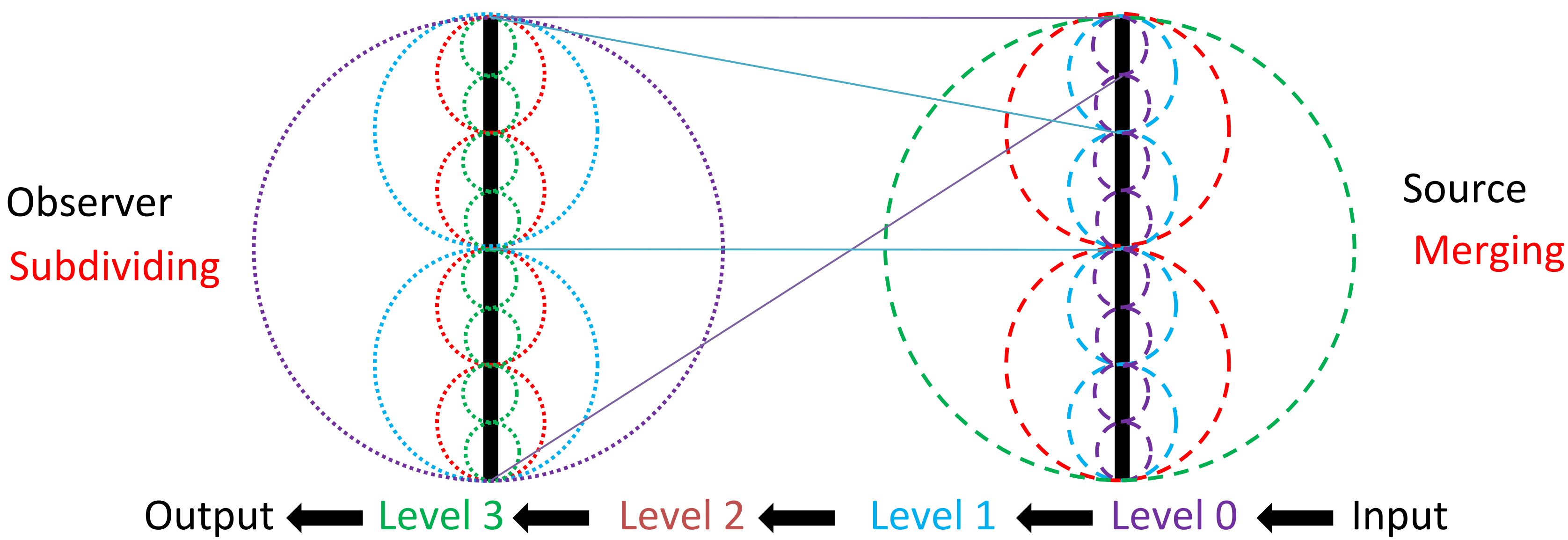
$$g(\boldsymbol{r},\boldsymbol{r}') = \frac{1}{4\pi}\frac{\exp(ik\,|\boldsymbol{r}-\boldsymbol{r}'|)}{|\boldsymbol{r}-\boldsymbol{r}'|}$$

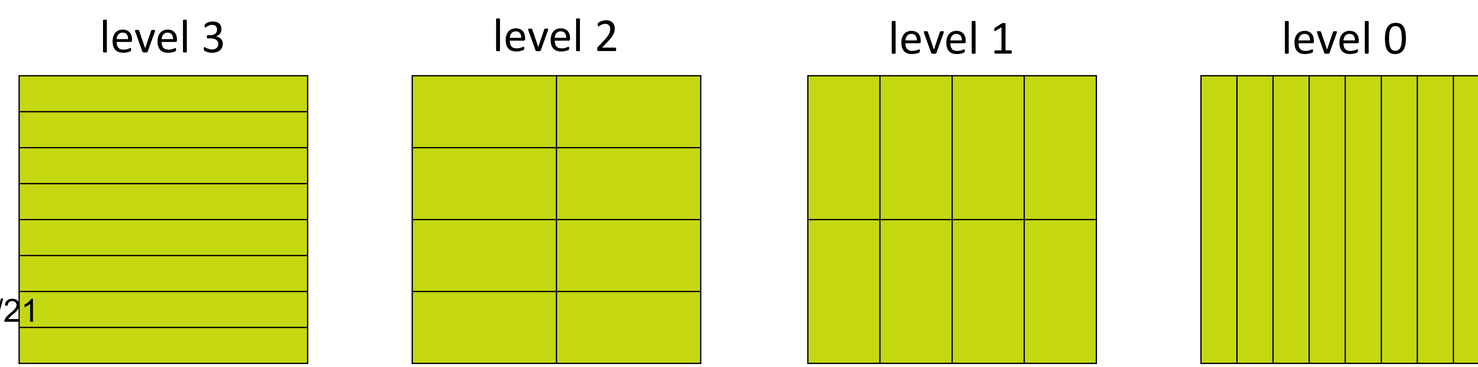


Physical interpretation of Butterfly

Degree of freedom (interaction rank): $2\text{D} \sim \dfrac{k\, a^s a^o}{d}, \quad 3D \sim \left(\dfrac{k\, a^s a^o}{d}\right)^2$

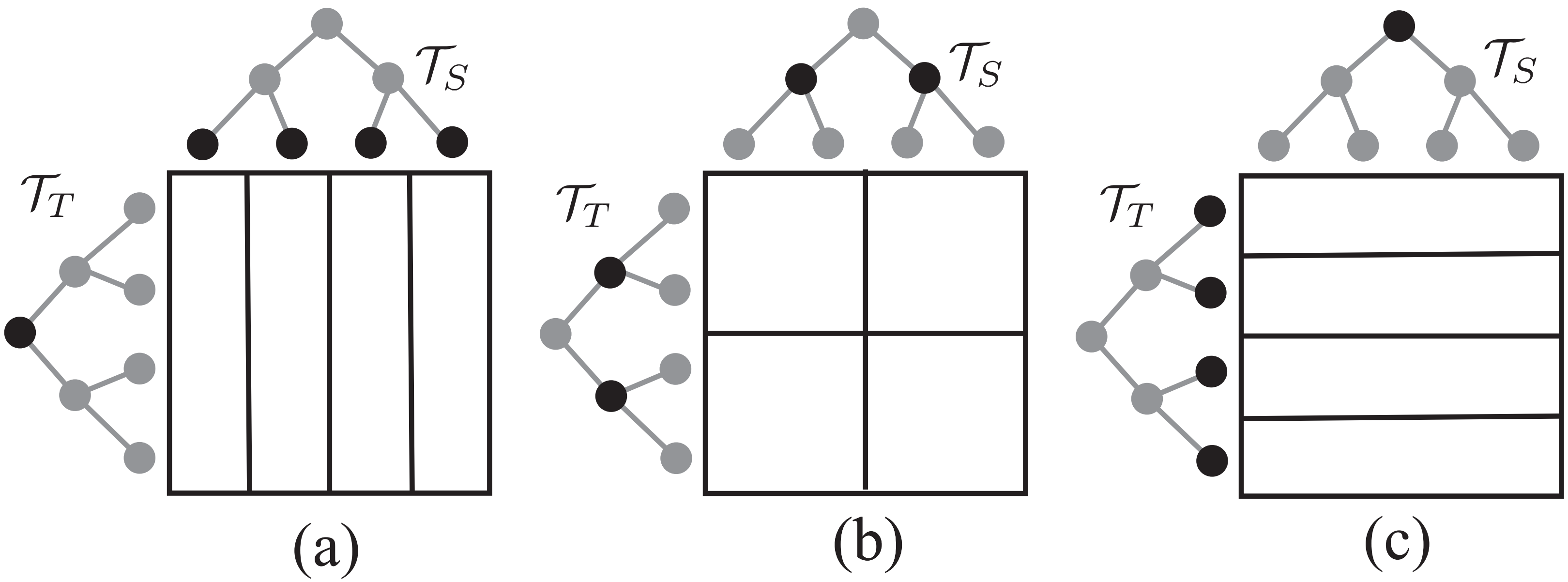
The ranks of all submatrices are r = constant (butterfly rank)





Hierarchical partitioning: Butterfly trees

Complementary low-rank property



Butterfly construction

Depending on how operator A is available

- Each entry can be evaluated in O(1) time

- Fast matvec available, e.g. in O(n logn) time

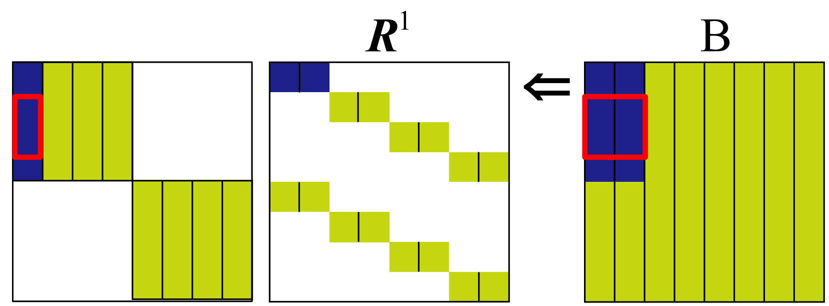
  Examples:
  - Compression of frontal matrices in sparse multifrontal solver
  - Conversion to butterfly from other FMM-like formats
  - Recompressing the composition of Fourier integrals
  - …

Butterfly Construction: entry-evaluation based

Let ***B*** has butterfly rank *r*, its *L*-level butterfly factorization is $\boldsymbol{B} = \boldsymbol{R}^L \ldots \boldsymbol{R}^1$

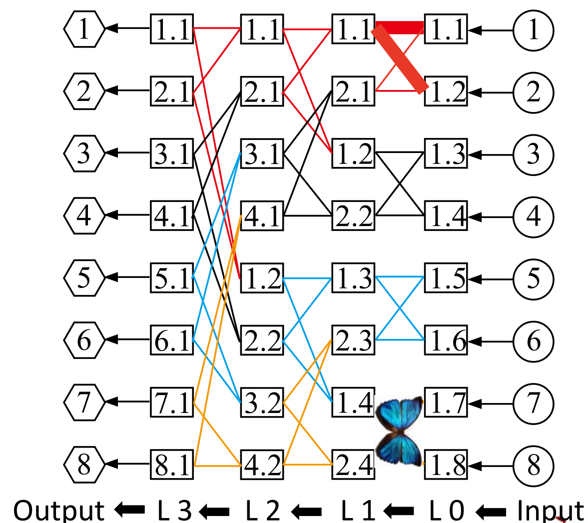
Compute LR compression for all judiciously selected submatrices

$R^{\ell}_{i,j}$ has size at most $r \times r$, Memory $O(n \log n)$, Flops $O(n \log n)$



$$\boldsymbol{R}^l = \mathrm{diag}(\boldsymbol{R}^l_1, \ldots, \boldsymbol{R}^l_{2^{l-1}})$$

$$\boldsymbol{R}^l_i = \begin{pmatrix} \boldsymbol{R}^l_{2i-1,1} \mid \boldsymbol{R}^l_{2i-1,2} & & \\ & \ddots & \\ & & \boldsymbol{R}^l_{2i-1,2^{L-l+1}-1} \mid \boldsymbol{R}^l_{2i-1,2^{L-l+1}} \\ \boldsymbol{R}^l_{2i,1} \mid \boldsymbol{R}^l_{2i,2} & & \\ & \ddots & \\ & & \boldsymbol{R}^l_{2i,2^{L-l+1}-1} \mid \boldsymbol{R}^l_{2i,2^{L-l+1}} \end{pmatrix}$$



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Let $\boldsymbol{B}$ has butterfly rank r, its L-level butterfly factorization is $\boldsymbol{B} = \boldsymbol{R}^L \ldots \boldsymbol{R}^1$

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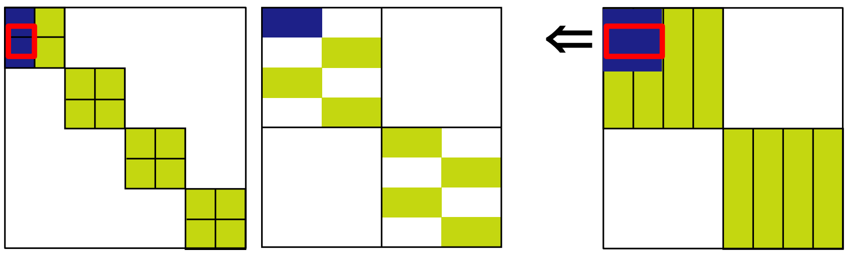
$\boldsymbol{R}^3$ $\quad$ $\boldsymbol{R}^2$



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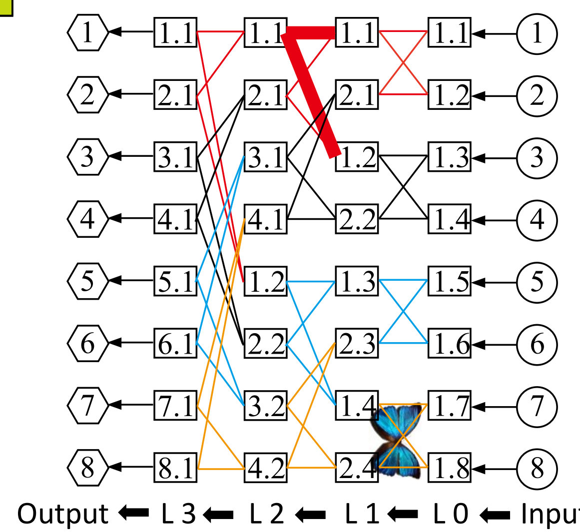

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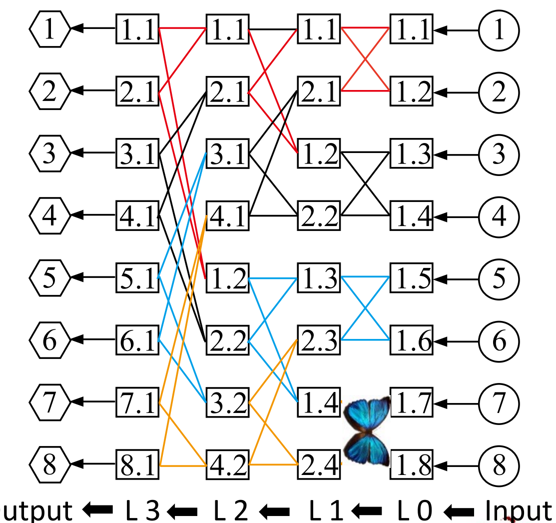
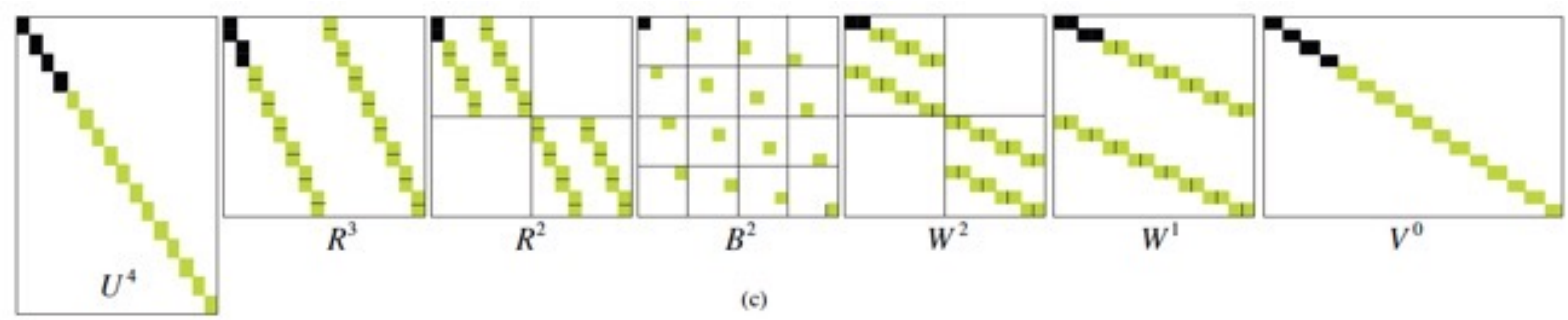
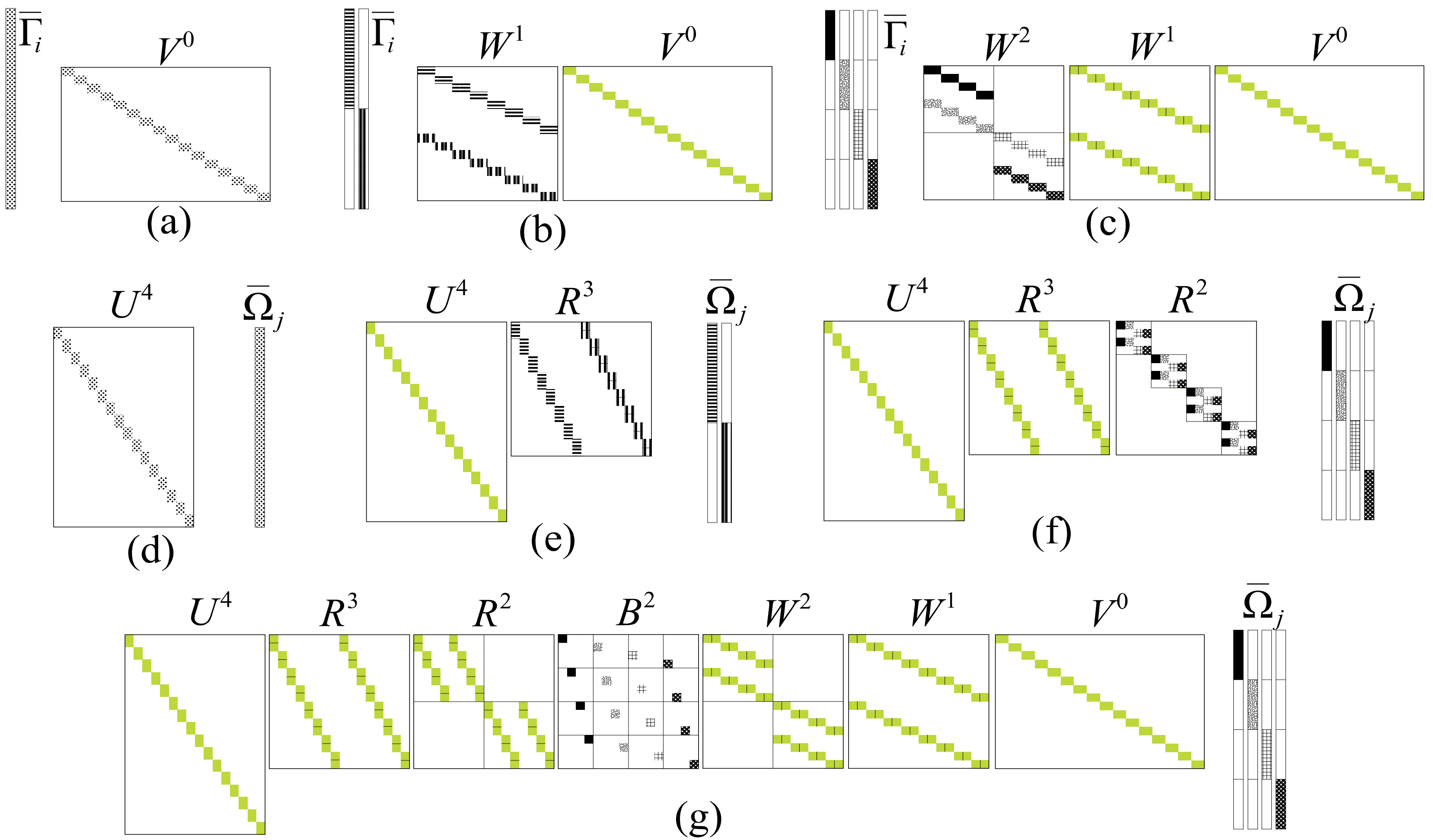


Hybrid form

- Column basis on the left, row basis on the right
- Meet at middle layer $l = L/2$



Butterfly Construction: random projection based

- BF_random_matvec : $O(n^{1.5}\log n)$ time, $O(n\log n)$ memory
- 

- For a $n\times n$ block A, $O(n^{0.5})$ vectors are needed
- Its L-level butterfly B satisfies: $||A-B||_F^2 \leq (L+2)\epsilon^2||A||_F^2$

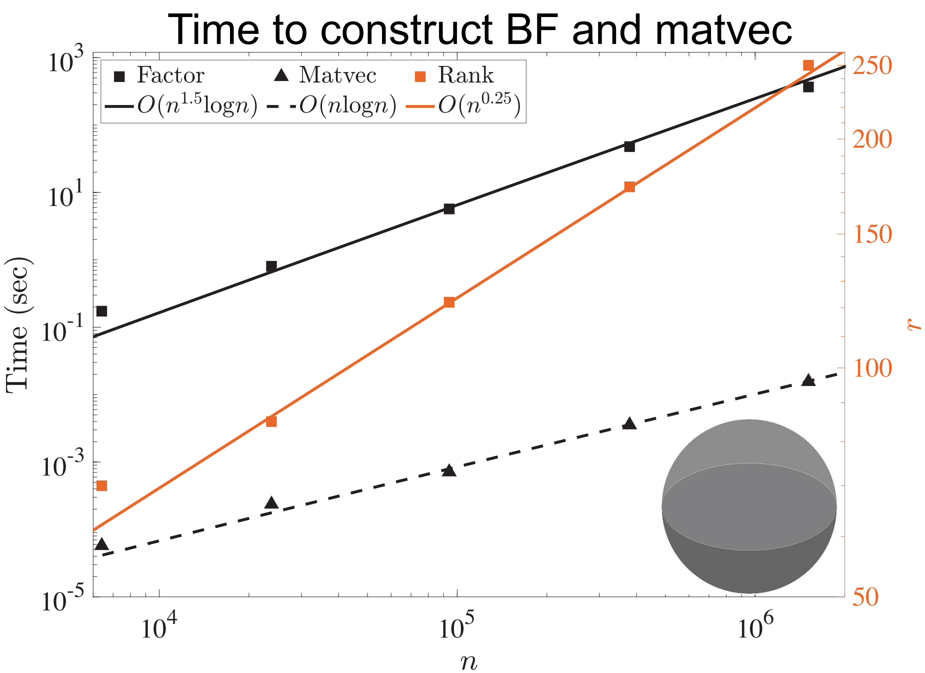
Butterfly Construction: randomized sketching based

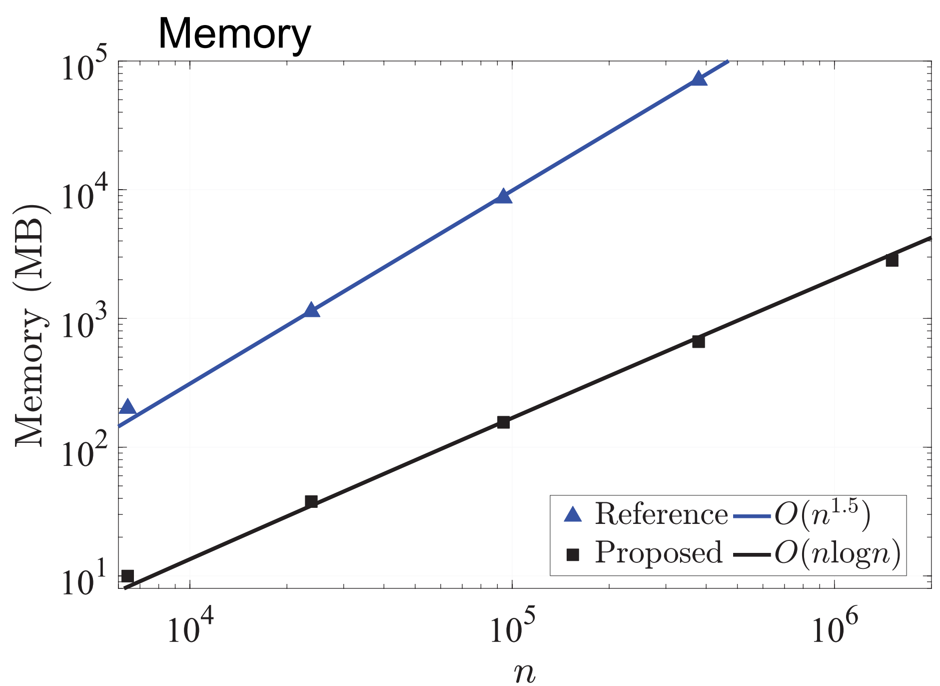
Liu, Xing, Guo, Michielssen, Ghysels, Li, 2021 (with parallelization)

3D Helmholtz kernel: interaction between two semi-sphere surfaces

BF to approximate:

$$A_{i,j} = \frac{\exp(i2\pi\kappa|\rho_i - \rho_j|)}{|\rho_i - \rho_j|}$$



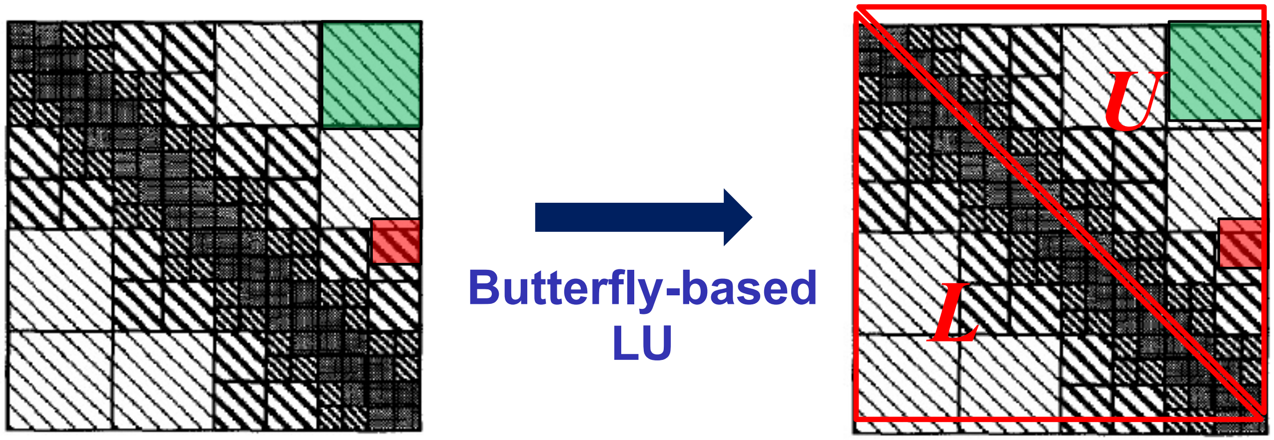


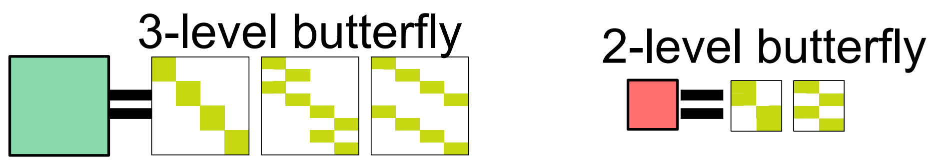
After construction, can do several operations

- Matrix-vector multiplication
  - Michielssen, Boag, 1996
  - Li, Yang, Martin, Ho, Ying, 2015
  - Poulson, Demanet , Maxwell, Ying, 2014 – parallelization

- Factorization / inversion
  - Liu, Guo, Michielssen, 2017
  - Liu, Xing, Guo, Michielssen, Ghysels, Li, 2020

Butterfly Solver: LU with H-BF





$$Z = \begin{bmatrix} Z_{11} & Z_{12} \\ Z_{21} & Z_{22} \end{bmatrix} = \begin{bmatrix} L_{11} & \\ L_{21} & L_{22} \end{bmatrix} \begin{bmatrix} U_{11} & U_{12} \\ & U_{22} \end{bmatrix}$$

(1) L_{11} and U_{11}: LU decompose $Z_{11} = L_{11}U_{11}$

(2) U_{12}: Triangular solve $Z_{12} = L_{11}U_{12}$

(3) L_{21}: Triangular solve $Z_{21} = L_{21}U_{11}$

(4) Update Z_{22}: $Z_{22} = Z_{22} - L_{21}U_{12}$

(5) L_{22} and U_{22}: LU decompose: $Z_{22} = L_{22}U_{22}$

Randomized butterfly operations:

Butterfly

$B = B_1 + B_2$

butterfly

$B = B_1 A$ or $B = AB_1$

Butterfly

$B = L^{-1}B_1$ or $B = B_1 U^{-1}$

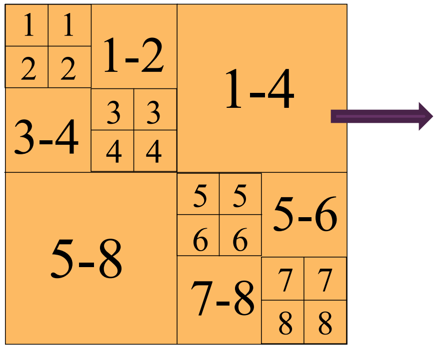
Lower triangular

Upper triangular

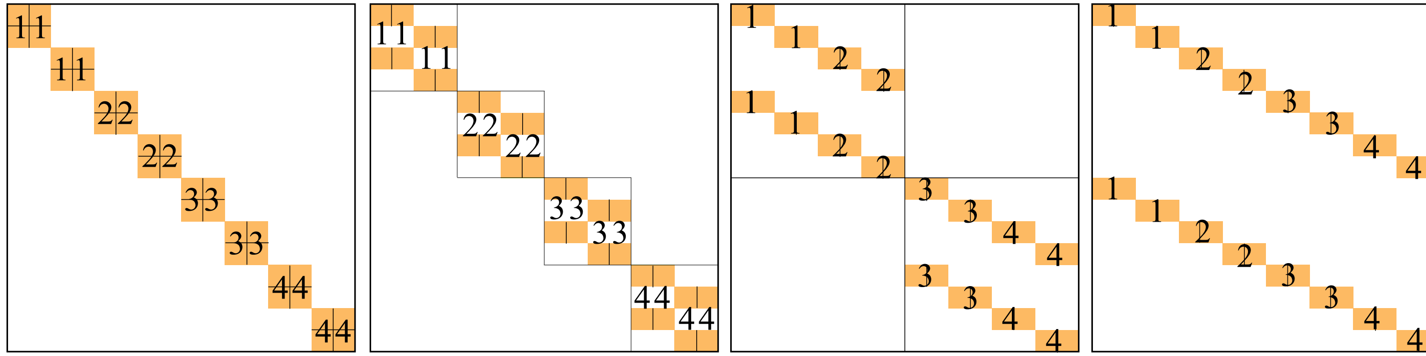
H. Guo, Y. Liu, J. Hu, and E. Michielssen, "A butterfly-based direct integral equation solver using hierarchical LU factorization for analyzing scattering from electrically large conducting objects", IEEE Trans. Antennas Propag., 2017

Distributed-memory Parallelization: BF construction via RS

- HODLR with Butterfly, symmetric bit-reversal ordering for each butterfly



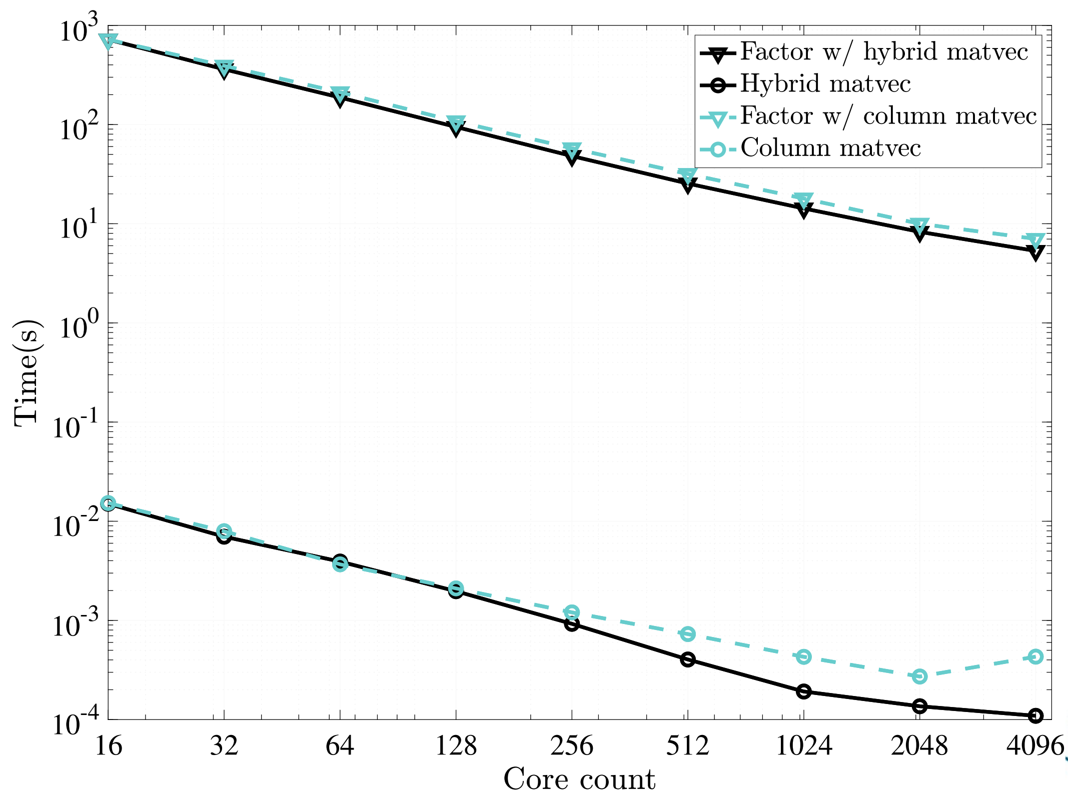
distributed



Distributed butterfly of $\boldsymbol{Z_{12}}$

$n = 2.56 \times 10^6$

core count: 16 - 4096



Outline

- Adaptive randomized sampling, error estimate, stopping criteria

  C. Gorman, G. Chavez, P. Ghysels, T. Mary, F.-H. Rouet, X.S. Li, "Robust and Accurate Stopping Criteria for Adaptive Randomized Sampling in Matrix-free Hierarchically Semiseparable Construction", SIAM J. Sci. Comput., 2019

- Butterfly compression for high frequency wave equations

  Y. Liu, X. Xing, H. Guo, E. Michielssen, P. Ghysels, X.S. Li, "Butterfly factorization via randomized matrix-vector multiplications'', SIAM J. Sci. Comput., 2021

- Sparse direct solver enhanced with data-sparse

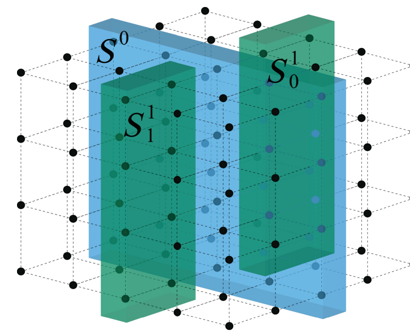
  Y. Liu, P. Ghysels, L. Claus, X.S. Li, "Sparse Approximate Multifrontal Factorization with Butterfly Compression for High Frequency Wave Equations", SIAM J. Sci. Comput., 2021

Sparse direct solver: STRUMPACK
Embedding LR data-sparse in multifrontal sparse factorization

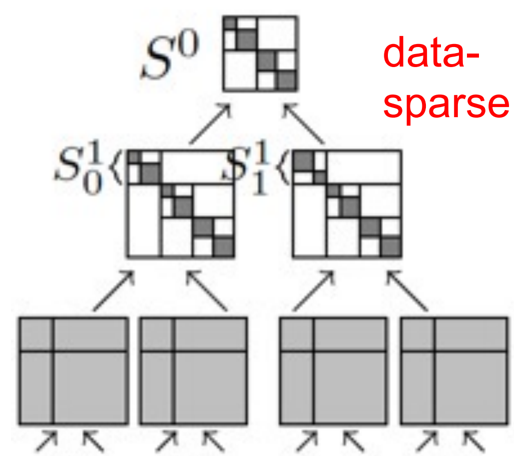
- Globally sparse, locally dense
  - Embed LR data-sparse in sparse multifrontal algorithm
- Baseline is a sparse multifrontal direct solver
- Nested Dissection ordering → separator tree
- In addition to structural sparsity, further apply LR data-sparsity to dense frontal matrices
- **Nested bases + randomized sampling** to achieve linear scaling in sparse case
  - **O(N logN) flops, O(N) memory for 3D elliptic PDEs**

    (as opposed to O(N^2) flops with exact factorization)

Nested dissection ordering

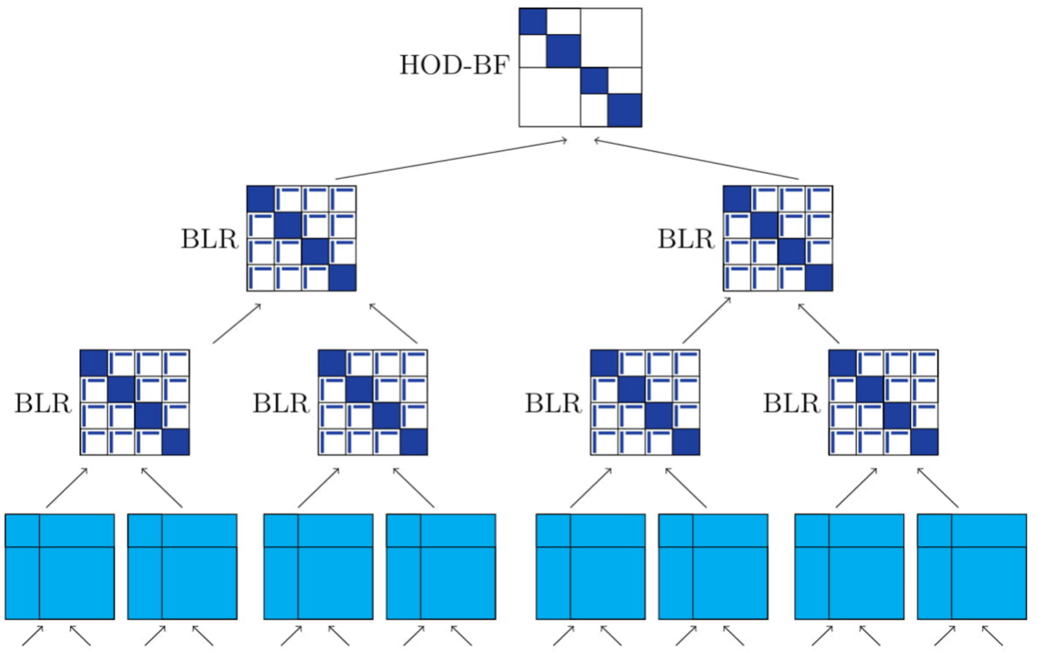


Multifrontal Separator tree



Sparse direct solver: combine multiple data-sparse

- Combining BLR and HOD-
  - Large fronts: HOD-BF
  - Medium fronts: BLR
  - Small fronts: no compr

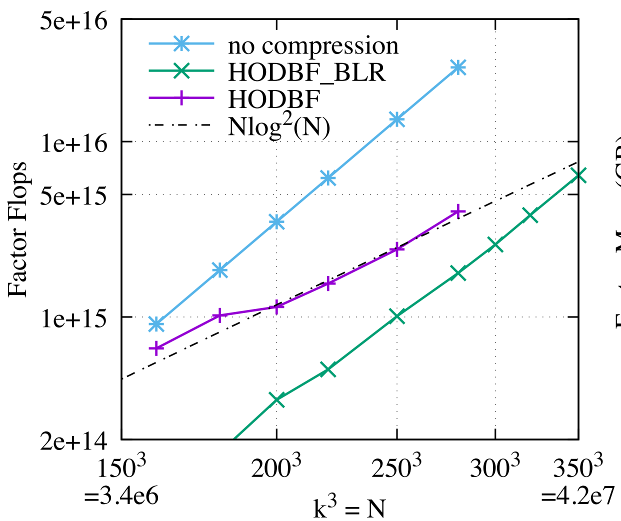


separator size(HOD-BF): 30k
separator size(BLR): 300

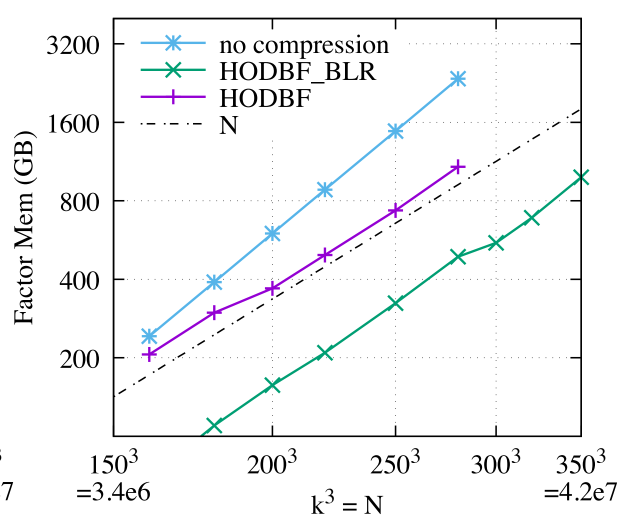
Sparse MF: HOD-BF/BLR: Finite Difference for 3D Helmholtz

$$\left(\sum_i \rho(\mathbf{x}) \frac{\partial}{\partial x_i} \frac{1}{\rho(\mathbf{x})} \frac{\partial}{\partial x_i}\right) p(\mathbf{x}) + \frac{\omega^2}{\kappa^2(\mathbf{x})} p(\mathbf{x}) = -f(\mathbf{x})$$

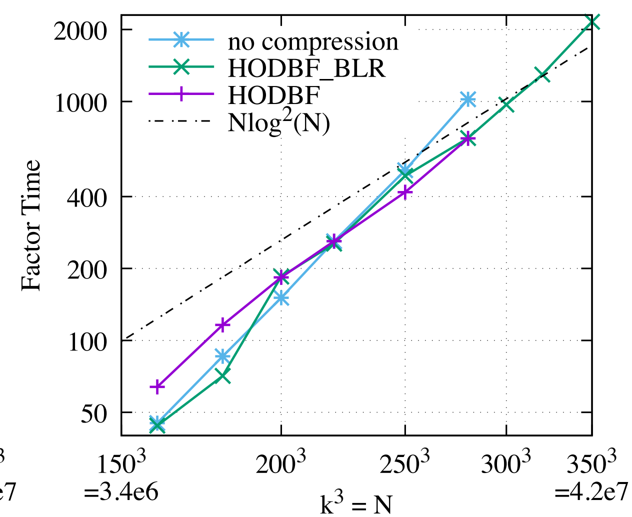
- 27-point finite difference stencil for 3D visco-acoustic propagation
- $v(\mathbf{x}) = 4000\mathrm{m/s}$, $\rho(\mathbf{x}) = 1\mathrm{kg/m}^3$, 15 points per wavelength
- Up to 64 Cori Haswell nodes (2048 cores)
- compression tolerance: 10^{-4} usually ~10 steps of GMRES



factor flops



factor size



Factor time

Sparse MF: HOD-BF vs. HSS

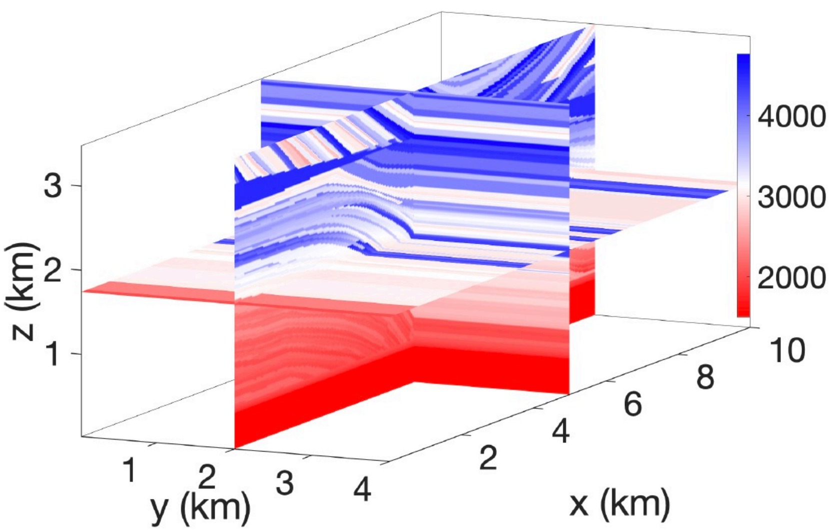
N = 250^3 , constant coefficients
32 Cori nodes (1024 cores)

Solver	Exact	HSS	HOD-BF	HOD-BF	HOD-BF
ε	-	10^{-3}	10^{-3}	10^{-2}	10^{-3}
$n_{\min}$	-	10K	10K	10K	7K
Compressed fronts	0	39	39	39	197
Dense fronts	1,869,841	1,869,802	1,869,802	1,869,802	1,869,644
$\boxed{\text{Factor time (sec)}}$	513	$\boxed{947}$	$\boxed{433}$	354	556
Factor flops (10^{15})	13.4	4.98	2.44	2.24	1.21
Flop Compression (%)	100	37.1	18.2	16.7	9.0
Factor mem (10^3 GB)	1.48	0.84	0.73	0.72	0.47
Mem Compression (%)	100	56.8	49.6	48.8	32.2
$\boxed{\text{Max. rank}}$	-	$\boxed{4698}$	$\boxed{364}$	153	389
Top 2 fronts					
Mem Compression (%)	-	21.9/14.6	7.29/3.54	4.4/1.89	6.3/3.6
Rank	-	4538/4698	154/242	121/213	177/255
Front time (sec)	37/108	172/195	52/88	42/60	46/70.6
GMRES its.	1	18	6	56	23
Solve flops (10^{12})	0.46	8.01	2.84	23.4	7.18
Solve time (sec)	0.72	19.2	3.5	30.1	13.2

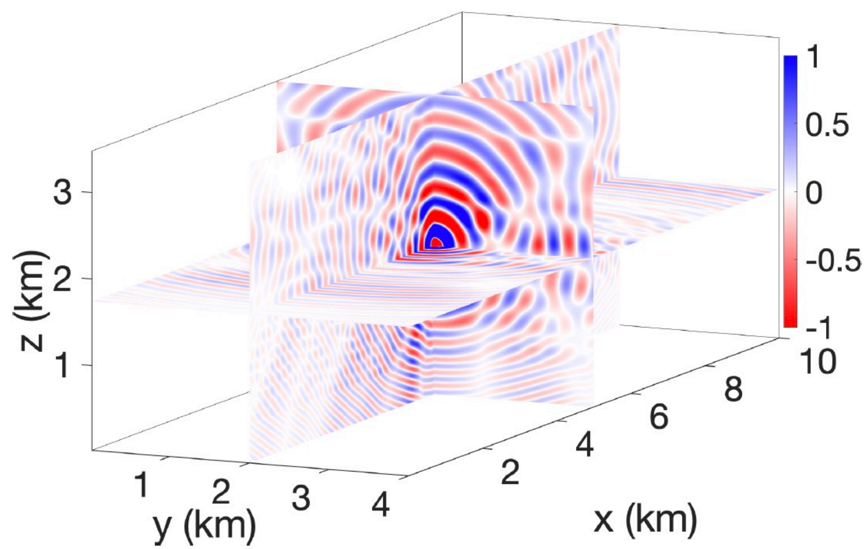
Sparse MF: HOD-BF: 3D Helmholtz, heterogeneous media

$$\left(\sum_i \rho(\mathbf{x})\frac{\partial}{\partial x_i}\frac{1}{\rho(\mathbf{x})}\frac{\partial}{\partial x_i}\right)p(\mathbf{x}) + \frac{\omega^2}{\kappa^2(\mathbf{x})}p(\mathbf{x}) = -f(\mathbf{x})$$

- 27-point finite difference stencil for 3D visco-acoustic propagation
- Marmousi2 P-wave velocity model $190\times216\times516, N = 21{,}176{,}640$, $\omega = 20\pi\mathrm{Hz}$, 7.5 points per wavelength
- 32 Cori Haswell nodes (1024 cores)



velocity model



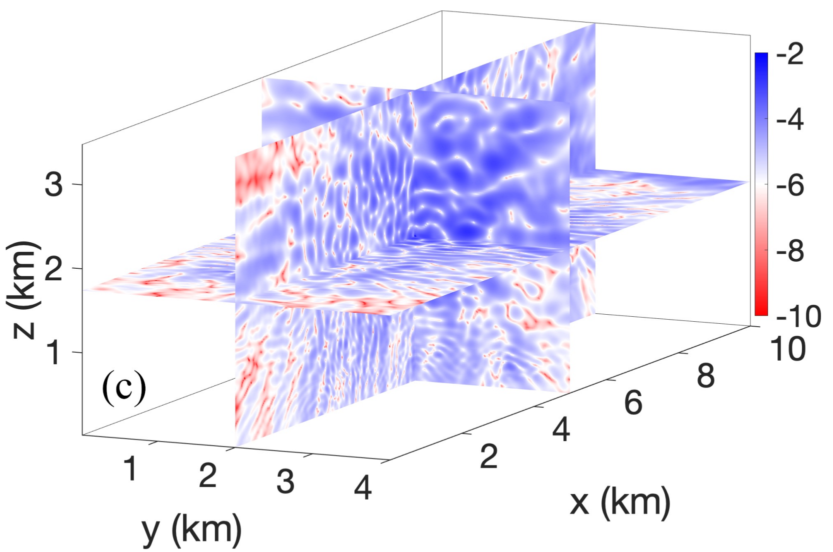
$\mathrm{Re}(p(\mathbf{x}))$

Sparse MF: HOD-BF: 3D Helmholtz, heterogeneous media

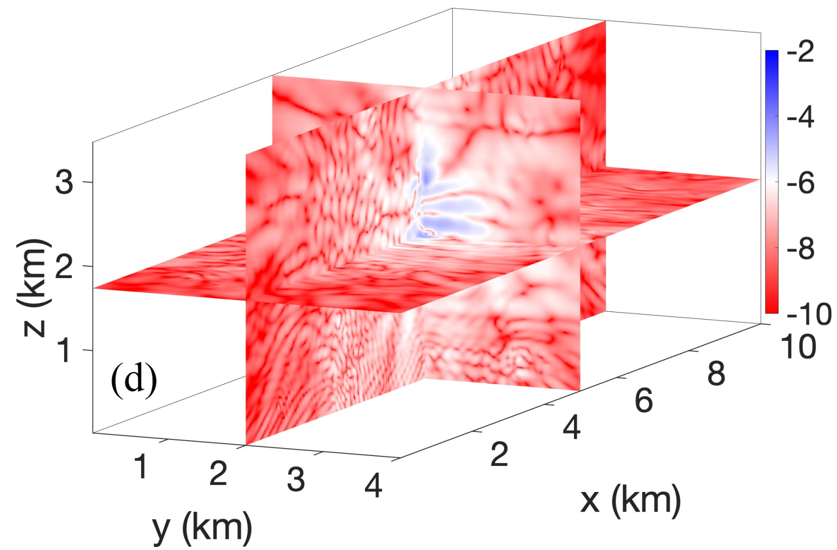
$$\left(\sum_i \rho(\mathbf{x})\frac{\partial}{\partial x_i}\frac{1}{\rho(\mathbf{x})}\frac{\partial}{\partial x_i}\right)p(\mathbf{x}) + \frac{\omega^2}{\kappa^2(\mathbf{x})}p(\mathbf{x}) = -f(\mathbf{x})$$

- Differences from truth in Re($p(\mathbf{x})$) with 2 tolerances

$\varepsilon = 10^{-4}$



$\varepsilon = 10^{-6}$



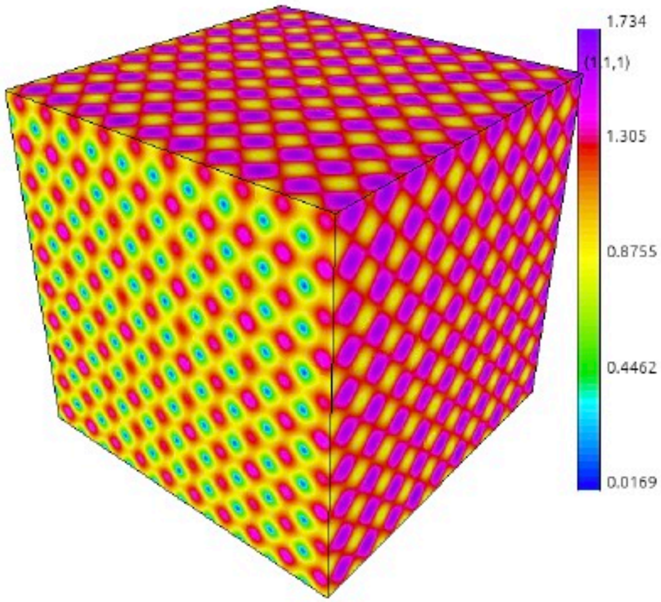
Sparse MF: HOD-BF: Finite Element for 3D Maxwell

$$\nabla \times \nabla \times \mathbf{E} - \Omega^2 \mathbf{E} = \mathbf{f}$$

- First-order Nedelec element discretization for 3D indefinite Maxwell in a homogenous cube
- $N = 14{,}827{,}904$, $\Omega = 16$, 24 points per wavelength
- 32 Cori Haswell nodes

ε	10^{-5}
HOD-BF fronts	6
Dense fronts	3,773,215
Factor time (sec)	581.1
Factor flops	$1.30 \cdot 10^{15}$
Flops fraction of direct (%)	61.3
Memory (GB)	426
Compression (%)	78.8
Maximum rank / front size	955 / 78203
GMRES its.	17
Solve flops	$5.73 \cdot 10^{12}$
Solve time (sec)	23.8

Solver breakdowns



$|\mathbf{E}(\mathbf{x})|$

Algorithm complexity (in bigO sense)

- Dense LU: $O(N^3)$
- Model PDEs with regular mesh, Nested Dissection ordering

	2D problems **$N = k^2$**			**3D problems** **$N = k^3$**		
	Factor flops	Solve flops	Memory	Factor flops	Solve flops	Memory
Exact sparse LU	$N^{3/2}$	$N \log(N)$	$N \log(N)$	N^2	$N^{4/3}$	$N^{4/3}$
STRUMPACK With LR compression	N	N	N	N^{α} polylog(N) ($\alpha < 2$)	$N \log(N)$	$N \log(N)$

Perspectives, future directions

- Techniques from structured matrices are very promising for preconditioning
  - LA tools: ID, randomization
  - Parallelism: coarse-grain (trees), fine-grain (dense submatrices)

- Caveat: wide spectrum of algorithms, not (yet) possible to have a decision tree of algorithm choices (e.g., iterative solution template book)
  - Problem-specific (esp. clustering)
  - Implementations are still being worked on for larger scale problems and machines

- Randomized LA is a very useful tool, rigorous error analyses are needed to understand approximation quality

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Questions?