Fast Construction of Hierarchically Low Rank Matrices Using Randomized Sketching

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Outline

- Background of hierarchical matrices
- Construction using randomization techniques
- Applications

Exploit STRUCTURES

1. Sparsity structure: defined by $\{0,1\}$ structure (Graphs).
   - Factors are denser (fill-in)
   - sparse LU: $O(N^2)$ flops and $O(N^{4/3})$ memory, for typical 3D PDEs

2. Low rank structure: in addition to structural sparsity, can find data-sparse structure in dense (sub)matrices (approximation)
   - Goal is to achieve $O(N)$ or $O(N\ polylog(N))$ memory & flops for compression, factorization ...
   - Hierarchical matrices: $\mathcal{H}$- & $\mathcal{H}^2$-matrix [Hackbusch et al. 1999] and their subclasses.

     [Bebendorf, Bini, Börm, Chandrasekaran, Chow, Darve, Dewilde, Grasedyck, Gu, Le Borne, Martinsson, Tygert, Van Barel, van der Veen, Vandebril, Xia, ..., MANY MORE]

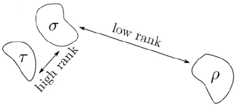
Application 1: Applying integral operator (N-body comput.)

$$(Kg)(x) = \int_Y K(x,y)g(y)dy, \quad \texttt{Kernel} \ K : X \times Y \to C$$

- Low rank property:

$$\texttt{admissible}(\tau, \sigma) = 1,$$

$$\textit{if} \ \frac{\texttt{Diam}(\tau) + \texttt{Diam}(\sigma)}{2} \le \eta \cdot \texttt{Dist}(\tau, \sigma)$$



- Many kernels have this property:
  - Gaussian kernel: $K(i,j) = \exp\left(-\frac{\|x_i - x_j\|_2^2}{2h^2}\right)$
  - Green's functions for Laplace equations:

$$\texttt{2D:} \ \log(||x_i - x_j|); \qquad \texttt{3D:} \ \frac{1}{(||x_i - x_j||)}$$

  - Green's functions for Helmholtz equations:

$$\texttt{2D:} \ H_0(k|x_i - x_j|); \qquad \texttt{3D:} \ \frac{e^{ik|x_i - x_j|}}{|x_i - x_j|}$$

  - Others: Fourier-type of kernel $e^{i\Phi(x,y)}$ where $\Phi(x,y)$ is smooth; e^{ixy}; Bessel function $J_0(xy)$

Hierarchical matrix approximation

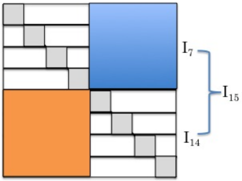
- Same mathematical foundation as FMM [Greengard/Rokhlin 1987], put in matrix form:
  - Diagonal block ("near field") represented exactly
  - Off-diagonal block ("far field") approximated via low-rank format

FMM separability of Green's function	Algebraic low rank off-diagonal
$G(x,y) \approx \sum_{\ell=1}^{r} f_\ell(x) g_\ell(y)$ $x \in X, y \in Y$	$A = \left[\begin{array}{c\|c} D_1 & U_1 B_1 V_2^T \\ \hline U_2 B_2 V_1^T & D_2 \end{array}\right]$

- Algebraic power: factorization, inversion, tensors, ...

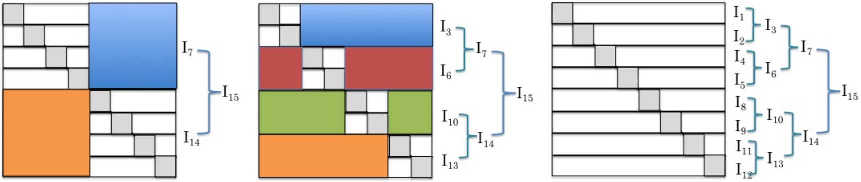
Hierarchical organization is key to optimal algorithm complexity

Example: Hierarchical Off-Diagonal Low Rank (HODLR)



Hierarchical organization is key to optimal algorithm complexity

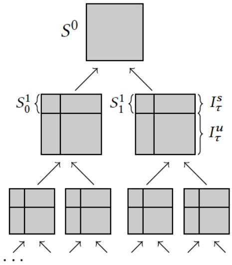
Example: Hierarchical Off-Diagonal Low Rank (HODLR)

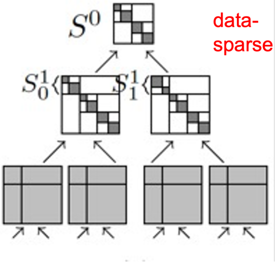


Algorithm can be top-down or bottom-up

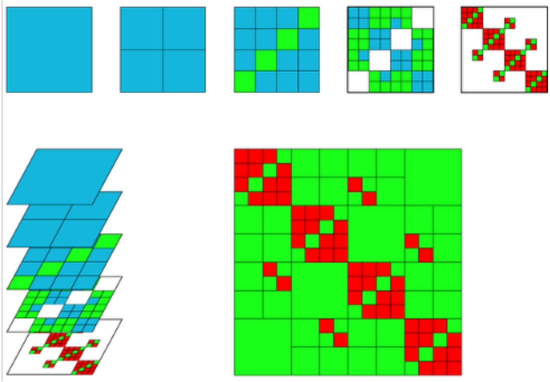
Application 2: discretized PDE

- Globally sparse, locally dense
  - Can embed LR data-sparse in sparse multifrontal algorithm
- In addition to structural sparsity, further apply LR data-sparsity to dense frontal matrices



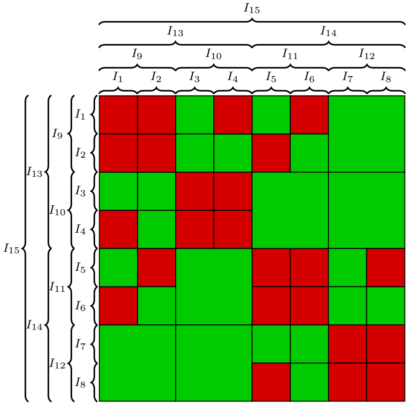


Hierrarchical matrix structure



1. Cluster the variables into a cluster tree
2. Define **admissibility condition** to determine whether a pair of clusters admits a low rank block
3. Hierarchically determine **admissible blocks** using a dual tree traversal on the cluster tree

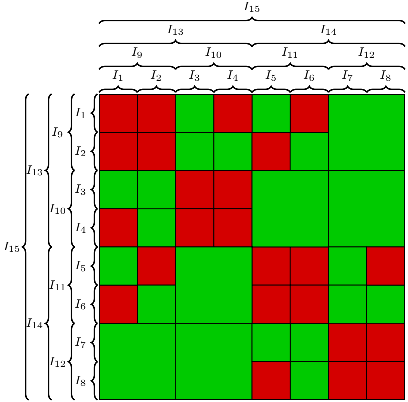
Cluster tree, Matrix tree

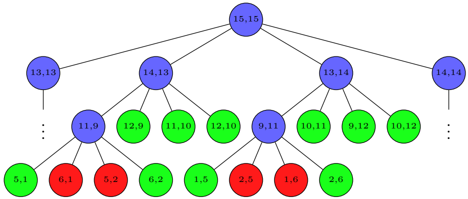


Cluster tree I: pairs of clusters define blocks in the matrix.

- Leaves form a block partitioning
- Red blocks = inadmissible leaves
- Green blocks = admissible blocks

Cluster tree, Matrix tree





Cluster tree I: pairs of clusters define blocks in the matrix.

- Leaves form a block partitioning
- Red blocks = inadmissible leaves
- Green blocks = admissible blocks

Matrix tree: generally not a complete tree

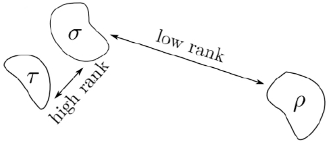
- Blue nodes = inadmissible blocks
- Red nodes = inadmissible leaves
- Green nodes = admissible leaves

Admissibility condition

$$\texttt{admissible}(\tau,\sigma) = 1,\ \textit{if}\ \frac{\texttt{Diam}(\tau)+\texttt{Diam}(\sigma)}{2} \le \eta \cdot \texttt{Dist}(\tau,\sigma)$$

Typically

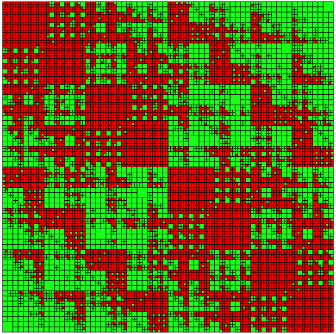
- weak admissibility: $\eta \ge 1$
  e.g., HODLR, HSS
- strong admissibility: $\eta \le 0.5$
  e.g., $\mathcal{H}$,$\mathcal{H}^2$



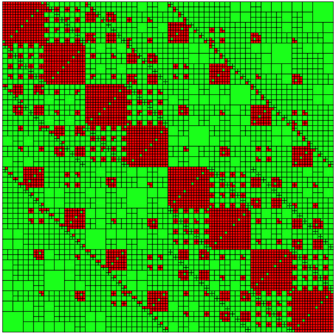
Admissibility condition

Example: block partitioning of a matrix associated with a set of $N = 2^{15}$ points in 3D geometry

Smaller η leads to more refined partitioning of off-diagonal blocks



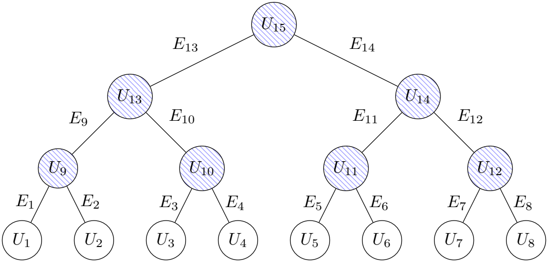
$\eta = 0.5$



$\eta = 0.7$

Nested basis leads to optimal complexity

- Represent parents in terms of their children using **transfer matrices**
  - $U_i^{l-1} = \begin{bmatrix} U_{i_1}^l & \\ & U_{i_2}^l \end{bmatrix} \begin{bmatrix} E_{i_1}^l \\ E_{i_1}^l \end{bmatrix}$
- Every low rank block has the form $A_{ts}^l = U_t^l S_{ts}^l {V_s^l}^T$
  - S_{ts}^l is the **coupling matrix**
- Assume we have an orthogonal basis: ${U_t^l}^T U_t^l = I$



Classes of hierarchical low rank matrices

	Strong admissibility	Weak admissibility
Indep. bases	$\mathcal{H}$	HODLR
Nested based	$\mathcal{H}^2$ Inverse FMM	HSS, HIF Recursive Skeletonization

Classes of hierarchical low rank matrices

	Strong admissibility	Weak admissibility
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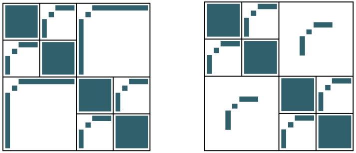
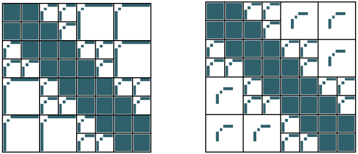
weak admissibility



strong admissibility



Deep dive: construction of hierarchical matrices

Low rank compression tool: adaptive randomized sketching

- Understanding probabilistic error

Low rank compression via randomized sketch

Approximate range of A:

1. Pick random matrix $\Omega_{n\times(k+p)}$, k target rank, p small, e.g. 10
2. Sample matrix $S = A\Omega$, with slight oversampling p
3. Compute $Q =$ ON-basis(S)

Benefits:

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

How to sketch only admissible blocks?

1. Preprocessing: Draw a big sketch using global A, $S = A\Omega$
   Sketching cost:
   - Dense matvec: $O(rN^2)$
   - FFT: $O(rN \log N)$ (e.g., Toeplitz)
   - FMM: $O(rN)$

   Can it be faster using structured random Ω?

[1] [Martinsson 2011; Xia 2013; Boukaram/Liu/Ghysels/L. 2025]

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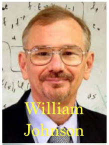
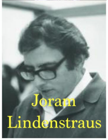
2. At each level, subtract small sketches corresponding to the inadmissible blocks [1]
   o Example: in HSS construction:
   block diagonal matrix at level ℓ: $D^{(\ell)} = diag(D_{\tau_1}, D_{\tau_2}, \ldots, D_{\tau_q})$

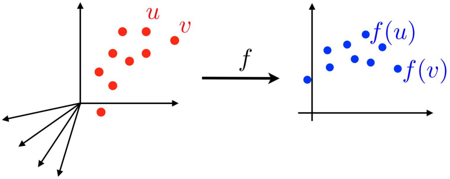
$$\text{Off-diagonal sketch: } S^{(\ell)} = \left(A - D^{(\ell)}\right)\Omega = S^r - D^{(\ell)}\Omega$$

[1] [Martinsson 2011; Xia 2013; Boukaram/Liu/Ghysels/L. 2025]

Unified view of sketching: Johnson-Lindenstrauss Lemma







Existence of good subspace embedding

JL-Lemma [Johnson-Lindenstrauss 1984]
Given $\varepsilon \in (0,1)$, let m and d be positive integers such that $d \geq 4(\varepsilon^2/2 - \varepsilon^3/3)^{-1} \log m$. For any set P of m points in $\mathbb{R}^n$ there exists $f : \mathbb{R}^n \to \mathbb{R}^d$ such that for all $u, v \in P$

$$(1-\varepsilon)\|u-v\|^2 \leq \|f(u)-f(v)\|^2 \leq (1+\varepsilon)\|u-v\|^2.$$

JL sketching operator: length preservation of a single vector

Suppose $\mathcal{D}$ is a distribution over matrices of size $d \times n$. We say that a matrix $R \sim \mathcal{D}$ is a $(n, d, \delta, \varepsilon)$-JL sketching operator if for any vector $x \in \mathbb{R}^n$ it satisfies

$$\Pr_{R \sim \mathcal{D}} \left[\frac{\left| \|Rx\|^2 - \|x\|^2 \right|}{\|x\|^2} > \varepsilon \right] < \delta.$$

- JL implies subspace embedding [Woodruff 2014]

Distributional JL family: drawn from certain distribution

Provided d sufficiently large, the following all satisfy JL sketching operator requirement:

- $R \sim Gaussian(n, d)$, i.i.d. normal distribution with mean 0, variance $1/d$ [Dasgupta/Gupta 2003]
- $R \sim SRHT(n, d), R = PHD$ [Halko/Martinsson/Tropp 2011]
  - P: sample d coordinates from n uniformly at random
  - H: Hadamard matrix
  - D: diagonal matrix, entries drawn from $\{+1, -1\}$ uniformly at random
- $R \sim SJLT(n, d, \alpha)$, Sparse JL Transform [Cohen/Jayrram/Nelson 2018]
  - α nonzero entries per row

Theory: Range-finder bound for general JL sketching operator

[Y. Yaniv, O.A. Malik, P. Ghysels, X.L.; CAMCoS 2025]

Theorem (Distributional JL implies Range-finder Bound)

Suppose $A \in \mathbb{C}^{m\times n}$ *is a matrix and let* $0 < r < \min(m, n)$ *be the target rank. If* R *is a* $(n, d, \frac{\delta}{2\max(5^{2r},n)}, \frac{\varepsilon}{12})$*-JL sketching operator with* $\varepsilon/12, \delta \in (0, 1)$ *and* $d = r + p$ *with* $p \geq 0$*, then the following holds with probability at least* $1 - \delta$*:*

$$||(I - P_Y)A|| \leq \left(\sqrt{1 + \frac{n(1+\varepsilon)}{(1-\varepsilon)}}\right)\sigma_{r+1}(A), \qquad (1)$$

where $Y = AR = Q\Omega$ *with* $P_Y = QQ^{\dagger}$*.*

Theory: Range-finder bound for special JL sketching operator: $R \sim Gaussian(n, d)$

Theorem ([Halko/Martinsson/Tropp 2011])

Choose oversampling parameter $p \geq 4$ *and target rank* $r \geq 2$, *where* $r + p \leq \min(m, n)$. *Draw* $R \in \mathbb{R}^{n\times(r+p)}$, $Y = AR = Q\Omega$ *and* $P_Y = QQ^*$, *t then the norm squared approximation error is*

$$||(I - P_Y)A|| \leq \left(1+16\sqrt{1 + \frac{r}{p+1}}\right)\sigma_{r+1}(A)+\frac{8\sqrt{r+p}}{p+1}\left(\sum_{j>r}\sigma_j^2(A)\right)^{1/2},$$

with probability at least $1 - 3e^{-p}$.

Theory: Range-finder bound for special JL sketching operator: $R \sim SJLT(n, d, \alpha)$

Theorem ([Yaniv/Malik/Ghysele/L. 2025])

A target rank $r < \min(m, n)$. Fix $\varepsilon, \delta \in (0, 1)$. If $\alpha = \Theta(\log^3(r/\delta)/\varepsilon)$, $d = \Omega(r \log^6(r/\delta)/\varepsilon^2)$, $Y = AR = Q\Omega$ and $P_Y = QQ^*$ then

$$||(I - P_Y)A|| \le \sigma_{r+1}(A)\sqrt{1 + \frac{1}{(1-\varepsilon)} \max\left(\frac{e^2 n\alpha}{d}, \log\left(\frac{2d}{\delta}\right) - \frac{n\alpha}{d}\right)}. \tag{2}$$

with probability $1 - \delta$.

Frobenius norm concentration bound for any JL sketching operator

- **Theorem** [Yaniv/Malik/Ghysele/L. 2025]
  Let $A \in \mathbb{R}^{m \times n}$ and $\varepsilon, \delta \in (0,1)$. If $R \in \mathbb{R}^{n \times d}$ is a $(n, d, \delta', \varepsilon)$-JL matrix where $\delta' = \delta/m$, then the following holds with probability at least $1 - \delta$:

$$(1-\varepsilon)\|A\|_F^2 \leq \|AR\|_F^2 \leq (1+\varepsilon)\|A\|_F^2.$$

- Furthermore, we established the following stochastic relationship between $||A||_F$ and $||S = AR||_F$: $\mathbb{E}\left[\frac{1}{\sqrt{d}}||S||_F^2\right] = ||A||_F^2$

- In practice, leads to robust stopping criteria in adaptive sketching
  Absolute: $||(I - QQ^*)A||_F \approx ||(I - QQ^*)S||_F \leq \varepsilon_a$
  Relative: $\frac{||((I-QQ^*)A||_F}{||A||_F} \approx \frac{||(I-QQ^*)S||_F}{||S||_F} \leq \varepsilon_r$

Sparse JLT is a highly structured random sparse matrix

Mitigate dense sampling cost

- SJLT [Kane/Nelson 2014; Cohen/Jayram/Nelson 2018]
  An SJLT matrix R of size $n \times d$ has a fixed number $\alpha \in [d]$ nonzero entries per row. The nonzero entries are drawn independently from two values $\{1/\sqrt{\alpha}, -1/\sqrt{\alpha}\}$ with equal probability. Example:

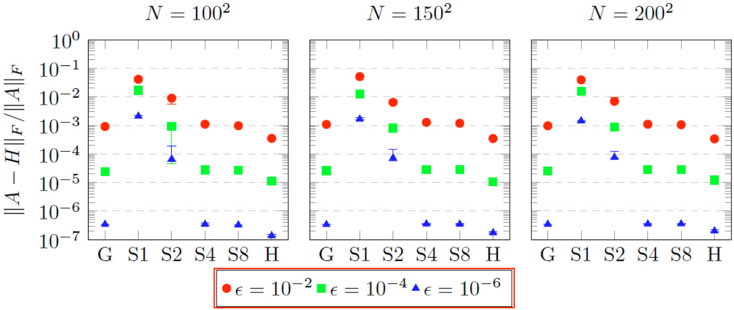
  $R \sim SJLT(4, 3, 2)$

$$R = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & -1 \\ 0 & -1 & -1 \\ 1 & -1 & 0 \\ 1 & 0 & 1 \end{bmatrix} = \frac{1}{\sqrt{2}} \left(\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 1 \end{bmatrix} - \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \right)$$

- Sketching AR only involves add/subtract; no multiplication
- Implementation is no harder than sparse matrix-vector multiplication

SJLT-sketching in HSS construction: accuracy & runtime

- Compared to Gaussian sketching; with varying sparsity level, varying compression tolerance
  Example: the top frontal matrix of 3D Poisson



$\alpha = 4$ **is sufficient!**

- Seral runtime up to 2.5X faster
- Parallel runtime with 32 MPI prrocesses:

  Sketching time up to 17X faster

  Total time up to 14X faster

Applications

- Iterative linear solvers:
  Hierarchical matrix-vector multiplication

- Direct linear solvers:
  Factoization/inversion: ULV, $\mathcal{H}$-LU, $\mathcal{H}^2$-LU [2], ...

[2] on GPU: [Boukaram/Keyes/L./Liu/Turkiyyah 2026]

STRUMPACK – STRUctured Matrices PACKage
http://portal.nersc.gov/project/sparse/strumpack/

- Fully algebraic solvers/preconditioners
- Dense: Can take user input of cluster tree & block partitioning
  - HSS, BLR, $\mathcal{H}^2$ (soon)
  - ButterflyPACK integration/interface: Butterfly, HODLR, HODBF
- Sparse multifrontal direct solver
- Approximate sparse factorization preconditioner
- C++, MPI + OpenMP + CUDA, real & complex, 32/64 bit integers
- BLAS, LAPACK, Metis
- Optional: MPI, ScaLAPACK, ParMETIS, (PT-)Scotch, cuBLAS/cuSOLVER, SLATE, ZFP

Kernel Ridge Regression: Ridge Regression + Kernel Trick

1. Training stage to compute model parameters:
Need to minimize the cost function:

$$argmin_w \, C(\mathbf{w}) = \sum_i (y_i - \mathbf{w}^T \mathbf{x}_i)^2 + \lambda \|\mathbf{w}\|^2$$

- x_i's are data points (rows of the data matrix $X^{n \times d}$)
- y_i's are their labels
- **w** is the normal vector to the target hyperplane

Can derive the optimal weights for the prediction model:

$$\mathbf{w} = X^T (\lambda I + X X^T)^{-1} \mathbf{y}$$

2. Prediction stage: given a new vector $\mathbf{x}_1$ from the test set, compute:

$$\begin{aligned} y_1 := \mathbf{w}^T \mathbf{x}_1 &= [(\lambda I + X X^T)^{-1} \mathbf{y}]^T X \mathbf{x}_1 \\ &\approx [(\lambda I + \mathcal{K}(X, X))^{-1} \mathbf{y}]^T \cdot \mathcal{K}(X, \mathbf{x}_1) \leftarrow \text{kernel trick} \end{aligned}$$

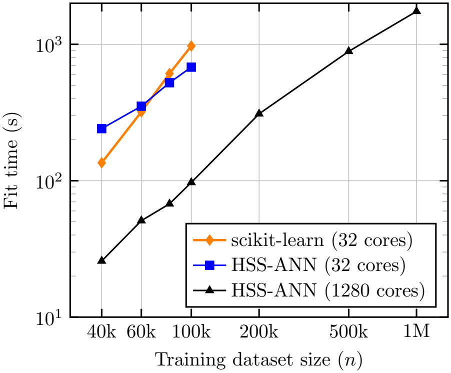
$\Longrightarrow$ Binary classification: class label predicted by the sign of y_1

STRUMPACK Python interface to Scikit-learn

- Scikit-learn: machine Learning in Python, http://scikit-learn.org/stable/
  - contains classifiers and regressors
  - but only provides shared-memory parallelism
- STRUMPACKKernel Python class:
  - derived from scikit-learn base classes BaseEstimator and ClassifierMixin
  - implements member functions: fit, predict and decision_function
  - can leverege all the other functions in scikit-learn

Time comparison between scikit-learn and HSS

Use Gaussian kernel $K(i,j) = \exp\left(-\frac{\|x_i - x_j\|_2^2}{2h^2}\right)$

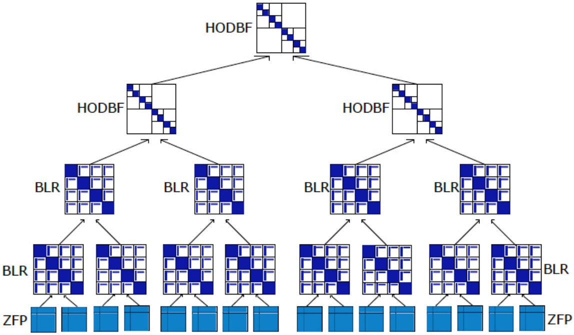


SUSY dataset (particle physics): classification to distinguish between a signal process which produces supersymmetric particles and a background process which does not

Rank structured multifrontal sparse factorization

Compressing large dense blocks in the multifrontal tree
Combining Hierarchically Off-Diagonal Butterfly (HODBF) and Block Low Rank (BLR)

- Largest: HODBF
- Medium: BLR
- Smaller: dense or lossy compression (ZFP)

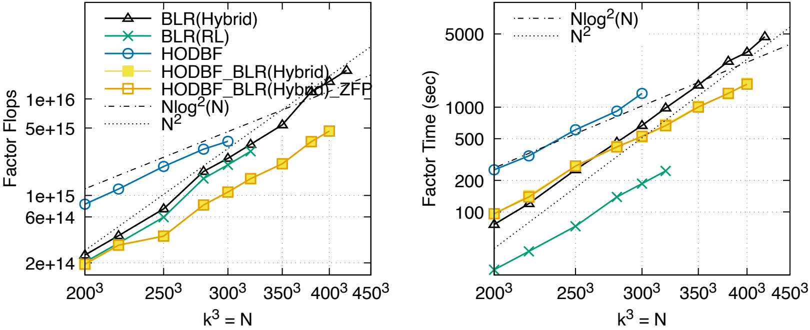


3D visco-acoustic wave propagation

Governed by the Helmholtz equation: $\mathbf{x} = (x_1, x_2, x_3)$

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

- Solution method: FD on staggered grids using a 27-point stencil, 8 PML absorbing boundary layers



Summary: Stages of operation

- Data clustering, matrix reordering
- Compression – usually dominating cost
  - Complexity depends on: black-box Av and $A^T v$, black-box entry evaluation $A(i,j)$
  - Goal: $O(N \, log^{\alpha} N)$
- Building solvers
  - Iterative solver: matrix-vector multiplication
  - Direct solvers: factorization (e.g., ULV, H-LU), solve, inversion
- Principal tool for efficient implementation and parallelization
  Sweeping through "trees" upward / downward: cluster tree, separator tree, ...

Open Problems

- How to choose α in $SJLT(n, d, \alpha)$?
- Subsampled randomized trig transform (SRTT), or Fourier transform (SRFT)
- Does it make sense to do $\mathcal{H}$, $\mathcal{H}^2$-QR? How?
- Spectral analysis for matrices preconditioned by low-rank factorization
- Data-sparse rank analysis for matrix inverse
- Data-sparse for tensor computations