A fast direct solver for non-oscillatory integral equations

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Model problem

- Laplace's equation with Dirichlet boundary conditions:

$$\Delta u = 0 \quad \text{in } \Omega \quad , \quad u = f \quad \text{on } \partial\Omega$$

- Fundamental to many areas of mathematical physics
- Solve using a Green's function representation (double-layer potential):

$$u(\mathbf{r}) = \int_{\partial\Omega} \frac{\partial G}{\partial \nu_{\mathbf{s}}}(\mathbf{r}, \mathbf{s})\, \sigma(\mathbf{s})\, dA_{\mathbf{s}} \quad \text{in } \Omega$$

- Integral equation for unknown surface density σ:

$$-\frac{1}{2}\sigma(\mathbf{r}) + \int_{\partial\Omega} \frac{\partial G}{\partial \nu_{\mathbf{s}}}(\mathbf{r}, \mathbf{s})\, \sigma(\mathbf{s})\, dA_{\mathbf{s}} = f(\mathbf{r}) \quad \text{on } \partial\Omega$$

- Discretize: $Ax = b$
- Good: well-conditioned, high-order, dimensional reduction
- Bad: dense matrices, computational cost

Let $A \in \mathbb{C}^{N \times N}$ discretize a non-oscillatory Green's function integral operator.

- Cost of applying A: $\mathcal{O}(N^2)$
- Cost of inverting A: $\mathcal{O}(N^3)$

Fast algorithms are required!

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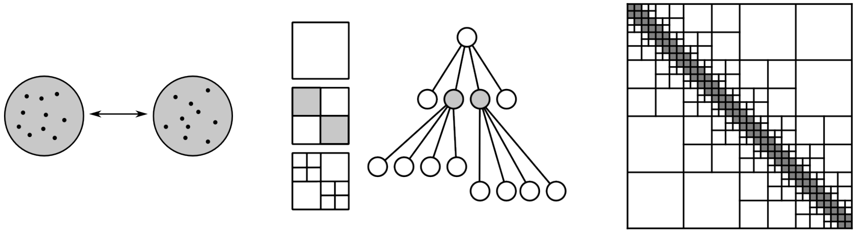
Fortunately, such matrices are structured.

- Analysis: non-oscillatory Green's functions have smooth far fields
- Algebra: separated off-diagonal matrix blocks are numerically low-rank



- Exploit smoothness with a hierarchical decomposition of space
- $\mathcal{O}(N \log N)$ matrix-vector multiplication (treecode, FMM, panel clustering)
- Combine with GMRES, BiCG, CGR, etc. for fast iterative solvers

Fast iterative solvers have been very successful, but they can still be inefficient:

- When A is ill-conditioned (multiphysics, singular geometries)
- When $Ax = b$ must be solved with many right-hand sides b or many perturbations of a base matrix A (optimization, design, time marching)

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One solution: fast direct solvers (construct A^{-1}).

- Robust: insensitive to conditioning, always works
- Fast solves and inverse updates following initial factorization

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Various approaches in recent years:

- $\mathscr{H}$- and $\mathscr{H}^2$-matrices (Hackbusch, Börm, Grasedyck, Bebendorf et al.)
- HSS matrices (Chandrasekaran, Gu, Xia, Li et al.)
- Skeletonization (Martinsson, Rokhlin, Gillman, Greengard, Bremer et al.)
  - BIEs in 2D
  - One-level BIEs in 3D

Here, we present a multilevel skeletonization-based fast direct solver in general dimension. For BIEs:

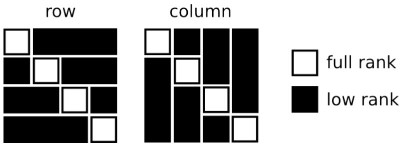
	2D	3D
precomp	$\mathcal{O}(N)$	$\mathcal{O}(N^{3/2})$
solve	$\mathcal{O}(N)$	$\mathcal{O}(N \log N)$

Main ideas/take-home messages :

- Kernel-independent: Laplace, Stokes, Yukawa, low-frequency Helmholtz
- Robust to geometry (e.g., boundary vs. volume, dimensionality)
- User-specified precision: trade accuracy for speed
- Naturally exposes the underlying sparsity of integral equation matrices
- Transparently takes advantage of sparse direct solver development
- Very fast solve times, beating the FMM by factors of 100–1000
- Simple framework: easy to analyze, implement, and optimize
- Somewhat similar in flavor to nested dissection

A block matrix A is block separable if

$$\underbrace{\begin{bmatrix} \times & \times \\ \times & \times \end{bmatrix}}_{A_{ij}} = \underbrace{\begin{bmatrix} \times \\ \times \end{bmatrix}}_{L_i} \underbrace{\begin{bmatrix} \times \end{bmatrix}}_{S_{ij}} \underbrace{\begin{bmatrix} \times & \times \end{bmatrix}}_{R_j} \quad , \qquad i \neq j.$$



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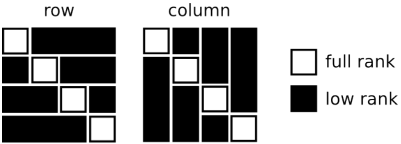
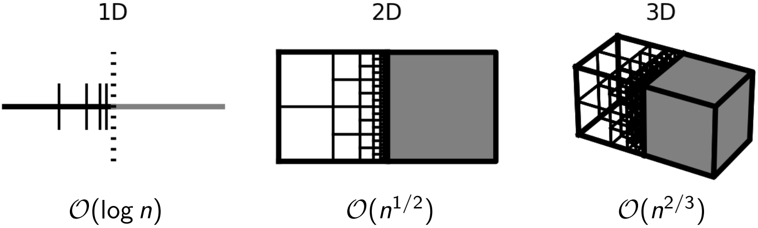


Integral equation matrices are block separable.



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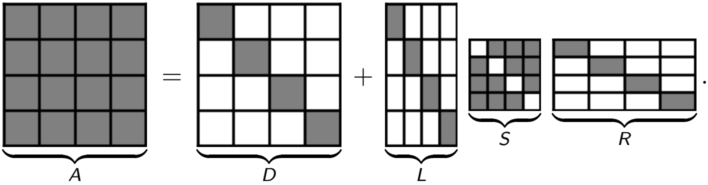

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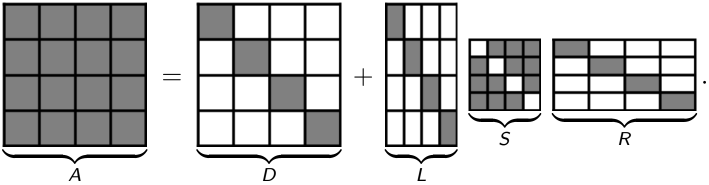


The inverse can be written in essentially the same form:

$$A^{-1} = \mathcal{D} + \mathcal{L}\mathcal{S}^{-1}\mathcal{R},$$

where

$$\mathcal{D} = D^{-1} - D^{-1}L\Lambda RD^{-1}, \quad \mathcal{L} = D^{-1}L\Lambda, \quad \mathcal{R} = \Lambda RD^{-1}, \quad \mathcal{S} = \Lambda + S,$$

with $\Lambda = \left(RD^{-1}L\right)^{-1}$.

- $\mathcal{D}$, $\mathcal{L}$, and $\mathcal{R}$ are block diagonal
- Reduces to inverting $\mathcal{S} \in \mathbb{C}^{K\times K}$, where typically $K \ll N$

We can also adopt a sparse matrix perspective. For

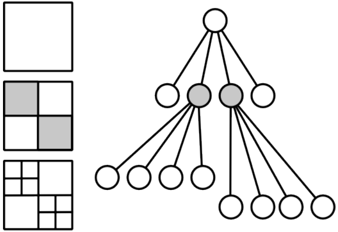
$$Ax = (D + LSR)\,x = b,$$

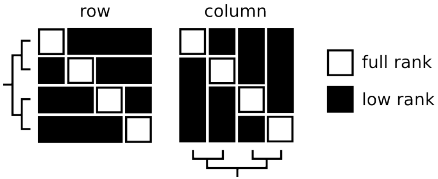
let $z \equiv Rx$ and $y \equiv Sz$. Then this is equivalent to the structured sparse system

$$\begin{bmatrix} D & L & \\ R & & -I \\ & -I & S \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} b \\ 0 \\ 0 \end{bmatrix}.$$

Factor using UMFPACK, SuperLU, MUMPS, Pardiso, etc.

Integral equation matrices are, in fact, hierarchically block separable, i.e., they are block separable at every level of an octree-type ordering.





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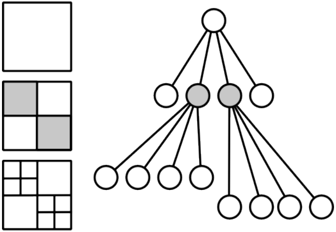

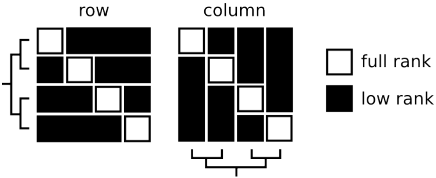

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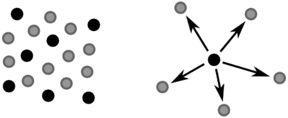
How to compress to block separable form?

An interpolative decomposition of a rank-k matrix is a representation

$$\underbrace{A}_{m\times n} = \underbrace{B}_{m\times k}\underbrace{P}_{k\times n},$$

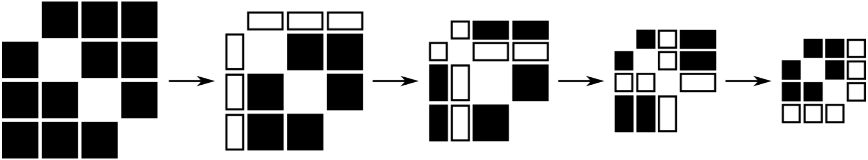
where B is a column-submatrix of A (with $\|P\|$ small).

- The ID compresses the column space; to compress the row space, apply the ID to A^{T}. We call the retained rows and columns skeletons.
- Adaptive algorithms can compute the ID to any specified precision $\epsilon > 0$.
- Related factorizations: RRQR, pseudoskeleton (CUR), ACA



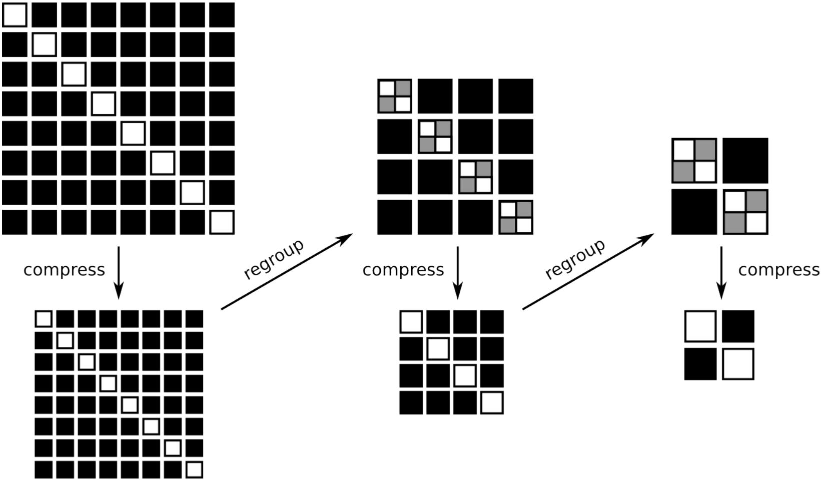
One-level matrix compression

- Compress the row space of each off-diagonal block row.
  Let the L_i be the corresponding row interpolation matrices.
- Compress the column space of each off-diagonal block column.
  Let the R_j be the corresponding column interpolation matrices.
- Approximate the off-diagonal blocks by $A_{ij} \approx L_i S_{ij} R_j$ for $i \neq j$.
- S is a skeleton submatrix of A

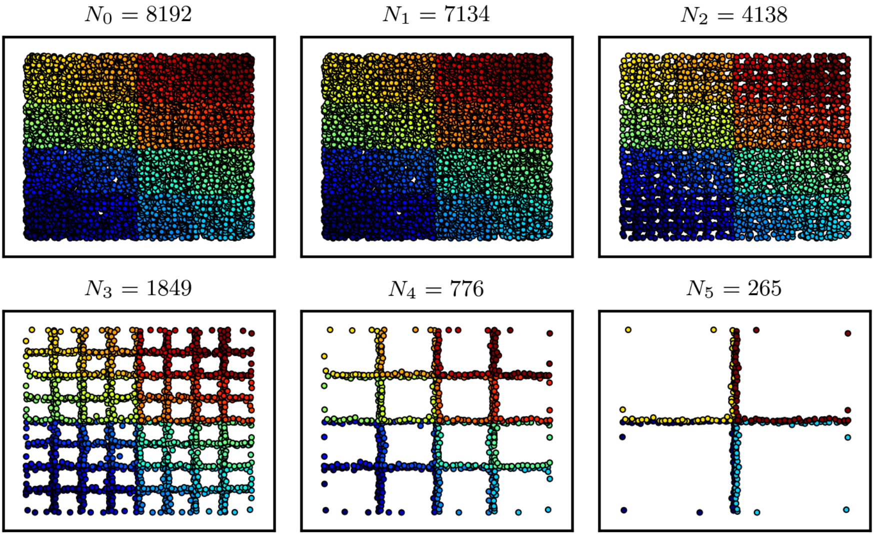


Skeletonization

Multilevel matrix compression



Recursive skeletonization



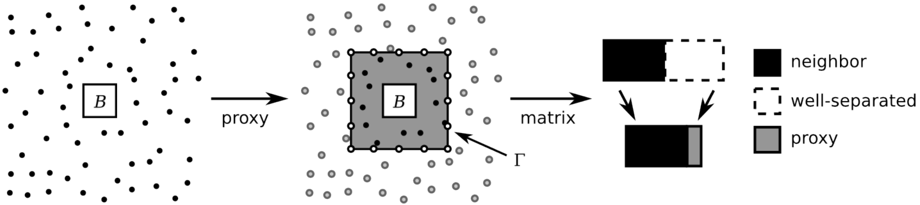
$$G(\mathbf{r}, \mathbf{s}) = -\frac{1}{2\pi} \log |\mathbf{r} - \mathbf{s}| \ , \quad \epsilon = 10^{-3}$$

Accelerated compression for PDEs

- General compression algorithm is global and so at least $\mathcal{O}(N^2)$
- For potential fields, use Green's theorem to accelerate:

$$u(\mathbf{r}) = \int_{\Gamma} \left[u(\mathbf{s}) \frac{\partial G}{\partial \nu_{\mathbf{s}}}(\mathbf{r}, \mathbf{s}) - G(\mathbf{r}, \mathbf{s}) \frac{\partial u}{\partial \nu}(\mathbf{s}) \right] dA_{\mathbf{s}}$$

- Represent well-separated points with a local proxy surface



Compressed matrix representation

Telescoping formula:

$$A \approx D^{(1)} + L^{(1)} \left[D^{(2)} + L^{(2)} \left(\cdots D^{(\lambda)} + L^{(\lambda)} S R^{(\lambda)} \cdots \right) R^{(2)} \right] R^{(1)}$$

- Efficient storage (data-sparse)

N	uncomp	comp
8192	537 MB	9.7 MB
131072	137 GB	184 MB

- Fast matrix-vector multiplication (generalized FMM)
- Fast matrix factorization and inverse application

Compressed matrix inversion

Recursively expand in sparse form:

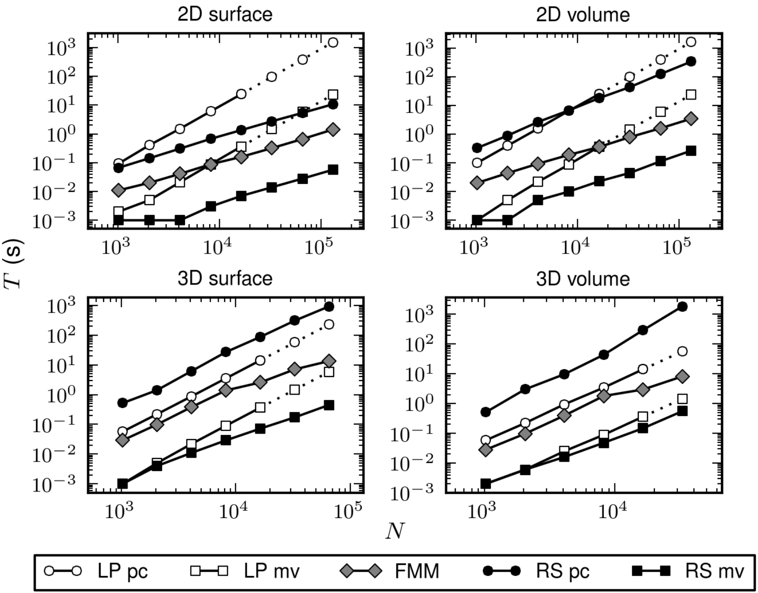
$$\begin{bmatrix} D^{(1)} & L^{(1)} & & & & & \\ R^{(1)} & & -I & & & & \\ & -I & D^{(2)} & L^{(2)} & & & \\ & & R^{(2)} & \ddots & \ddots & & \\ & & & \ddots & D^{(\lambda)} & L^{(\lambda)} & \\ & & & & R^{(\lambda)} & & -I \\ & & & & & -I & S \end{bmatrix} \begin{bmatrix} x \\ y^{(1)} \\ z^{(1)} \\ \vdots \\ \vdots \\ y^{(\lambda)} \\ z^{(\lambda)} \end{bmatrix} = \begin{bmatrix} b \\ 0 \\ 0 \\ \vdots \\ \vdots \\ 0 \\ 0 \end{bmatrix}.$$

This can be treated efficiently using any standard sparse direct solver.

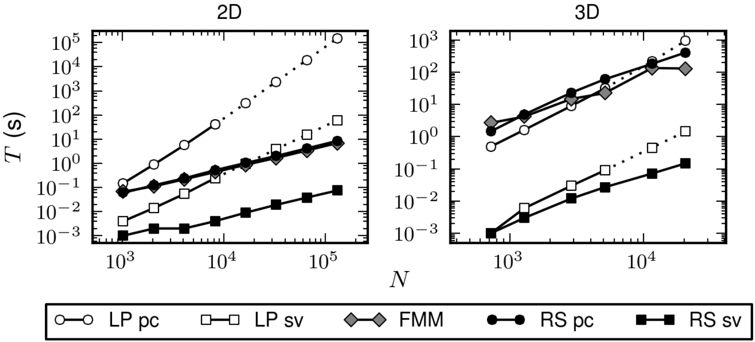
Multilevel inversion formula (for analysis):

$$A^{-1} \approx \mathcal{D}^{(1)} + \mathcal{L}^{(1)} \left[\mathcal{D}^{(2)} + \mathcal{L}^{(2)} \left(\cdots D^{(\lambda)} + \mathcal{L}^{(\lambda)} \mathcal{S}^{-1} \mathcal{R}^{(\lambda)} \cdots \right) \mathcal{R}^{(2)} \right] \mathcal{R}^{(1)}$$

Laplace FMM


2D surface
2D volume
3D surface
3D volume
T (s)
N
LP pc
LP mv
FMM
RS pc
RS mv

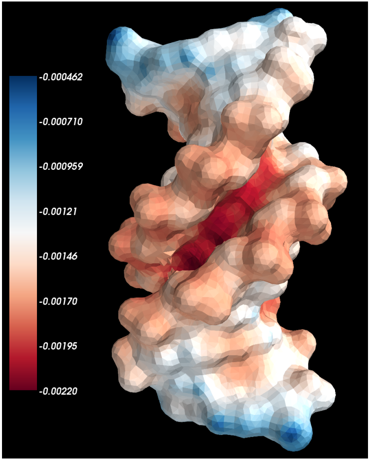
Laplace BIE solver



- Less memory-efficient than FMM/GMRES
- Each solve is extremely fast (in elements/sec)

ϵ	10^{-3}	10^{-6}	10^{-9}
2D	3.3×10^6	2.0×10^6	1.7×10^6
3D	6.0×10^5	1.4×10^5	6.2×10^4

Poisson electrostatics

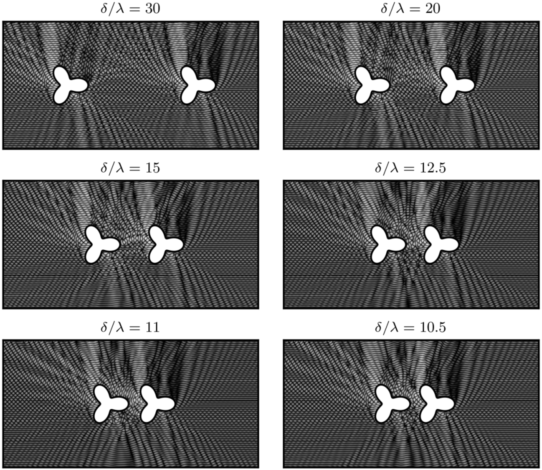


$$
\begin{aligned}
-\Delta\varphi &= 0 && \text{in } \Omega_0 \\
-\Delta\varphi &= \frac{1}{\varepsilon_1}\sum_i q_i \delta\left(\mathbf{r} - \mathbf{r}_i\right) && \text{in } \Omega_1 \\
[\varphi] = \left[\varepsilon \frac{\partial \varphi}{\partial \nu}\right] &= 0 && \text{on } \Sigma
\end{aligned}
$$

N	7612	19752
FMM/GMRES	12.6 s	26.9 s
RS precomp	151 s	592 s
RS solve	0.03 s	0.08 s

Break-even point: 10–25 solves

Multiple scattering



- Each object: 10λ

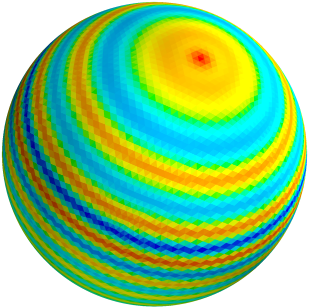
$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$$

- FMM/GMRES with block preconditioner via RS

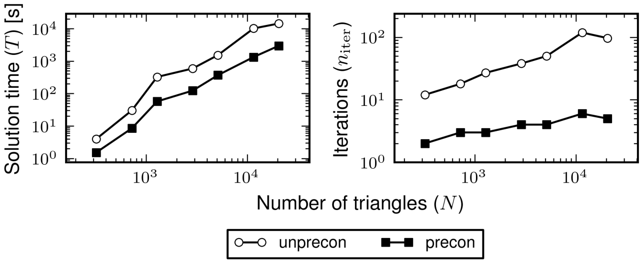
$$\begin{bmatrix} A_{11}^{-1} & \\ & A_{22}^{-1} \end{bmatrix}$$

- Unprecon: 700 iterations
- Precon: 10 iterations
- $50\times$ speedup

Helmholtz preconditioning



- $N = 20480$, 10λ
- Precondition with low-precision inverse ($\epsilon = 10^{-3}$)
- Iterate for full accuracy ($\epsilon = 10^{-12}$)
- Unprecon: 190 iterations
- Precon: 6 iterations
- $10\times$ speedup



Summary

Complexities in d dimensions (BIEs in $d+1$ dimensions):

$$\text{precomp} \sim \begin{cases} N & \text{if } d = 1, \\ N^{3(1-1/d)} & \text{if } d > 1, \end{cases} \qquad \text{solve} \sim \begin{cases} N & \text{if } d = 1, \\ N \log N & \text{if } d = 2, \\ N^{2(1-1/d)} & \text{if } d > 2 \end{cases}$$

- Mild assumptions: low-rank off-diagonal blocks, Green's theorem
- Based only on numerical linear algebra
- Kernel-independent: Laplace, Stokes, Yukawa, low-frequency Helmholtz
- Very fast solves following precomputation (~ 0.1 s)
- Highly effective for preconditioning
- Reveals connection with sparse matrices (Chandrasekaran, Gu et al.)
- Naturally parallelizable via block-sweep structure
- Extensions: low-rank updates, least squares, other matrix decompositions
- Similar ideas also apply for PDE formulations (Xia, Gillman et al.)