Hierarchical Algorithms for Computational Linear Algebra

Yuval Harness - INRIA Team HiePACS

INVENTORS FOR THE DIGITAL WORLD

Joint work of the FastLA Associate Team members

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The FastLA Associate Team

Fast and Scalable Hierarchical Algorithms for Computational Linear Algebra

Collaboration

- INRIA project-team HiePacs.
- Scientific Computing Group, LBNL.
- Mechanics and Computation Group, Stanford.

Theme

- Study & design hierarchical parallel & scalable numerical techniques.
- Applications: N-body interaction calculations and the solution of large sparse linear systems.
- Implementation: heterogeneous manycore platforms by using task based runtime systems.

Outline

Hierarchical Numerical Techniques

The Basics

Introduction

Motivation

- Problem: solution/factorization of extremeley large dense linear systems:

$$Ax = b$$

- Consider a matrix of dimesnion $n \times n$:

$$\begin{array}{lcl} \text{Sparse} & \Rightarrow & \mathcal{O}(n) \text{ storage units} \\ \text{Dense} & \Rightarrow & \mathcal{O}(n^2) \text{ storage units} \end{array}$$

- Memory consumption in the dense case is a major bottleneck in extending our capability to handle larger and more challenging linear systems.

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- Memory consumption in the dense case is a major bottleneck in extending our capability to handle larger and more challenging linear systems.

Remarks

- In typical applications, forming A explicitly is prohibitive.
- Such matrices also emerege while solving large sparse systems.

Hierarchical Matrices

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- **Hierarchical matrix (H-matrix)** is a data sparse approximation of a non-sparse matrix.

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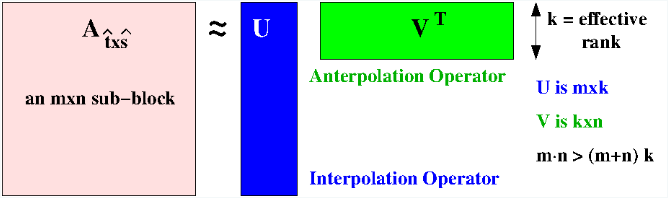
- **Basic principles**
  1. perform rows and columns permutations
  2. replace sub-blocks by low-rank factorizations.

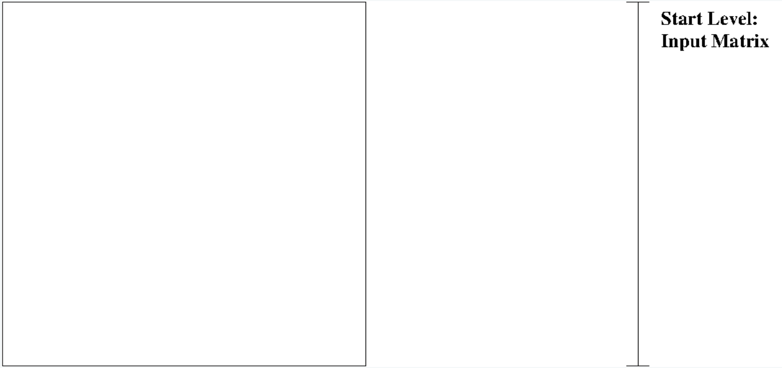


  $A_{\hat{t}\times\hat{s}}$ is a sub-block of $A \in \mathbb{F}^{N\times N}$, $\hat{s}, \hat{t} \subset \mathcal{I} = \{1, 2, ..., N\}$.

  3. **Hierarchical partitioning** $\Rightarrow$ almost linear complexity.

Hierarchical Partitioning

Strong Hierarchical Partitioning



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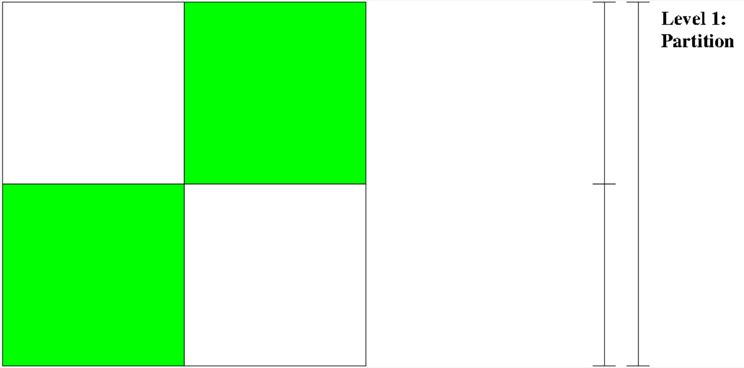

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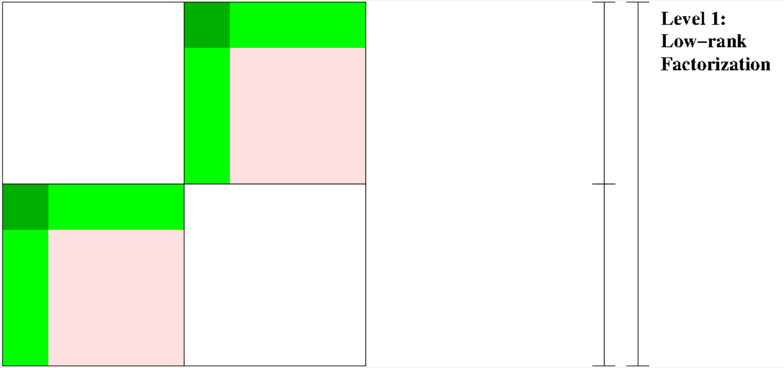

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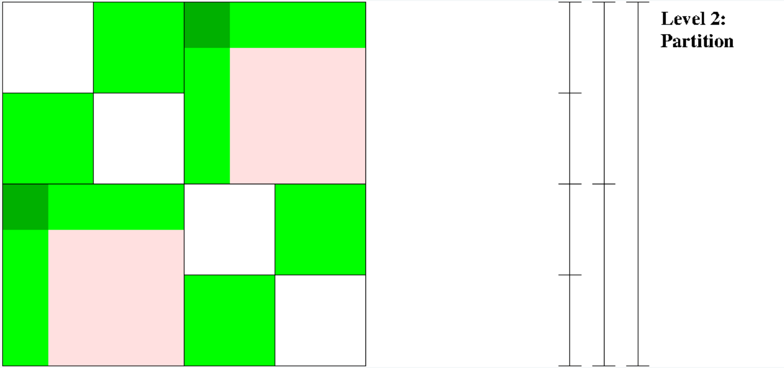

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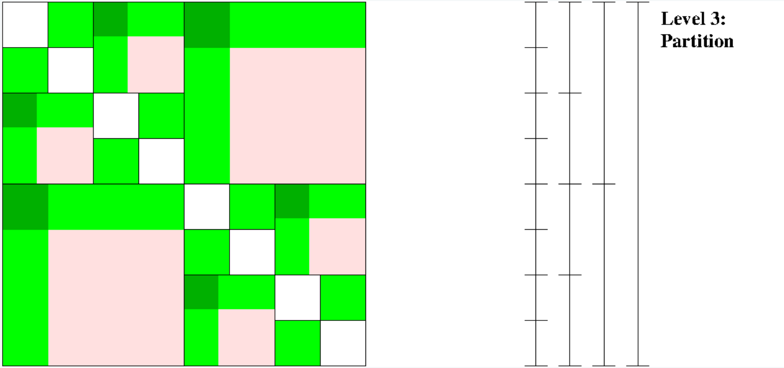

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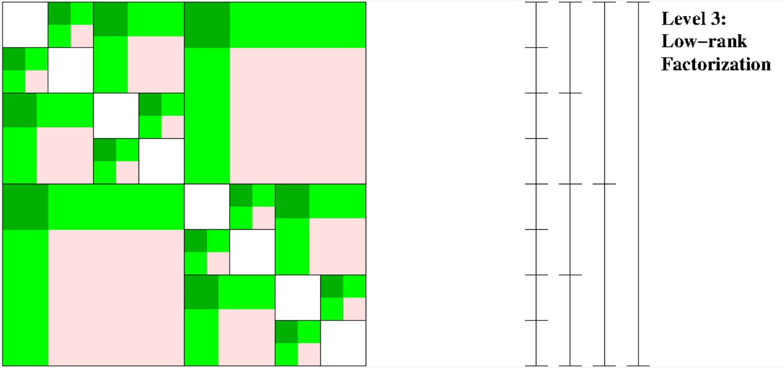

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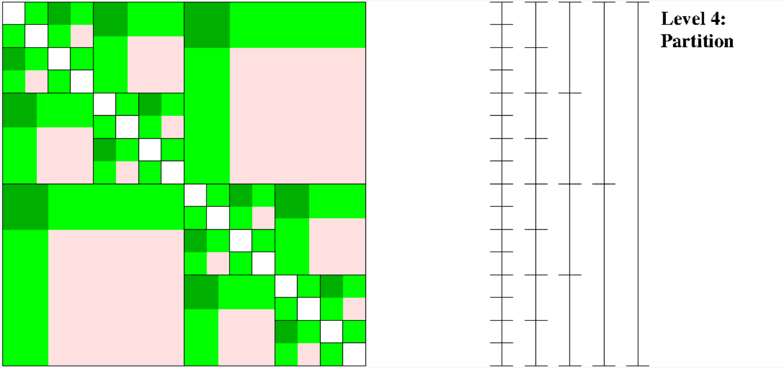

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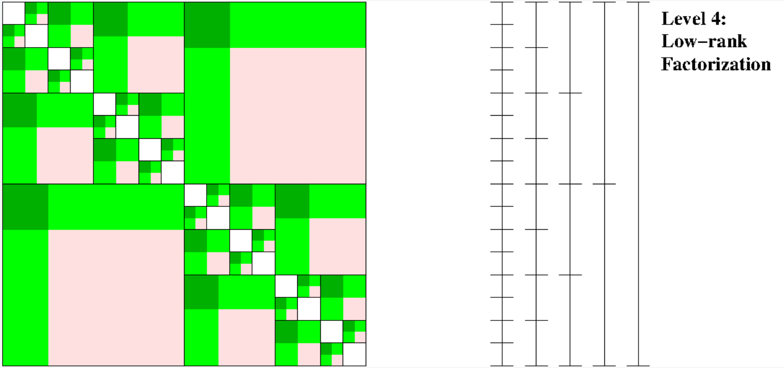

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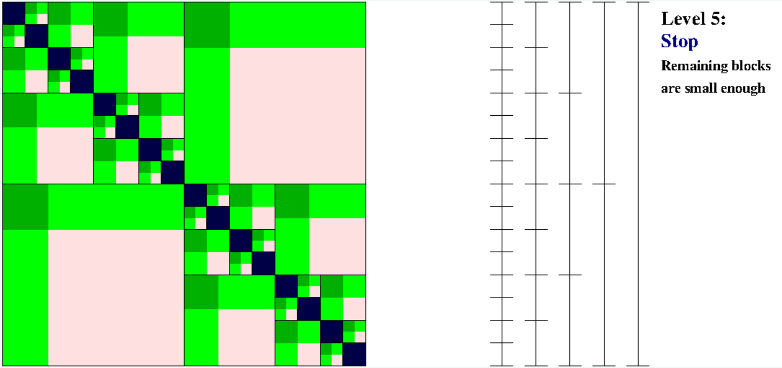

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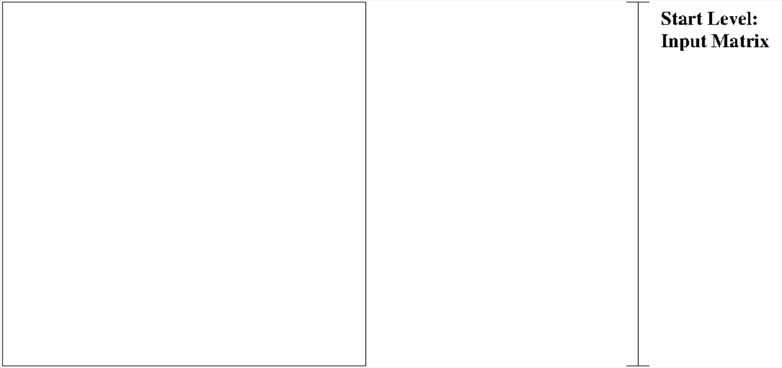

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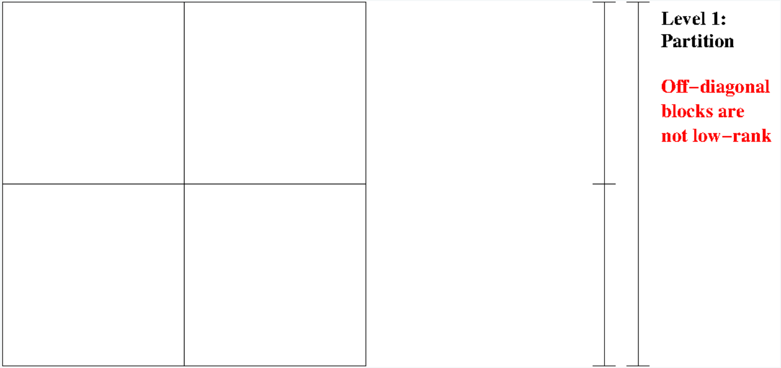

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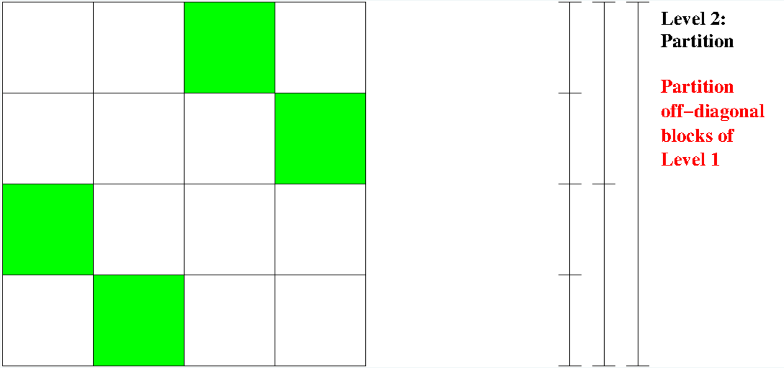

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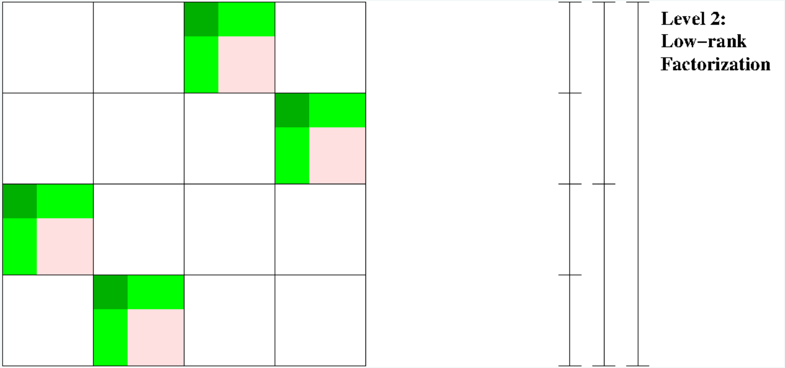

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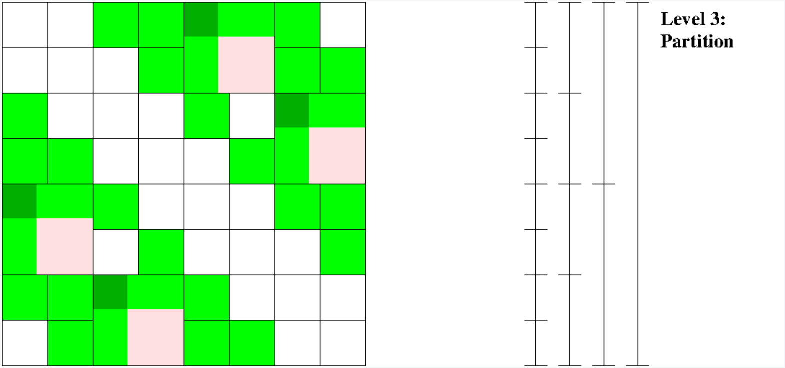

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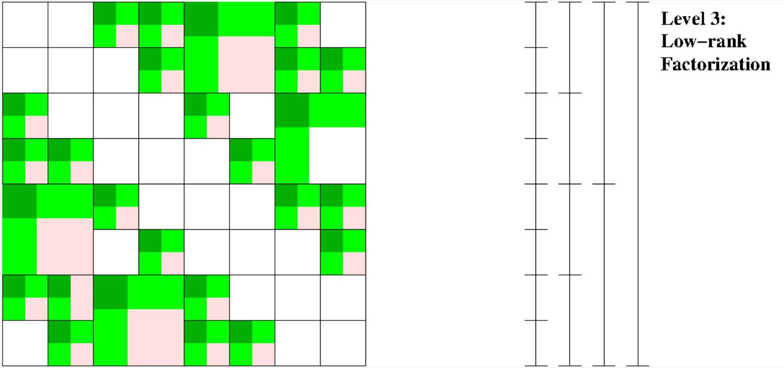

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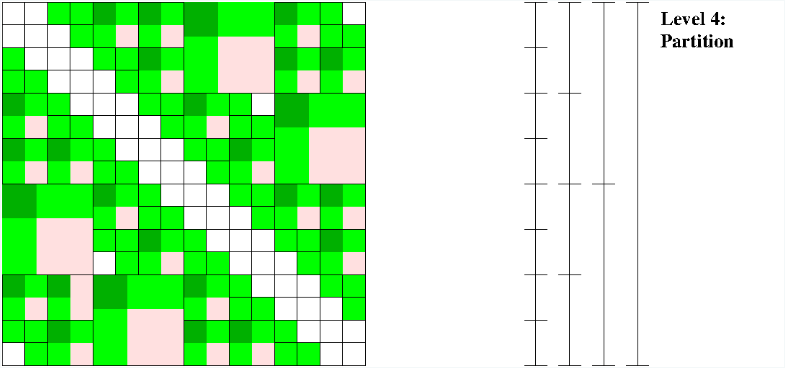

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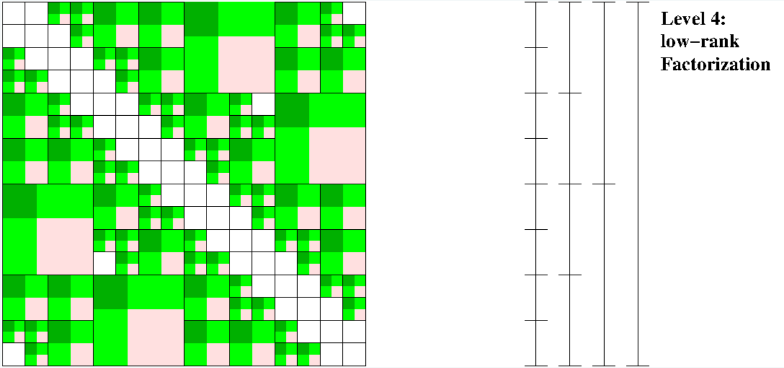

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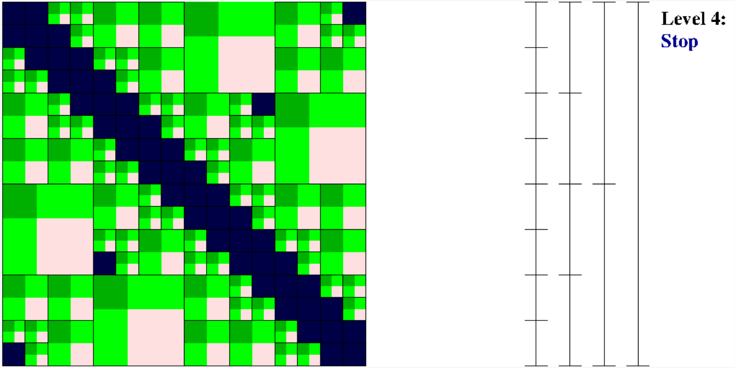

Compression, Complexity and Challenges

Matrix Compression

- Essentially H-matrix approximation is a matrix compression method.
- Works well for discretizations of Integral equations and elliptic PDEs.

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Complexity of operations

- Complexity of obtaining the hierarchical matrix should be almost linear:

$$\mathcal{O}\left(N \log^{\alpha} N\right), \quad \alpha \text{ is 'small'}$$

- Arithmetics $(+, -, \cdot, \mathrm{inv})$ should be possible in almost linear complexity.
- Hierarchical techniques a.k.a. Fast hierarchical methods.

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Challenges

- Fast identification & factorization of low-rank structures.
- Prohibitively expensive to form the large dense blocks.

Fast Methods for Geostatistics

H-matrix accelerated Randomized SVD

Introduction

Collaborators

Pierre Blanchard, Olivier Coulaud (INRIA) & Eric Darve (Stanford)

Problem: Generation of Gaussian Random Fields

- $\mathbf{Y} \sim \mu(\mathbf{0}, \mathbf{C})$ is a multivariate Gaussian random field (GRF).
- The covariance $\mathbf{C} \in \mathbb{R}^{N \times N}$ can be prescribed as a kernel matrix

$$\mathbf{C} = \{k(\|\mathbf{x}_i - \mathbf{x}_j\|_2)\}_{i,j=1\dots N}$$

  - $\mathbf{x}$: large and highly heterogenous 3D grid
  - k: correlation kernel such as

$$k_{1/2}(r) = e^{-r/\ell} \quad \text{or} \quad k_{\infty}(r) = e^{-r^2/(2\ell^2)}$$

- Generating $\mathbf{Y}$ requires computing a square root $\mathbf{A}$

$$\mathbf{C} = \mathbf{A}\mathbf{A}^{\mathsf{T}} \quad \rightarrow \quad \mathbf{Y} = \mathbf{A} \cdot \mathbf{X} \quad : \quad \mathbf{X} \sim \mu(\mathbf{0}, \mathbf{I}_N)$$

H-matrix accelerated Randomized SVD

Standard Methods: (Often become computationally prohibitive for large N)

- Cholesky ($\mathcal{O}(N^3)$).
- circulant embedding ($\mathcal{O}(N \log N)$ for equispaced grids)
- turning bands method (approximate).

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Solution: H-matrix accelerated Randomized SVD

- Randomized range evaluation:

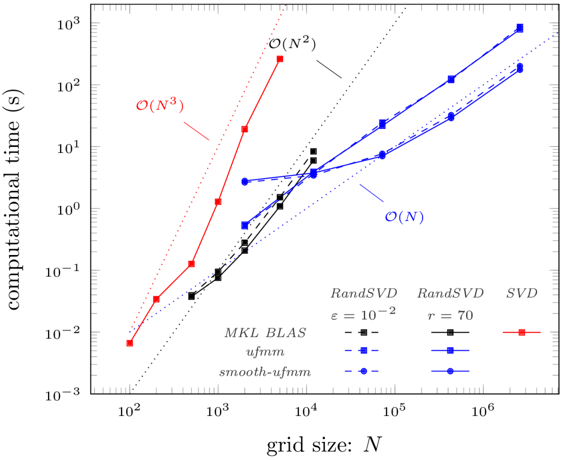
$$\mathbf{Z} = \mathbf{C} \cdot \mathbf{\Omega} \quad : \quad \mathbf{\Omega} \in \mathbb{R}^{N \times r} \text{ is a random Gaussian matrix}.$$

- Approximate Square root:

$$\mathbf{Z} = \mathbf{QR} \quad \rightarrow \quad \mathbf{A} = \mathbf{QU\Sigma}^{1/2} \, : \, \mathbf{U\Sigma U}^T = \mathbf{Q}^T\mathbf{CQ} \in \mathbb{R}^{r \times r}.$$

- H-matrix matrix product acceleration: $\mathbf{C} \rightarrow \mathbf{C}^{\mathcal{H}}$
  - Approximating A in $\mathcal{O}(r^2 \times N)$ operations.
  - Matrix-free method with $\mathcal{O}(r \times N)$ memory footprint.
  - Handles highly heterogeneous grids more efficiently than standard methods.

H-matrix accelerated Randomized SVD: time=f(n)



H-Matrices in Sparse Direct Solvers

Low-rank Operations in a Supernodal Solver

Introduction

Collaborators

Gregoire Pichon, Mathieu Faverge, Pierre Ramet, Jean Roman (INRIA) & Eric Darve (Stanford)

Problem: Solve $Ax = b$ where $A = A^T$ is large and sparse

- Cholesky: factorize $A = LL^T$ (symmetric pattern for LU)
- Solve $Ly = b$
- Solve $L^T x = y$

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Solution: Direct Solver

- Expensive with respect to iterative solvers.
- More robust, and allow to tackle hard problems.
- "Fill-ins" $\Rightarrow$ dense blocks $\Rightarrow$ high memory consumption.

Reducing Fill-ins with Nested Dissection

Objective

- Reorder A to reduce Fill-ins.

Nested Dissection

- Associate A as a graph: $G = (V, E, \sigma_p)$

  V: vertices, E: edges, σ_p: unknowns permutation
- The Algorithm: (computing σ_p)
  1. Partition $V = A \cup B \cup C$
  2. Order C with larger numbers: $V_A < V_C$ and $V_B < V_C$
  3. Apply the process recursively on A and B

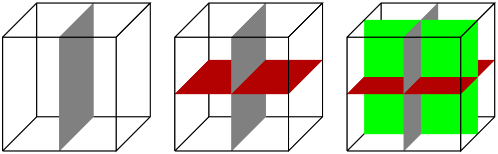
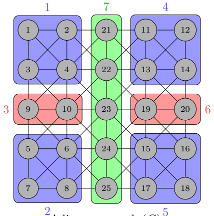


Figure : Three-levels of nested dissection on a regular cube

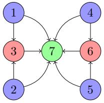
Reducing Fill-ins with Nested Dissection

Symbolic Factorization

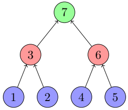
1. Build a partition with the nested dissection process.
2. Compute block elimination tree thanks to the block quotient graph.



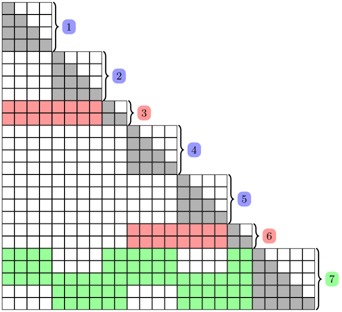
Adjacency graph (G).



Quotient graph $(G^*/P) = (G/P)^*$



Elimination tree (T).



Factorized matrix (L).

Block-Low-Rank Compression

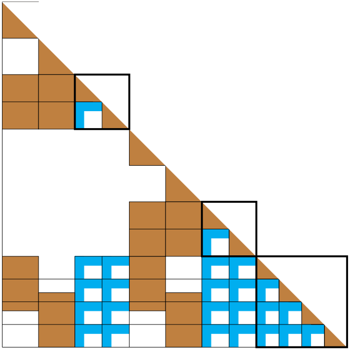
Definition

Block-Low-Rank (BLR) compression of a dense block:

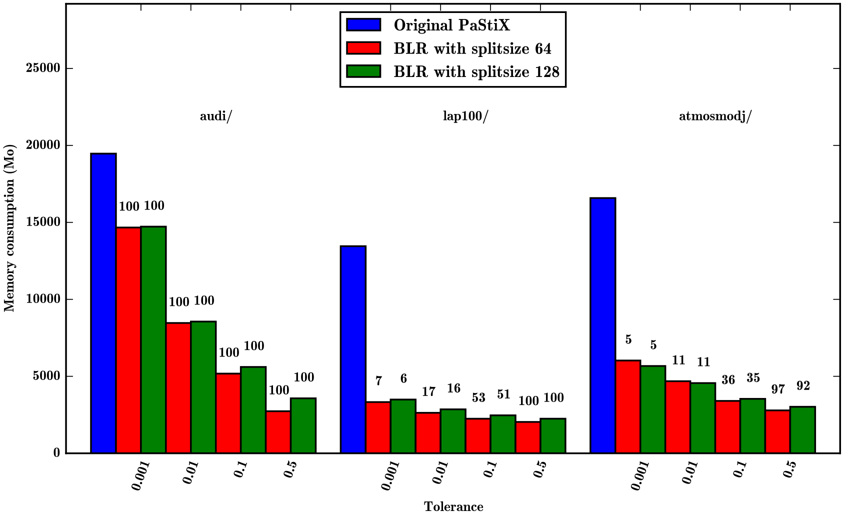
- dividing the block into equally sized sub-blocks.
- replacing each sub-block by a low-rank factorization.

Current Implementation

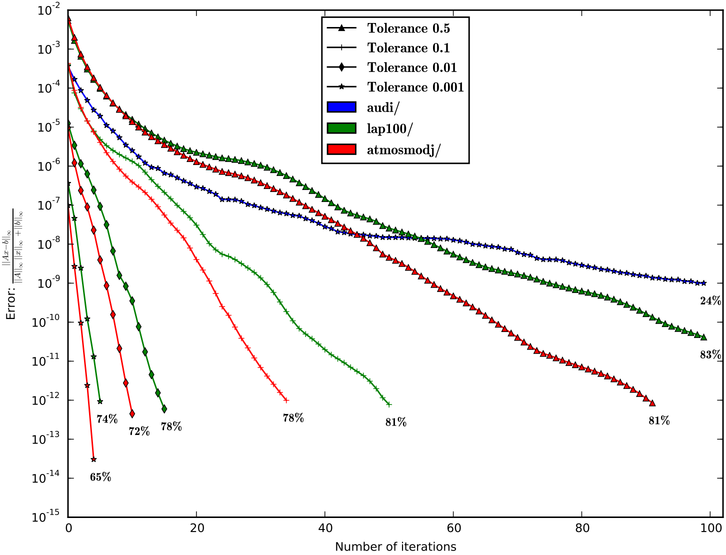
- Use BLR representation for large off-diagonal blocks
- Ordering strategy and kernels will form the foundation for future extensions.



Memory Consumption depending on Tolerance



Accuracy depending on Tolerance, Blocksize=128



Hierarchical Multilevel Preconditioning

Spectral Analysis

Introduction

Collaborators

Yuval Harness, Emanuel Agullo, Luc Giraud (INRIA) &
Eric Darve (Stanford)

Problem: Solve $Ax = b$ where $A = A^T > 0$ is **extremely** large and sparse

- The problem is too big for a direct solver.

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Solution: Algebraic Domain Decomposition

$$A = \left(\begin{array}{cccc|c} A_{I_1 I_1} & & & & A_{I_1 \Gamma} \\ & A_{I_2 I_2} & & & A_{I_2 \Gamma} \\ & & \ddots & & \vdots \\ & & & A_{I_p I_p} & A_{I_p \Gamma} \\ \hline A_{\Gamma I_1} & A_{\Gamma I_2} & \cdots & A_{\Gamma I_p} & A_{\Gamma \Gamma} \end{array}\right)$$

- Each $A_{I_j I_j}$ can be inverted in parallel by a direct solver.

The Schur System

The (Global) Schur System

$$Ax = \begin{pmatrix} A_{II} & A_{I\Gamma} \\ A_{\Gamma I} & A_{\Gamma\Gamma} \end{pmatrix} \begin{pmatrix} x_I \\ x_\Gamma \end{pmatrix} = \begin{pmatrix} b_I \\ b_\Gamma \end{pmatrix}$$

- $A_{II} \leftrightarrow$ interior subdomains, $A_{\Gamma\Gamma} \leftrightarrow$ separators.
- If x_Γ is known $\Rightarrow x_I = A_{II}^{-1}(b_I - A_{I\Gamma}x_\Gamma)$.
- The dense Schur system: $Sx_\Gamma = b_\Gamma$, $S = A_{\Gamma\Gamma} - A_{\Gamma I}A_{II}^{-1}A_{I\Gamma}$.

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Iterative Solution

- $Sx_\Gamma = b_\Gamma$ is solved iteratively.
- $\kappa(S) < \kappa(A)$.
- S is never formed, but assembled at each iteration:

$$Sx_\Gamma = \sum_{i=1}^{N} R_i^T S_i R_i x_\Gamma \quad : \quad R_i : \mathbb{R}^N \to \mathbb{R}^{n_i}$$

- All the local components, $\{S_i\}$, are computed in parallel.

Hierarchical Matrix Preconditioning

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- Further preconditioning for Krylov iterations.

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- Let $\widehat{S}$ be an H-matrix approximation of $S = S^T > 0$.
- The preconditioned system: $\widehat{S}^{-1/2} S \widehat{S}^{-1/2} y = \widehat{S}^{-1/2} b$.
- How do we guarantee $\widehat{S}$ is SPD as well?
- Can we estimate/control the condition number?

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Notes

- Consider S be close to singularity: $\|S\| < \epsilon$.
- If $\|S - \widehat{S}\| \geq \epsilon \Rightarrow \widehat{S}$ can be arbitrarily close to singularity.
- We want $\widehat{S}$ to be inaccurate as possible.

Two-Level Analysis

Objective: estimation of spectral bounds

$$\alpha := \inf_{x \neq 0} \frac{x^T \widehat{S} x}{x^T S x}, \quad \beta := \sup_{x \neq 0} \frac{x^T \widehat{S} x}{x^T S x}.$$

- $\alpha > 0 \Leftrightarrow \widehat{S}$ is SPD.
- β / α is the spectral condition number, $\kappa(\widehat{S}^{-1/2} S \widehat{S}^{-1/2})$.

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The Two-Level Problem

$$S = \left(\begin{array}{c|c} S_1 & M \\ \hline M^T & S_2 \end{array}\right), \quad \widehat{A} = \left(\begin{array}{c|c} \widehat{S}_1 & \widehat{M} \\ \hline \widehat{M}^T & \widehat{S}_2 \end{array}\right),$$

- The matrices S, S_1 and S_2 are SPD.
- The matrices $\widehat{S}_1$ and $\widehat{S}_2$ are symmetric as well, and satisfy:

$$\forall x_i \;\; 0 < \alpha_i \leq \frac{x_i^T\widehat{S}_i x_i}{x_i^T S_i x_i} \leq \beta_i \quad \Leftrightarrow \quad \alpha_i S_i \leq \widehat{S}_i \leq \beta_i S_i .$$

Two-Level Analysis

Assumptions

Let $\widehat{M}$ be a GSVD truncation of M,

$$\widehat{M} = \widehat{S}_1^{1/2}\widehat{\mathcal{M}}\widehat{S}_2^{1/2} \quad : \quad \widehat{\mathcal{M}} = \mathcal{U}_p \Sigma_p \mathcal{V}_p^T \approx \mathcal{M} = \widehat{S}_1^{-1/2} M \widehat{S}_2^{-1/2},$$

and assume that $\underline{S} = \left(\begin{array}{c|c} \frac{1}{\beta_1}\widehat{S}_1 & M \\ \hline M^T & \frac{1}{\beta_2}\widehat{S}_2 \end{array}\right) > 0.$

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Main Result

$$\frac{x^T \widehat{S} x}{x^T S x} \leq \max\left\{ \frac{\beta_{\max} - \sqrt{\beta_1\beta_2}\sigma_1}{1 - \sqrt{\beta_1\beta_2}\sigma_1}, \frac{\beta_{\max}}{1 - \sqrt{\beta_1\beta_2}\sigma_{p+1}} \right\} \geq \beta_{\max},$$

$$\frac{x^T \widehat{S} x}{x^T S x} \geq \min\left\{ \frac{\alpha_{\min} - \sqrt{\alpha_1\alpha_2}\sigma_1}{1 - \sqrt{\alpha_1\alpha_2}\sigma_1}, \frac{\alpha_{\min}}{1 + \sqrt{\alpha_1\alpha_2}\sigma_{p+1}} \right\} \leq \alpha_{\min}.$$

The singular value of $\mathcal{M}$: $\sigma_1 \geq \sigma_2 \geq \ldots$.

Multi-Level Implementation

The Multi-Level case

$$\widehat{S} = \widehat{S}_1^{(0)}, \quad \widehat{S}_k^{(\ell)} = \left(\begin{array}{c|c} \widehat{S}_{2k-1}^{(\ell+1)} & \widehat{M}_k^{(\ell)} \\ \hline \widehat{M}_k^{(\ell)^T} & \widehat{S}_{2k}^{(\ell+1)} \end{array} \right) \in \mathbb{R}^{n_k^{(\ell)} \times n_k^{(\ell)}},$$

$$S = S_1^{(0)}, \quad S_k^{(\ell)} = \left(\begin{array}{c|c} S_{2k-1}^{(\ell+1)} & M_k^{(\ell)} \\ \hline M_k^{(\ell)^T} & S_{2k}^{(\ell+1)} \end{array} \right) \in \mathbb{R}^{n_k^{(\ell)} \times n_k^{(\ell)}},$$

Recursive Estimation

$$\alpha_k^{(\ell)} = \frac{1 - \sqrt{\frac{\alpha_{k,\max}^{(\ell)}}{\alpha_{k,\min}^{(\ell)}}} \sigma_{k,1}^{(\ell)}}{\frac{1}{\alpha_{k,\min}^{(\ell)}} - \sqrt{\frac{\alpha_{k,\max}^{(\ell)}}{\alpha_{k,\min}^{(\ell)}}} \sigma_{k,1}^{(\ell)}} \leq \frac{1 - \sqrt{\frac{\beta_{k,\min}^{(\ell)}}{\beta_{k,\max}^{(\ell)}}} \sigma_{k,1}^{(\ell)}}{\frac{1}{\beta_{k,\max}^{(\ell)}} - \sqrt{\frac{\beta_{k,\min}^{(\ell)}}{\beta_{k,\max}^{(\ell)}}} \sigma_{k,1}^{(\ell)}} = \beta_k^{(\ell)},$$

where $\alpha_{k,\min}^{(\ell)} = \min\left\{\alpha_{2k-1}^{(\ell+1)}, \alpha_{2k}^{(\ell+1)}\right\}$, $\beta_{k,\max}^{(\ell)} = \max\left\{\beta_{2k-1}^{(\ell+1)}, \beta_{2k}^{(\ell+1)}\right\}$.

Concluding Remarks

Summary, Conclusions and Future Study

Concluding Remarks

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- Hierarchical Matrices.
- Applications & Challenges in Computational Linear Algebra.

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- Direct Solvers: move from BLR to better compression schemes.
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- Main difficulty is to do it in a 'reasonable' complexity.

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Thank You