Rank-structured preconditioners for two- and three-dimensional integral and differential equations

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Overview

1. $\mathcal{H}^2$-matrices
2. $\mathcal{H}^2$-matrix arithmetic operations
3. Summary

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Model problem

Goal: Given an asymptotically smooth kernel function, solve

$$\int_\Omega g(x,y)u(y)\,dy = f(x) \qquad \text{for all } x \in \Omega.$$

Discretization leads to system $Gu = b$ with a matrix $G \in \mathbb{R}^{\mathcal{I}\times\mathcal{I}}$.

$$g_{ij} = \int_\Omega \varphi_i(x) \int_\omega g(x,y)\varphi_j(y)\,dy\,dx \quad \text{or}$$
$$g_{ij} = g(x_i, y_j) \qquad \text{for } i,j \in \mathcal{I}.$$

Problem: High accuracy requires large number of basis functions.

Idea: Approximate G by a matrix that can be represented efficiently.

Uniform $\mathcal{H}$-matrix

Idea: Locally approximate kernel function, e.g., by interpolation

$$g_{ij} = g(x_i, y_j) \approx \sum_{\nu=1}^{k} \sum_{\mu=1}^{k} \mathcal{L}_{\tau,\nu}(x_i) g(\xi_{\tau,\nu}, \xi_{\sigma,\mu}) \mathcal{L}_{\sigma,\mu}(y_j).$$

for clusters $\tau, \sigma \subseteq \Omega$, $x_i \in \tau$ and $y_j \in \sigma$.

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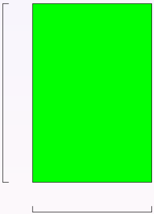
Block approximation by three-term factorization

$$G|_{\hat\tau\times\hat\sigma} \approx V_\tau S_{\tau\sigma} W_\sigma^*.$$

with $\hat\tau := \{i \in \mathcal{I} \;:\; x_i \in \tau\}$ and $\hat\sigma := \{j \in \mathcal{I} \;:\; y_j \in \sigma\}$.



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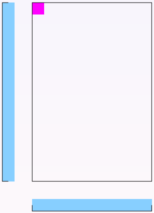

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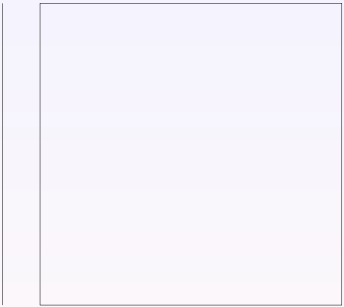
Cluster bases: V_τ depends only on τ, W_σ only on σ.

Coupling matrices $S_{\tau\sigma}$ are $k \times k$-matrices.

Block tree

Problem: Since the kernel function is only locally smooth, split $\Omega \times \Omega$ into subdomains $\tau \times \sigma$ admitting an approximation.



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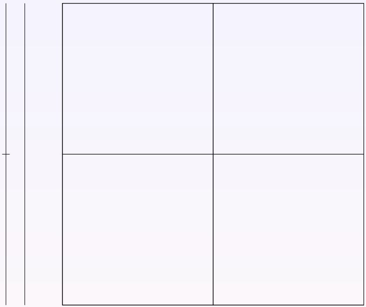

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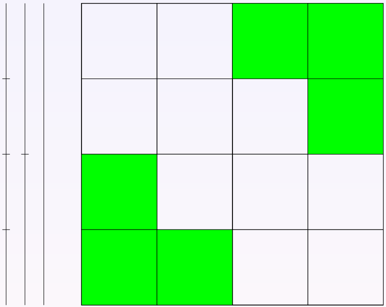

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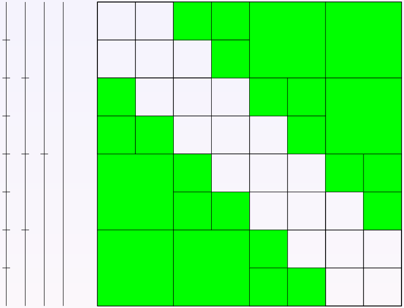

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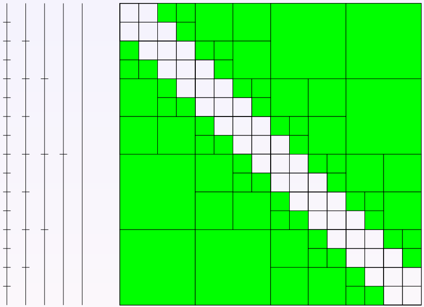

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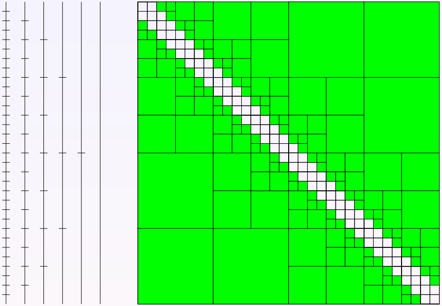

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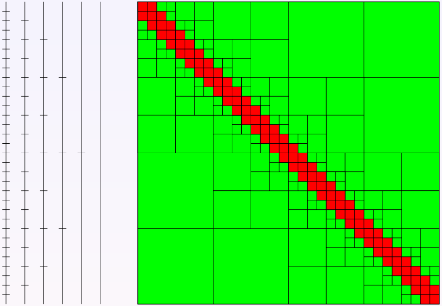

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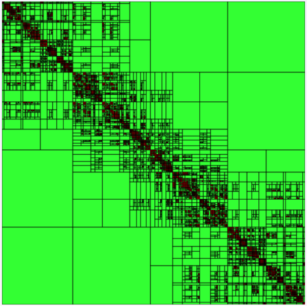

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General case: Block structure can be significantly more involved.

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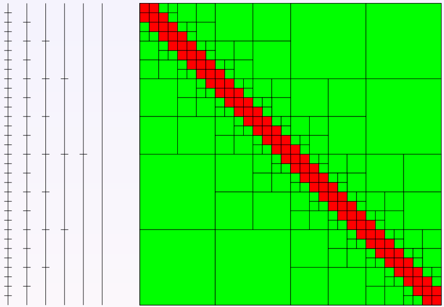

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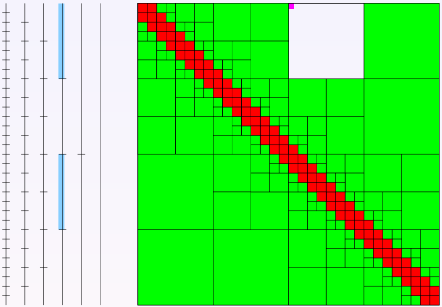

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$$G|_{\hat\tau \times \hat\sigma} \approx V_\tau S_{\tau\sigma} W_\sigma^*.$$

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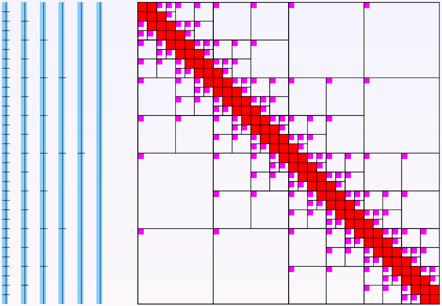

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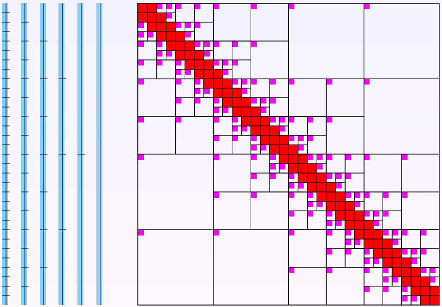

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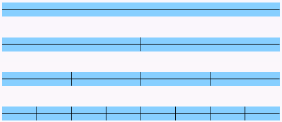
Result: $\mathcal{O}(nk)$ storage for coupling matrices $(S_{\tau\sigma})$, but $\mathcal{O}(nk \log n)$ for cluster bases (V_τ) and (W_σ).

Cluster basis

Challenge: Cluster basis $(V_\tau)_\tau$ requires storage $\sim nk \log n$.



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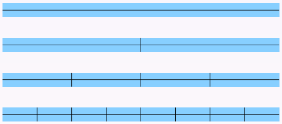

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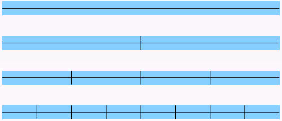

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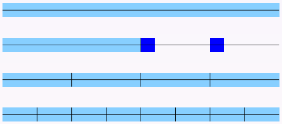
Transfer matrices can be stored instead of V_τ:

$$V_\tau = \begin{pmatrix} V_{\tau_1} E_{\tau_1} \\ V_{\tau_2} E_{\tau_2} \end{pmatrix}, \qquad \mathrm{sons}(\tau) = \{\tau_1, \tau_2\}.$$



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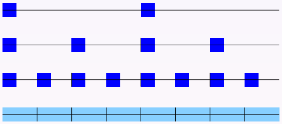

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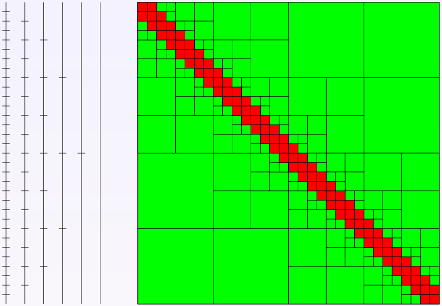
Result: Storage $\sim nk$.

$\mathcal{H}^2$-matrix



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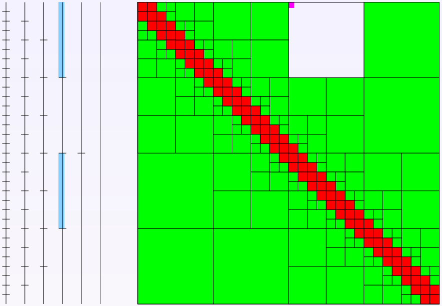

Admissible blocks represented by coupling matrices

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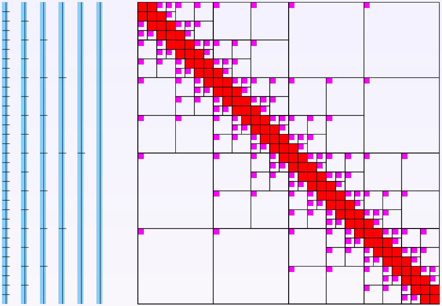

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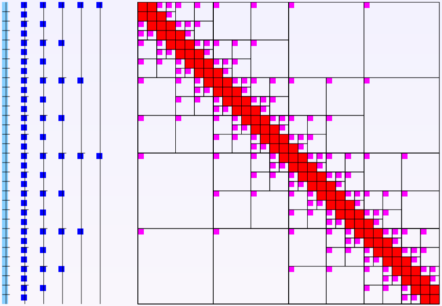

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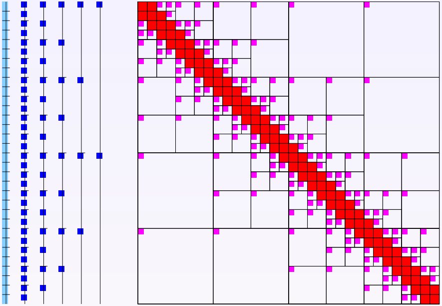

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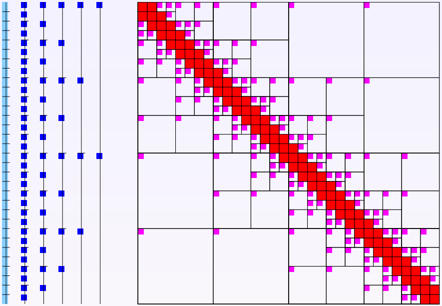

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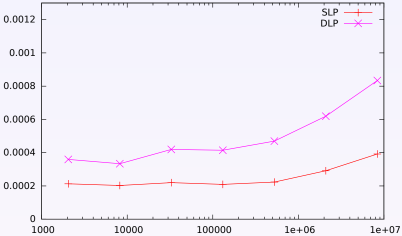
$\mathcal{H}^2$-matrices are the algebraic counterparts of fast multipole representations.

Experiment: Unit sphere

Example: Dirichlet problem on the unit sphere, direct formulation.



Time for setup:

Less than 1+2 hours for
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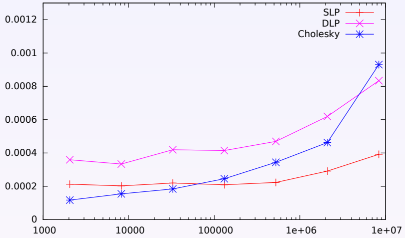

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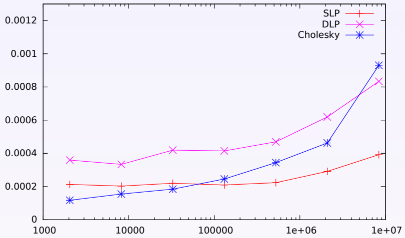

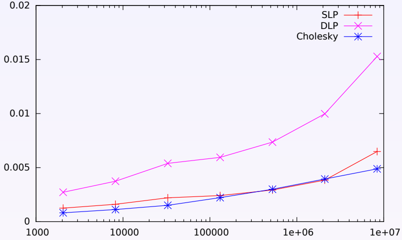

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Storage for matrices:
Less than 55+128 GB for
more than 8 million triangles.

$\mathcal{H}$-Cholesky preconditioner:
More than 41 GB.

Overview

LR factorization

Goal: Given an $\mathcal{H}^2$-matrix G, compute its LR factorization $G = LR$.

Approach: If G is inadmissible, compute $G = LR$ directly.
Otherwise, use submatrices

$$\begin{pmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{pmatrix} = \begin{pmatrix} L_{11} & \\ L_{21} & L_{22} \end{pmatrix} \begin{pmatrix} R_{11} & R_{12} \\ & R_{22} \end{pmatrix}$$

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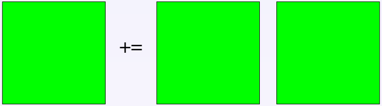
This is equivalent to

$$G_{11} = L_{11} R_{11},$$
$$G_{12} = L_{11} R_{12}, \qquad G_{21} = L_{21} R_{11},$$
$$G_{22} - L_{21} R_{12} = L_{22} R_{22}.$$

If we can compute $Z \leftarrow Z + \alpha XY$, we can find the LR factorization.

Multiplication

Goal: Perform update $Z|_{\hat{\tau}\times\hat{\rho}} \leftarrow Z|_{\hat{\tau}\times\hat{\rho}} + \alpha X|_{\hat{\tau}\times\hat{\sigma}} Y|_{\hat{\sigma}\times\hat{\rho}}$ efficiently.



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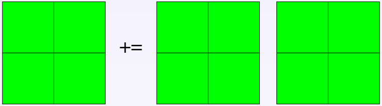

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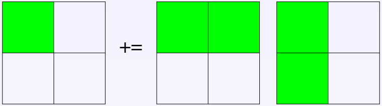

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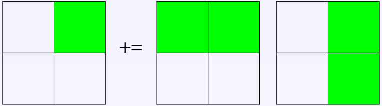

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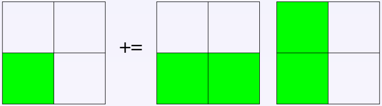

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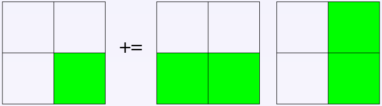

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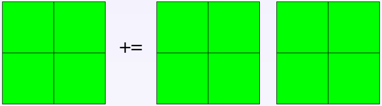

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Important case: What happens if one of the factors is not subdivided?

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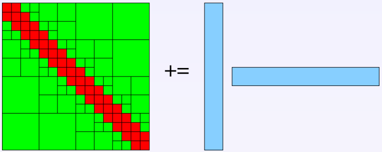
General case: If (τ, σ) or (σ, ρ) are leaves, the product $X|_{\hat\tau\times\hat\sigma} Y|_{\hat\sigma\times\hat\rho}$ is always a low-rank matrix in factorized representation.

Low-rank update

Goal: Approximate $Z + AB^*$.



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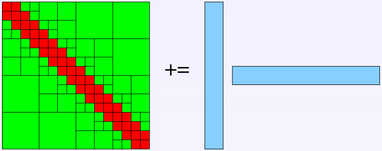

Idea: Result $Z + AB^*$ is an $\mathcal{H}^2$-matrix: for admissible (τ, σ) we have

$$
\begin{aligned}
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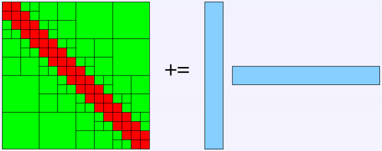

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Challenge: Each update increases storage requirements, although actual numerical rank may be low. $\rightarrow$ Recompression required.

Recompression

Goal: Given an $\mathcal{H}^2$-matrix with unnecessarily high rank, construct a more efficient approximation.

Row basis: Find orthogonal $(Q_\tau)_\tau$ such that

$$Q_\tau Q_\tau^* G|_{\tau\times\sigma} \approx G|_{\tau\times\sigma} \qquad \text{for all admissible } (\tau,\sigma).$$

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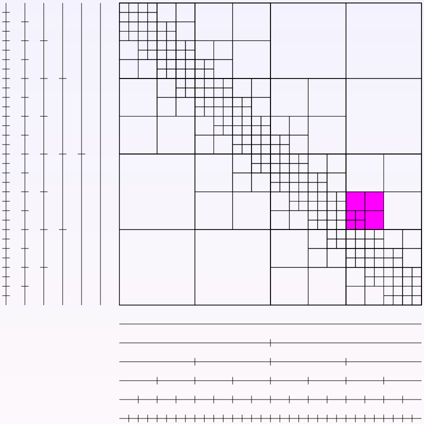
Result: Cluster bases can be constructed in $\mathcal{O}(nk^2)$ operations, using $\mathcal{O}(nk)$ units of auxiliary storage, e.g., for $(Z_\tau)_\tau$.
Conversion of $\mathcal{H}^2$-matrix to new bases takes $\mathcal{O}(nk^2)$ operations.

Local low-rank update

Goal: Approximate local update $Z|_{\hat{\tau}\times\hat{\sigma}} + AB^*$.



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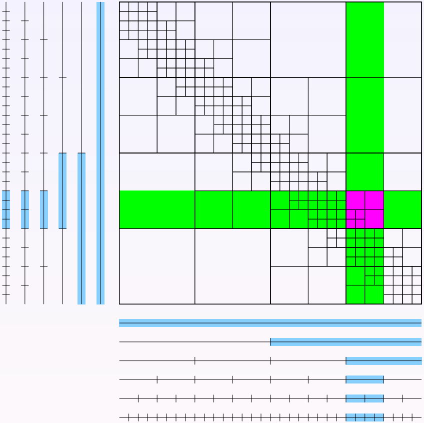

Cluster bases: Changes affect entire block rows and columns.

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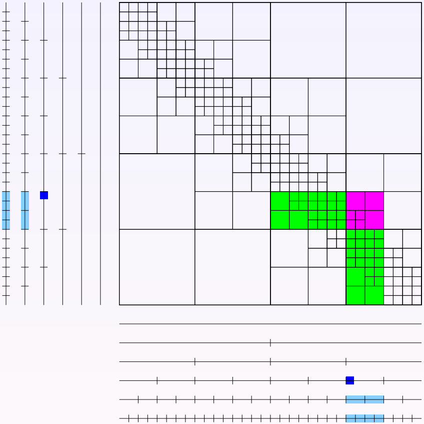

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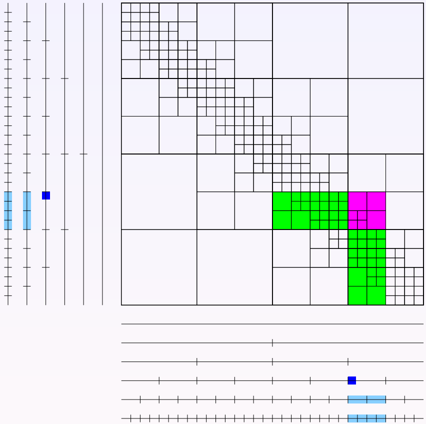

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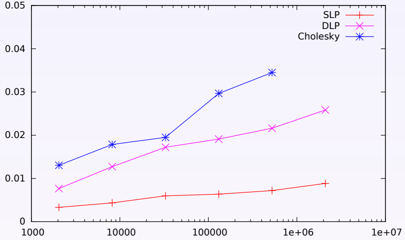
Solution: Use transfer matrices to limit the effect.

Result: Only $\mathcal{O}(k^2(\#\hat\tau + \#\hat\sigma))$ operations required.

Multiplication and factorization in $\mathcal{O}(nk^2 \log n)$ operations.

Experiment: Unit sphere

Example: Dirichlet problem on the unit sphere, direct formulation.



Time for setup:

Less than 6+15 hours for more than 2 million triangles.

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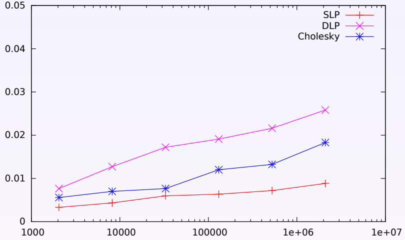

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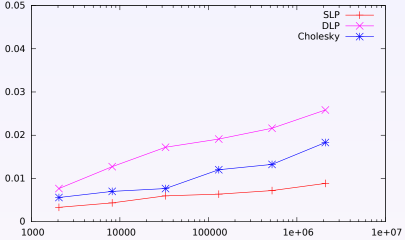

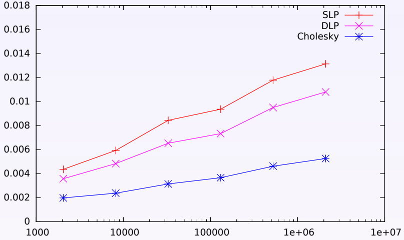

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Storage for matrices:
Less than 28+23 GB for more than 2 million triangles.

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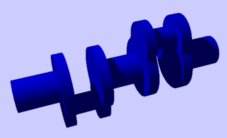
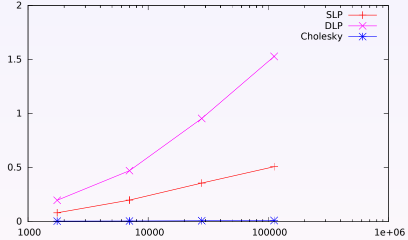
Experiment: Crank shaft

Example: Dirichlet problem on the NetGen "crank shaft" geometry, direct formulation.





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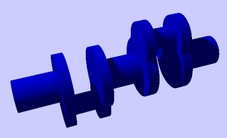

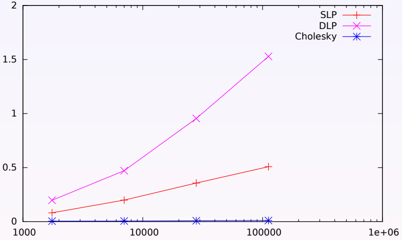

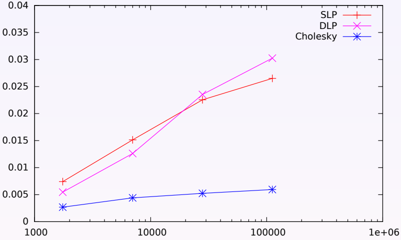

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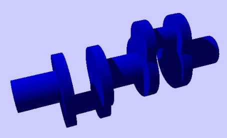

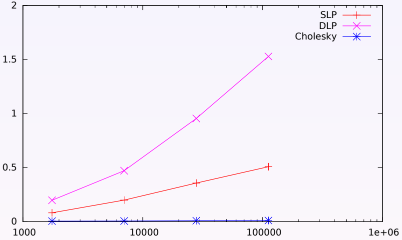

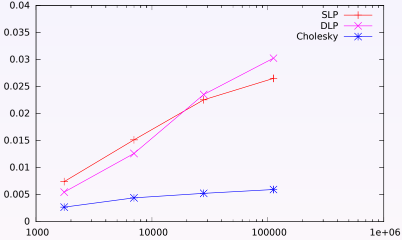

Due to very high quadrature orders, the cost of constructing the $\mathcal{H}^2$-Cholesky preconditioner is almost negligible.

Summary

$\mathcal{H}^2$-matrices:

- Admissible blocks in factorized form $G|_{\hat{\tau}\times\hat{\sigma}} = V_\tau S_{\tau\sigma} W_\sigma^*$.
- Cluster bases in nested form $V_\tau = \begin{pmatrix} V_{\tau_1} E_{\tau_1} \\ V_{\tau_2} E_{\tau_2} \end{pmatrix}$.
- Storage requirements $\mathcal{O}(nk)$.

Arithmetic operations:

- Factorization expressed by multiplications
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Resources

References

- W. Hackbusch, B. N. Khoromskij, S. A. Sauter:
  On $\mathcal{H}^2$-matrices (2000)
- S. B., W. Hackbusch:
  Data-sparse approximation by adaptive $\mathcal{H}^2$-matrices (2002)
- S. B.:
  Efficient numerical methods for non-local operators (2010)
- S. B., K. Reimer:
  Efficient arithmetic operations for rank-structured matrices based on hierarchical low-rank updates (2015)
- S. B., S. Christophersen:
  Approximation of integral operators by Green quadrature and nested cross approximation, arXiv preprint (2015)

Software

- H2Lib, open source, available at GitHub