Algorithmic aspects of hierarchical matrices

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Christian-Albrechts-Universität zu Kiel

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Overview

1. Introduction
2. Algorithms
3. Parallelization

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Goal

Dense matrices are required by important applications, e.g.,

- when discretizing integral equations,
- when solving partial differential equations, or
- when approximating matrix functions like $\exp(A)$.

Problem: Standard representation requires n^2 units of storage.

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Approach: Use data-sparse approximation of G.

- Storage $\mathcal{O}(nk \log(n))$,
- matrix-vector product $\mathcal{O}(nk \log(n))$,
- approximated matrix-matrix product $\mathcal{O}(nk^2 \log^2(n))$,
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Challenge: Still very time-consuming, has to be parallelized.

Model problem

Integral operator approximated by Nystrøm's method leads to matrix $G \in \mathbb{R}^{n \times n}$ with

$$g_{ij} = \gamma(x_i, x_j), \qquad \gamma : [0,1] \times [0,1] \to \mathbb{R} \qquad \text{for all } i, j \in [1:n],$$

where $x_1, \ldots, x_n \in [0,1]$.

Challenge: Dense matrix, have to store n^2 coefficients.

Low-rank approximation

Idea: Given intervals $t, s \subseteq [0,1]$ with $\operatorname{diam}(t) \leq \operatorname{dist}(t,s)$, we have

$$\gamma(x,y) \approx \sum_{\nu=0}^{k-1} \frac{(x-x_t)^\nu}{\nu!} \frac{\partial^\nu \gamma}{\partial x^\nu}(x_t,y) \text{ for all } x \in t,\ y \in s.$$

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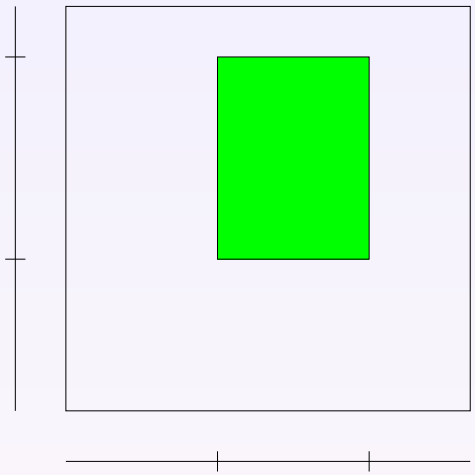
Low-rank factorization given by

$$G|_{\hat{t}\times\hat{s}} \approx A_{ts} B_{ts}^*$$

with $\hat{t} := \{i \in [1:n] \ : \ x_i \in t\}$ and



$$a_{ts,i\nu} := \frac{(x_i - x_t)^\nu}{\nu!}, \qquad b_{ts,j\nu} := \frac{\partial^{\nu+\mu}\gamma}{\partial x^\nu \partial y^\mu}(x_t, y_j).$$

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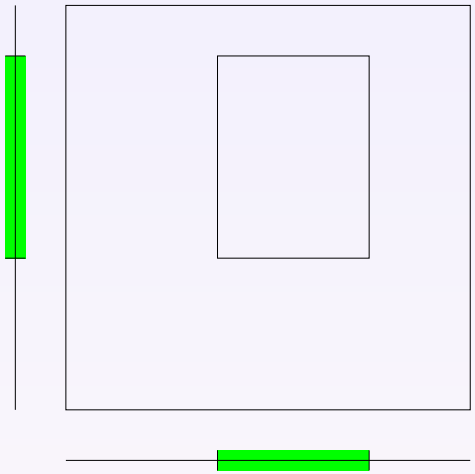

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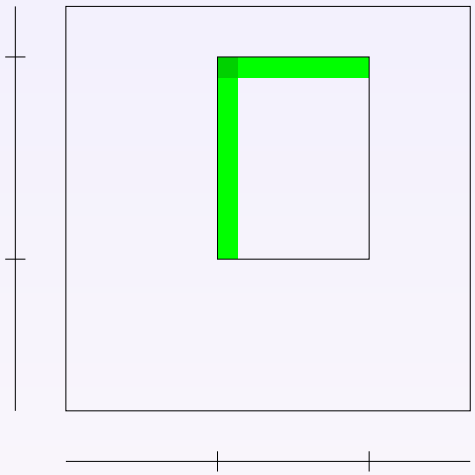

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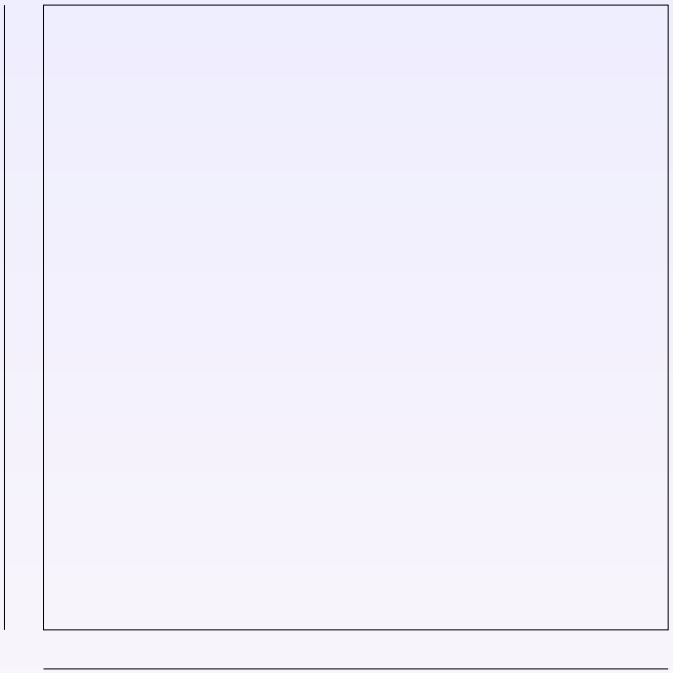
Hierarchical matrix



Goal: Split matrix into submatrices that can be approximated

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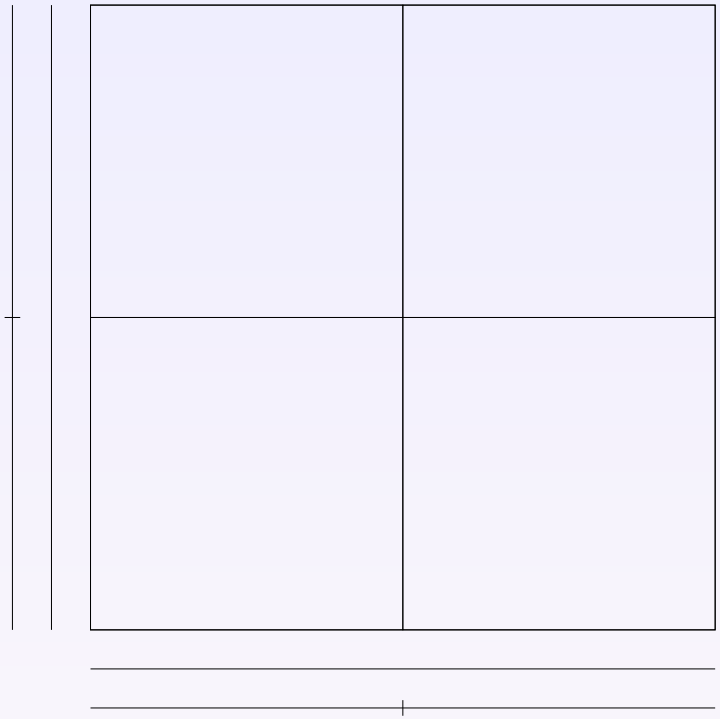

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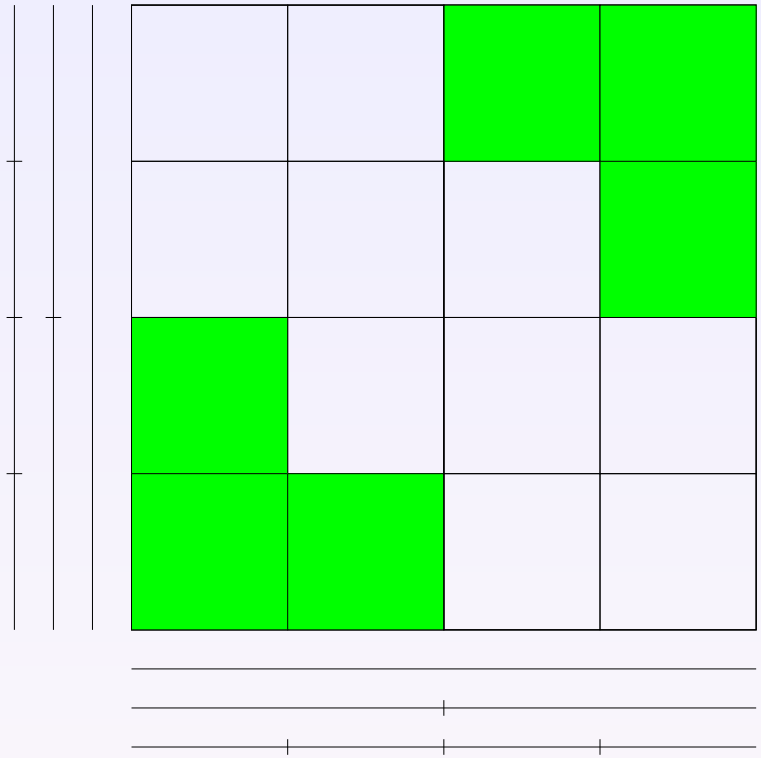

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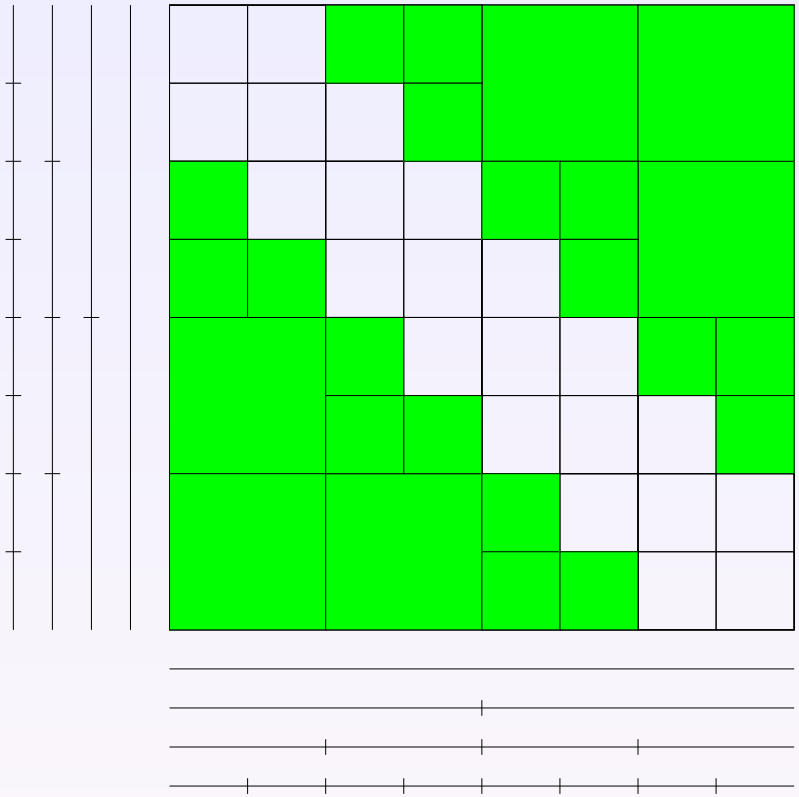

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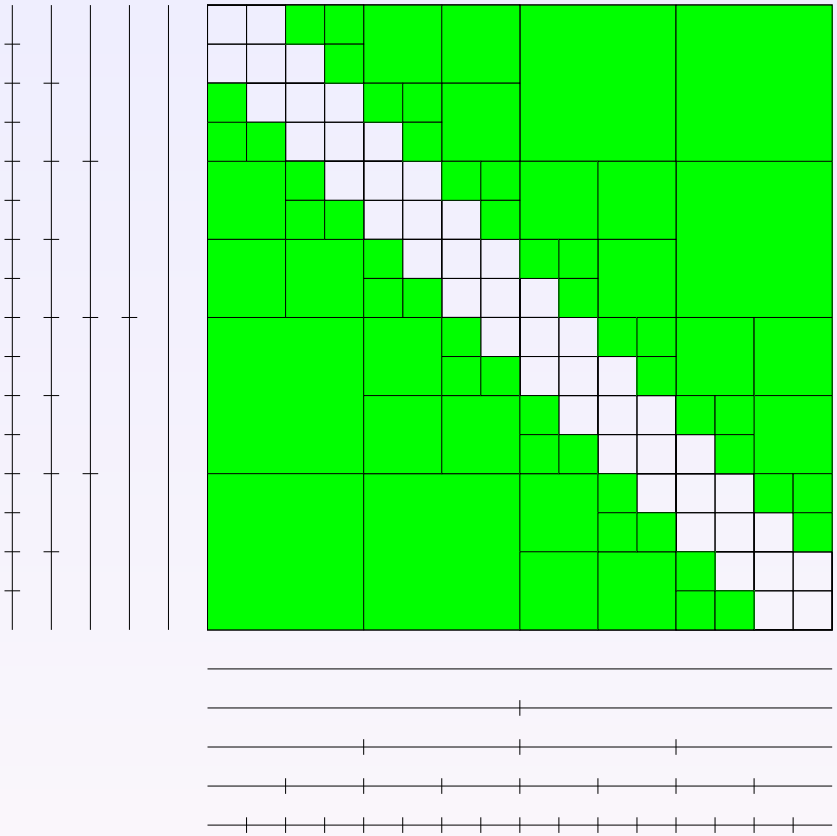

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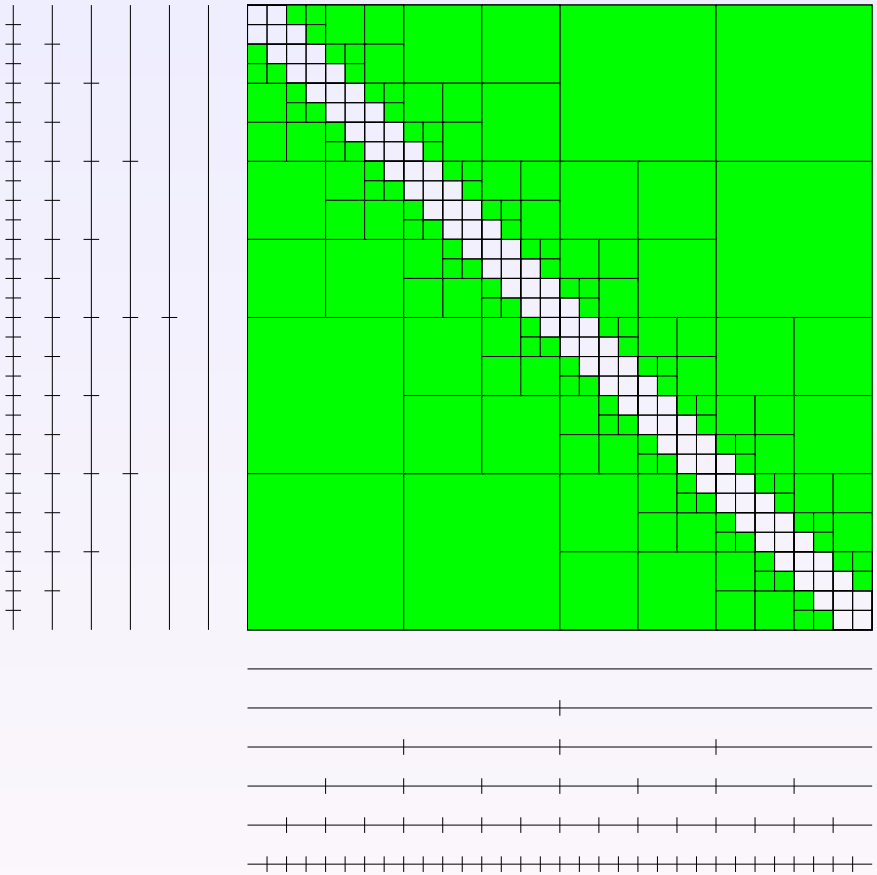

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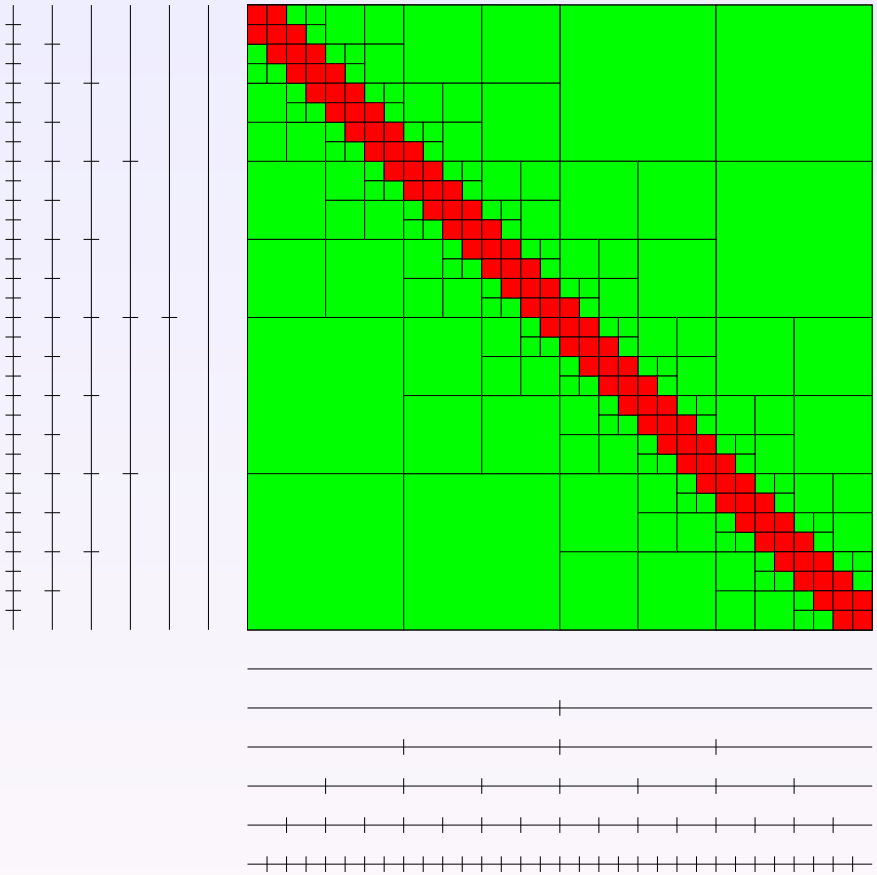

Goal: Split matrix into submatrices that can be approximated and a sparse remainder matrix.

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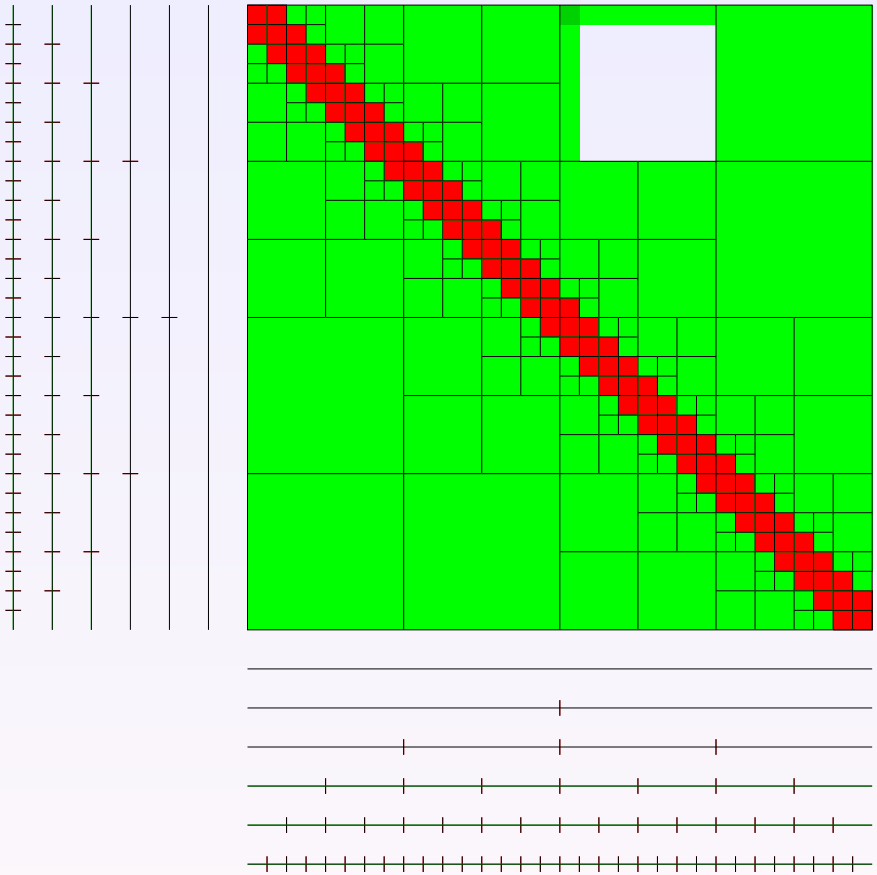

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Approximate submatrices by factorization

$$G|_{\hat{t}\times\hat{s}} \approx A_{ts} B_{ts}^*.$$

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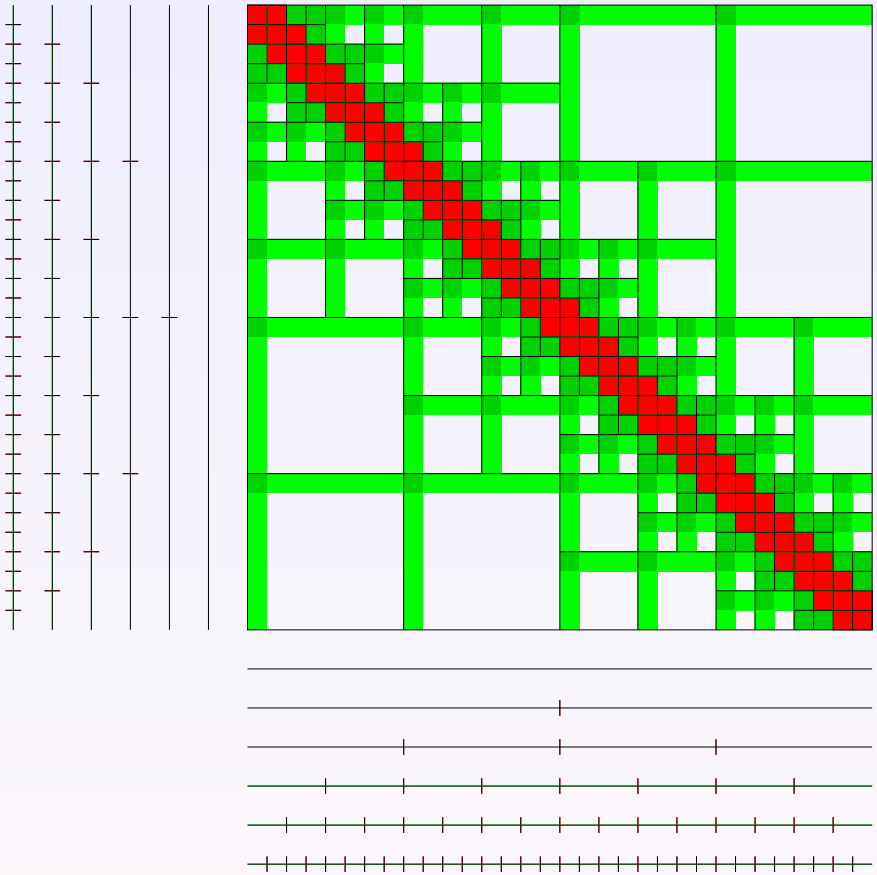

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Result: Storage $\mathcal{O}(nk\log(n))$.

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Fundamental operations

Matrix-vector multiplication: Split into two products

$$y = A_{ts} B_{ts}^* x \qquad \Longleftrightarrow \qquad z = B_{ts}^* x \wedge y = A_{ts} z.$$

Complexity $\mathcal{O}(k(\#\hat{t} + \#\hat{s}))$ for one submatrix, $\mathcal{O}(nk \log(n))$ for entire hierarchical matrix.

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Truncated update: Best approximation of

$$A_{ts} B_{ts}^* + C_{ts} D_{ts}^* = \begin{pmatrix} A_{ts} & C_{ts} \end{pmatrix} \begin{pmatrix} B_{ts} & D_{ts} \end{pmatrix}^*$$

can be found in $\mathcal{O}(k^2(\#\hat{t} + \#\hat{s}))$ for one submatrix, $\mathcal{O}(nk^2 \log(n))$ for entire hierarchical matrix.

Matrix multiplication

Goal: Compute update

$$Z|_{\hat{t}\times\hat{r}} \leftarrow Z|_{\hat{t}\times\hat{r}} + \alpha X|_{\hat{t}\times\hat{s}} Y|_{\hat{s}\times\hat{r}}$$

Recursion can be used as long as $X|_{\hat{t}\times\hat{s}}$ and $Y|_{\hat{s}\times\hat{r}}$ are subdivided.

$$\begin{pmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{pmatrix} \begin{pmatrix} Y_{11} & Y_{12} \\ Y_{21} & Y_{22} \end{pmatrix} = \begin{pmatrix} X_{11}Y_{11} + X_{12}Y_{21} & \\ & \end{pmatrix}$$

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Factorization is crucial if one factor has low rank.

$$Z|_{\hat{t}\times\hat{r}} \leftarrow Z|_{\hat{t}\times\hat{r}} + \alpha\ X|_{\hat{t}\times\hat{s}} A_{sr}\ B_{sr}^*.$$

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$$Z|_{\hat{t}\times\hat{r}} \leftarrow Z|_{\hat{t}\times\hat{r}} + \alpha(X|_{\hat{t}\times\hat{s}} A_{sr}) B_{sr}^*.$$

Reduces to k matrix-vector multiplications and a low-rank update.

Complexity $\mathcal{O}(k^2(\#\hat{t} + \#\hat{s} + \#\hat{r})\log(n))$ for one update,
$\mathcal{O}(nk^2\log^2(n))$ for entire multiplication.

LU factorization

Goal: Find $G|_{\hat{t}\times\hat{t}} = LU$ with lower triangular L and upper triangular U.

Approach: Block representation

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

yields recursive algorithm

$$G_{11} = L_{11} U_{11},$$

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$$G_{11} = L_{11} U_{11},$$
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Similar: Inversion, Cholesky factorization.

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Task graph

Goal: Parallelize matrix operations like the LU factorization.

Our approach: Construct a task graph representing the dependencies between operations.

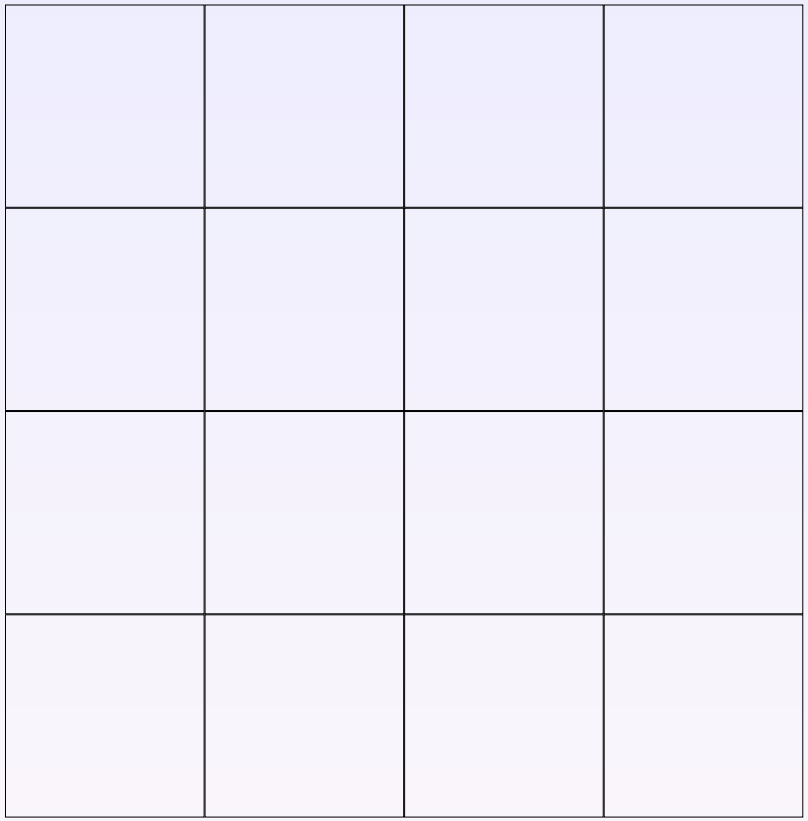
$$G_{11} \xrightarrow{\text{decomp}} L_{11}, U_{11}$$

$$G_{12}, L_{11} \xrightarrow{\text{lsolve}} U_{12}, \qquad G_{21}, R_{11} \xrightarrow{\text{usolve}} L_{21}$$

$$G_{22}, L_{21}, R_{12} \xrightarrow{\text{decomp}} L_{22}, U_{22}.$$

Problem: Straightforward approach offers only very limited potential for parallelization.

Recursive LU decomposition



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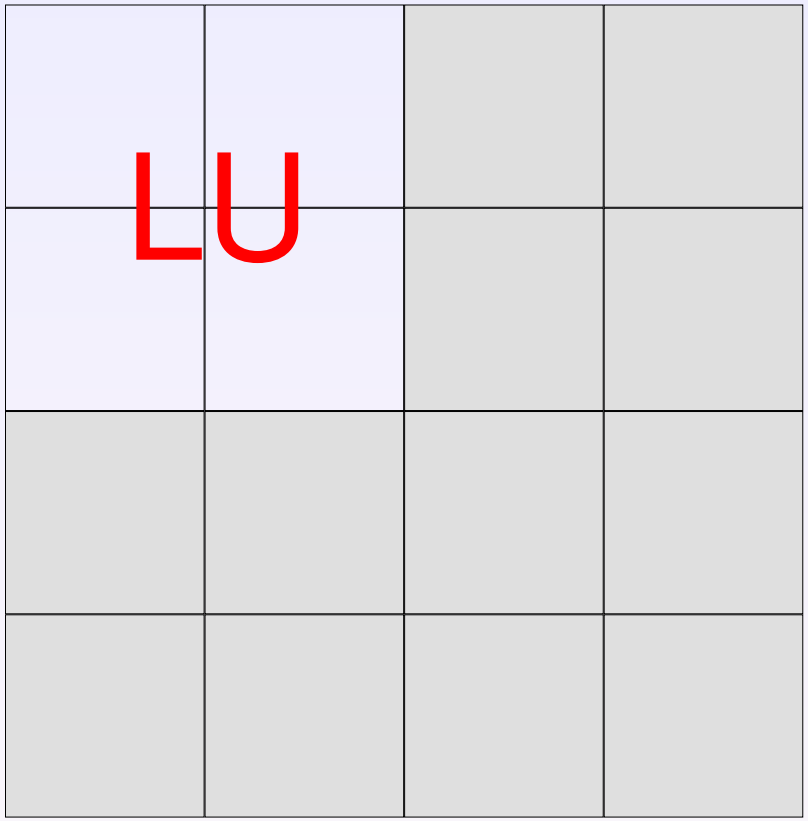

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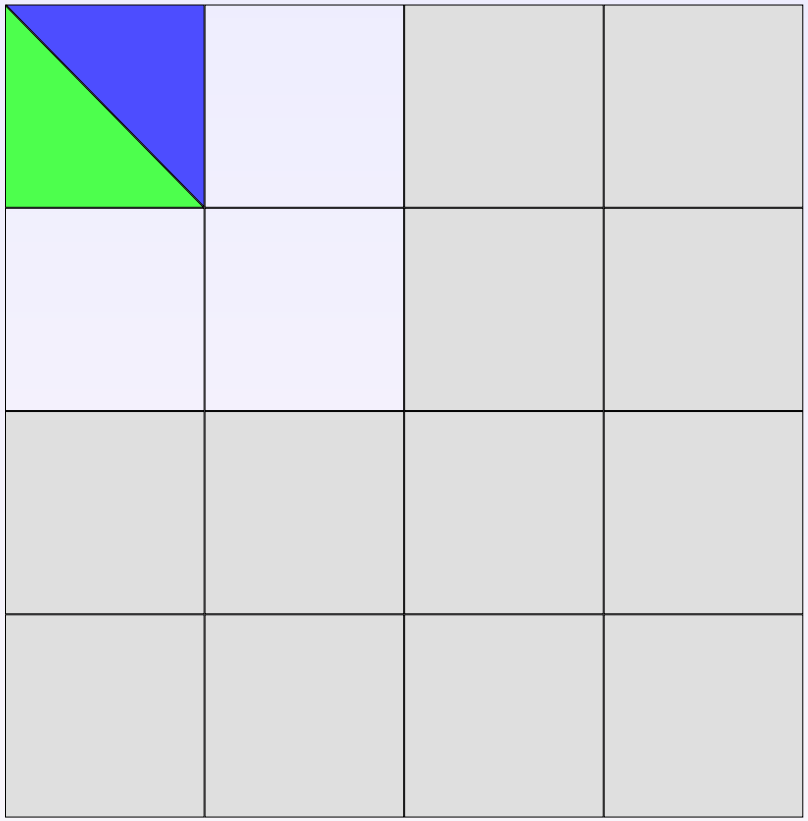

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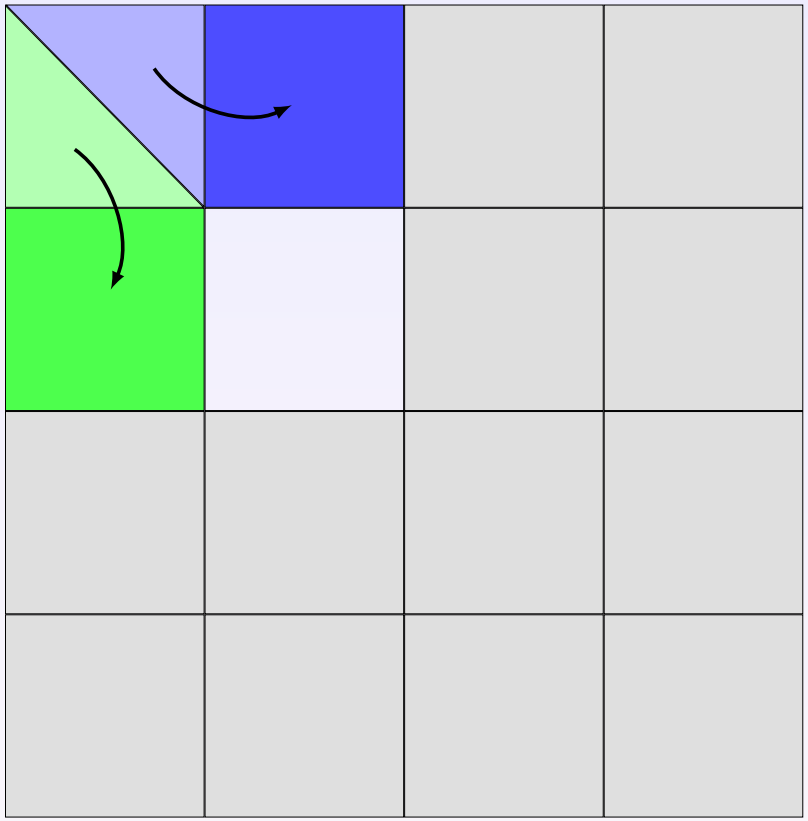

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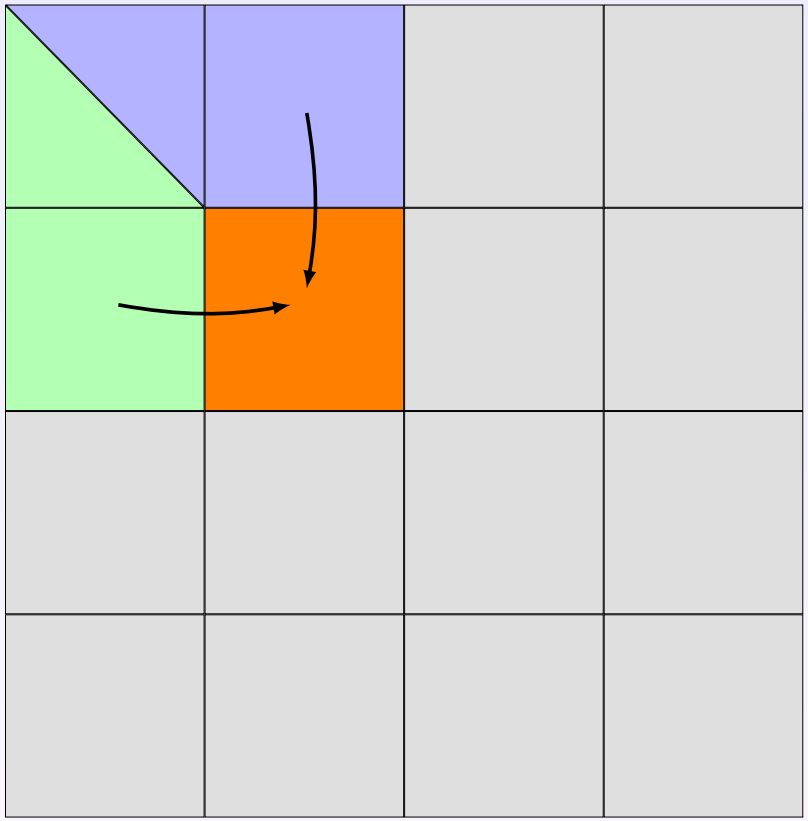

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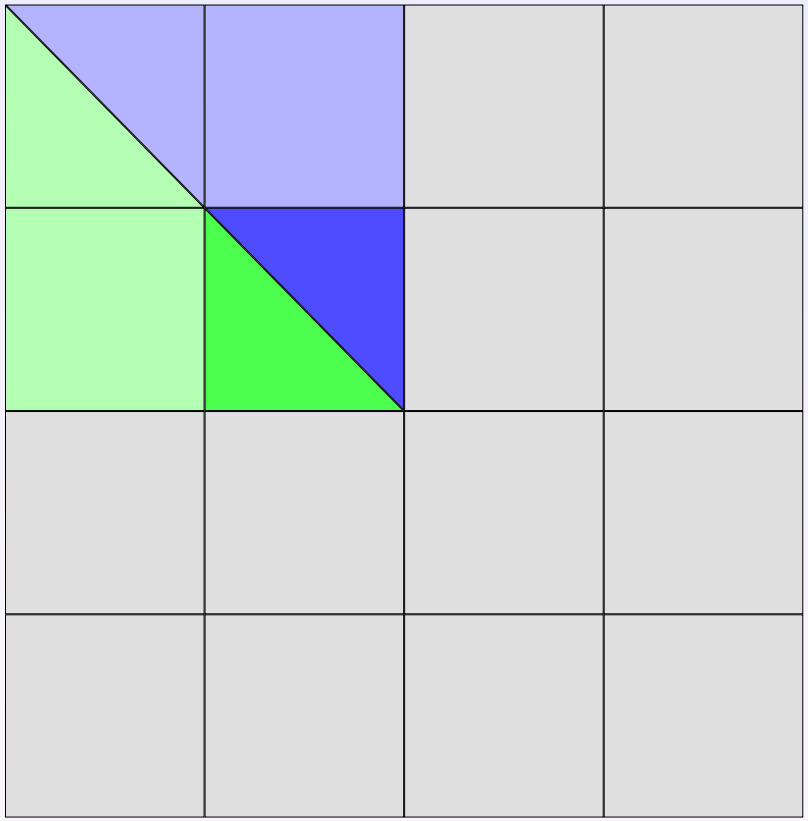

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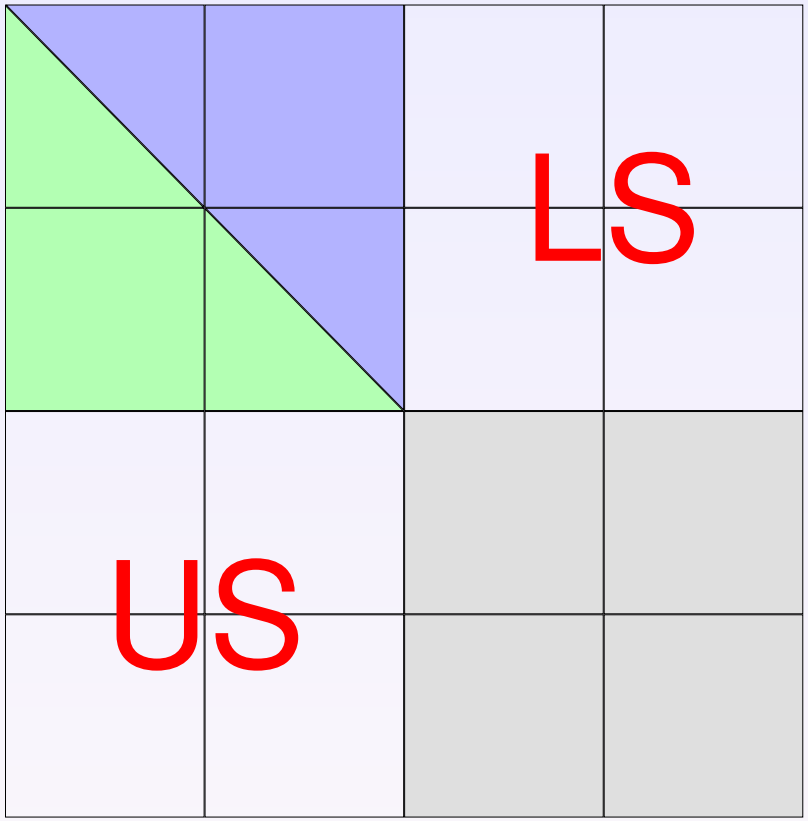

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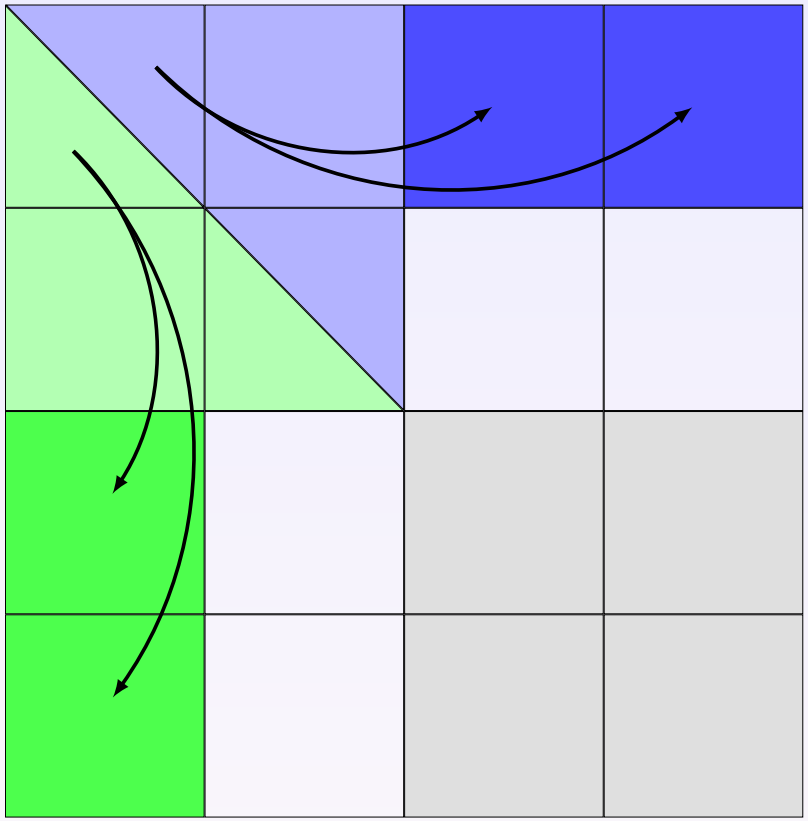

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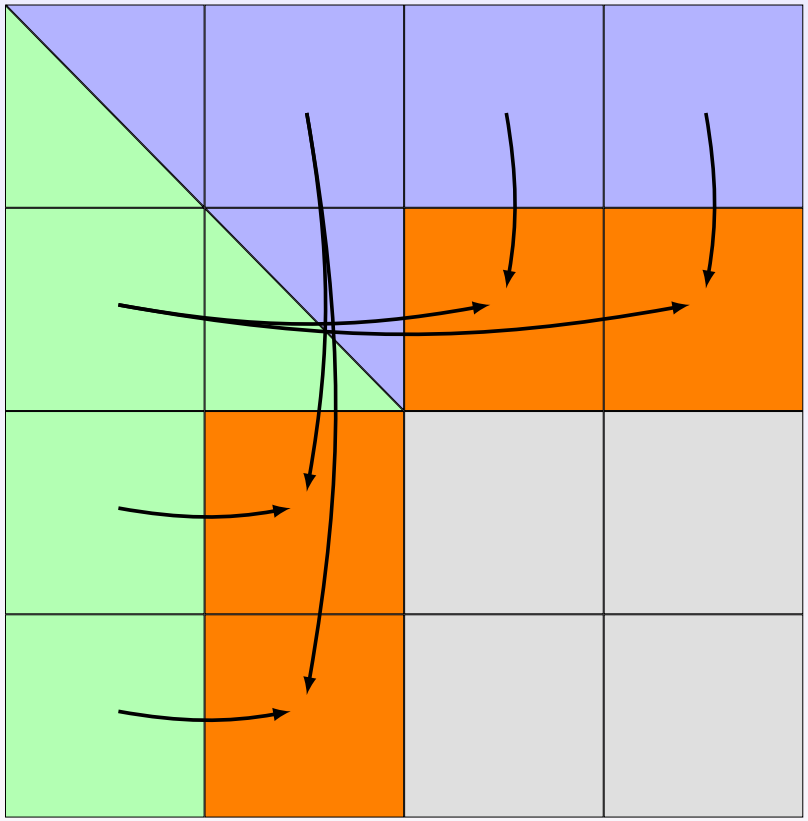

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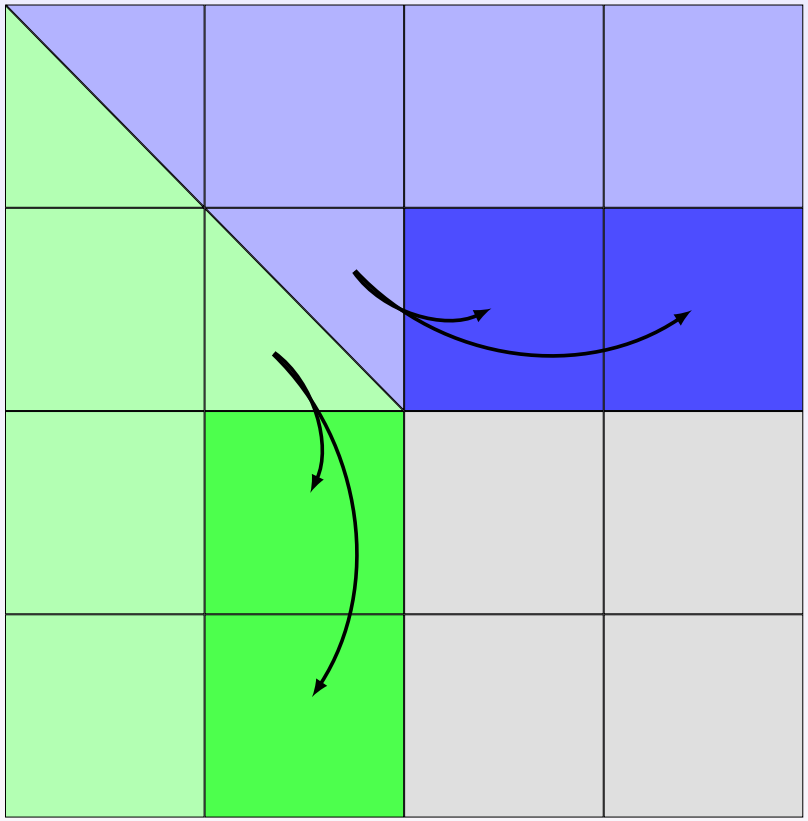

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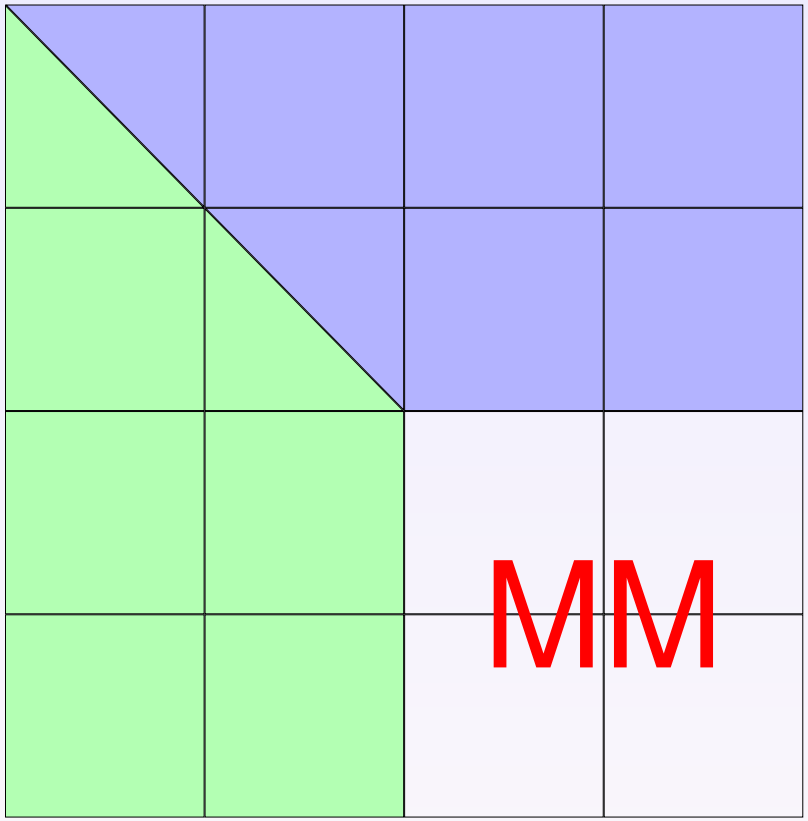

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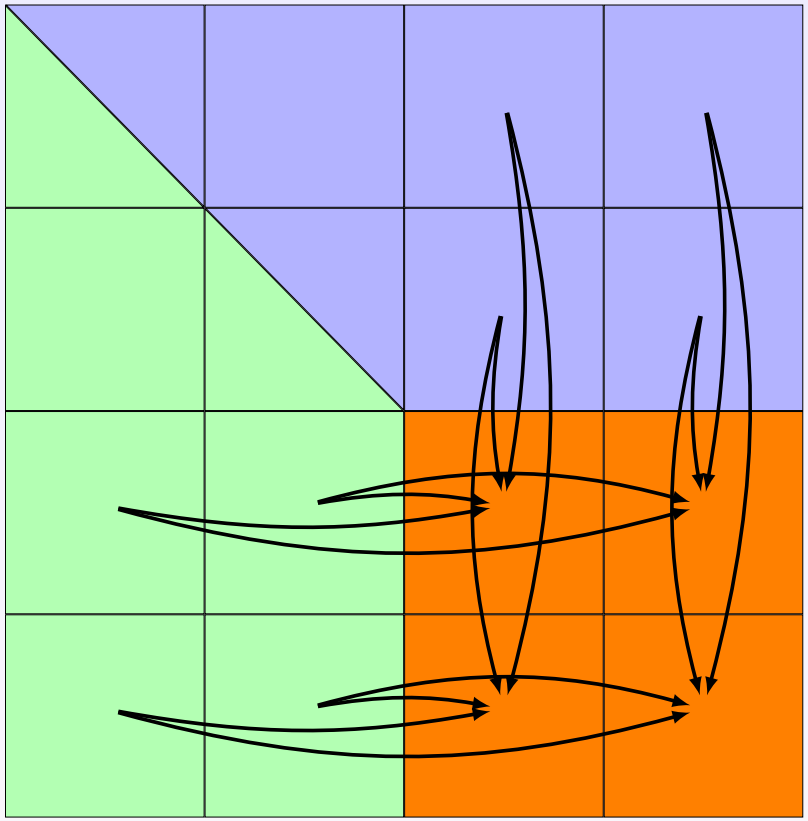

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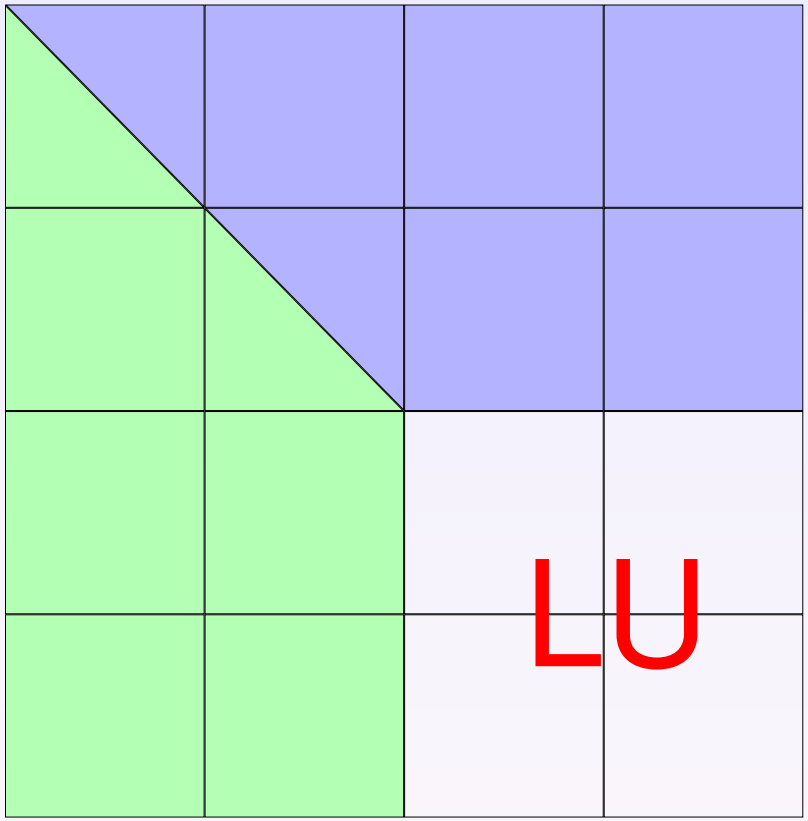

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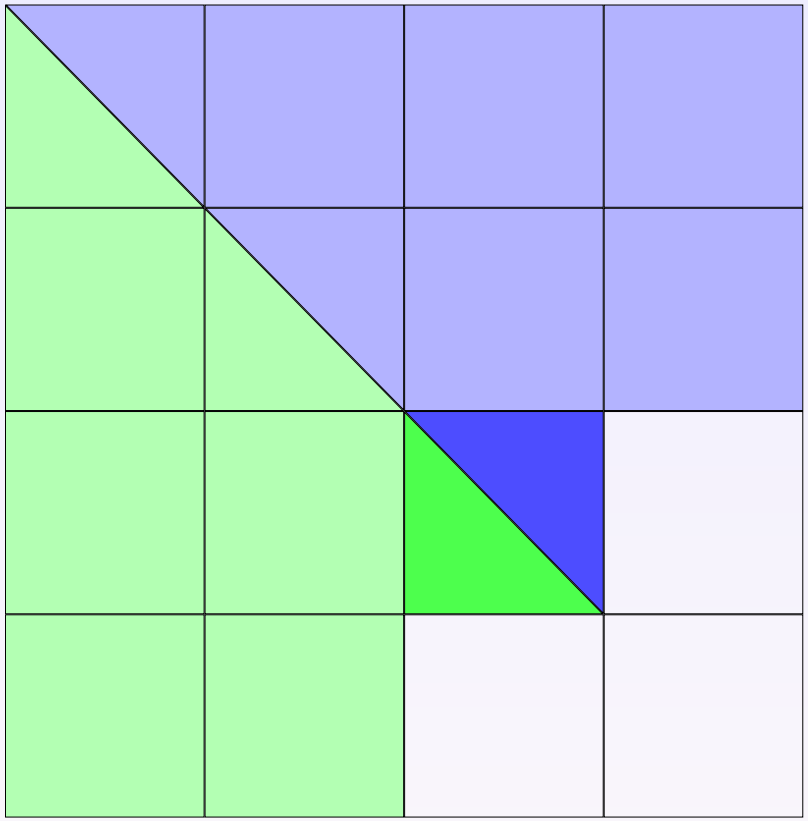
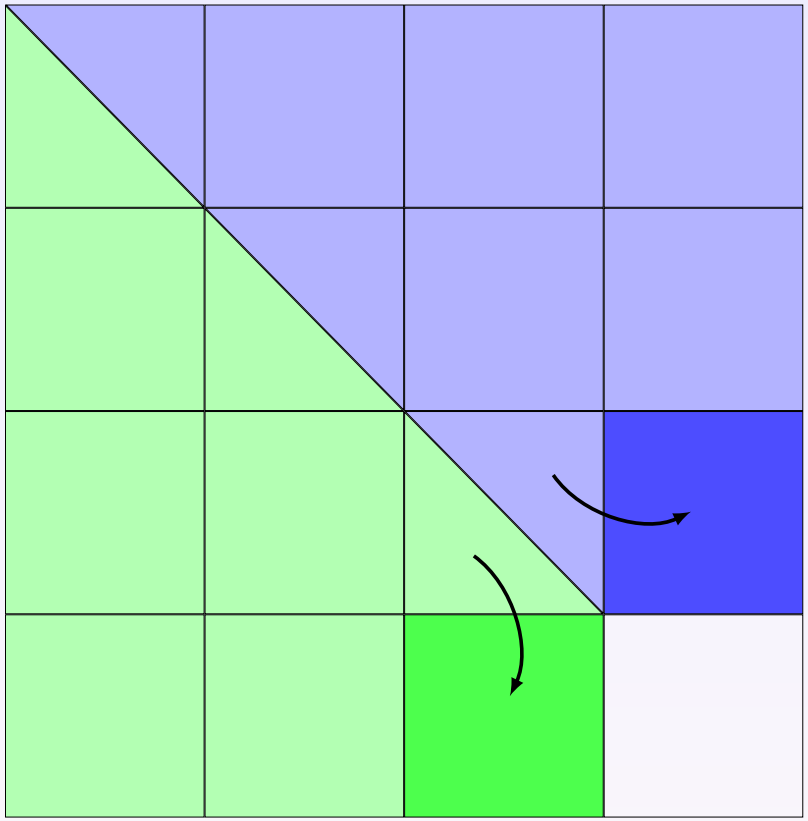
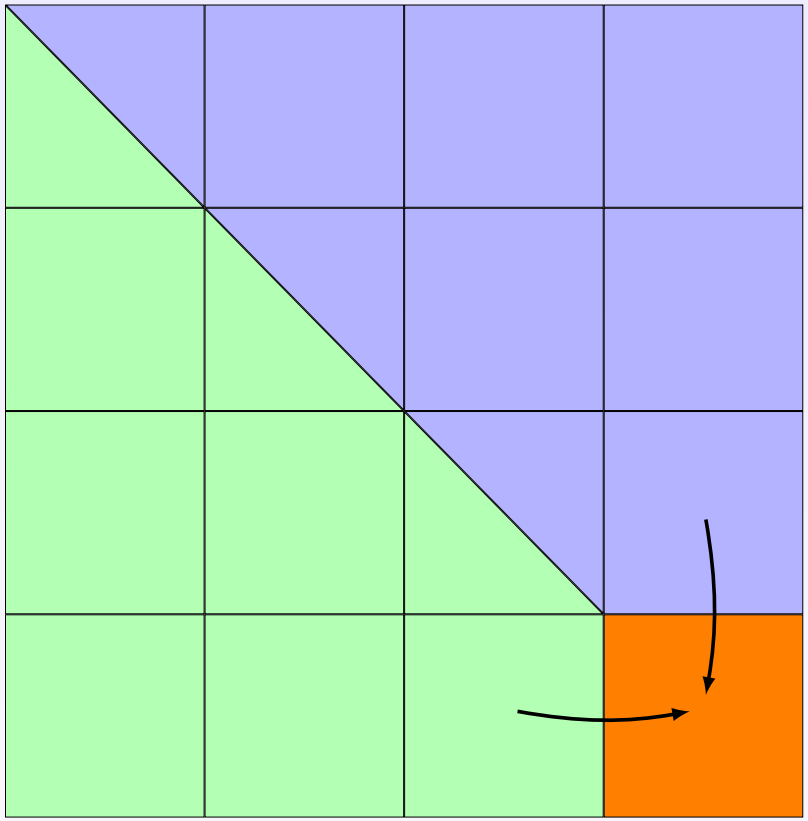


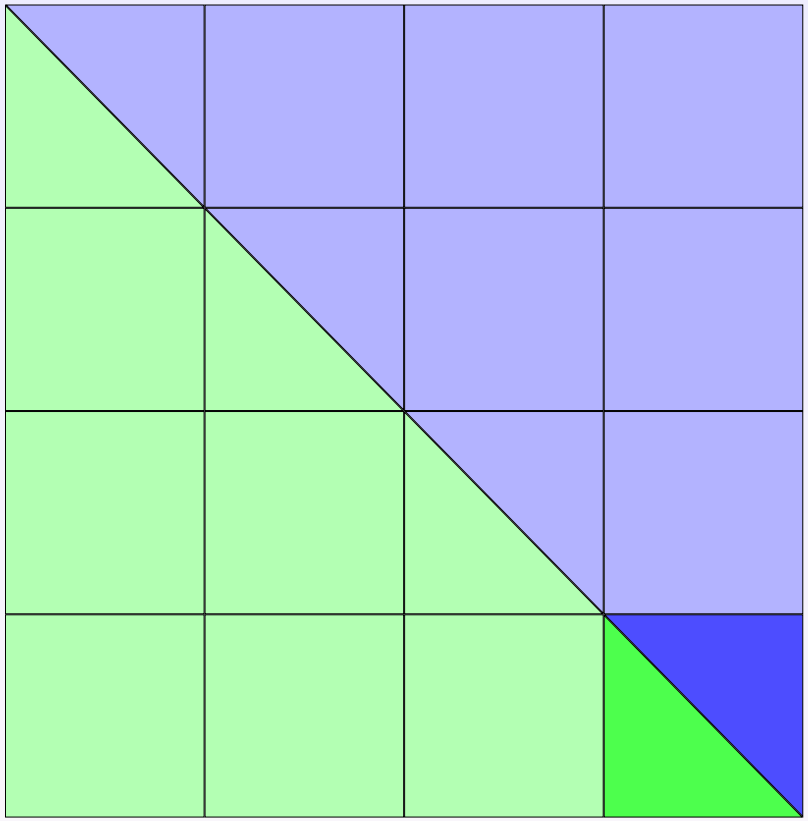
Recursive LU decomposition



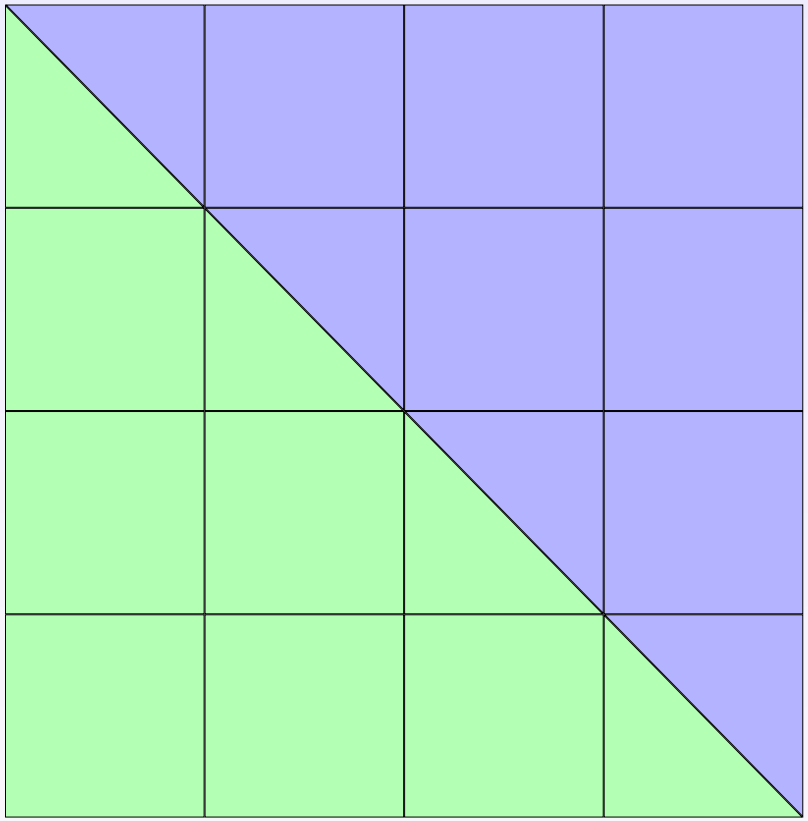
Recursive LU decomposition



Recursive LU decomposition



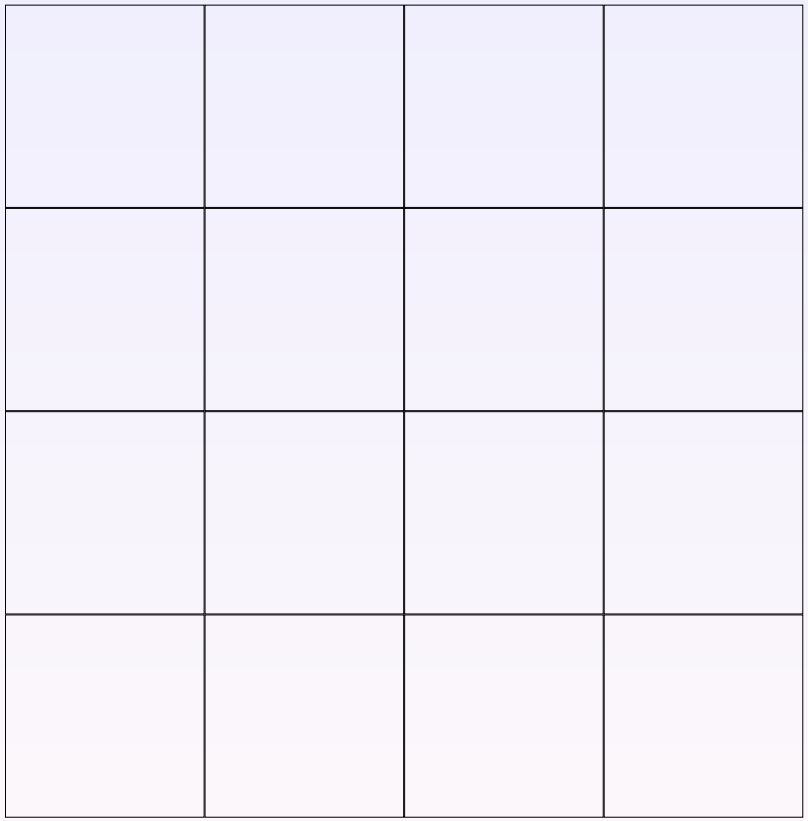
Recursive LU decomposition



Problem: Recursive structure introduces artificial dependencies between “super-tasks” that are unnecessary and harm parallelization.

Flattened task graph

Idea: Eliminate super-tasks and expose only the necessary dependencies between sub-tasks.



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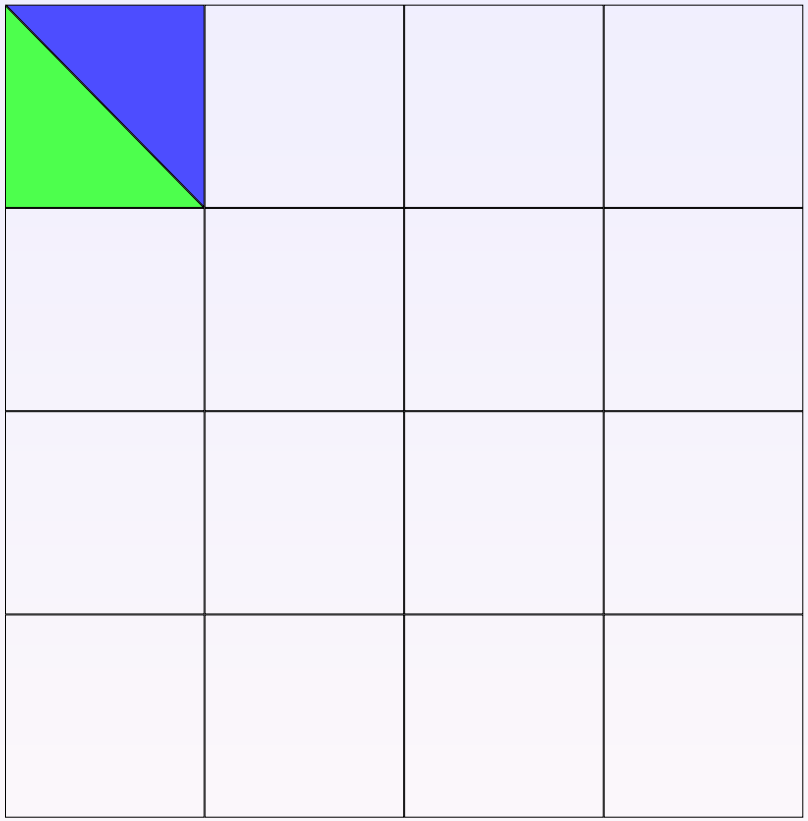

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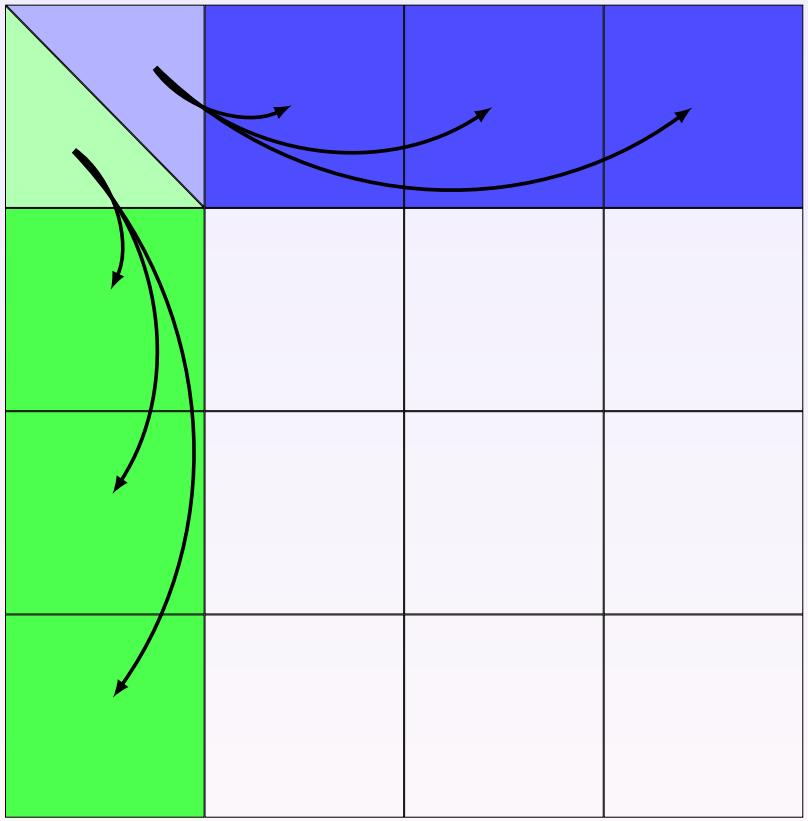

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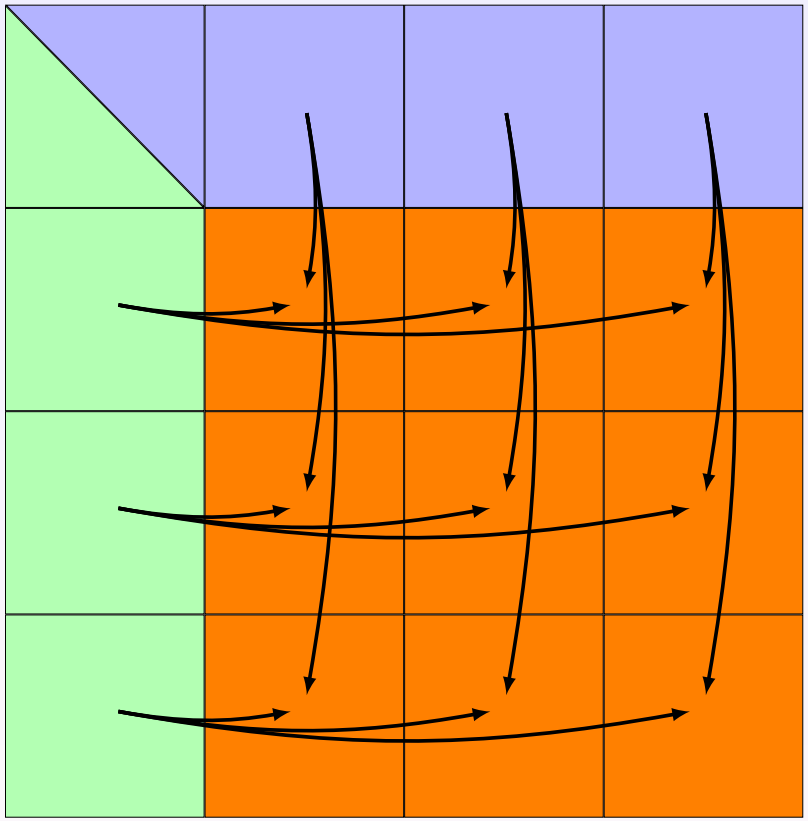

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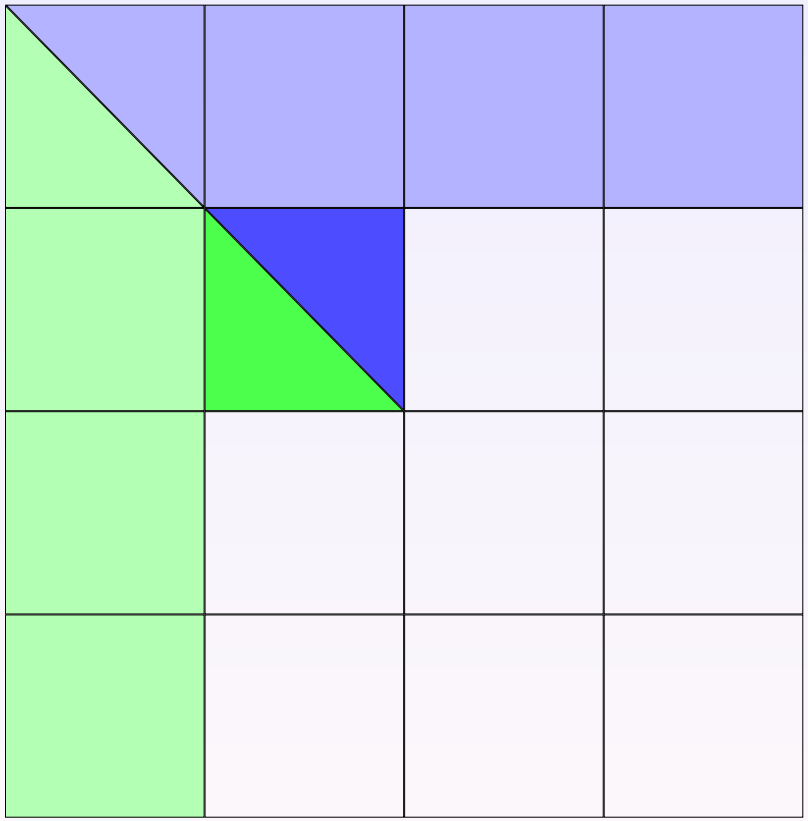

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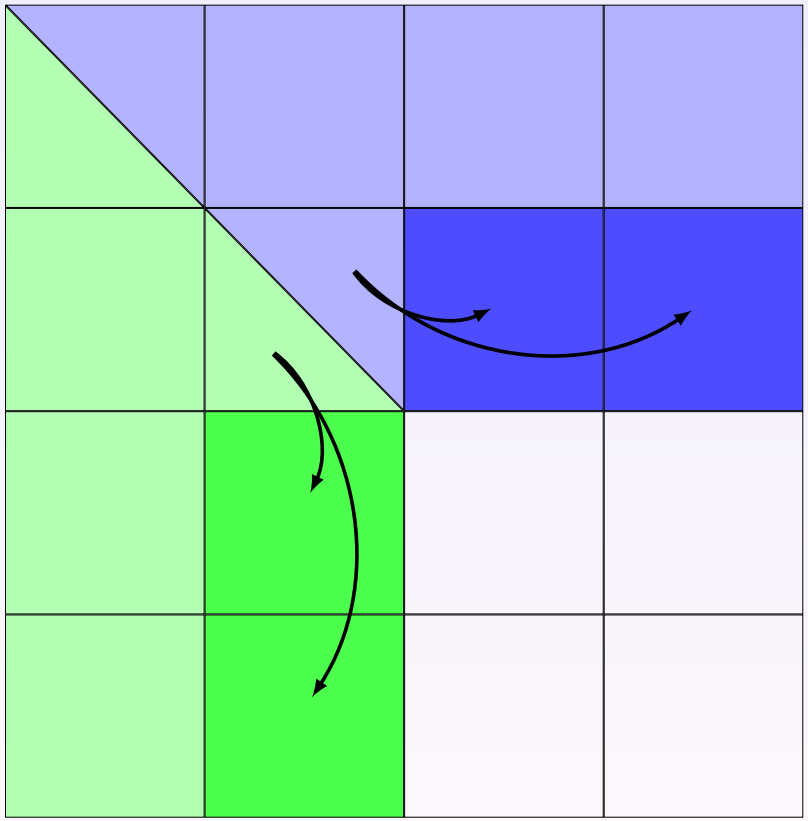

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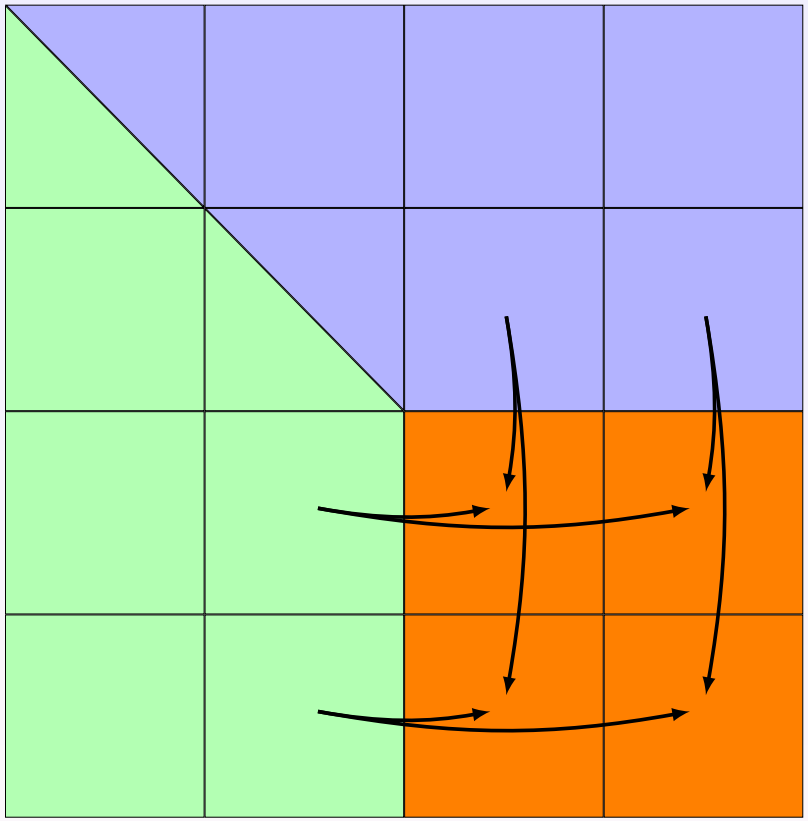

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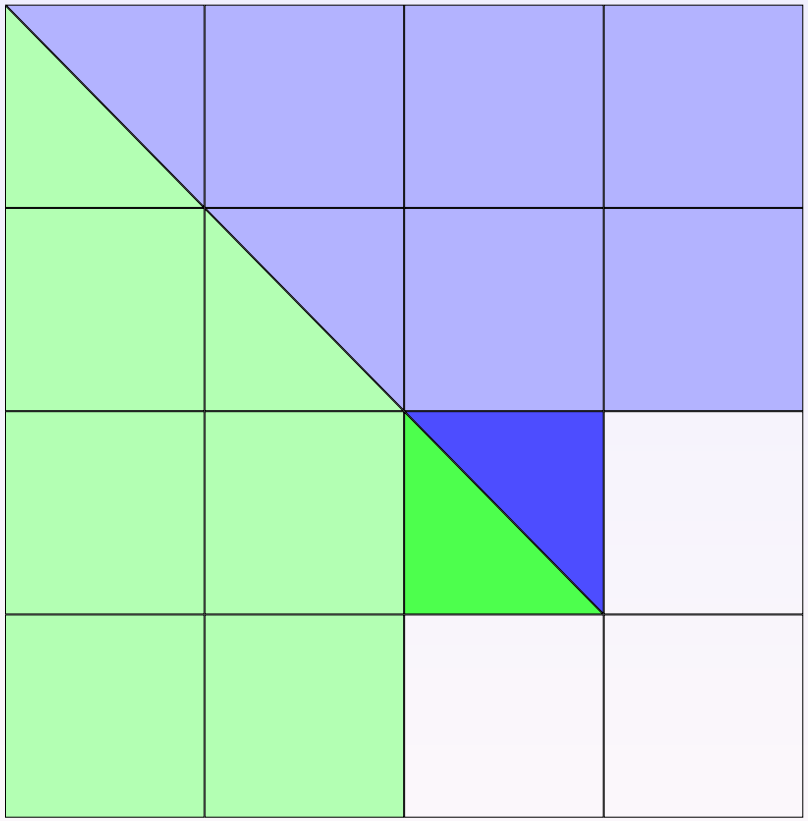

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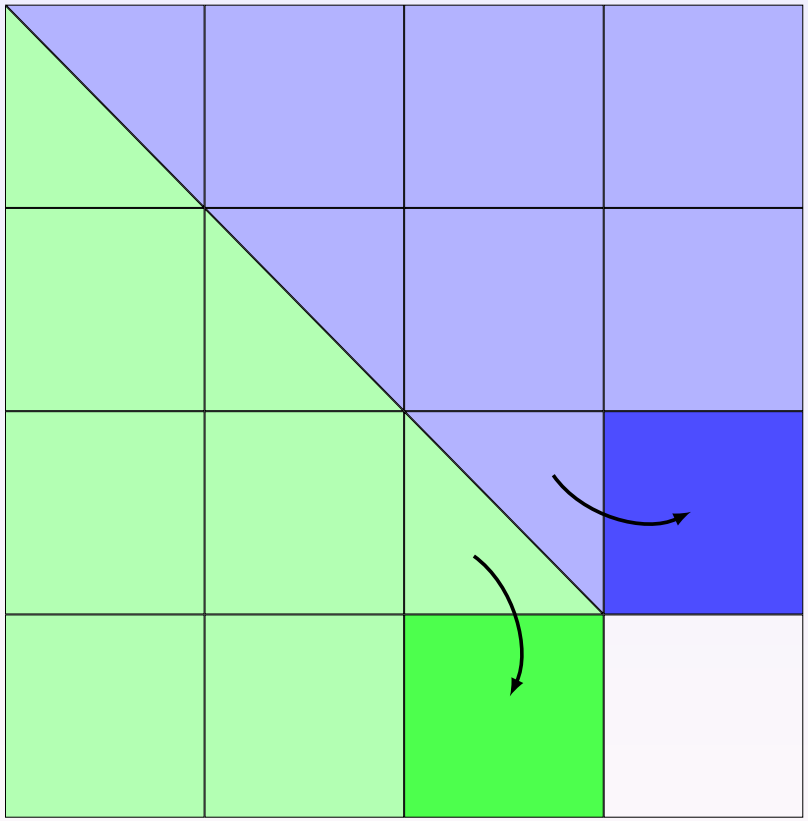

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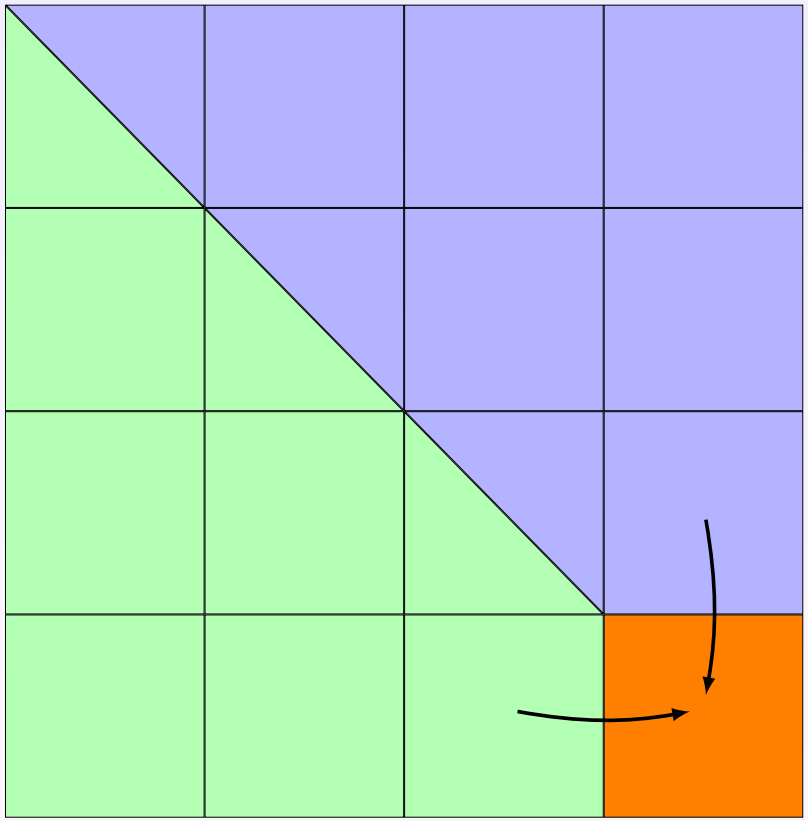

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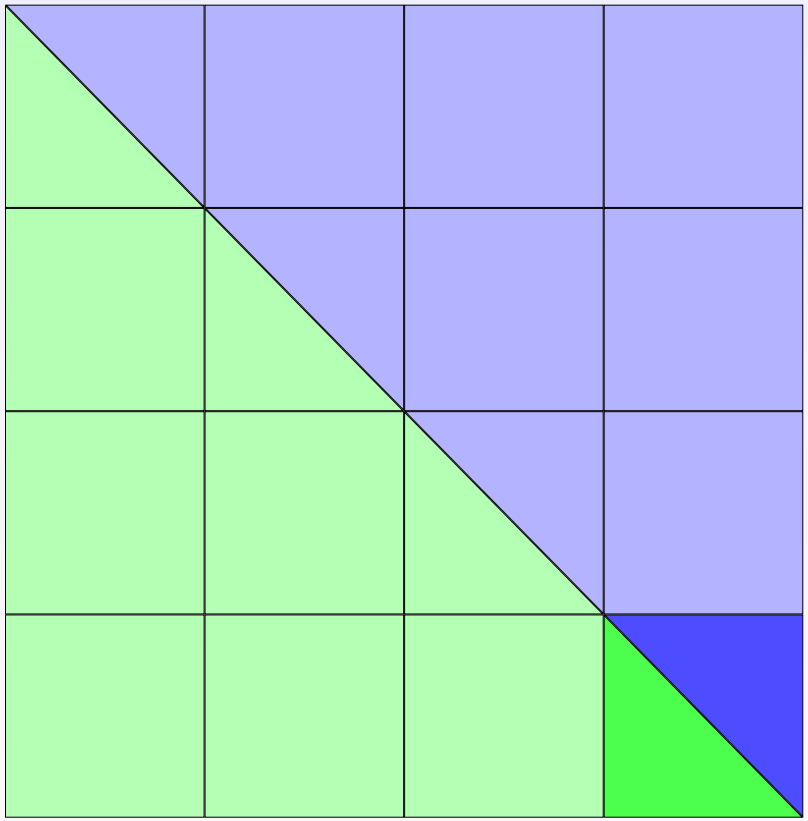

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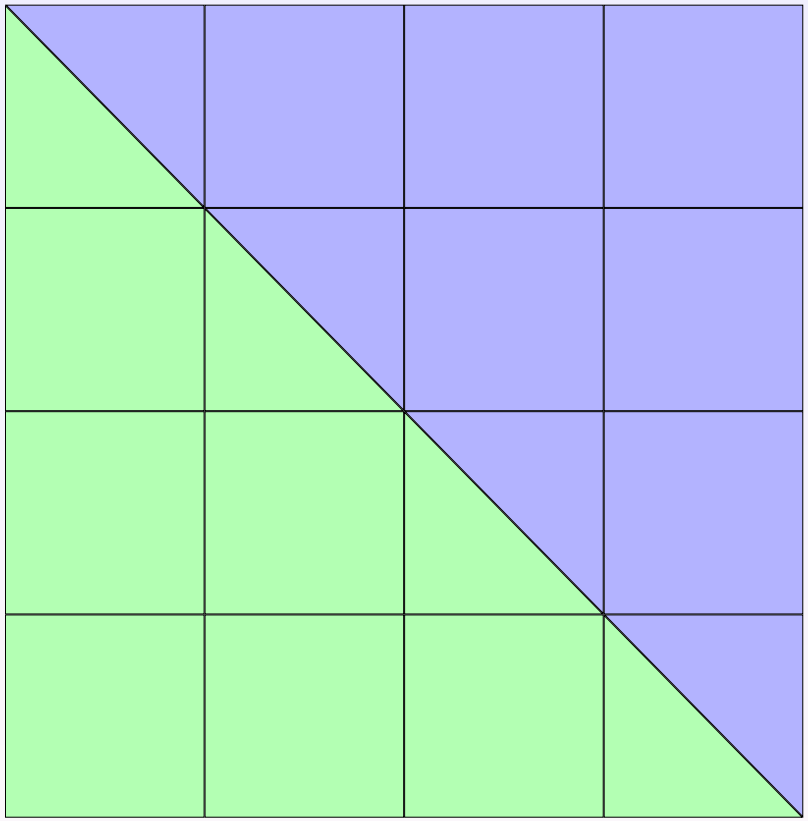

Open Questions

Scheduling: How can we employ multiple processors?

Data locality: How can we reduce data transfers between remote memory segments? How can we take advantage of caches?

Dynamic scheduling: Can we avoid setting up the entire (large) task graph prior to scheduling?

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