Technische Universität Braunschweig

Institute for Computational Mathematics

High Performance Block Incomplete LU Factorization

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Sparse Days @ Cerfacs 2017, Toulouse, September 8, 2017

Outline

- Motivation
- Block ILUs
- Setting Up and Improving the Block Structures
- Numerical Results
- Numerical Results — Symmetric Indefinite Case
- Conclusions

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  - solving large–scale sparse linear systems

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  where L, U^T unit lower triangular, D diagonal
- $Ax = b$: Iterative solution (preconditioned Krylov subspace method, e.g. PCG, GMRES,...)
- $\mathcal{D}(A^{-1})$: selectively invert LDU, supplemented with low-rank deflation using singular vectors

Motivation — Fast (approximate) *LU* Factorization

Modern sparse direct solvers (e.g. PARDISO, MA48, UMFPACK, MUMPS, SuperLU, ...) are hard to beat, they

- (may) improve diagonal dominance and reduce pivoting in advance
- use fill-reducing orderings
- apply combinatorial techniques to detect dense blocks (supernodes/multifrontal) [Duff,Erisman,Reid'17]
- make heavily use of dense matrix kernels (level–3 BLAS, LAPACK)

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To compete with direct methods, ILUs should

- produce drastically less fill–in (ILUs in general with modest drop tolerance)
- compute robust factorizations (e.g. ILUPACK)
- make use of dense matrix kernels, if possible (that is what this talk is about)

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A Block Incomplete *LU* Factorization method

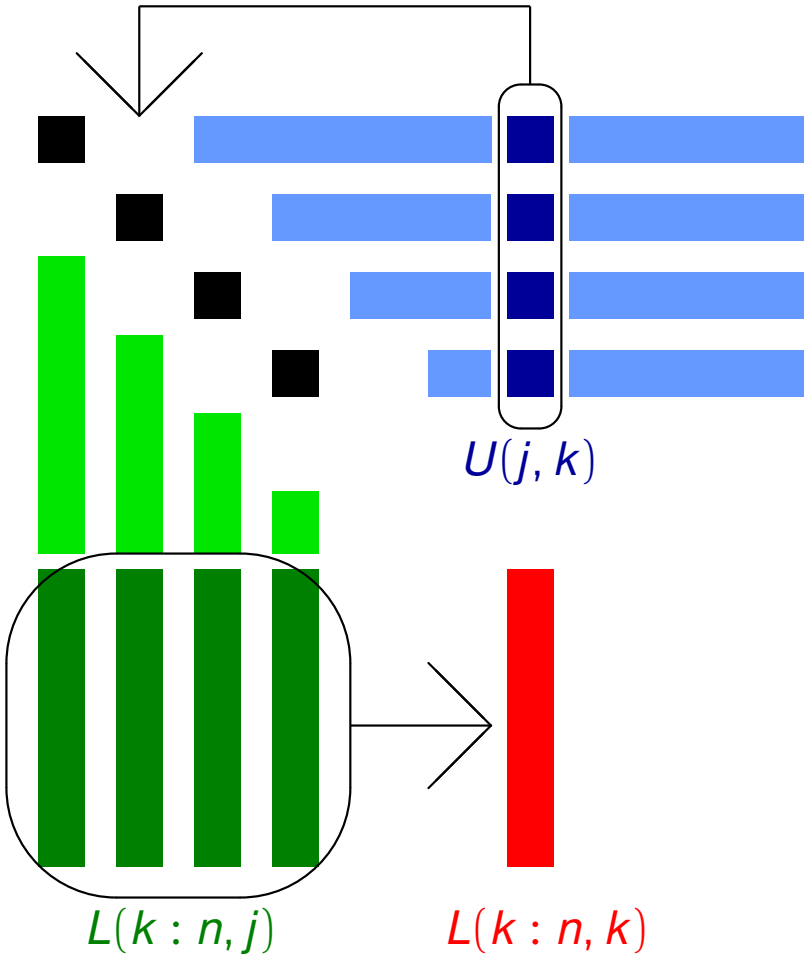
A generic meta block ILU approach

Suppose that some preprocessing has been done in advance:

- improve diagonal dominance by scaling and permuting the system matrix A
- reduce fill–in by using a fill–reducing method
- suppose that the (block) ILU will not break down
- suppose that an initial block structure is provided

$\longrightarrow$ (block) ILU with no worries

Basics: the Crout ILU



Basics: the Crout ILU for Sparse Matrices

Suppose that A is sparse.

- initially, $L(k:n,k)$ is sparse
- downdating $L(k:n,k)$ can be implemented efficiently:
  - use a linked list to quickly discover those j such that $U(j,k) \neq 0$ are required
  - `AXPY`-like operation in sparse mode
- dropping and scaling is cheap
- hopefully, $L(k:n,k)$ remains sparse after all
- analogous arguments apply to U

The Crout Block ILU

- replace scalars by blocks in the Crout ILU
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- diagonal blocks stored as dense matrices
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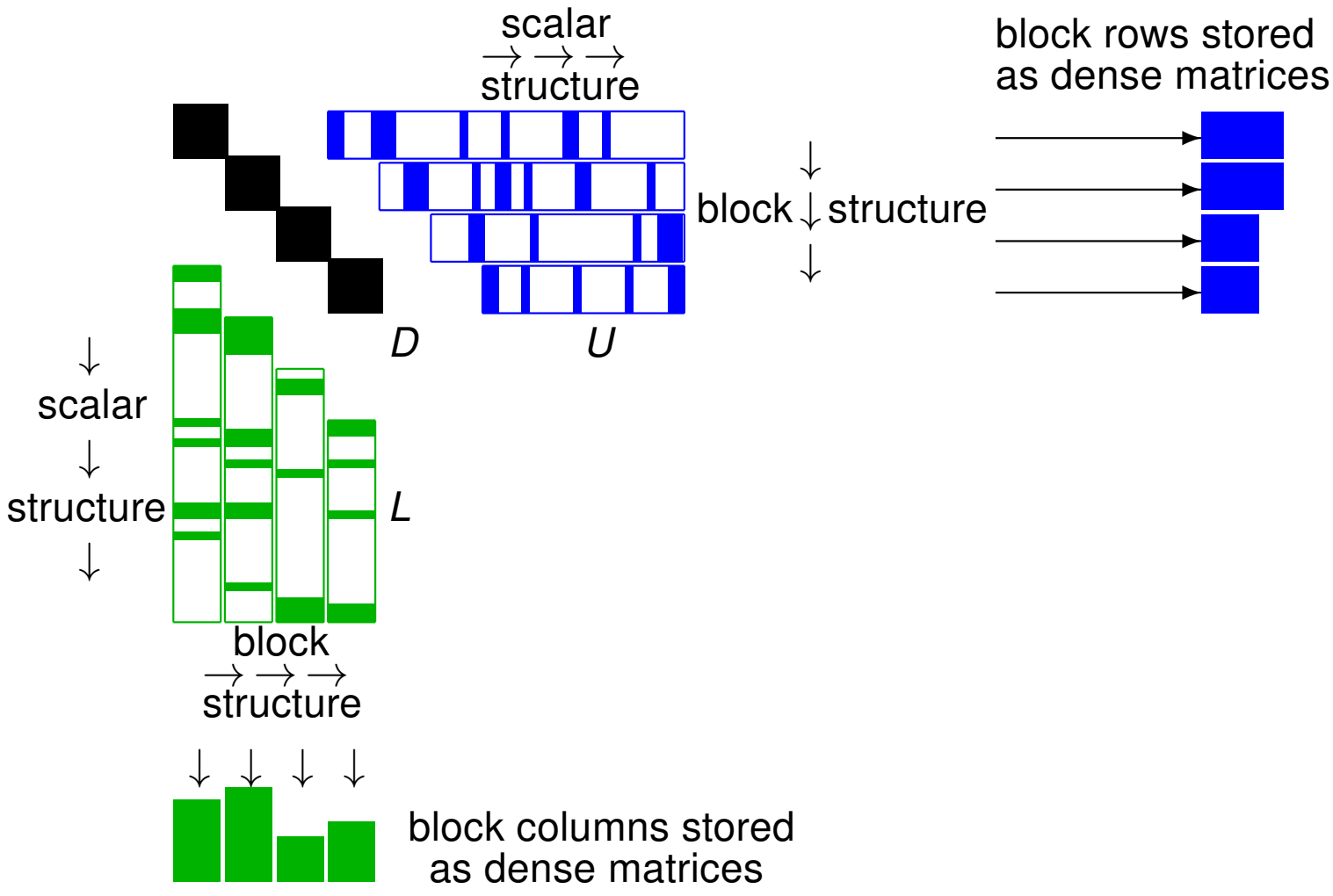
  - L: $\rightarrow$ block columns, $\downarrow$ scalar rows
  - U: $\downarrow$ block rows, $\rightarrow$ scalar columns

The Crout Block ILU



The Crout Block ILU

- dropping: $\|L(i,k) \cdot L(k,k)^{-1}\| \leqslant \tau$
  $\|U(k,k)^{-1} \cdot U(k,i)\| \leqslant \tau$
- downdating: $L(k:n,k) \leftarrow L(k:n,k) - L(k:n,j) \cdot U(j,k)$
  1. `gather` from $L(k:n,k)$
  2. use dense matrix kernel (level–3 BLAS `GEMM`)
  3. `scatter` back to $L(k:n,k)$

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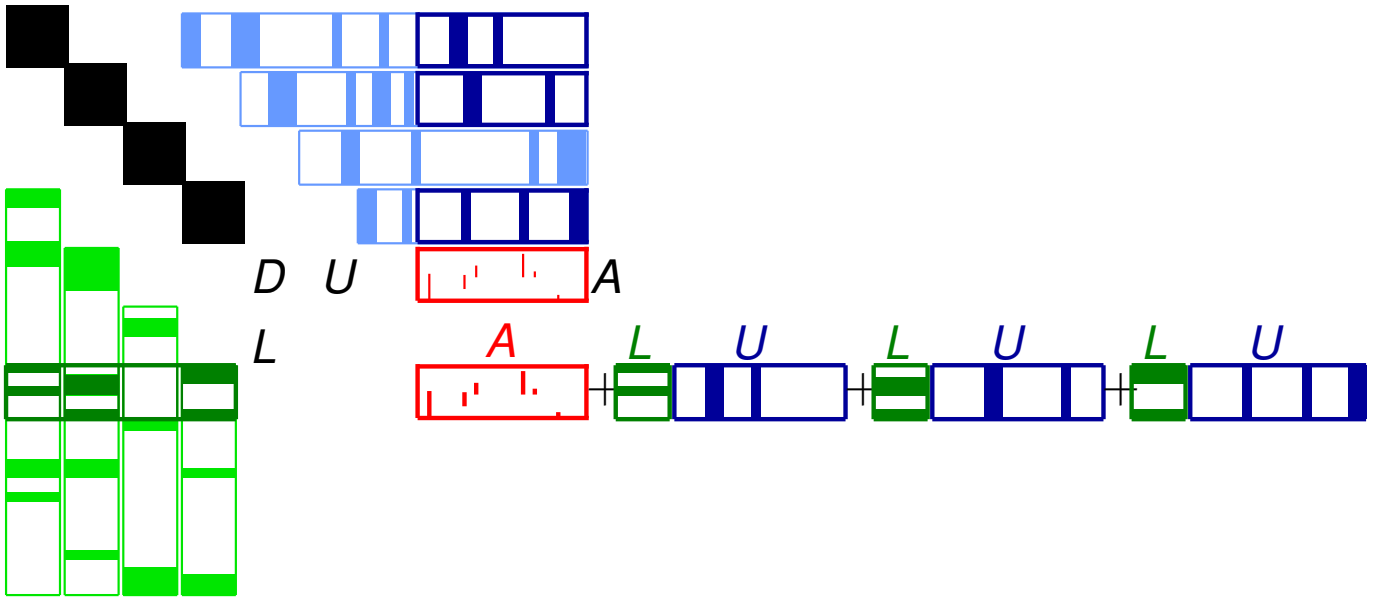

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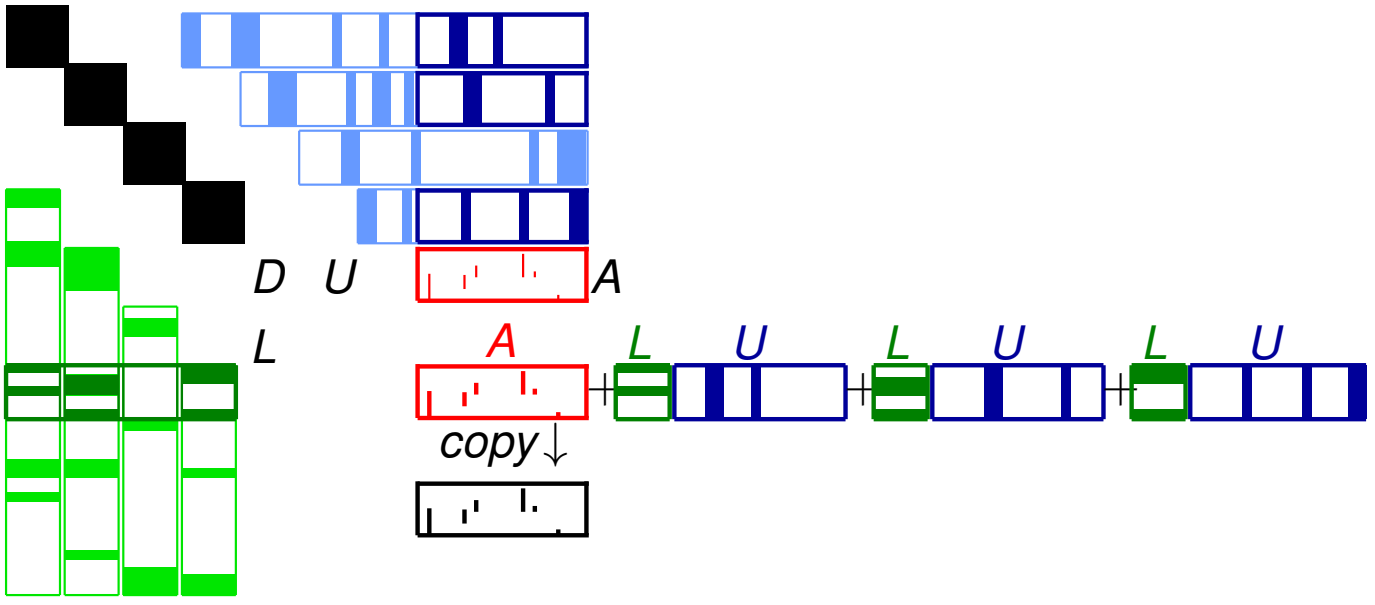

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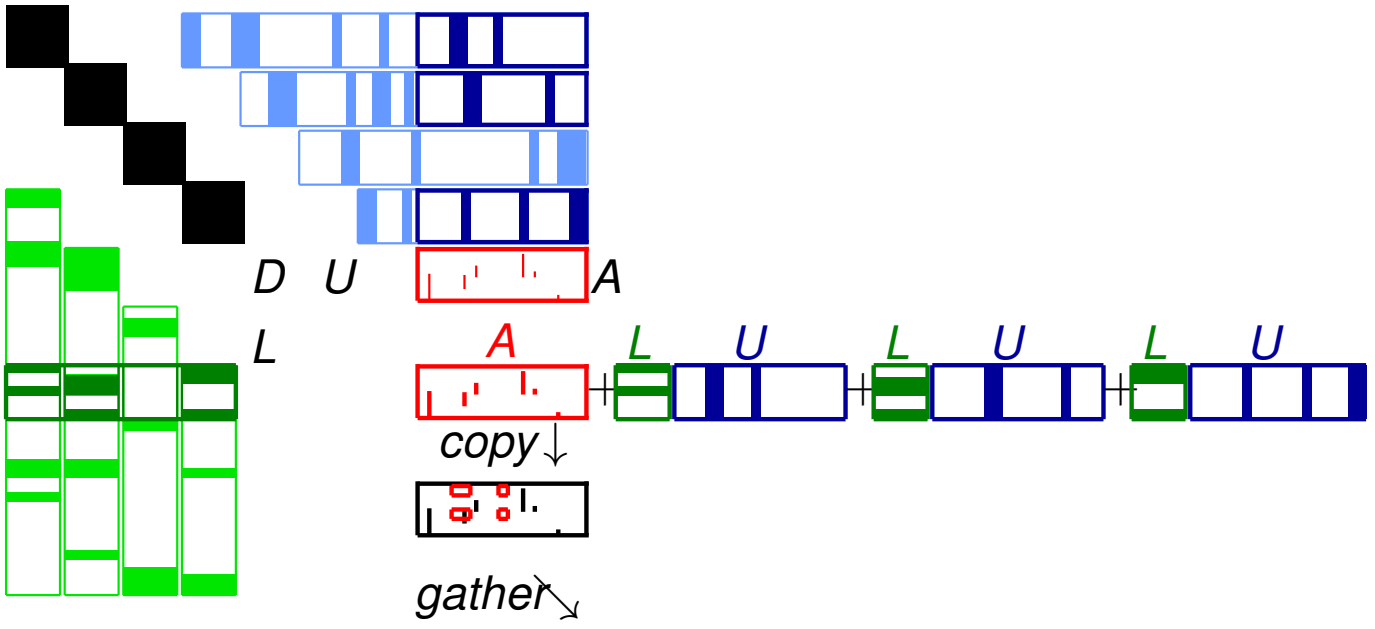

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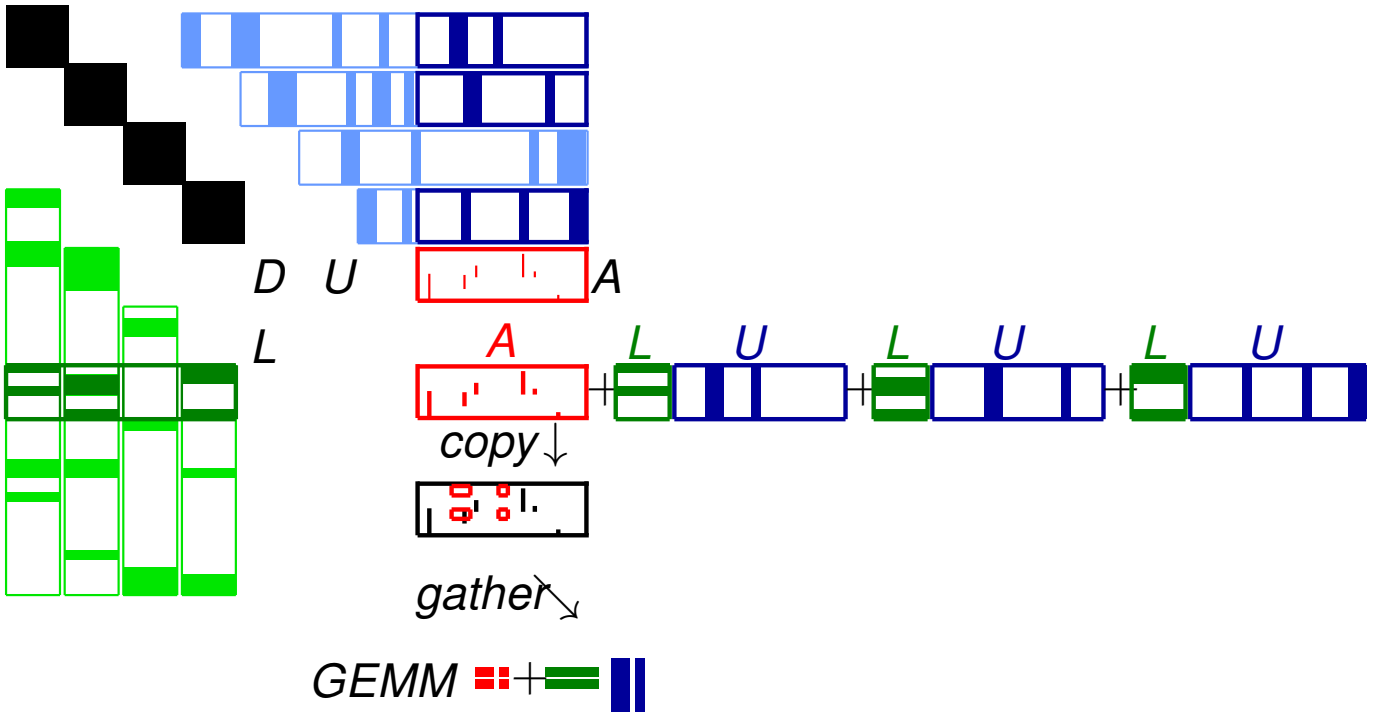

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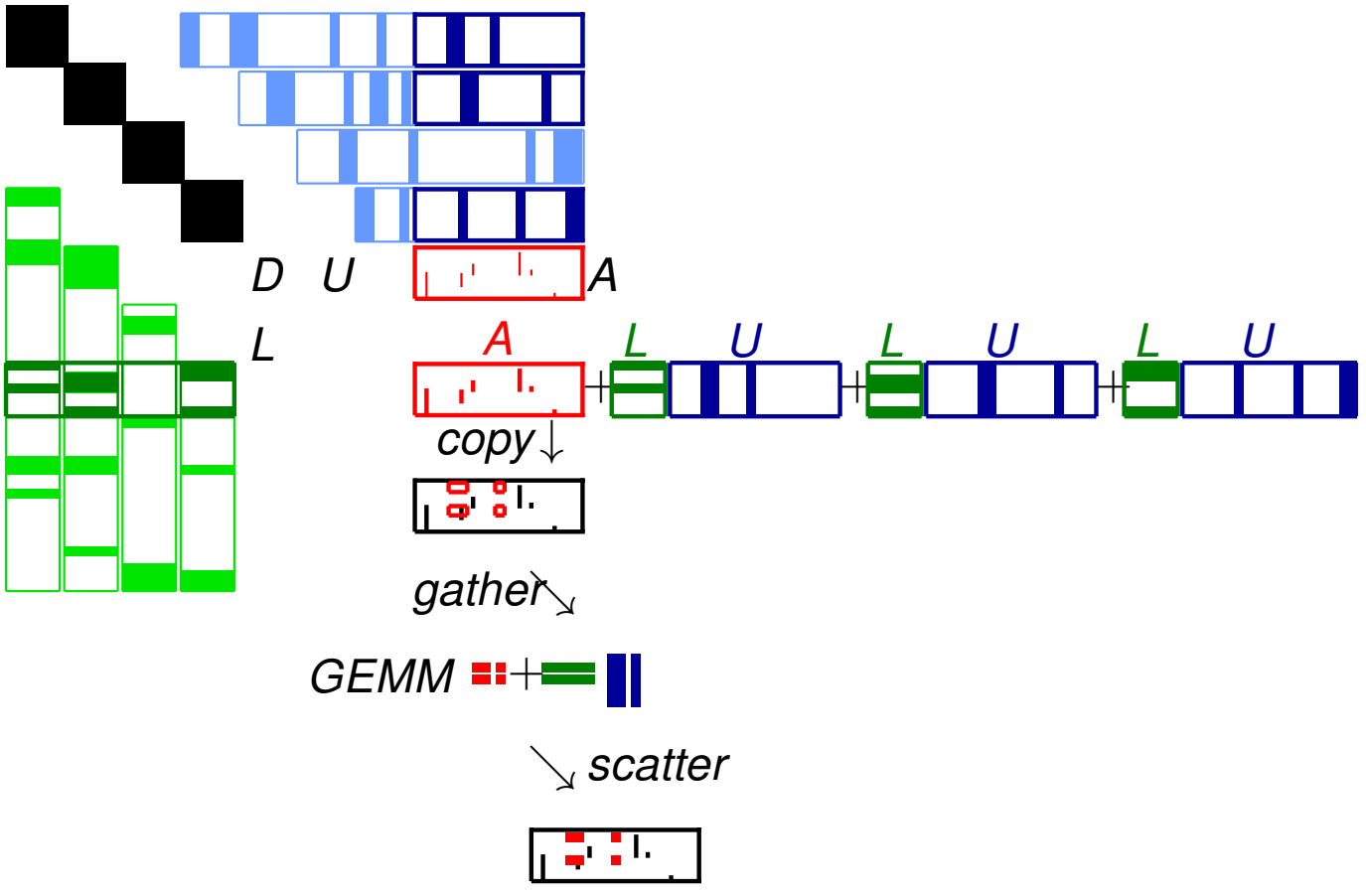

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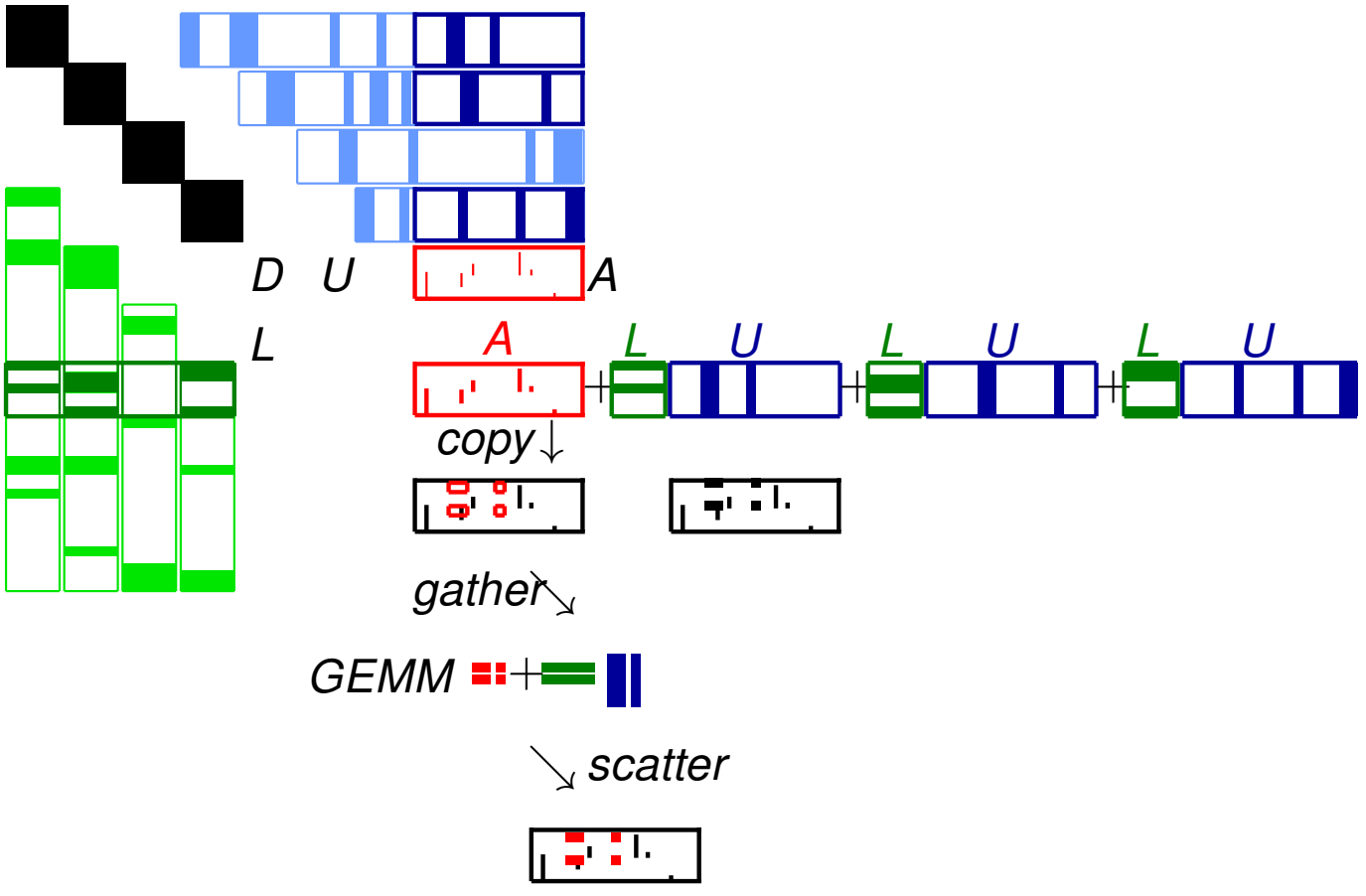

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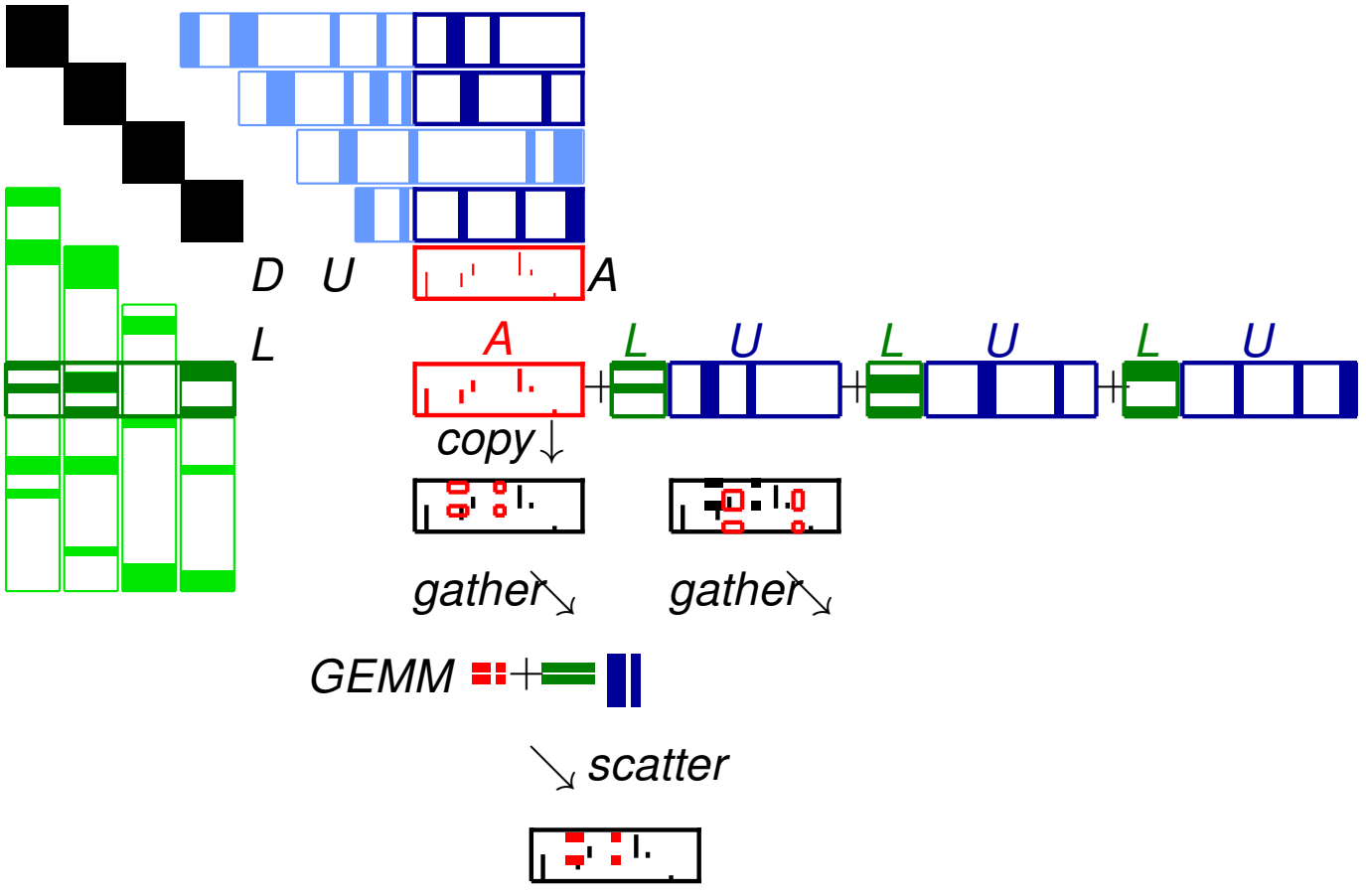

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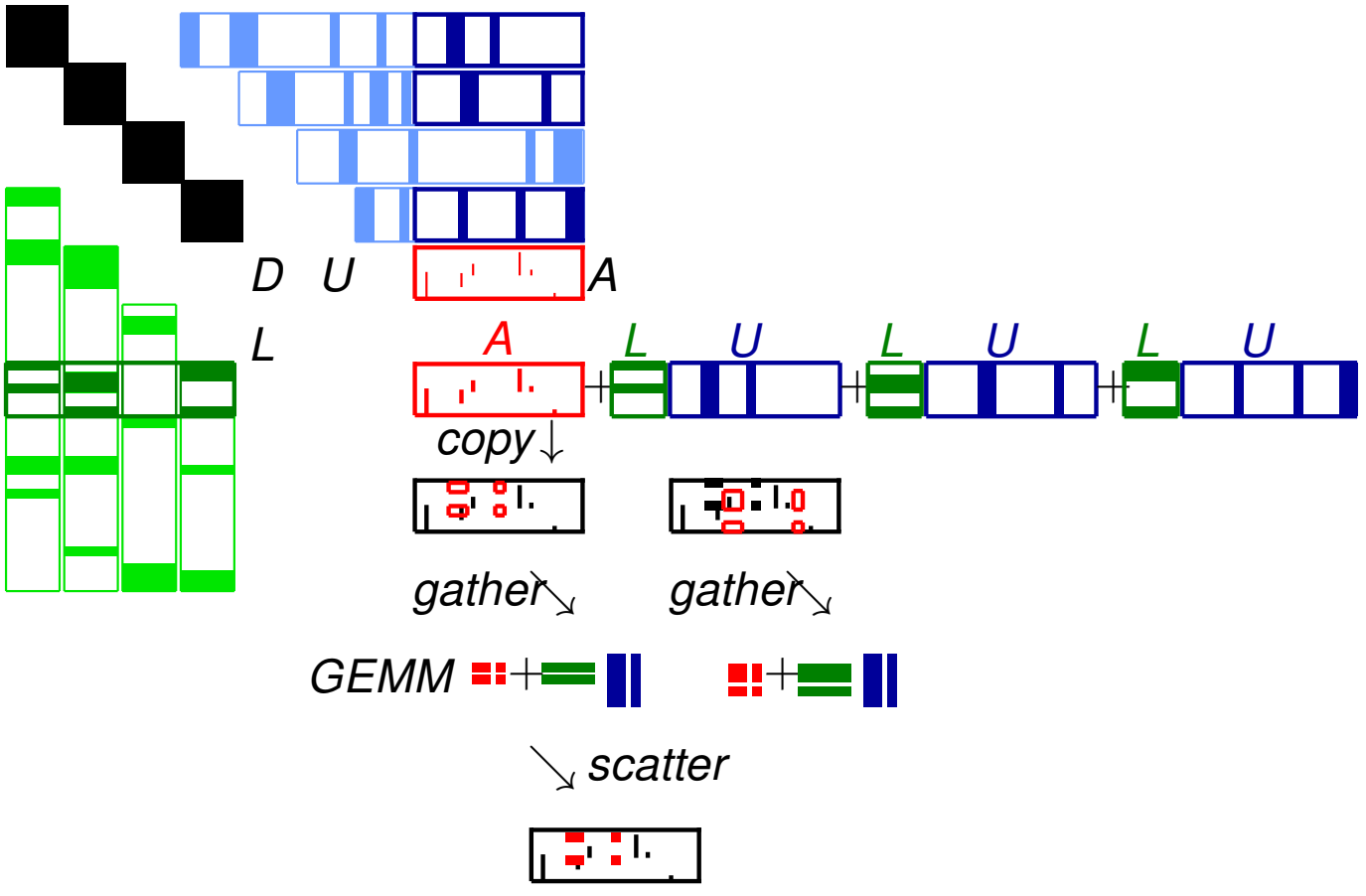

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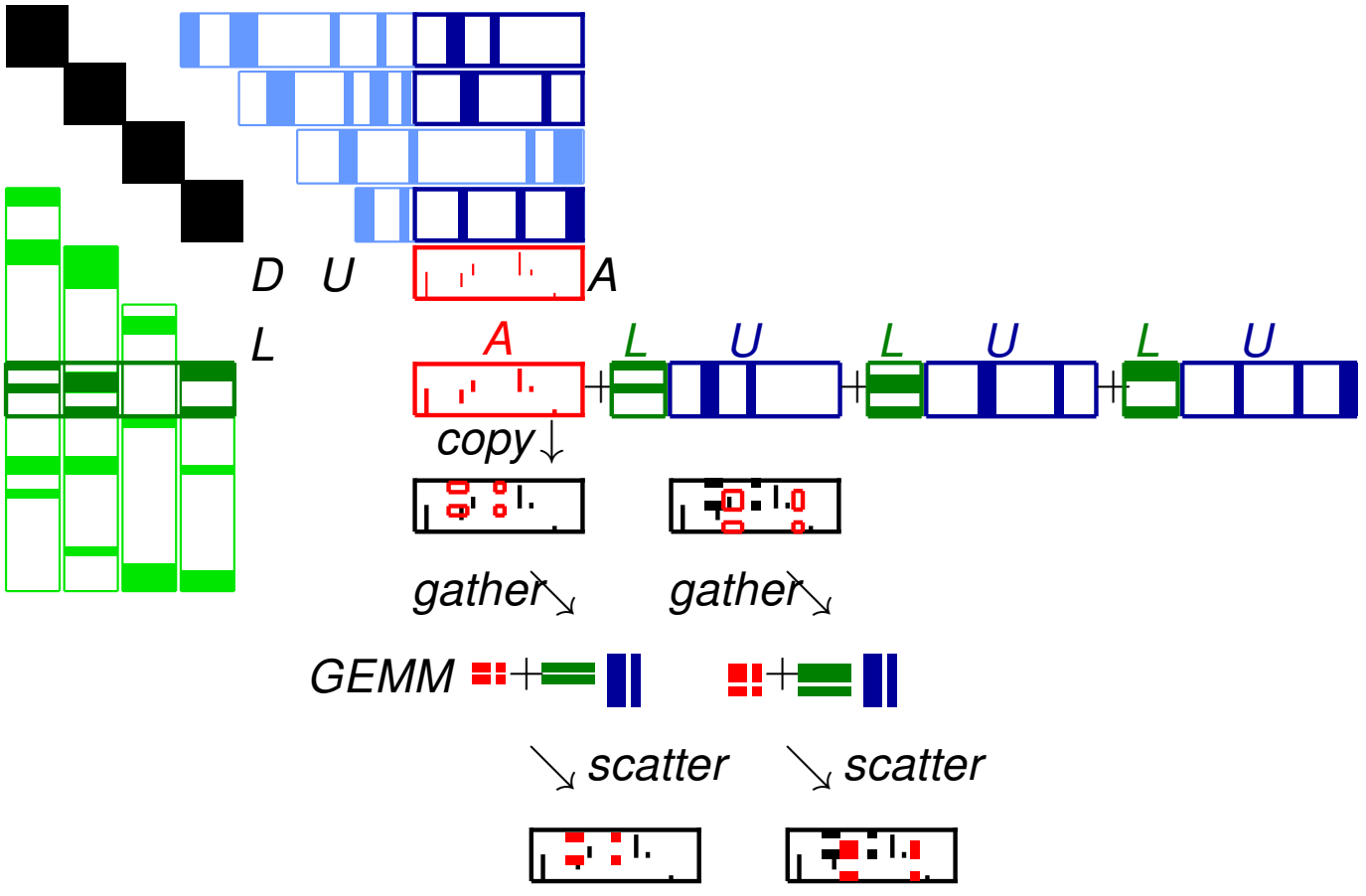

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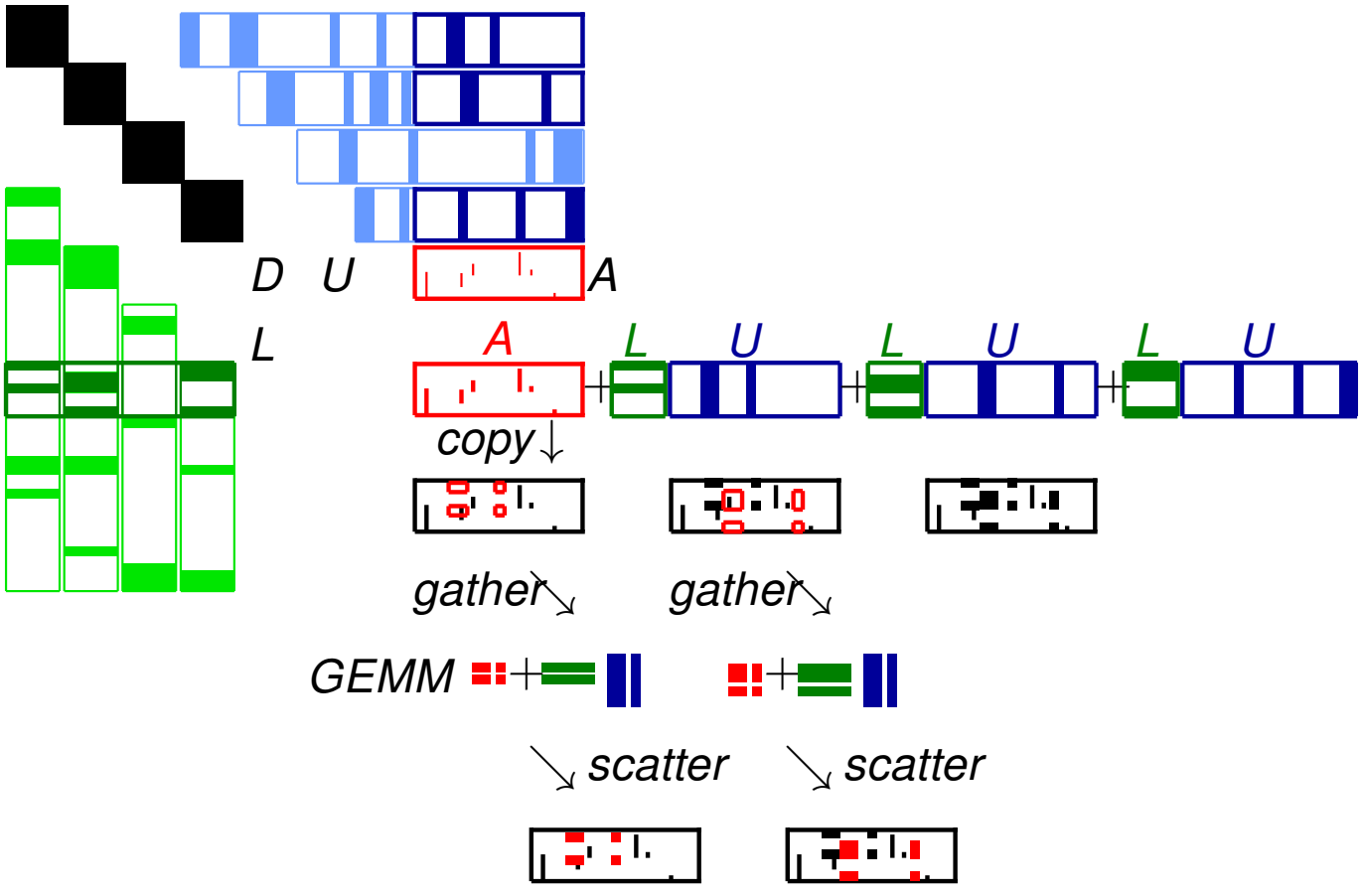

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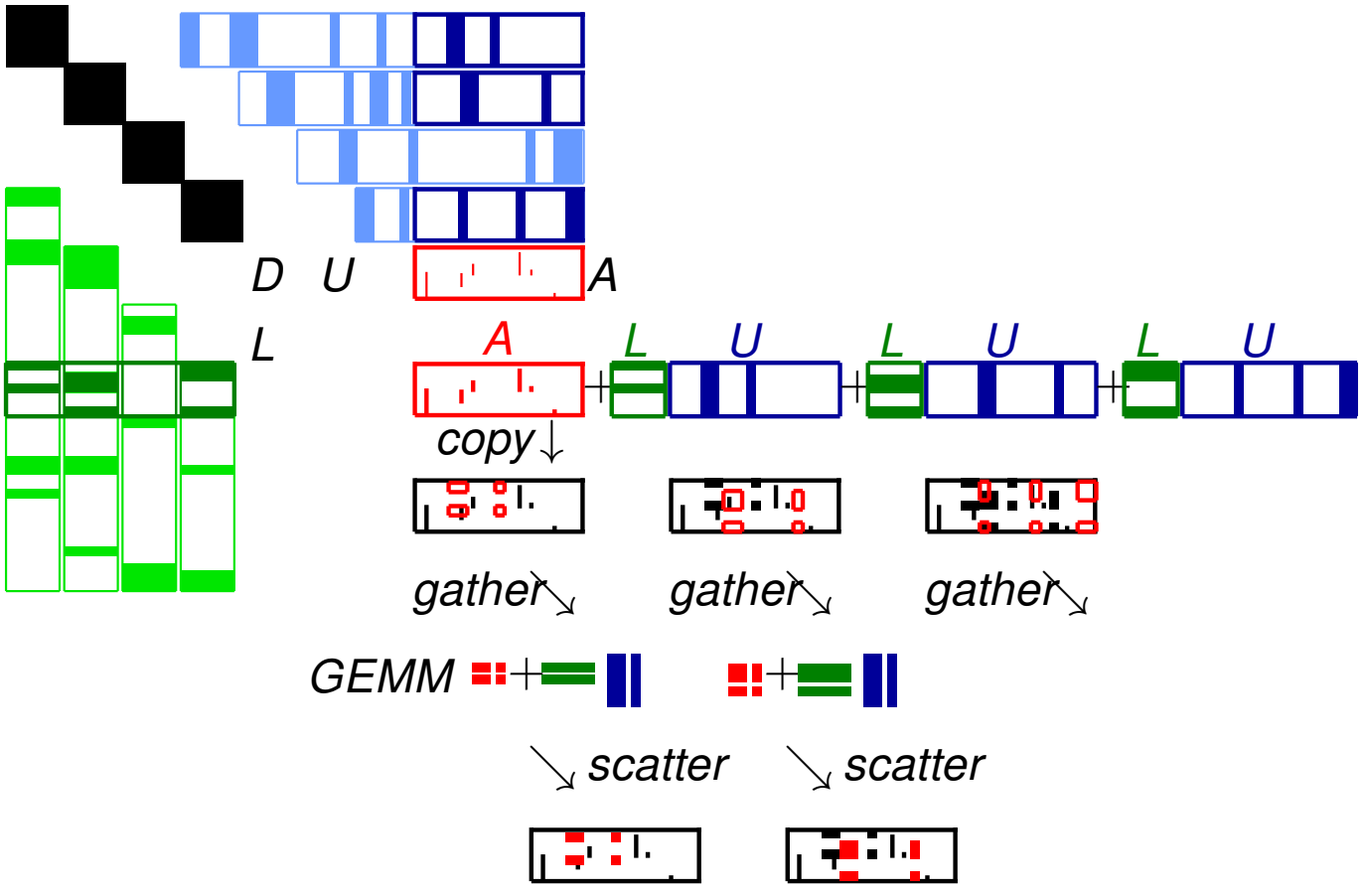

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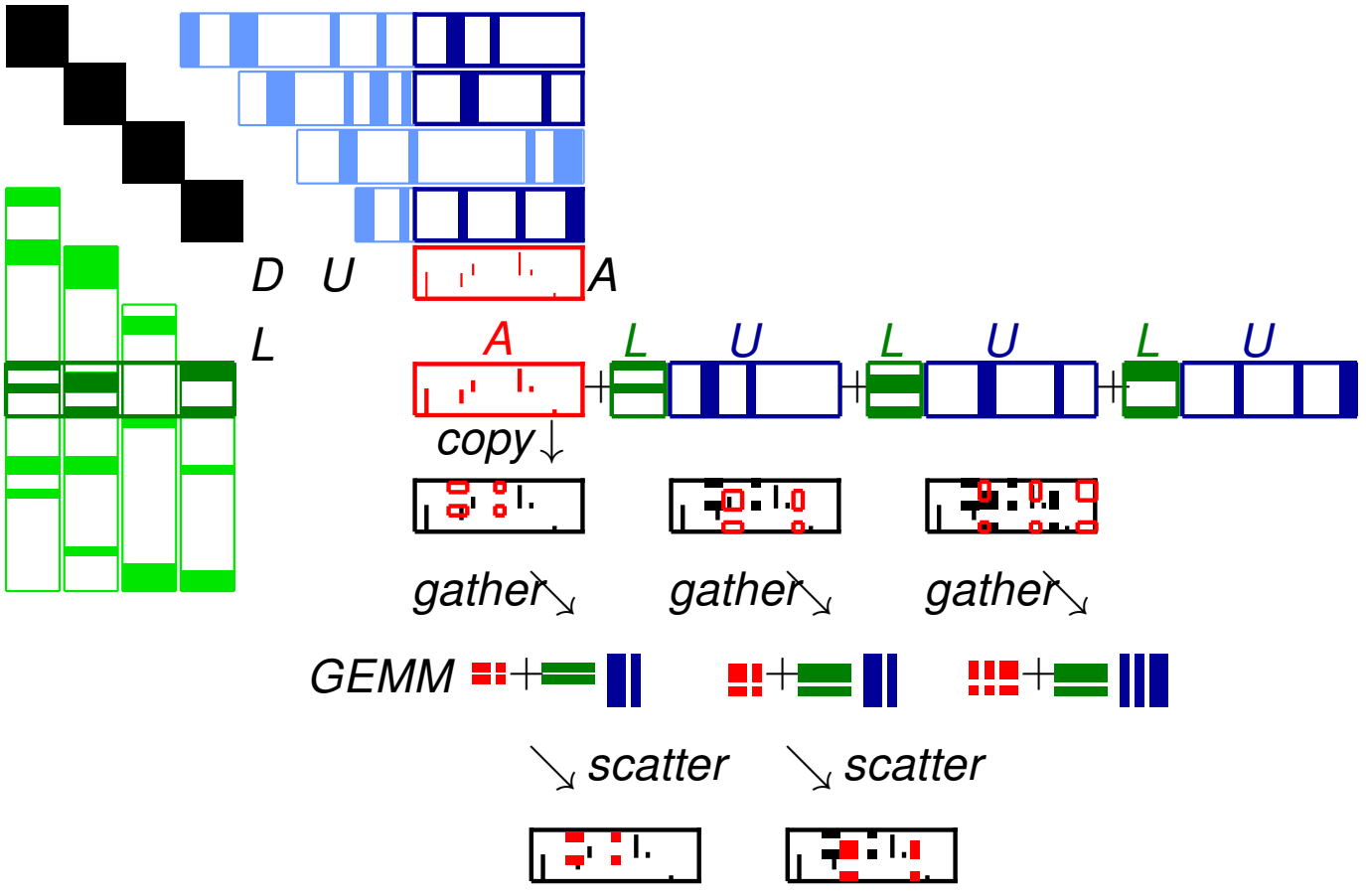

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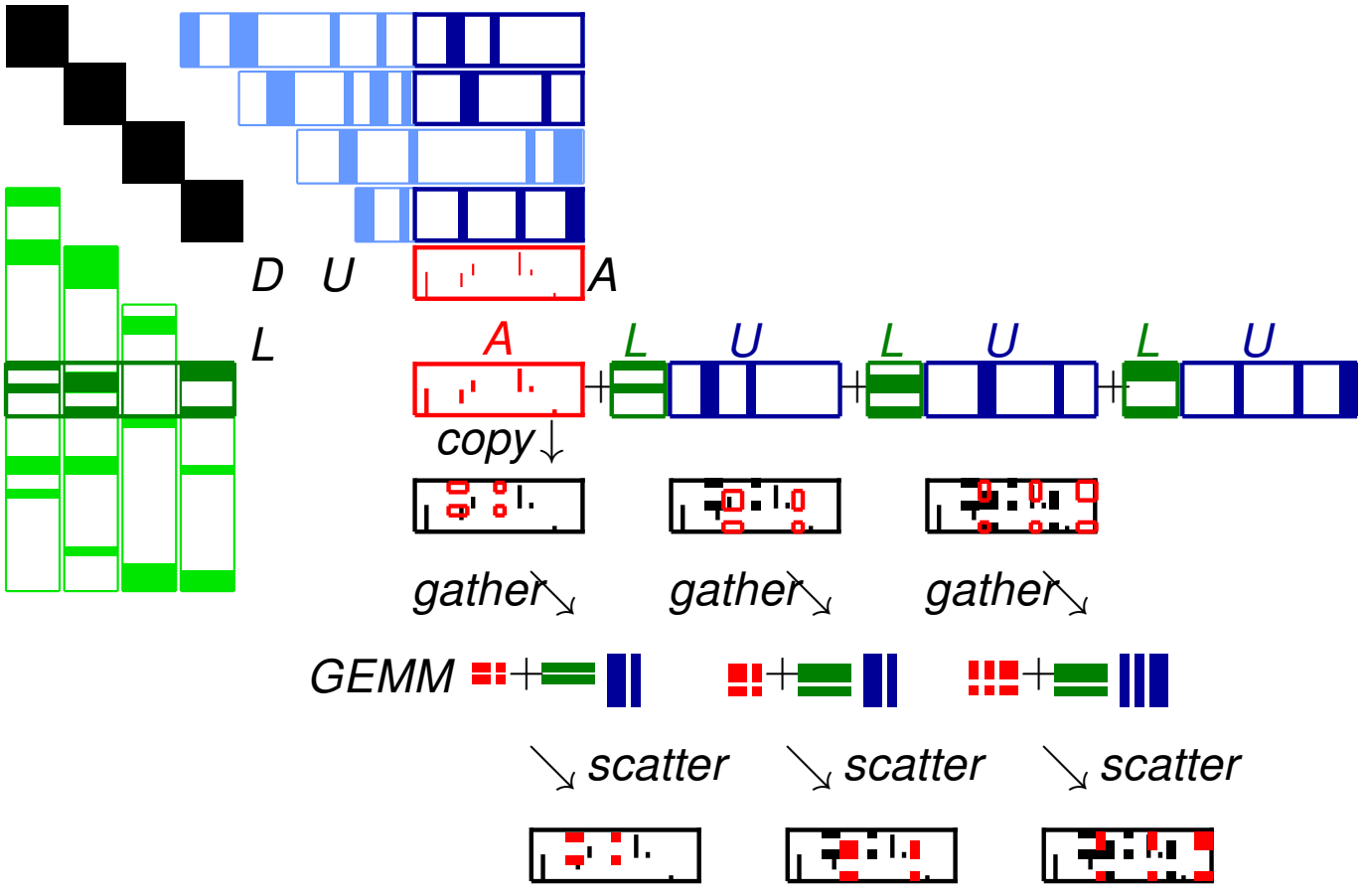

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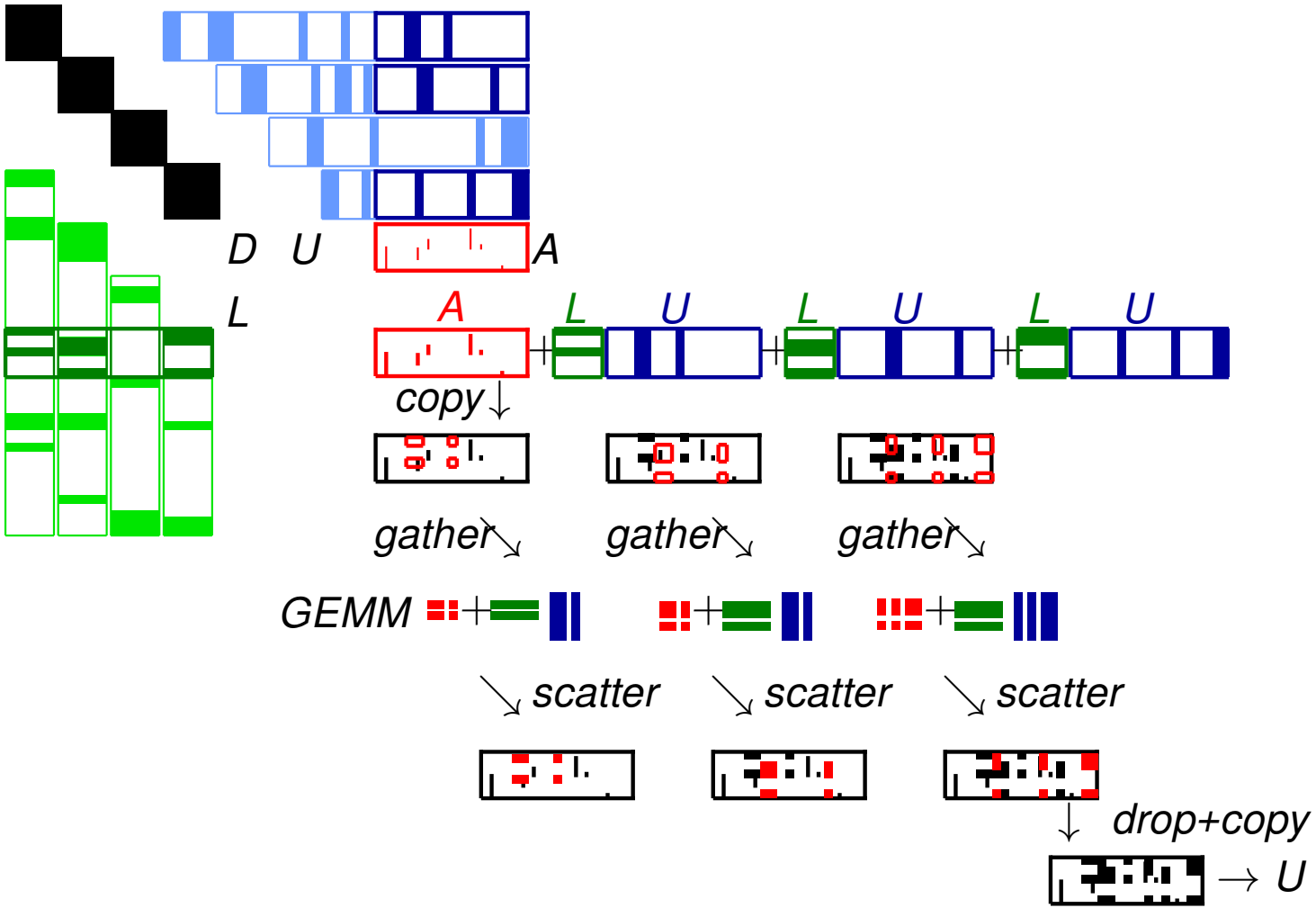

The Crout Block ILU

- downdating performed in two passes
  1. first pass: set up and merge nonzero index list for $L(k:n,k)$ (resp. $(U(k,k:n))$
  2. second pass: downdate $L(k:n,k)$
- As much as possible: multithreaded Intel MKL is used
  1. BLAS (level 1, 2 and 3)
  2. LAPACK
  3. gather, scatter
  4. sparse `dot` and `axpy`
- level–3 BLAS update used whenever sensible, scatter/gather skipped whenever possible
- scalar update bypasses level–3 BLAS and uses sparse `axpy` instead (similar bypasses for rank–1 update and blocks of small size)

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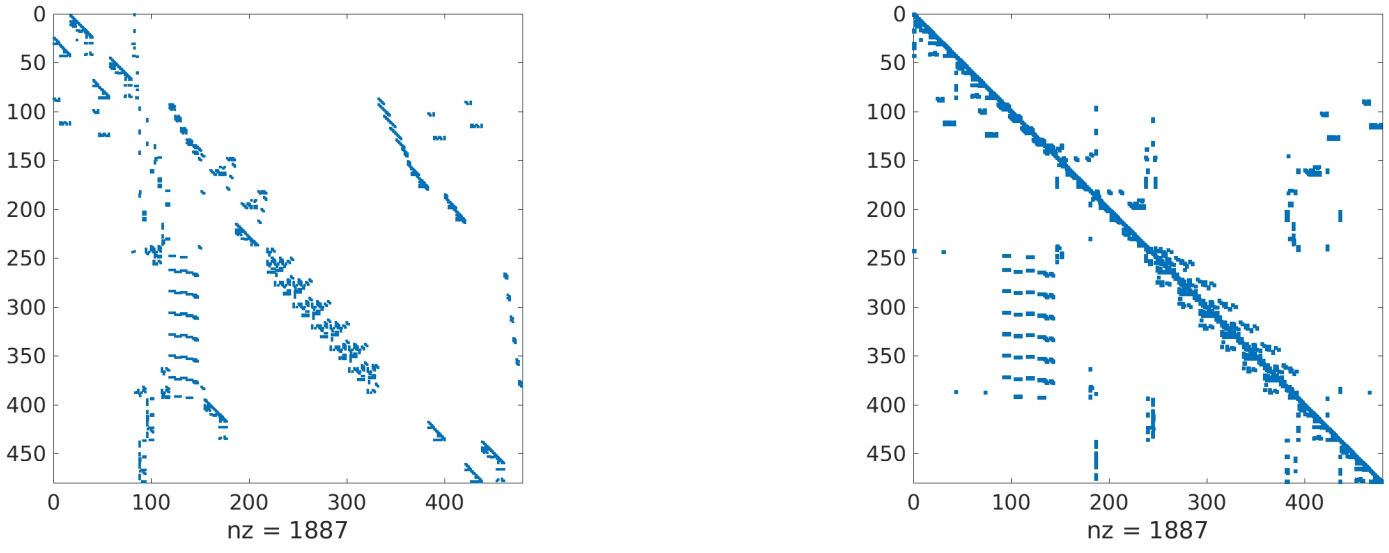
Maximum Weight Matchings

Maximum weight matchings: combinatorial algorithm (MC64 [Duff ,Koster'99]) to improve the diagonal dominance

$$A \rightarrow D_l A D_r \Pi$$

D_l, D_r diagonal scalings, Π permutation



initial matrix versus permuted and rescaled matrix

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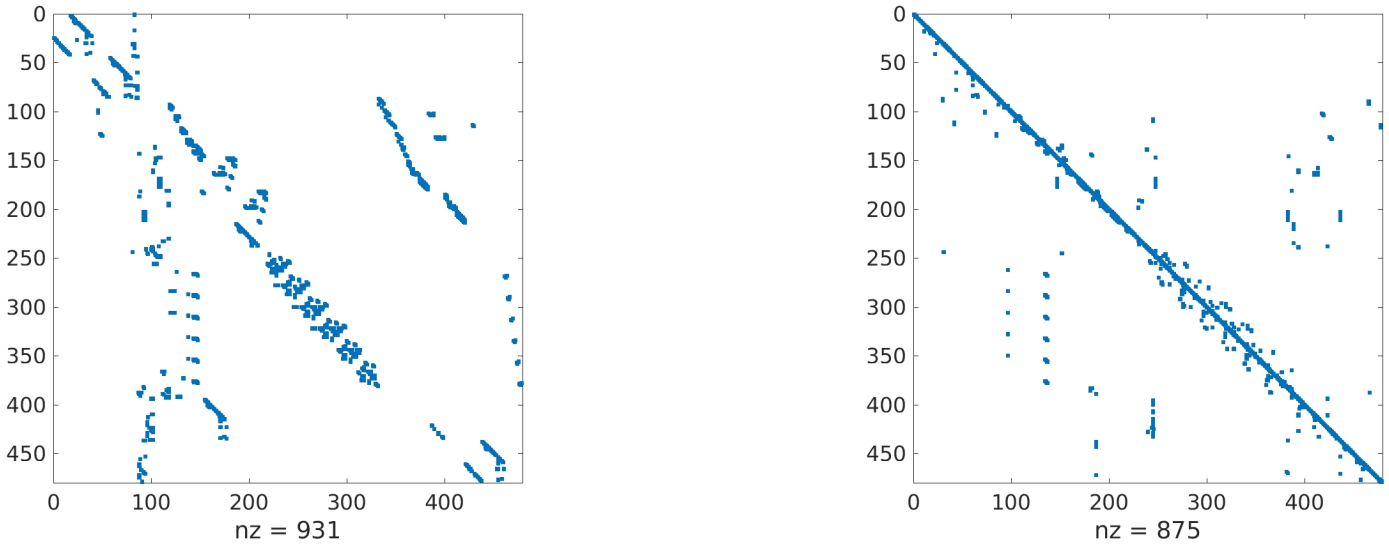

largest entries in modulus: initial matrix versus permuted and rescaled matrix

Cosine–Based Blocking

Idea: merge rows to block rows the their pattern is similar [Saad'03]

$$C := \text{pattern}(A),\ C = \begin{bmatrix} c_1^T \\ \vdots \\ c_n^T \end{bmatrix}$$

rows c_i^T and c_j^T are considered to have a similar pattern if

$$\frac{\|c_i\|_2 \cdot \|c_j\|_2}{c_i^T c_j} \geqslant \tau,\ \text{e.g.,}\ \tau = 0.8$$

- ratio refers to cosine of the angle between two rows
- integer–based algorithm (only counting)
- extremely fast if AA^T is sparse as well, otherwise simplifications required
- not always usefull

Cosine–Based Blocking — Example

sample matrix A (**venkat50**) from the SuiteSparse Matrix Collection.

- size $n = 62'424$, $nz = 1'717'777$ nonzero entries (approx. $\frac{nz}{n} = 27.5$ nonzeros per row/column)
- system arises from the discretization of the 2D compressible Euler equations. (velocity u, v, pressure p, density ρ)

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1. initially apply maximum weight matching (scalings+permutation)
2. apply cosine–based blocking.

system size	# dgl. blocks	max. size	avg. size	std. deviation
$62'424$	$15'723$	4	3.97	0.297

Fill–Reducing Symmetric Orderings

$$A \rightarrow P^T AP, \;\; P \text{ permutation}$$

- standard permutation routines to reduce the fill–in, e.g. approximate minimum degree [Amestoy,Davis,  '96], nested dissection [Karypis,Kumar'98], [LaSalle,Karypis'13] ...
- cosine–based blocking is preserved (apply permutation to the compressed graph)

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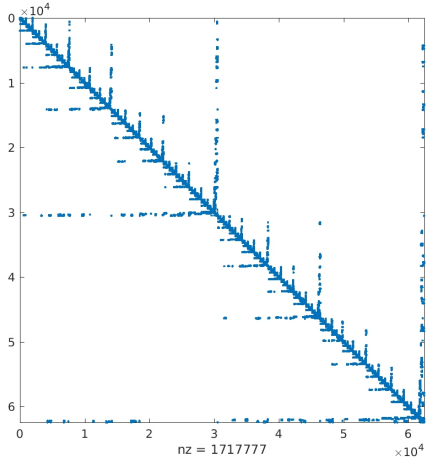

Matrix **venkat50** after maximum weight matching, cosine–based blocking and (MT-)METIS reordering based on the compressed graph

Block Pattern via Simplified ILU

- direct solvers build their blocks using combinatorial methods (elimination tree, supernodes)
- often these block structures are too big/too dense for ILUs.
- instead use a simplified quick–&–dirty ILU to guess a larger block pattern.

  rough idea: locally use ILU(1), i.e., roughly perform ILU on the pattern of A^2 with some drop tolerance τ and detect denser blocks
  $\longrightarrow$ ILU(1,τ)–blocking

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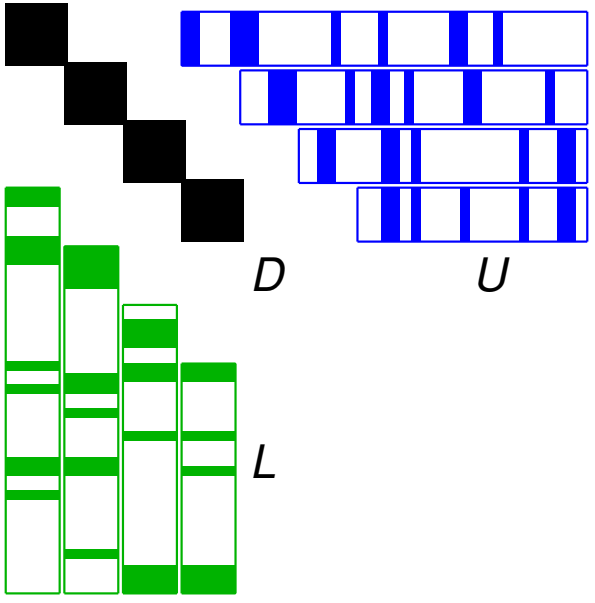
sample matrix A (**venkat50**)

	# blocks	max. size	avg. size	std. deviation
only cosine	15′723	4	3.97	0.297
only ILU(1,10^{-2})	24′138	16	2.59	2.15
cosine+ILU(1,10^{-2})	13′786	16	4.53	1.50

Progressive Aggregation

- improve block size during the factorization
- merge two consecutive block columns/row, when the additional fill is small



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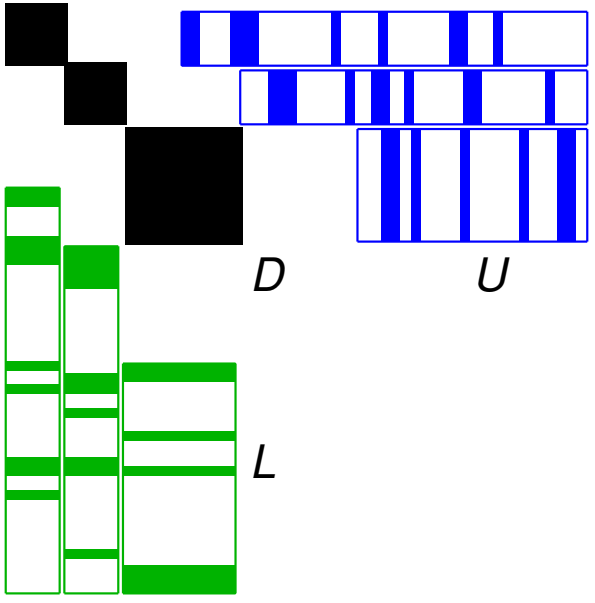

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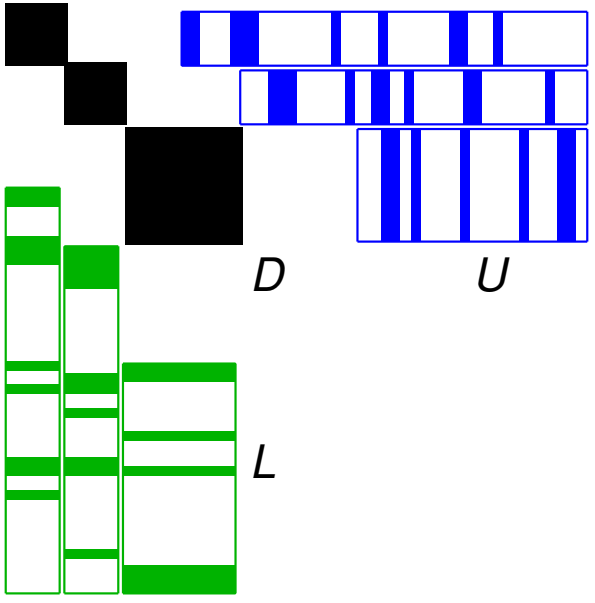

	# blocks	max. size	avg. size	std. deviation
cosine	15′723	4	3.97	0.297
ILU(1,10^{-2})	24′138	16	2.59	2.15
progr. aggr.	32′996	13	1.89	1.59
cosine+ILU(1,10^{-2})+progr.	8′259	44	7.56	5.23

Combined Approach

Sample matrix A (`venkat50`)

- use scalings + permutation by maximum weight matching (MC64[ ,Koster'99])
- use nested dissection (MT-METIS)
- iterative solution by GMRES(30)[Saad,Schultz'86], preconditioned by block ILU ('B ILU')

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blockings

- cosine-based 'c'
- ILU(1,τ)-based 'i'
- progressive aggregation 'p'

$\longrightarrow$ B ILU(cip), B ILU(c--), ...

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	time ILU[sec]	$\frac{nz(L+U)}{nz(A)}$	time GMRES[sec]	# steps
B ILU(c--)	1.9	4.3	3.0	29
B ILU(-i-)	3.9	4.0	4.0	31
B ILU(--p)	3.7	3.5	7.4	52
B ILU(cip)	1.9	4.9	2.3	26

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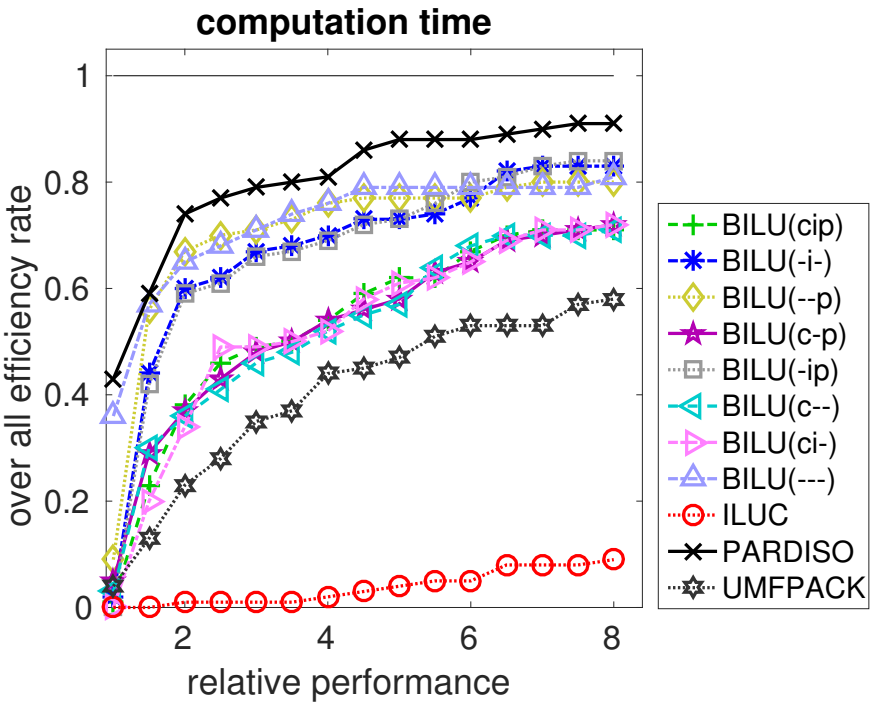
Numerical Results

- 1 TB main memory, 4 Intel Xeon E7-4880 v2 @ 2.5 GHz processors each of them having 12 cores on a socket leading to 60 cores in total.
- MATLAB R2015b as front end using Intel MKL 11.1/11.2
- Numerical methods
  - PARDISO, UMFPACK (as implemented in MATLAB)
  - B ILU(***) + GMRES(30) with relative residual of 10^{-6}
  - MATLAB's Crout ILU (referred to as "ILUC") + GMRES(30) with relative residual of 10^{-6}
- 100 matrices of size $\geqslant 10'000$ from the SuiteSparse Matrix Collection
- performance profile

Numerical Results — Performance Profiles



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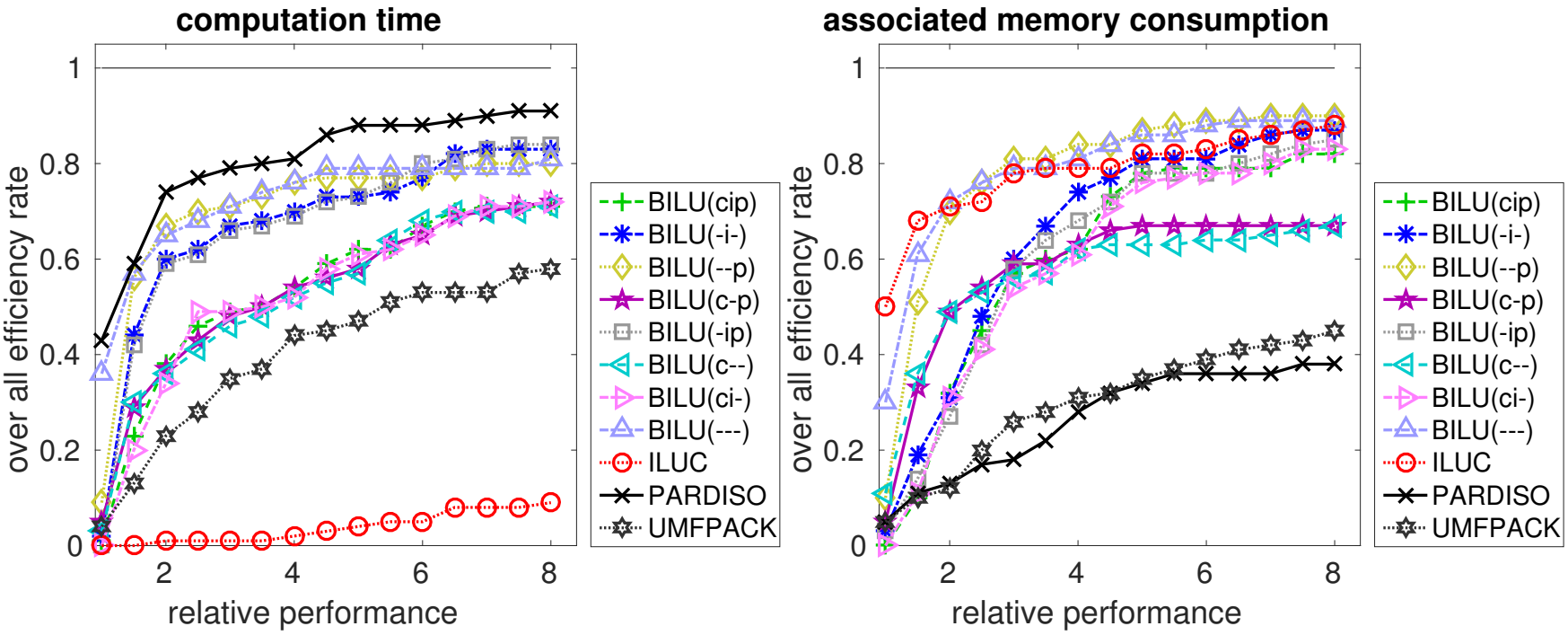
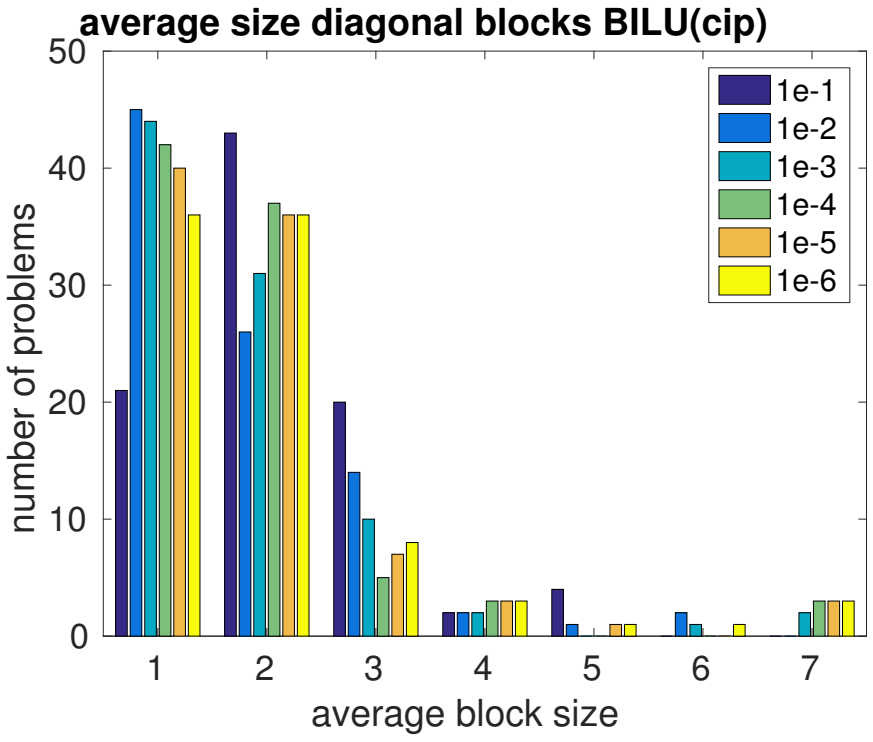


Numerical Results — Block Size of Diagonal Blocks



Average block size of B ILU(cip) depending on the drop tolerance.

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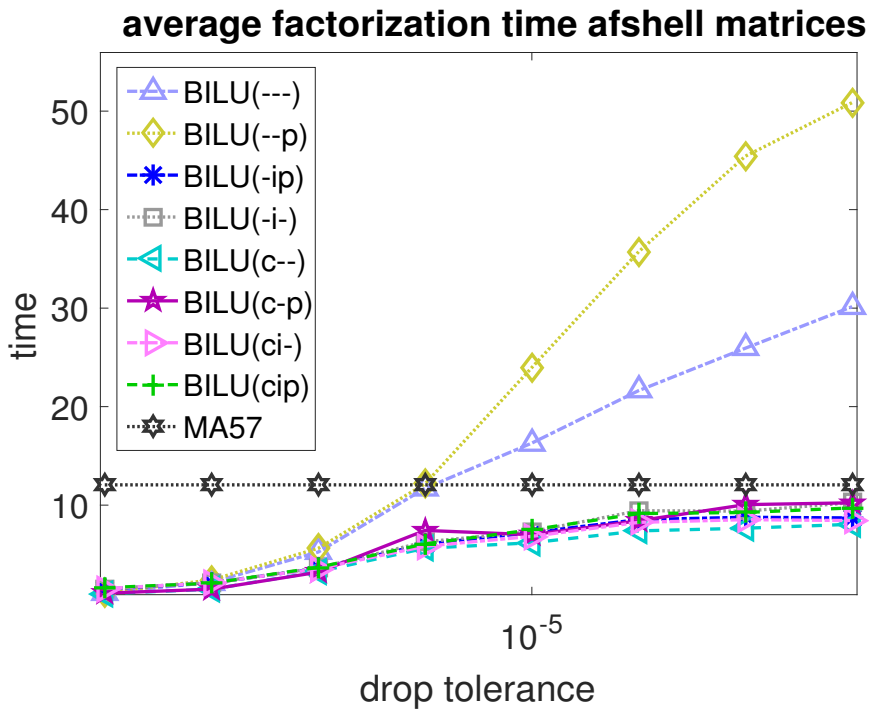
Setup Indefinite Case

- Symmetrized maximum weight matching [Duff,Pralet'05]
- symmetric reordering applied to the compressed graph (2×2 pivots are collapsed), e.g. (MT-)METIS, AMD
- apply symmetric indefinite variant of B ILU $\rightarrow$ B ILDL
- iterative solver simplified QMR [Freund,Nachtigal'95],[Freund,Jarre'97]
- use symmetrized version of blocking strategies (cosine, BILDL(1,τ), progressive aggregation)
- compare B ILDL with MA57 [

et al.] as implemented in MATLAB

Results Indefinite Case



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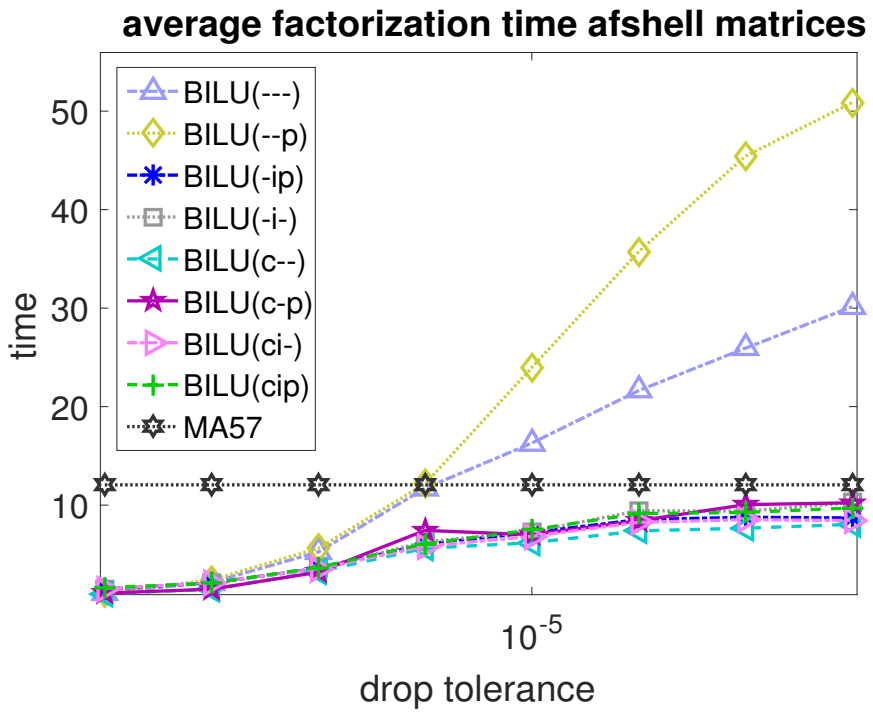
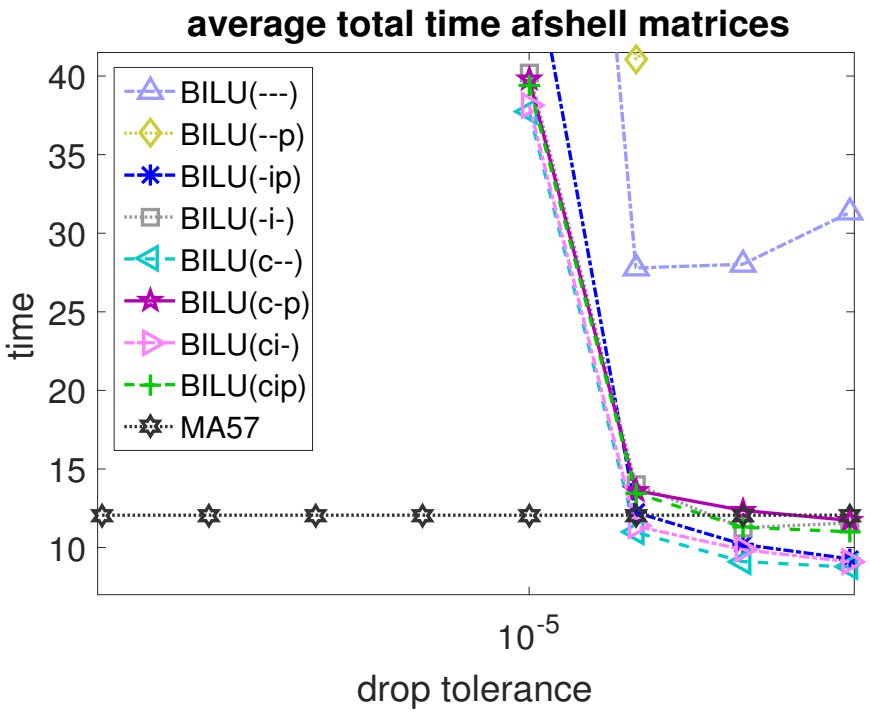
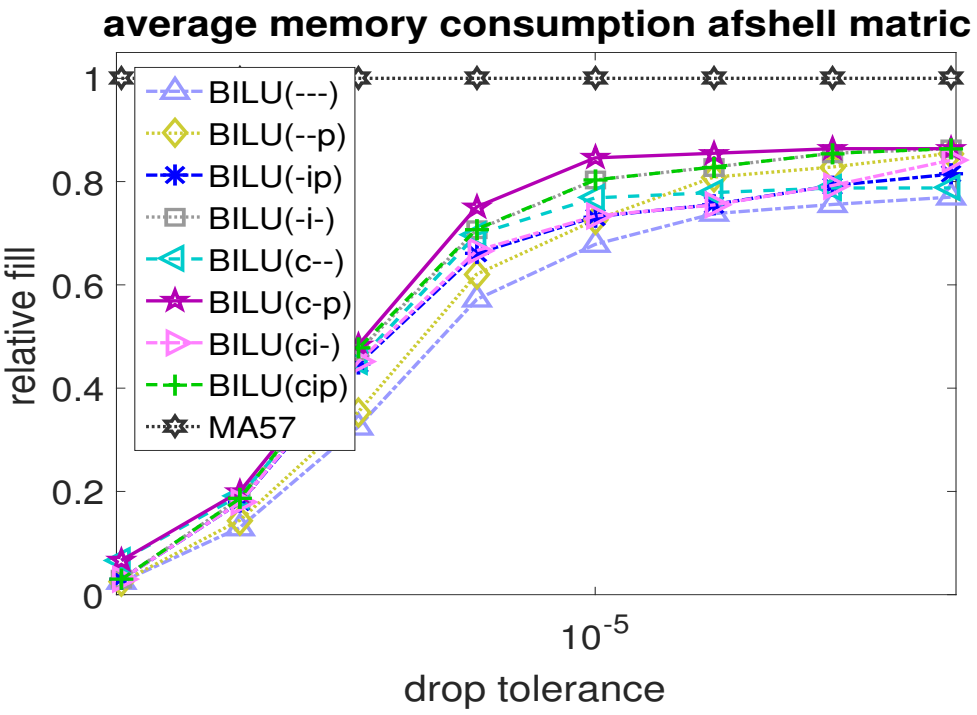




Results Indefinite Case



Outline

- Motivation
- Block ILUs
- Setting Up and Improving the Block Structures
- Numerical Results
- Numerical Results — Symmetric Indefinite Case
- **Conclusions**

Conclusions

- B ILU leads to a high performance ILU method
- major impact: efficient use of blocking strategies, level–3 BLAS and multithreading
- drawback: straightforward approach (no pivoting, just perturbations)
- general case (real/complex) and SPD case (real/complex), and symmetric indefinite case (real/complex) implemented
- used as template as part of an approximate selective inversion method and inside a large–scale sparse inverse covariance matrix estimation approach

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Epilogue

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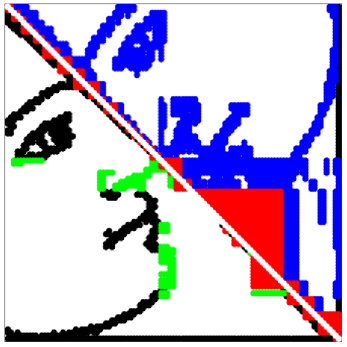

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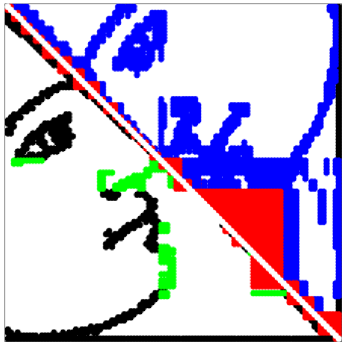

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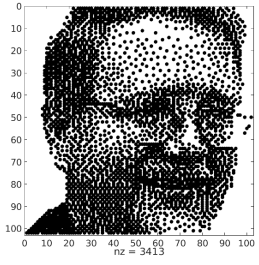

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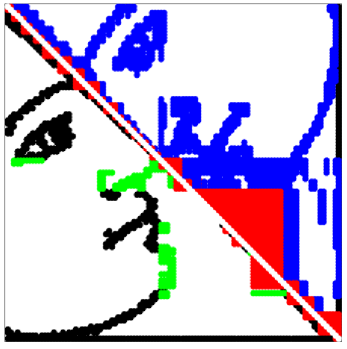

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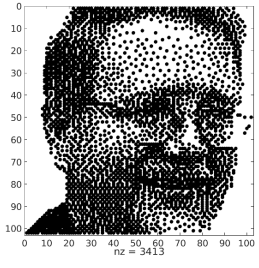

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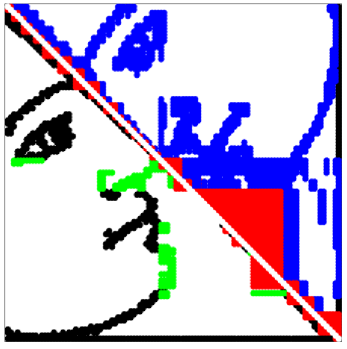

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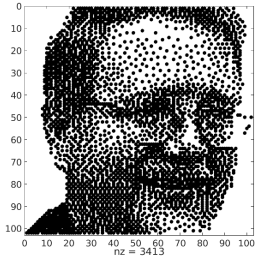

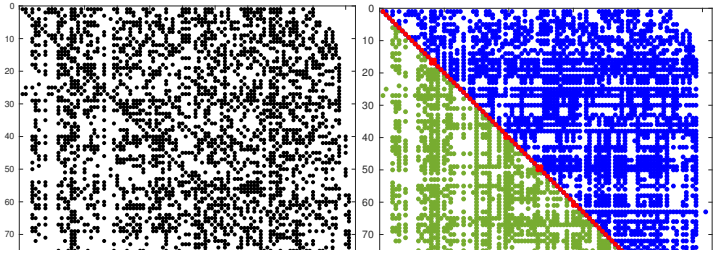

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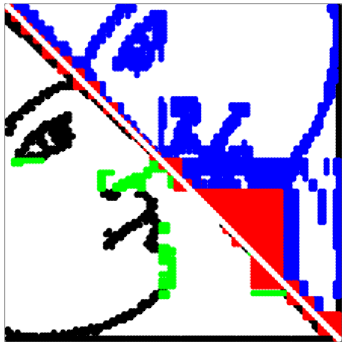

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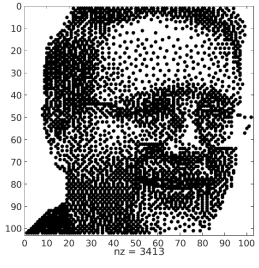

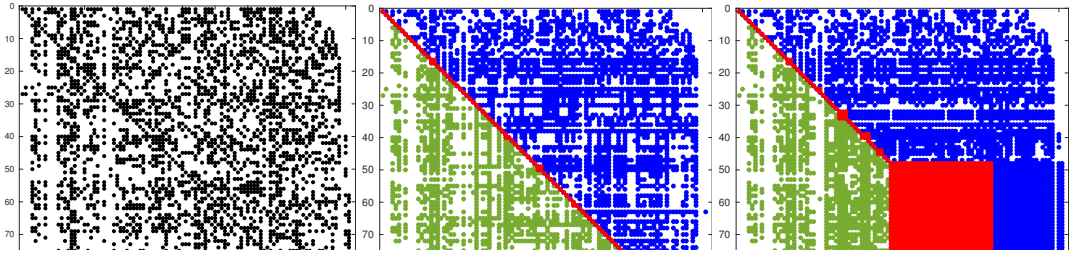

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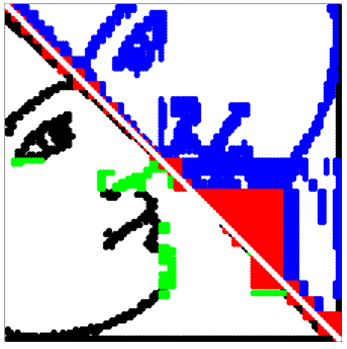

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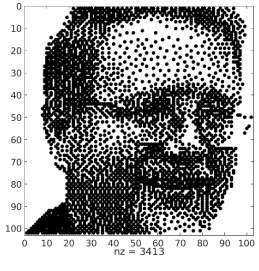

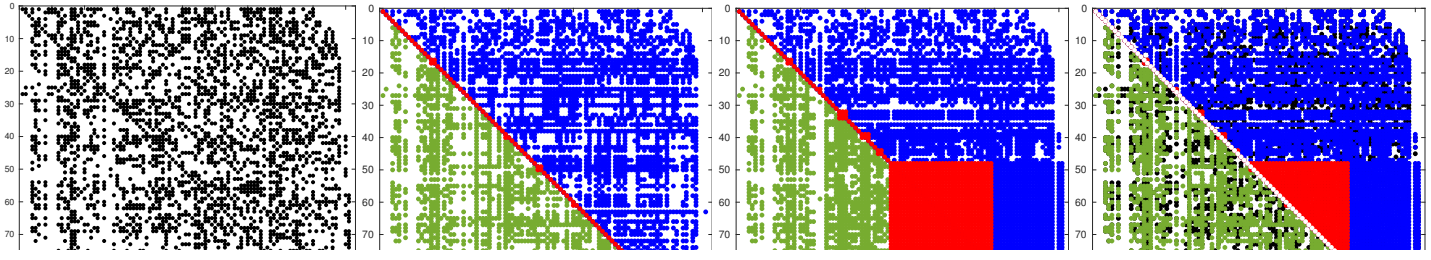

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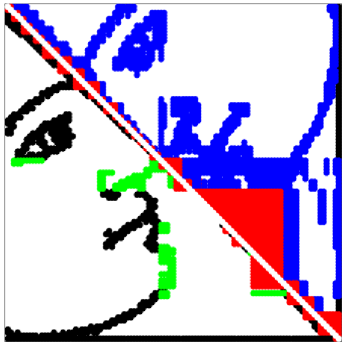

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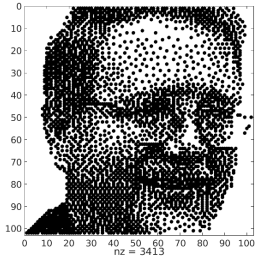

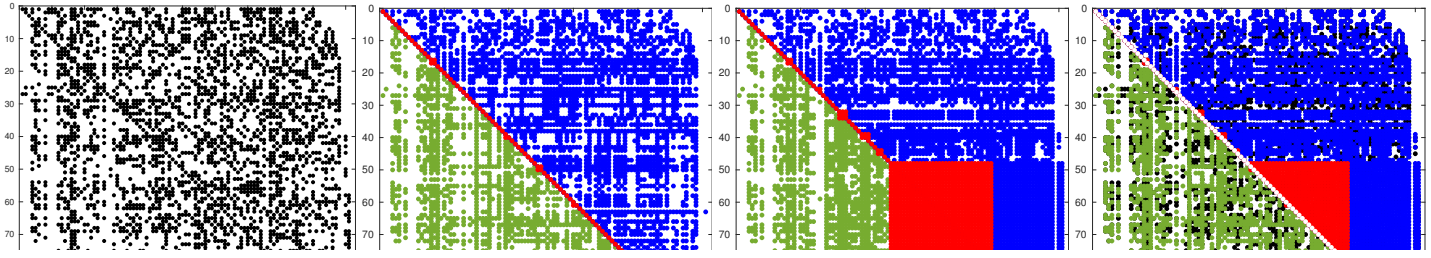

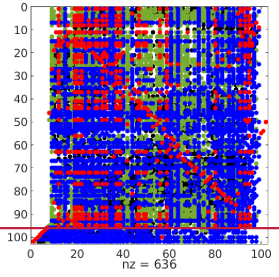

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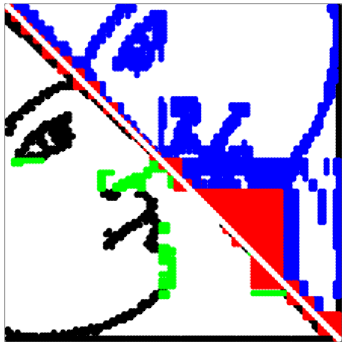

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