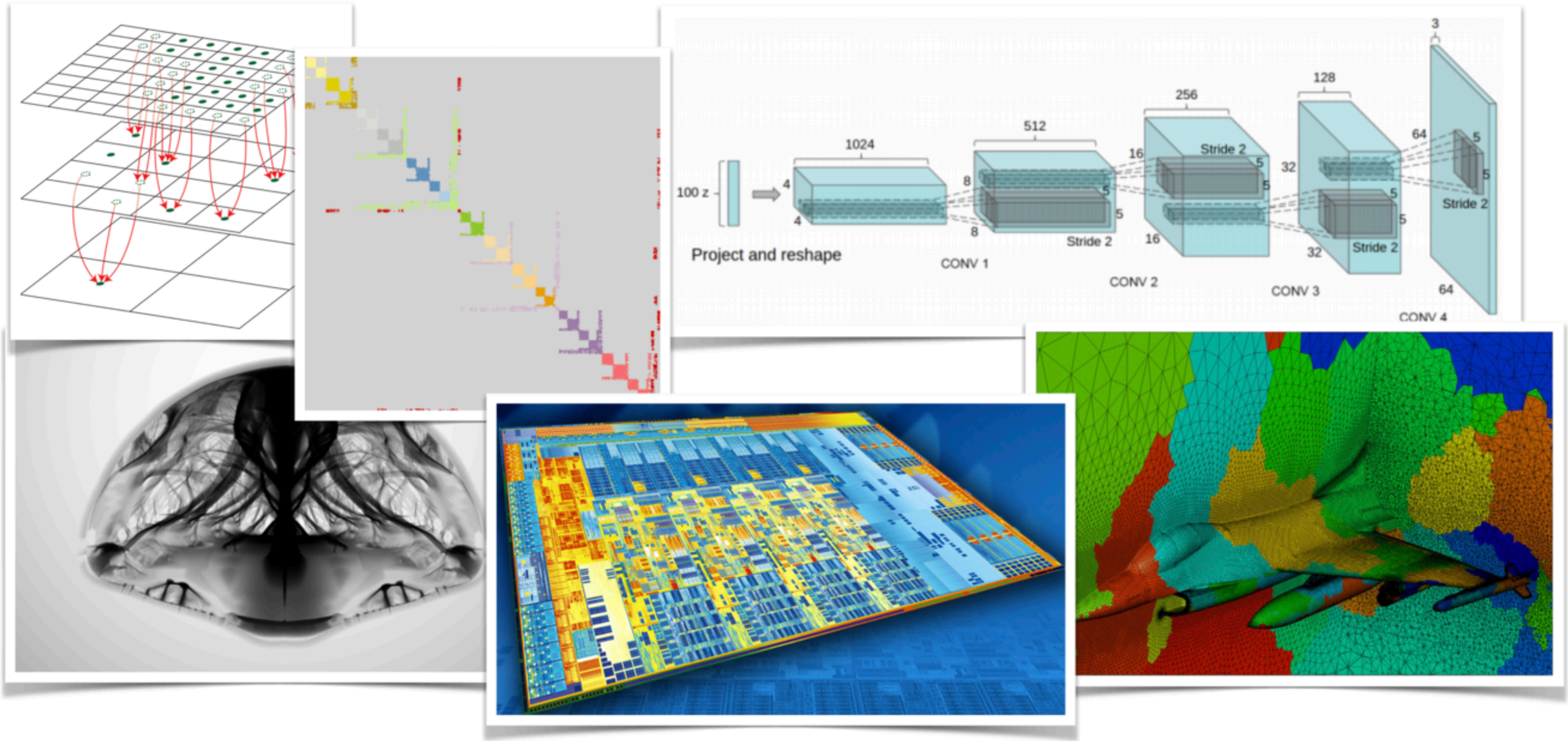


Lecture 19: Sparse Direct Solvers. Mathematical Concepts, Challenges to Parallelism, and creative remedies (in MKL PARDISO).

Tuesday April 4th 2023

Today's lecture

- Discussion of *sparse direct* system solvers.
- Mathematical concepts, and challenges to parallelism
- High-level discussion of the tricks and methods that MKL PARDISO employs to engineer parallelism (both via multithreading, and vectorization opportunities)

Recap

We did a walk-through of PARDISO, a solver library within Intel MKL.
PARDISO facilitates the solution of linear systems ***Ax=b*** *for which:*

- The coefficient matrix ***A*** *is sparse (as opposed to LAPACK and many BLAS Level 3 routines that operate on dense matrices)*

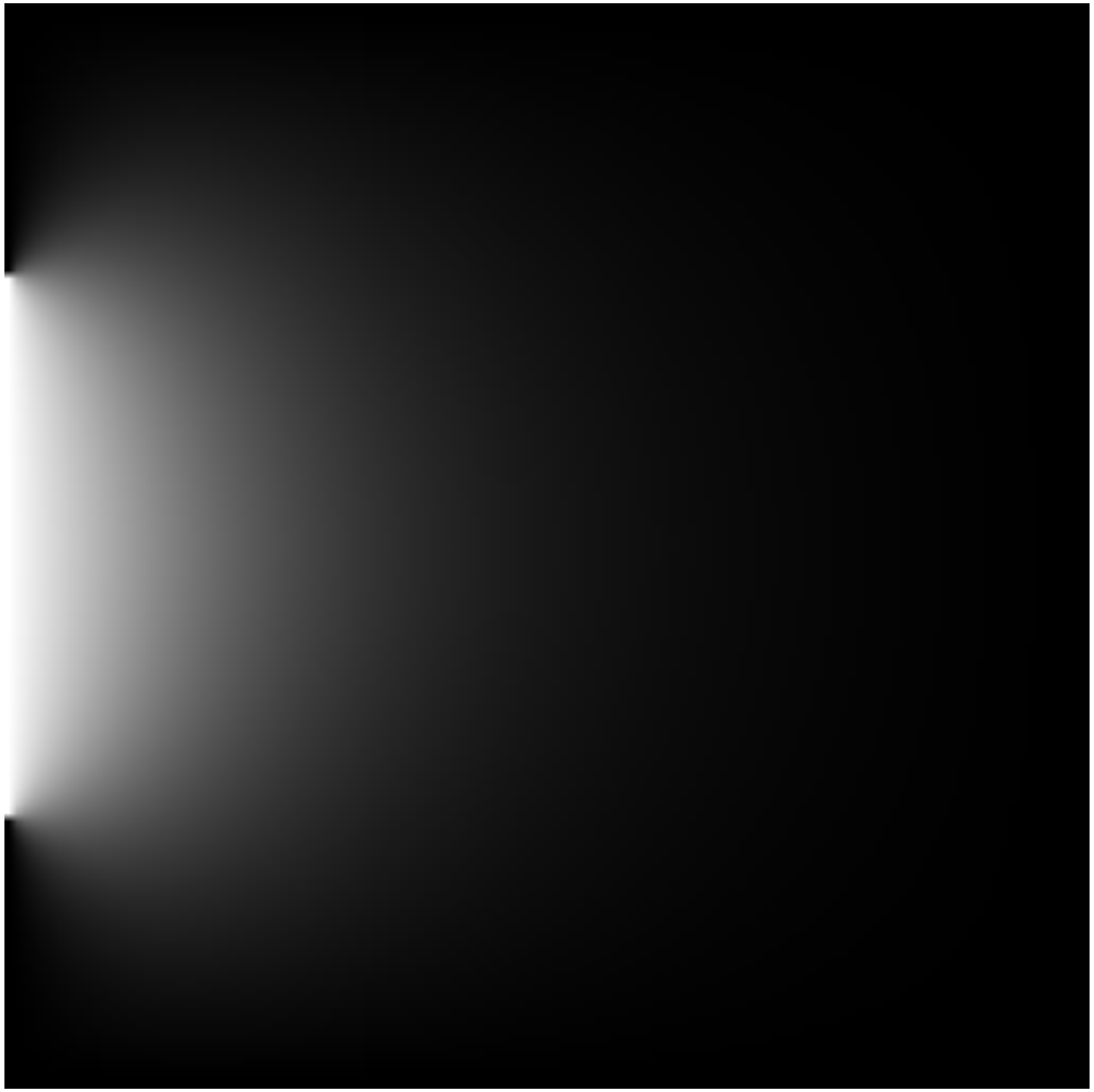
- The solver works for several different types of matrices, but is particularly efficient for symmetric (and, ideally, positive definite) matrices for which a factorization of ***A*** *is computed once (the "Cholesky" decomposition, when applicable) and re-used at low-cost for solving with different right-hand-sides*

- The solver is "direct", in that it computes the entire solution without the need for iteration

PARDISO operates on CSR-encoded matrices - same as we used before (but when used with symmetric matrices expects to be given just "half" matrix)

Result of direct solver

SparseDirect/LaplacePARDISO_0_0



A deeper look - Solver stages

PARDISO Phase 1 : Reorder the matrix to generate favorable properties
No numerical operations done in this stage - values of matrix entries don’t matter, the only thing that matters is the sparsity pattern
(we’ll see what those “favorable properties” are)

PARDISO solver (DirectSolver.cpp)

SparseDirect/LaplacePARDISO_0_0

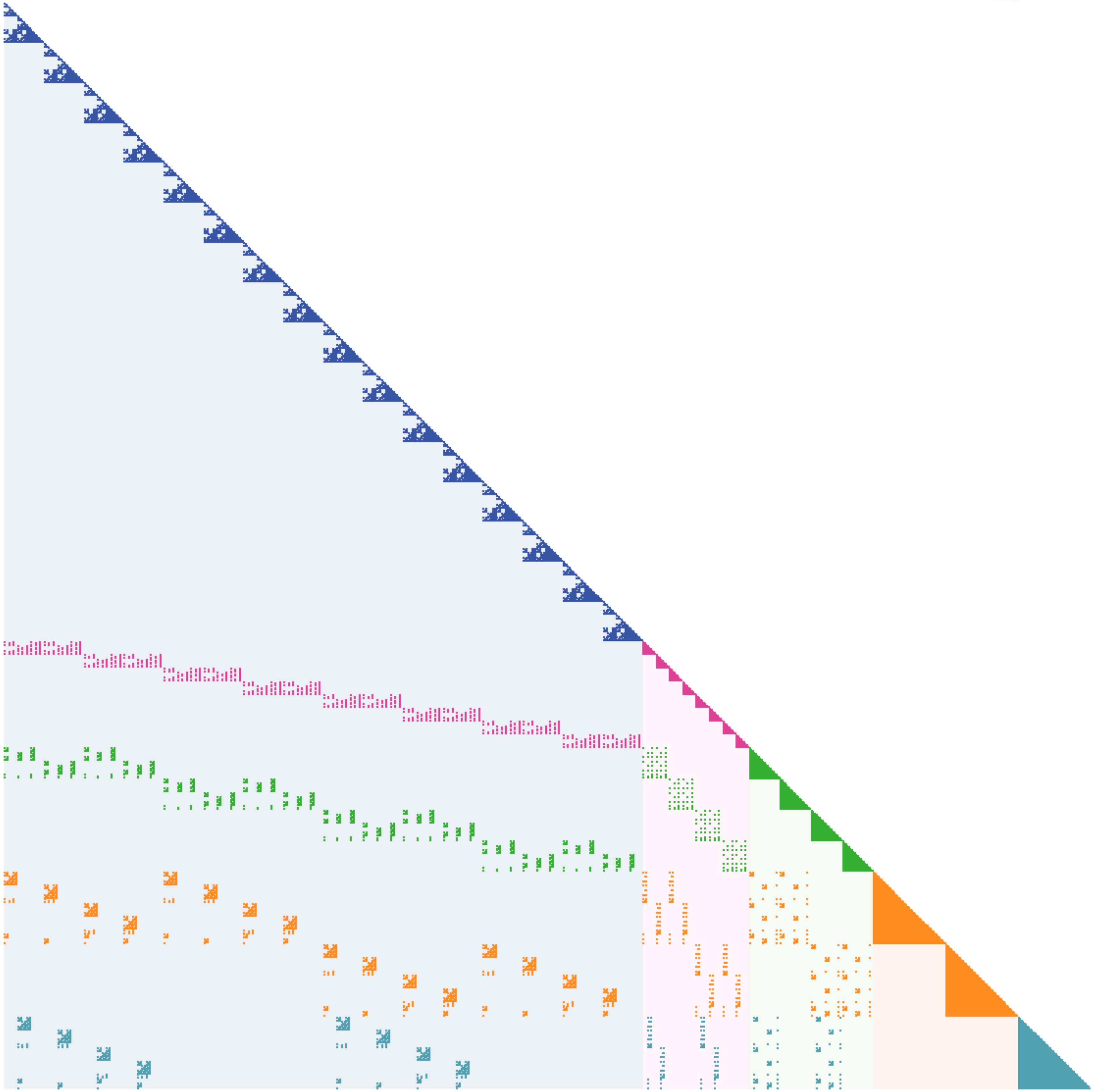
```
}

// Reordering and Symbolic Factorization. This step also allocates
// all memory that is necessary for the factorization
phase = 11; StartPhase, EndPhase. 11 runs only the first phase
PARDISO (pt, &maxfct, &mnum, &mtype, &phase, &n,
    matrix.GetValues(), matrix.GetRowOffsets(), matrix.GetColumnIndices(),
    &idum, &nrhs, iparm, &msglvl, &ddum, &ddum, &error);
if ( error != 0 )
    throw std::runtime_error("PARDISO error during symbolic factorization");

std::cout << "Reordering completed ... " << std::endl;
std::cout << "Number of nonzeros in factors = " <<  iparm[17] << std::endl;
std::cout << "Number of factorization MFLOPS = " << iparm[18] << std::endl;

// Numerical factorization
phase = 22;
PARDISO (pt, &maxfct, &mnum, &mtype, &phase, &n,
    matrix.GetValues(), matrix.GetRowOffsets(), matrix.GetColumnIndices(),
    &idum, &nrhs, iparm, &msglvl, &ddum, &ddum, &error);
if ( error != 0 )
    throw std::runtime_error("PARDISO error during numerical factorization");

std::cout << "Factorization completed ... " << std::endl;

// Back substitution and iterative refinement
phase = 33;
iparm[7] = 0;         // Max numbers of iterative refinement steps
PARDISO (pt, &maxfct, &mnum, &mtype, &phase, &n,
```

Laplacian - Initial equation ordering

Banded diagonal matrix with a maximum of 7 entries per row

$$
\begin{pmatrix}
-6 & 1 & & & 1 & & & & 1 & & & \\
1 & -6 & 1 & & & 1 & & & & \ddots & & \\
 & 1 & -6 & 1 & & & \ddots & & & & \ddots & \\
 & & \ddots & \ddots & \ddots & & & \ddots & & & & 1 \\
1 & & & \ddots & \ddots & \ddots & & & \ddots & & & \\
 & 1 & & & \ddots & \ddots & \ddots & & & \ddots & & \\
 & & \ddots & & & \ddots & \ddots & \ddots & & & 1 & \\
 & & & \ddots & & & \ddots & \ddots & \ddots & & & 1 \\
1 & & & & \ddots & & & \ddots & \ddots & \ddots & & \\
 & \ddots & & & & \ddots & & & 1 & -6 & 1 & \\
 & & \ddots & & & & 1 & & & 1 & -6 & 1 \\
 & & & 1 & & & & 1 & & & 1 & -6
\end{pmatrix}
\mathbf{x} = \mathbf{b}
$$

Laplacian - Pattern after a possible reordering



SparseDirect/LaplacePARDISO_0_0

Execution:

```
Summary: ( reordering phase )
================
Times:
======
Time spent in calculations of symmetric matrix portrait (fulladj): 0.046880 s
Time spent in reordering of the initial matrix (reorder)         : 1.529101 s
Time spent in symbolic factorization (symbfct)                   : 2.171409 s
Time spent in data preparations for factorization (parlist)      : 0.202028 s
Time spent in allocation of internal data structures (malloc)    : 0.498570 s
Time spent in additional calculations                            : 0.455895 s
Total time spent                                                 : 4.903884 s
Statistics:
===========
Parallel Direct Factorization is running on 20 OpenMP
< Linear system Ax = b >
             number of equations:           2097152
             number of non-zeros in A:      8050652
             number of non-zeros in A (%): 0.00018
             number of right-hand sides:    1
< Factors L and U >
             number of columns for each panel: 96
             number of independent subgraphs:  0
             number of supernodes:                    1409897
             size of largest supernode:               16591
             number of non-zeros in L:                2065304266
             number of non-zeros in U:                1
             number of non-zeros in L+U:              2065304267
Reordering completed ...
Number of nonzeros in factors = 2065304267
Number of factorization MFLOPS = 22854214
```

About 10% of overall runtime (typically: at least that much)

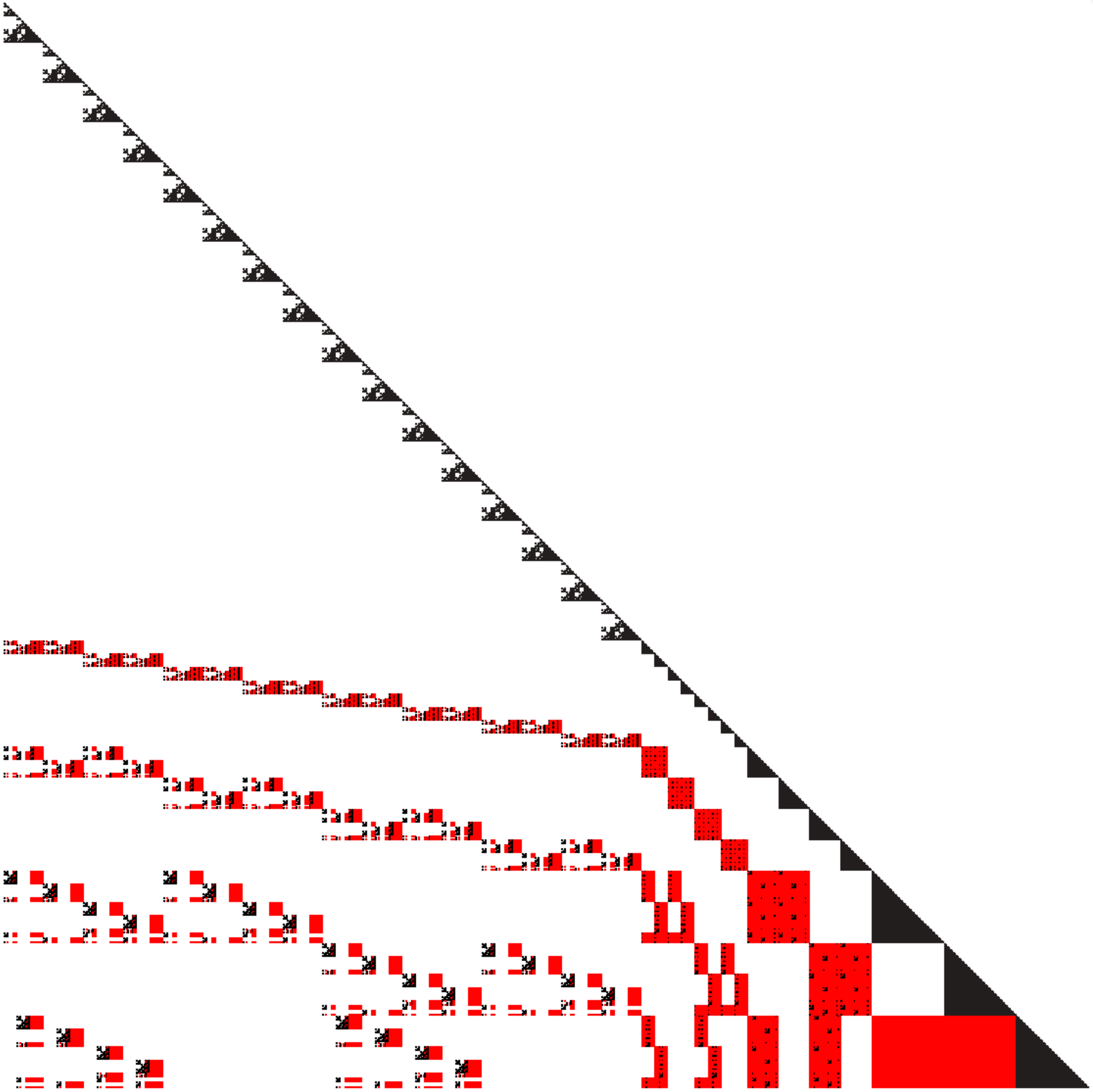
still better than nnz in dense which would be 2097152^2

A deeper look - Solver stages

PARDISO Phase 1 : Reorder the matrix to generate favorable properties
No numerical operations done in this stage - values of matrix entries don’t matter, the only thing that matters is the sparsity pattern
(we’ll see what those “favorable properties” are)

PARDISO Phase 2 : Perform the actual Cholesky Decomposition (factorization)
This is the computation-heavy part of the algorithm, and the most expensive part of the execution, for typical (large) matrix sizes.
Note: In accordance with theory, the Cholesky factor ***L*** *includes all of the entries in the sparsity pattern of* ***A*** *in its own, plus some more*
(hopefully as few as possible; reordering influences that)

Sparsity of Cholesky Factor (L) vs. Laplacian Matrix



SparseDirect/LaplacePARDISO_0_0

PARDISO solver (DirectSolver.cpp)

Execution:

```
Summary: ( factorization phase )
================
Times:
======
Time spent in copying matrix to internal data structure (A to LU): 0.000000 s
Time spent in factorization step (numfct)                         : 44.352600 s
Time spent in allocation of internal data structures (malloc)     : 0.022322 s
Time spent in additional calculations                             : 0.000002 s
Total time spent                                                  : 44.374928 s
Statistics:
===========
Parallel Direct Factorization is running on 20 OpenMP
< Linear system Ax = b >
             number of equations:           2097152
             number of non-zeros in A:      8050652
             number of non-zeros in A (%): 0.000183
             number of right-hand sides:    1
< Factors L and U >
             number of columns for each panel: 96
             number of independent subgraphs:  0
             number of supernodes:                    1410153
             size of largest supernode:               16591
             number of non-zeros in L:                2057589566
             number of non-zeros in U:                1
             number of non-zeros in L+U:              2057589567
             gflop   for the numerical factorization: 22775.748047
             gflop/s for the numerical factorization: 513.515503

Factorization completed ...
 PARDISO (pt, &maxfct, &mnum, &mtype, &phase, &n,
```

About 90% of overall runtime (sometimes less)

Almost 25% of peak arithmetic utilization

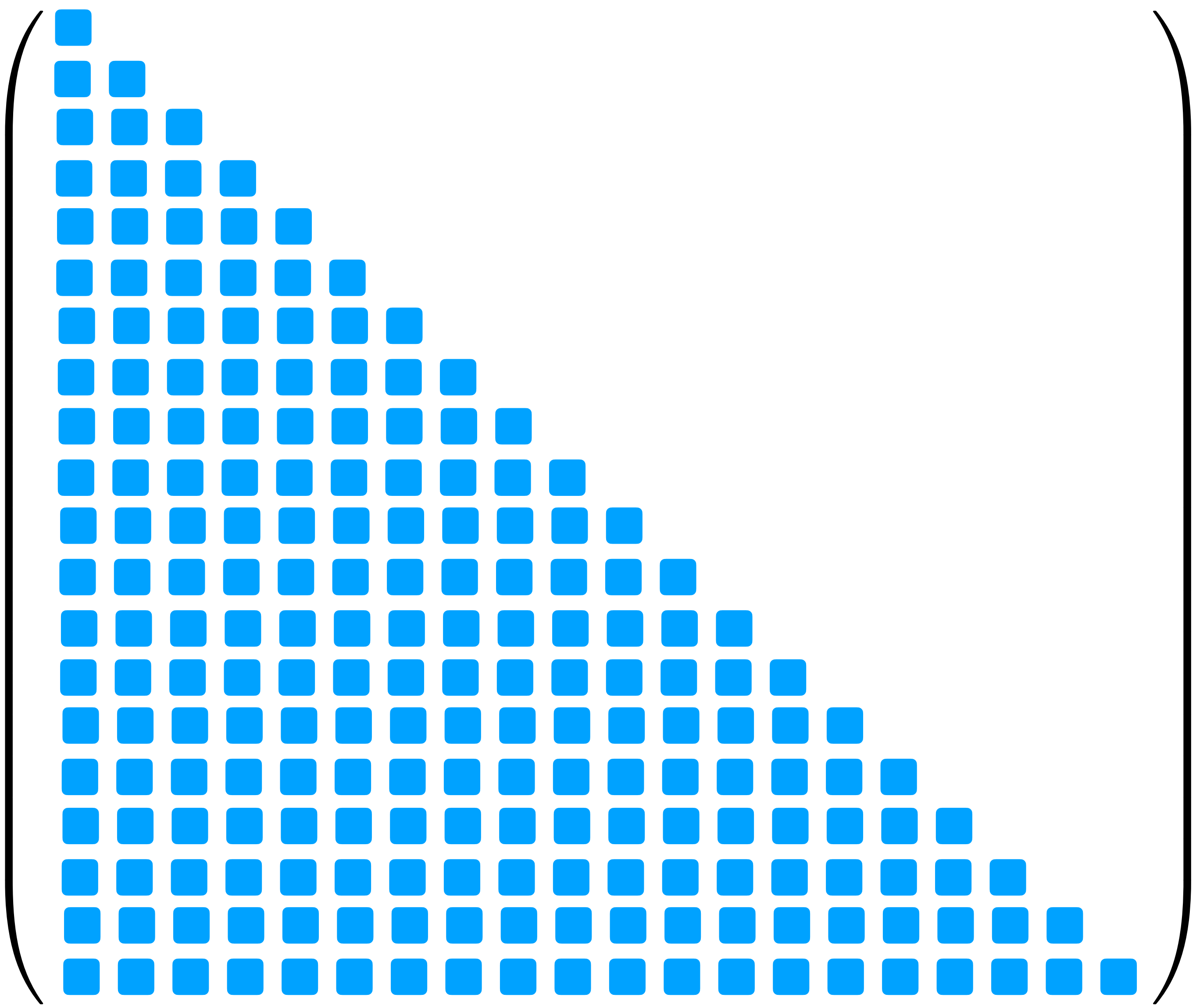
Obstacles to performance & parallelism

*<u>Matrix Density</u> : The number of required operations scale (super-linearly …) with the number of non-zero entries in **L** … thus, ensuring sparser **L** factors has an immediate effect on performance*

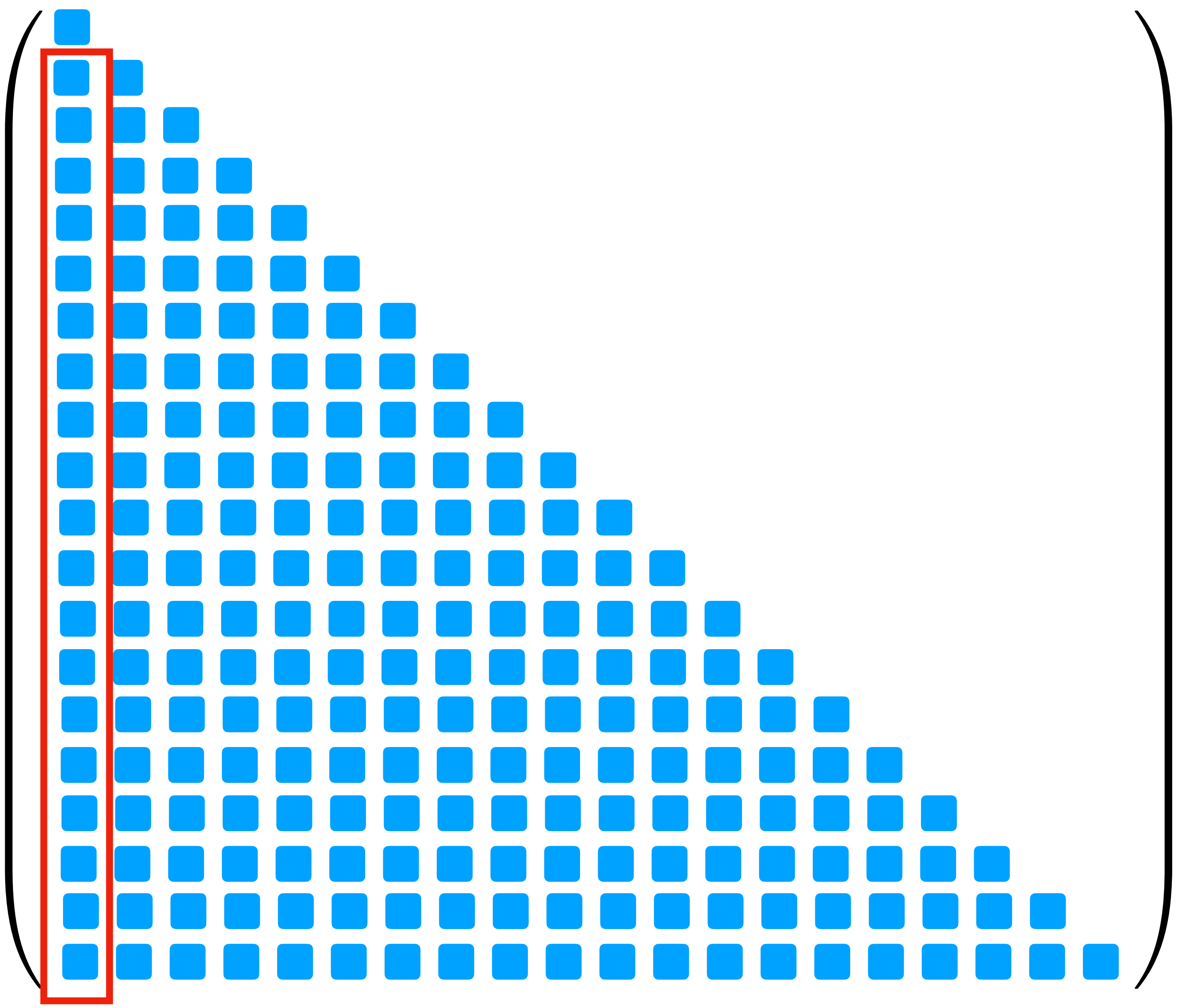
Linear scaling with nnz.

<u>Multithreading</u> : Cholesky, similar to Gauss Elimination, is seemingly a very "serial" algorithm (significant dependencies between steps/loops). We must find some way to cope with this apparent limitation.

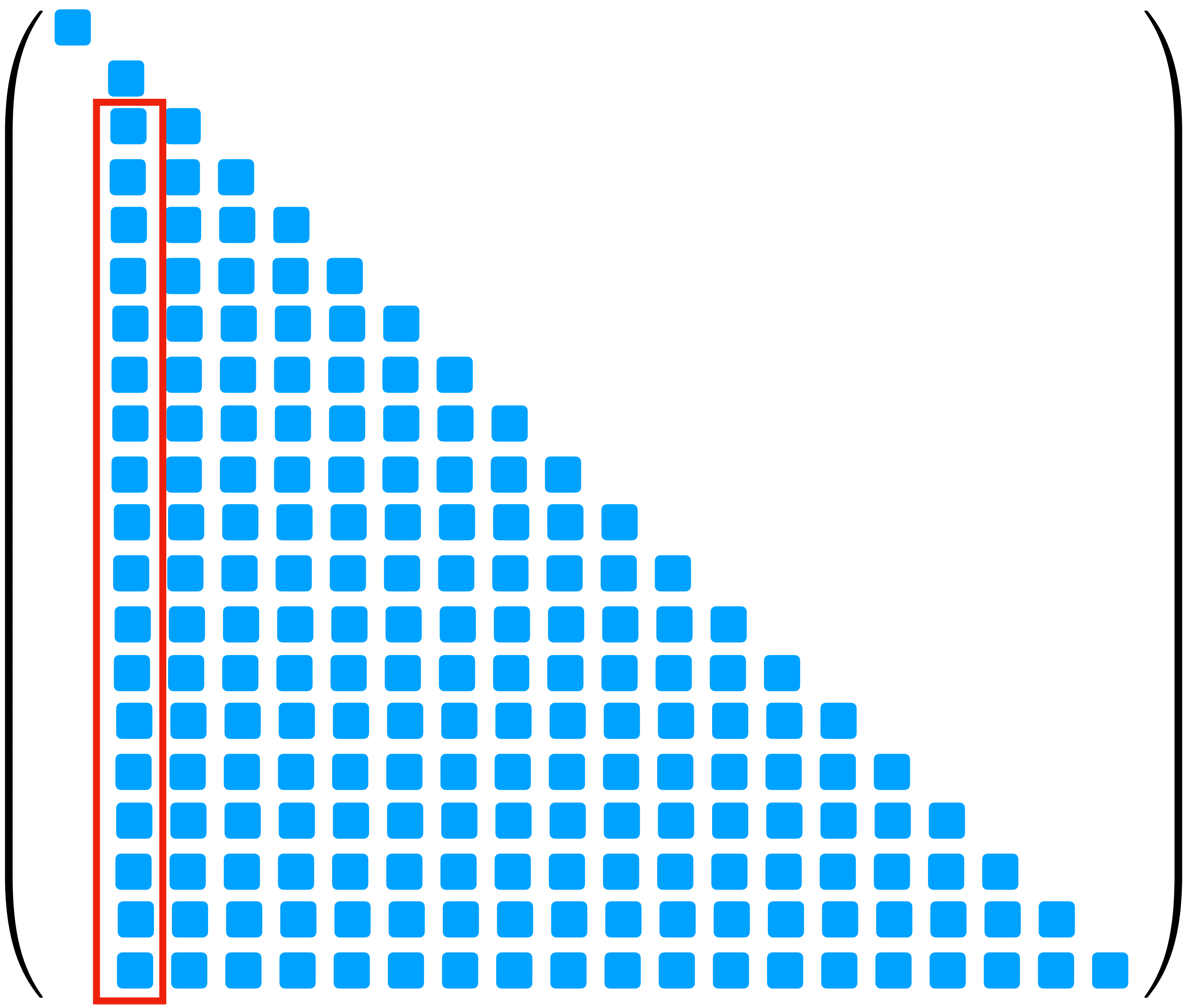
1. Factor L as sparse as possible through algebra. Eg: Lower Triangular
2. Exploit opportunities for multithreading
3. Exploit opportunities for vectorization



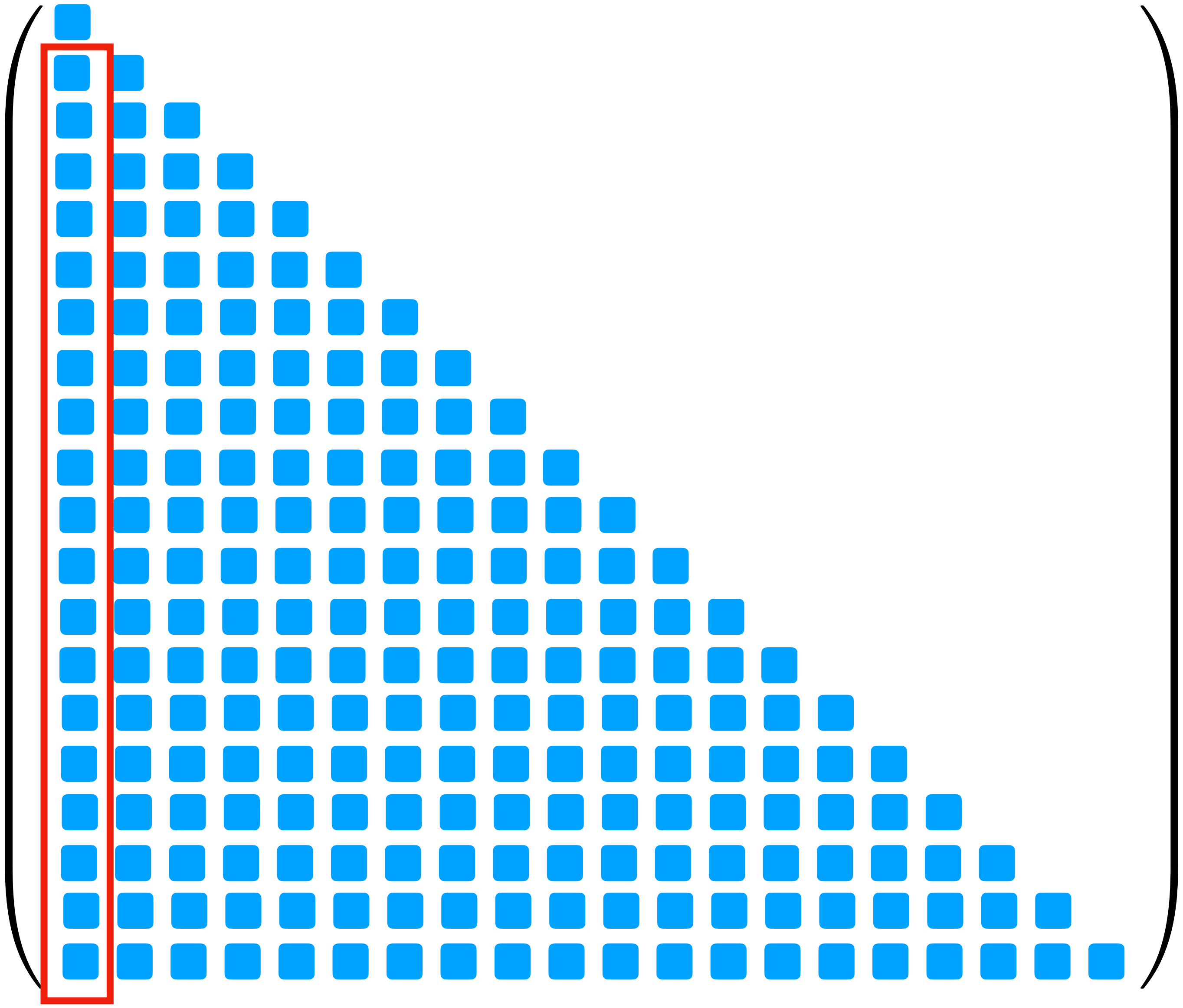
Consider Gauss Elimination …



We need to make all these entries zero …



… and then continue to the next column



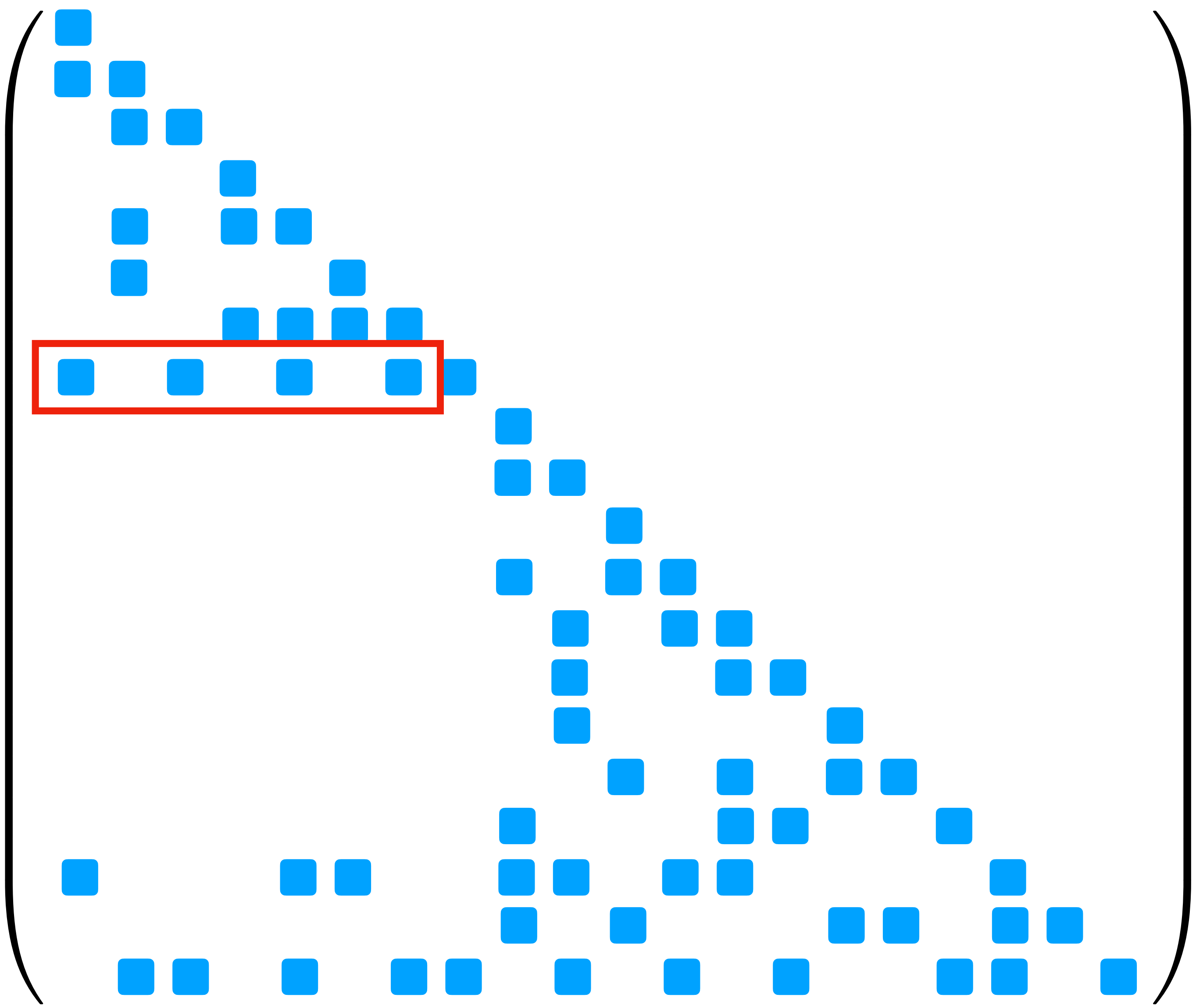
We can do each row of this operation in parallel … but we need to wait for this column before moving to the next (… in principle)

Obstacles to performance & parallelism

*<u>Matrix Density</u> : The number of required operations scale (super-linearly …) with the number of non-zero entries in **L** … thus, ensuring sparser **L** factors has an immediate effect on performance*

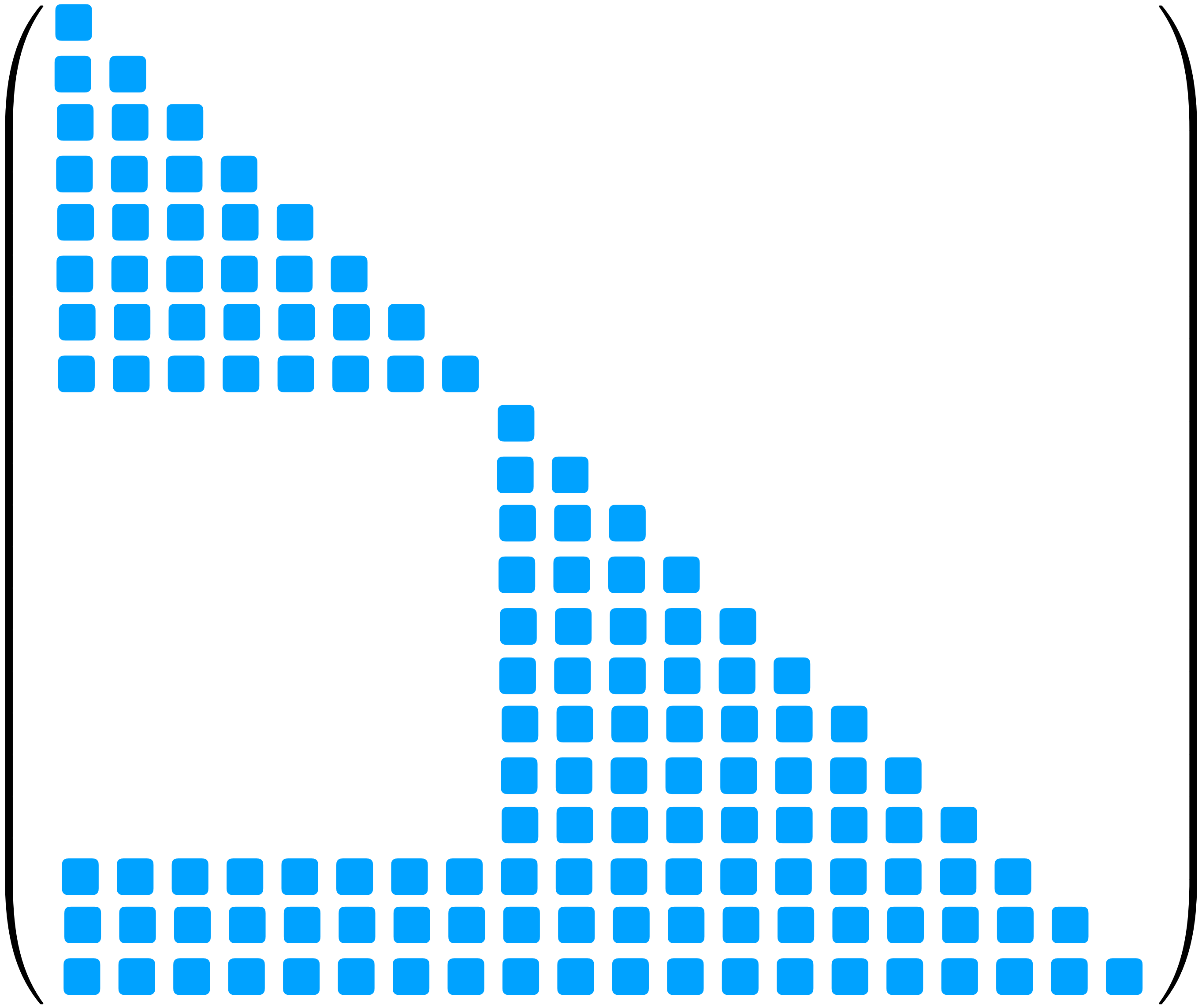
<u>Multithreading</u> : Cholesky, similar to Gauss Elimination, is seemingly a very "serial" algorithm (significant dependencies between steps/loops). We must find some way to cope with this apparent limitation.

<u>Vectorization/SIMD</u> : Sparse matrices don't have the regularity that SIMD operations require; we need to "engineer" such regularity if possible



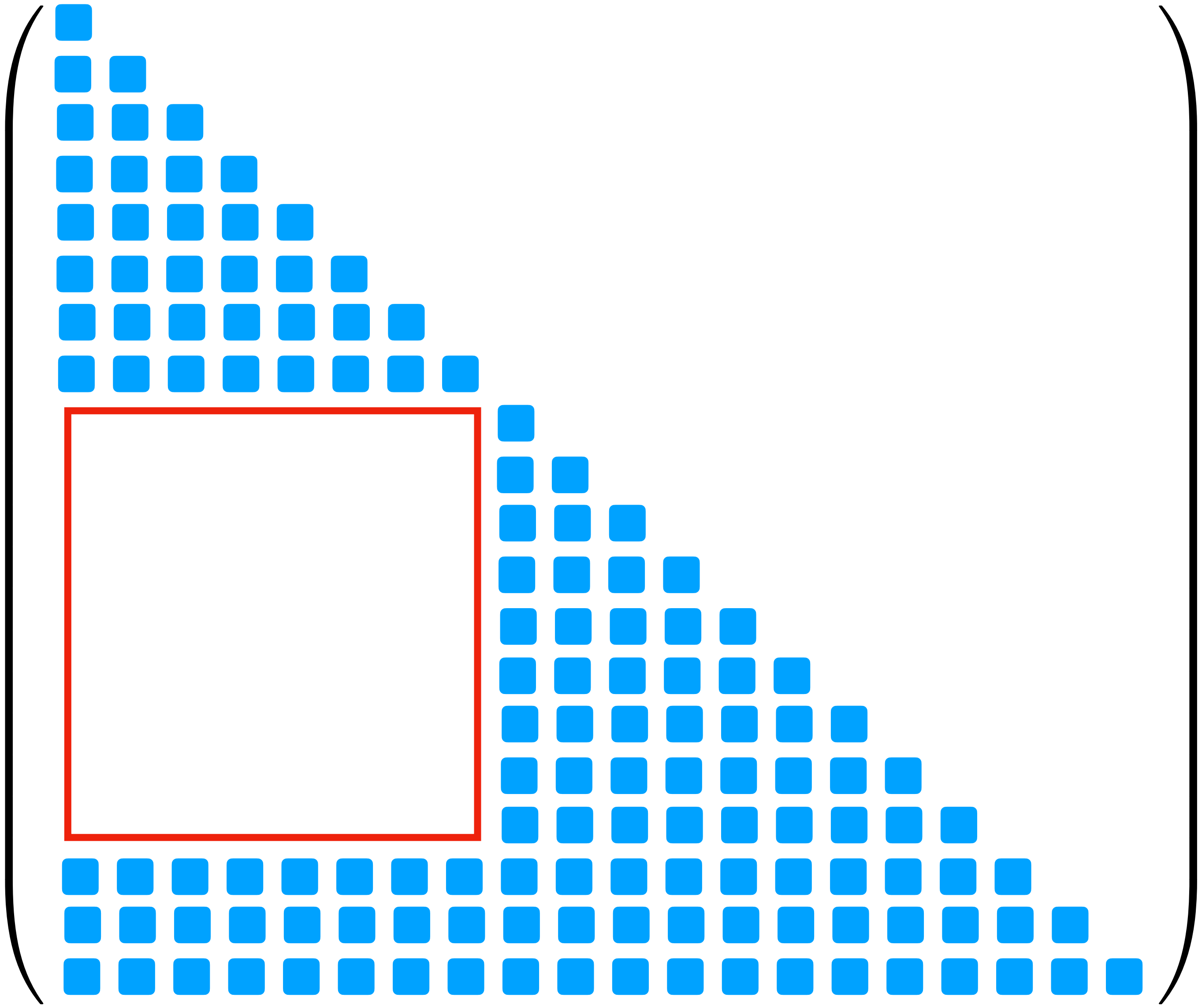
Tasks that we would normally consider candidates for SIMD are not at all regular …

Engineering/Maximizing Sparsity



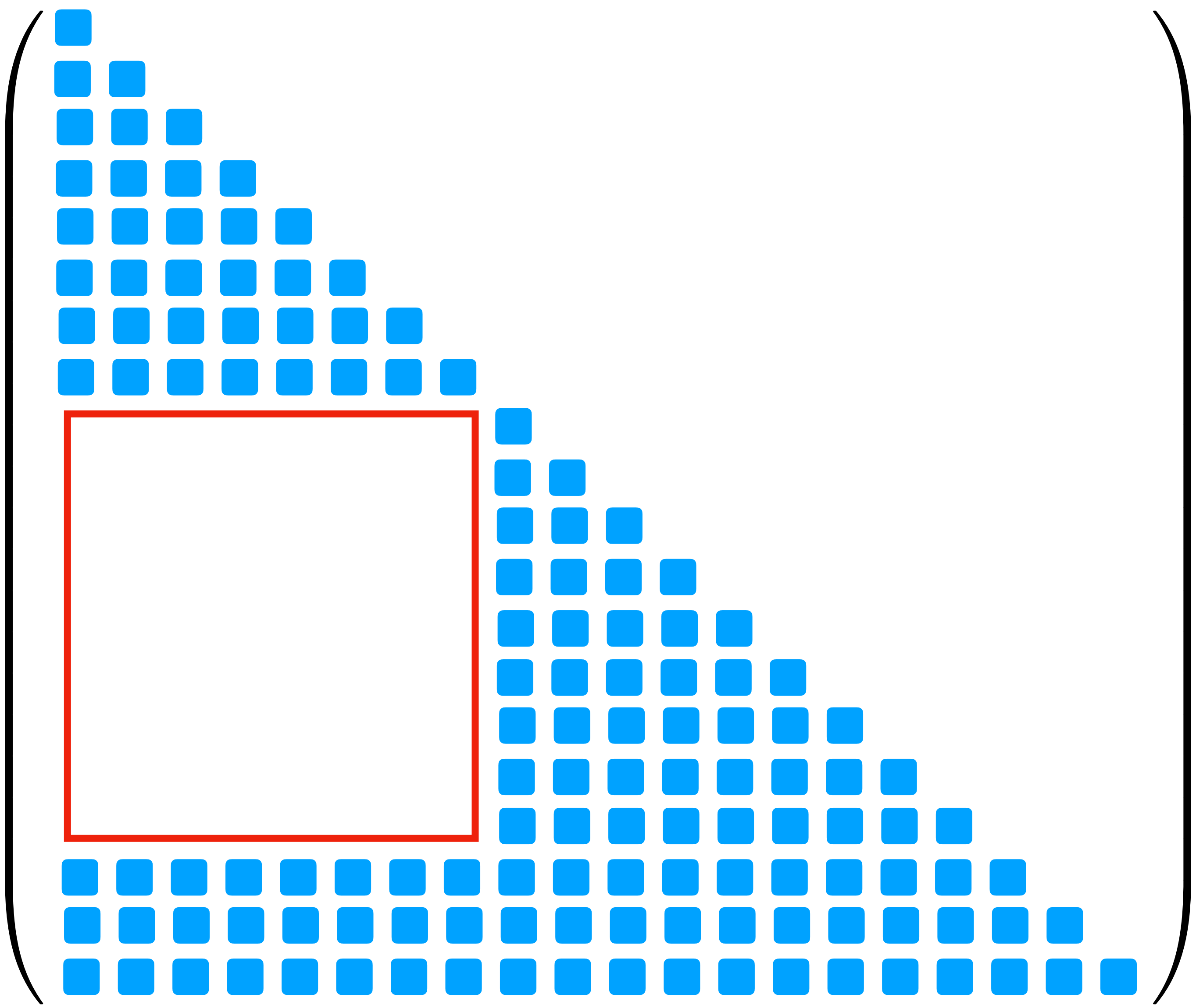
*Sparsity pattern of **A***
(lower-triangular part only)

Engineering/Maximizing Sparsity



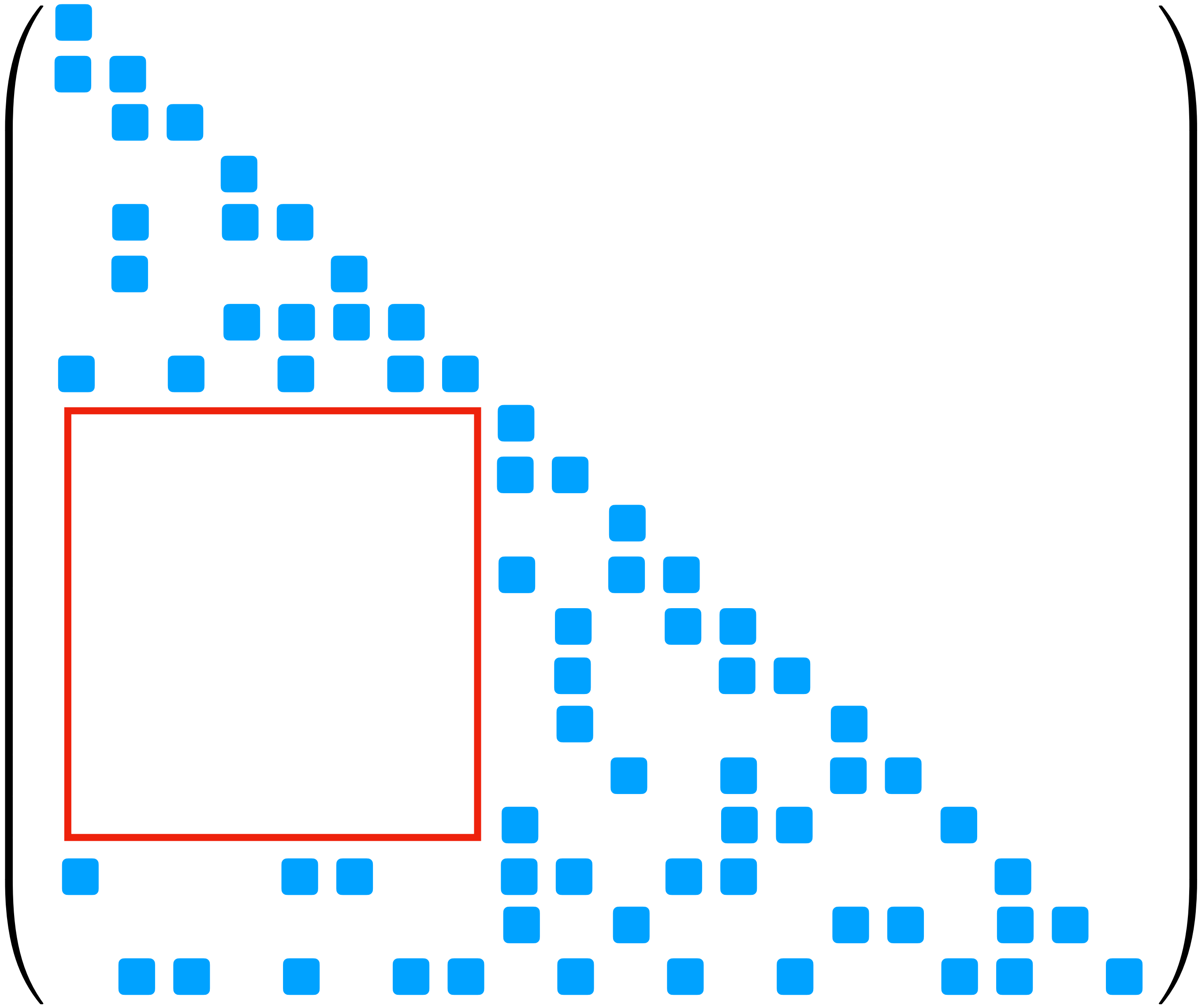
Theory can prove that:
If there's a rectangular gap in the sparsity pattern of ***A*** *…*

Engineering/Maximizing Sparsity



Theory can prove that:
… that gap will also be present
*in the Cholesky factor **L***

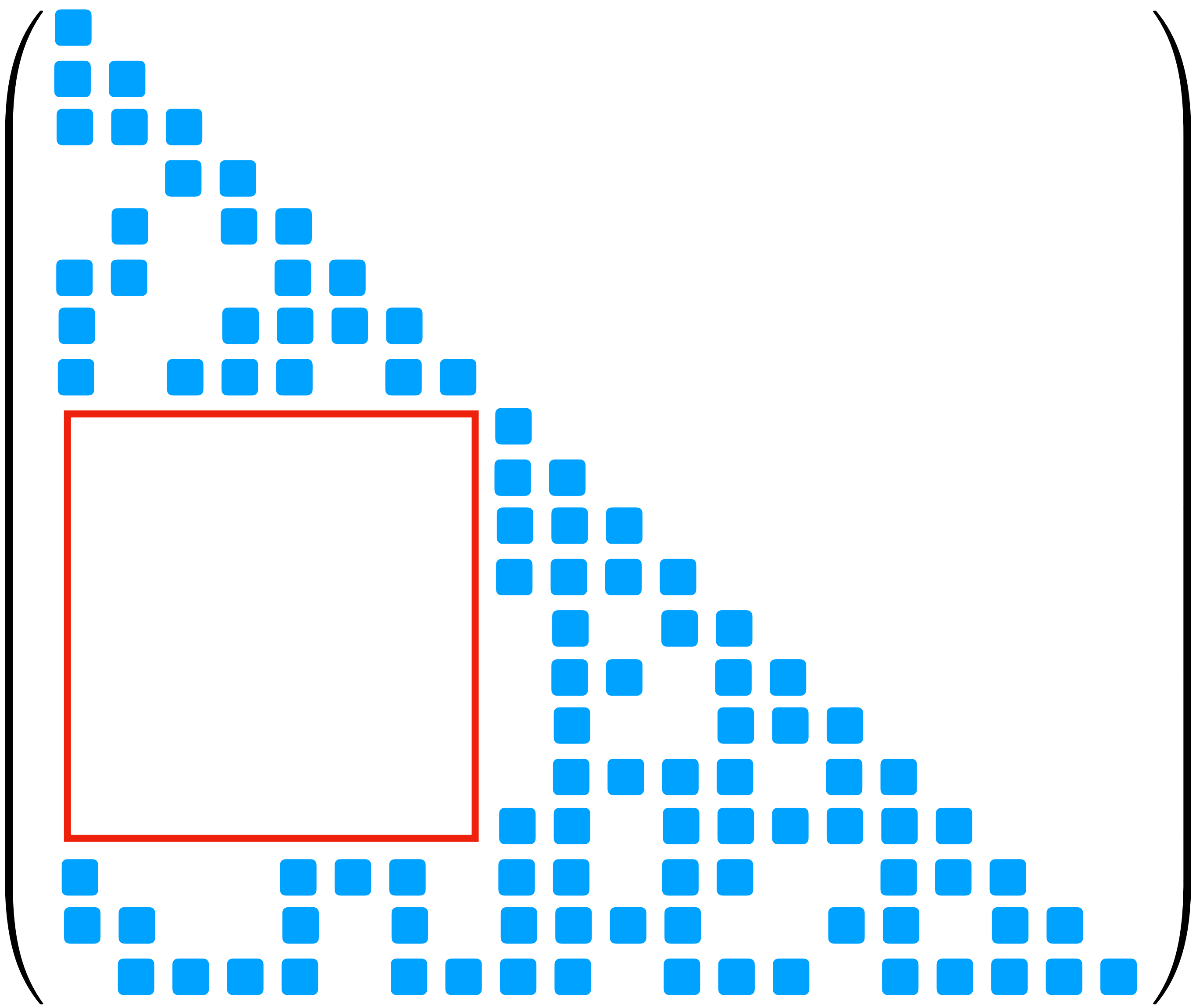
Engineering/Maximizing Sparsity



Edge to diagonal

*A sparse matrix **A** can have such gaps without being "dense" elsewhere …*

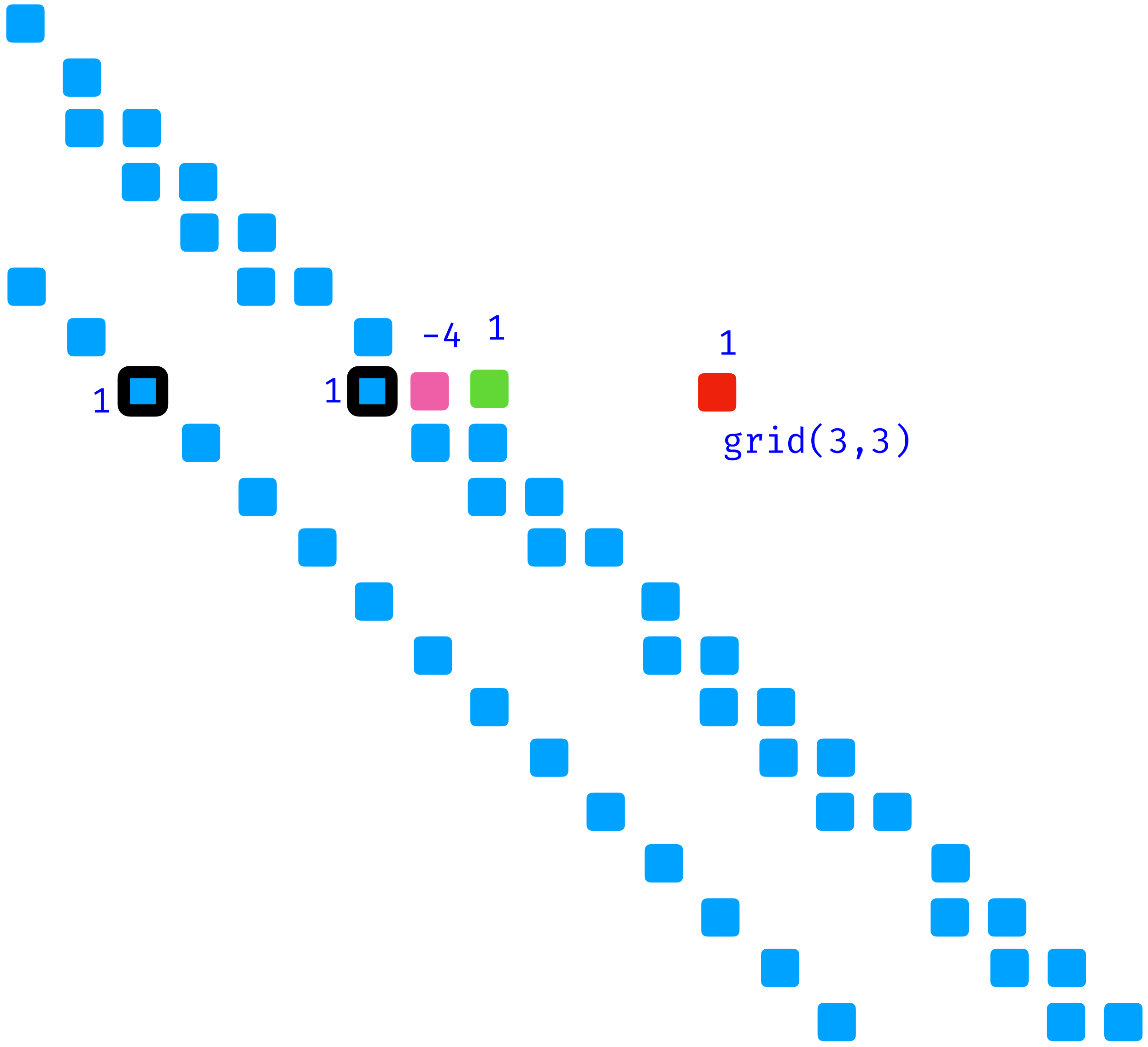
Engineering/Maximizing Sparsity



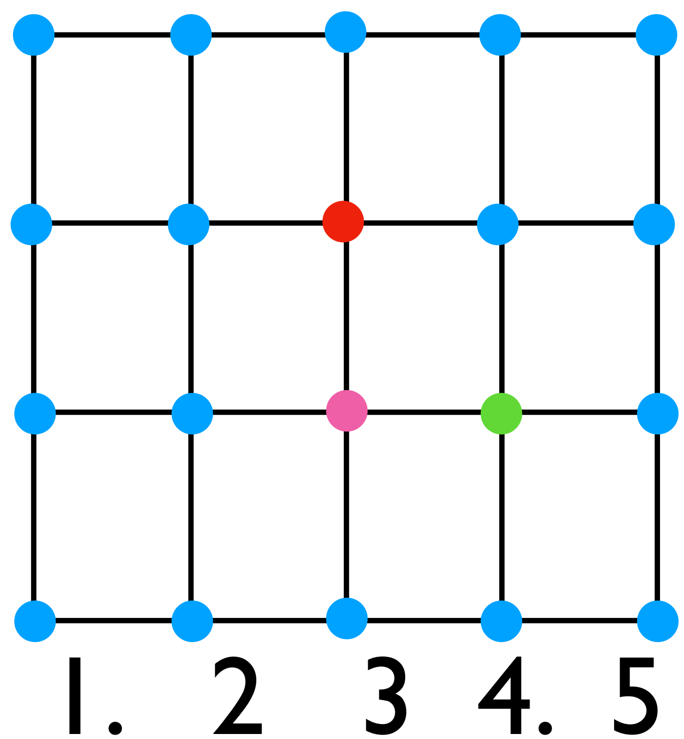
Harvest sparsity in blocks (dependent on algorithm)

*… and the corresponding factor **L** (even if it becomes denser away from such gaps) does retain these "holes" in its sparsity pattern*

In PARDISO, we only consider one section of the triangular matrix.
This image is wrong, refer to redrawn on next slide

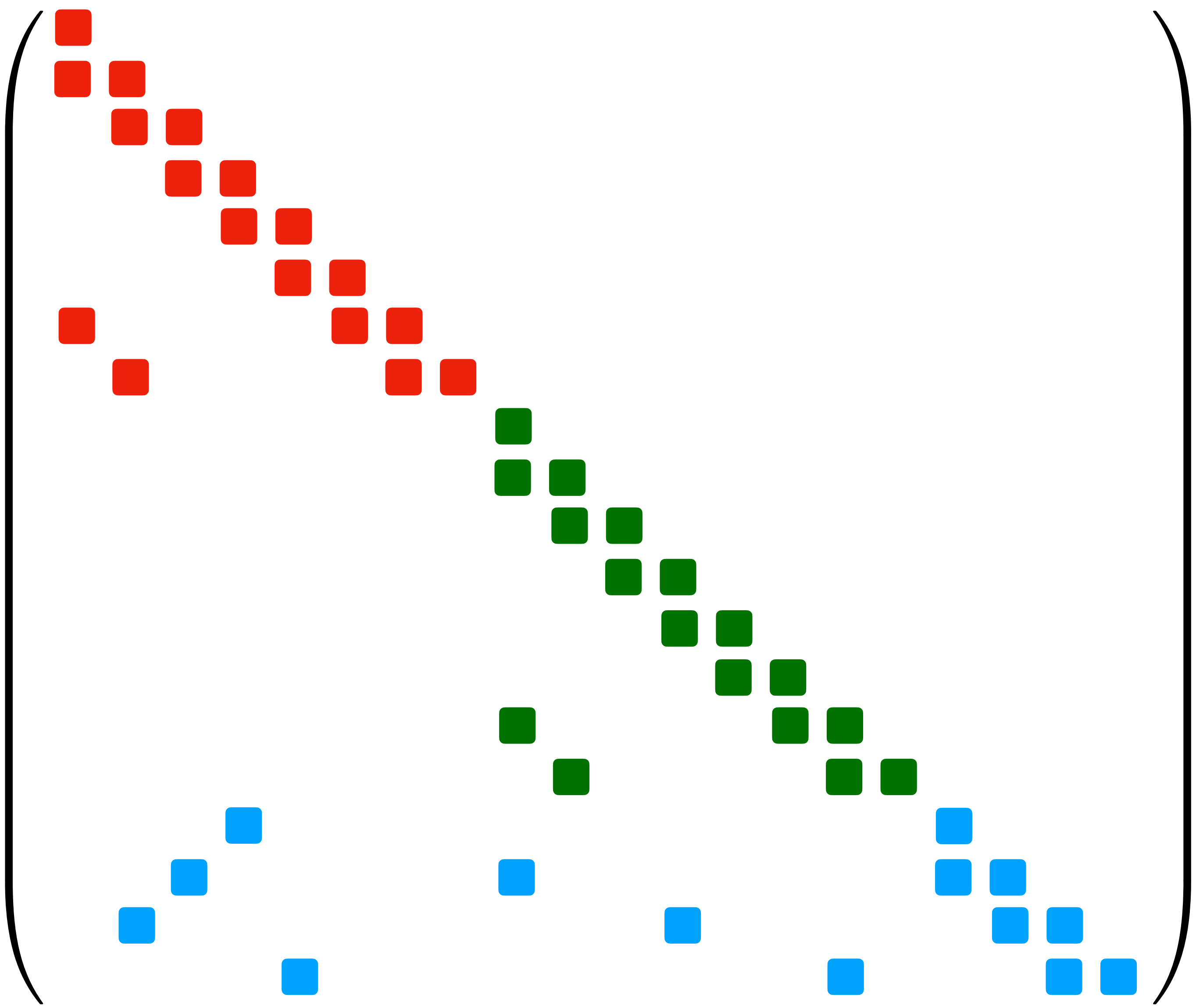


The grid has no hoelx

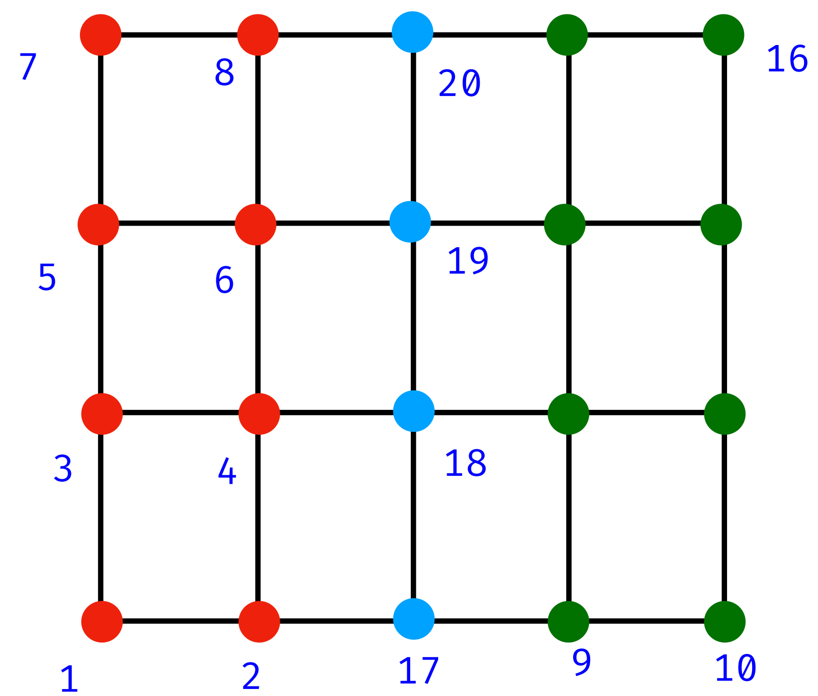


Laplacian stencil of the element on diagonal (in pink). Orange is 5 spots away from pink and is represented by counting 5 from left to right.

Engineering/Maximizing Sparsity

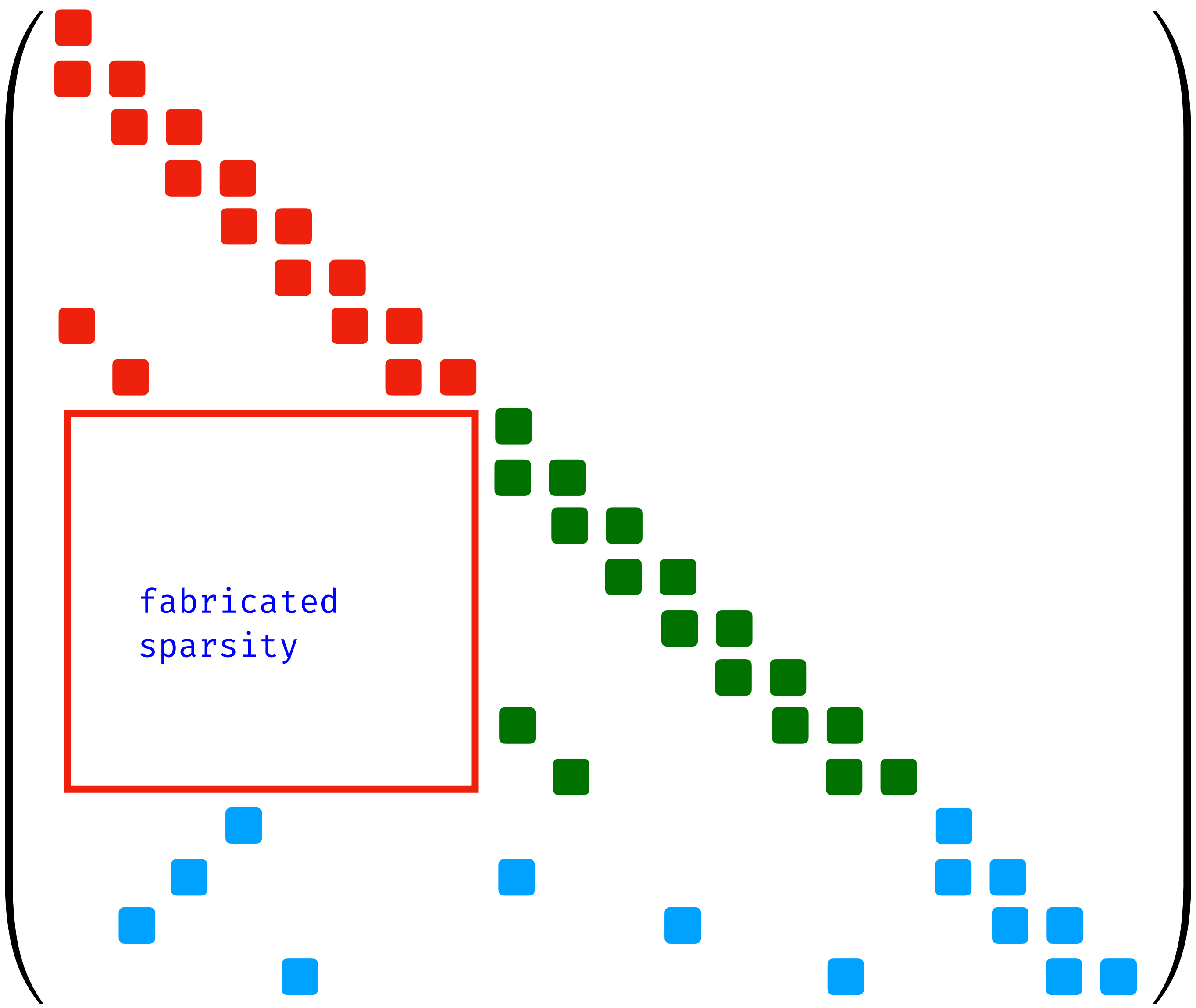


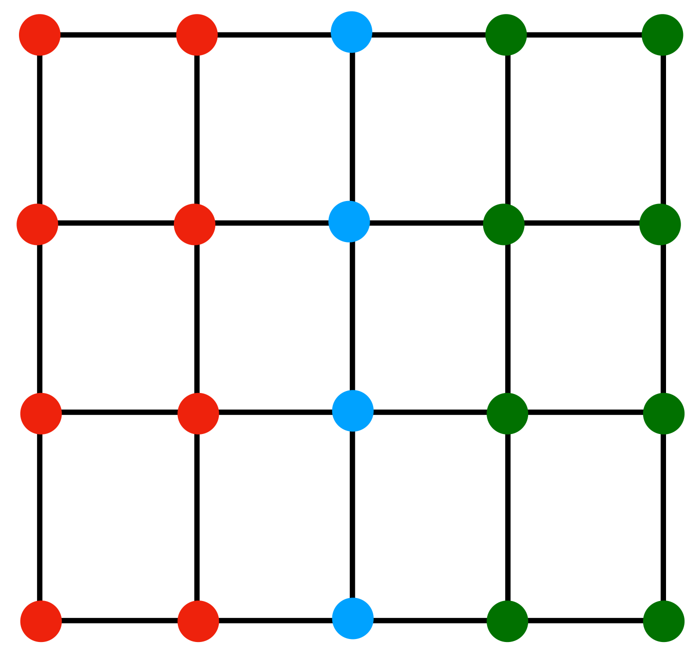
Stencil to Matrix conversion involves enumeration of the nnz elements



achieved by swapping rows in the matrix which only changes the bookkeeping involved

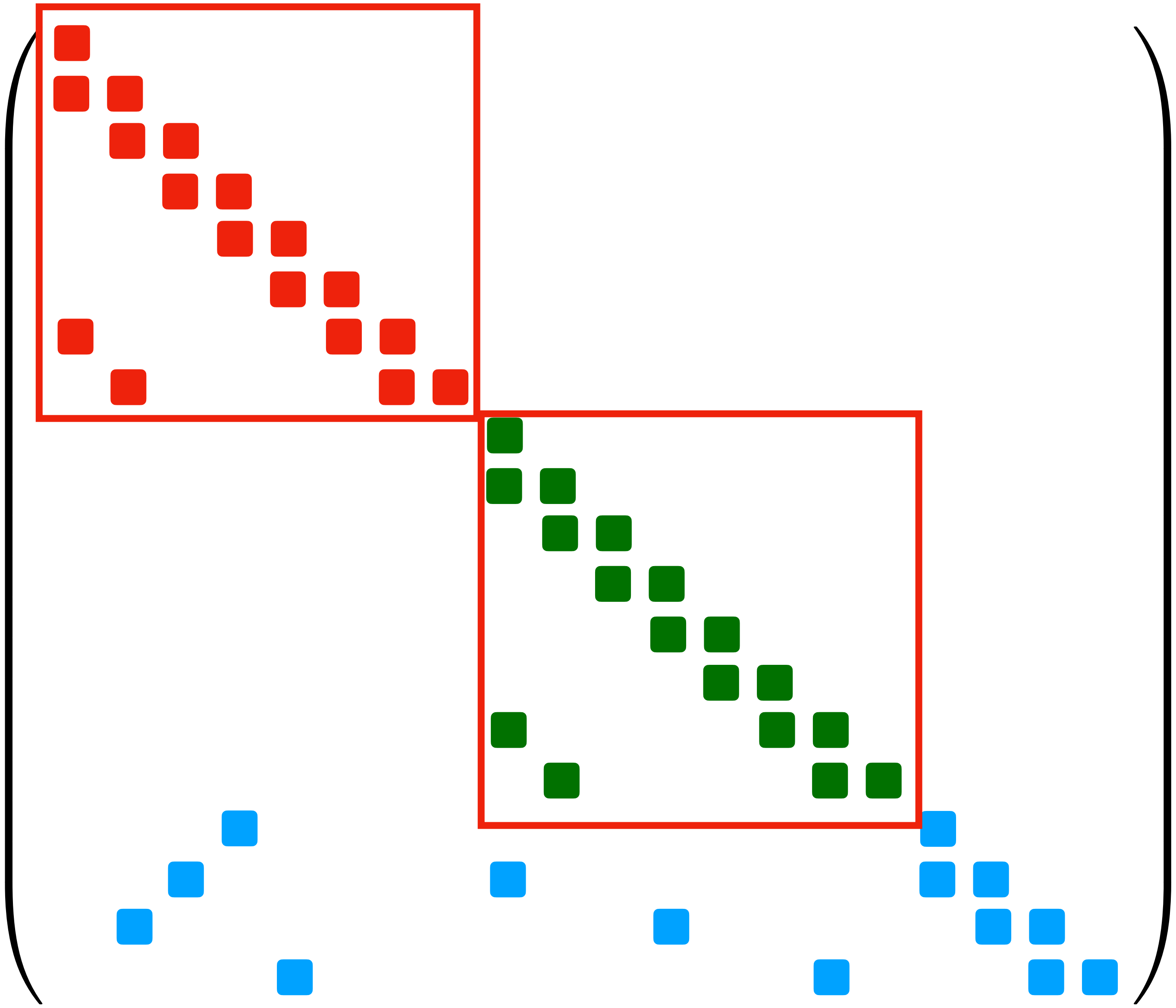
Engineering/Maximizing Sparsity





Vectorization

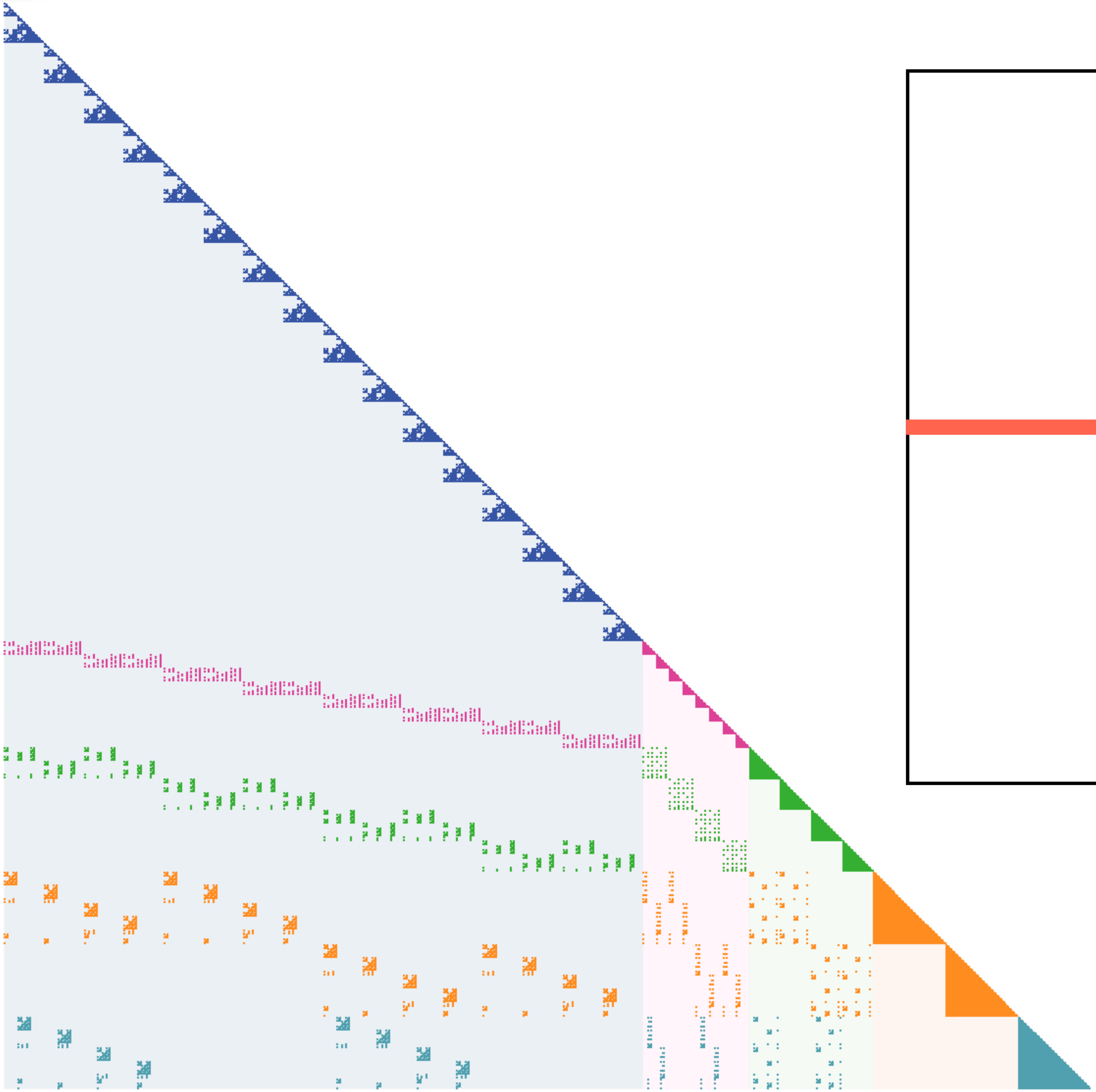
Engineering/Maximizing Sparsity

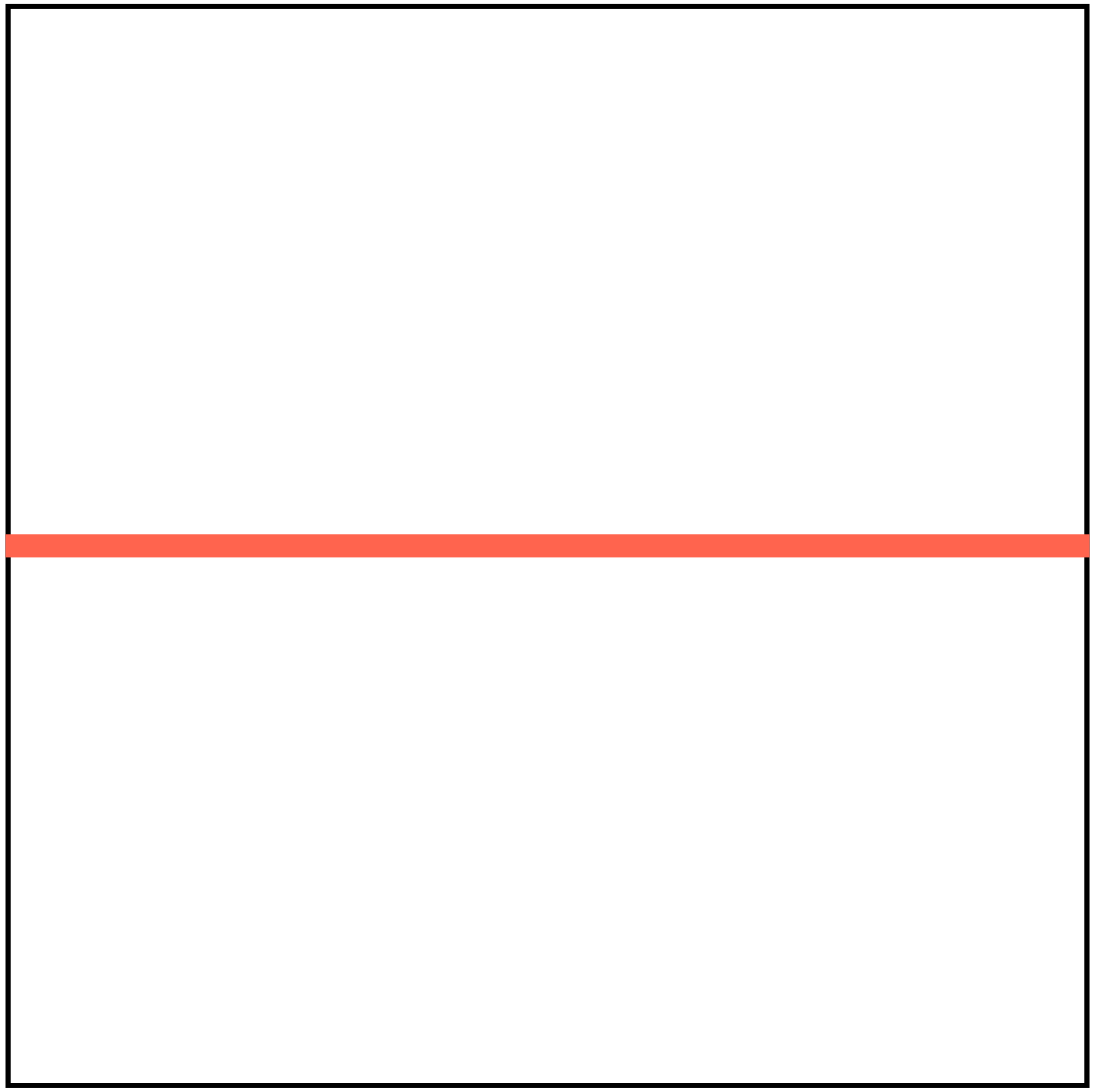


Second benefit:
Cholesky can process each of these two blocks in-parallel!

Multi-threading

Laplacian - Pattern after a possible reordering





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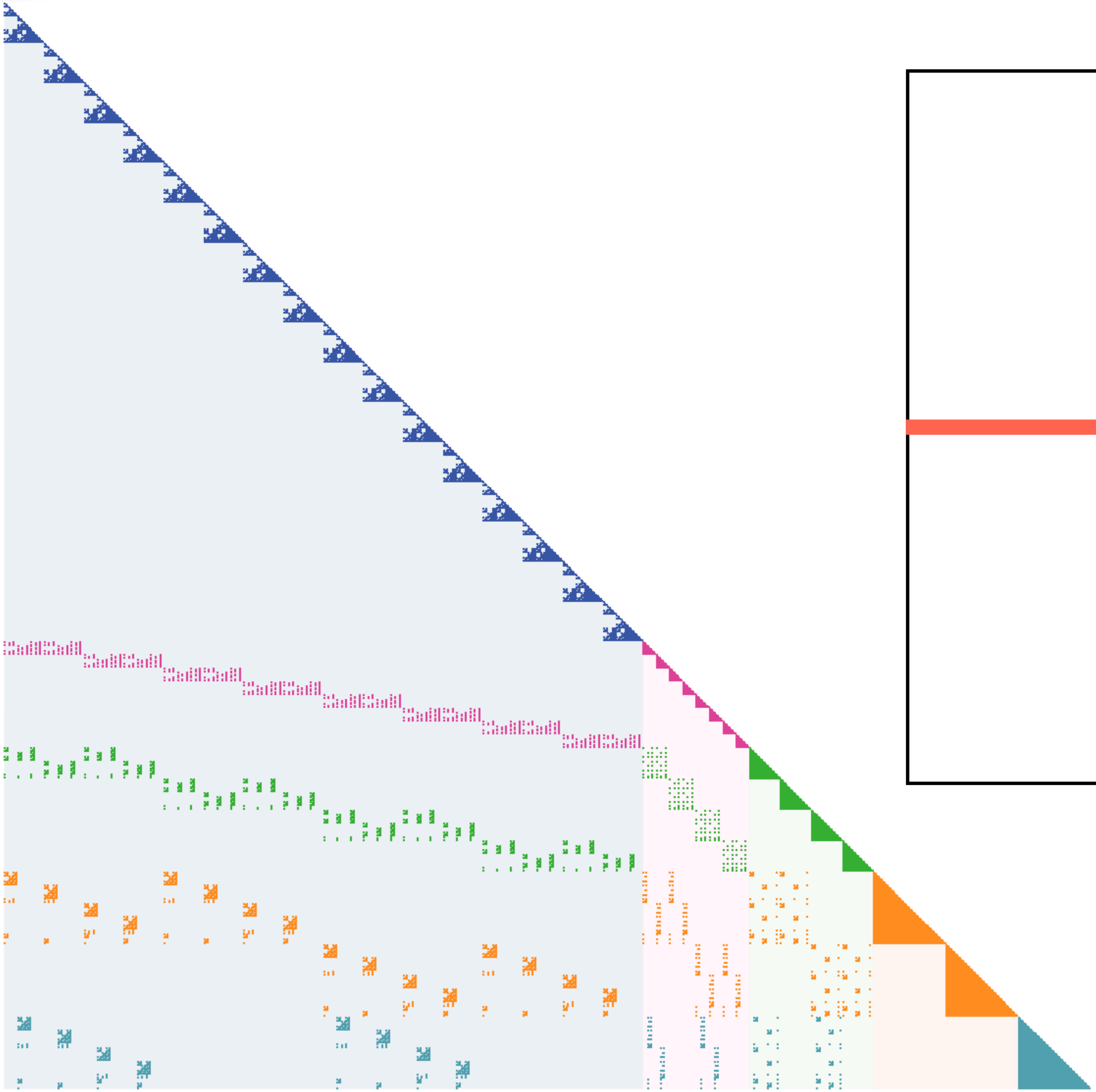

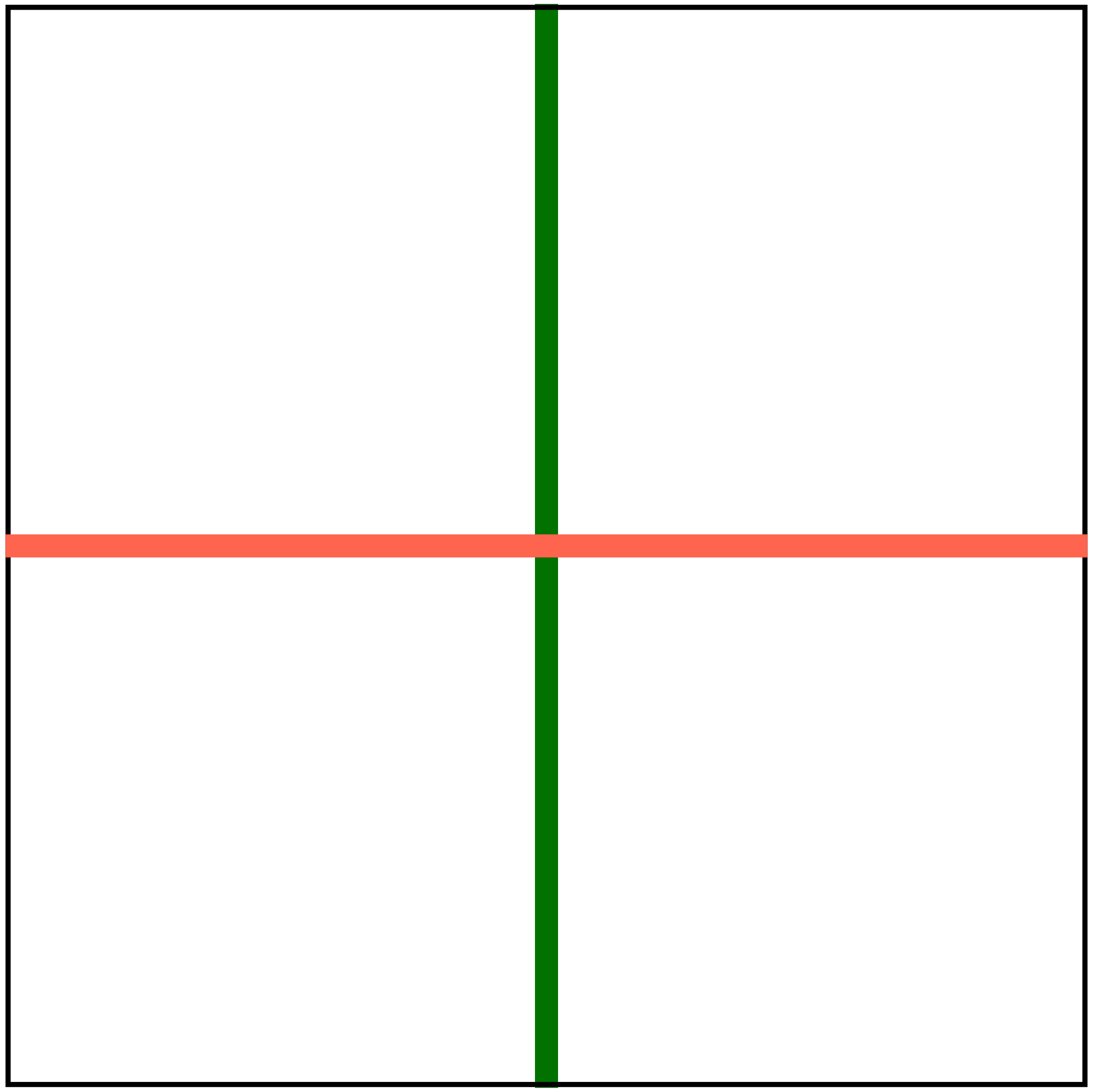

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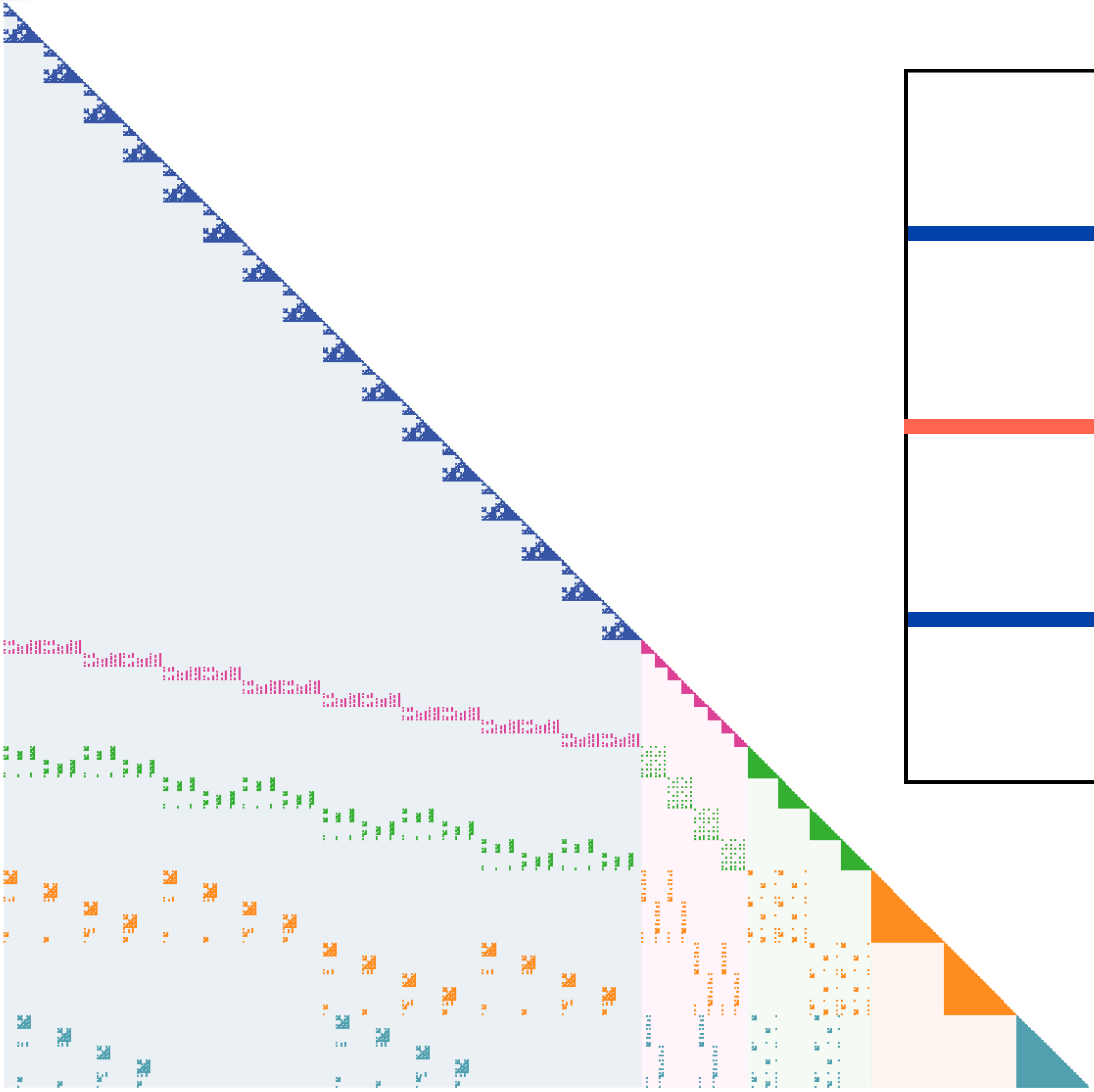
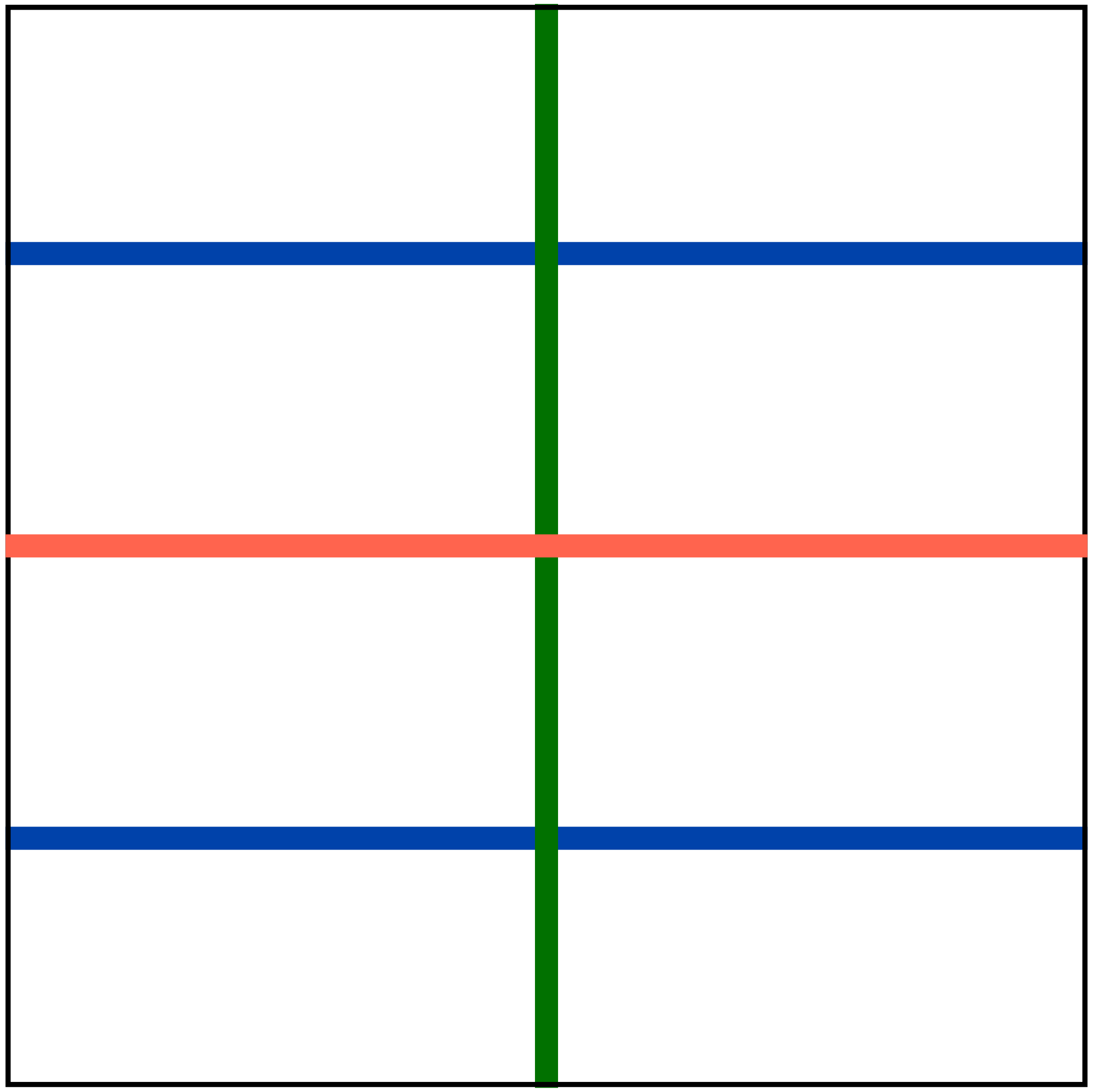
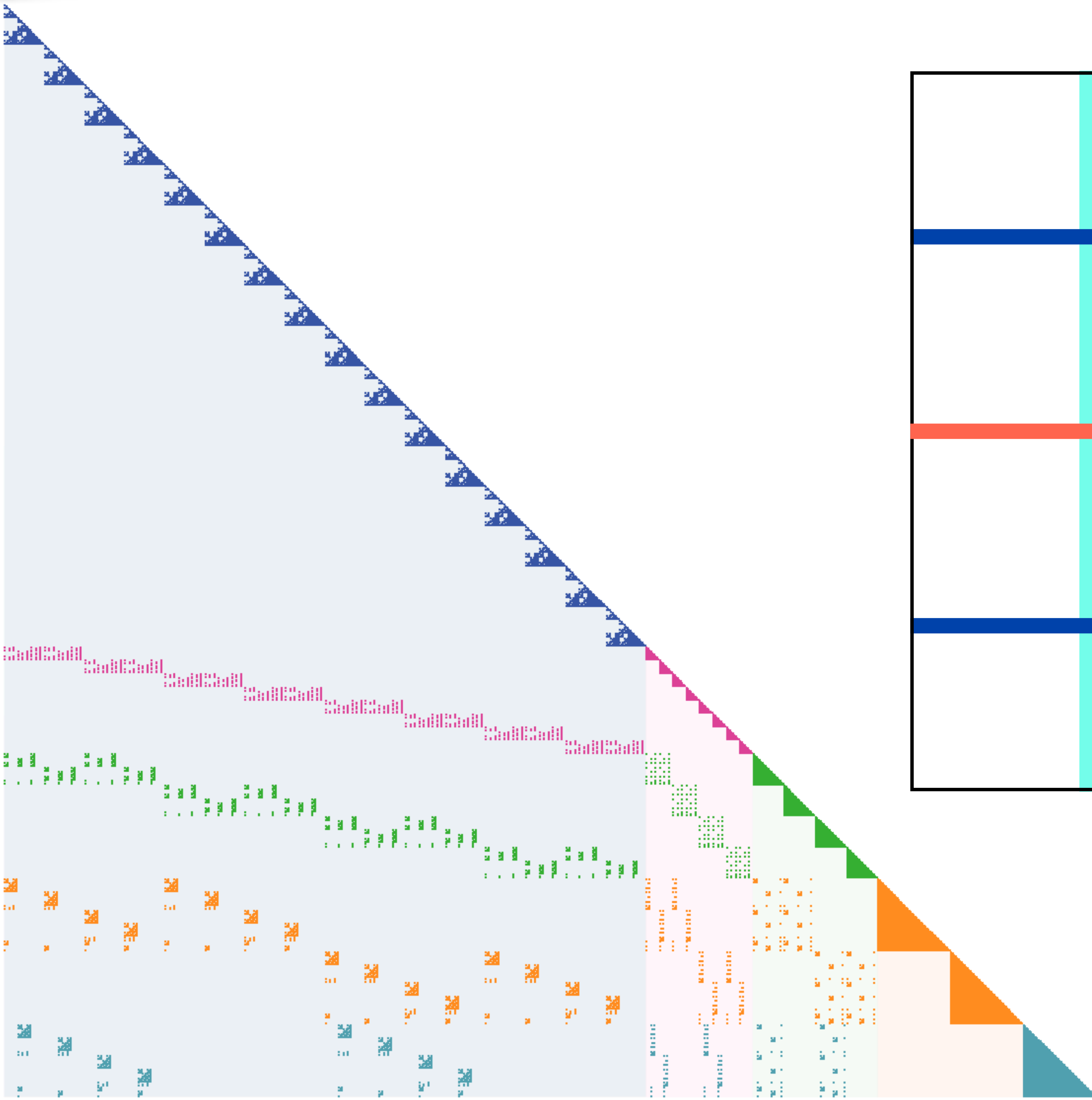
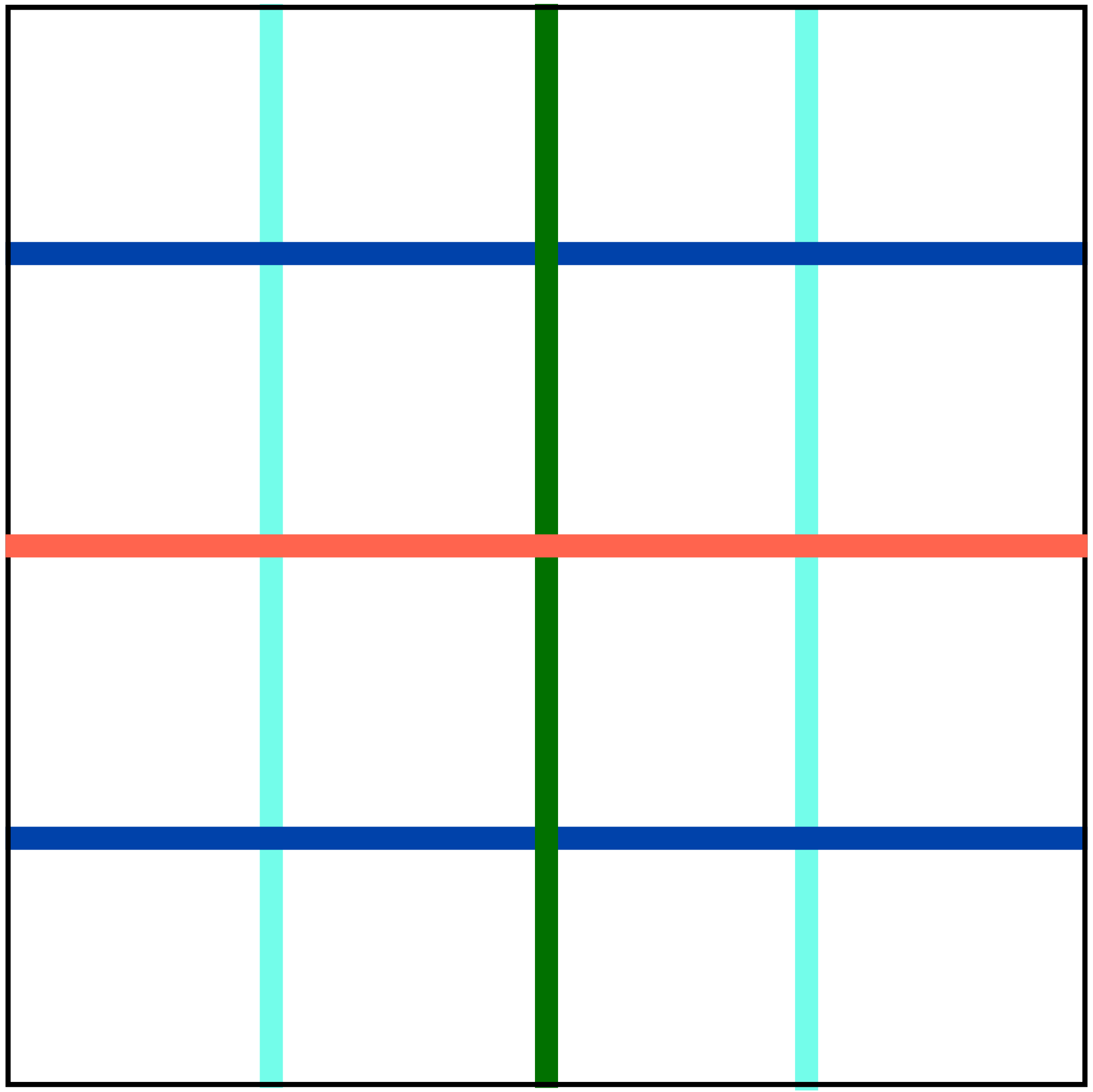


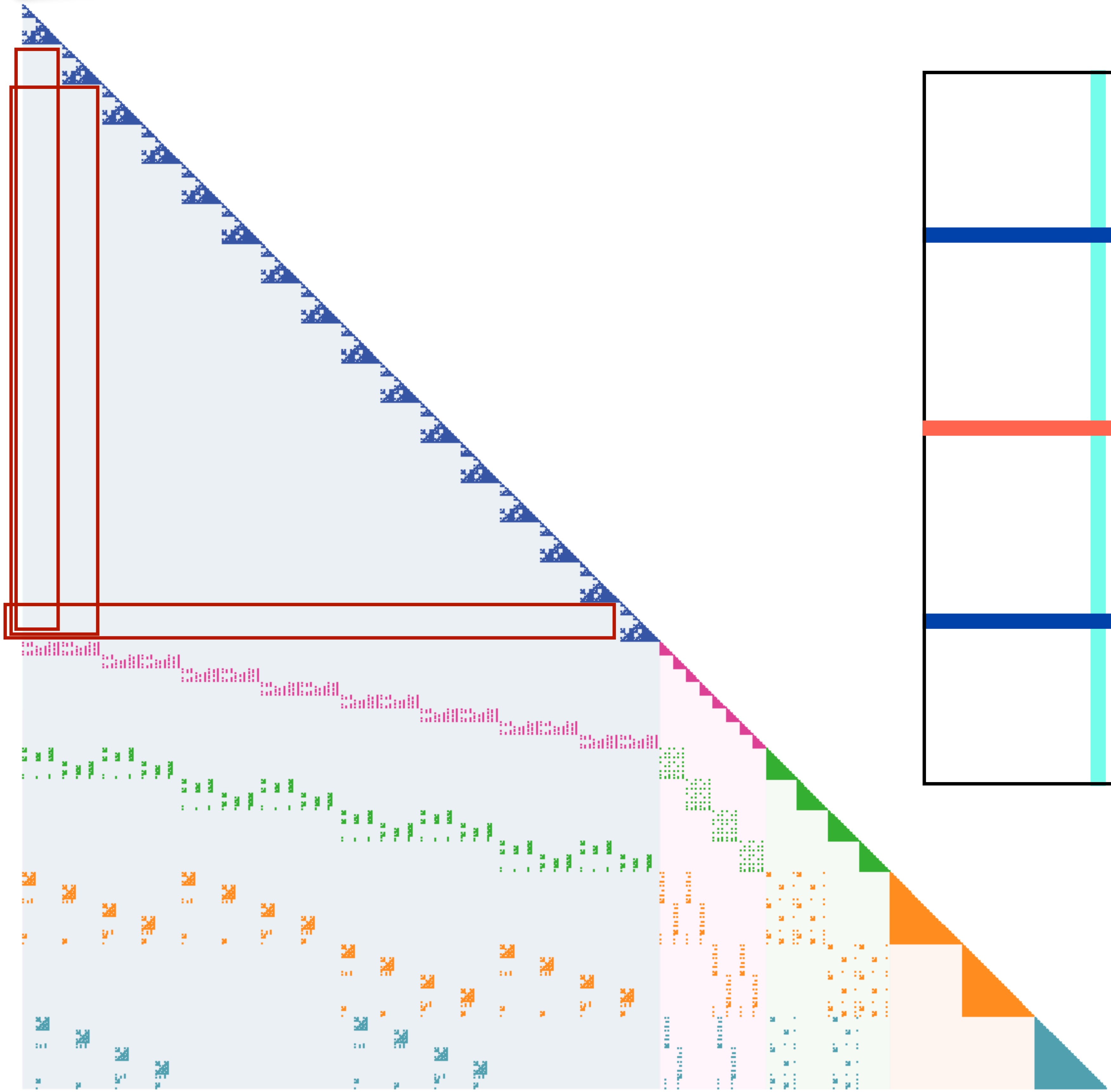


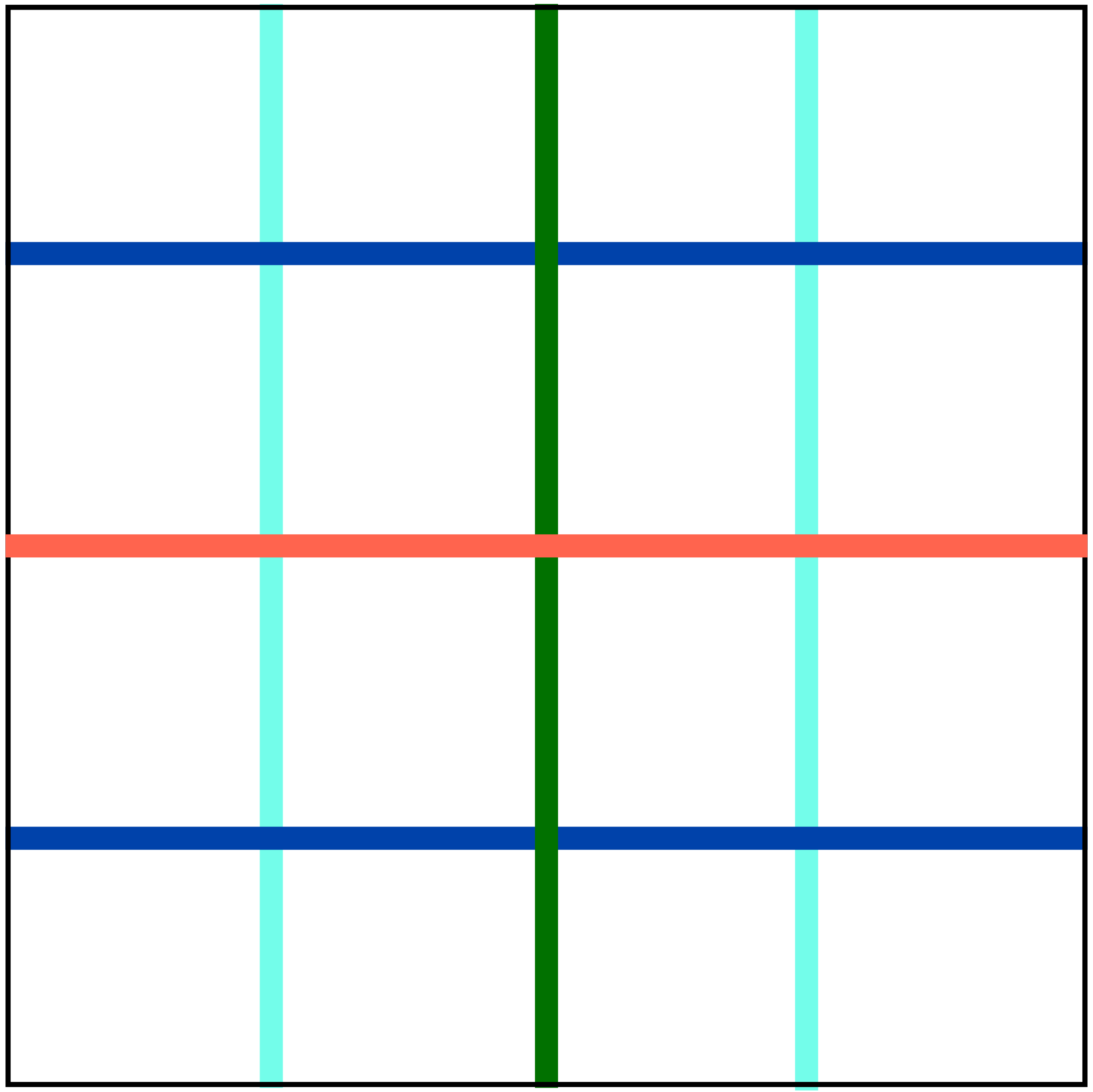
Laplacian - Pattern after a possible reordering



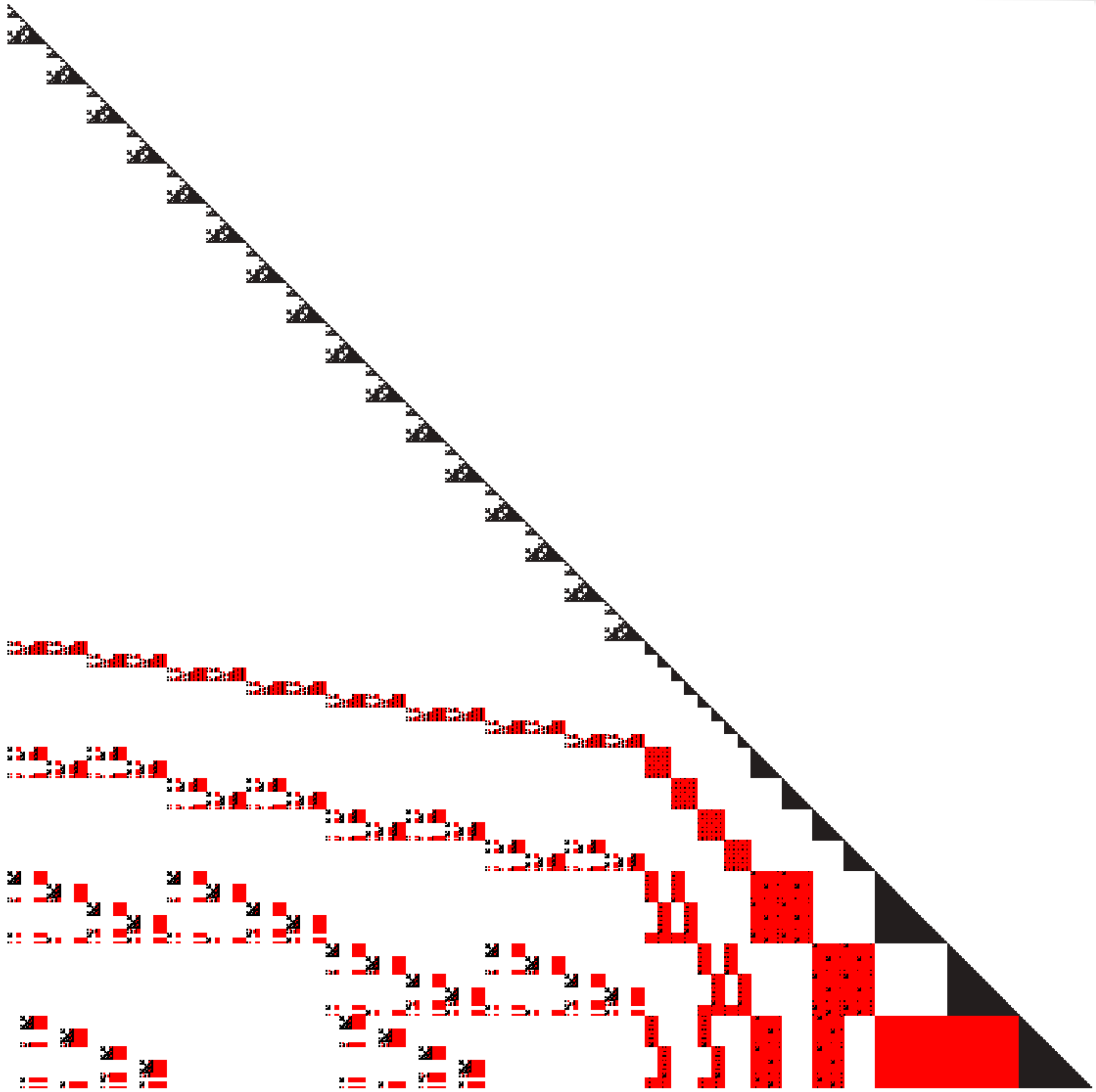


Laplacian - Pattern after a possible reordering

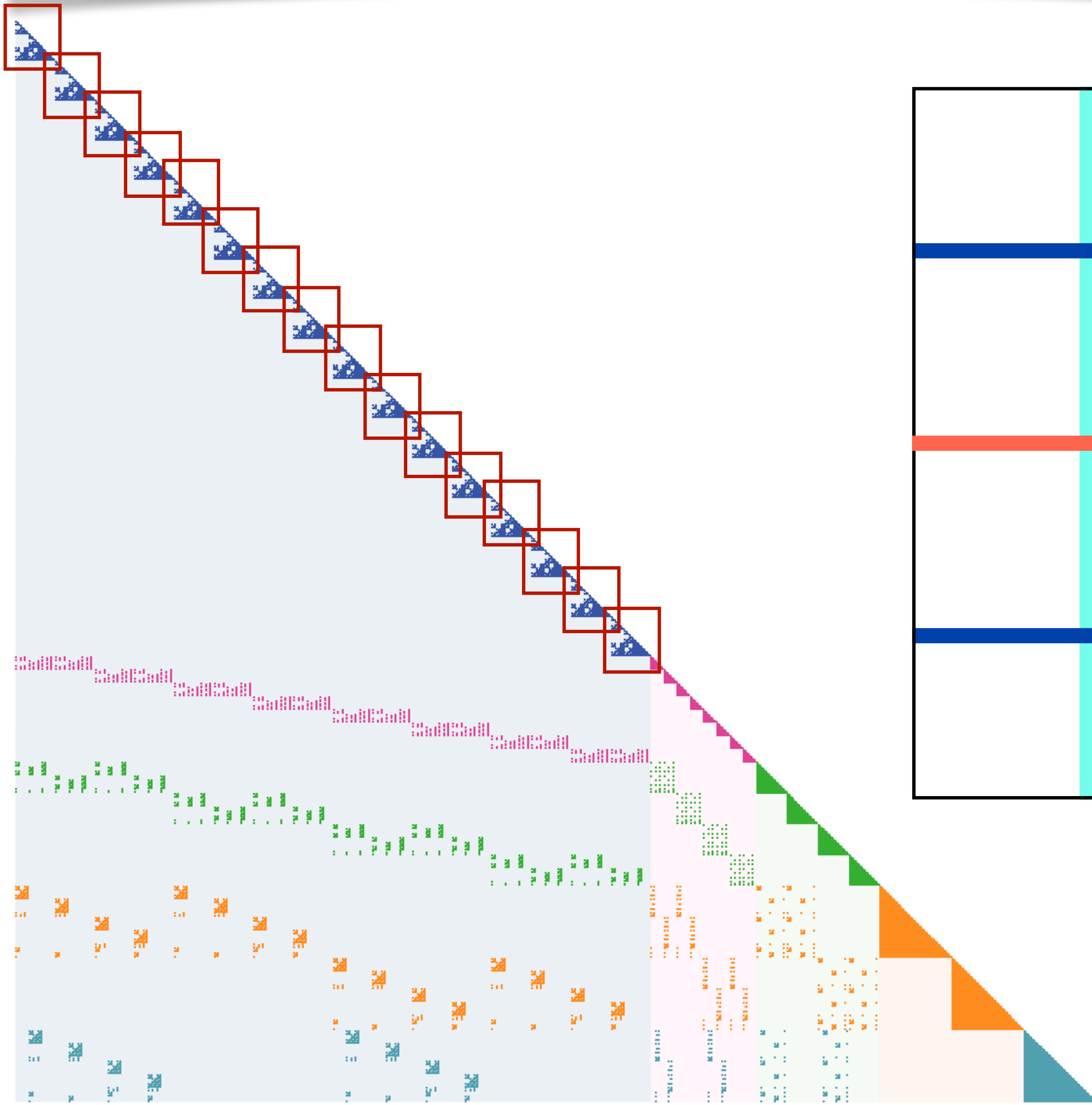


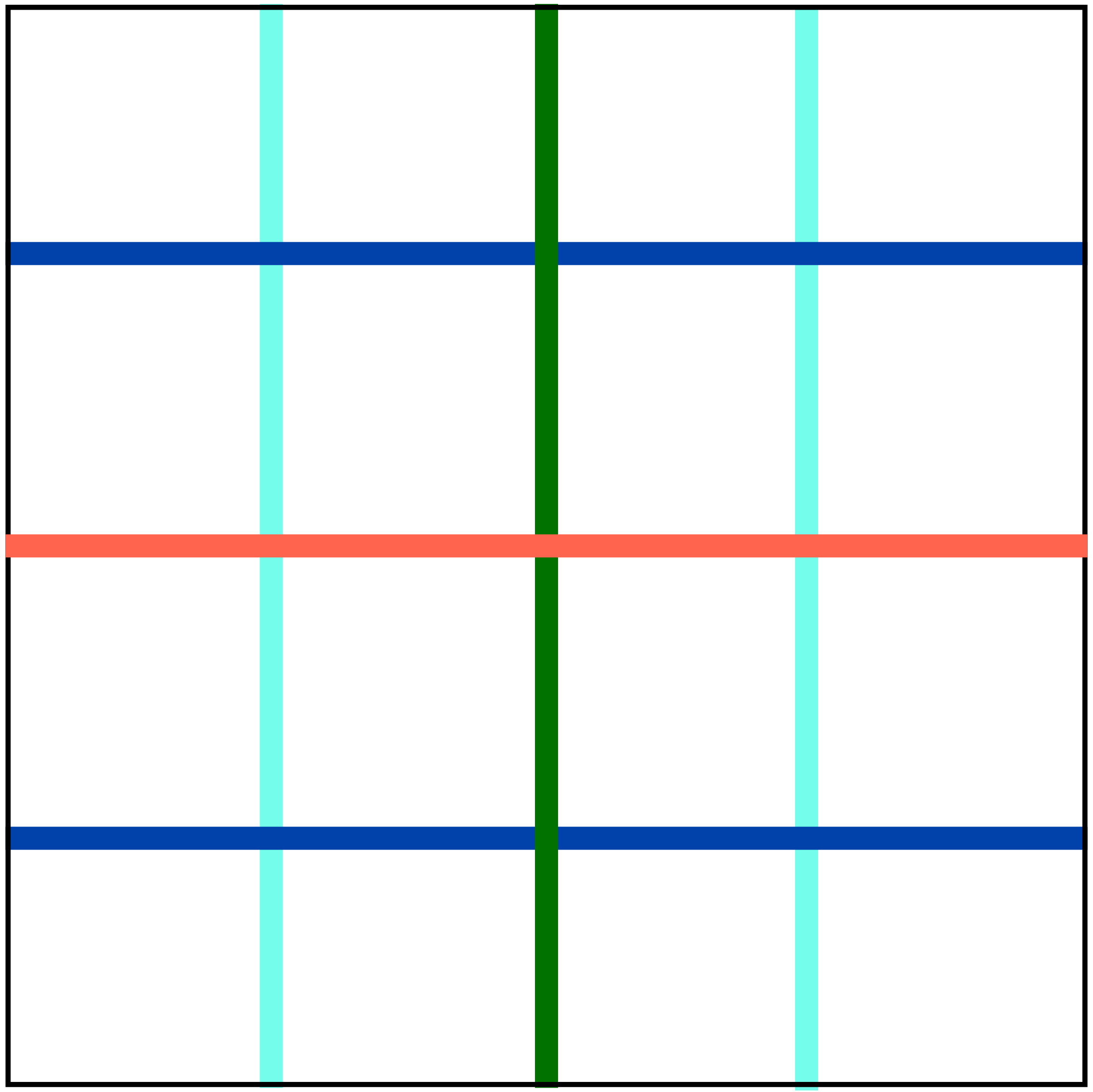


Sparsity of Cholesky Factor (L) vs. Laplacian Matrix



Laplacian - Pattern after a possible reordering





These blocks, too, can be processed in parallel

PARDISO solver (DirectSolver.cpp)

Execution:

```
Summary: ( factorization phase )
================
Times:
======
Time spent in copying matrix to internal data structure (A to LU): 0.000000 s
Time spent in factorization step (numfct)                         : 44.352600 s
Time spent in allocation of internal data structures (malloc)     : 0.022322 s
Time spent in additional calculations                             : 0.000002 s
Total time spent                                                  : 44.374928 s
Statistics:
===========
Parallel Direct Factorization is running on 20 OpenMP
< Linear system Ax = b >
             number of equations:           2097152
             number of non-zeros in A:      8050652
             number of non-zeros in A (%): 0.000183
             number of right-hand sides:    1
< Factors L and U >
             number of columns for each panel: 96
             number of independent subgraphs:  0
             number of supernodes:                    1410153
             size of largest supernode:               16591
             number of non-zeros in L:                2057589566
             number of non-zeros in U:                1
             number of non-zeros in L+U:              2057589567
             gflop   for the numerical factorization: 22775.748047
             gflop/s for the numerical factorization: 513.515503

Factorization completed ...
 PARDISO (pt, &maxfct, &mnum, &mtype, &phase, &n,
```

About 90% of overall runtime (sometimes less)

Almost 25% of peak arithmetic utilization

Obstacles to performance & parallelism

Matrix Density : *The number of required operations scale (super-linearly …) with the number of non-zero entries in **L** … thus, ensuring sparser **L** factors has an immediate effect on performance*

Multithreading : *Cholesky, similar to Gauss Elimination, is seemingly a very “serial” algorithm (significant dependencies between steps/loops). We must find some way to cope with this apparent limitation.*

Vectorization/SIMD : *Sparse matrices don’t have the regularity that SIMD operations require; we need to “engineer” such regularity if possible*