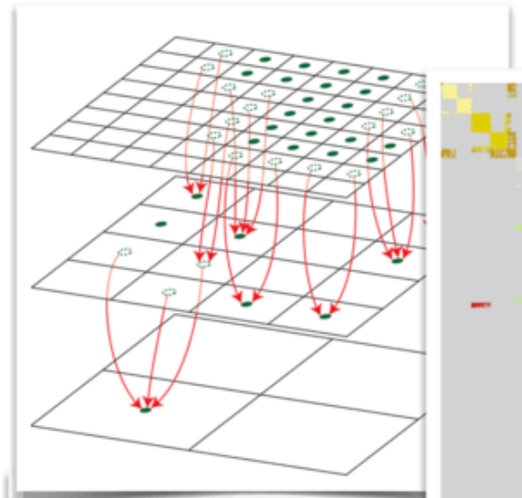
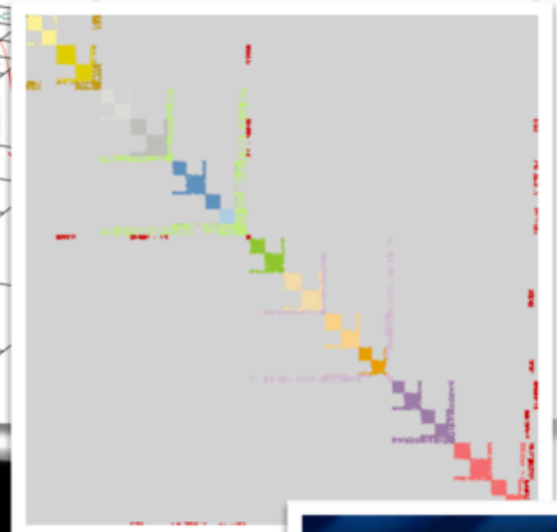
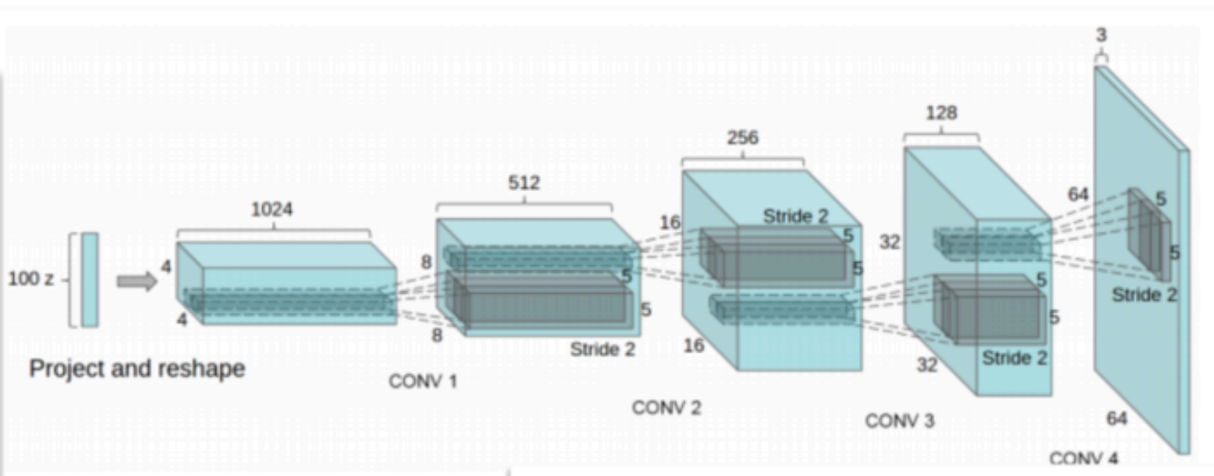
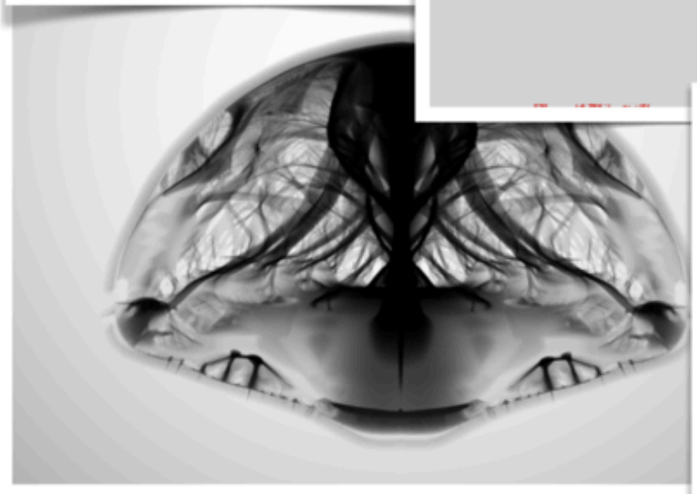
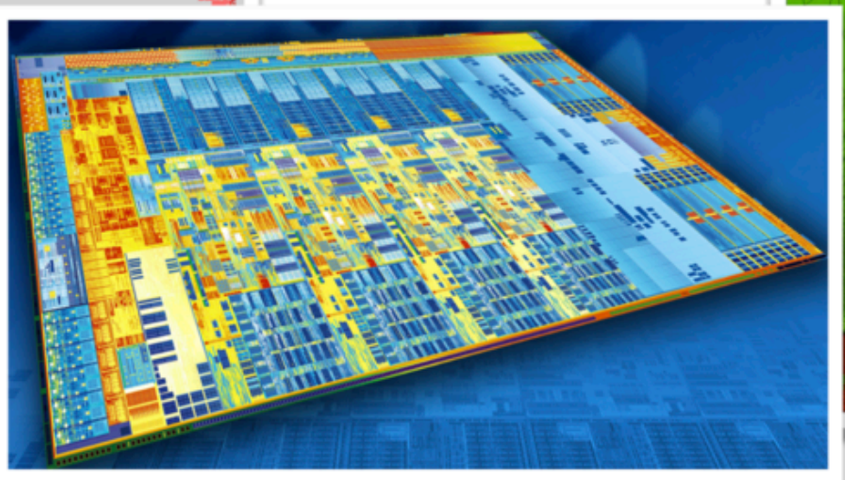
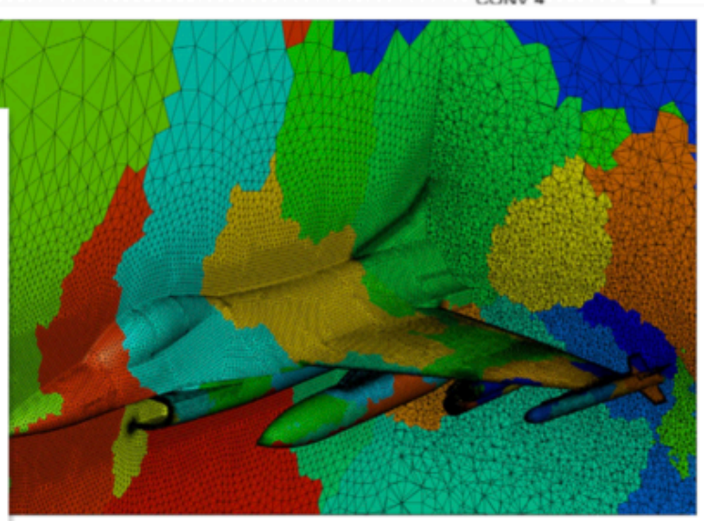












Lecture 20: Engineering regularity and vectorization potential in MKL PARDISO. Sparse direct solvers wrap-up A first look at indirect array access & prefetching.

Tuesday April 13th 2021

Logistics

- HW#4 to be released this week
- Working through grading backlog (thanks for your patience!) Expect midterm and HW1 by end-of-week, HW2/3 by next.

Today's lecture

- Wrapping-up discussion of *sparse direct* system solvers.

- High-level discussion of the tricks and methods that MKL PARDISO employs to engineer parallelism (primarily ways to engineer regularity, and expose and vectorization opportunities)

- A first look at a "Sparse Saxpy" workload, as an exemplar of indirect array access, and prefetching implications

Sparse Factorizations:
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.

SparseDirect/LaplacePARDISO_0_0

PARDISO solver (DirectSolver.cpp)

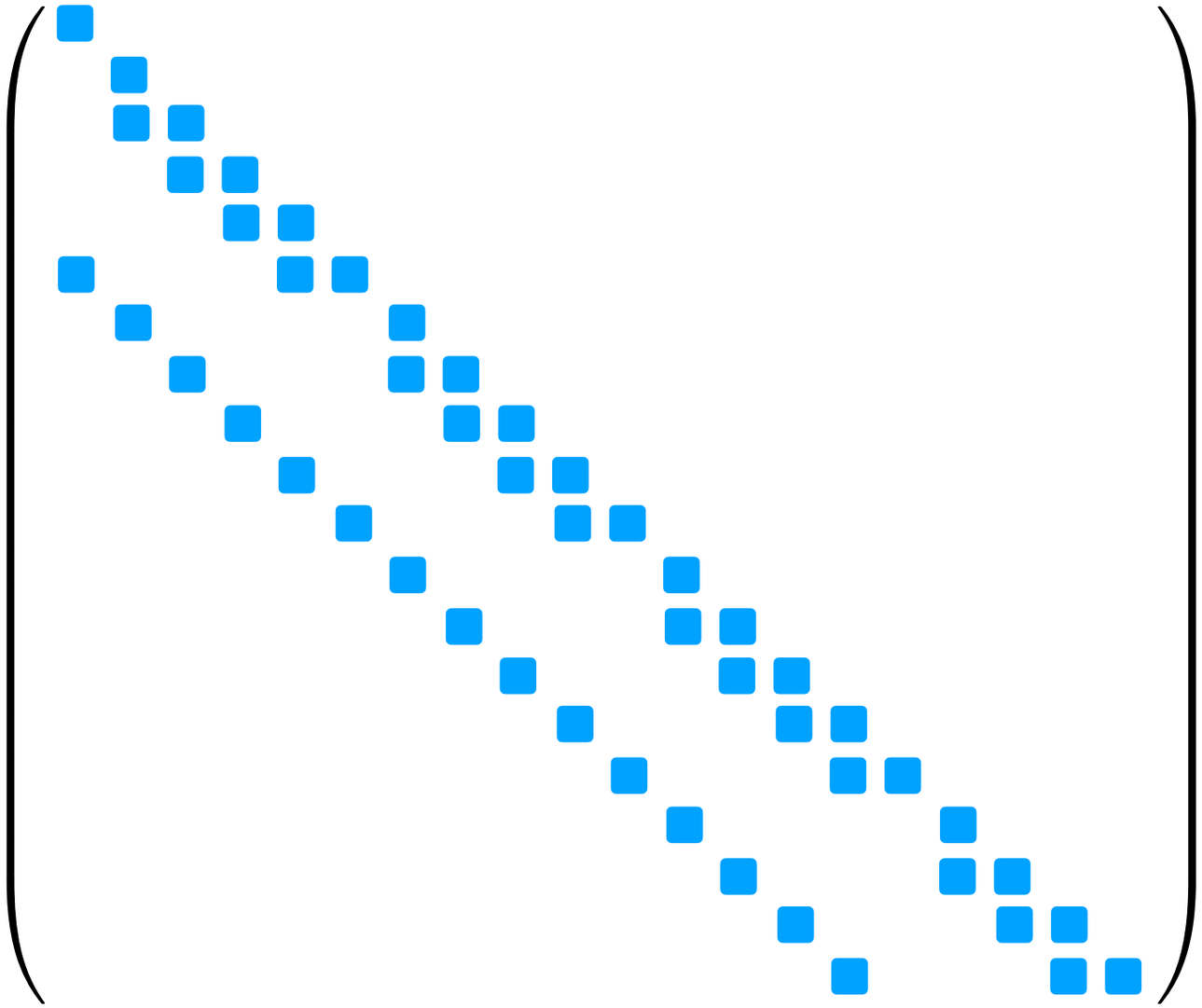
Execution:

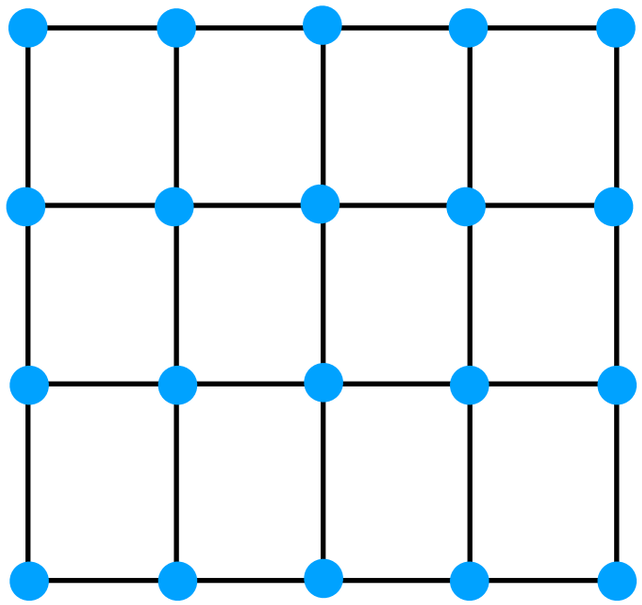
```
Summary: ( factorization phase )
================
Times:
======
Time spent in copying matrix to internal data structure (A to LU): 0.000000 s
Time spent in factorization step (numfct)                        : 44.352600 s
Time spent in allocation of internal data structures (malloc)    : 0.022322 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)

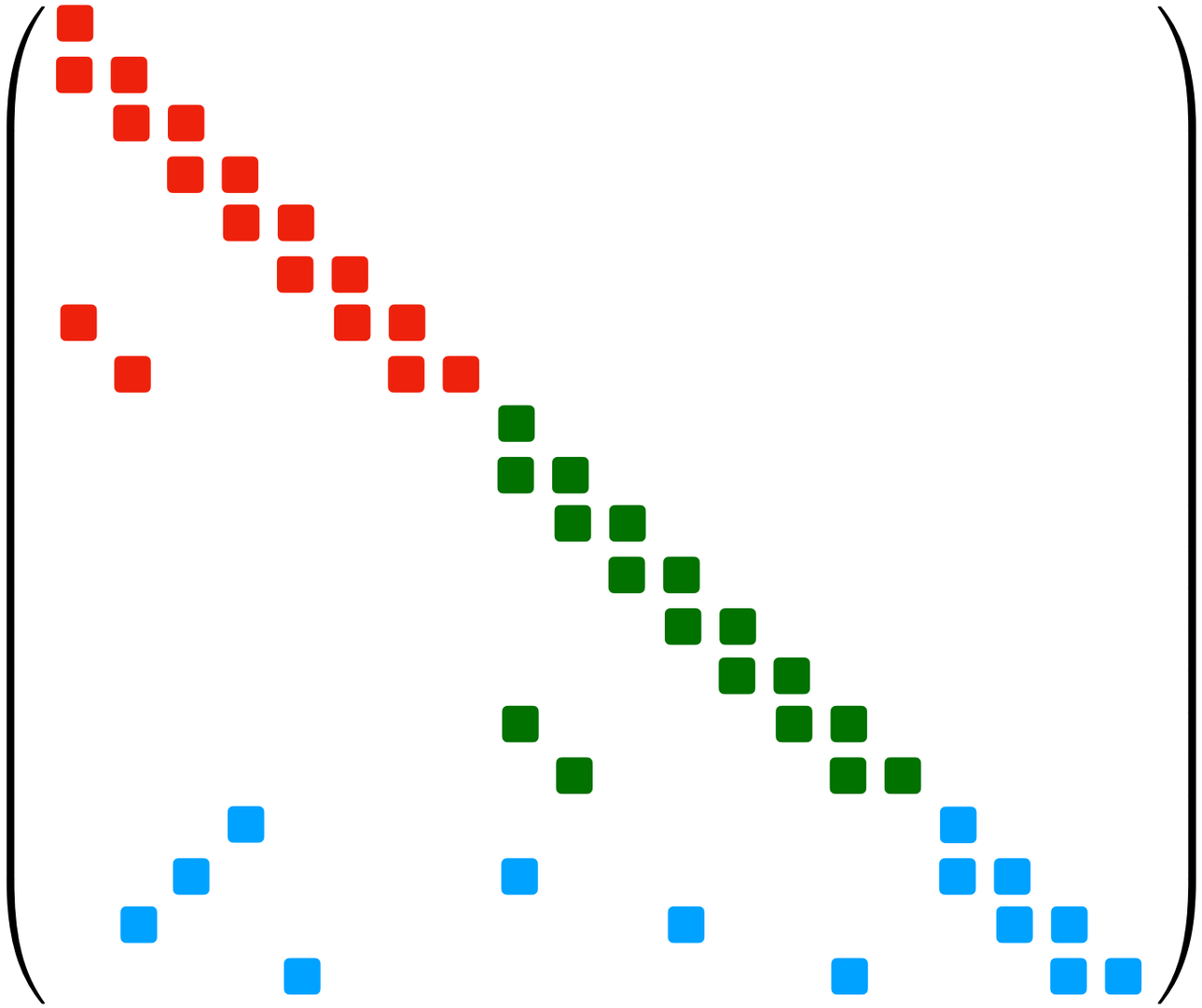
Almost 25% of peak arithmetic utilization

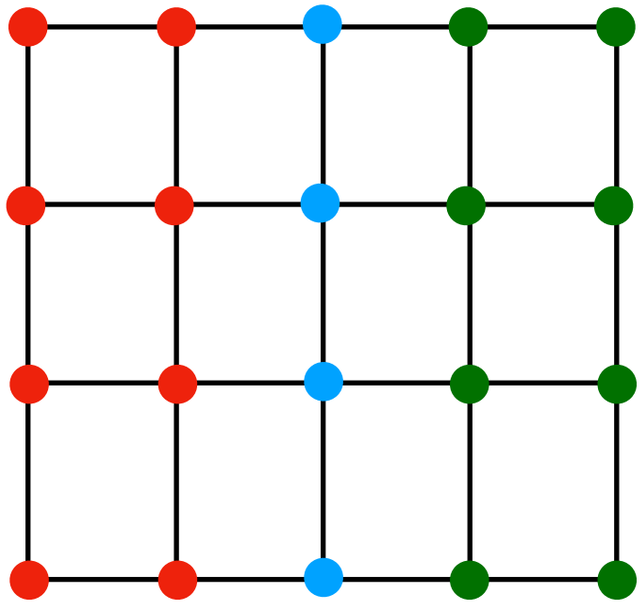
Engineering/Maximizing Sparsity



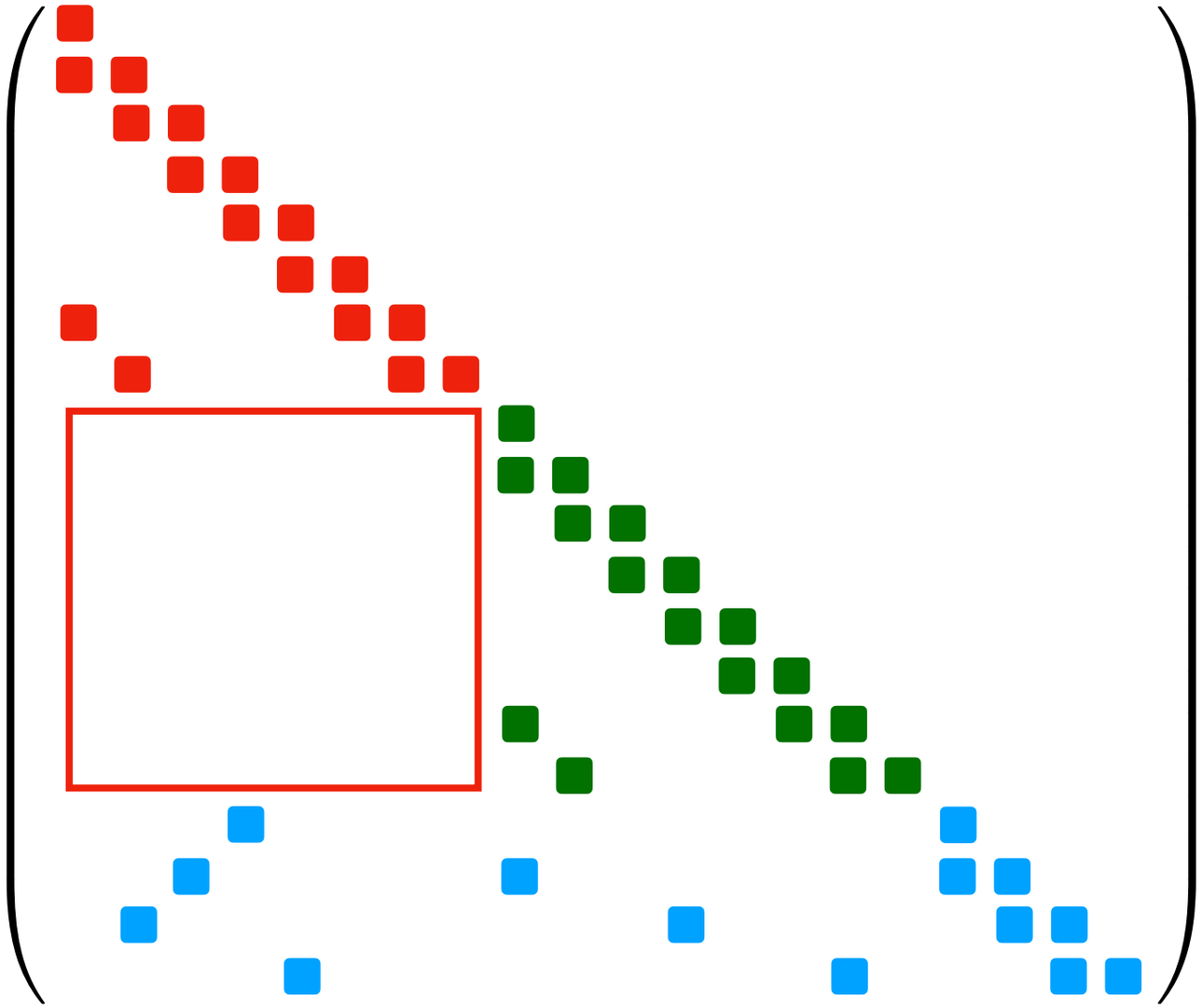


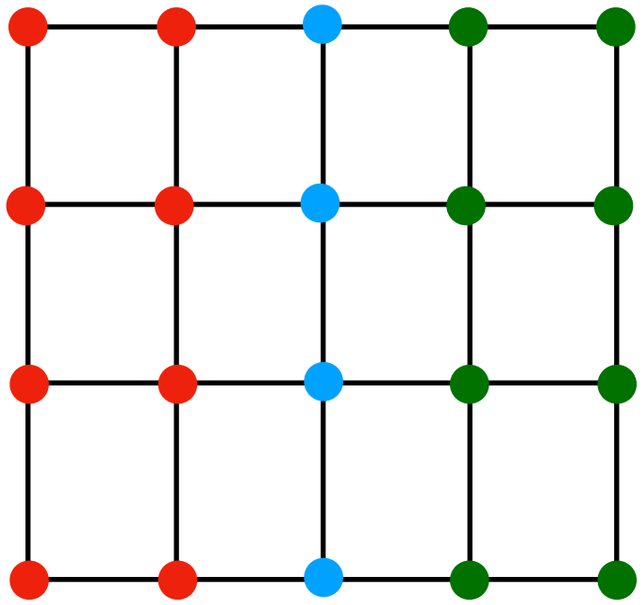
Engineering/Maximizing Sparsity





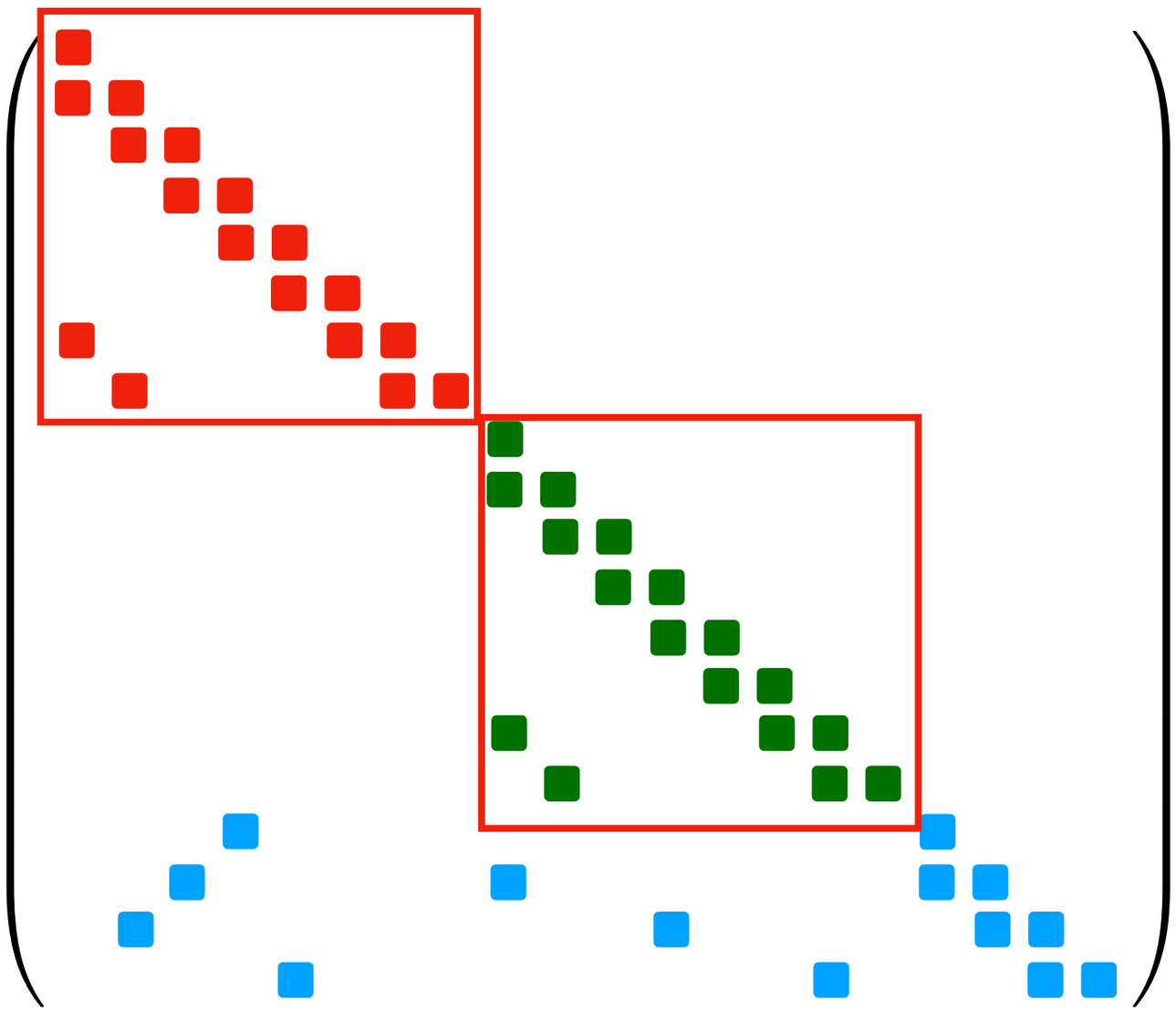
Engineering/Maximizing Sparsity





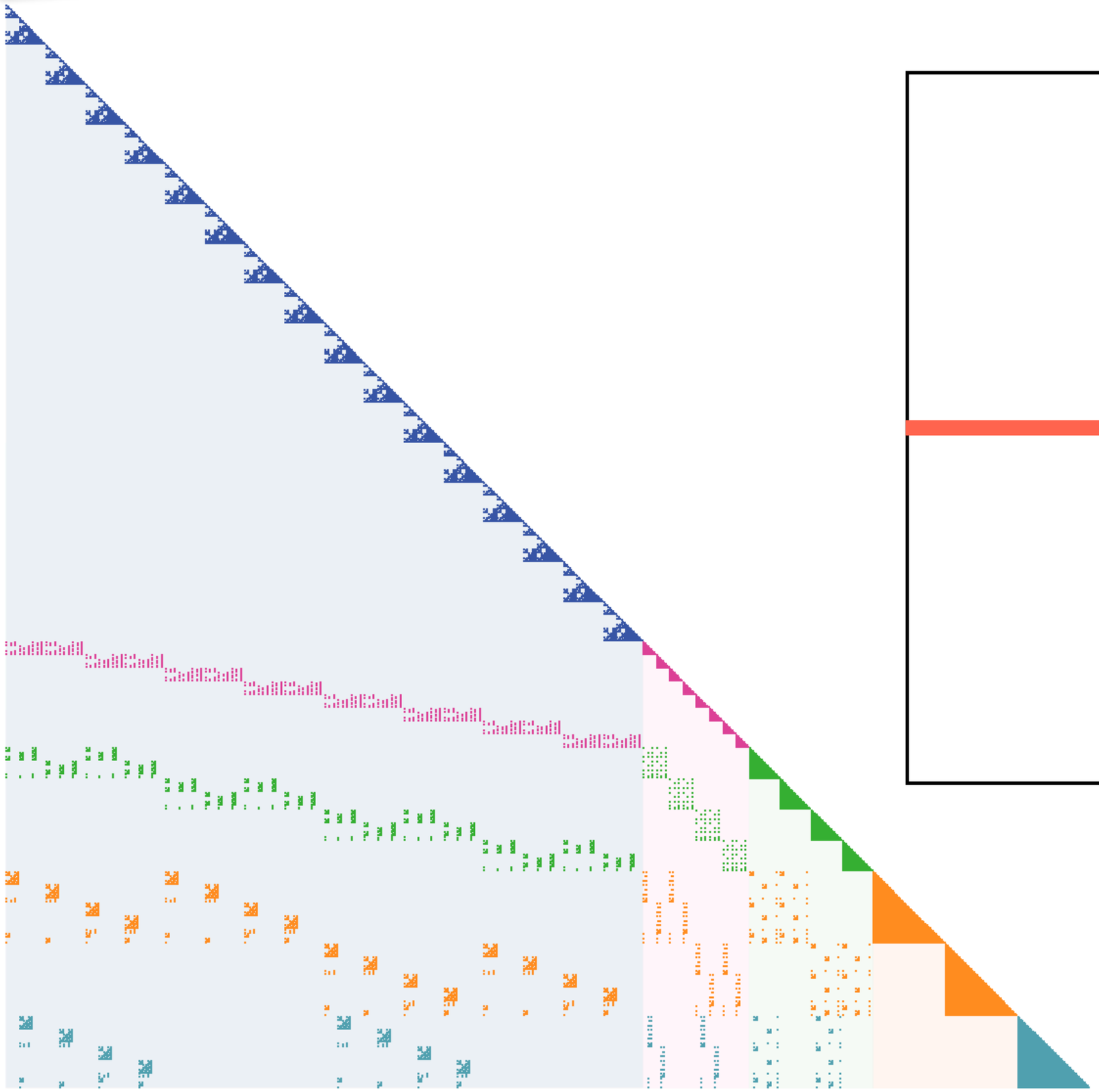
Cholesky splits matrix into two factors which are triangular, A=LL^T. The gaps are introduced by changing the numbering from the lexicographical order. The benefit of this is that any entry of the matrix at row i and col j will be non zero iff they have a spoke in the grid. It also allows doing the red and green parts independently, for instance performing Gaussian Elimination.

Engineering/Maximizing Sparsity

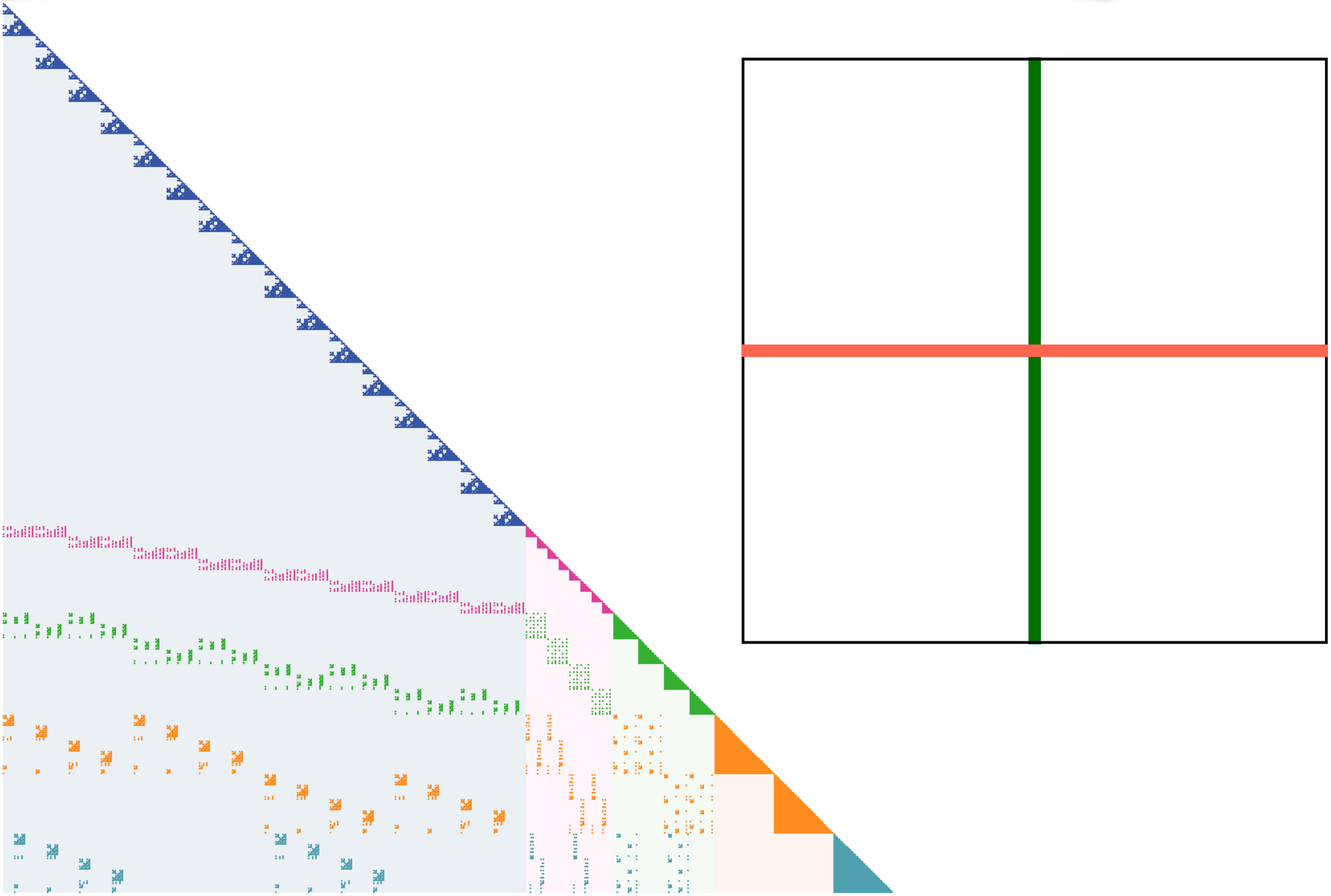


Second benefit:
Cholesky can process each of these two blocks in-parallel!

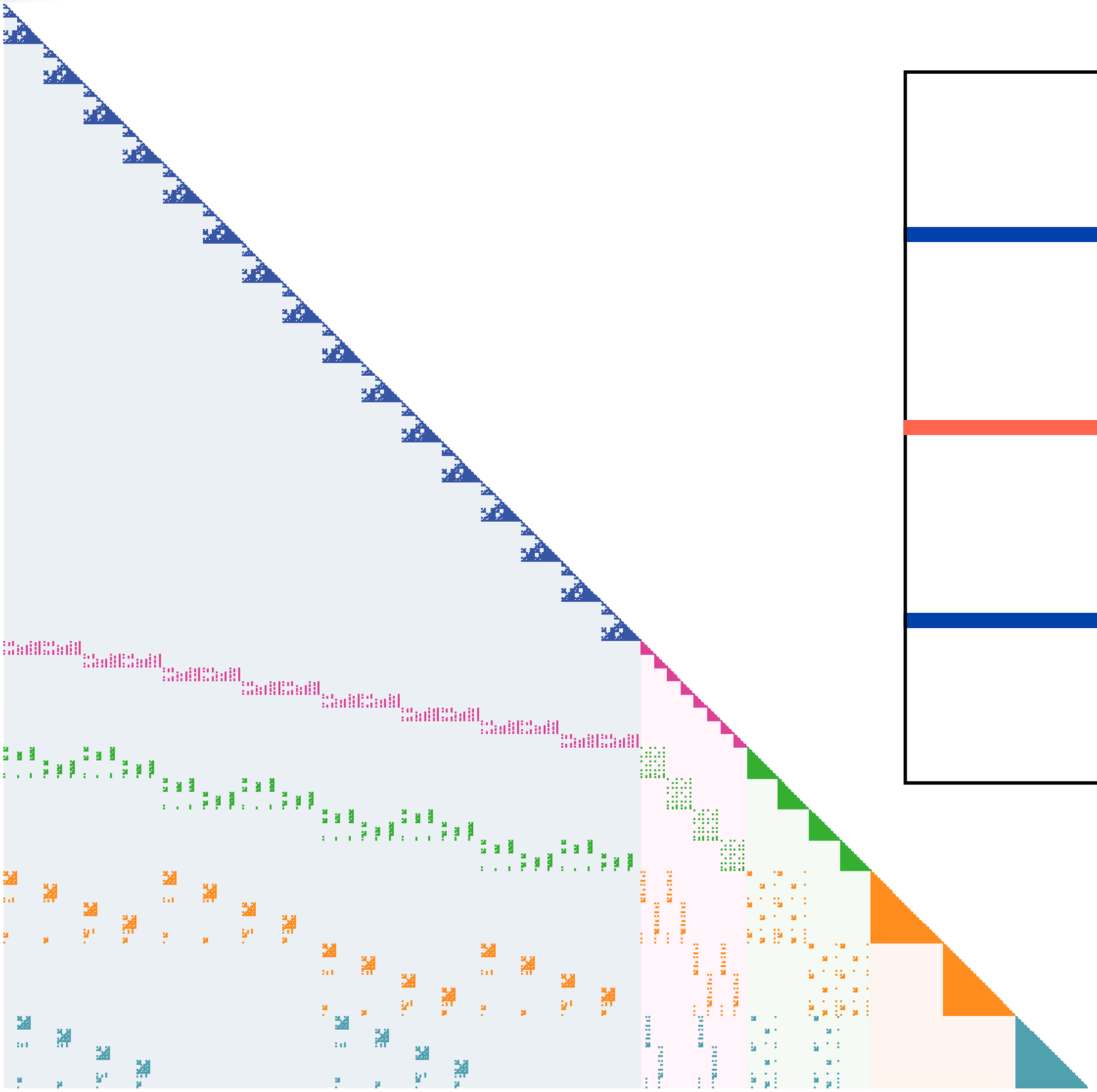
Laplacian - Pattern after a possible reordering

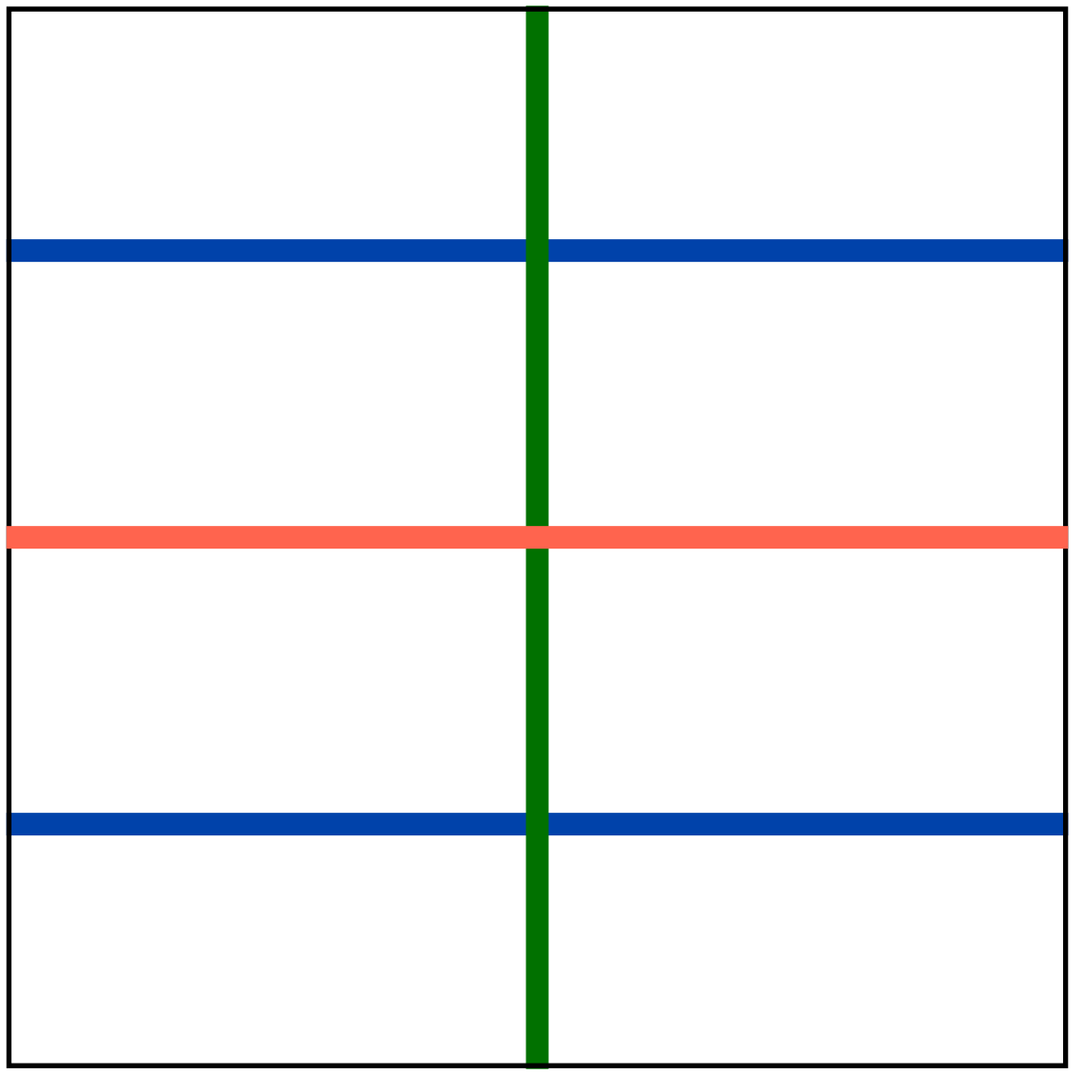


Laplacian - Pattern after a possible reordering

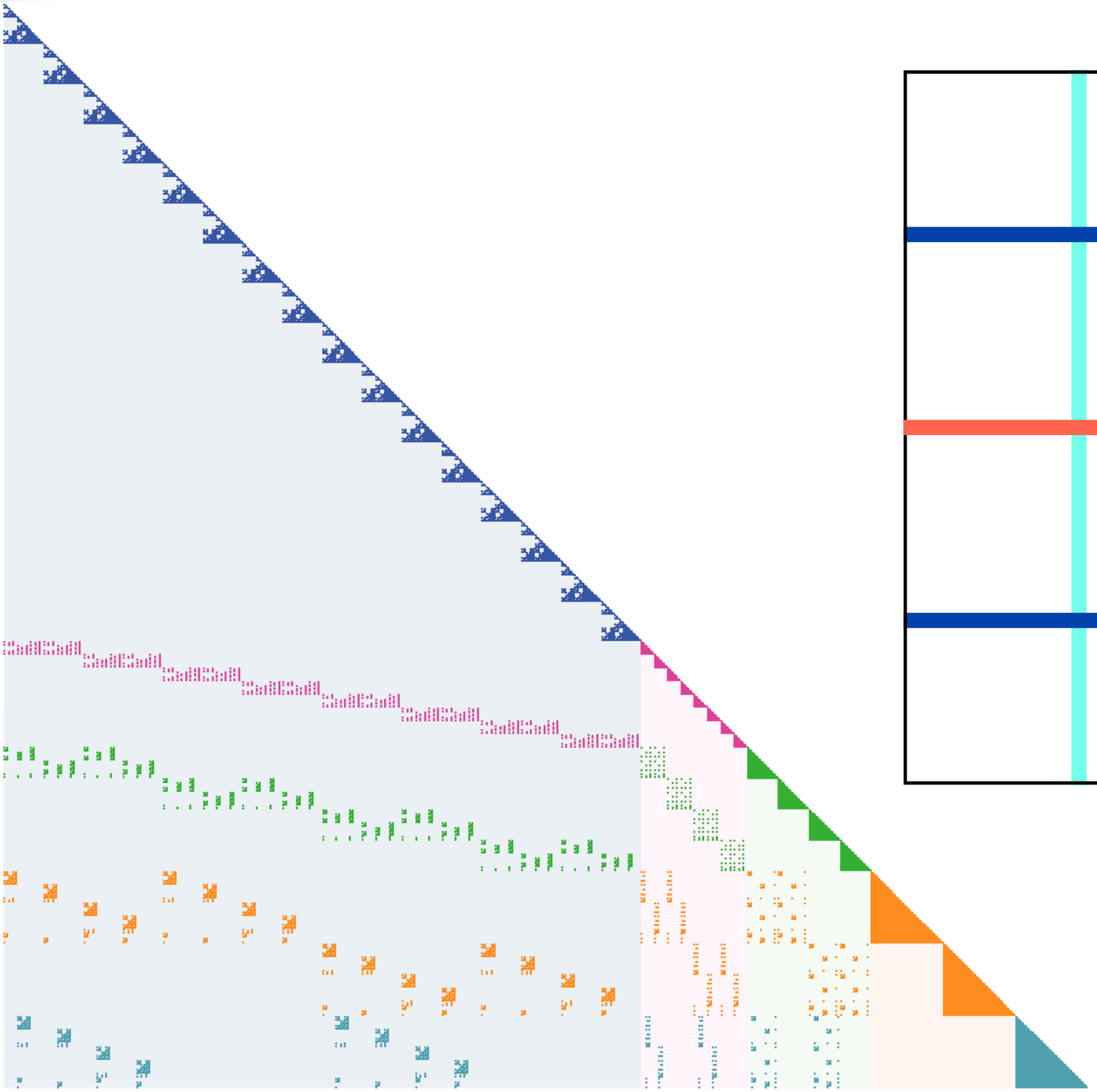


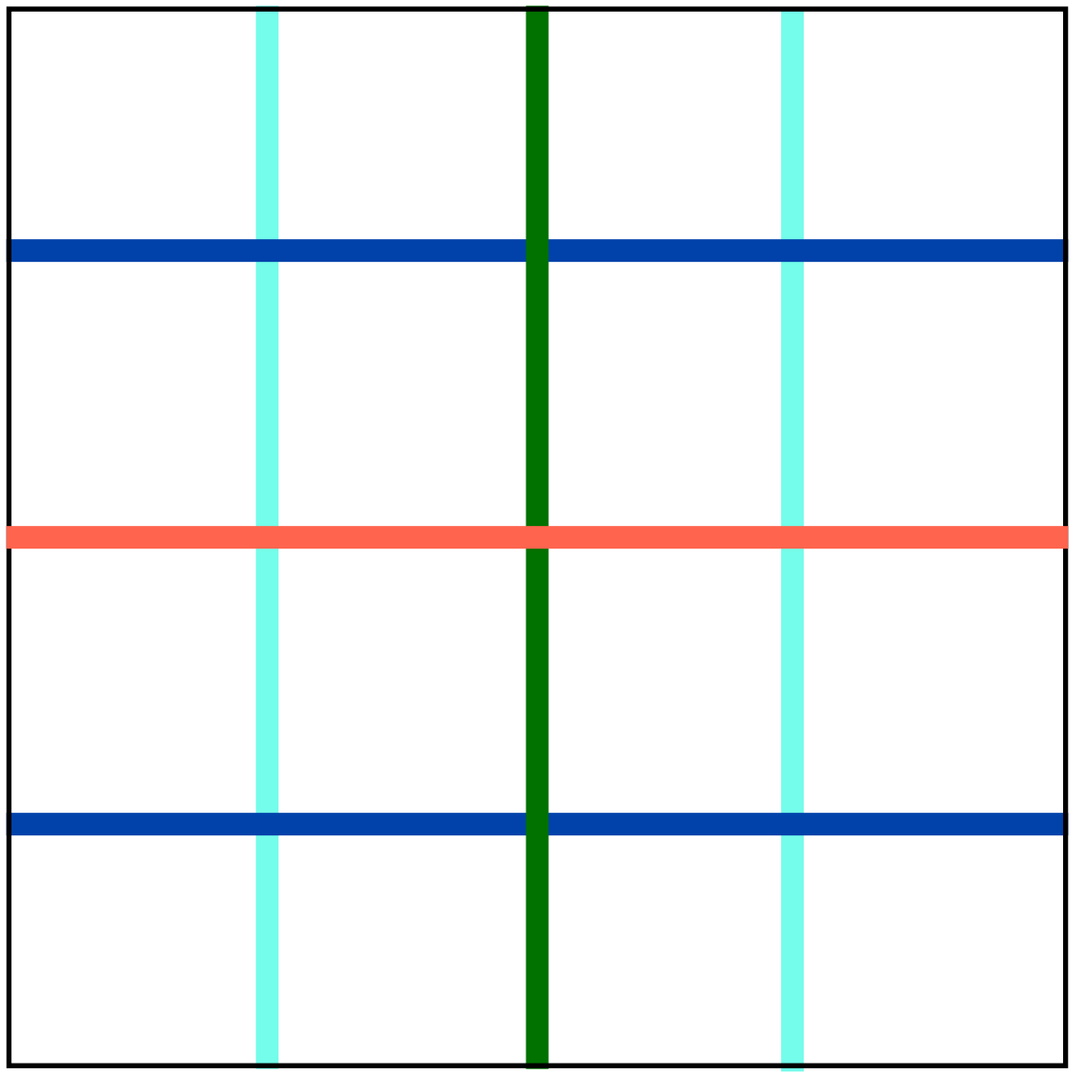
Laplacian - Pattern after a possible reordering



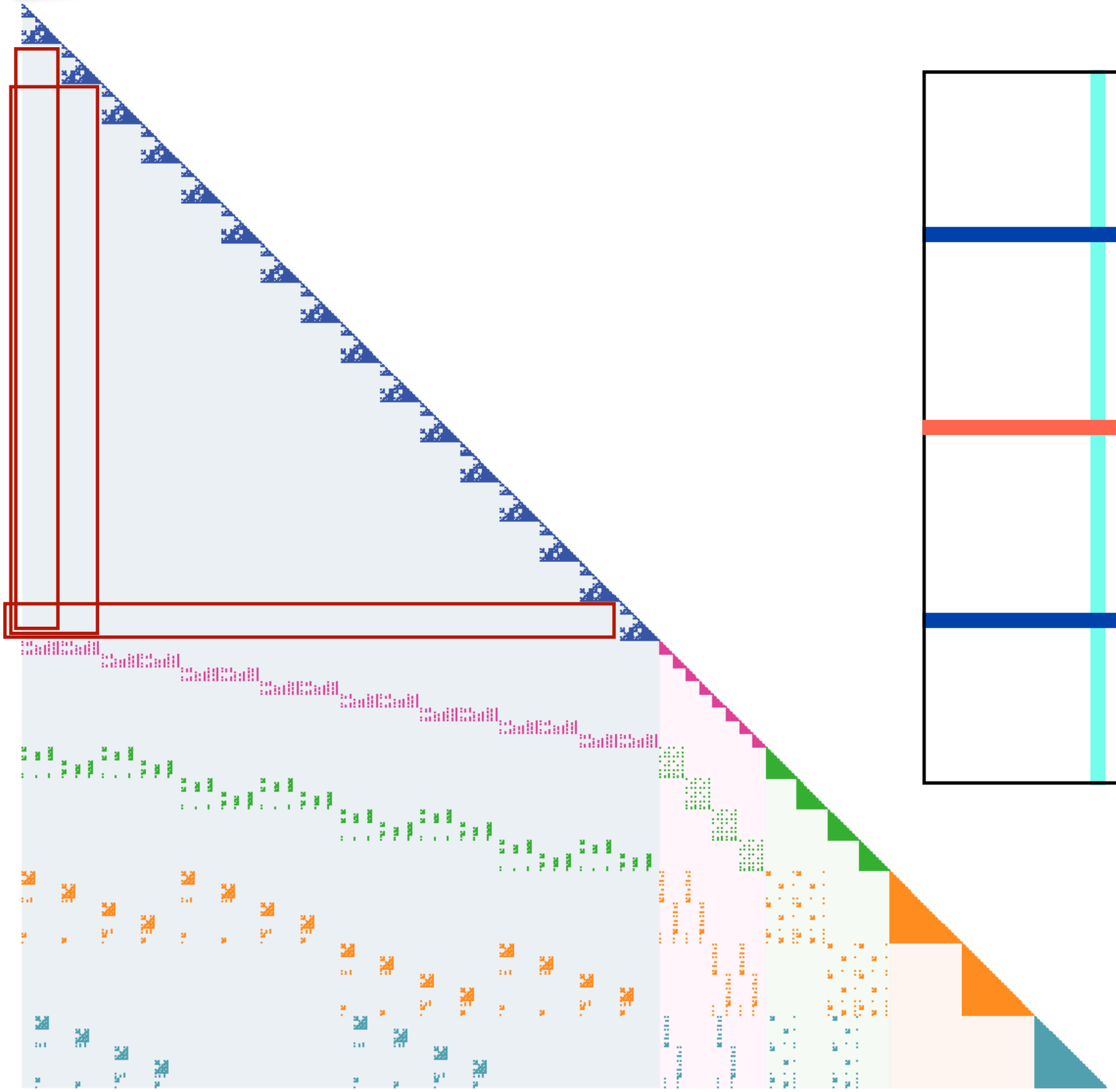


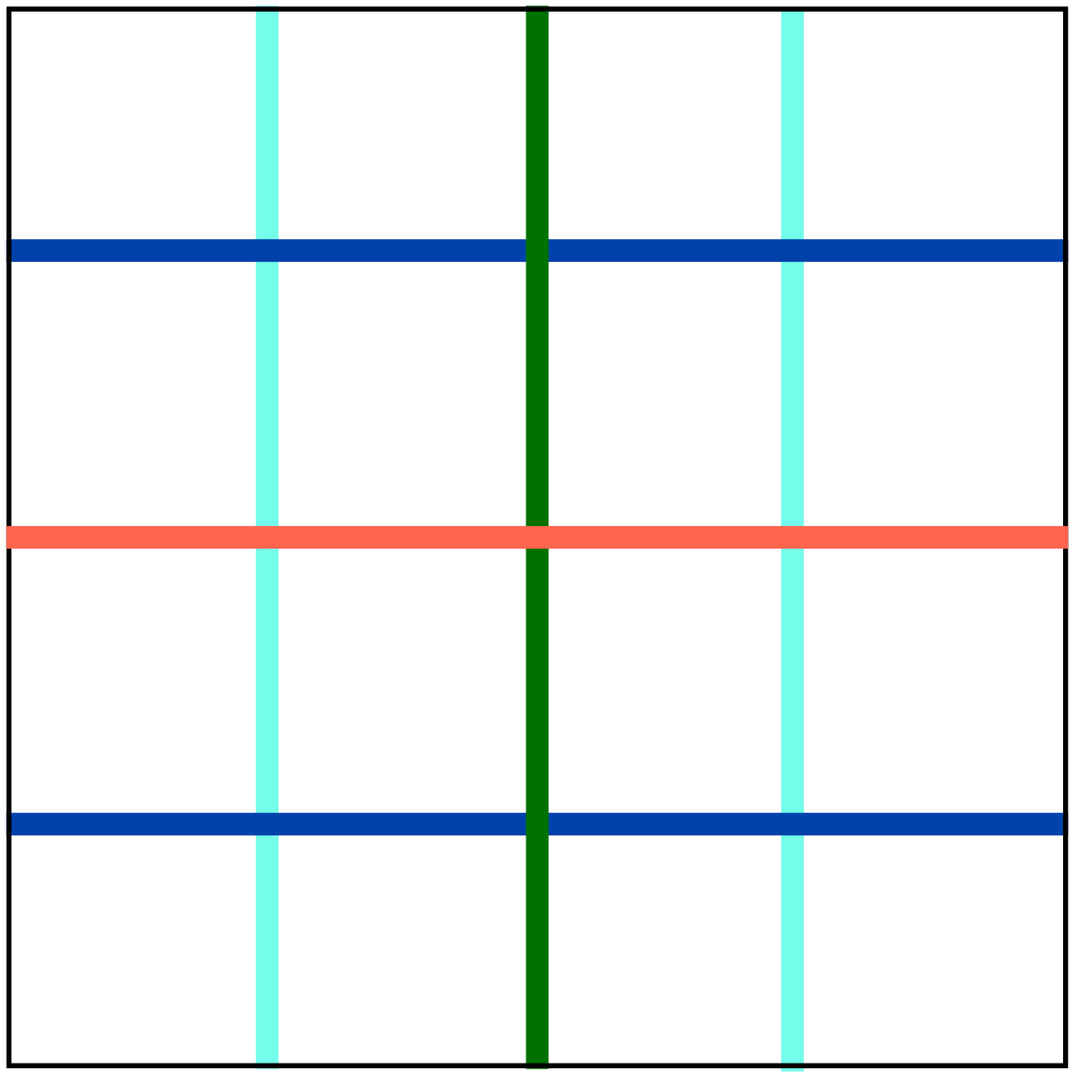
Laplacian - Pattern after a possible reordering



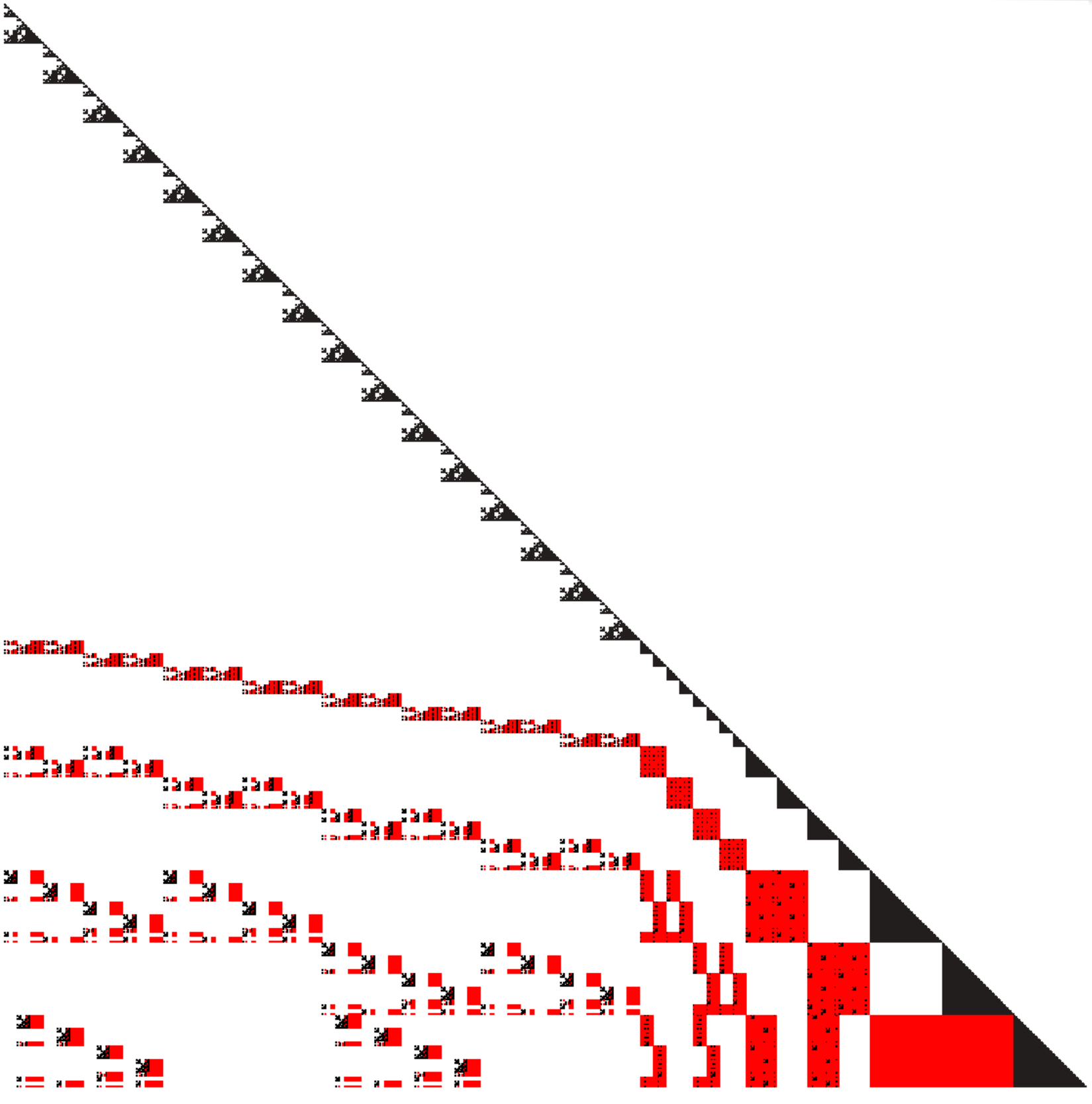


Laplacian - Pattern after a possible reordering

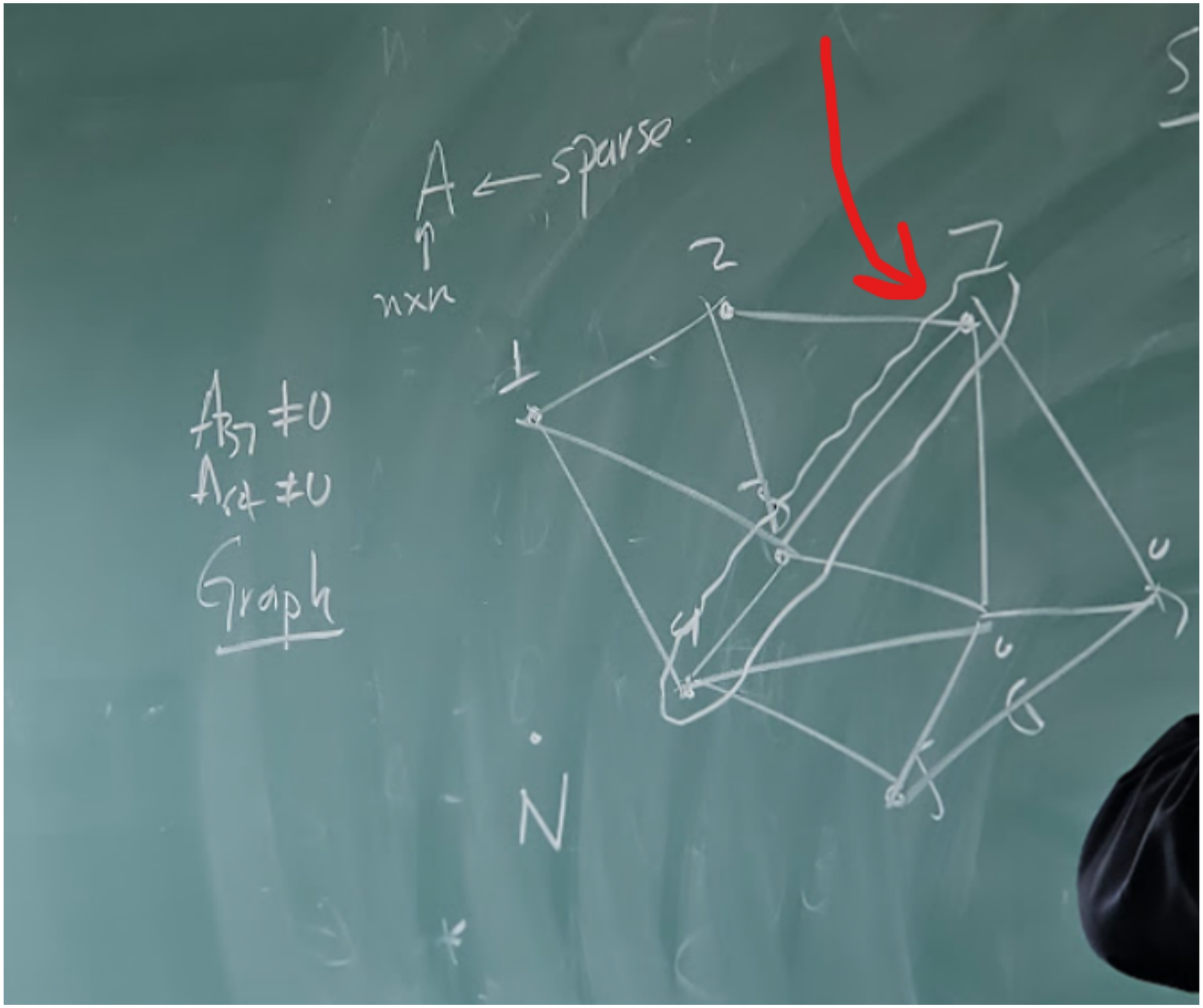




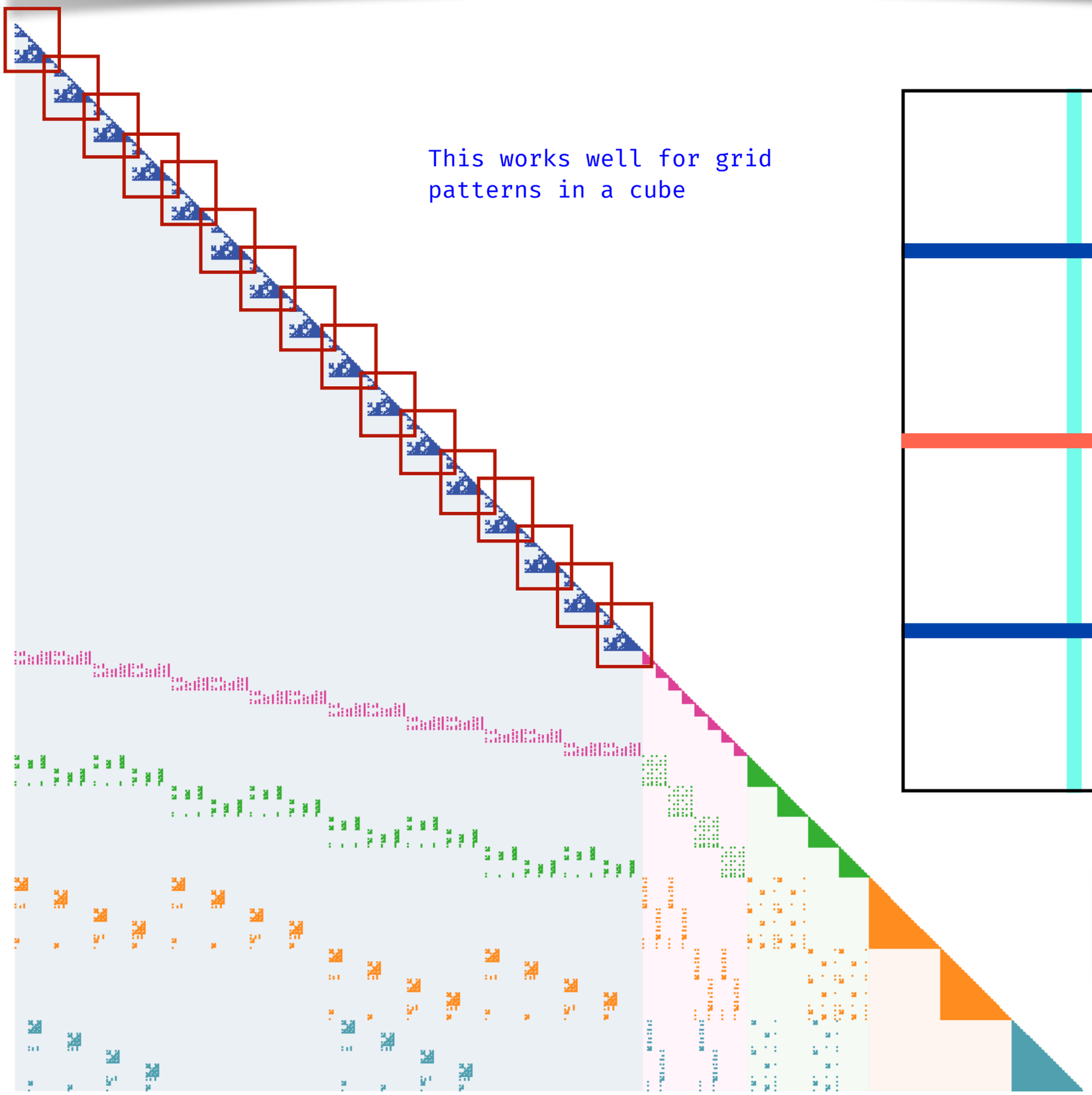
Sparsity of Cholesky Factor (L) vs. Laplacian Matrix



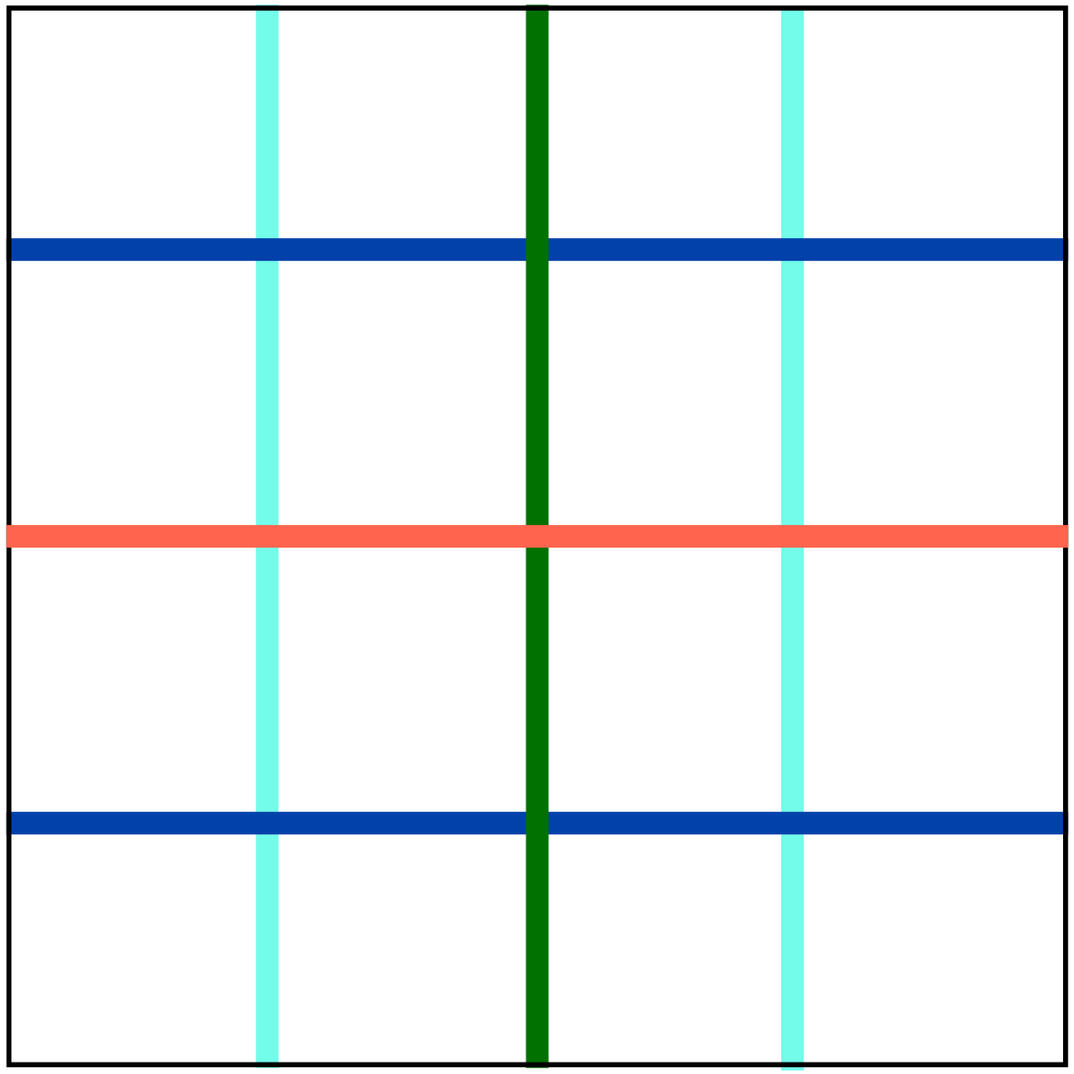
Separation possible in graphs for independent parallelism



Laplacian - Pattern after a possible reordering



This works well for grid patterns in a cube



These blocks, too, can be processed in parallel

Obstacles to performance & parallelism

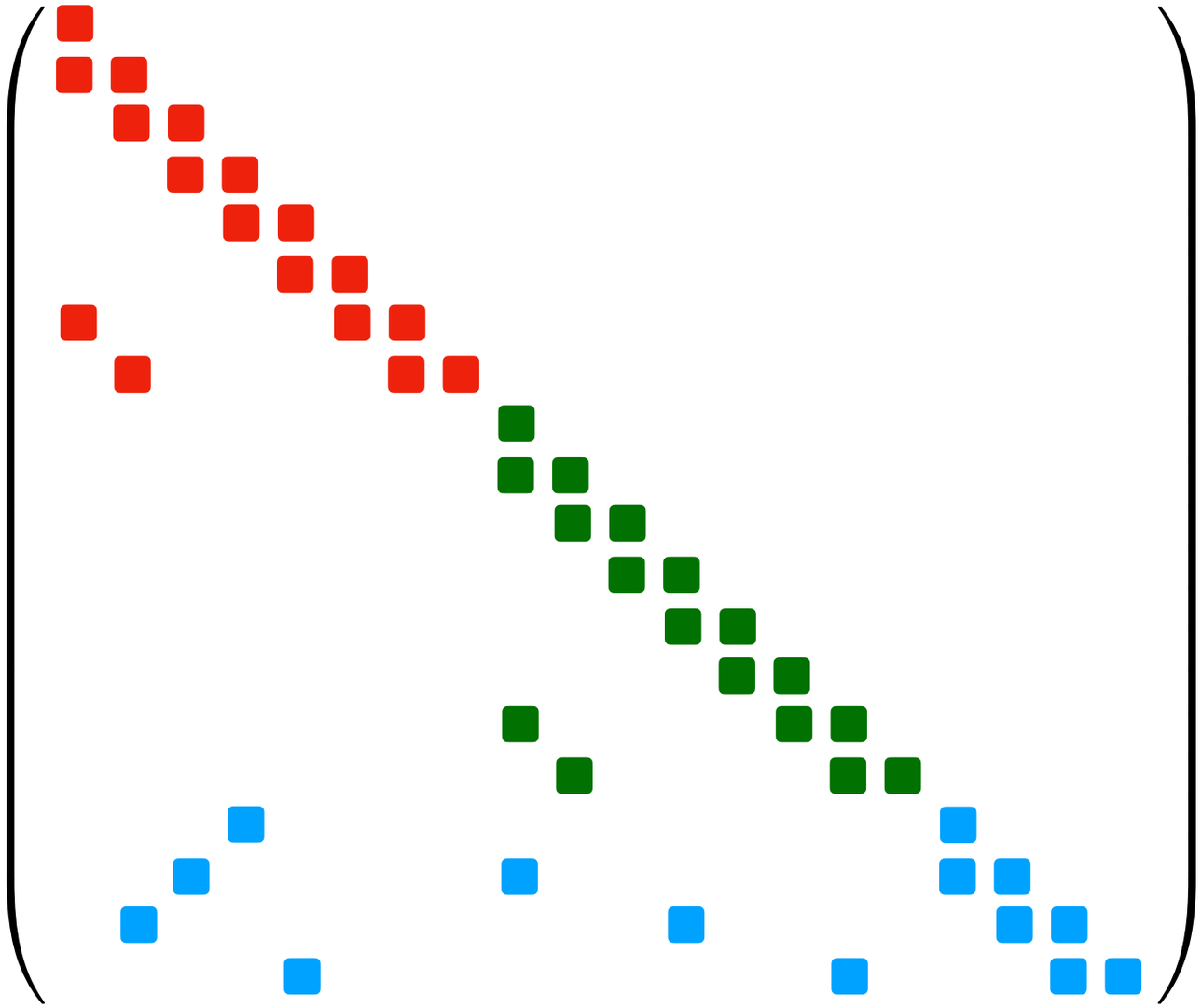
*Matrix Density : The number of required operations scale (super-linearly …) with the number of non-zero entries in **L** … thus, ensuring sparser **L** factors has an immediate effect on performance*

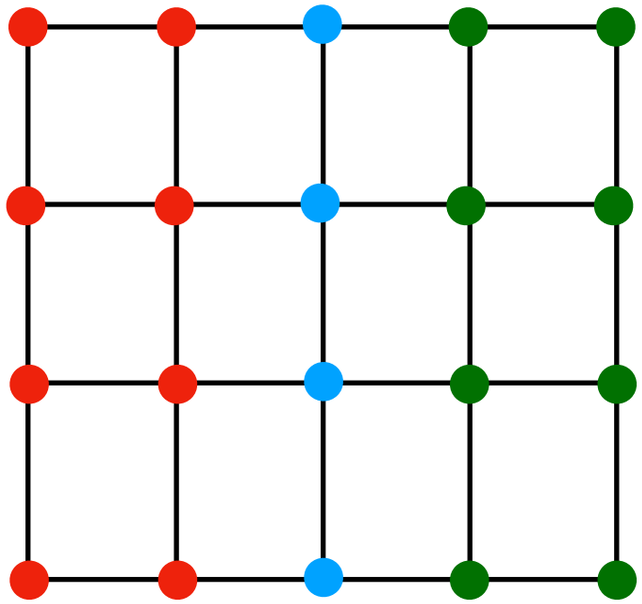
Multithreading : Cholesky, similar to Gauss Elimination, is seemingly a very "serial" algorithm (significant dependencies between steps/loops). We must find some way to cope with this apparent limitation.

```
Requires more regularity than parallelism not just independence like before
```

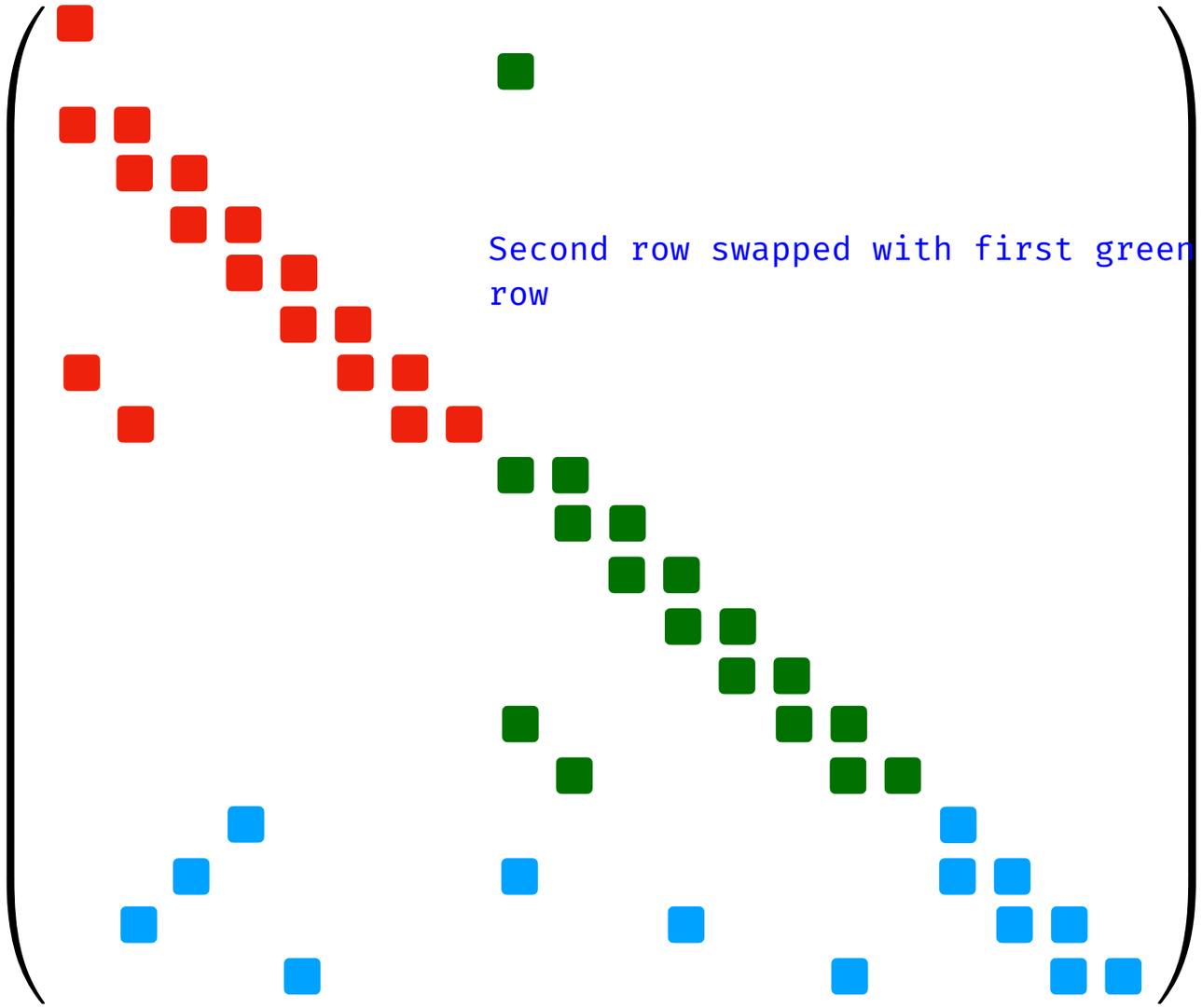
Vectorization/SIMD : Sparse matrices don't have the regularity that SIMD operations require; we need to "engineer" such regularity if possible

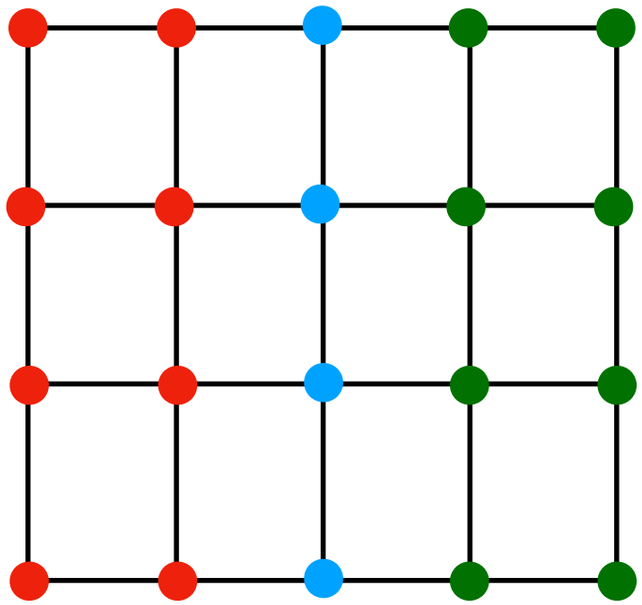
Engineering/Maximizing Sparsity



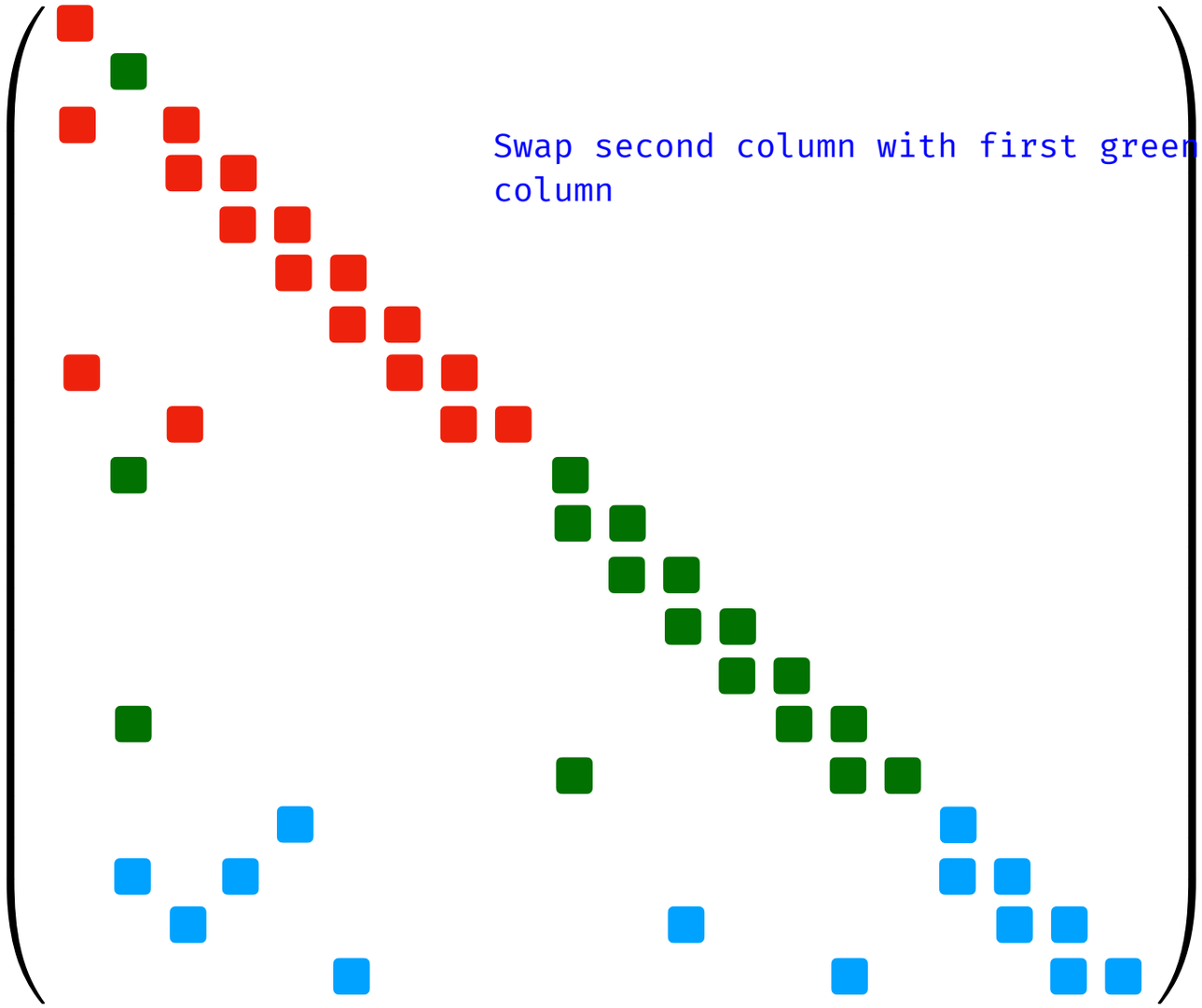


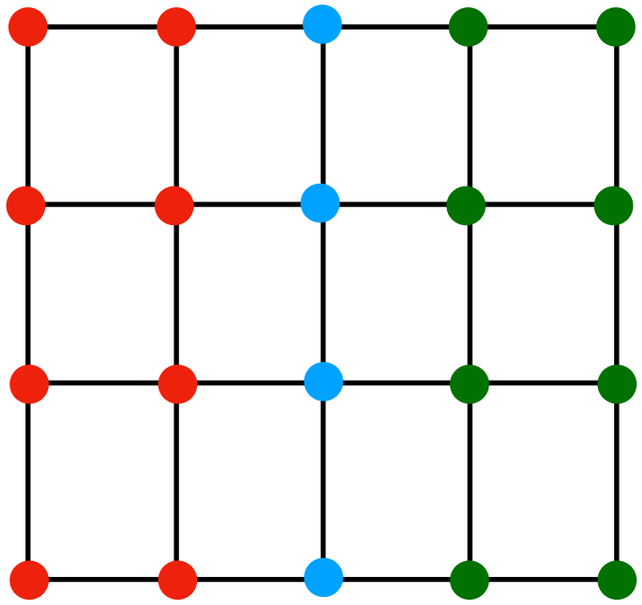
Engineering/Maximizing Sparsity



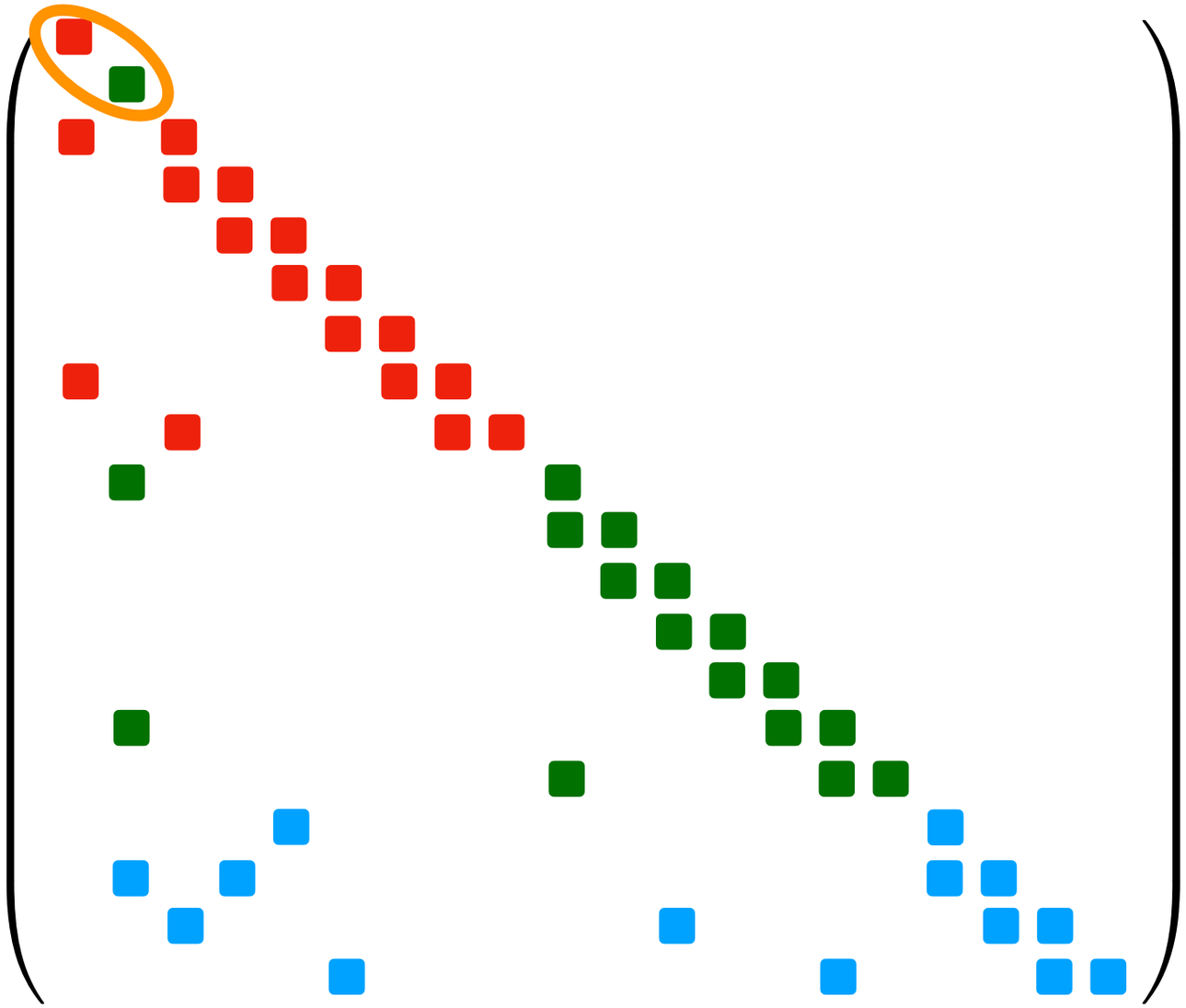


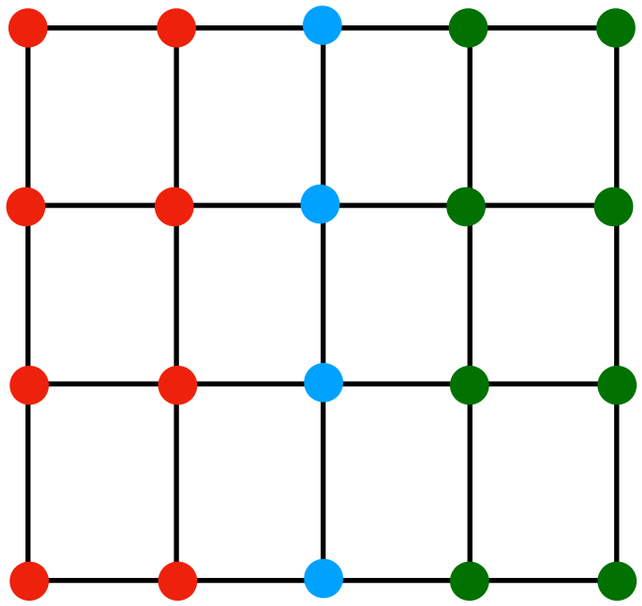
Engineering/Maximizing Sparsity





Engineering/Maximizing Sparsity





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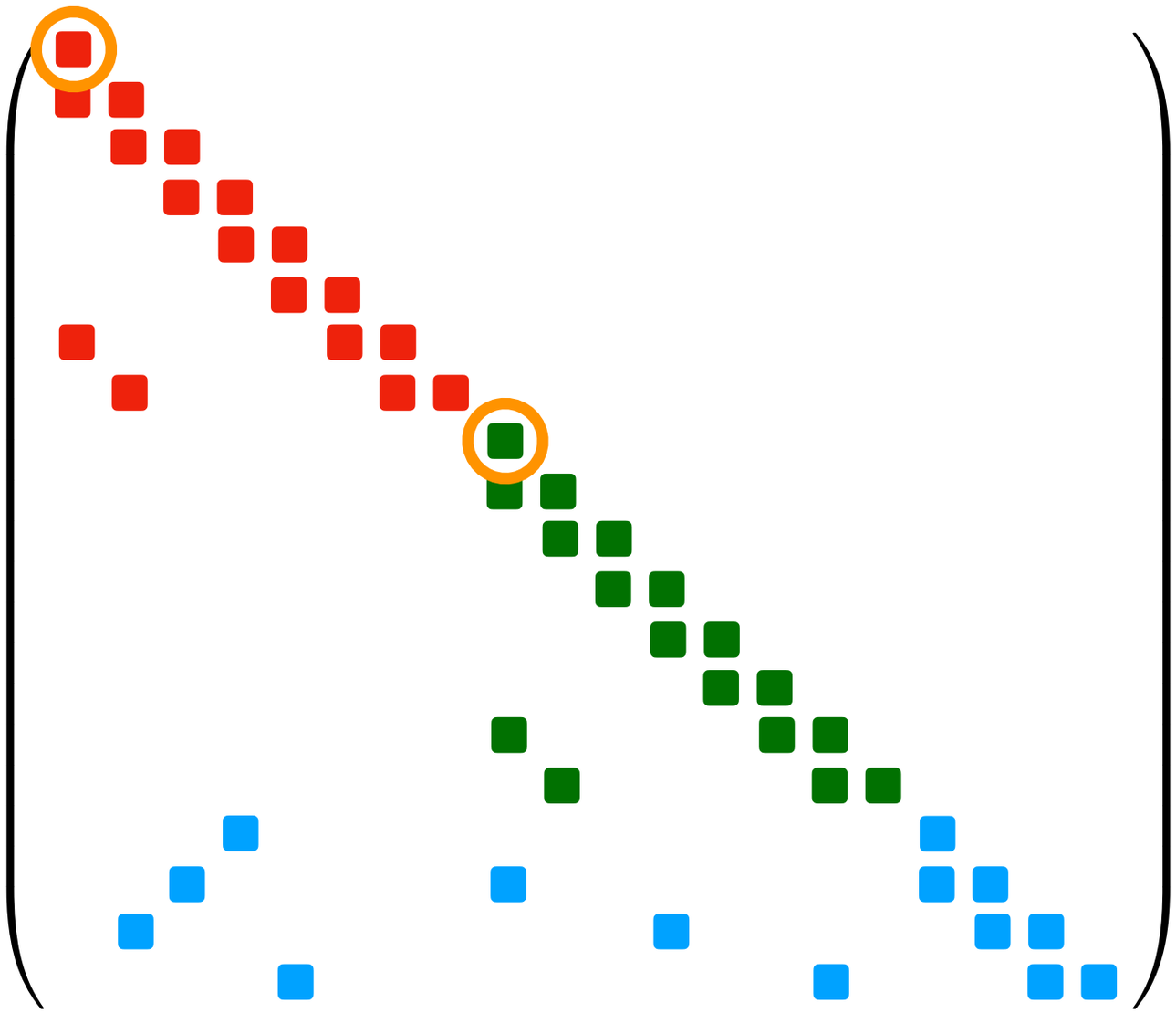

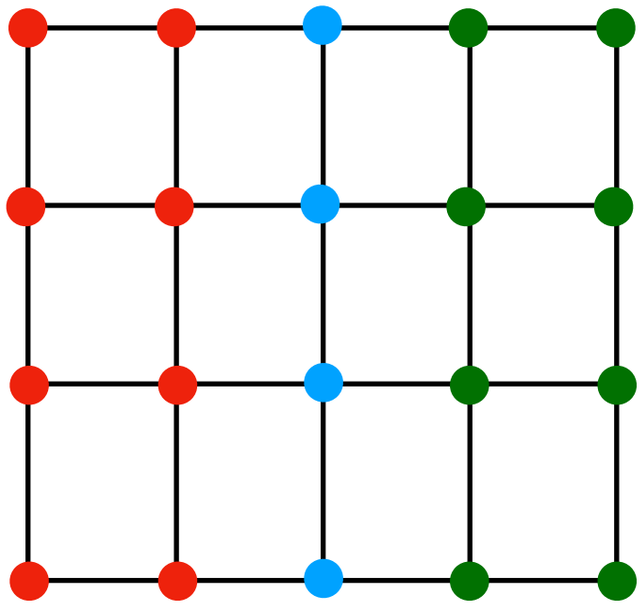

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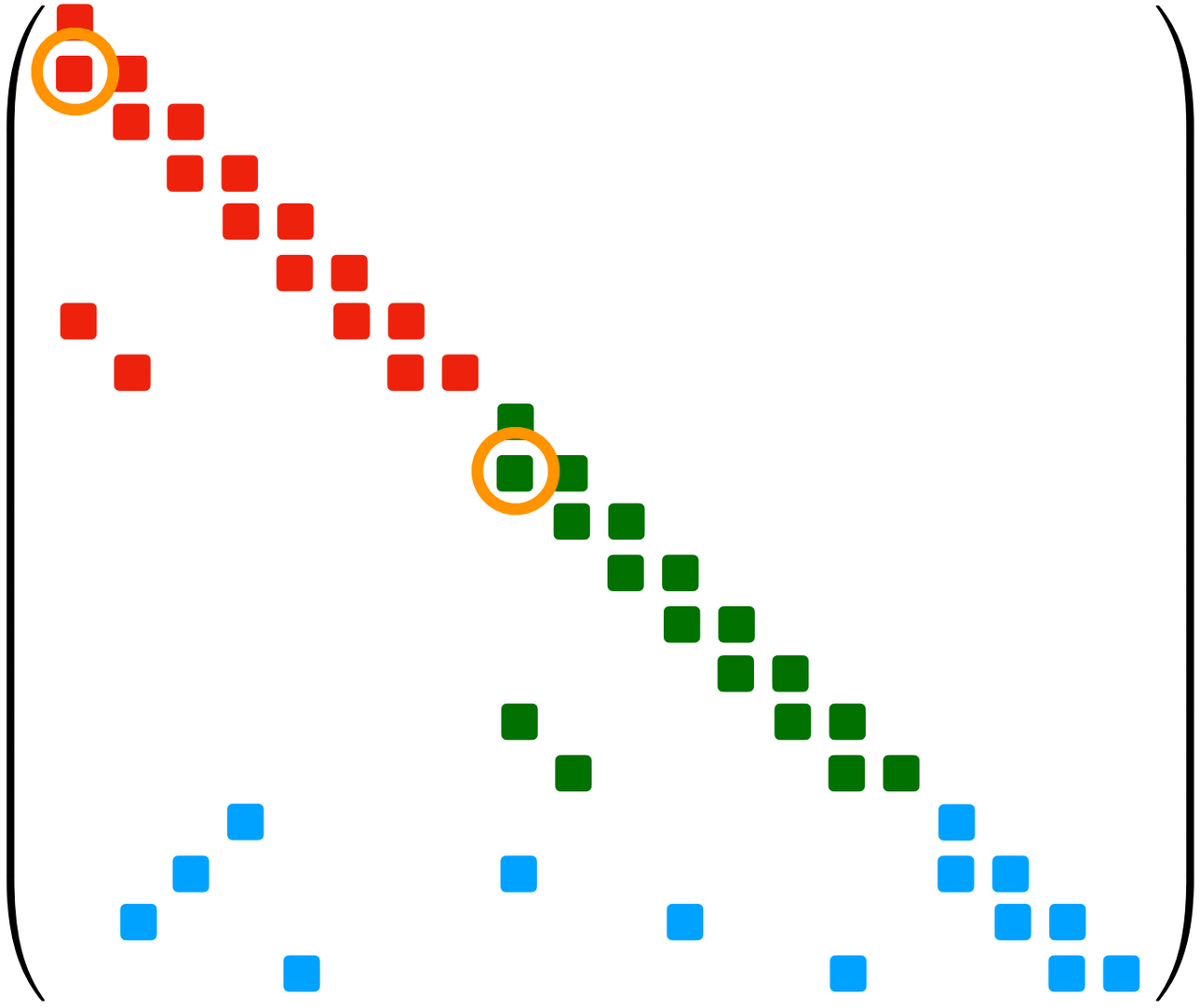

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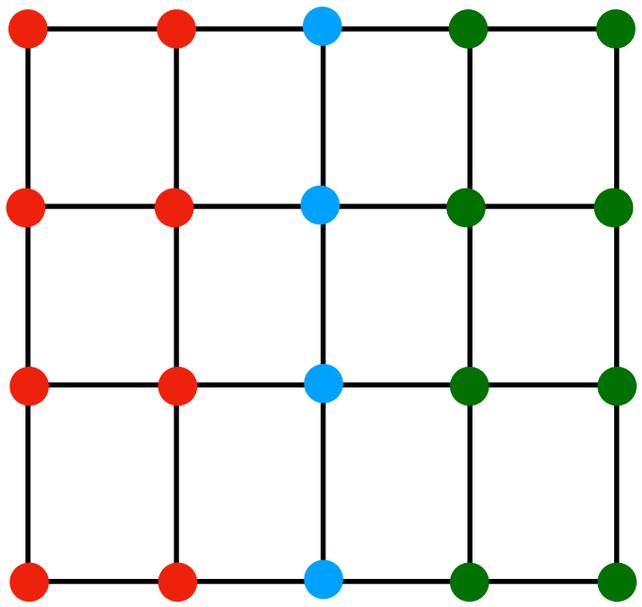

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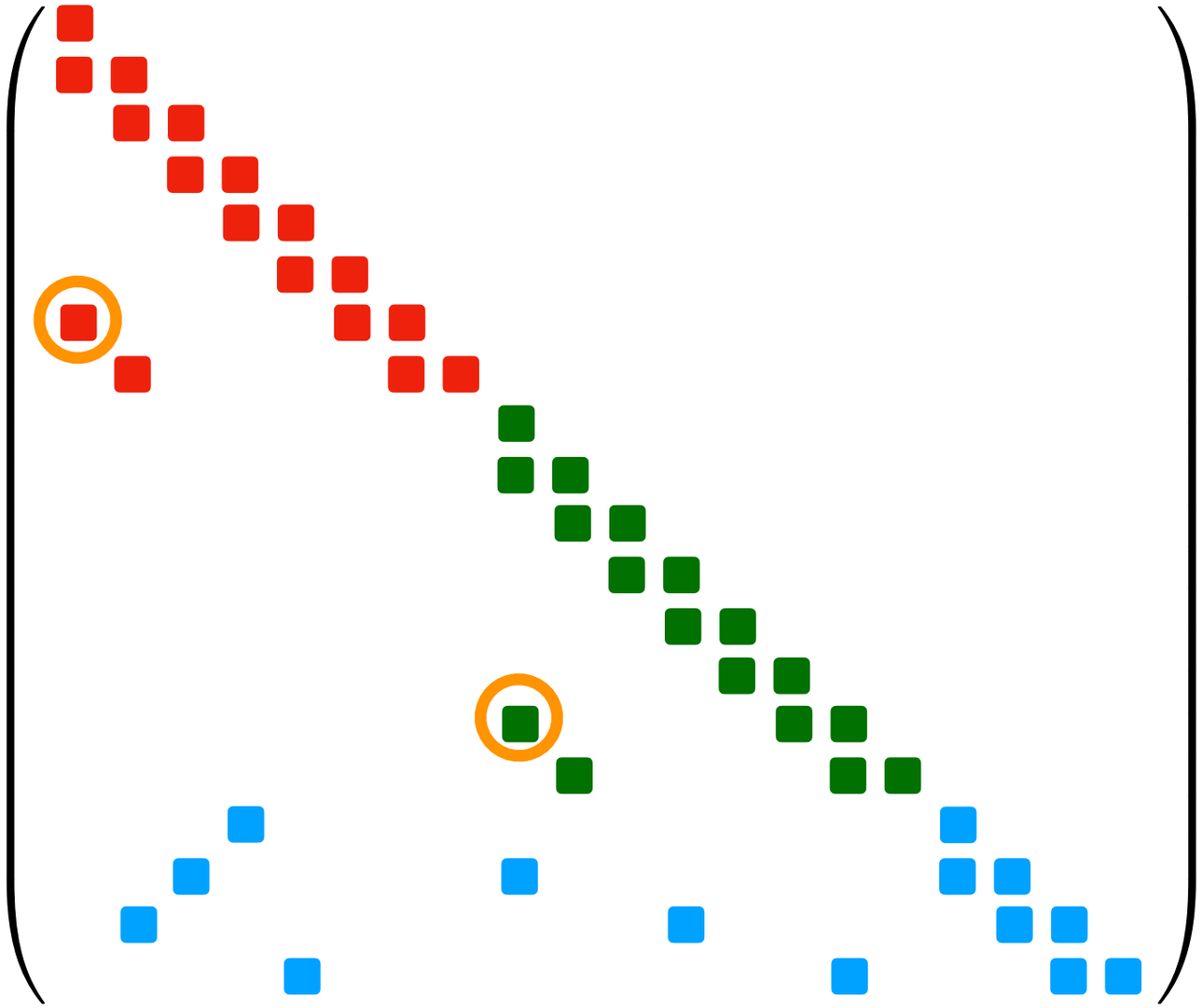

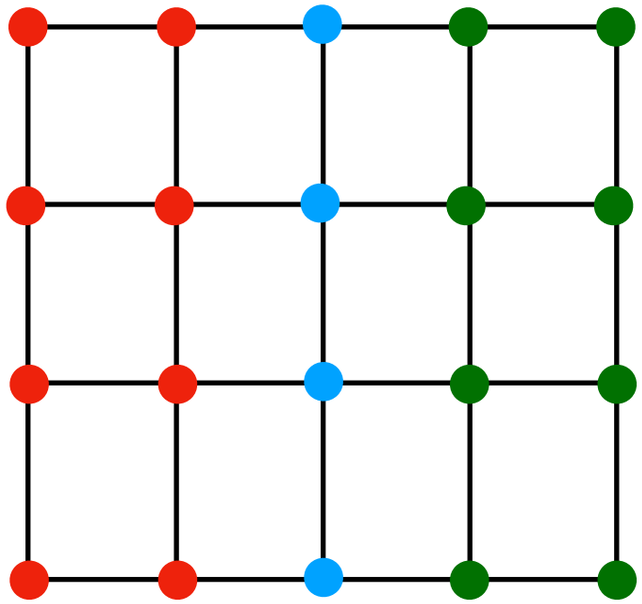

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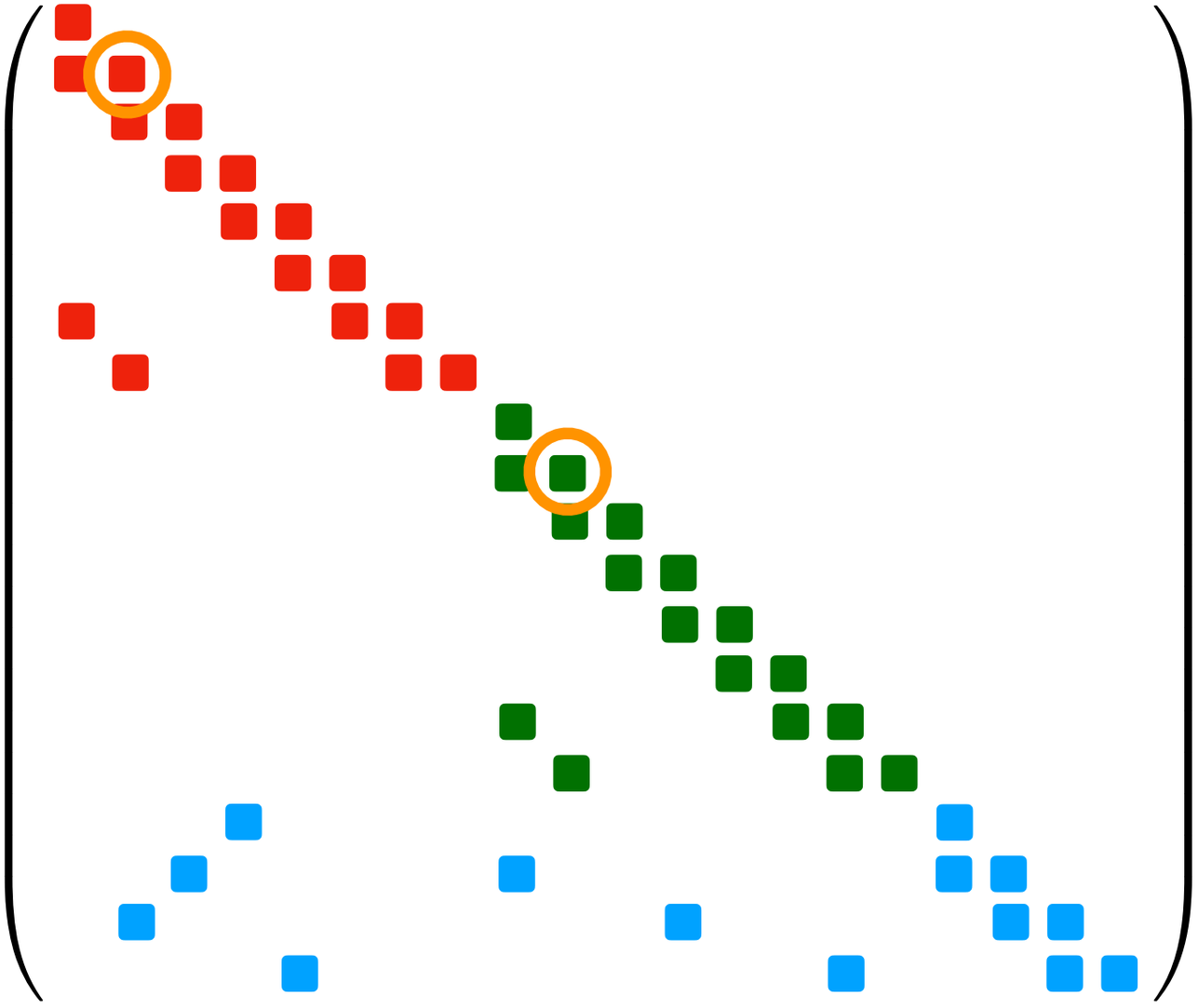
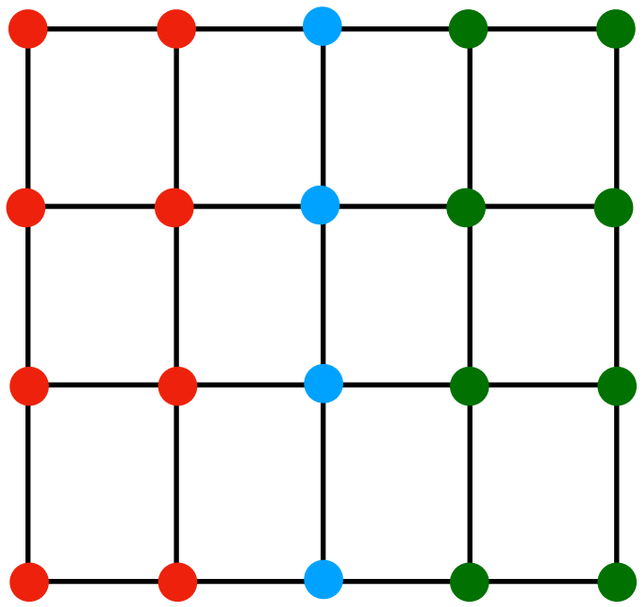
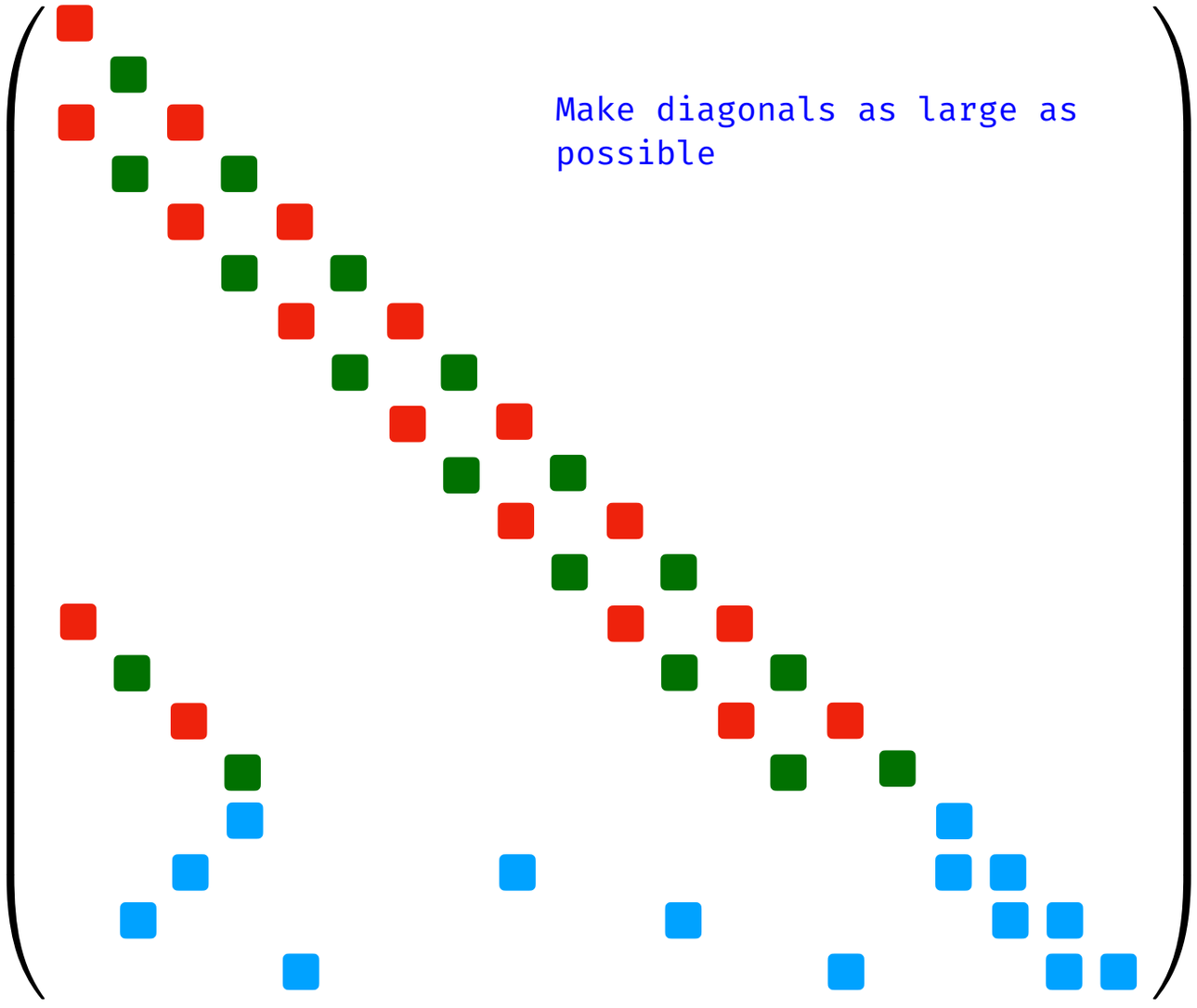


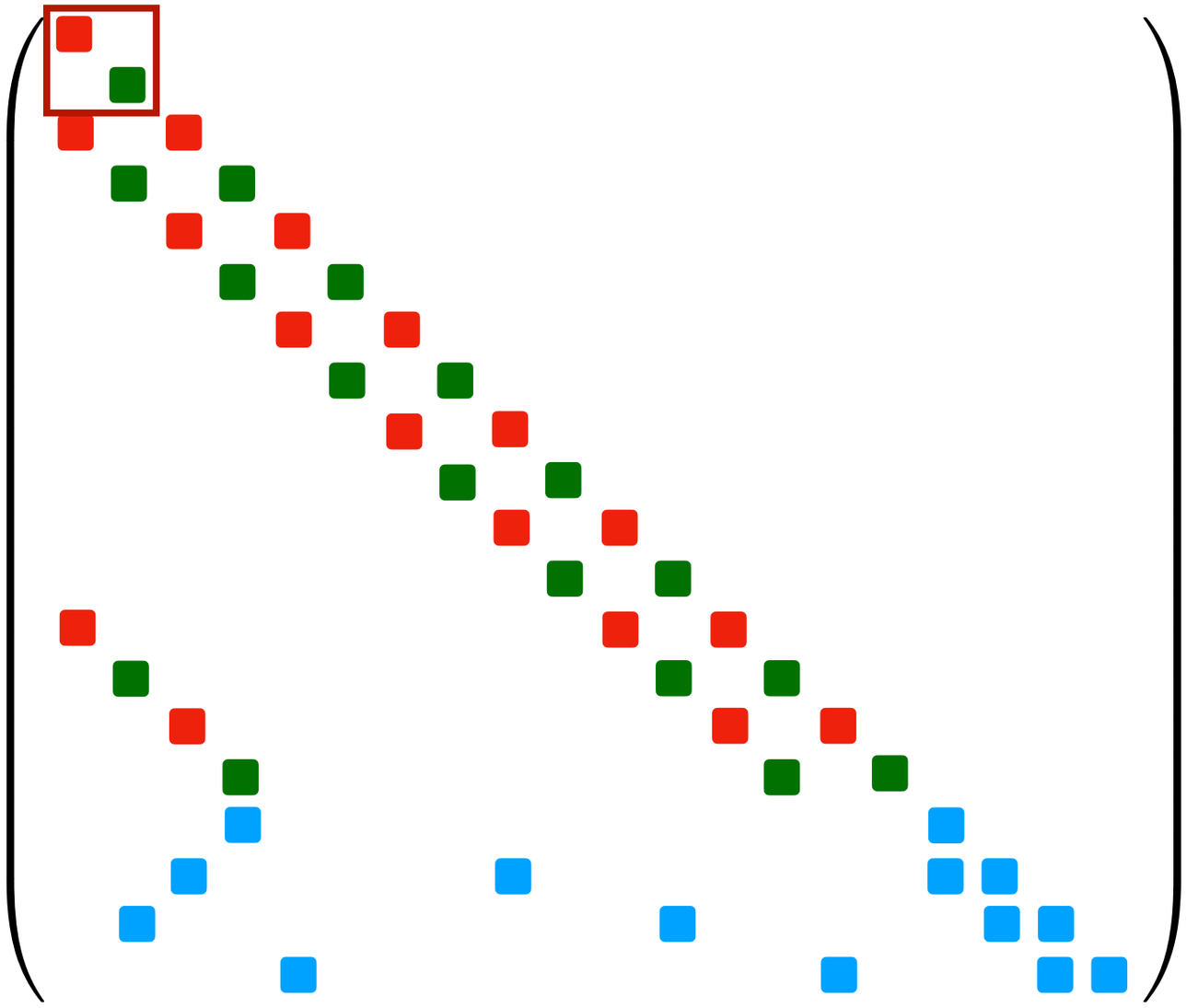


Engineering/Maximizing Sparsity



After reordering:
Sparsity pattern becomes a (sparse) collection of diagonal ***blocks***

Engineering/Maximizing Sparsity



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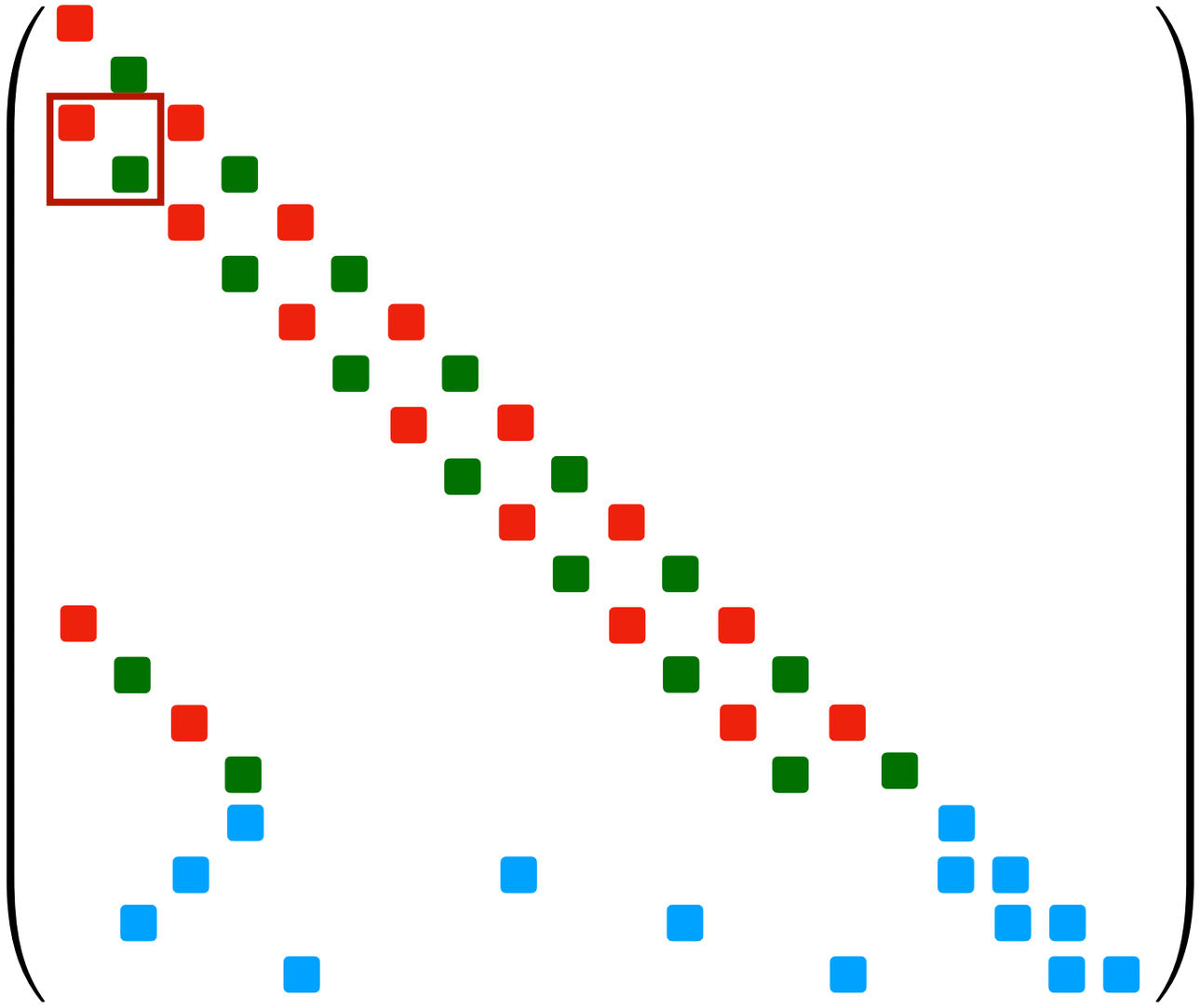
Engineering/Maximizing Sparsity



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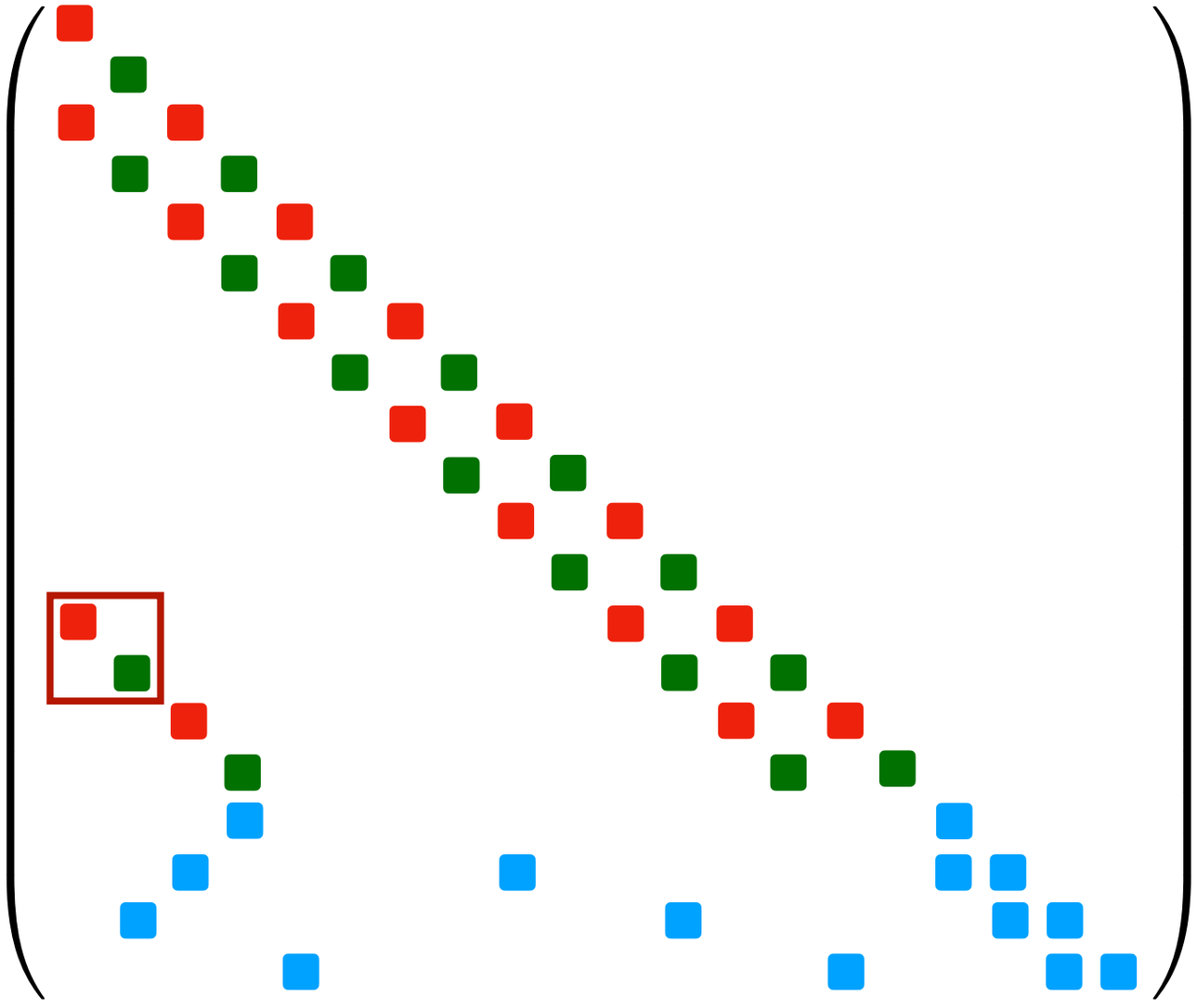

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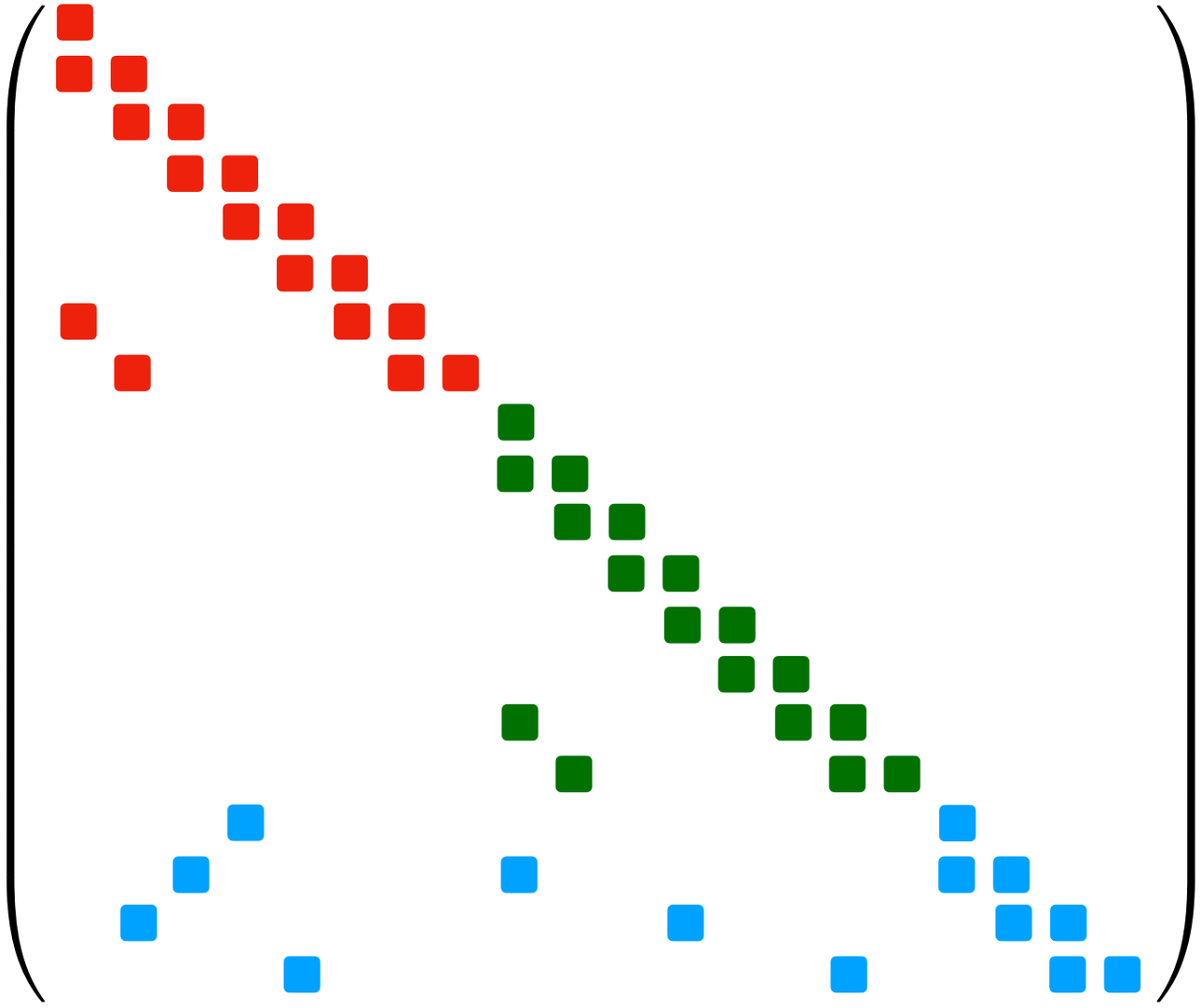
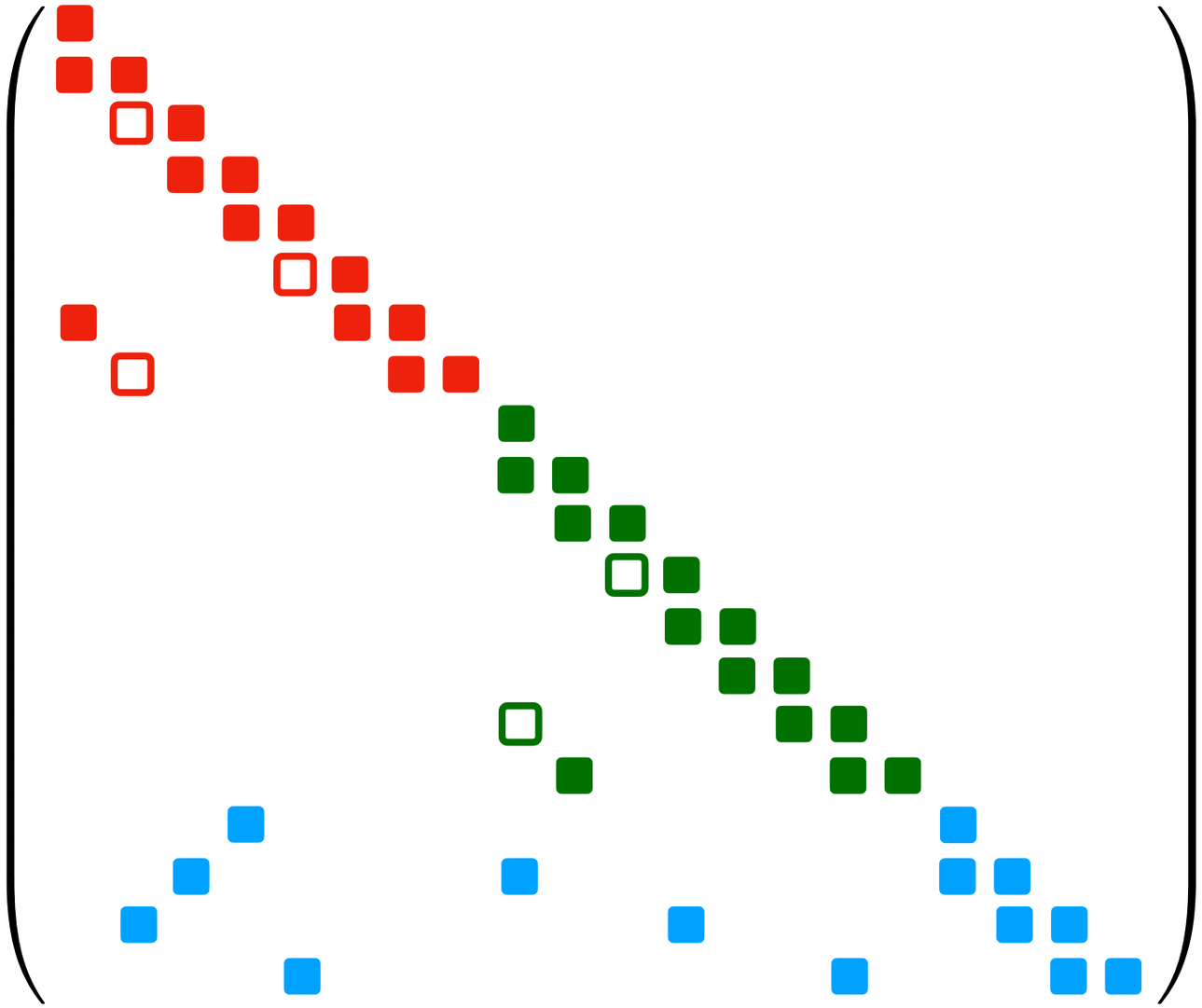


The patterns identified here are to be looked as fractals in larger matrices. That is when they are good for performance.

This transformation was predicated on the grid "partitions" having the same sparsity pattern …

Engineering/Maximizing Sparsity

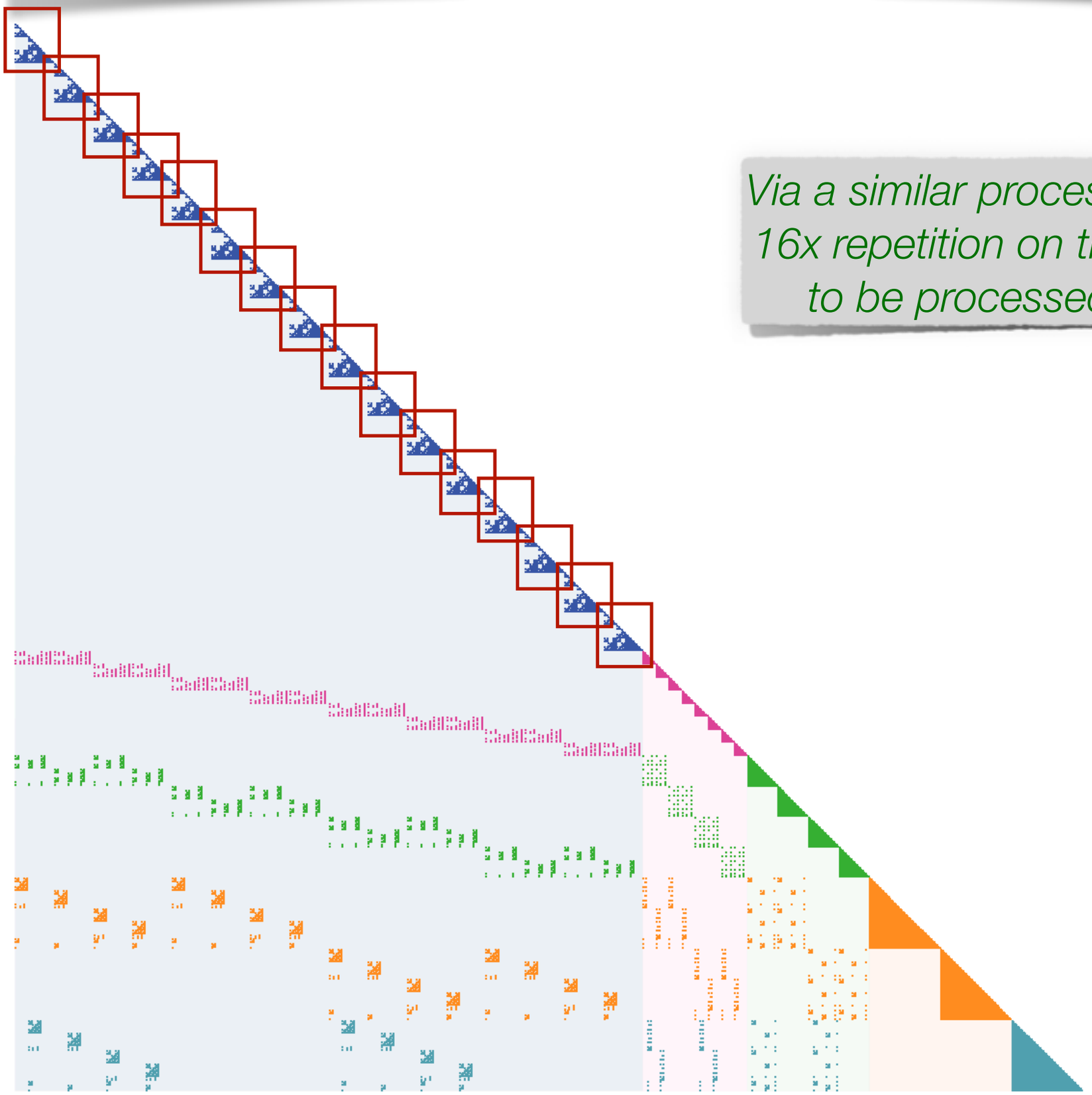


Padding to make the sparsity pattern uniform

… but can be made to work even if the sparsity patterns are "almost" the same (this near-similarity needs to be discovered…)

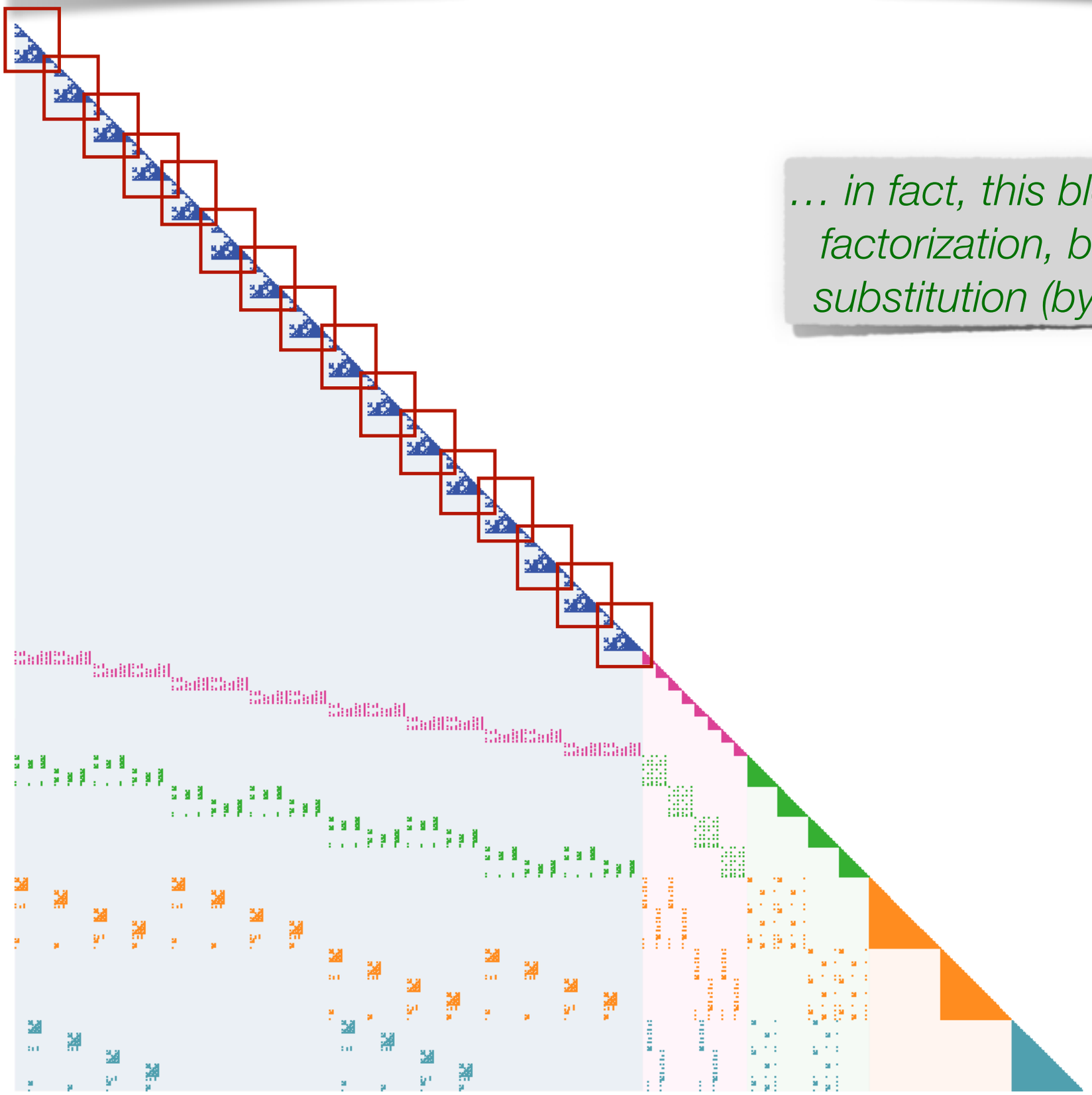
Reordering: reduces sparsity of factors, creates independent blocks with similar sparsity patterns, allows serial operation like Gaussian elimination to be better

Laplacian - Pattern after a possible reordering



Via a similar process … any patterns that exhibit 16x repetition on this layout, can be engineered to be processed in parallel using SIMD …

Laplacian - Pattern after a possible reordering



… in fact, this blocking accelerates not only factorization, but also forward/backward substitution (by allowing SIMD operation)

PARDISO solver (DirectSolver.cpp)

SparseDirect/LaplacePARDISO_0_0

```
// 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,
    matrix.GetValues(), matrix.GetRowOffsets(), matrix.GetColumnIndices(),
    &idum, &nrhs, iparm, &msglvl, static_cast<void*>(&f[0][0][0]), &x[0][0][0], &error);
if ( error != 0 )
    throw std::runtime_error("PARDISO error during solution phase");

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

// Termination and release of memory.
phase = -1;            // Release internal memory
PARDISO (pt, &maxfct, &mnum, &mtype, &phase, &n,
    &ddum, matrix.GetRowOffsets(), matrix.GetColumnIndices(),
    &idum, &nrhs, iparm, &msglvl, &ddum, &ddum, &error);

if (writeOutput) WriteAsImage("x", x, 0, 0, XDIM/2);
}
```

$Ax=b$

$LL^Tx=b$

$Lw = b$: Forward

$L^Tx = w$: Back

PARDISO solver (DirectSolver.cpp)

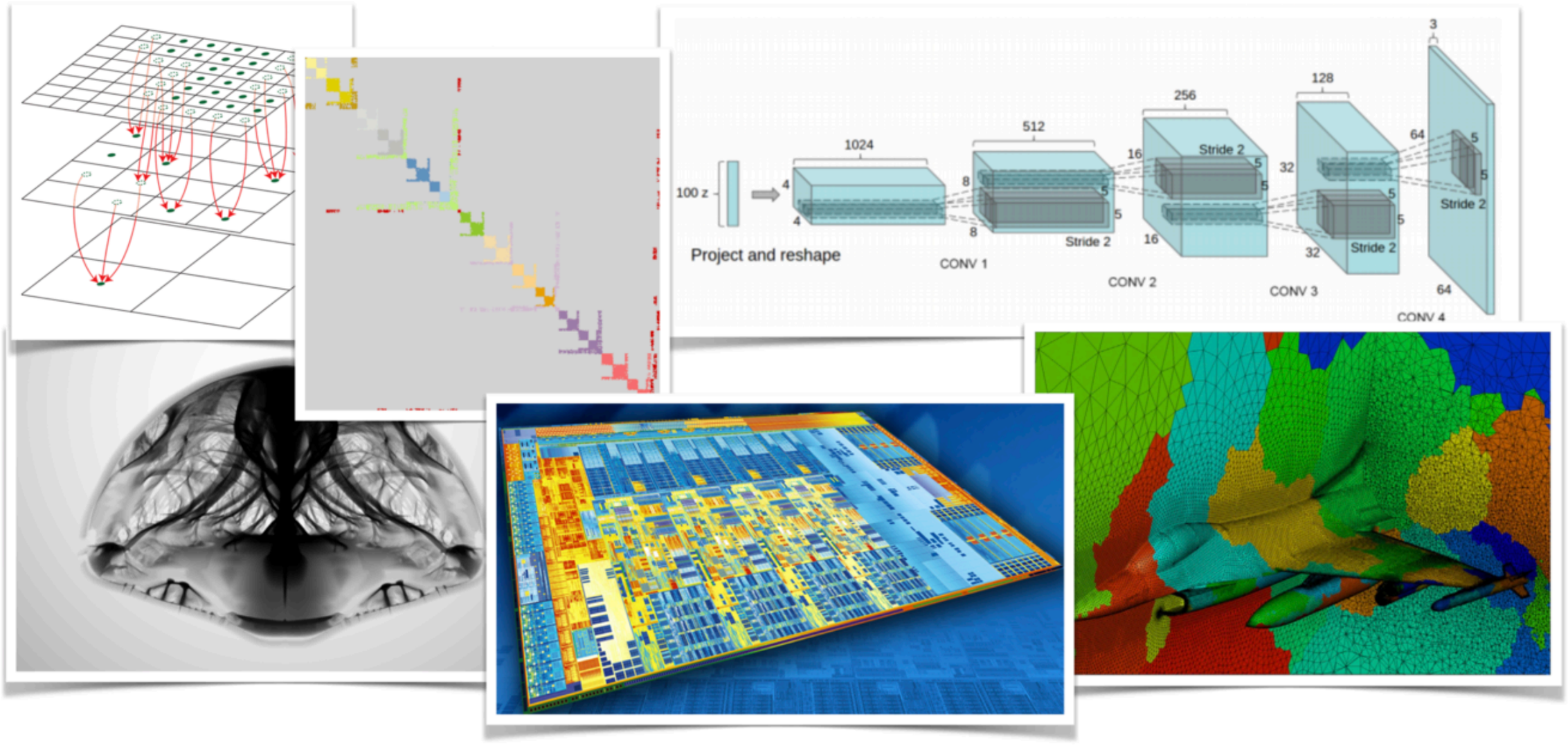
SparseDirect/LaplacePARDISO_0_0

Execution:

```
Summary: ( solution phase )
================
Times:
======
Time spent in direct solver at solve step (solve)                : 0.463208 s
Time spent in additional calculations                            : 0.021776 s
Total time spent                                                 : 0.484984 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:                    1407769
             size of largest supernode:               16591
             number of non-zeros in L:                2080602470
             number of non-zeros in U:                1
             number of non-zeros in L+U:              2080602471
             gflop   for the numerical factorization: 23028.583984
             gflop/s for the numerical factorization: 512.041504
```

Almost <1-2% of the factorization cost (which is what we hope!)

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

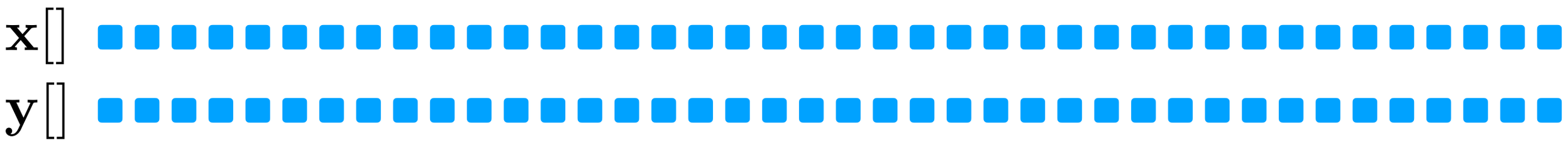


Lecture 20: Engineering regularity and vectorization potential in MKL PARDISO. Sparse direct solvers wrap-up

A first look at indirect array access & prefetching.

(Dense) Saxpy

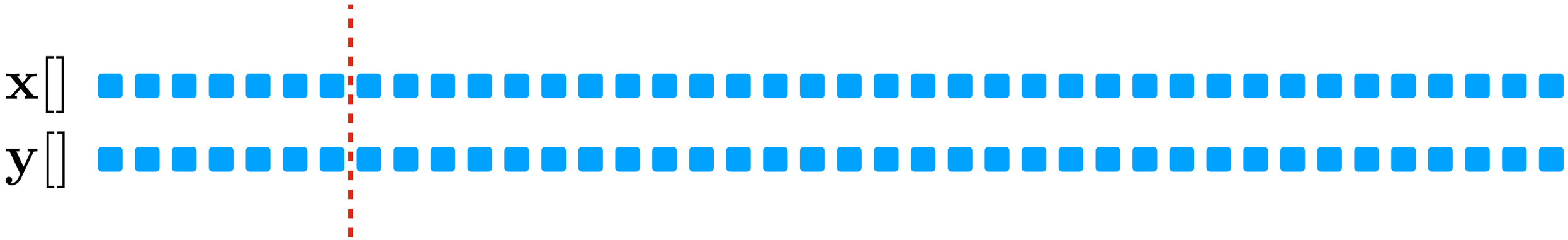
$$\texttt{for}\ \ i = 0, \ldots, N$$
$$\mathbf{y}[i] \mathrel{+}= \alpha \mathbf{x}[i]$$



(Dense) Saxpy

$$\texttt{for}\ \ i = 0, \ldots, N$$
$$\mathbf{y}[i] \mathrel{+}= \alpha \mathbf{x}[i]$$

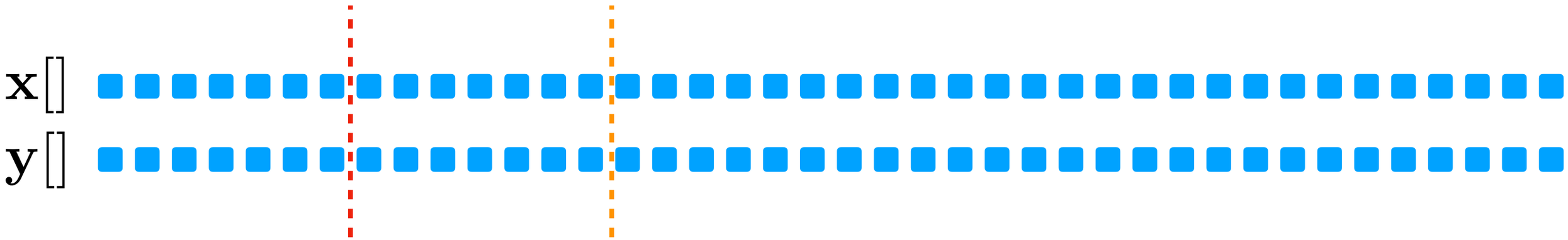
For full-bandwidth use:
If computation is here …



(Dense) Saxpy

$$\texttt{for} \;\; i = 0, \ldots, N$$
$$\mathbf{y}[i] \mathrel{+}= \alpha \mathbf{x}[i]$$

For full-bandwidth use:
If computation is here …



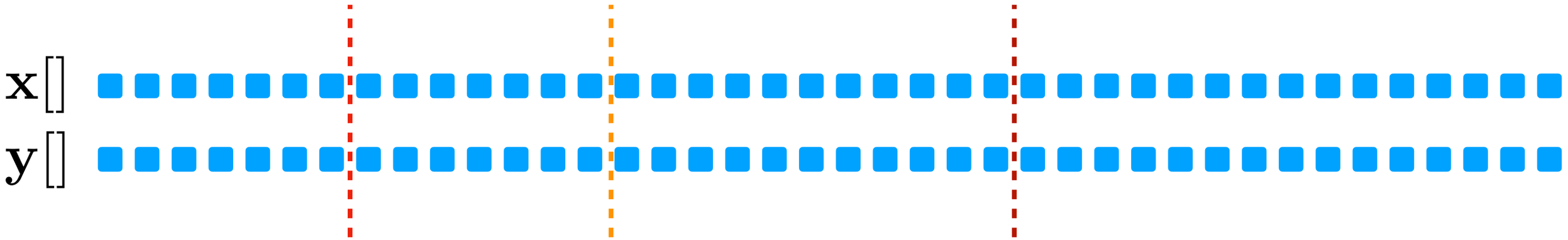
Then, data up to here better be in L1 Cache …

(Dense) Saxpy

$$\texttt{for}\ \ i = 0, \ldots, N$$
$$\mathbf{y}[i] \mathrel{+}= \alpha \mathbf{x}[i]$$

For full-bandwidth use:
If computation is here …

… and everything up to here already in L2 cache

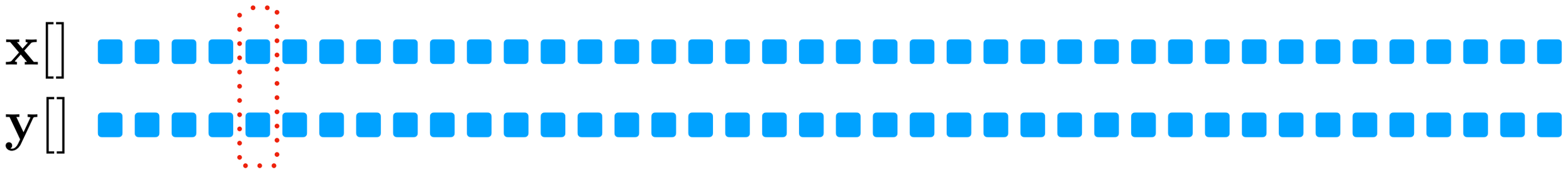


Then, data up to here better be in L1 Cache …

(Dense) Saxpy

$$\texttt{for} \;\; i = 0, \ldots, N$$
$$\mathbf{y}[i] \mathrel{+}= \alpha \mathbf{x}[i]$$

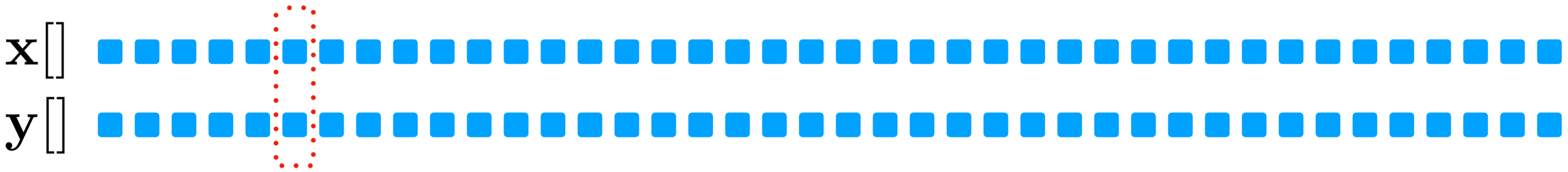
Hardware prefetching:
If following a certain
stride while accessing memory



(Dense) Saxpy

$$\texttt{for} \;\; i = 0, \ldots, N$$
$$\mathbf{y}[i] \mathrel{+}= \alpha \mathbf{x}[i]$$

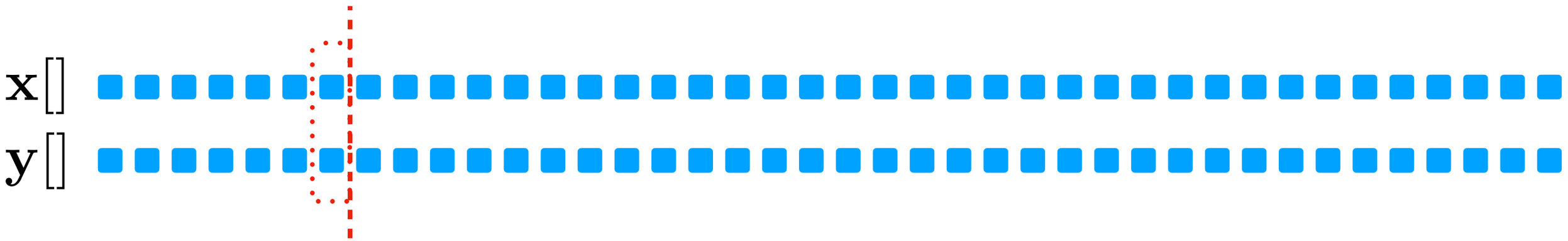
Hardware prefetching:
If following a certain
stride while accessing memory



(Dense) Saxpy

$$\texttt{for} \;\; i = 0, \ldots, N$$
$$\mathbf{y}[i] \mathrel{+}= \alpha \mathbf{x}[i]$$

Hardware prefetching:
If following a certain
stride while accessing memory

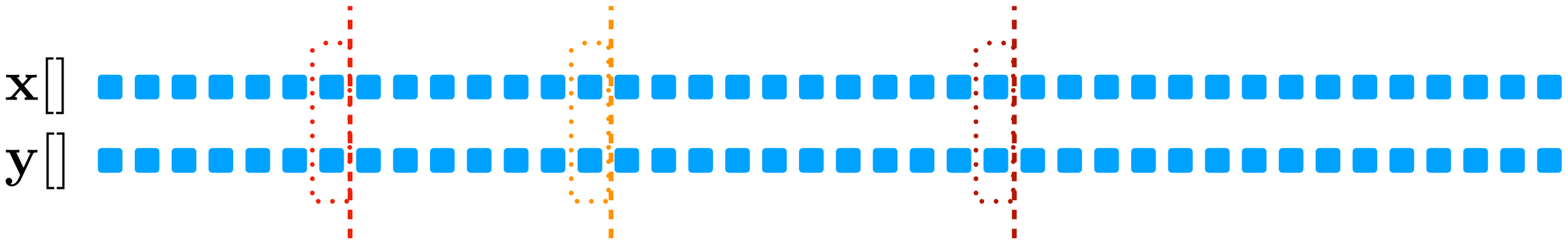


(Dense) Saxpy

$$\texttt{for } \; i = 0, \ldots, N$$
$$\mathbf{y}[i] \mathrel{+}= \alpha \mathbf{x}[i]$$

Hardware prefetching: If following a certain stride while accessing memory

… the CPU automatically "looks ahead" and prefetches according to the same ("apparent") stride into caches

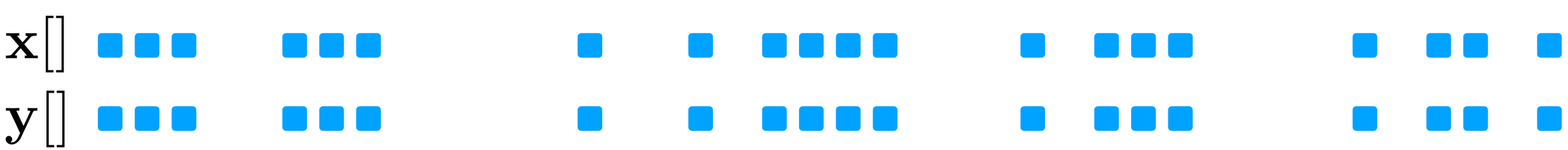


Sparse Saxpy

for $i =$ (some indices)

$$\mathbf{y}[i] \mathrel{+}= \alpha \mathbf{x}[i]$$

Effective hardware prefetching is hard:
- We don't know what to prefetch
- Even if we guess, good chance what's prefetched will be wasted

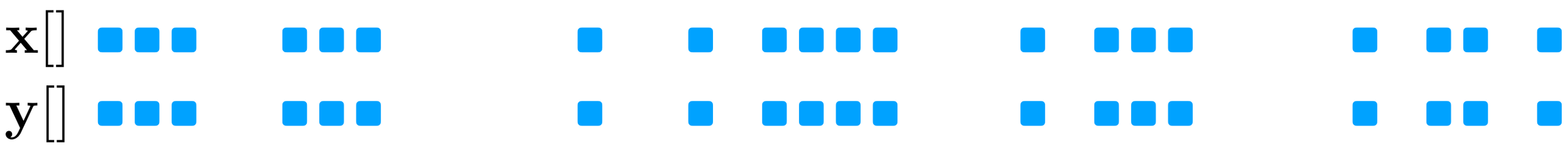


Our specific benchmark : Indirectly indexed Saxpy

$$\texttt{for } \; i = 0, \ldots, N$$

$$\mathbf{y}[\text{offset}[i]] \mathrel{+}= \alpha \mathbf{x}[\text{offset}[i]]$$

*Indices originate from array **offsets[]***
- There is a logic of where to prefetch from (the offsets array has that information)
- But the compiler/CPU cannot infer that; the user might have to help



Main routine (main.cpp)

Prefetching/SparseSaxpy_0_0

```
#include "Timer.h"
#include "Utilities.h"
#include "PointwiseOps.h"

int main(int argc, char *argv[])
{
    std::vector<int> blockOffsets;
    float *x;
    float *y;

    InitializeArrays(blockOffsets, x, y);

    // Initialization
    for (int run = 0; run < 30; run++)
    {
        Timer timer;
        timer.Start();
        SparseSaxpy(blockOffsets, x, y, 3.14f);
        timer.Stop("SparseSaxpy time : ");
    }

    return 0;
}
```

Initialization utilities (Utilities.h/cpp)

```
#pragma once

#include <vector>

#include "Parameters.h"

void* AlignedAllocate(const std::size_t size, const std::size_t alignment);
void InitializeArrays(std::vector<int>& blockOffsets, float *&x, float *&y);
```

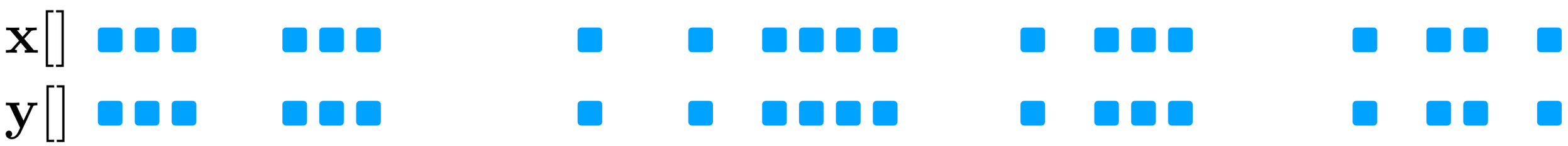
Benchmark Parameters (Parameters.h)

```
#pragma once

#define BLOCK_SIZE 16
#define MAX_CLUSTER_SIZE 4
#define MAX_CLUSTER_DISTANCE 32
#define NUMBER_OF_BLOCKS 4*1024*1024
```

Sparse Saxpy

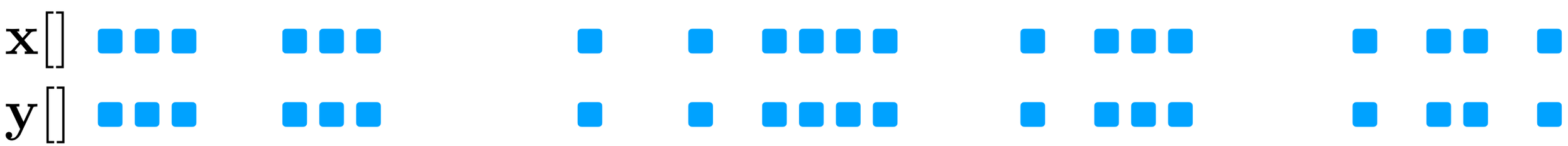
Our test collection of array entries comes in chunks of aligned 16-tuples (for simplicity)
Each "square" in the illustration below corresponds to 16-contiguous entries
(16 = BLOCK_SIZE in Parameters.h)



Sparse Saxpy

*Array **blockOffsets[]** contains the location of where each block-of-16 entries starts*

MAX_CLUSTER_SIZE is the maximum of how many blocks to “bundle/cluster” together (layout is randomly initialized)
while MAX_CLUSTER_DISTANCE is the average distance between block clusters



Stock saxpy routine (PointwiseOps.cpp)

Prefetching/SparseSaxpy_0_0

```
#include "PointwiseOps.h"

void SparseSaxpy(std::vector<int>& blockOffsets, const float *x, float *y, const float scale)
{
#pragma omp parallel for
    for (int b = 0; b < blockOffsets.size(); b++)
        for (int i = 0; i < BLOCK_SIZE; i++)
            y[blockOffsets[b]+i] += scale * x[blockOffsets[b]+i];
}
```

Stock saxpy routine (PointwiseOps.cpp)

Prefetching/SparseSaxpy_0_0

```
#include "
void Spars                                                    at scale)
{
#pragma om
    for (i
        fo

}
```

Execution:

```
Allocated total of 4194304 blocks (67108864 entries; 256MB of actual data)
   in a span of 1946.55MB
[SparseSaxpy time : 33.5354ms]
[SparseSaxpy time : 25.3708ms]
[SparseSaxpy time : 25.3139ms]
[SparseSaxpy time : 24.32ms]
[SparseSaxpy time : 25.3662ms]
[SparseSaxpy time : 24.3337ms]
[SparseSaxpy time : 24.3135ms]
[SparseSaxpy time : 26.3057ms]
[SparseSaxpy time : 25.3865ms]
[SparseSaxpy time : 24.3556ms]
[SparseSaxpy time : 25.3534ms]
[SparseSaxpy time : 24.1806ms]
[SparseSaxpy time : 24.1684ms]
[SparseSaxpy time : 25.1663ms]
[SparseSaxpy time : 24.1898ms]
[SparseSaxpy time : 25.138ms]
```

Stock saxpy routine (PointwiseOps.cpp)

Prefetching/SparseSaxpy_0_1

```
#include "PointwiseOps.h"
#include "immintrin.h"

void SparseSaxpy(std::vector<int>& blockOffsets, const float *x, float *y, const float scale)
{
    static constexpr int L2_PREFETCH_DISTANCE = 64;
    static constexpr int L1_PREFETCH_DISTANCE = 8;

#pragma omp parallel for
    for (int b = 0; b < blockOffsets.size(); b++) {
        _mm_prefetch ( &x[blockOffsets[b+L2_PREFETCH_DISTANCE]], _MM_HINT_T2 );
        _mm_prefetch ( &x[blockOffsets[b+L1_PREFETCH_DISTANCE]], _MM_HINT_T1 );
        _mm_prefetch ( &y[blockOffsets[b+L2_PREFETCH_DISTANCE]], _MM_HINT_T2 );
        _mm_prefetch ( &y[blockOffsets[b+L1_PREFETCH_DISTANCE]], _MM_HINT_T1 );
#pragma omp simd
        for (int i = 0; i < BLOCK_SIZE; i++)
            y[blockOffsets[b]+i] += scale * x[blockOffsets[b]+i];
    }
}
```

Stock saxpy routine (PointwiseOps.cpp)

Prefetching/SparseSaxpy_0_1

```
#include "PointwiseOps.h"
#include "immintrin.h"

void SparseSaxpy(std::vector<int>& blockOffsets, const float *x, float *y, const float scale)
{
    static constexpr int L2_PREFETCH_DISTANCE = 64;
    static constexpr int L1_PREFETCH_DISTANCE = 8;

#pragma omp parallel for
    for (int b = 0; b < blockOffsets.size(); b++) {
        _mm_prefetch ( &x[blockOffsets[b+L2_PREFETCH_DISTANCE]], _MM_HINT_T2 );
        _mm_prefetch ( &x[blockOffsets[b+L1_PREFETCH_DISTANCE]], _MM_HINT_T1 );
        _mm_prefetch ( &y[blockOffsets[b+L2_PREFETCH_DISTANCE]], _MM_HINT_T2 );
        _mm_prefetch ( &y[blockOffsets[b+L1_PREFETCH_DISTANCE]], _MM_HINT_T1 );
#pragma omp simd
        for (int i = 0; i < BLOCK_SIZE; i++)
            y[blockOffsets[b]+i] += scale * x[blockOffsets[b]+i];
    }
}
```

Temporal prefetch hints. Preserves the line in cache indicating reuse

We provide explicit prefetching hints for both L1 and L2 caches (note: prefetch typically does not fault if given an invalid memory)

Prefetching/SparseSaxpy_0_1

Stock saxpy routine (PointwiseOps.cpp)

```
#include "PointwiseOps.h"
#include "immintrin.h"

void Sparse                                                    scale)
{
    static
    static
#pragma omp
    for (in
        _mm
        _mm
        _mm
        _mm
#pragma omp
        for
    }
}
```

Execution:

```
Allocated total of 4194304 blocks (67108864 entries; 256MB of actual data)
in a span of 1945.54MB
[SparseSaxpy time : 21.6707ms]
[SparseSaxpy time : 12.3966ms]
[SparseSaxpy time : 12.3517ms]
[SparseSaxpy time : 12.3327ms]
[SparseSaxpy time : 12.3688ms]
[SparseSaxpy time : 12.3316ms]
[SparseSaxpy time : 12.333ms]
[SparseSaxpy time : 12.3355ms]
[SparseSaxpy time : 12.3285ms]
[SparseSaxpy time : 12.333ms]
[SparseSaxpy time : 12.3489ms]
[SparseSaxpy time : 12.3211ms]
[SparseSaxpy time : 12.3352ms]
[SparseSaxpy time : 12.3222ms]
[SparseSaxpy time : 12.3475ms]
[SparseSaxpy time : 12.3308ms]
```

Prefetching/SparseSaxpy_0_1

Stock saxpy routine (PointwiseOps.cpp)

```
#include "PointwiseOps.h"
#include "immintrin.h"

void Sparse                                                    scale)
{
    static
    static
#pragma omp
    for (in
        _mm
        _mm
        _mm
        _mm
#pragma omp
        for
    }
}
```

Execution:

```
Allocated total of 4194304 blocks (67108864 entries; 256MB of actual data)
in a span of 1945.54MB
[SparseSaxpy time : 21.6707ms]
[SparseSaxpy time : 12.3966ms]
[SparseSaxpy time : 12.3517ms]
[SparseSaxpy time : 12.3327ms]
[SparseSaxpy time : 12.3688ms]
[SparseSaxpy time : 12.3316ms]
[SparseSaxpy time : 12.333ms]
[SparseSaxpy time : 12.3355ms]
[SparseSaxpy time : 12.3285ms]
[SparseSaxpy time : 12.333ms]
[SparseSaxpy time : 12.3489ms]
[SparseSaxpy time : 12.3211ms]
[SparseSaxpy time : 12.3352ms]
[SparseSaxpy time : 12.3222ms]
[SparseSaxpy time : 12.3475ms]
[SparseSaxpy time : 12.3308ms]
```

Note: Performance boost is highly variable depending on compiler, CPU, optimization level, and context!