CBMS Conference on Fast Direct Solvers

Dartmouth College

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Lecture 9: Direct Solvers for Integral Equations

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Research support by:

In this lecture, we develop a direct solver for an integral equations such as

$$\alpha\, q(\boldsymbol{x}) + \int_\Gamma k(\boldsymbol{x},\boldsymbol{y})\, q(\boldsymbol{y})\, dS(\boldsymbol{y}) = f(\boldsymbol{x}), \qquad \boldsymbol{x} \in \Gamma, \tag{1}$$

where Γ is a contour in $\mathbb{R}^2$ or a surface in $\mathbb{R}^3$. We'll do 2D first, and will then generalize.

Upon Nyström discretization (see Lecture 7), the BIE (1) turns into the linear system

$$\underset{N\times N}{\mathbf{A}} \quad \underset{N\times 1}{\mathbf{q}} \quad = \quad \underset{N\times 1}{\mathbf{f}},$$

where $\mathbf{A}$ is a dense $N \times N$ matrix.

Standard approach: Use an iterative solver (e.g. GMRES, CG), combined with an $O(N)$ method for evaluating $\mathbf{x} \mapsto \mathbf{A}\mathbf{x}$ such as the Fast Multipole Method (FMM) or panel clustering. When convergence is fast, optimal $O(N)$ complexity results.

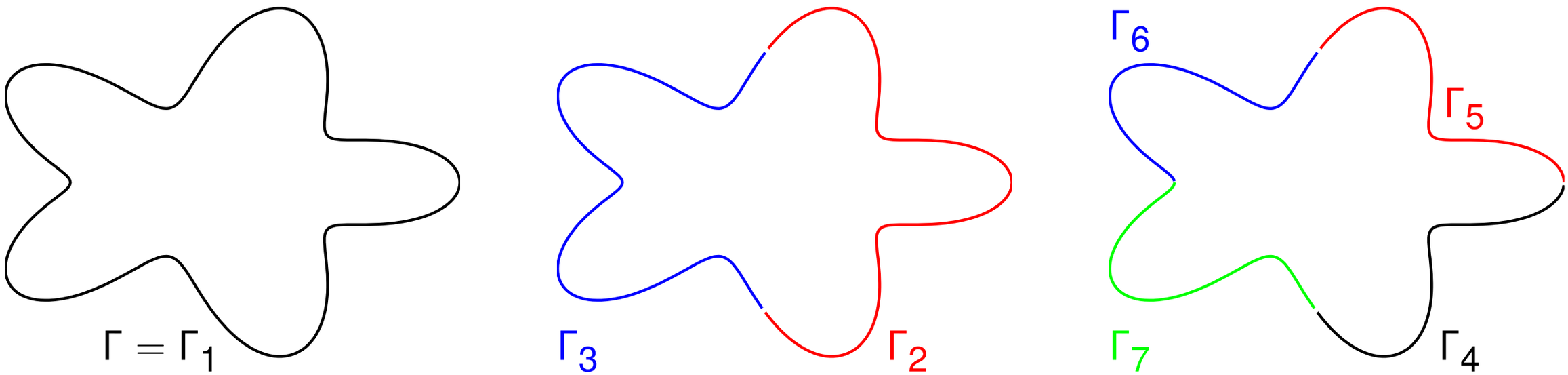
New approach: We seek to construct a direct solver which in a single sweep constructs a data-sparse representation of an operator $\mathbf{B}$ such that $\mathbf{B} \approx \mathbf{A}^{-1}$. Why?

- Can solve problems for which iterative methods converge slowly or not at all.
- Very fast when solving a sequence of equations with the same operator.
- Well suited for modern computers (low communication, memory and flops are cheap).

Key observation: The off-diagonal blocks of $\mathbf{A}$ tend to have low numerical rank.
(Note that for high-frequency problems, other structure in $\mathbf{A}$ is used.)

The direct solvers are (like the FMM, panel clustering, $\mathcal{H}$-matrices, ...) based on hierarchical partitioning of the physical domain.

Example: Consider a BIE defined on a contour $\Gamma \subset \mathbb{R}^2$.



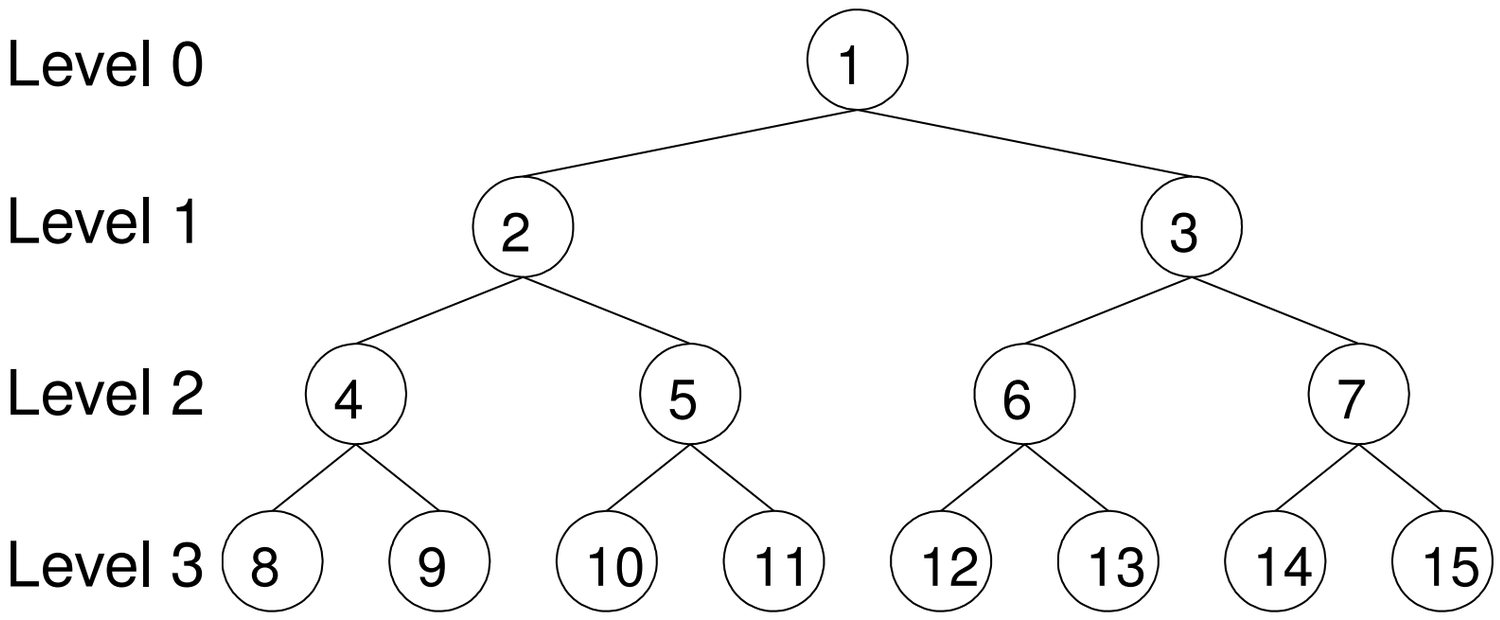
Let $\Gamma = \Gamma_1$ denote the root of a tree.

Partition Γ_1 into two pieces $\Gamma_1 = \Gamma_2 \cup \Gamma_3$.

Further partition $\Gamma_2 = \Gamma_4 \cup \Gamma_5$ and $\Gamma_3 = \Gamma_6 \cup \Gamma_7$.

The tree partitioning corresponds to a partitioning of the index vector $I = [1, 2, 3, \ldots, N]$.

For instance, if $N = 400$, and we use a tree with 4 levels, and split the index vector by halves each time, we get:



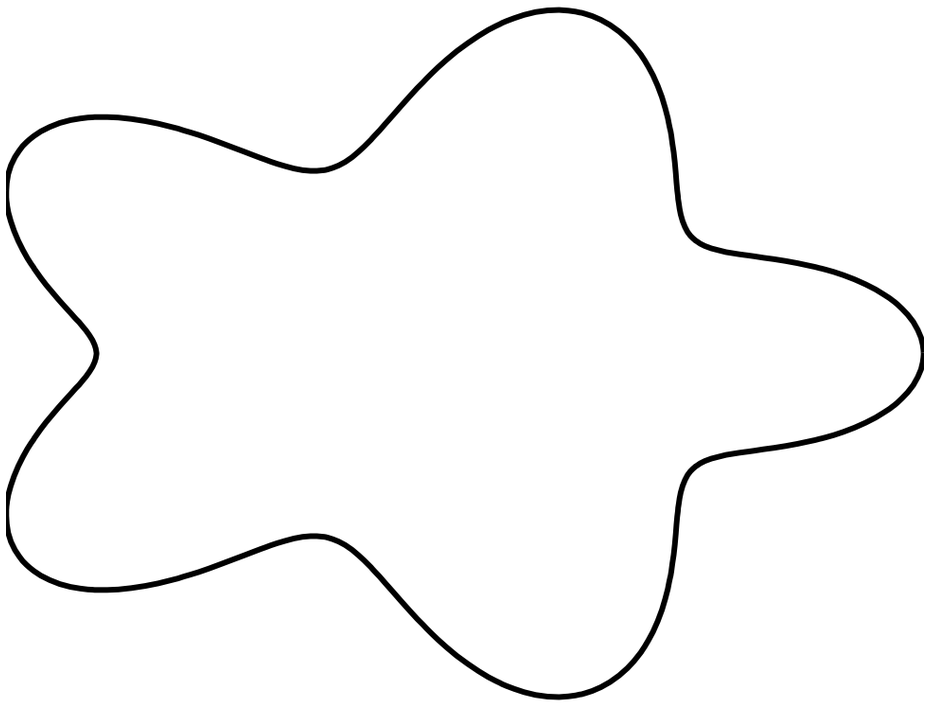
Note: *This simplistic illustration would be accurate for a simple curve.*

For complicated curves, for surfaces/volumes, etc, the index vectors are not contiguous.

The key is to subdivide based on locations $\{\boldsymbol{x}_i\}_{i=1}^{N}$ *in physical space.*

Claim: The matrix **A** resulting upon discretization of a BIE on a curve can often be represented as an "$\mathcal{S}$-matrix" with low or moderate ranks.

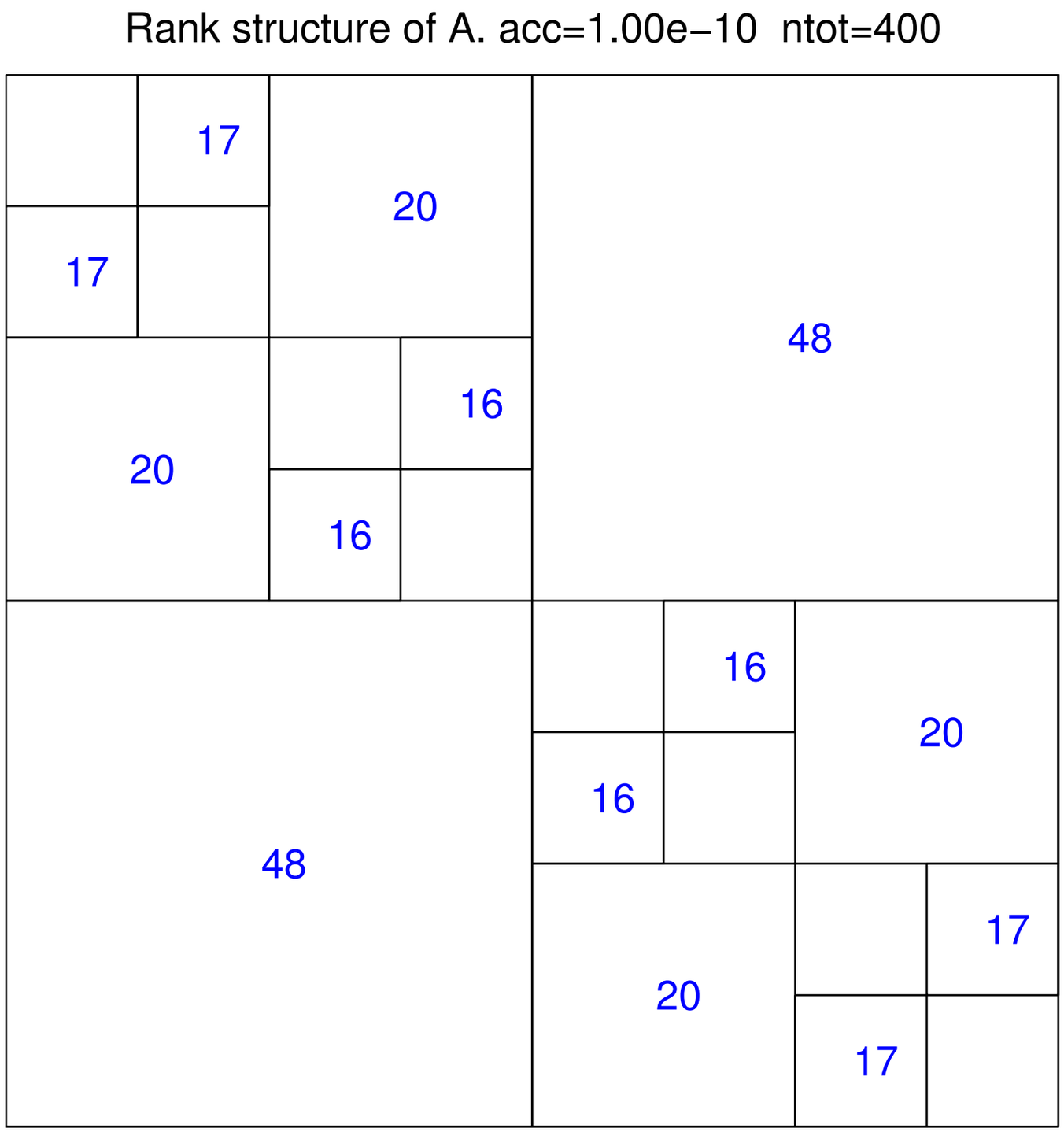
Example 1: Laplace problem discretized with Kolm-Rokhlin quadrature, $n = 400$.



The contour.

"Combined field" kernel:

$$K(\boldsymbol{x}, \boldsymbol{x}') = \log|\boldsymbol{x}-\boldsymbol{x}'| + \frac{\boldsymbol{n}' \cdot (\boldsymbol{x} - \boldsymbol{x}')}{|\boldsymbol{x} - \boldsymbol{x}'|}.$$



Ranks of off-diagonal blocks.

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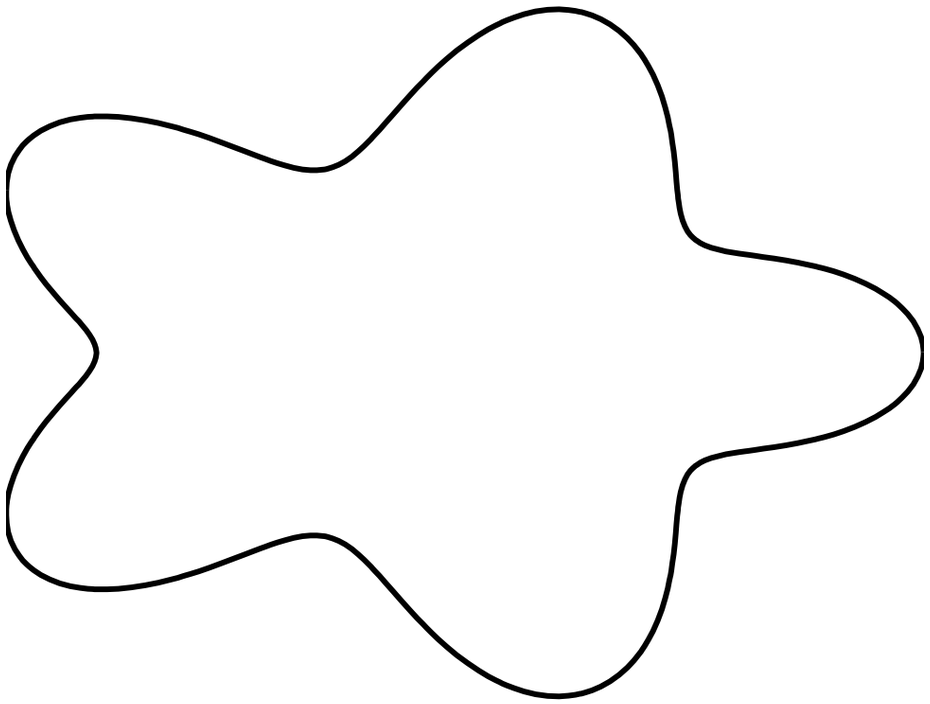

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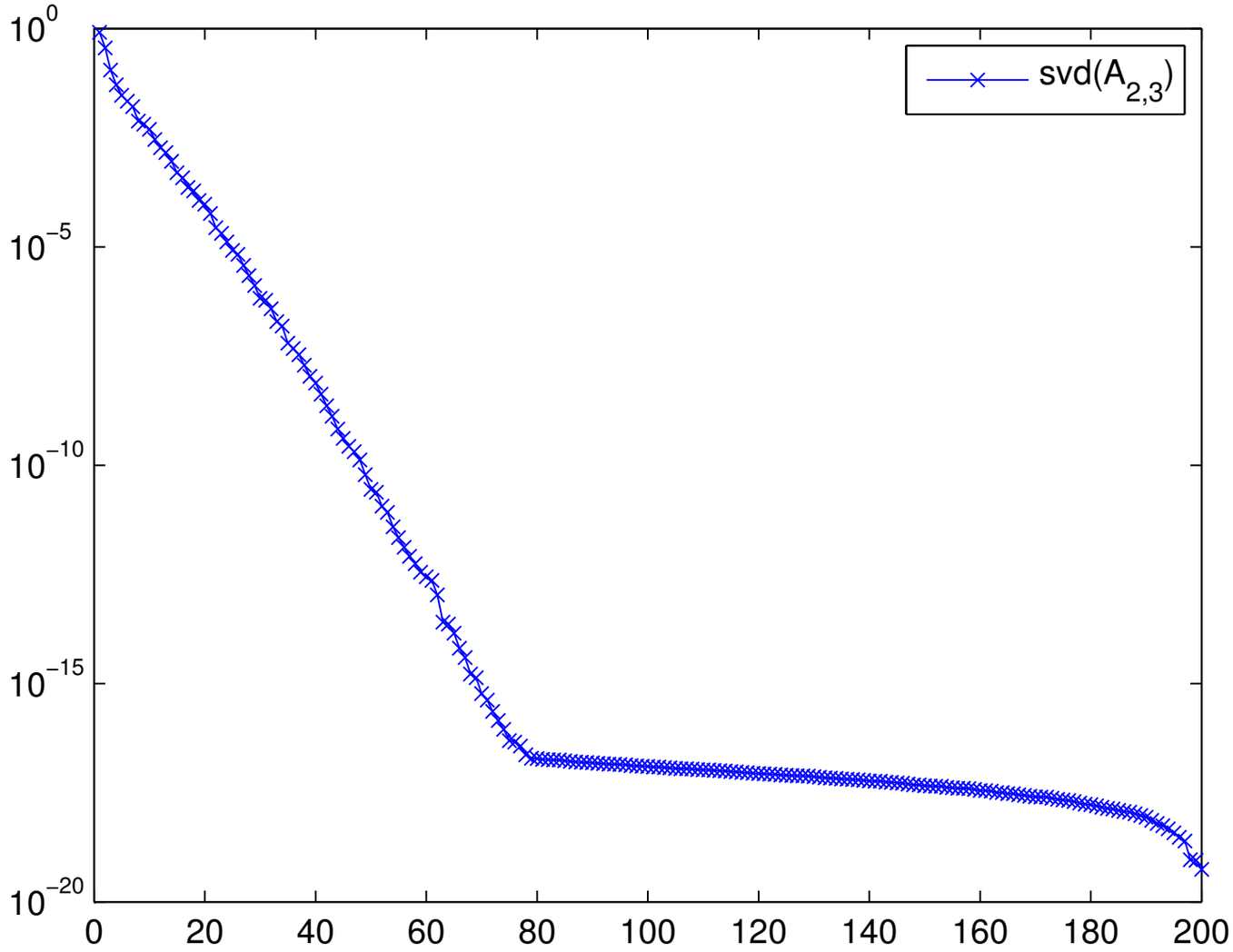
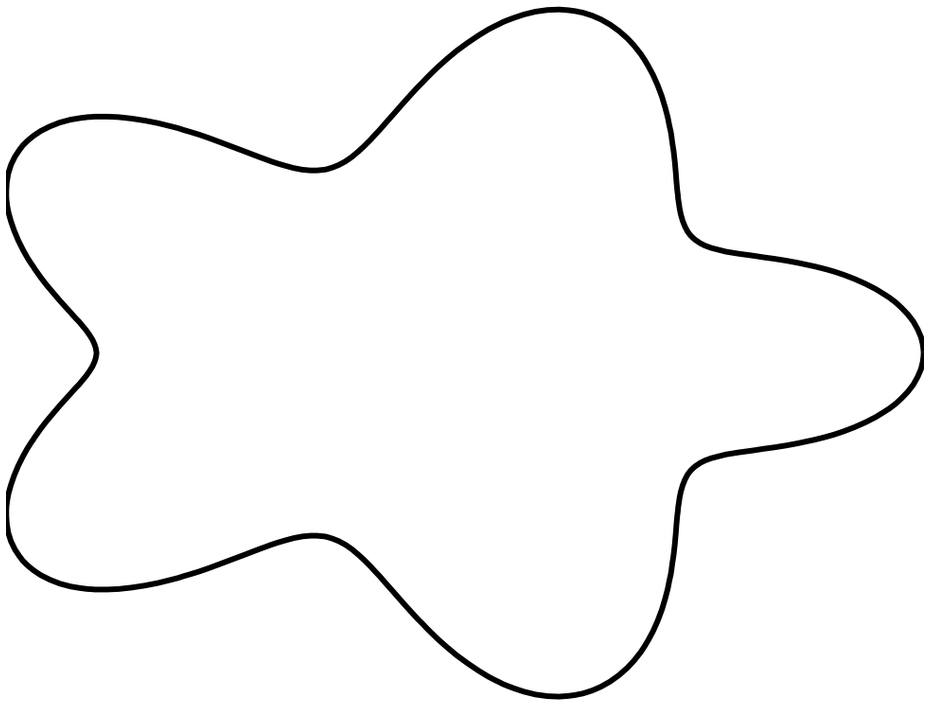


Singular values of $\mathbf{A}_{2,3}$

(top right quadrant of $\mathbf{A}$*)*

Example 2: Helmholtz problem discretized with Kolm-Rokhlin quadrature, $n = 400$.

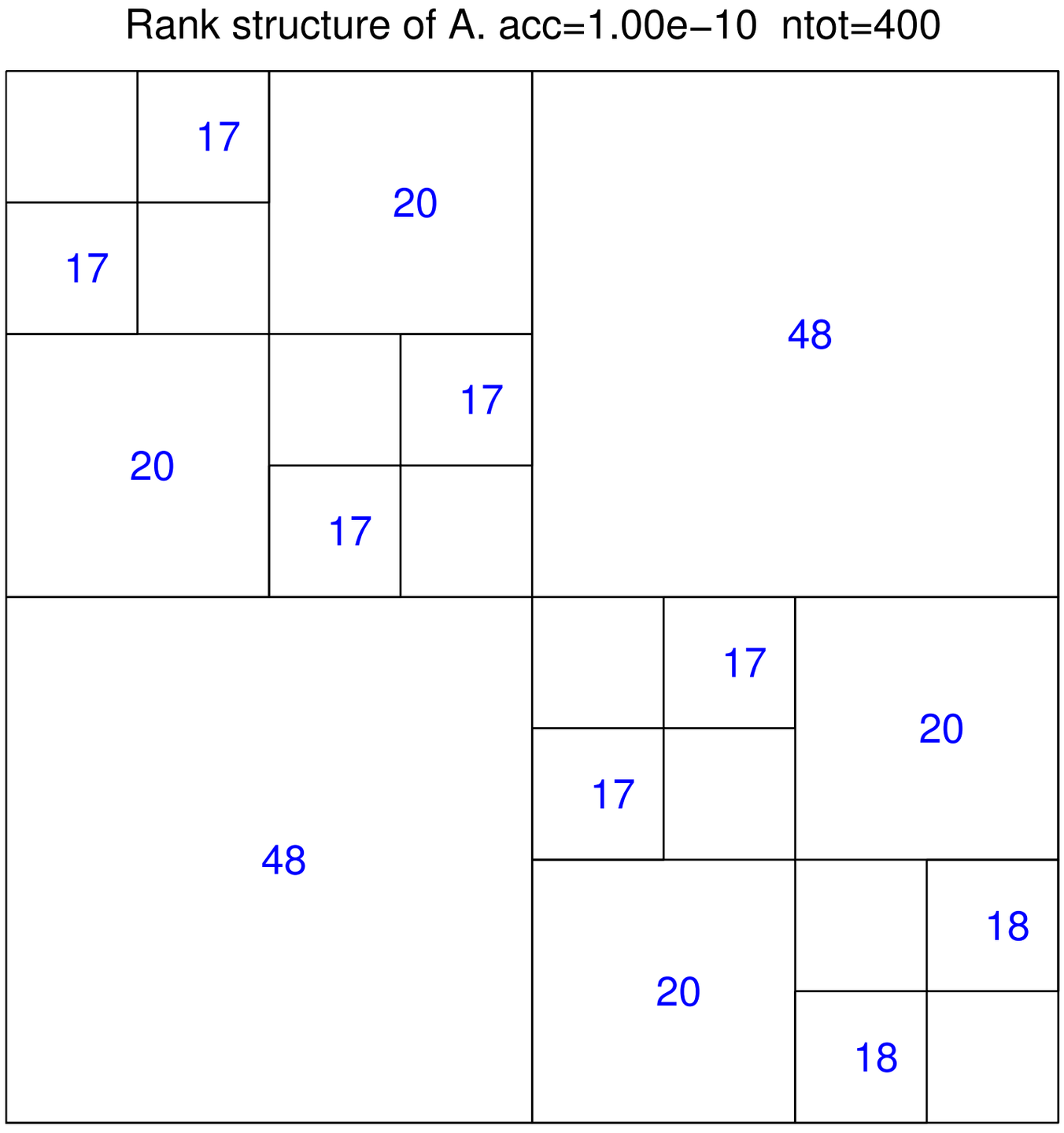


The contour, diameter = 1.2λ.

"Combined field" kernel:

$$K(\boldsymbol{x}, \boldsymbol{x}') = i\,\kappa\, H_0(\kappa|\boldsymbol{x} - \boldsymbol{x}'|) + \partial_{\boldsymbol{n}'} H_0(\kappa|\boldsymbol{x} - \boldsymbol{x}'|).$$

(the weights might be off...)



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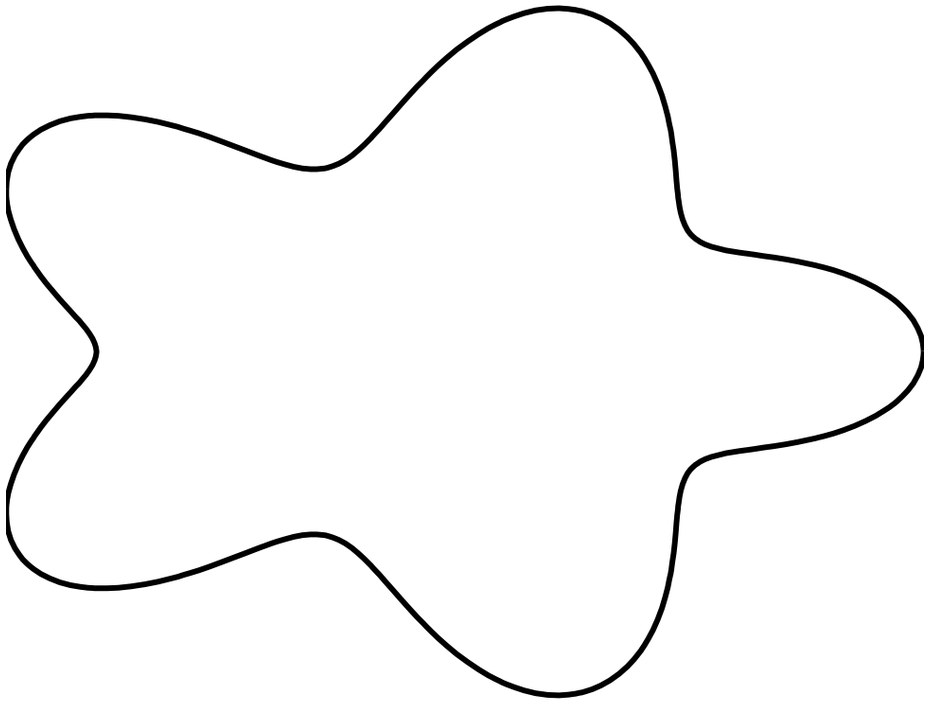

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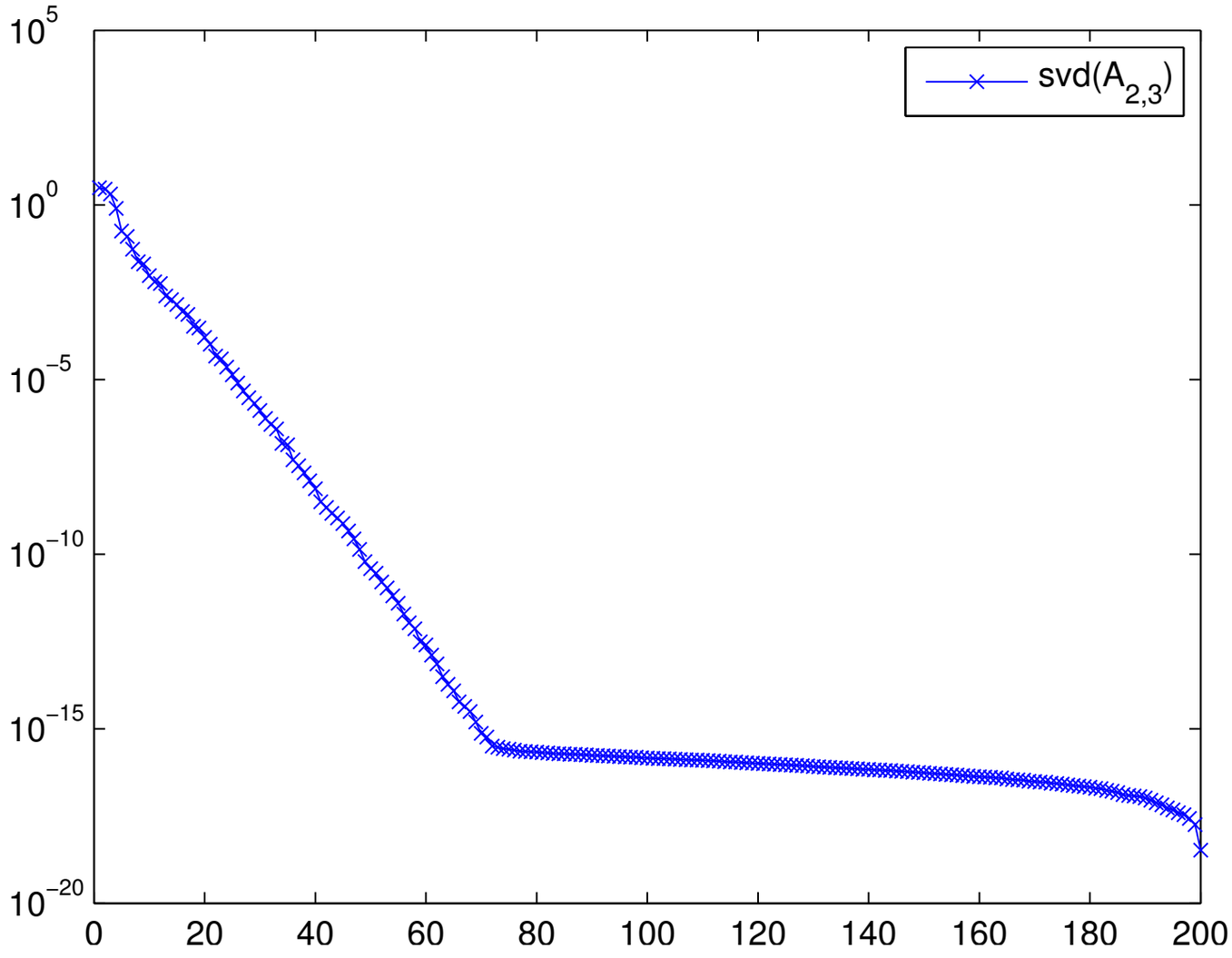

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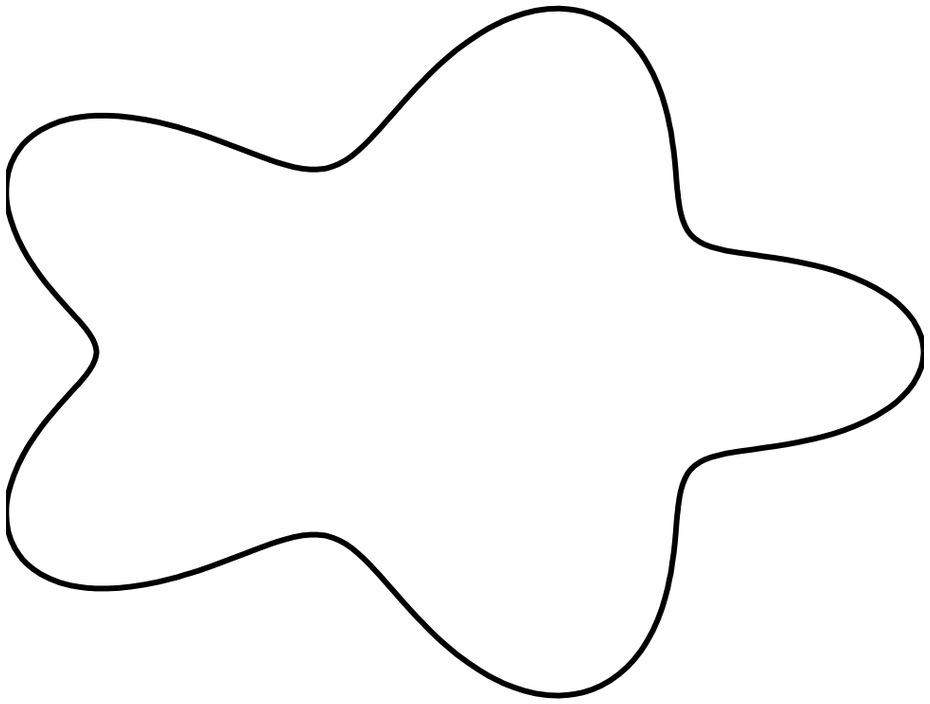
Example 3: *medium-frequency* Helmholtz, Kolm-Rokhlin quadrature, $n = 400$.



The contour, diameter = 29λ.

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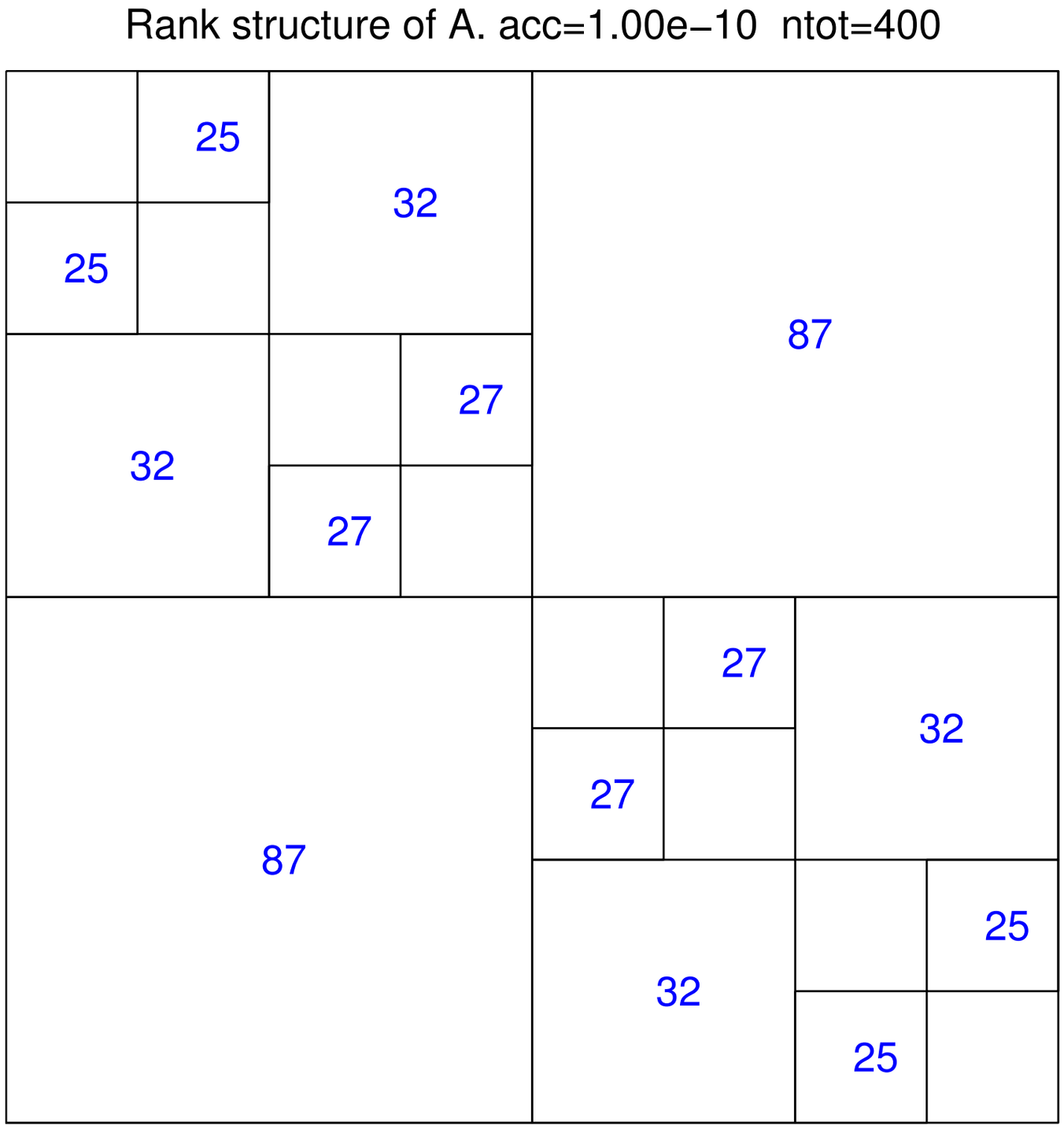

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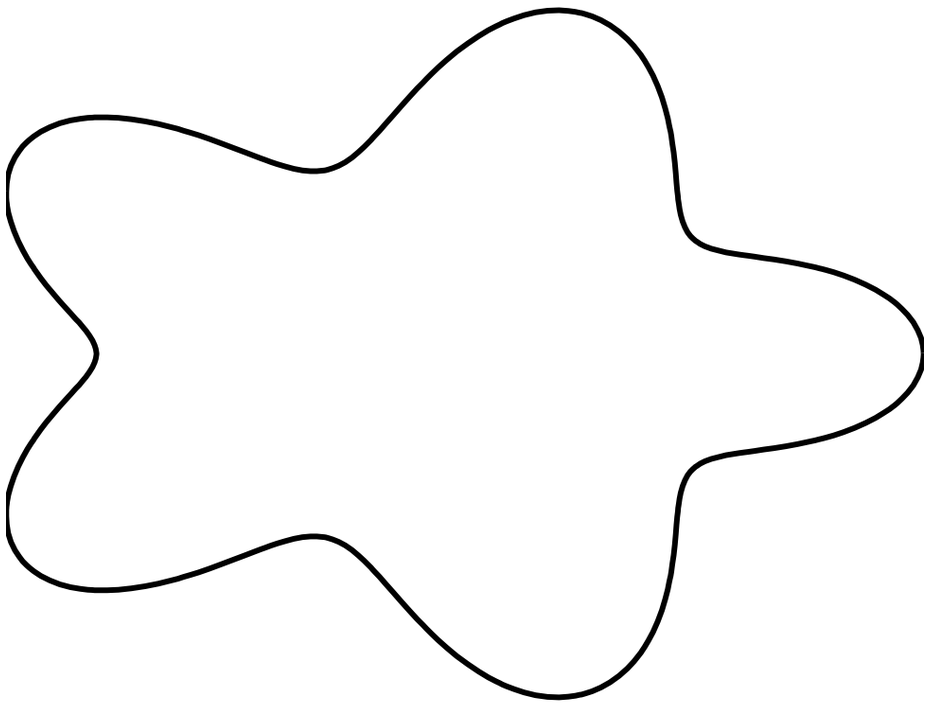

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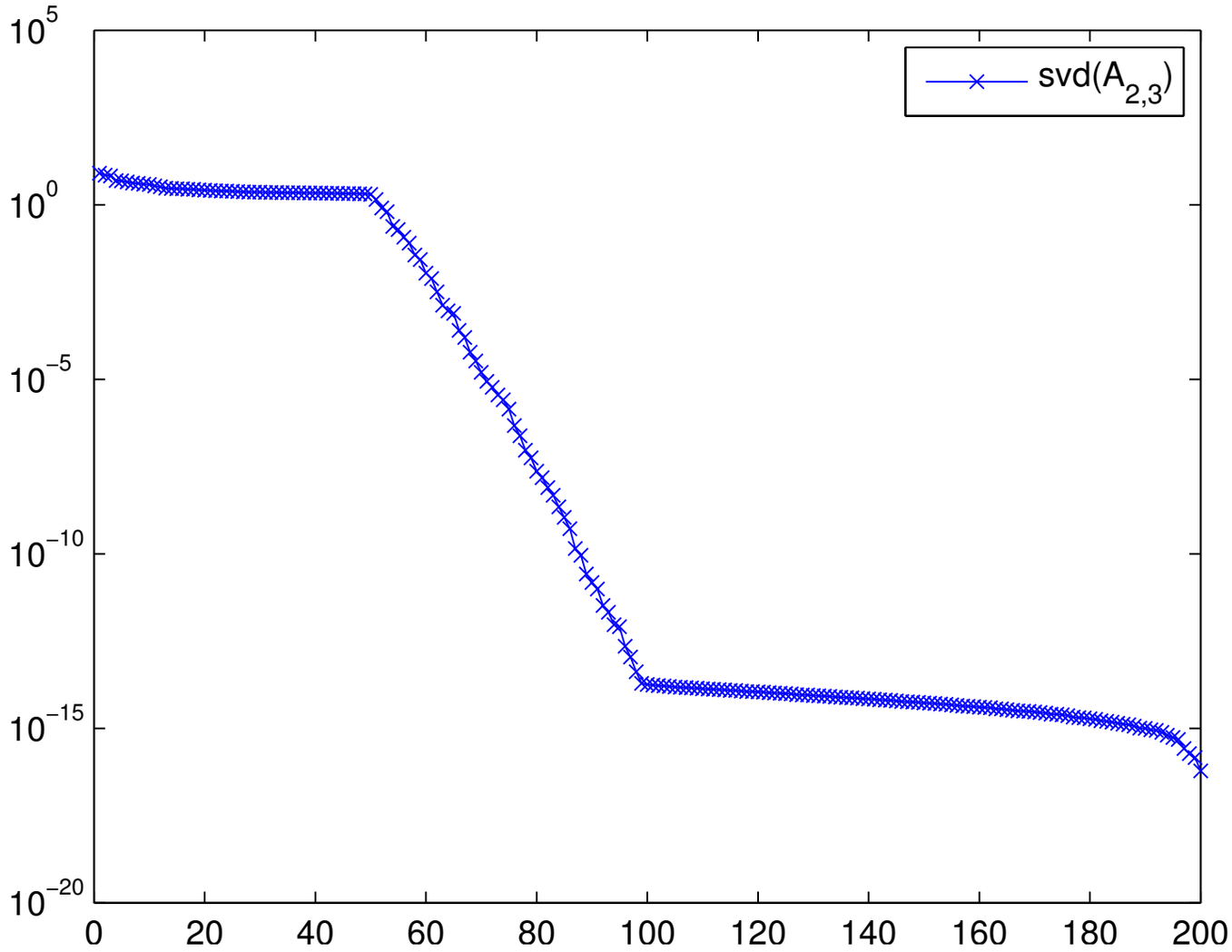


Singular values of $\mathbf{A}_{2,3}$

(top right quadrant of $\mathbf{A}$*)*

The "simple" $\mathcal{S}$-matrix format can be used for to build direct solvers for BIEs, but we will use a more efficient format called the *Hierarchically Block Separable (HBS)* format (sometimes called "Hierarchically Semi Separable (HSS)" format).

First we introduce *block separable* matrices. Consider a linear system

$$\mathbf{A}\,\mathbf{q} = \mathbf{f},$$

where $\mathbf{A}$ is a "block-separable" matrix consisting of $p \times p$ blocks of size $n \times n$:

$$\mathbf{A} = \begin{bmatrix} \mathbf{D}_4 & \mathbf{A}_{45} & \mathbf{A}_{46} & \mathbf{A}_{47} \\ \mathbf{A}_{54} & \mathbf{D}_5 & \mathbf{A}_{56} & \mathbf{A}_{57} \\ \mathbf{A}_{64} & \mathbf{A}_{65} & \mathbf{D}_6 & \mathbf{A}_{67} \\ \mathbf{A}_{74} & \mathbf{A}_{75} & \mathbf{A}_{76} & \mathbf{D}_7 \end{bmatrix}. \qquad \text{(Shown for } p = 4.\text{)}$$

Core assumption: Each off-diagonal block $\mathbf{A}_{ij}$ admits the factorization

$$\begin{array}{ccccc} \mathbf{A}_{ij} & = & \mathbf{U}_i & \tilde{\mathbf{A}}_{ij} & \mathbf{V}_j^* \\ n \times n & & n \times k & k \times k & k \times n \end{array}$$

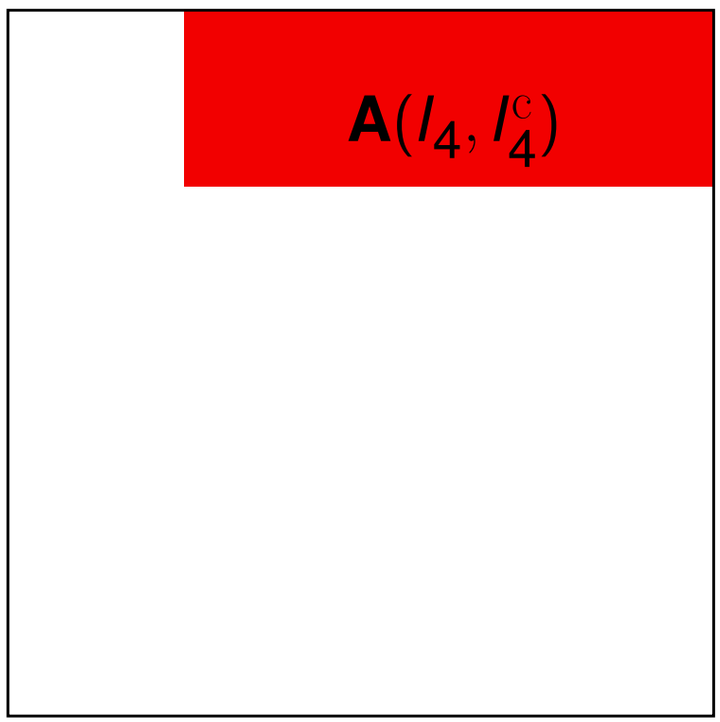
where the rank k is significantly smaller than the block size n.

The critical part of the assumption is that all off-diagonal blocks in the i'th row use the same basis matrices $\mathbf{U}_i$ for their column spaces (and analogously all blocks in the j'th column use the same basis matrices $\mathbf{V}_j$ for their row spaces).

What is the role of the basis matrices $\mathbf{U}_\tau$ *and* $\mathbf{V}_\tau$*?*

Recall our toy example: $\mathbf{A} = \begin{bmatrix} \mathbf{D}_4 & \mathbf{U}_4 \tilde{\mathbf{A}}_{45} \mathbf{V}_5^* & \mathbf{U}_4 \tilde{\mathbf{A}}_{46} \mathbf{V}_6^* & \mathbf{U}_4 \tilde{\mathbf{A}}_{47} \mathbf{V}_7^* \\ \mathbf{U}_5 \tilde{\mathbf{A}}_{54} \mathbf{V}_4^* & \mathbf{D}_5 & \mathbf{U}_5 \tilde{\mathbf{A}}_{56} \mathbf{V}_6^* & \mathbf{U}_5 \tilde{\mathbf{A}}_{57} \mathbf{V}_7^* \\ \mathbf{U}_6 \tilde{\mathbf{A}}_{64} \mathbf{V}_4^* & \mathbf{U}_6 \tilde{\mathbf{A}}_{65} \mathbf{V}_5^* & \mathbf{D}_6 & \mathbf{U}_6 \tilde{\mathbf{A}}_{67} \mathbf{V}_7^* \\ \mathbf{U}_7 \tilde{\mathbf{A}}_{74} \mathbf{V}_4^* & \mathbf{U}_7 \tilde{\mathbf{A}}_{75} \mathbf{V}_5^* & \mathbf{U}_7 \tilde{\mathbf{A}}_{76} \mathbf{V}_6^* & \mathbf{D}_7 \end{bmatrix}$.

We see that the columns of $\mathbf{U}_4$ must span the column space of the matrix $\mathbf{A}(I_4, I_4^c)$ where I_4 is the index vector for the first block and $I_4^c = I \backslash I_4$.



The matrix $\mathbf{A}$

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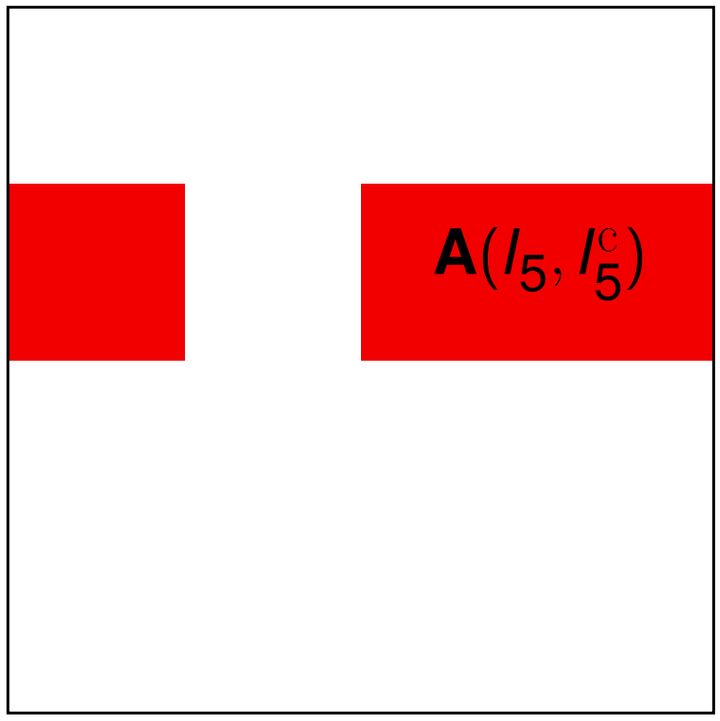
We see that the columns of $\mathbf{U}_5$ must span the column space of the matrix $\mathbf{A}(I_5, I_5^{\mathrm{c}})$ where I_5 is the index vector for the first block and $I_5^{\mathrm{c}} = I \backslash I_5$.



The matrix $\mathbf{A}$

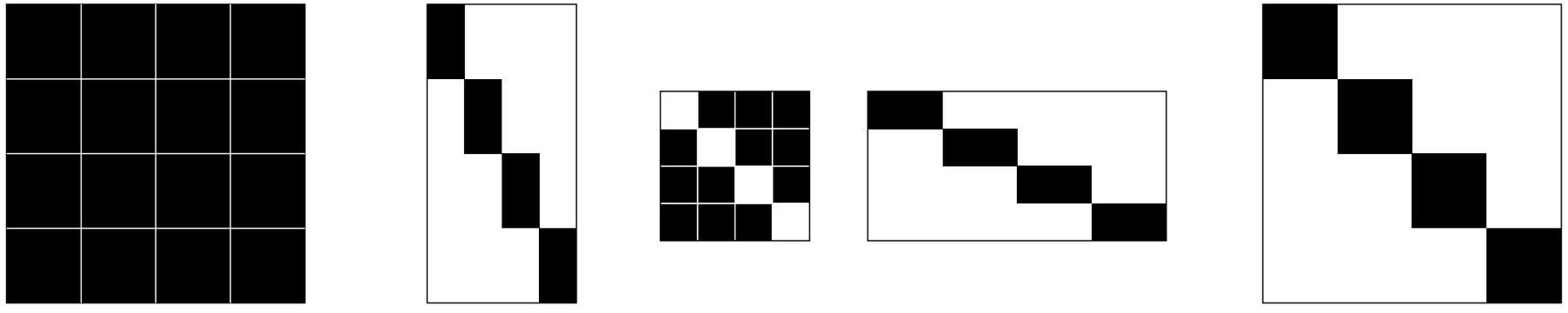
Recall $\mathbf{A} = \begin{bmatrix} \mathbf{D}_4 & \mathbf{U}_4\tilde{\mathbf{A}}_{45}\mathbf{V}_5^* & \mathbf{U}_4\tilde{\mathbf{A}}_{46}\mathbf{V}_6^* & \mathbf{U}_4\tilde{\mathbf{A}}_{47}\mathbf{V}_7^* \\ \mathbf{U}_5\tilde{\mathbf{A}}_{54}\mathbf{V}_4^* & \mathbf{D}_5 & \mathbf{U}_5\tilde{\mathbf{A}}_{56}\mathbf{V}_6^* & \mathbf{U}_5\tilde{\mathbf{A}}_{57}\mathbf{V}_7^* \\ \mathbf{U}_6\tilde{\mathbf{A}}_{64}\mathbf{V}_4^* & \mathbf{U}_6\tilde{\mathbf{A}}_{65}\mathbf{V}_5^* & \mathbf{D}_6 & \mathbf{U}_6\tilde{\mathbf{A}}_{67}\mathbf{V}_7^* \\ \mathbf{U}_7\tilde{\mathbf{A}}_{74}\mathbf{V}_4^* & \mathbf{U}_7\tilde{\mathbf{A}}_{75}\mathbf{V}_5^* & \mathbf{U}_7\tilde{\mathbf{A}}_{76}\mathbf{V}_6^* & \mathbf{D}_7 \end{bmatrix}.$

Then $\mathbf{A}$ admits the factorization:

$$\mathbf{A} = \underbrace{\begin{bmatrix} \mathbf{U}_4 & & & \\ & \mathbf{U}_5 & & \\ & & \mathbf{U}_6 & \\ & & & \mathbf{U}_7 \end{bmatrix}}_{=\mathbf{U}} \underbrace{\begin{bmatrix} \mathbf{0} & \tilde{\mathbf{A}}_{45} & \tilde{\mathbf{A}}_{46} & \tilde{\mathbf{A}}_{47} \\ \tilde{\mathbf{A}}_{54} & \mathbf{0} & \tilde{\mathbf{A}}_{56} & \tilde{\mathbf{A}}_{57} \\ \tilde{\mathbf{A}}_{64} & \tilde{\mathbf{A}}_{65} & \mathbf{0} & \tilde{\mathbf{A}}_{67} \\ \tilde{\mathbf{A}}_{74} & \tilde{\mathbf{A}}_{75} & \tilde{\mathbf{A}}_{76} & \mathbf{0} \end{bmatrix}}_{=\tilde{\mathbf{A}}} \underbrace{\begin{bmatrix} \mathbf{V}_4^* & & & \\ & \mathbf{V}_5^* & & \\ & & \mathbf{V}_6^* & \\ & & & \mathbf{V}_7^* \end{bmatrix}}_{=\mathbf{V}^*} + \underbrace{\begin{bmatrix} \mathbf{D}_4 & & & \\ & \mathbf{D}_5 & & \\ & & \mathbf{D}_6 & \\ & & & \mathbf{D}_7 \end{bmatrix}}_{=\mathbf{D}}$$

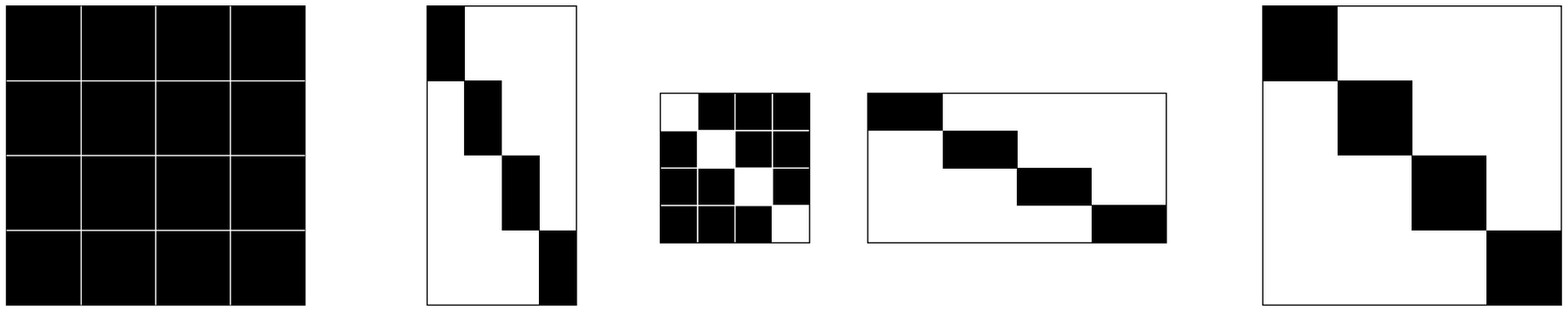
or

$$\underset{pn \times pn}{\mathbf{A}} = \underset{pn \times pk}{\mathbf{U}} \; \underset{pk \times pk}{\tilde{\mathbf{A}}} \; \underset{pk \times pn}{\mathbf{V}^*} + \underset{pn \times pn}{\mathbf{D}},$$



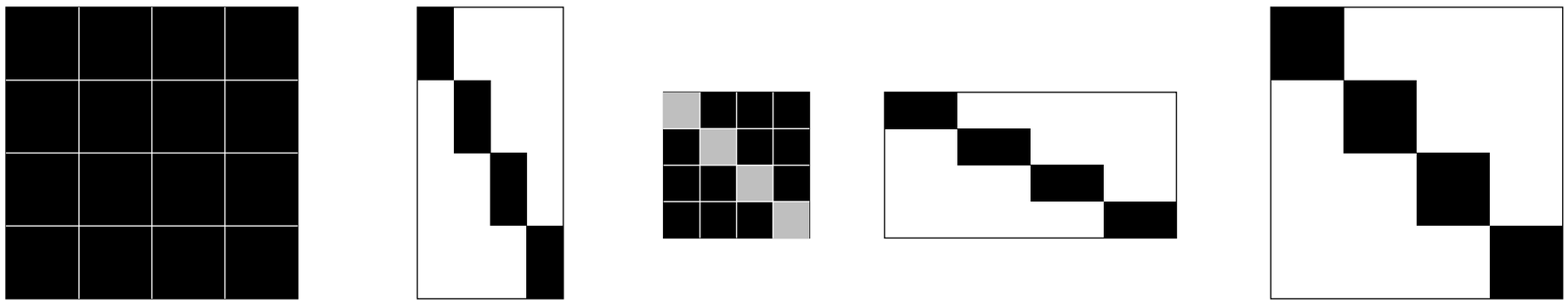
Lemma: [Variation of Woodbury] If an $N \times N$ matrix $\mathbf{A}$ admits the factorization

$$\underset{pn\times pn}{\mathbf{A}} = \underset{pn\times pk}{\mathbf{U}}\ \underset{pk\times pk}{\tilde{\mathbf{A}}}\ \underset{pk\times pn}{\mathbf{V}^*} + \underset{pn\times pn}{\mathbf{D}},$$



then

$$\underset{pn\times pn}{\mathbf{A}^{-1}} = \underset{pn\times pk}{\mathbf{E}}\ \underset{pk\times pk}{(\tilde{\mathbf{A}}+\hat{\mathbf{D}})^{-1}}\ \underset{pk\times pn}{\mathbf{F}^*} + \underset{pn\times pn}{\mathbf{G}},$$



where (provided all intermediate matrices are invertible)

$$\hat{\mathbf{D}} = \left(\mathbf{V}^*\,\mathbf{D}^{-1}\,\mathbf{U}\right)^{-1}, \quad \mathbf{E} = \mathbf{D}^{-1}\,\mathbf{U}\,\hat{\mathbf{D}}, \quad \mathbf{F} = \left(\hat{\mathbf{D}}\,\mathbf{V}^*\,\mathbf{D}^{-1}\right)^*, \quad \mathbf{G} = \mathbf{D}^{-1} - \mathbf{D}^{-1}\,\mathbf{U}\,\hat{\mathbf{D}}\,\mathbf{V}^*\,\mathbf{D}^{-1}.$$

Note: All matrices set in blue are block diagonal.

Classical Woodbury: $\left(\mathbf{D}+\mathbf{U}\tilde{\mathbf{A}}\mathbf{V}^*\right)^{-1} = \mathbf{D}^{-1} - \mathbf{D}^{-1}\mathbf{U}\left(\tilde{\mathbf{A}}+\mathbf{V}^*\mathbf{D}^{-1}\mathbf{U}\right)^{-1}\mathbf{V}^*\mathbf{D}^{-1}.$

Derivation of "our" Woodbury: We consider the linear system

$$\begin{bmatrix} \mathbf{D}_4 & \mathbf{U}_4\tilde{\mathbf{A}}_{45}\mathbf{V}_5^* & \mathbf{U}_4\tilde{\mathbf{A}}_{46}\mathbf{V}_6^* & \mathbf{U}_4\tilde{\mathbf{A}}_{47}\mathbf{V}_7^* \\ \mathbf{U}_5\tilde{\mathbf{A}}_{54}\mathbf{V}_4^* & \mathbf{D}_5 & \mathbf{U}_5\tilde{\mathbf{A}}_{56}\mathbf{V}_6^* & \mathbf{U}_5\tilde{\mathbf{A}}_{57}\mathbf{V}_7^* \\ \mathbf{U}_6\tilde{\mathbf{A}}_{64}\mathbf{V}_4^* & \mathbf{U}_6\tilde{\mathbf{A}}_{65}\mathbf{V}_5^* & \mathbf{D}_6 & \mathbf{U}_6\tilde{\mathbf{A}}_{67}\mathbf{V}_7^* \\ \mathbf{U}_7\tilde{\mathbf{A}}_{74}\mathbf{V}_4^* & \mathbf{U}_7\tilde{\mathbf{A}}_{75}\mathbf{V}_5^* & \mathbf{U}_7\tilde{\mathbf{A}}_{76}\mathbf{V}_6^* & \mathbf{D}_7 \end{bmatrix} \begin{bmatrix} \mathbf{q}_4 \\ \mathbf{q}_5 \\ \mathbf{q}_6 \\ \mathbf{q}_7 \end{bmatrix} = \begin{bmatrix} \mathbf{f}_4 \\ \mathbf{f}_5 \\ \mathbf{f}_6 \\ \mathbf{f}_7 \end{bmatrix}.$$

Introduce *reduced variables* $\tilde{\mathbf{q}}_i = \mathbf{V}_i^* \mathbf{q}_i$.

The system $\sum_j \mathbf{A}_{ij}\mathbf{q}_j = \mathbf{f}_i$ then takes the form

$$\left[\begin{array}{cccc|cccc} \mathbf{D}_4 & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{U}_4\tilde{\mathbf{A}}_{45} & \mathbf{U}_4\tilde{\mathbf{A}}_{46} & \mathbf{U}_4\tilde{\mathbf{A}}_{47} \\ \mathbf{0} & \mathbf{D}_5 & \mathbf{0} & \mathbf{0} & \mathbf{U}_5\tilde{\mathbf{A}}_{54} & \mathbf{0} & \mathbf{U}_5\tilde{\mathbf{A}}_{56} & \mathbf{U}_5\tilde{\mathbf{A}}_{57} \\ \mathbf{0} & \mathbf{0} & \mathbf{D}_6 & \mathbf{0} & \mathbf{U}_6\tilde{\mathbf{A}}_{64} & \mathbf{U}_6\tilde{\mathbf{A}}_{65} & \mathbf{0} & \mathbf{U}_6\tilde{\mathbf{A}}_{67} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{D}_7 & \mathbf{U}_7\tilde{\mathbf{A}}_{74} & \mathbf{U}_7\tilde{\mathbf{A}}_{75} & \mathbf{U}_7\tilde{\mathbf{A}}_{76} & \mathbf{0} \\ \hline -\mathbf{V}_4^* & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & -\mathbf{V}_5^* & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{I} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & -\mathbf{V}_6^* & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & -\mathbf{V}_7^* & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{I} \end{array}\right] \begin{bmatrix} \mathbf{q}_4 \\ \mathbf{q}_5 \\ \mathbf{q}_6 \\ \mathbf{q}_7 \\ \tilde{\mathbf{q}}_4 \\ \tilde{\mathbf{q}}_5 \\ \tilde{\mathbf{q}}_6 \\ \tilde{\mathbf{q}}_7 \end{bmatrix} = \begin{bmatrix} \mathbf{f}_4 \\ \mathbf{f}_5 \\ \mathbf{f}_6 \\ \mathbf{f}_7 \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix}.$$

Now form the Schur complement to eliminate the $\mathbf{q}_j$'s.

After eliminating the "fine-scale" variables $\mathbf{q}_i$, we obtain

$$\begin{bmatrix} \mathbf{I} & \mathbf{V}_4^* \tilde{\mathbf{A}}_{44}^{-1} \mathbf{U}_4 \tilde{\mathbf{A}}_{45} & \mathbf{V}_4^* \tilde{\mathbf{A}}_{44}^{-1} \mathbf{U}_4 \tilde{\mathbf{A}}_{46} & \mathbf{V}_4^* \tilde{\mathbf{A}}_{44}^{-1} \mathbf{U}_4 \tilde{\mathbf{A}}_{47} \\ \mathbf{V}_5^* \tilde{\mathbf{A}}_{55}^{-1} \mathbf{U}_5 \tilde{\mathbf{A}}_{54} & \mathbf{I} & \mathbf{V}_5^* \tilde{\mathbf{A}}_{55}^{-1} \mathbf{U}_5 \tilde{\mathbf{A}}_{56} & \mathbf{V}_5^* \tilde{\mathbf{A}}_{55}^{-1} \mathbf{U}_5 \tilde{\mathbf{A}}_{57} \\ \mathbf{V}_6^* \tilde{\mathbf{A}}_{66}^{-1} \mathbf{U}_6 \tilde{\mathbf{A}}_{61} & \mathbf{V}_6^* \tilde{\mathbf{A}}_{66}^{-1} \mathbf{U}_6 \tilde{\mathbf{A}}_{65} & \mathbf{I} & \mathbf{V}_6^* \tilde{\mathbf{A}}_{66}^{-1} \mathbf{U}_6 \tilde{\mathbf{A}}_{67} \\ \mathbf{V}_7^* \tilde{\mathbf{A}}_{77}^{-1} \mathbf{U}_7 \tilde{\mathbf{A}}_{74} & \mathbf{V}_7^* \tilde{\mathbf{A}}_{77}^{-1} \mathbf{U}_7 \tilde{\mathbf{A}}_{75} & \mathbf{V}_7^* \tilde{\mathbf{A}}_{77}^{-1} \mathbf{U}_7 \tilde{\mathbf{A}}_{76} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{q}}_4 \\ \tilde{\mathbf{q}}_5 \\ \tilde{\mathbf{q}}_6 \\ \tilde{\mathbf{q}}_7 \end{bmatrix} = \begin{bmatrix} \mathbf{V}_4^* \mathbf{D}_4^{-1} \mathbf{f}_4 \\ \mathbf{V}_5^* \mathbf{D}_5^{-1} \mathbf{f}_5 \\ \mathbf{V}_6^* \mathbf{D}_6^{-1} \mathbf{f}_6 \\ \mathbf{V}_7^* \mathbf{D}_7^{-1} \mathbf{f}_7. \end{bmatrix}.$$

We set

$$\tilde{\mathbf{A}}_{ii} = \left(\mathbf{V}_i^* \, \mathbf{D}_{ii}^{-1} \, \mathbf{U}_i \right)^{-1},$$

and multiply line i by $\tilde{\mathbf{A}}_{ii}$ to obtain the reduced system

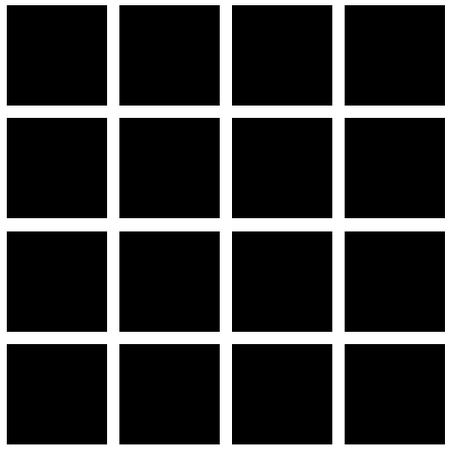
$$\begin{bmatrix} \tilde{\mathbf{A}}_{44} & \tilde{\mathbf{A}}_{45} & \tilde{\mathbf{A}}_{46} & \tilde{\mathbf{A}}_{47} \\ \tilde{\mathbf{A}}_{54} & \tilde{\mathbf{A}}_{55} & \tilde{\mathbf{A}}_{56} & \tilde{\mathbf{A}}_{57} \\ \tilde{\mathbf{A}}_{64} & \tilde{\mathbf{A}}_{65} & \tilde{\mathbf{A}}_{66} & \tilde{\mathbf{A}}_{67} \\ \tilde{\mathbf{A}}_{74} & \tilde{\mathbf{A}}_{75} & \tilde{\mathbf{A}}_{76} & \tilde{\mathbf{A}}_{77} \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{q}}_4 \\ \tilde{\mathbf{q}}_5 \\ \tilde{\mathbf{q}}_6 \\ \tilde{\mathbf{q}}_7 \end{bmatrix} = \begin{bmatrix} \tilde{\mathbf{f}}_4 \\ \tilde{\mathbf{f}}_5 \\ \tilde{\mathbf{f}}_6 \\ \tilde{\mathbf{f}}_7 \end{bmatrix}.$$

where

$$\tilde{\mathbf{f}}_i = \tilde{\mathbf{A}}_{ii} \, \mathbf{V}_i^* \, \mathbf{D}_{ii}^{-1} \, \mathbf{f}_i.$$

Before compression, we have a $pn \times pn$ linear system

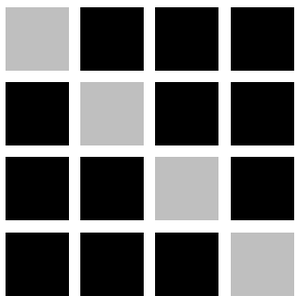
$$\sum_{j=1}^{p} \mathbf{A}_{ij}\mathbf{q}_j = \mathbf{f}_i, \quad i = 1, 2, \ldots, p.$$



The original matrix

After compression, we have a $pk \times pk$ linear system

$$\mathbf{D}_{ii}\tilde{\mathbf{q}}_i + \sum_{i \neq j} \tilde{\mathbf{A}}_{ij}\tilde{\mathbf{q}}_j = \tilde{\mathbf{f}}_i, \quad i = 1, 2, \ldots, p.$$



The reduced matrix

Recall that k is the ε-rank of $\mathbf{A}_{i,j}$ for $i \neq j$.

The point is that $k < n$.

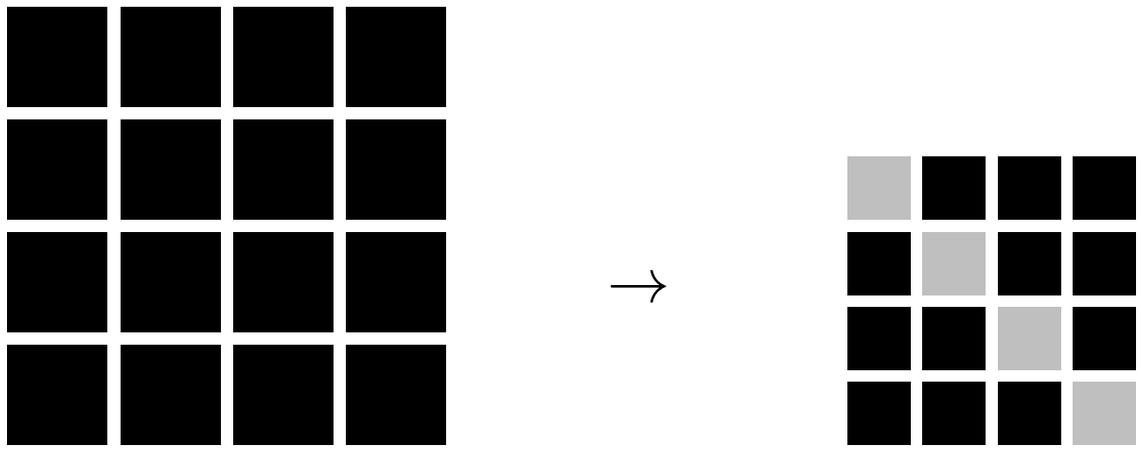
The compression algorithm needs to execute the following steps:

- Compute $\mathbf{U}_i$, $\mathbf{V}_i$, $\tilde{\mathbf{A}}_{ij}$ so that $\mathbf{A}_{ij} = \mathbf{U}_i \, \tilde{\mathbf{A}}_{ij} \, \mathbf{V}_j^*$.
- Compute the new diagonal matrices $\hat{\mathbf{D}}_{ii} = \left(\mathbf{V}_i^* \, \mathbf{A}_{ii}^{-1} \, \mathbf{U}_i\right)^{-1}$.
- Compute the new loads $\tilde{\mathbf{q}}_i = \hat{\mathbf{D}}_{ii} \, \mathbf{V}_i^* \, \mathbf{A}_{ii}^{-1} \, \mathbf{q}_i$.

For the algorithm to be efficient, it has to be able to carry out these steps *locally*.

To achieve this, we use interpolative representations, then $\tilde{\mathbf{A}}_{i,j} = \mathbf{A}(\tilde{I}_i, \tilde{I}_j)$.

We have built a scheme for reducing a system of size $pn \times pn$ to one of size $pk \times pk$.

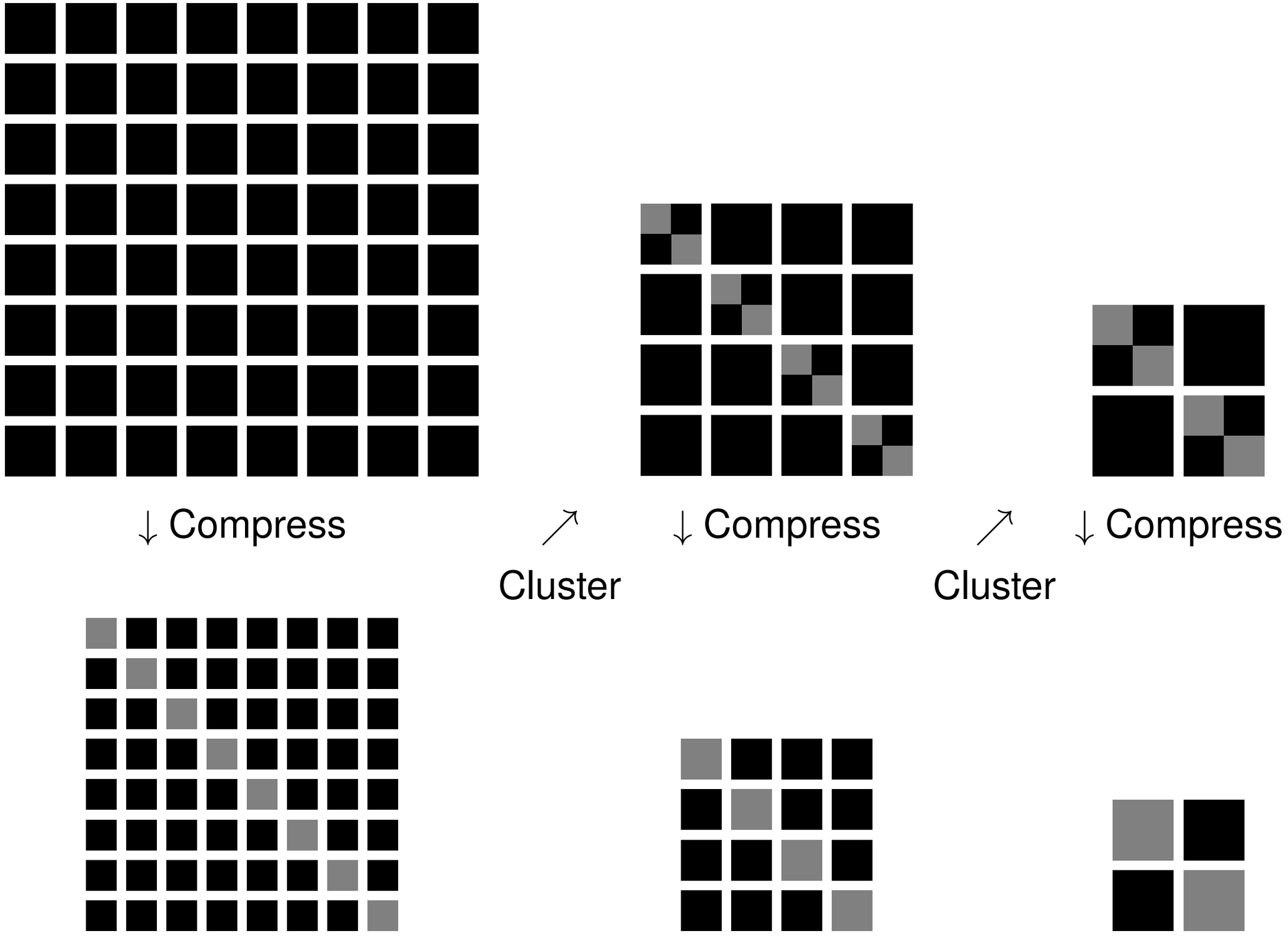


The computational gain is $(k/n)^3$. Good, but not earth-shattering.

Question: How do we get to $O(N)$?

Answer: It turns out that the reduced matrix is itself compressible. Recurse!

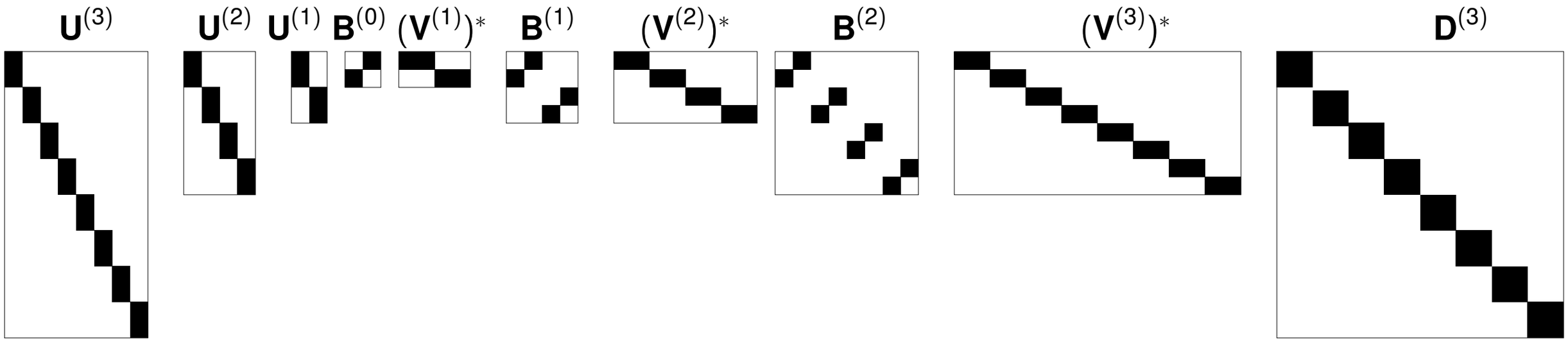
A globally $O(N)$ algorithm is obtained by hierarchically repeating the process:



Formally, one can view this as a telescoping factorization of $\mathbf{A}$:

$$\mathbf{A} = \mathbf{U}^{(3)}\big(\mathbf{U}^{(2)}\big(\mathbf{U}^{(1)}\,\mathbf{B}^{(0)}\,(\mathbf{V}^{(1)})^* + \mathbf{B}^{(1)}\big)(\mathbf{V}^{(2)})^* + \mathbf{B}^{(2)}\big)(\mathbf{V}^{(3)})^* + \mathbf{D}^{(3)}.$$

Expressed pictorially, the factorization takes the form



The *inverse of A* then takes the form

$$\mathbf{A}^{-1} = \mathbf{E}^{(3)}\big(\mathbf{E}^{(2)}\big(\mathbf{E}^{(1)}\,\hat{\mathbf{D}}^{(0)}\,(\mathbf{F}^{(1)})^* + \hat{\mathbf{D}}^{(1)}\big)(\mathbf{F}^{(2)})^* + \hat{\mathbf{D}}^{(2)}\big)(\mathbf{V}^{(3)})^* + \hat{\mathbf{D}}^{(3)}.$$

All matrices are block diagonal except $\hat{\mathbf{D}}^{(0)}$*, which is small.*

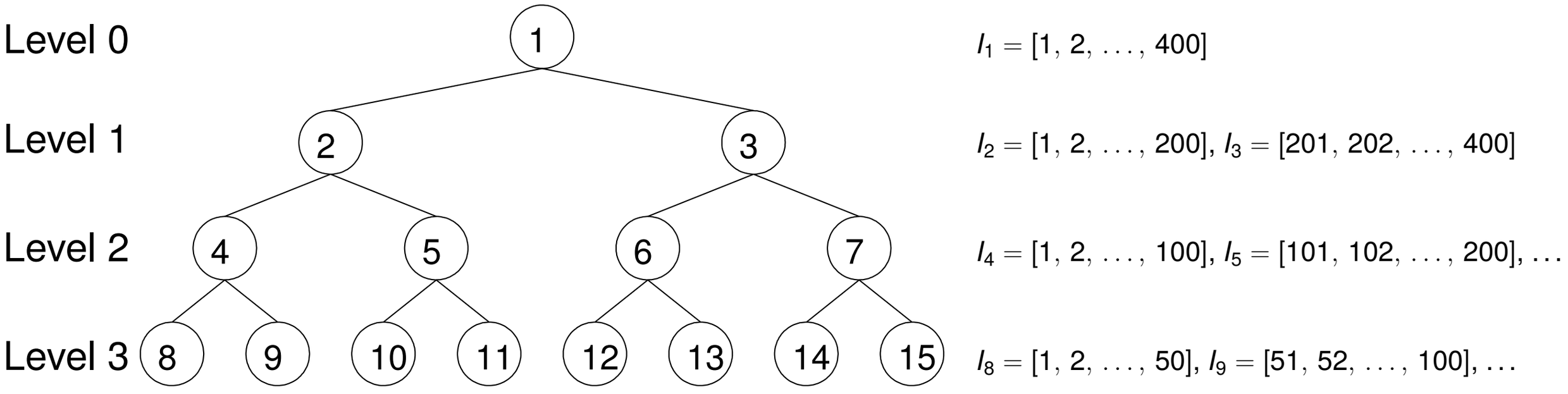
Formal definition of an HBS matrix

Let us first recall the concept of a binary tree on the index vector:

Let **A** be an $N \times N$ matrix.

Suppose $\mathcal{T}$ is a binary tree on the index vector $I = [1, 2, 3, \ldots, N]$.

For a node τ in the tree, let I_τ denote the corresponding index vector.



For nodes σ and τ on the same level, set $\mathbf{A}_{\sigma,\tau} = \mathbf{A}(I_\sigma, I_\tau)$.

Formal definition of an HBS matrix

Suppose $\mathcal{T}$ is a binary tree.

For a node τ in the tree, let I_τ denote the corresponding index vector.

For leaves σ and τ, set $\mathbf{A}_{\sigma,\tau} = \mathbf{A}(I_\sigma, I_\tau)$ and suppose that all off-diagonal blocks satisfy

$$\begin{array}{cccccc} \mathbf{A}_{\sigma,\tau} & = & \mathbf{U}_\sigma & \tilde{\mathbf{A}}_{\sigma,\tau} & \mathbf{V}_\tau^* & \sigma \neq \tau \\ n \times n & & n \times k & k \times k & k \times n & \end{array}$$

For non-leaves σ and τ, let $\{\sigma_1, \sigma_2\}$ denote the children of σ, and let $\{\tau_1, \tau_2\}$ denote the children of τ. Set

$$\mathbf{A}_{\sigma,\tau} = \begin{bmatrix} \tilde{\mathbf{A}}_{\sigma_1,\tau_1} & \tilde{\mathbf{A}}_{\sigma_1,\tau_2} \\ \tilde{\mathbf{A}}_{\sigma_2,\tau_1} & \tilde{\mathbf{A}}_{\sigma_2,\tau_2} \end{bmatrix}$$

Then suppose that the off-diagonal blocks satisfy

$$\begin{array}{cccccc} \mathbf{A}_{\sigma,\tau} & = & \mathbf{U}_\sigma & \tilde{\mathbf{A}}_{\sigma,\tau} & \mathbf{V}_\tau^* & \sigma \neq \tau \\ 2k \times 2k & & 2k \times k & k \times k & k \times 2k & \end{array}$$

An HBS matrix **A** *associated with a tree* $\mathcal{T}$ *is specified by the following factors:*

	Name:	Size:	Function:
For each leaf	$\mathbf{D}_\tau$	$n \times n$	The diagonal block $\mathbf{A}(I_\tau, I_\tau)$.
node τ:	$\mathbf{U}_\tau$	$n \times k$	Basis for the columns in the blocks in row τ.
	$\mathbf{V}_\tau$	$n \times k$	Basis for the rows in the blocks in column τ.
For each parent	$\mathbf{B}_\tau$	$2k \times 2k$	Interactions between the children of τ.
node τ:	$\mathbf{U}_\tau$	$2k \times k$	Basis for the columns in the (reduced) blocks in row τ.
	$\mathbf{V}_\tau$	$2k \times k$	Basis for the rows in the (reduced) blocks in column τ.

Inversion of an HBS matrix

loop over all levels, finer to coarser, $\ell = L, L-1, \ldots, 1$

  loop over all boxes τ on level ℓ,

    if τ is a leaf node

      $\mathbf{X} = \mathbf{D}_\tau$

    else

      Let σ_1 and σ_2 denote the children of τ.

      $$\mathbf{X} = \begin{bmatrix} \mathbf{D}_{\sigma_1} & \mathbf{B}_{\sigma_1,\sigma_2} \\ \mathbf{B}_{\sigma_2,\sigma_1} & \mathbf{D}_{\sigma_2} \end{bmatrix}$$

    end if

    $\mathbf{D}_\tau = \left(\mathbf{V}_\tau^* \mathbf{X}^{-1} \mathbf{U}_\tau\right)^{-1}$.

    $\mathbf{E}_\tau = \mathbf{X}^{-1} \mathbf{U}_\tau \mathbf{D}_\tau$.

    $\mathbf{F}_\tau^* = \mathbf{D}_\tau \mathbf{V}_\tau^* \mathbf{X}^{-1}$.

    $\mathbf{G}_\tau = \mathbf{X}^{-1} - \mathbf{X}^{-1} \mathbf{U}_\tau \mathbf{D}_\tau \mathbf{V}_\tau^* \mathbf{X}^{-1}$.

  end loop

end loop

$$\mathbf{G}_1 = \begin{bmatrix} \mathbf{D}_2 & \mathbf{B}_{2,3} \\ \mathbf{B}_{3,2} & \mathbf{D}_3 \end{bmatrix}^{-1}.$$

```
function EFG = OMNI_invert_HBS_nsym(NODES)
nboxes = size(NODES,2);
EFG = cell(3,nboxes);
ATD_VEC = cell(1,nboxes);
% Loop over all nodes, from finest to coarser.
for ibox = nboxes:(-1):2
   % Assemble the diagonal matrix.
   if (NODES{5,ibox}==0) % ibox is a leaf.
      AD = NODES{40,ibox};
   elseif (NODES{5,ibox}==2) % ibox has precisely two children
      ison1 = NODES{4,ibox}(1);
      ison2 = NODES{4,ibox}(2);
      AD = [ATD_VEC{ison1},NODES{46,ison1};NODES{46,ison2},ATD_VEC{ison2}];
   end
   % Extract the matrices U and V.
   U = NODES{38,ibox};
   V = NODES{39,ibox};
   % Construct the various projection maps.
   ADinv = inv(AD);
   ATD = inv(V'*ADinv*U);
   ATD_VEC{ibox} = ATD;
   EFG{1,ibox} = ADinv*U*ATD;
   EFG{2,ibox} = ATD*(V')*ADinv;
   EFG{3,ibox} = ADinv - EFG{1,ibox}*(V'*ADinv);
end
% Assemble the "top matrix" and invert it:
AT = [ATD_VEC{2},NODES{46,2};NODES{46,3},ATD_VEC{3}];
EFG{3,1} = inv(AT);
return
```

Now let us return to the question of how to compute a block-separable factorization of a matrix $\mathbf{A}$, where the low-rank factorization is based on an *interpolative decomposition.*

Example: Consider an $N \times N$ matrix $\mathbf{A}$, and a partitioning of the index vector

$$I = \{1, 2, 3, \ldots, N\} = I_4 \cup I_5 \cup I_6 \cup I_7.$$

We then seek to determine matrices $\{\mathbf{U}_\tau, \mathbf{V}_\tau\}_{\tau=4}^{7}$ and index vectors $\tilde{I}_\kappa \subset I_\kappa$ such that

$$\mathbf{A}(I_\tau, I_\sigma) = \mathbf{U}_\tau \, \tilde{\mathbf{A}}_{\tau,\sigma} \, \mathbf{V}_\sigma^*, \qquad \sigma \neq \tau,$$

where $\tilde{\mathbf{A}}_{\tau,\sigma} = \mathbf{A}(\tilde{I}_\tau, \tilde{I}_\sigma)$ is a submatrix of $\mathbf{A}_{\tau,\sigma}$.

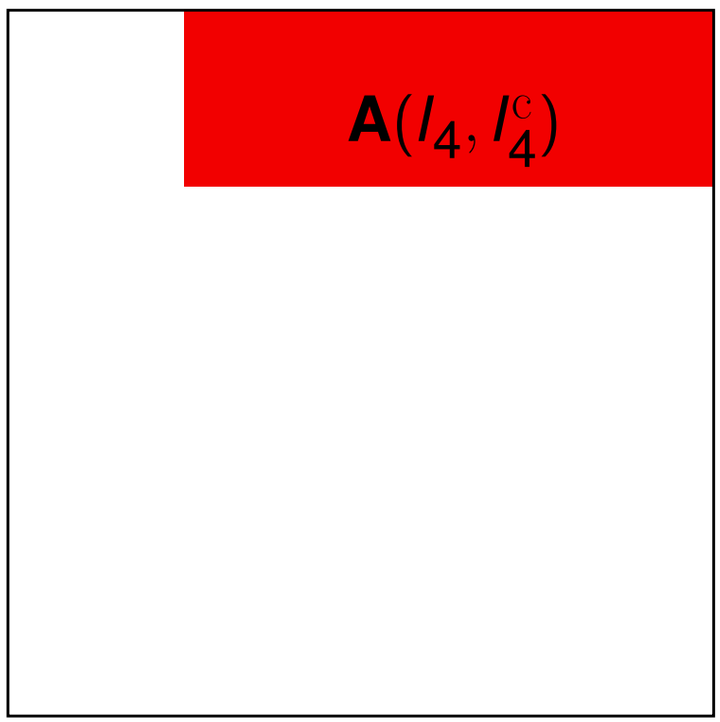
In other words, we seek a factorization

$$\mathbf{A} = \underbrace{\begin{bmatrix} \mathbf{U}_4 & & & \\ & \mathbf{U}_5 & & \\ & & \mathbf{U}_6 & \\ & & & \mathbf{U}_7 \end{bmatrix}}_{=\mathbf{U}} \underbrace{\begin{bmatrix} \mathbf{0} & \tilde{\mathbf{A}}_{45} & \tilde{\mathbf{A}}_{46} & \tilde{\mathbf{A}}_{47} \\ \tilde{\mathbf{A}}_{54} & \mathbf{0} & \tilde{\mathbf{A}}_{56} & \tilde{\mathbf{A}}_{57} \\ \tilde{\mathbf{A}}_{64} & \tilde{\mathbf{A}}_{65} & \mathbf{0} & \tilde{\mathbf{A}}_{67} \\ \tilde{\mathbf{A}}_{74} & \tilde{\mathbf{A}}_{75} & \tilde{\mathbf{A}}_{76} & \mathbf{0} \end{bmatrix}}_{=\tilde{\mathbf{A}}} \underbrace{\begin{bmatrix} \mathbf{V}_4^* & & & \\ & \mathbf{V}_5^* & & \\ & & \mathbf{V}_6^* & \\ & & & \mathbf{V}_7^* \end{bmatrix}}_{=\mathbf{V}^*} + \underbrace{\begin{bmatrix} \mathbf{D}_4 & & & \\ & \mathbf{D}_5 & & \\ & & \mathbf{D}_6 & \\ & & & \mathbf{D}_7 \end{bmatrix}}_{=\mathbf{D}}.$$

What is the role of the basis matrices $\mathbf{U}_\tau$ *and* $\mathbf{V}_\tau$*?*

Recall our toy example: $\mathbf{A} = \begin{bmatrix} \mathbf{D}_4 & \mathbf{U}_4 \tilde{\mathbf{A}}_{45} \mathbf{V}_5^* & \mathbf{U}_4 \tilde{\mathbf{A}}_{46} \mathbf{V}_6^* & \mathbf{U}_4 \tilde{\mathbf{A}}_{47} \mathbf{V}_7^* \\ \mathbf{U}_5 \tilde{\mathbf{A}}_{54} \mathbf{V}_4^* & \mathbf{D}_5 & \mathbf{U}_5 \tilde{\mathbf{A}}_{56} \mathbf{V}_6^* & \mathbf{U}_5 \tilde{\mathbf{A}}_{57} \mathbf{V}_7^* \\ \mathbf{U}_6 \tilde{\mathbf{A}}_{64} \mathbf{V}_4^* & \mathbf{U}_6 \tilde{\mathbf{A}}_{65} \mathbf{V}_5^* & \mathbf{D}_6 & \mathbf{U}_6 \tilde{\mathbf{A}}_{67} \mathbf{V}_7^* \\ \mathbf{U}_7 \tilde{\mathbf{A}}_{74} \mathbf{V}_4^* & \mathbf{U}_7 \tilde{\mathbf{A}}_{75} \mathbf{V}_5^* & \mathbf{U}_7 \tilde{\mathbf{A}}_{76} \mathbf{V}_6^* & \mathbf{D}_7 \end{bmatrix}$.

We see that the columns of $\mathbf{U}_4$ must span the column space of the matrix $\mathbf{A}(I_4, I_4^c)$ where I_4 is the index vector for the first block and $I_4^c = I \backslash I_4$.

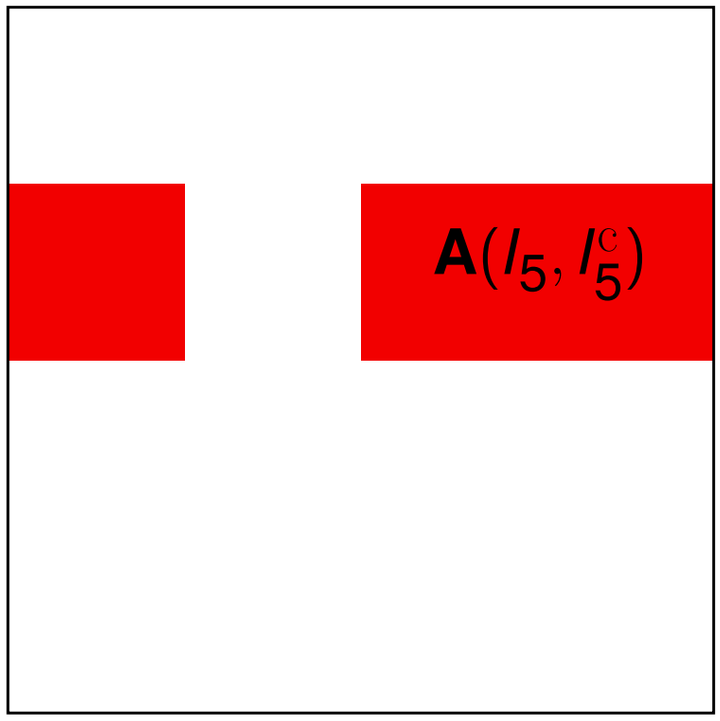


The matrix $\mathbf{A}$

What is the role of the basis matrices $\mathbf{U}_\tau$ and $\mathbf{V}_\tau$?

Recall our toy example: $\mathbf{A} = \begin{bmatrix} \mathbf{D}_4 & \mathbf{U}_4\tilde{\mathbf{A}}_{45}\mathbf{V}_5^* & \mathbf{U}_4\tilde{\mathbf{A}}_{46}\mathbf{V}_6^* & \mathbf{U}_4\tilde{\mathbf{A}}_{47}\mathbf{V}_7^* \\ \mathbf{U}_5\tilde{\mathbf{A}}_{54}\mathbf{V}_4^* & \mathbf{D}_5 & \mathbf{U}_5\tilde{\mathbf{A}}_{56}\mathbf{V}_6^* & \mathbf{U}_5\tilde{\mathbf{A}}_{57}\mathbf{V}_7^* \\ \mathbf{U}_6\tilde{\mathbf{A}}_{64}\mathbf{V}_4^* & \mathbf{U}_6\tilde{\mathbf{A}}_{65}\mathbf{V}_5^* & \mathbf{D}_6 & \mathbf{U}_6\tilde{\mathbf{A}}_{67}\mathbf{V}_7^* \\ \mathbf{U}_7\tilde{\mathbf{A}}_{74}\mathbf{V}_4^* & \mathbf{U}_7\tilde{\mathbf{A}}_{75}\mathbf{V}_5^* & \mathbf{U}_7\tilde{\mathbf{A}}_{76}\mathbf{V}_6^* & \mathbf{D}_7 \end{bmatrix}$.

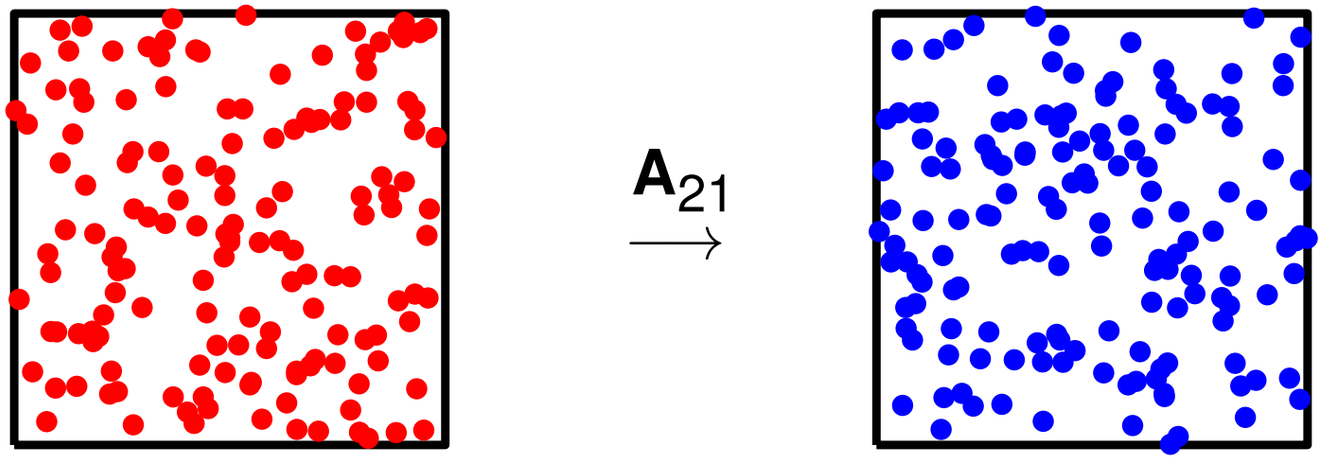
We see that the columns of $\mathbf{U}_5$ must span the column space of the matrix $\mathbf{A}(I_5, I_5^{\mathrm{c}})$ where I_5 is the index vector for the first block and $I_5^{\mathrm{c}} = I \backslash I_5$.



The matrix $\mathbf{A}$

As mentioned earlier, it is handy to use the *interpolative decomposition (ID)*, in which $\mathbf{U}_\tau$ and $\mathbf{V}_\tau$ contain identity matrices. To review how this works, consider a situation with n sources in a domain Ω_1 inducing m potentials in a different domain Ω_2.

Source locations $\{\boldsymbol{y}_j\}_{j=1}^n$ *Target locations* $\{\boldsymbol{x}_i\}_{i=1}^m$



Let $\mathbf{A}_{21}$ denote the $m \times n$ matrix with entries $\mathbf{A}_{21}(i,j) = \log|\boldsymbol{x}_i - \boldsymbol{y}_j|$. Then

$$\begin{array}{ccccc} \mathbf{f} & = & \mathbf{A}_{21} & \mathbf{q} \\ m \times 1 & & m \times n & n \times 1 \end{array}$$

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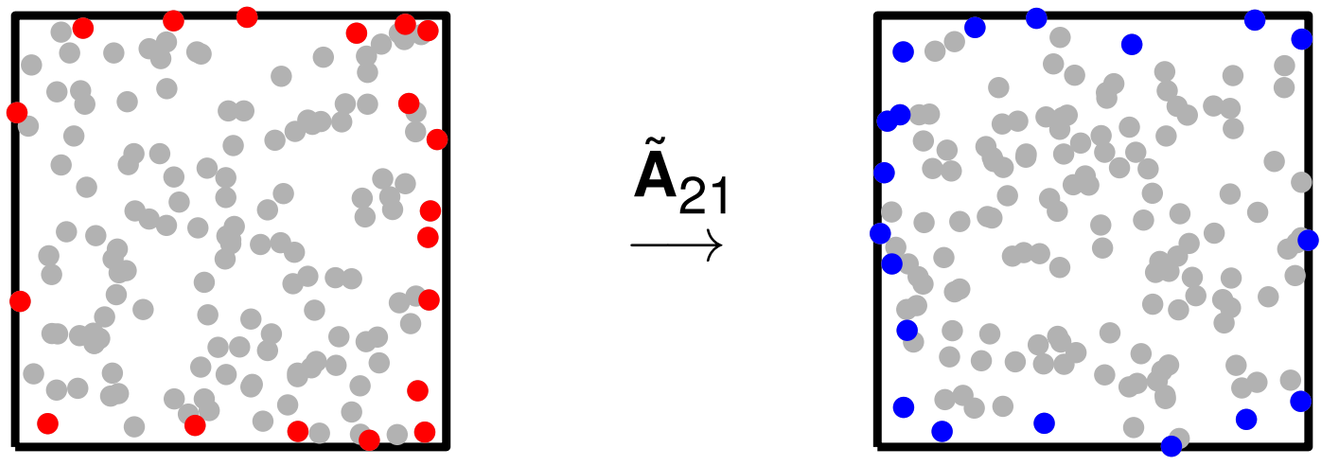

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$$\begin{array}{ccccccccc} \mathbf{f} & = & \mathbf{A}_{21} & \mathbf{q} & = & \mathbf{U}_2 & \tilde{\mathbf{A}}_{21} & \mathbf{V}_1^* & \mathbf{q} \\ m \times 1 & & m \times n & n \times 1 & & m \times k & k \times k & k \times n & n \times 1 \end{array}$$

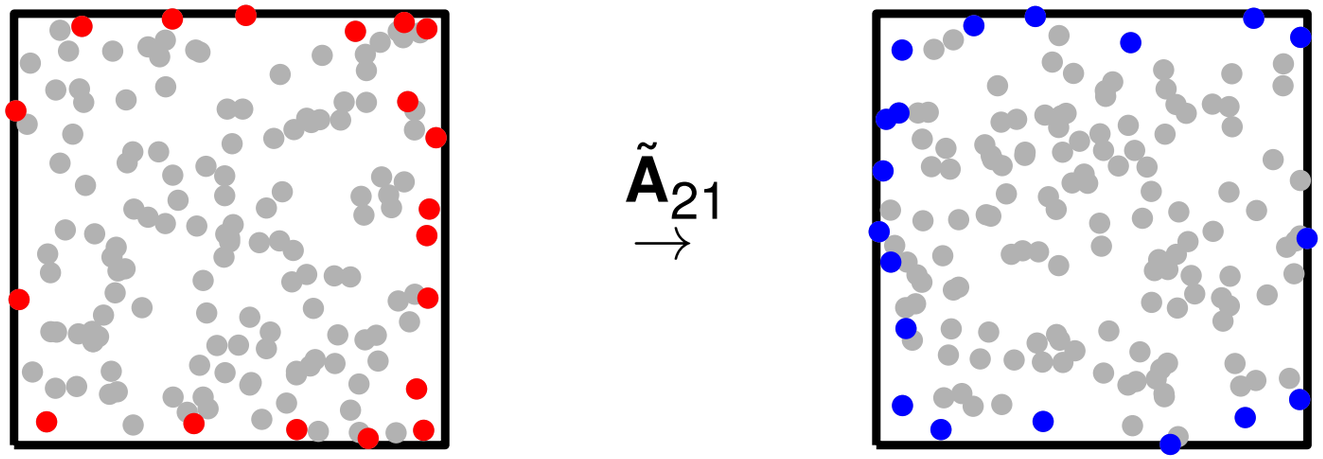
where $\tilde{\mathbf{A}}_{21} = \mathbf{A}_{21}(\tilde{I}_2, \tilde{I}_1)$ is a $k \times k$ submatrix of $\mathbf{A}$.

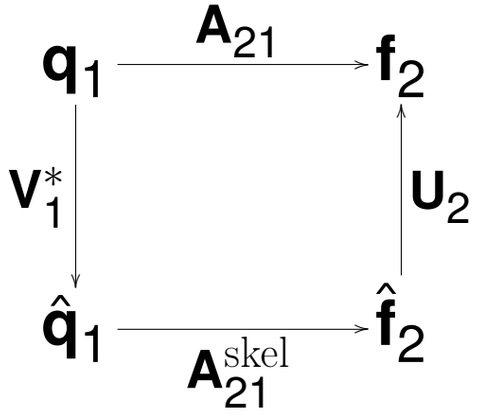
The index vector $\tilde{I}_1 \subseteq \{1, 2, \ldots, n\}$ marks the chosen *skeleton source locations.*

The index vector $\tilde{I}_2 \subseteq \{1, 2, \ldots, m\}$ marks the chosen *skeleton target locations.*

Review of ID: Consider a rank-k factorization of an $m \times n$ matrix: $\mathbf{A}_{21} = \mathbf{U}_2 \, \tilde{\mathbf{A}}_{21} \, \mathbf{V}_1^*$

Sources in Ω_1 *Targets in* Ω_2



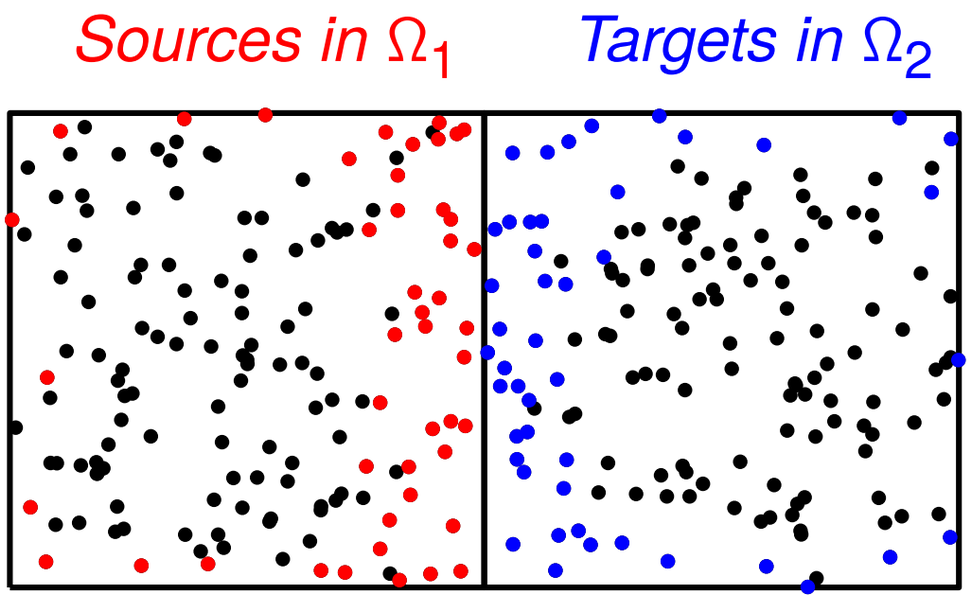


To precision 10^{-10}*, the rank is* 19.

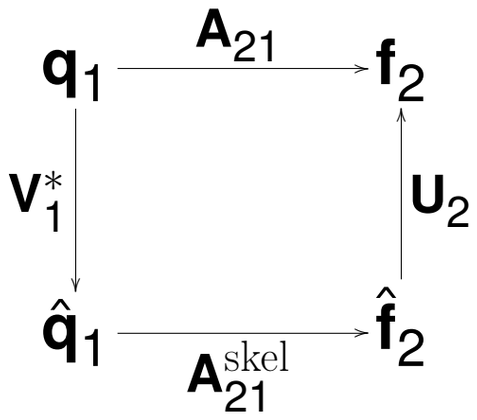
Advantages of the ID:

- The rank is k is typically close to optimal.
- Applying $\mathbf{V}_1^*$ and $\mathbf{U}_2$ is cheap — they both contain $k \times k$ identity matrices.
- The matrices $\mathbf{V}_1^*$ and $\mathbf{U}_2$ are well-conditioned.
- Finding the k points is cheap — simply use Gaussian elimination.
- The map $\tilde{\mathbf{A}}_{12}$ is simply a restriction of the original map $\mathbf{A}_{12}$.
  (We loosely say that "the physics of the problem is preserved".)
- Interaction between **adjacent** boxes can be compressed (no buffering required).

Review of ID: Consider a rank-k factorization of an $m \times n$ matrix: $\mathbf{A}_{21} = \mathbf{U}_2 \, \tilde{\mathbf{A}}_{21} \, \mathbf{V}_1^*$



To precision 10^{-10}*, the rank is* 46.



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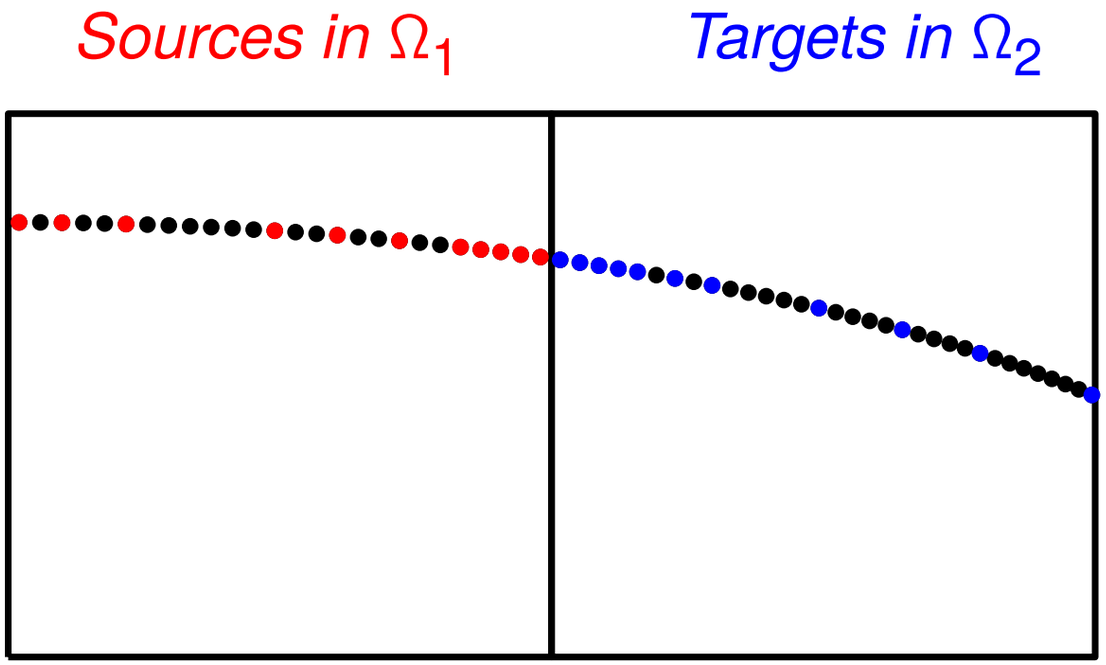
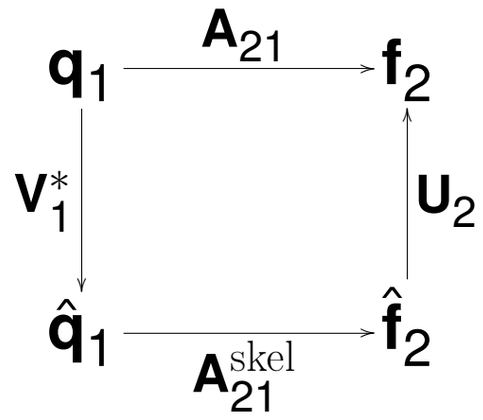
Review of ID: Consider a rank-k factorization of an $m \times n$ matrix: $\mathbf{A}_{21} = \mathbf{U}_2 \, \tilde{\mathbf{A}}_{21} \, \mathbf{V}_1^*$



To precision 10^{-10}*, the rank is* 11.



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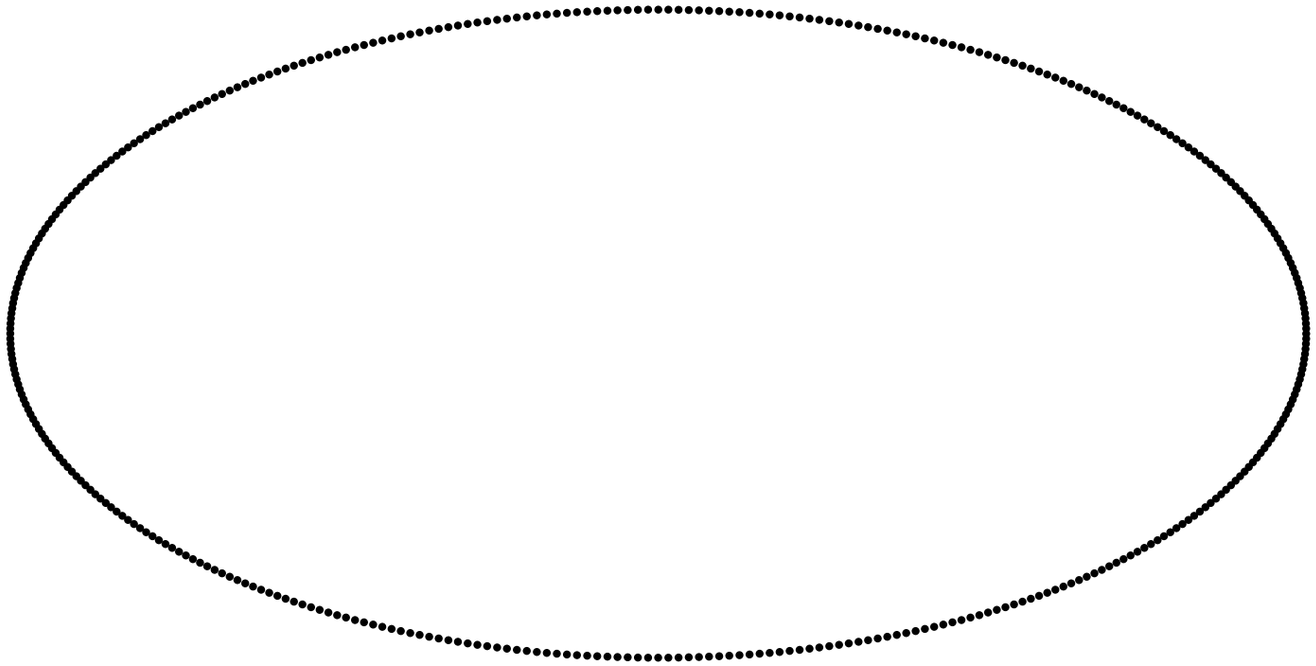
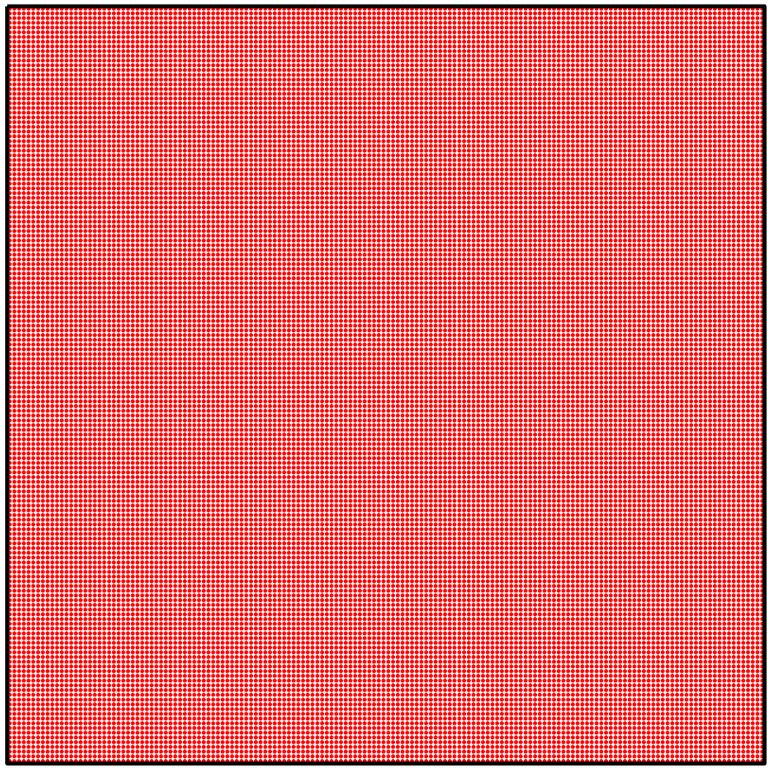
- The matrices $\mathbf{V}_1^*$ and $\mathbf{U}_2$ are well-conditioned.
- Finding the k points is cheap — simply use Gaussian elimination.
- The map $\tilde{A}_{12}$ is simply a restriction of the original map A_{12}.
  (We loosely say that "the physics of the problem is preserved".)
- Interaction between **adjacent** boxes can be compressed (no buffering required).

Model problem: Consider a collection of points $\{\boldsymbol{x}_i\}_{i=1}^N$ along a contour Γ.

Let $\mathbf{A}$ be the $N \times N$ matrix with entries $\mathbf{A}(i,j) = \log|\boldsymbol{x}_i - \boldsymbol{x}_j|$ for $i \neq j$.



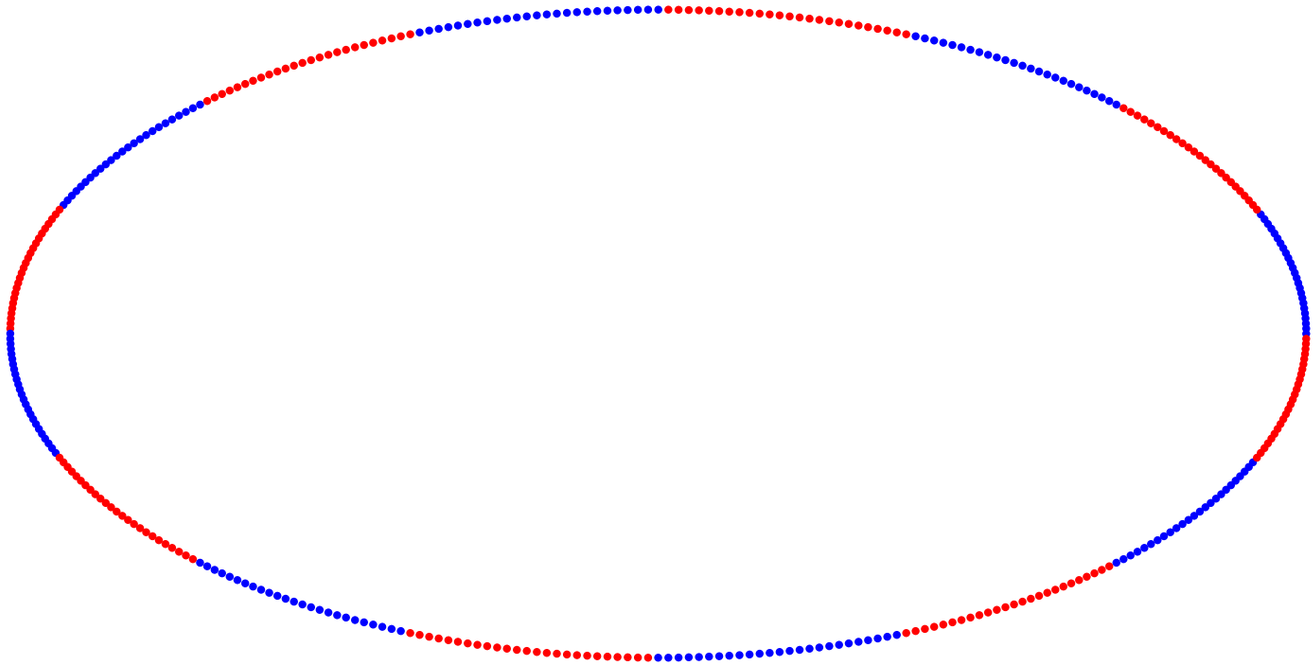
The contour



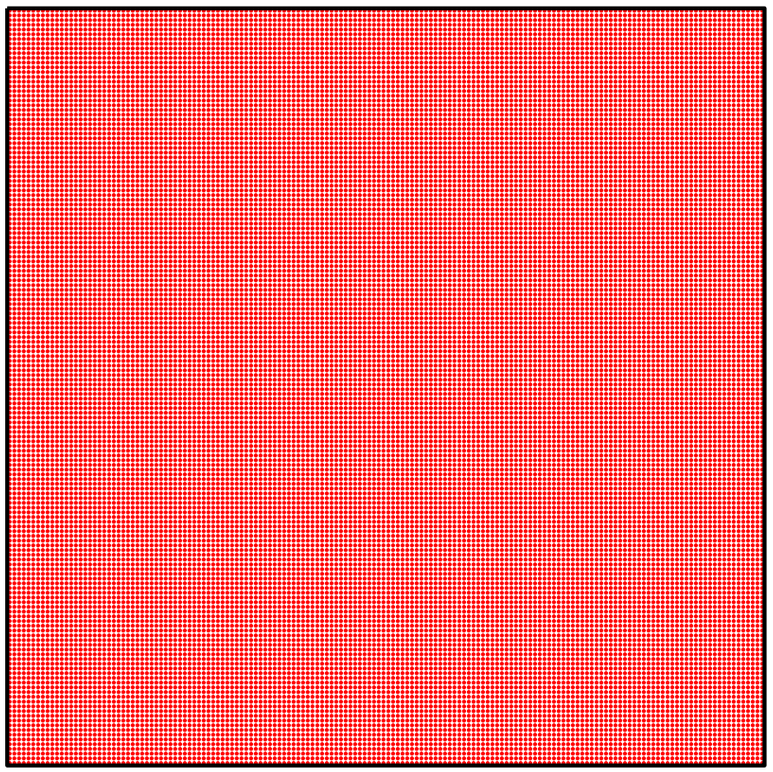
The matrix

Model problem: Consider a collection of points $\{\boldsymbol{x}_i\}_{i=1}^N$ along a contour Γ.

Let $\mathbf{A}$ be the $N \times N$ matrix with entries $\mathbf{A}(i,j) = \log|\boldsymbol{x}_i - \boldsymbol{x}_j|$ for $i \neq j$.



The contour

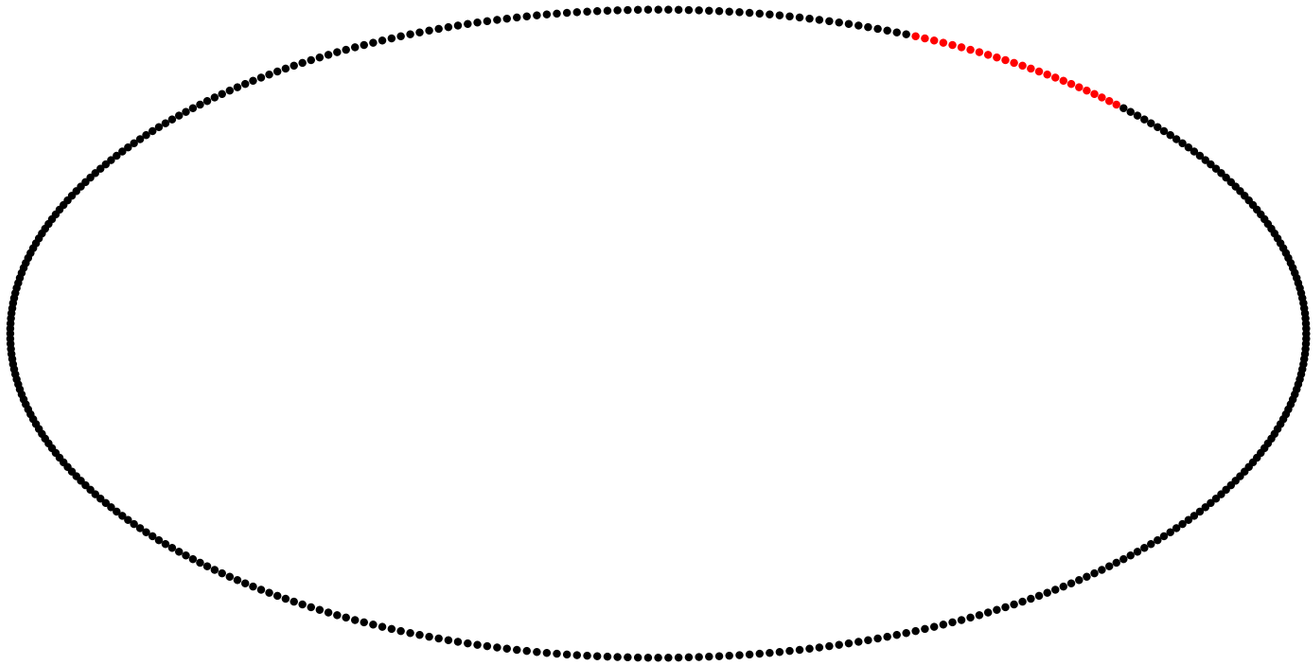


The matrix

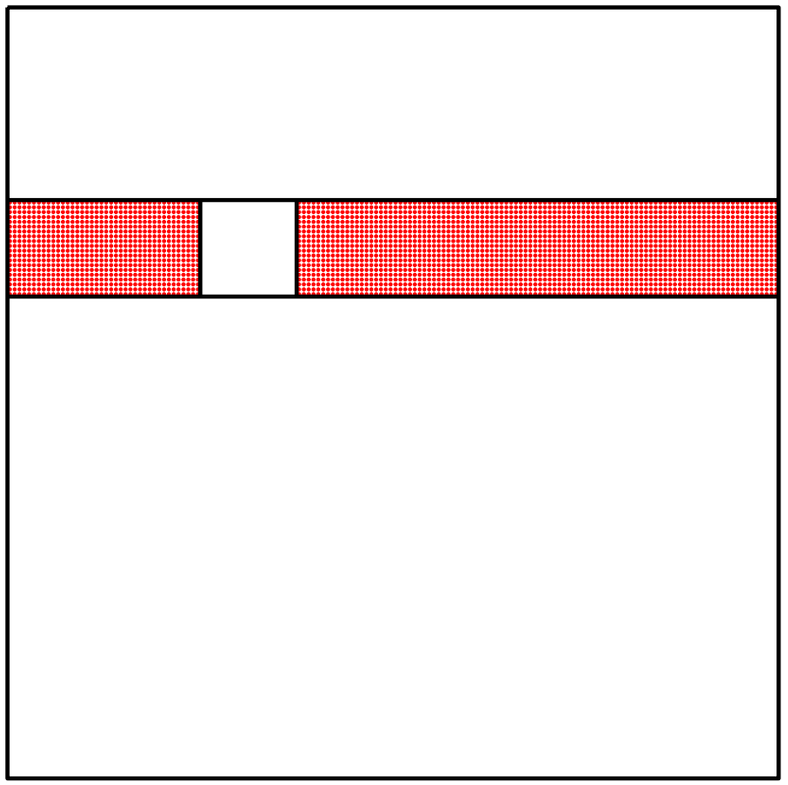
Partition the contour into 16 leaves.

Model problem: Consider a collection of points $\{\boldsymbol{x}_i\}_{i=1}^N$ along a contour Γ.

Let $\mathbf{A}$ be the $N \times N$ matrix with entries $\mathbf{A}(i,j) = \log|\boldsymbol{x}_i - \boldsymbol{x}_j|$ for $i \neq j$.



The contour



The block $\mathbf{A}(I_\tau, I_\tau^c)$ shown in red.

Now let us focus on a single panel Γ_τ associated with index vector I_τ.

Our task is to determine a basis matrix $\mathbf{U}_\tau$ and an index vector $\tilde{I}_\tau \subset I_\tau$ such that

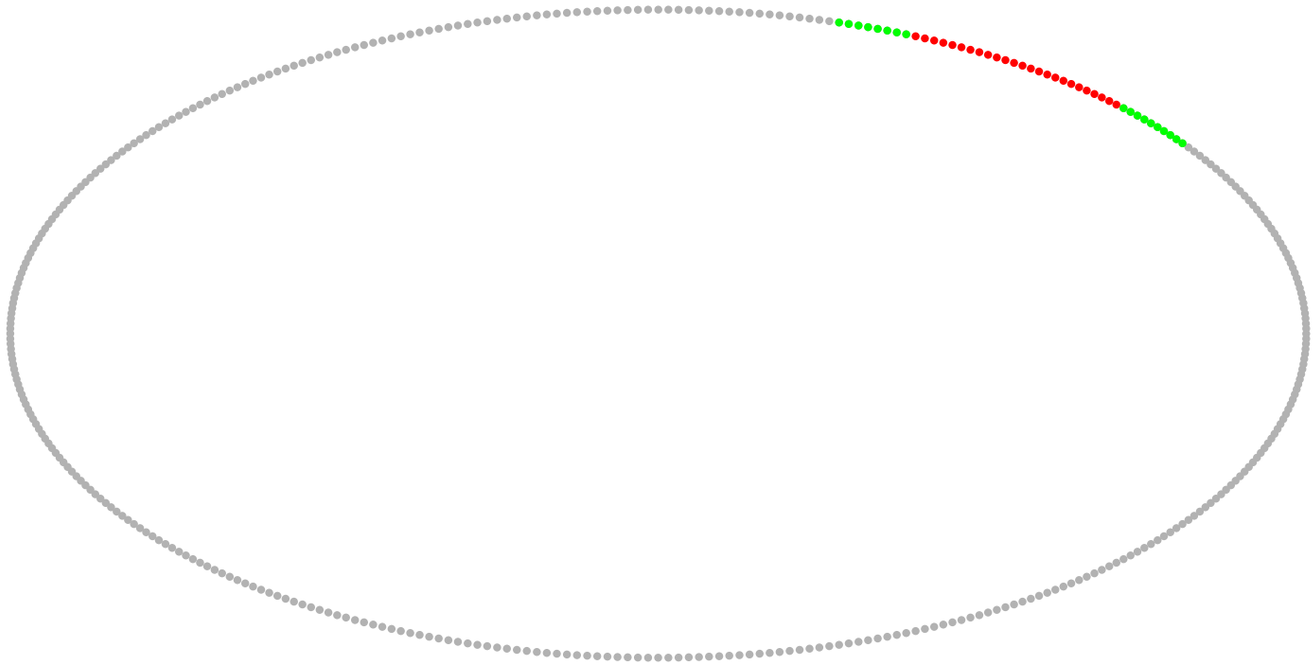
$$\begin{array}{ccccc} \mathbf{A}(I_\tau, I_\tau^c) & = & \mathbf{U}_\tau & & \mathbf{A}(\tilde{I}_\tau, I_\tau^c) \\ n \times (N-n) & & n \times k & & k \times (N-n) \end{array}$$

The most direct way of doing this is to perform Gram-Schmidt on the rows of $\mathbf{A}(I_\tau, I_\tau^c)$.

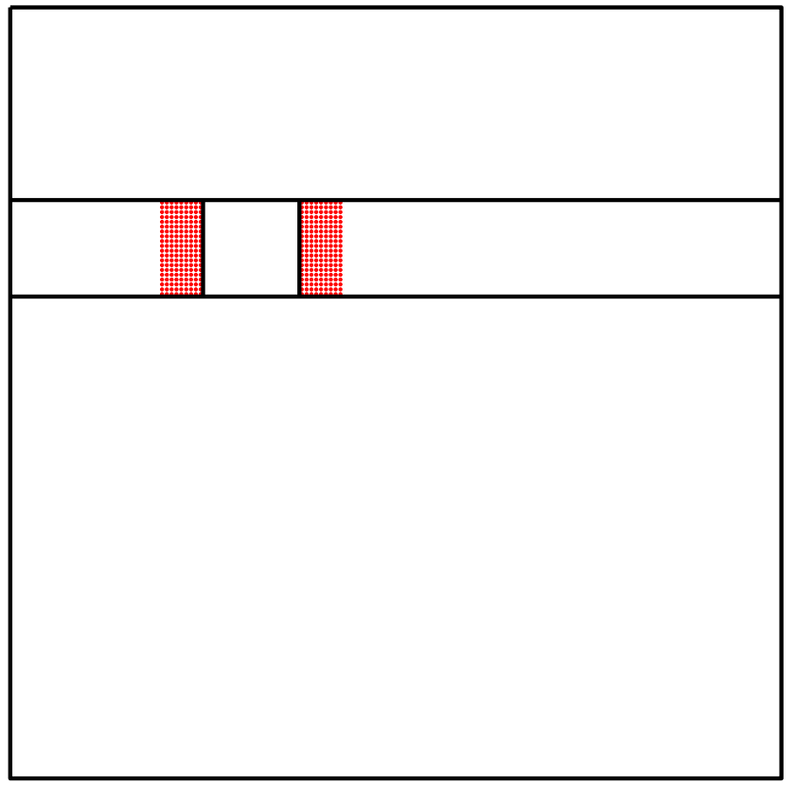
This works great, but it is expensive, since $\mathbf{A}(I_\tau, I_\tau^c)$ is big. We seek a *local* procedure.

Model problem: Consider a collection of points $\{\boldsymbol{x}_i\}_{i=1}^N$ along a contour Γ.

Let $\mathbf{A}$ be the $N \times N$ matrix with entries $\mathbf{A}(i,j) = \log|\boldsymbol{x}_i - \boldsymbol{x}_j|$ for $i \neq j$.



The contour



The block $\mathbf{A}(I_\tau, I_\tau^{(\text{near})})$ shown in red.

Idea (bad): Ignore all charges in the far-field!

Let $I_\tau^{(\text{near})}$ denote the near-field points.

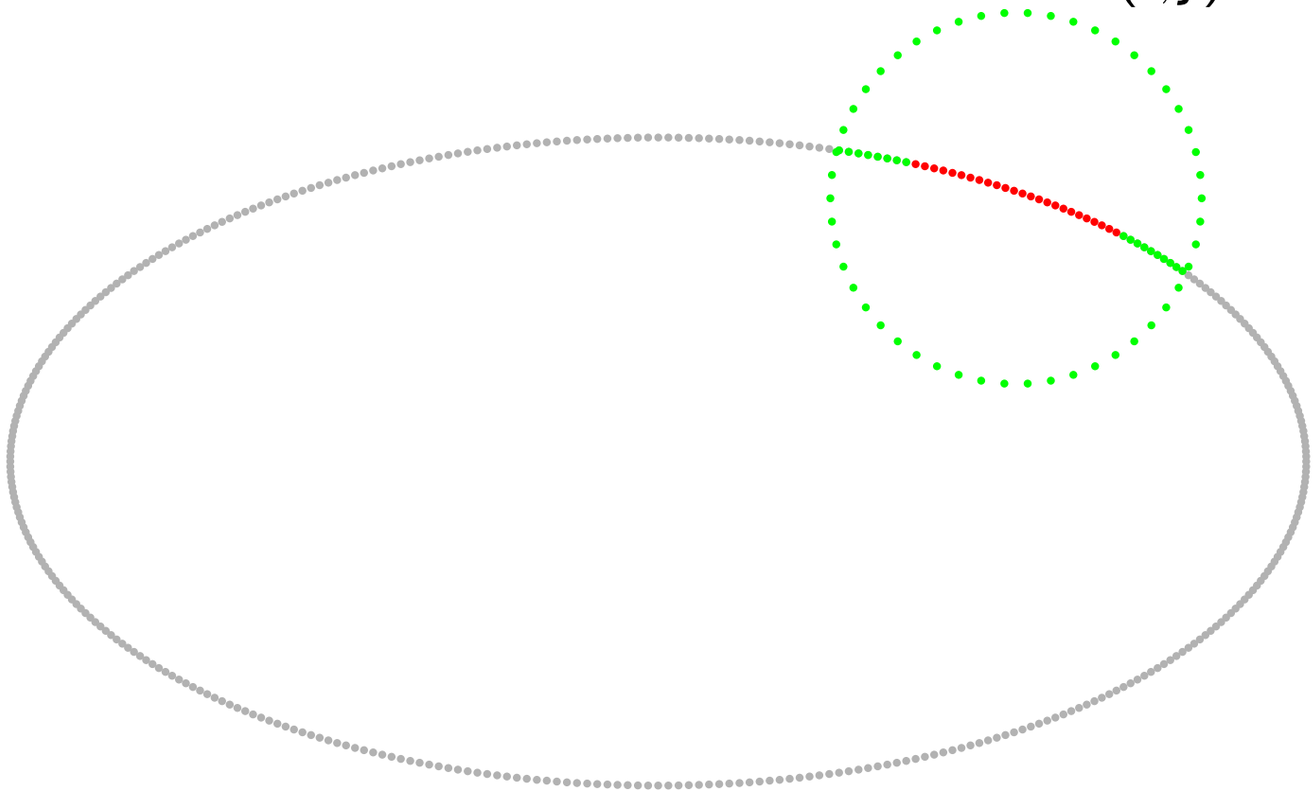
Then factor the smaller matrix $\mathbf{B} = \mathbf{A}(I_\tau, I_\tau^{(\text{near})})$:

$$\begin{array}{ccccc} \mathbf{B} & = & \mathbf{U}_\tau & & \mathbf{B}(J,:) \\ n \times n_{\text{near}} & & n \times k & & k \times n_{\text{near}} \end{array}$$

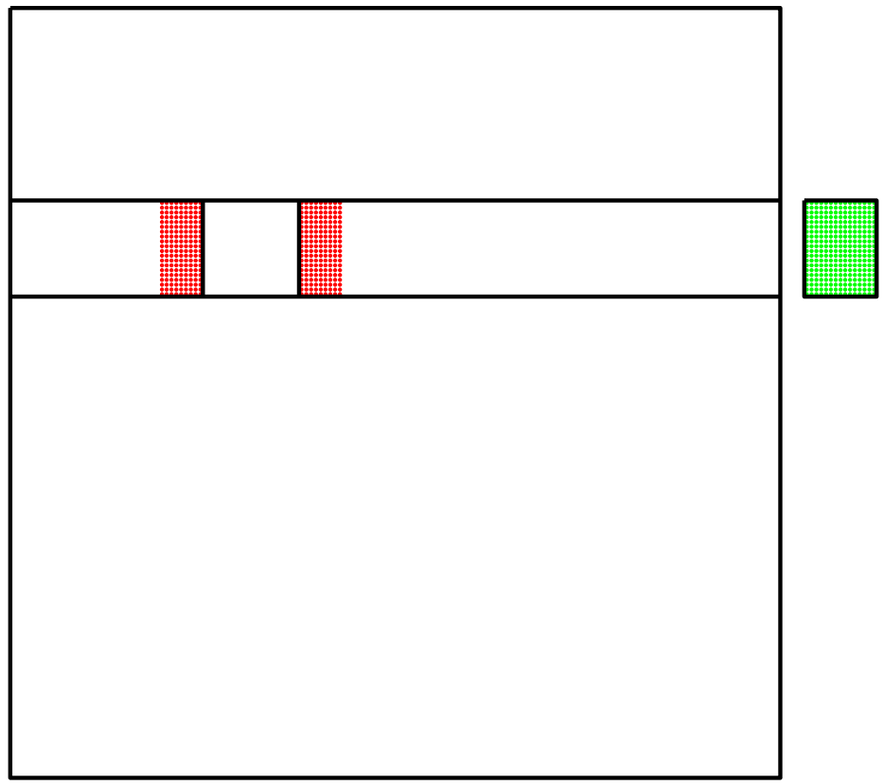
and set $\tilde{I}_\tau = I_\tau(J)$.

Model problem: Consider a collection of points $\{\boldsymbol{x}_i\}_{i=1}^{N}$ along a contour Γ.

Let $\mathbf{A}$ be the $N \times N$ matrix with entries $\mathbf{A}(i,j) = \log|\boldsymbol{x}_i - \boldsymbol{x}_j|$ for $i \neq j$.



The contour



The block $\mathbf{A}(I_\tau, I_\tau^{(\text{near})})$ shown in red. The block $\mathbf{G}$ shown in green.

Idea: Replace charges in the far-field by "proxy" charges.

Let $I_\tau^{(\text{near})}$ denote the near-field points and let $\mathbf{G}$ denote a matrix of size $n \times n_{\text{proxy}}$ that maps charges on the proxy locations to potentials on Γ_τ.

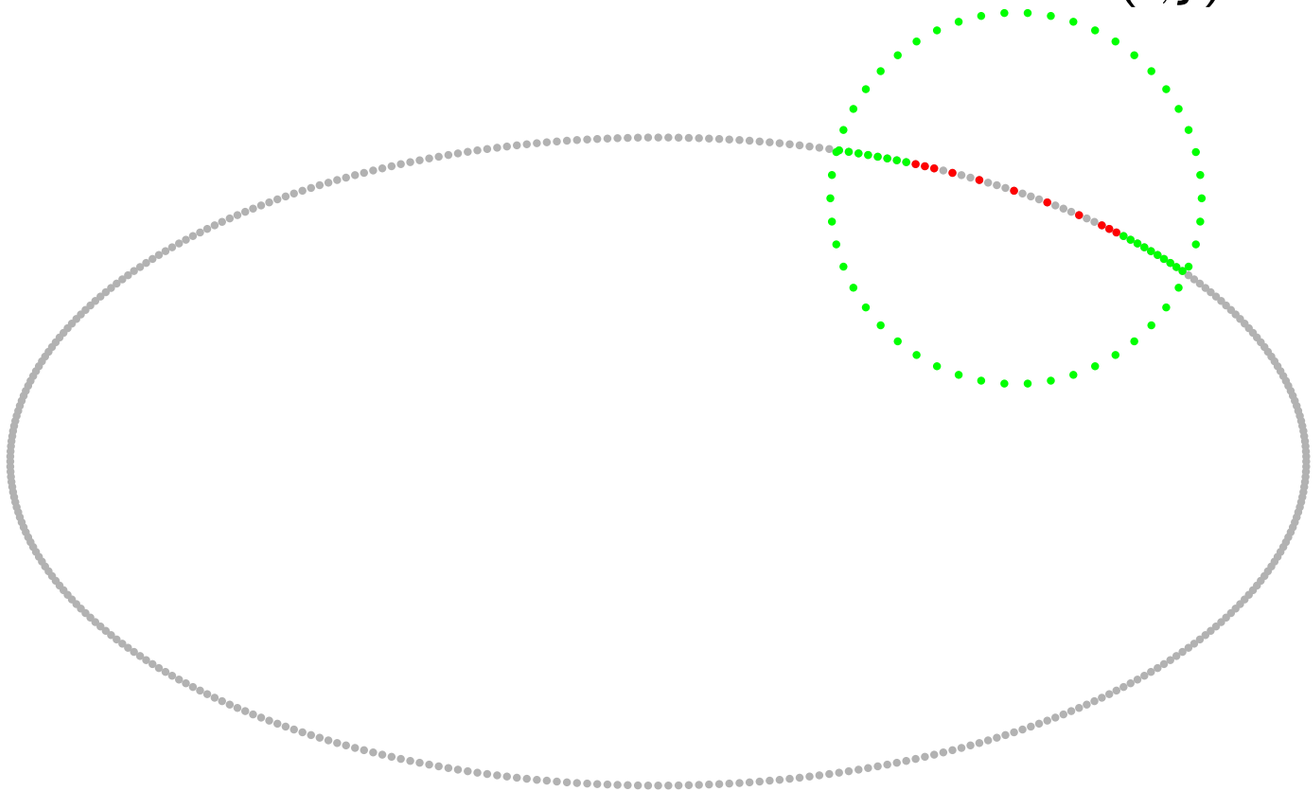
Then factor the smaller matrix $\mathbf{B} = [\mathbf{A}(I_\tau, I_\tau^{(\text{near})}),\ \mathbf{G}]$:

$$\underset{n \times (n_{\text{near}} + n_{\text{proxy}})}{\mathbf{B}} = \underset{n \times k}{\mathbf{U}_\tau} \quad \underset{k \times (n_{\text{near}} + n_{\text{proxy}})}{\mathbf{B}(J,:)}$$

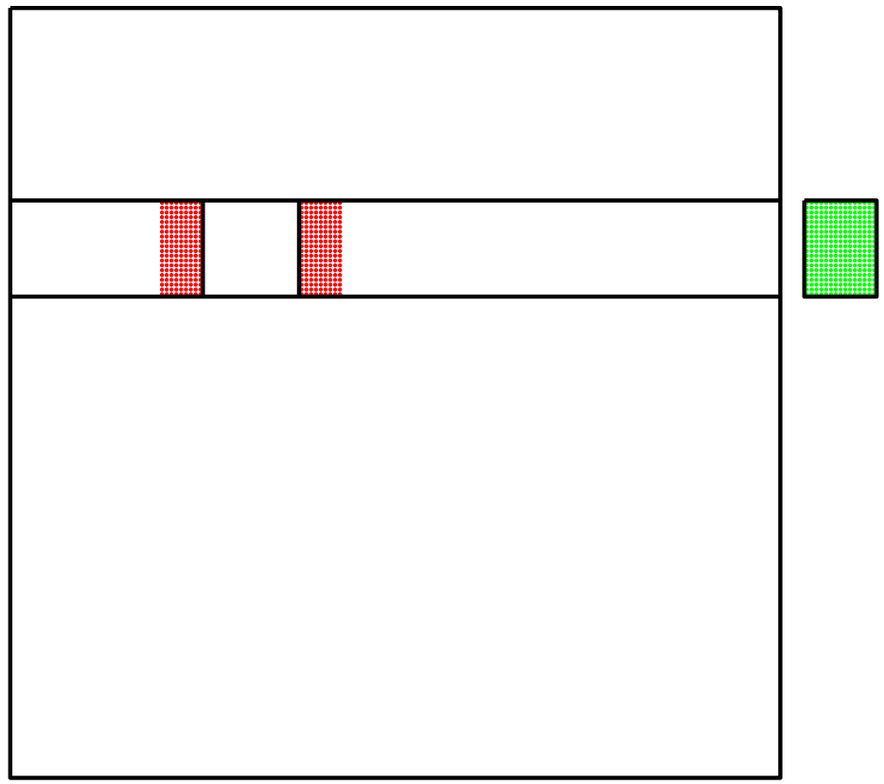
and set $\tilde{I}_\tau = I_\tau(J)$.

Model problem: Consider a collection of points $\{\boldsymbol{x}_i\}_{i=1}^{N}$ along a contour Γ.

Let $\mathbf{A}$ be the $N \times N$ matrix with entries $\mathbf{A}(i,j) = \log|\boldsymbol{x}_i - \boldsymbol{x}_j|$ for $i \neq j$.



The contour



The block $\mathbf{A}(I_\tau, I_\tau^{(\text{near})})$ shown in red. The block $\mathbf{G}$ shown in green.

Idea: Replace charges in the far-field by "proxy" charges.

Let $I_\tau^{(\text{near})}$ denote the near-field points and let $\mathbf{G}$ denote a matrix of size $n \times n_{\text{proxy}}$ that maps charges on the proxy locations to potentials on Γ_τ.

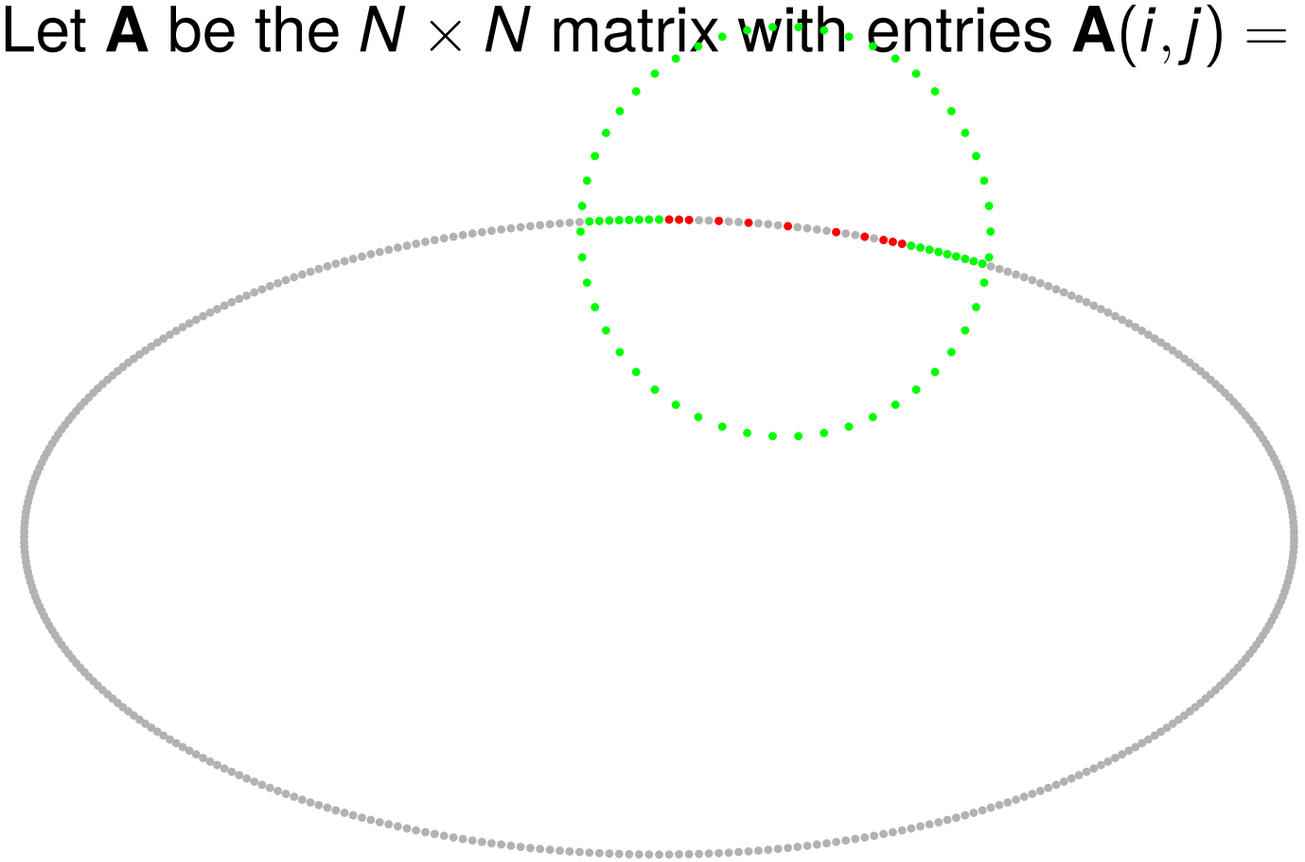
Then factor the smaller matrix $\mathbf{B} = [\mathbf{A}(I_\tau, I_\tau^{(\text{near})}),\ \mathbf{G}]$:

$$\underset{n \times (n_{\text{near}} + n_{\text{proxy}})}{\mathbf{B}} = \underset{n \times k}{\mathbf{U}_\tau} \quad \underset{k \times (n_{\text{near}} + n_{\text{proxy}})}{\mathbf{B}(J,:)}$$

and set $\tilde{I}_\tau = I_\tau(J)$.

Model problem: Consider a collection of points $\{\boldsymbol{x}_i\}_{i=1}^{N}$ along a contour Γ.

Let $\mathbf{A}$ be the $N \times N$ matrix with entries $\mathbf{A}(i,j) = \log|\boldsymbol{x}_i - \boldsymbol{x}_j|$ for $i \neq j$.



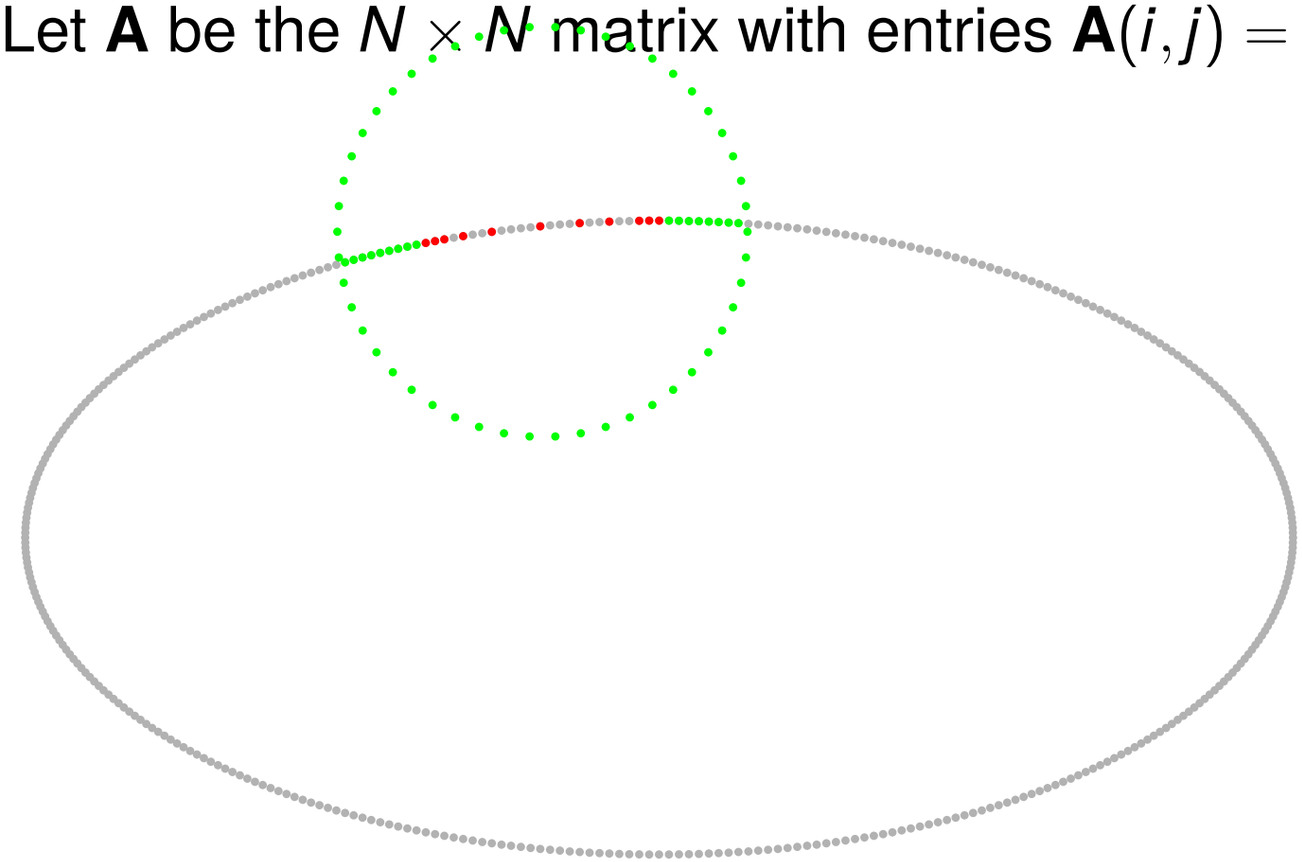
The contour

Idea: Replace charges in the far-field by "proxy" charges.

... execute the same steps for the next panel ...

Model problem: Consider a collection of points $\{\boldsymbol{x}_i\}_{i=1}^N$ along a contour Γ.

Let $\mathbf{A}$ be the $N \times N$ matrix with entries $\mathbf{A}(i,j) = \log|\boldsymbol{x}_i - \boldsymbol{x}_j|$ for $i \neq j$.



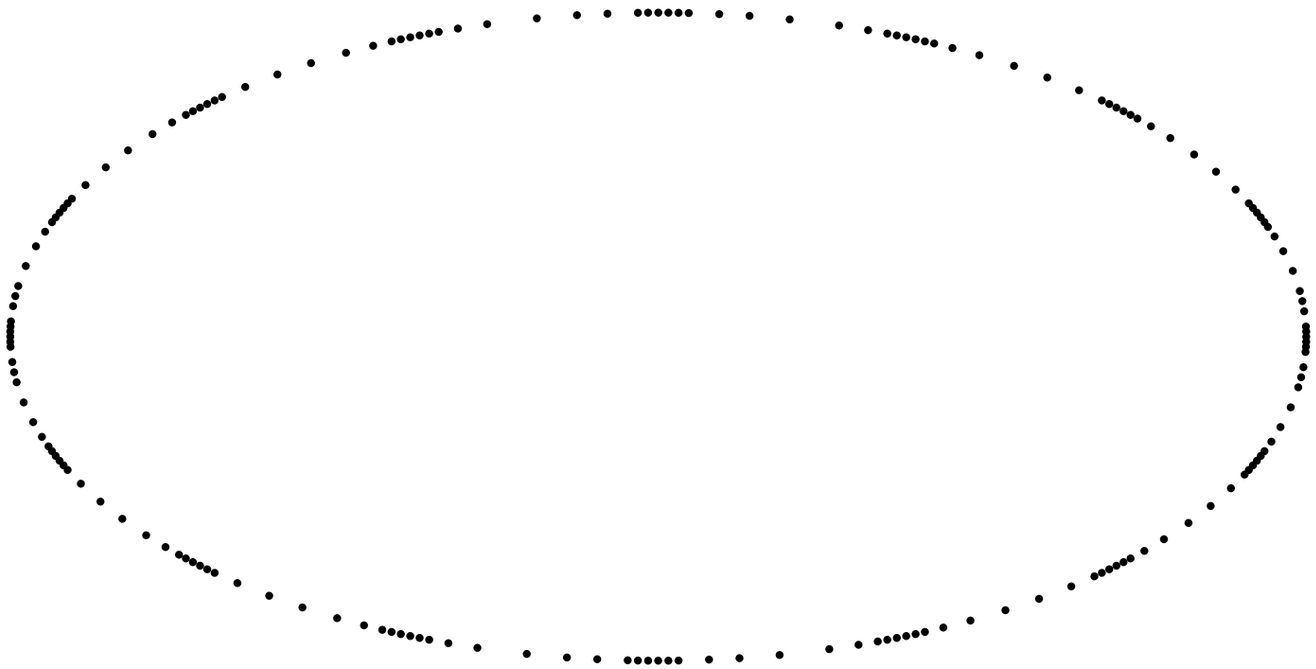
The contour

Idea: Replace charges in the far-field by "proxy" charges.

... and the next ...

Model problem: Consider a collection of points $\{\boldsymbol{x}_i\}_{i=1}^N$ along a contour Γ.

Let $\mathbf{A}$ be the $N \times N$ matrix with entries $\mathbf{A}(i,j) = \log|\boldsymbol{x}_i - \boldsymbol{x}_j|$ for $i \neq j$.

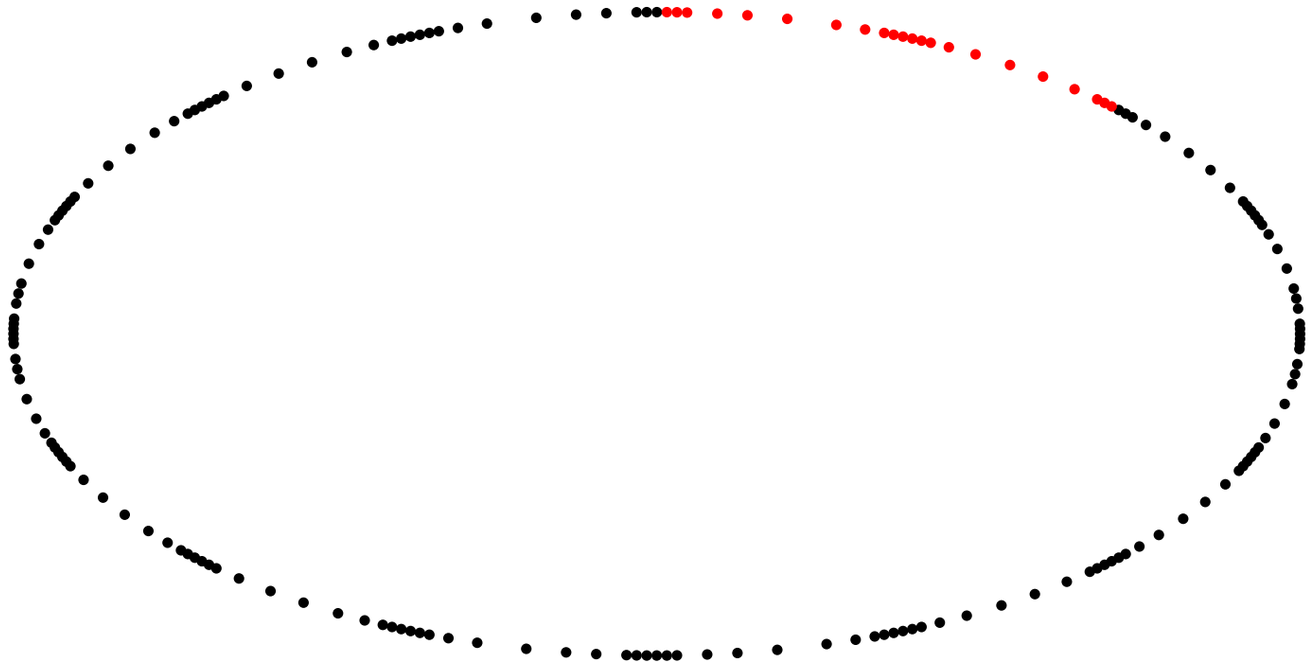


The contour

Once all leaves have been processed, we have in effect eliminated a bunch of points.

Model problem: Consider a collection of points $\{\boldsymbol{x}_i\}_{i=1}^{N}$ along a contour Γ.

Let $\mathbf{A}$ be the $N \times N$ matrix with entries $\mathbf{A}(i,j) = \log|\boldsymbol{x}_i - \boldsymbol{x}_j|$ for $i \neq j$.



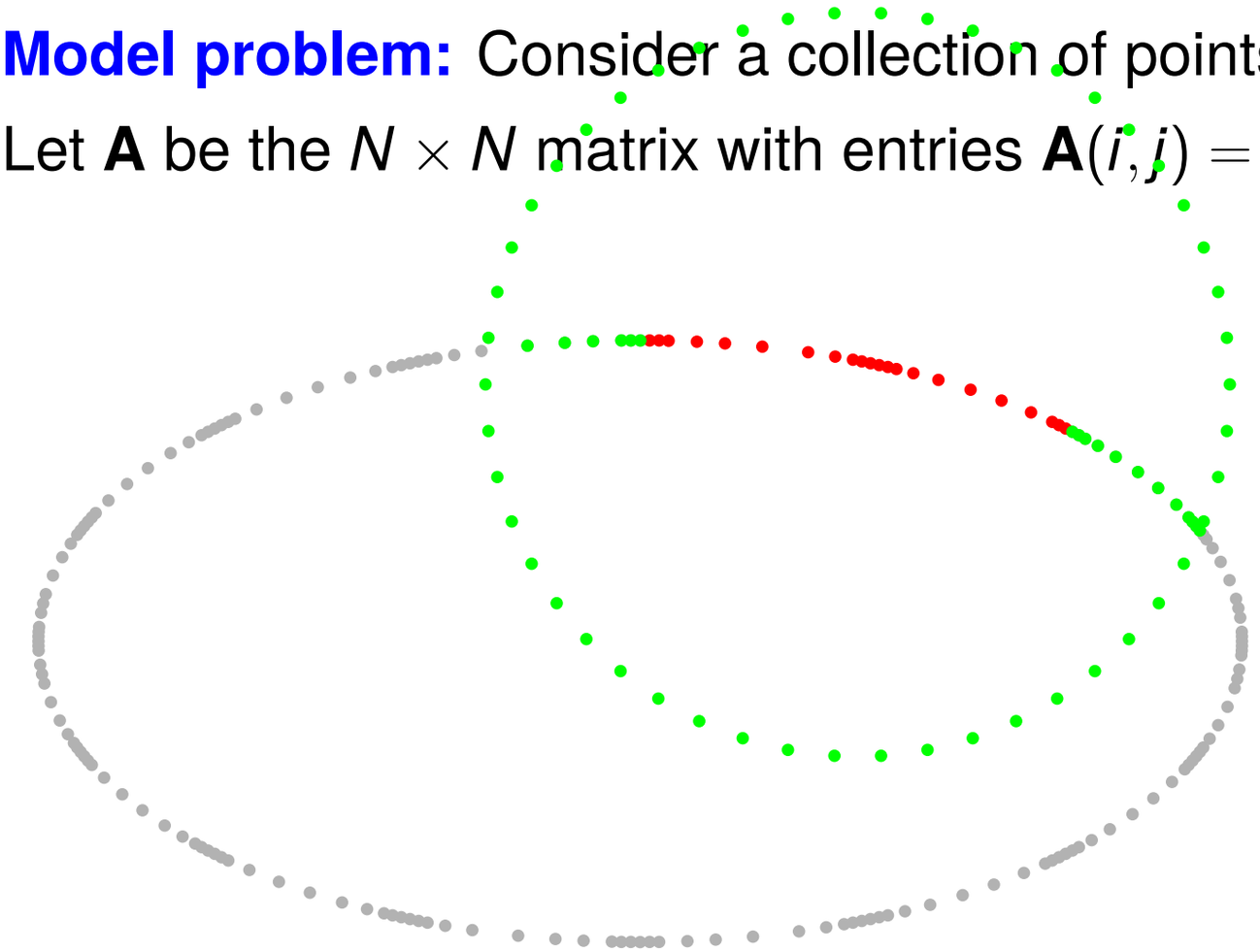
The contour

The matrix

Now consider compression of a parent node.

Model problem: Consider a collection of points $\{\boldsymbol{x}_i\}_{i=1}^N$ along a contour Γ.

Let $\mathbf{A}$ be the $N \times N$ matrix with entries $\mathbf{A}(i,j) = \log|\boldsymbol{x}_i - \boldsymbol{x}_j|$ for $i \neq j$.

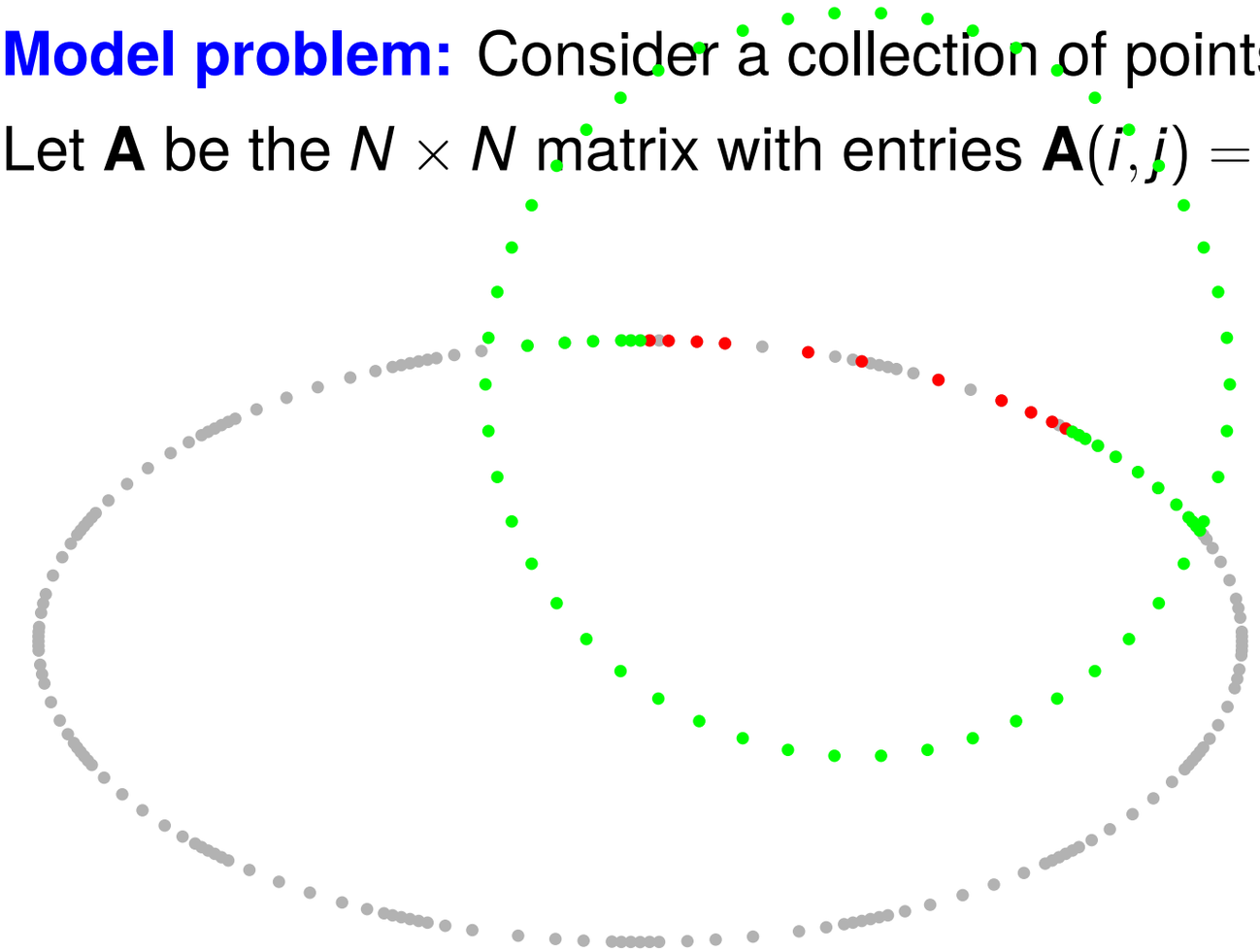


The contour

Replace far-field nodes by a small set of proxy charges.

Model problem: Consider a collection of points $\{\boldsymbol{x}_i\}_{i=1}^N$ along a contour Γ.

Let $\mathbf{A}$ be the $N \times N$ matrix with entries $\mathbf{A}(i,j) = \log|\boldsymbol{x}_i - \boldsymbol{x}_j|$ for $i \neq j$.

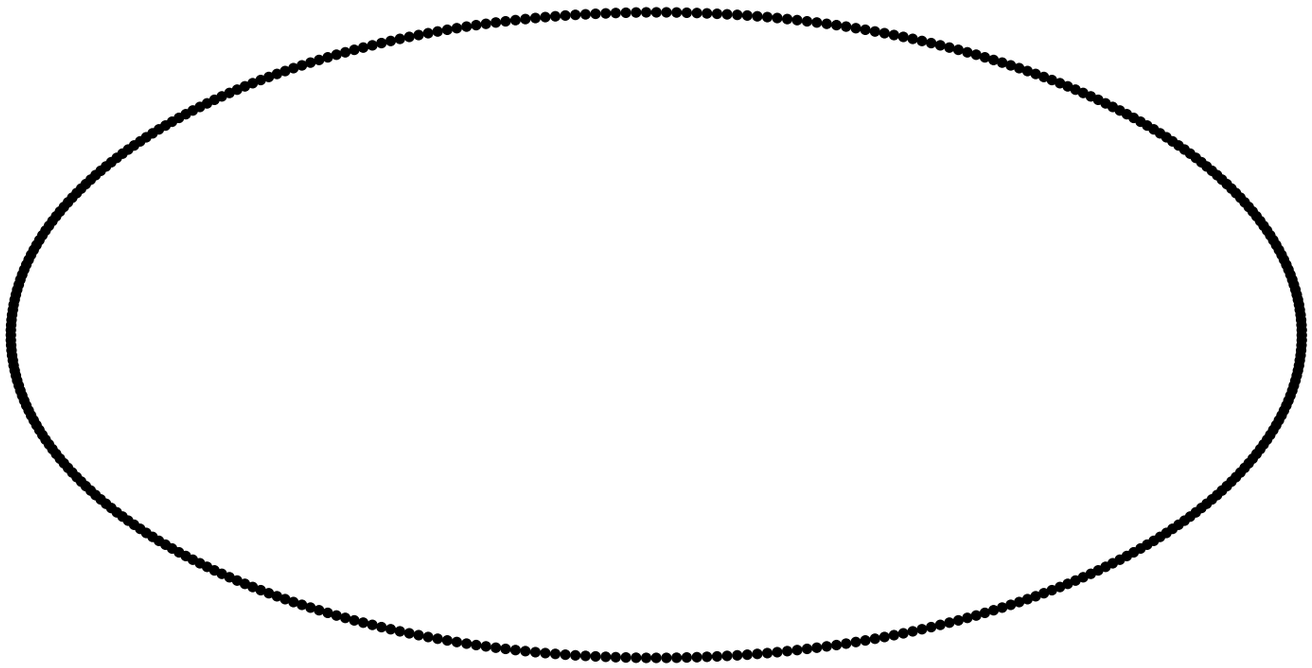


The contour

Points remaining after compression.

Model problem: Consider a collection of points $\{\boldsymbol{x}_i\}_{i=1}^N$ along a contour Γ.

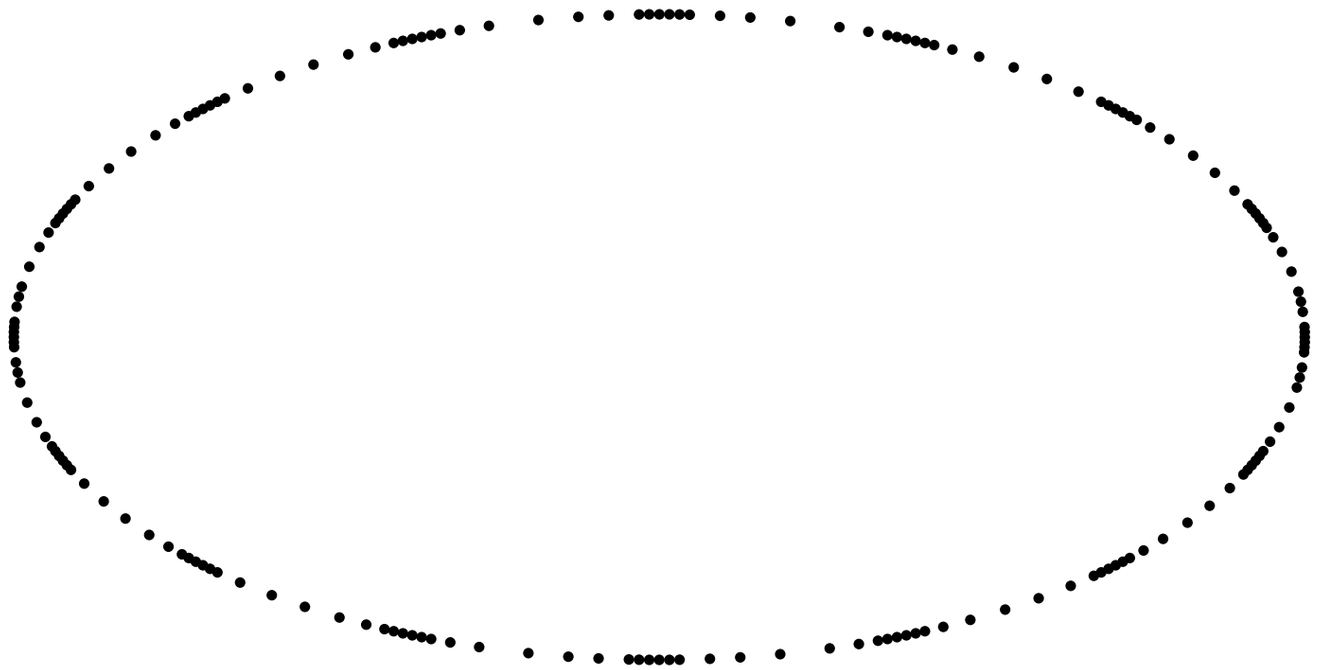
Let $\mathbf{A}$ be the $N \times N$ matrix with entries $\mathbf{A}(i,j) = \log|\boldsymbol{x}_i - \boldsymbol{x}_j|$ for $i \neq j$.



All points

Model problem: Consider a collection of points $\{\boldsymbol{x}_i\}_{i=1}^N$ along a contour Γ.

Let $\mathbf{A}$ be the $N \times N$ matrix with entries $\mathbf{A}(i,j) = \log|\boldsymbol{x}_i - \boldsymbol{x}_j|$ for $i \neq j$.



After level 4 compression.

Model problem: Consider a collection of points $\{\boldsymbol{x}_i\}_{i=1}^N$ along a contour Γ.

Let $\mathbf{A}$ be the $N \times N$ matrix with entries $\mathbf{A}(i,j) = \log|\boldsymbol{x}_i - \boldsymbol{x}_j|$ for $i \neq j$.

After level 3 compression.

Model problem: Consider a collection of points $\{\boldsymbol{x}_i\}_{i=1}^N$ along a contour Γ.

Let $\mathbf{A}$ be the $N \times N$ matrix with entries $\mathbf{A}(i,j) = \log|\boldsymbol{x}_i - \boldsymbol{x}_j|$ for $i \neq j$.

After level 2 compression.

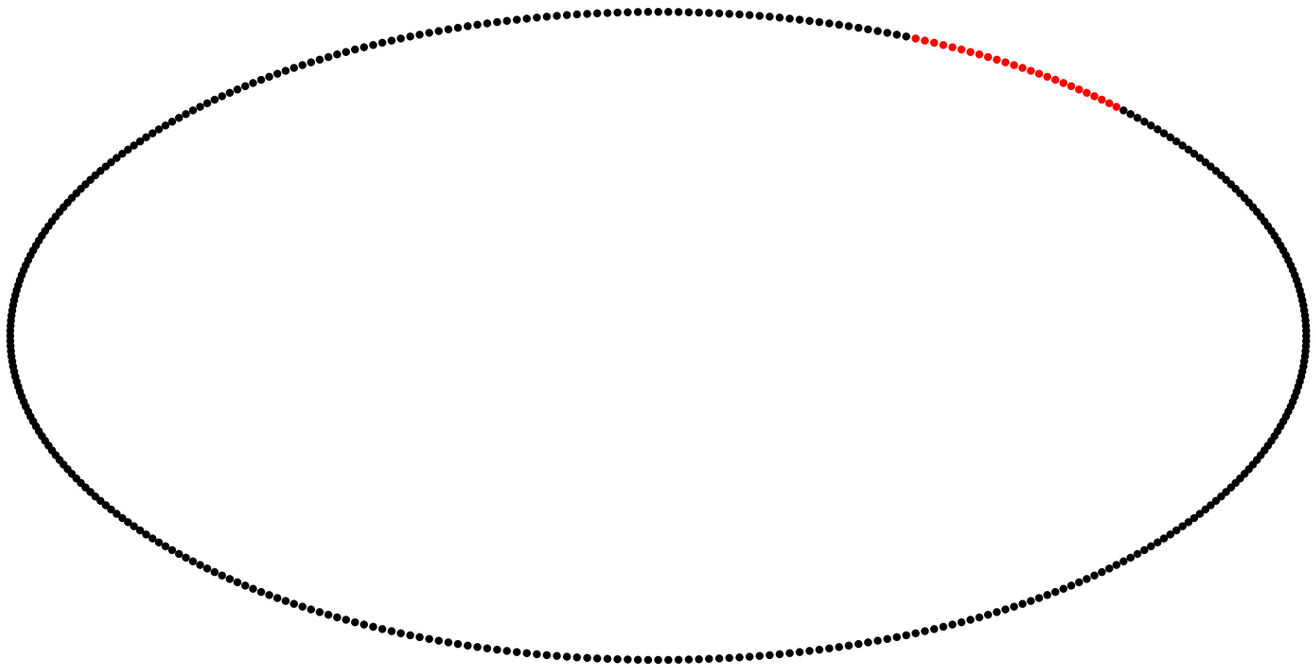
Model problem: Consider a collection of points $\{\boldsymbol{x}_i\}_{i=1}^N$ along a contour Γ.

Let $\mathbf{A}$ be the $N \times N$ matrix with entries $\mathbf{A}(i,j) = \log|\boldsymbol{x}_i - \boldsymbol{x}_j|$ for $i \neq j$.

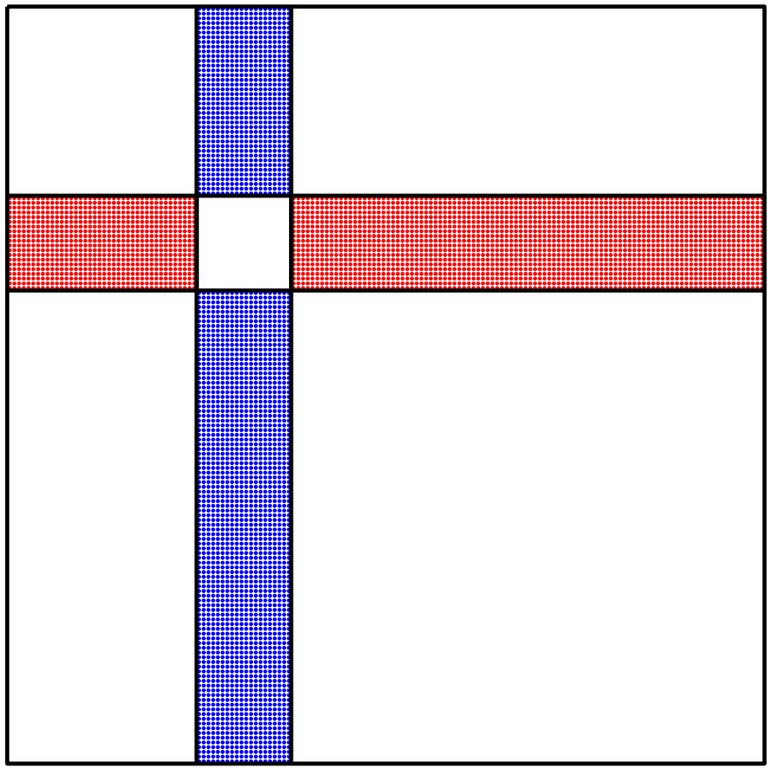
After level 1 compression.

Model problem (non-sym): Consider a collection of points $\{\boldsymbol{x}_i\}_{i=1}^N$ along a contour Γ.

Let $\mathbf{A}$ be the $N \times N$ *non-symmetric* matrix with entries $\mathbf{A}(i,j) = \dfrac{(\boldsymbol{x}_i - \boldsymbol{x}_j) \cdot \boldsymbol{n}_j}{|\boldsymbol{x}_i - \boldsymbol{x}_j|^2}$ for $i \neq j$.



The contour



$\mathbf{A}(I_\tau, I_\tau^c)$ *in red.*
$\mathbf{A}(I_\tau^c, I_\tau)$ *in blue.*

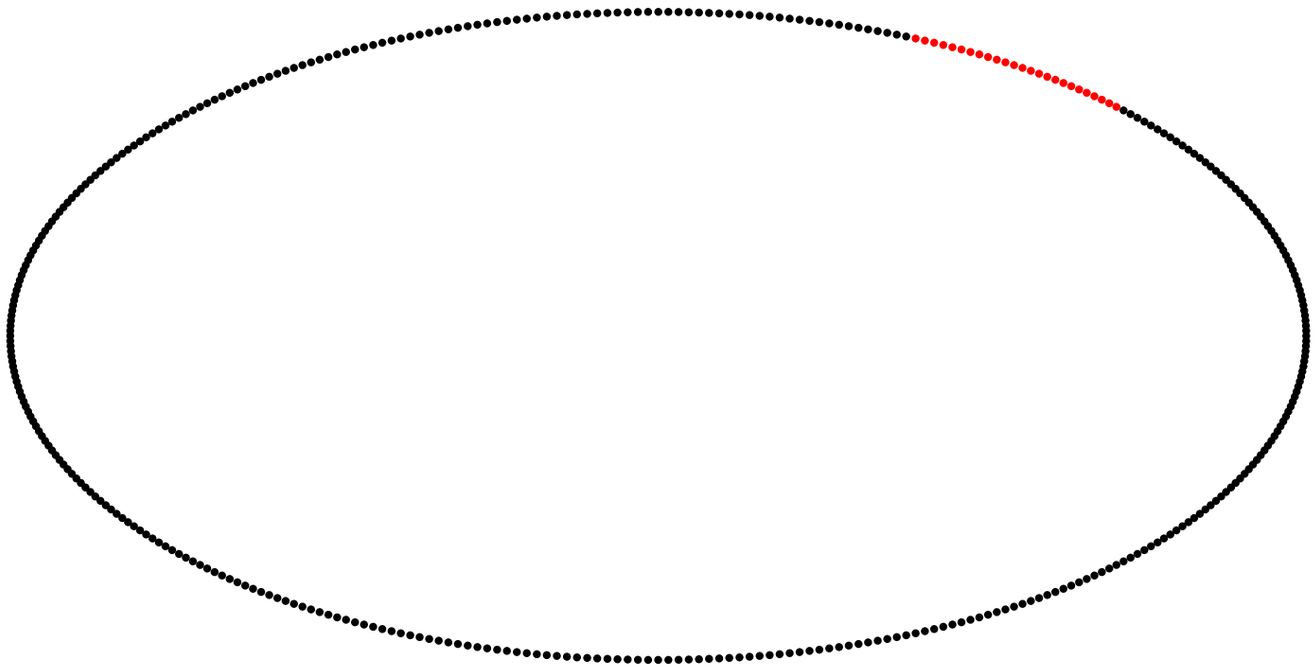
Let Γ_τ be a panel associated with an index vector I_τ.

Our task is to determine basis matrices $\mathbf{U}_\tau$, $\mathbf{V}_\tau$ and index vectors $\tilde{I}_\tau$, $\hat{I}_\tau$, s.t.

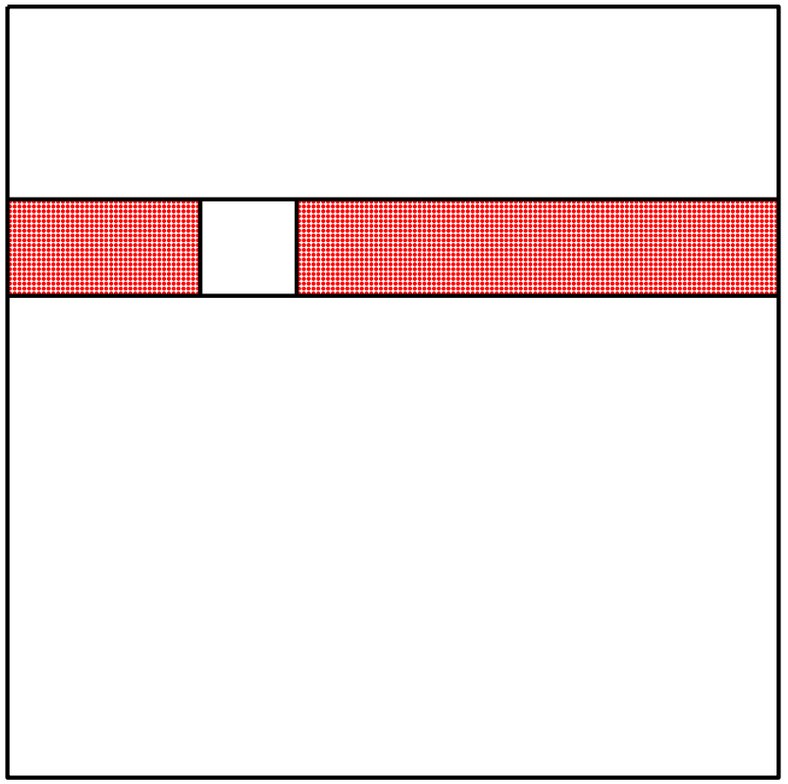
$$\underset{n \times (N-n)}{\mathbf{A}(I_\tau, I_\tau^c)} = \underset{n \times k}{\mathbf{U}_\tau} \; \underset{k \times (N-n)}{\mathbf{A}(\tilde{I}_\tau, I_\tau^c)} \quad \text{and} \quad \underset{(N-n) \times n}{\mathbf{A}(I_\tau^c, I_\tau)} = \underset{(N-n) \times k}{\mathbf{A}(I_\tau^c, \hat{I}_\tau)} \; \underset{k \times n}{\mathbf{V}_\tau^*}$$

Model problem (non-sym): Consider a collection of points $\{\boldsymbol{x}_i\}_{i=1}^N$ along a contour Γ.

Let $\mathbf{A}$ be the $N \times N$ *non-symmetric* matrix with entries $\mathbf{A}(i,j) = \dfrac{(\boldsymbol{x}_i - \boldsymbol{x}_j) \cdot \boldsymbol{n}_j}{|\boldsymbol{x}_i - \boldsymbol{x}_j|^2}$ for $i \neq j$.



The contour



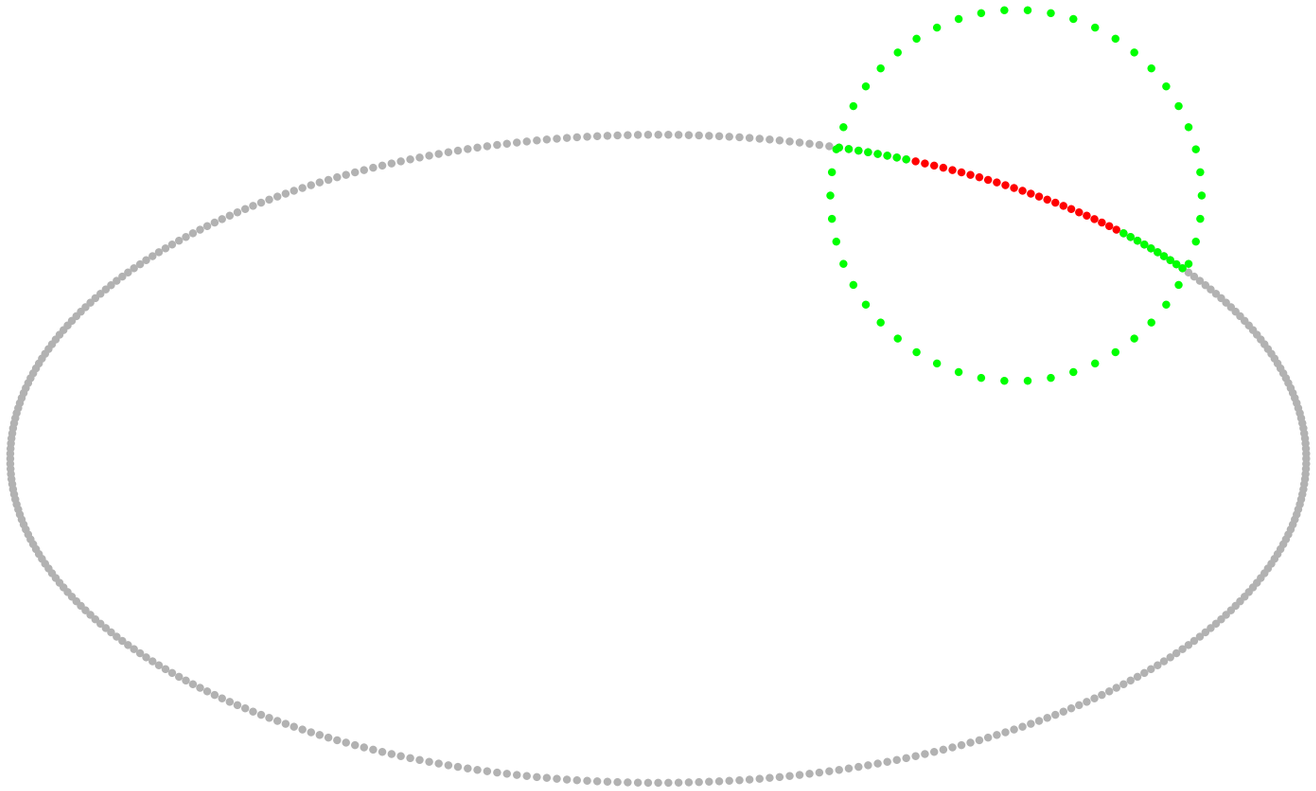
$\mathbf{A}(I_\tau, I_\tau^{\mathrm{c}})$ *in red.*

Let us first consider the task of finding $\mathbf{U}_\tau$. We need to factor

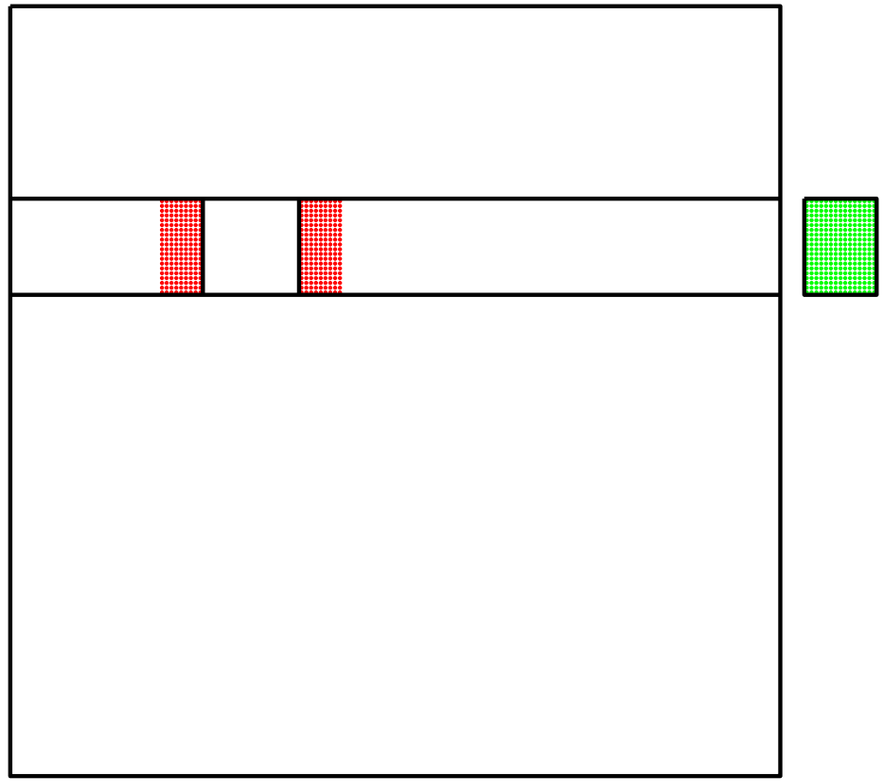
$$\begin{array}{ccccc} \mathbf{A}(I_\tau, I_\tau^{\mathrm{c}}) & = & \mathbf{U}_\tau & & \mathbf{A}(\tilde{I}_\tau, I_\tau^{\mathrm{c}}) \\ n \times (N-n) & & n \times k & & k \times (N-n) \end{array}$$

Model problem (non-sym): Consider a collection of points $\{\boldsymbol{x}_i\}_{i=1}^N$ along a contour Γ.

Let $\mathbf{A}$ be the $N \times N$ *non-symmetric* matrix with entries $\mathbf{A}(i,j) = \dfrac{(\boldsymbol{x}_i - \boldsymbol{x}_j) \cdot \boldsymbol{n}_j}{|\boldsymbol{x}_i - \boldsymbol{x}_j|^2}$ for $i \neq j$.



The contour



The block $\mathbf{A}(I_\tau, I_\tau^{(\text{near})})$ *shown in red.*
The block $\mathbf{G}$ *shown in green.*

Everything works the same!

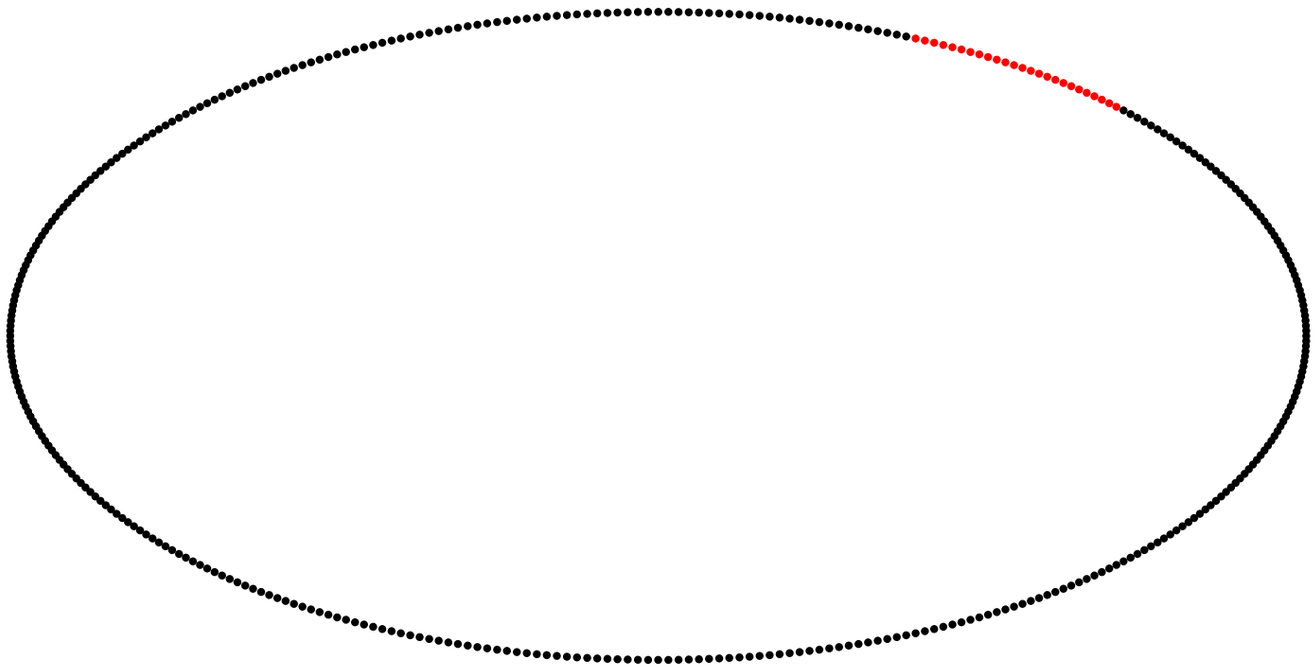
Replace charges in the far-field by "proxy" charges, let $I_\tau^{(\text{near})}$ denote the near-field points and let $\mathbf{G}$ denote a matrix of size $n \times n_{\text{proxy}}$ that maps *monopole* charges on the proxy locations to potentials on Γ_τ. Then factor the smaller matrix $\mathbf{B} = [\mathbf{A}(I_\tau, I_\tau^{(\text{near})}), \mathbf{G}]$:

$$\underset{n \times (n_{\text{near}} + n_{\text{proxy}})}{\mathbf{B}} = \underset{n \times k}{\mathbf{U}_\tau} \; \underset{k \times (n_{\text{near}} + n_{\text{proxy}})}{\mathbf{B}(J,:)}$$

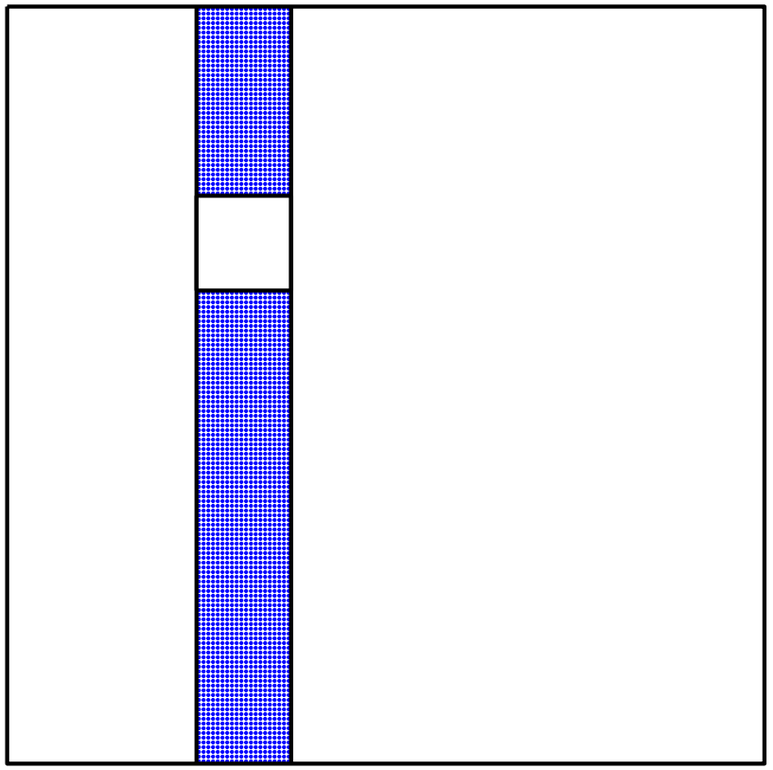
and set $\tilde{I}_\tau = I_\tau(J)$.

Model problem (non-sym): Consider a collection of points $\{\boldsymbol{x}_i\}_{i=1}^N$ along a contour Γ.

Let $\mathbf{A}$ be the $N \times N$ *non-symmetric* matrix with entries $\mathbf{A}(i,j) = \dfrac{(\boldsymbol{x}_i - \boldsymbol{x}_j) \cdot \boldsymbol{n}_j}{|\boldsymbol{x}_i - \boldsymbol{x}_j|^2}$ for $i \neq j$.



The contour



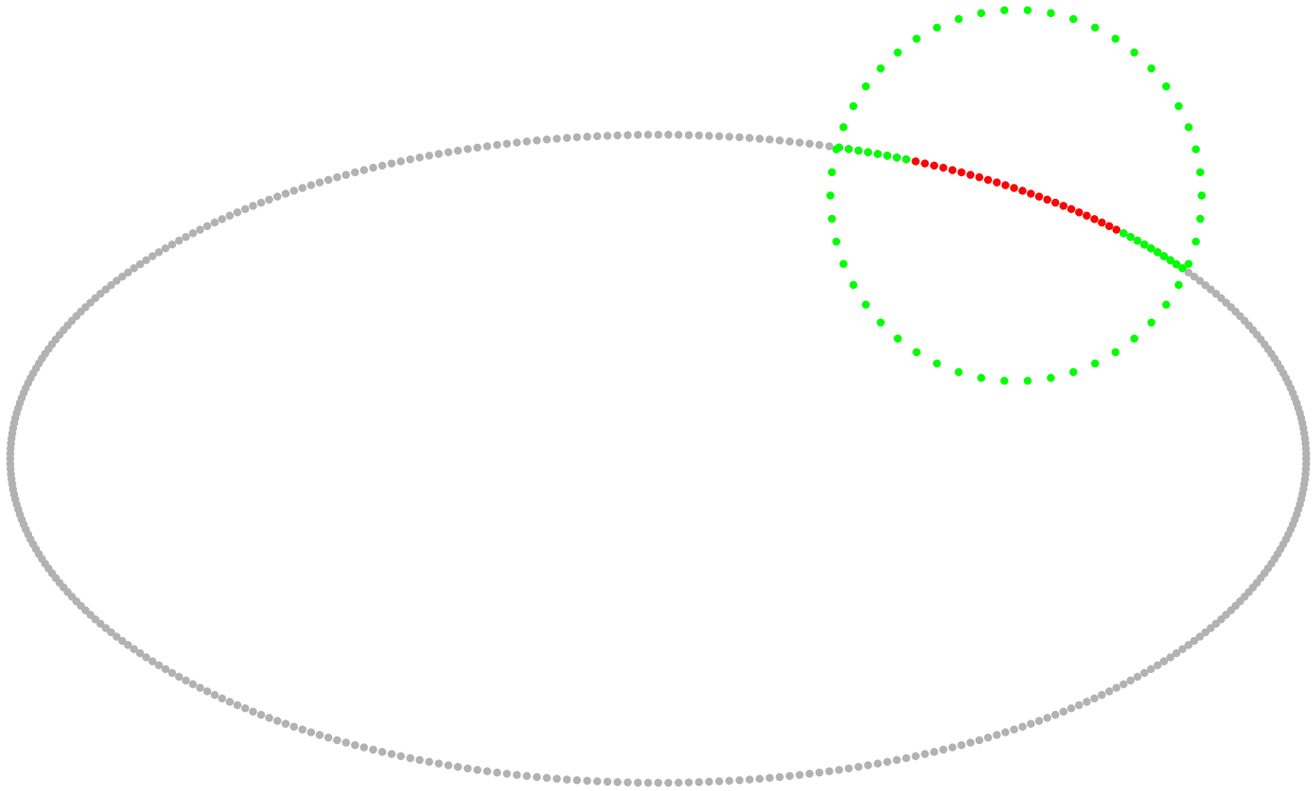
$\mathbf{A}(I_\tau^{\mathrm{c}}, I_\tau)$ *in blue.*

Next we consider the task of finding $\mathbf{V}_\tau$. We need to factor

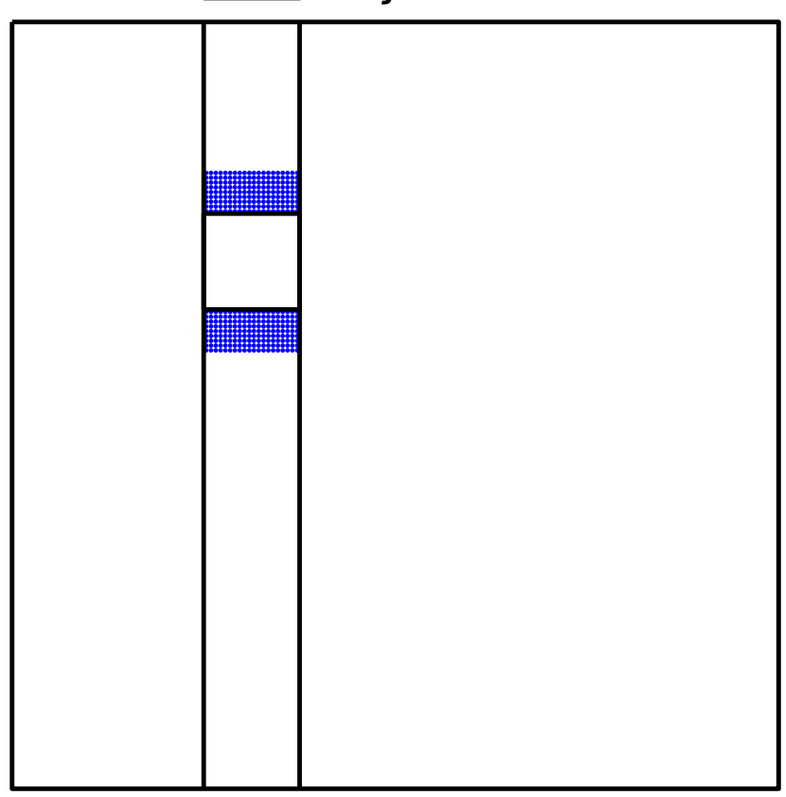
$$\begin{array}{ccccc} \mathbf{A}(I_\tau^{\mathrm{c}}, I_\tau) & = & \mathbf{A}(I_\tau^{\mathrm{c}}, \hat{I}_\tau) & \mathbf{V}_\tau^* \\ (N-n) \times n & & (N-n) \times k & k \times n \end{array}$$

Model problem (non-sym): Consider a collection of points $\{\boldsymbol{x}_i\}_{i=1}^N$ along a contour Γ.

Let $\mathbf{A}$ be the $N \times N$ *non-symmetric* matrix with entries $\mathbf{A}(i,j) = \dfrac{(\boldsymbol{x}_i - \boldsymbol{x}_j) \cdot \boldsymbol{n}_j}{|\boldsymbol{x}_i - \boldsymbol{x}_j|^2}$ for $i \neq j$.



The contour



$\mathbf{A}(I_\tau^{\mathrm{c}}, I_\tau)$ *in blue.*
$\mathbf{G}$ *in magenta.*

Things work *almost* the same . . .

Replace charges in the far-field by "proxy" charges, let $I_\tau^{(\mathrm{near})}$ denote the near-field points and let $\mathbf{G}$ denote a matrix of size $n \times n_{\mathrm{proxy}}$ that maps *dipole* charges on Γ_τ to potentials on the proxy points. Then factor the smaller problem:

$$\begin{bmatrix} \mathbf{A}(I_\tau^{(\mathrm{near})}, I_\tau) \\ \mathbf{G} \end{bmatrix} = \begin{bmatrix} \mathbf{A}(I_\tau^{(\mathrm{near})}, \hat{I}_\tau) \\ \mathbf{G}(:, J) \end{bmatrix} \mathbf{V}_\tau^*.$$

Notes:

- There are in fact two potentially different sets of skeleton points:
  1. The *incoming skeleton points* resulting from an ID of the *rows* of $\mathbf{A}(I_\tau, I_\tau^c)$.
  2. The *outgoing skeleton points* resulting from an ID of the *columns* of $\mathbf{A}(I_\tau^c, I_\tau)$.

  It is possible, and often practical, to enforce that these skeletons be the same.

  This can be done by constructing an ID for the rows of $[\mathbf{A}(I_\tau, I_\tau^c),\ \mathbf{A}(I_\tau^c, I_\tau)^*]$.

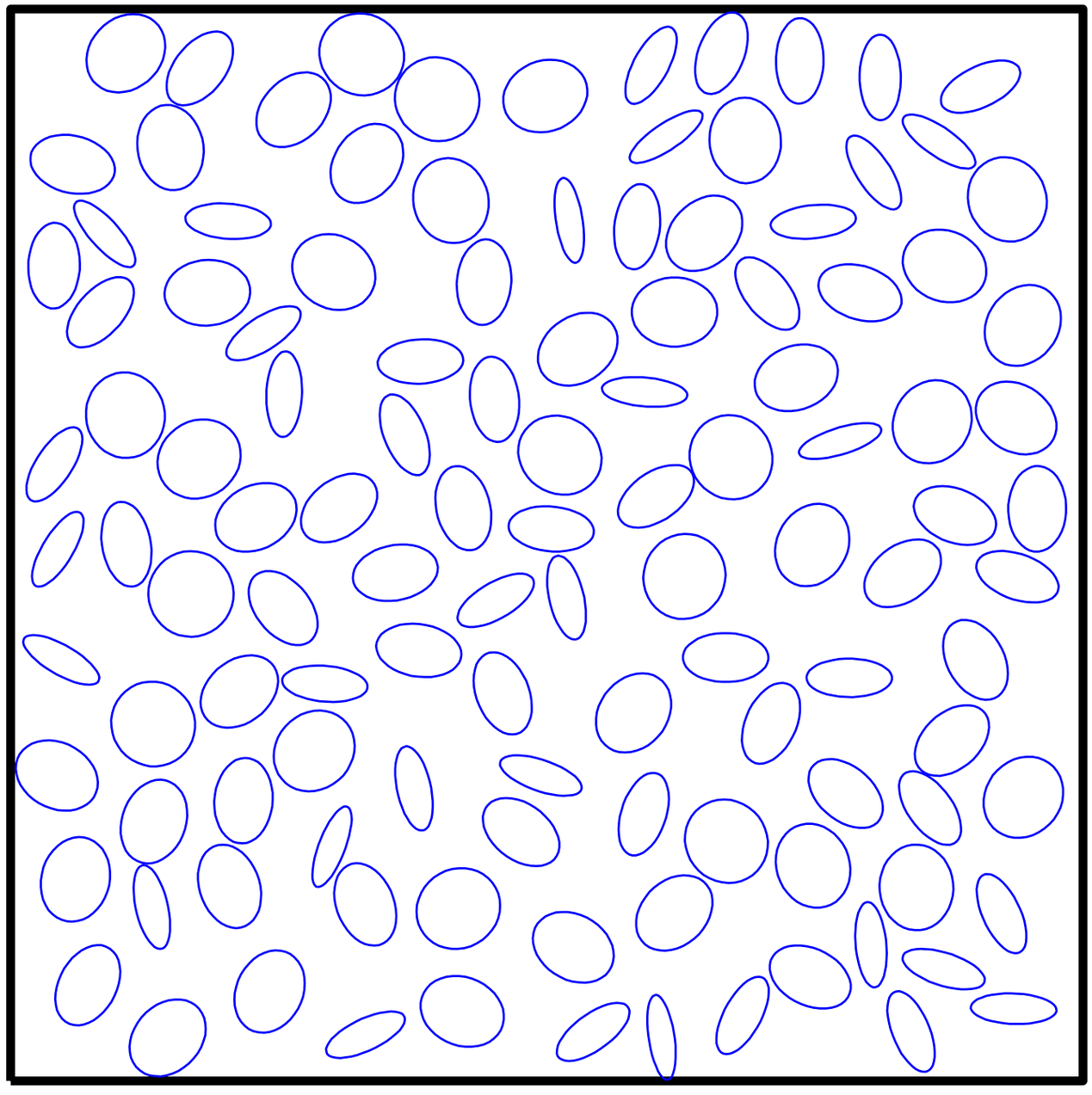
- In real life, the presence of quadrature corrections for "near-diagonal" elements slightly complicates matters. However, these complications can all be handled.

- For *Helmholtz*, the compression technique based on a proxy domain (e.g. circle) to account for the far-field has to be modifed to avoid the possibility of resonances (avoid using resonant radii, or, use *two* concentric sets of proxy circles separated by a distance $\lambda/4$, or, use both monopoles and dipoles on the proxy surface, etc).

- For other elliptic PDEs (Stokes, elasticity, time-harmonic Maxwell, etc), analogous representations can be worked out. Each case has its own subtleties, but the basic ideas carry over. (At least, it currently appears that they do!)

- Some care is necessary in determining how finely to sample the proxy surface, in particular for Helmholtz.

A "volume filling" domain: Now consider a contour like this:

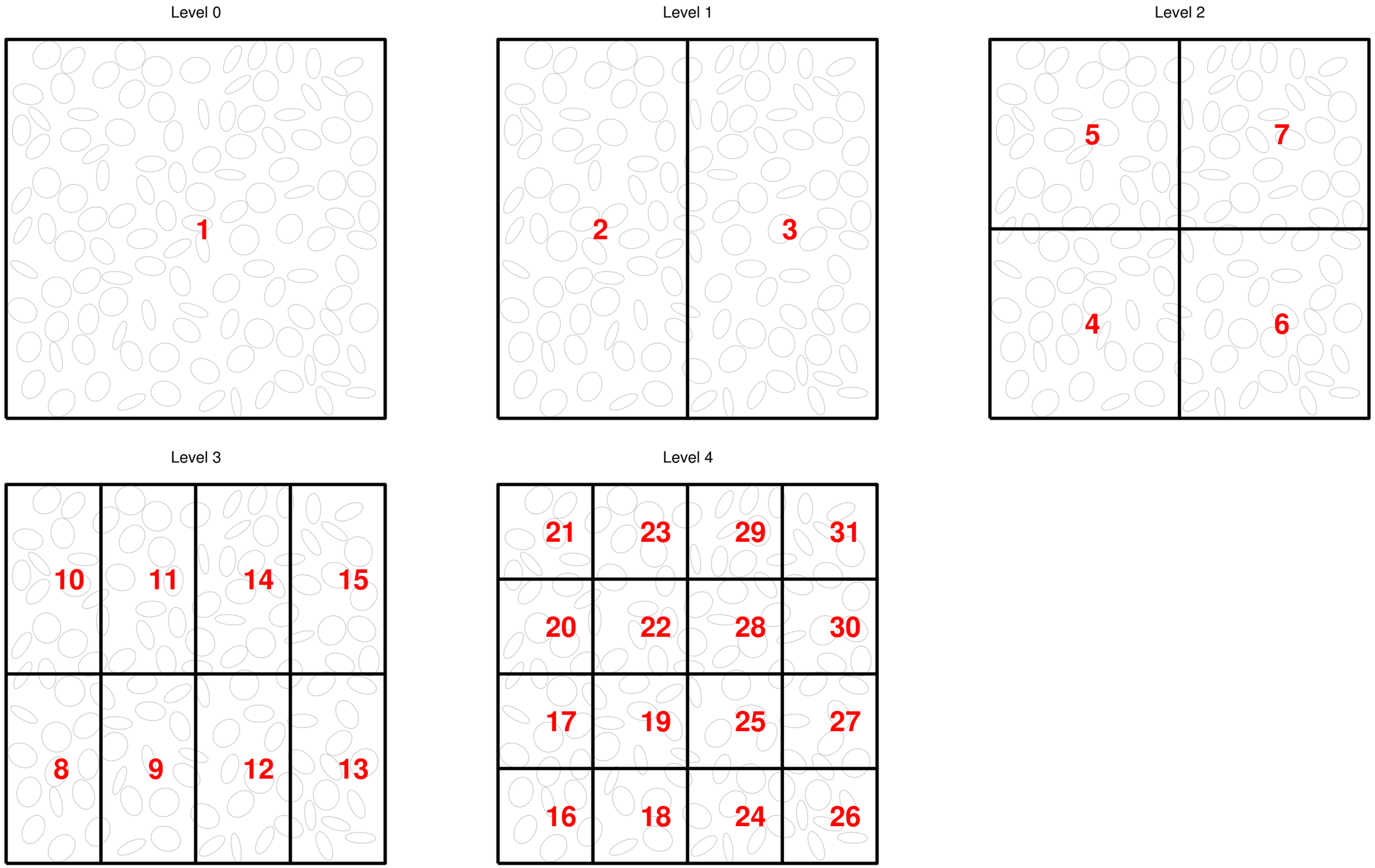


Let **A** denote an $N \times N$ matrix arising upon discretizing a boundary integral operator

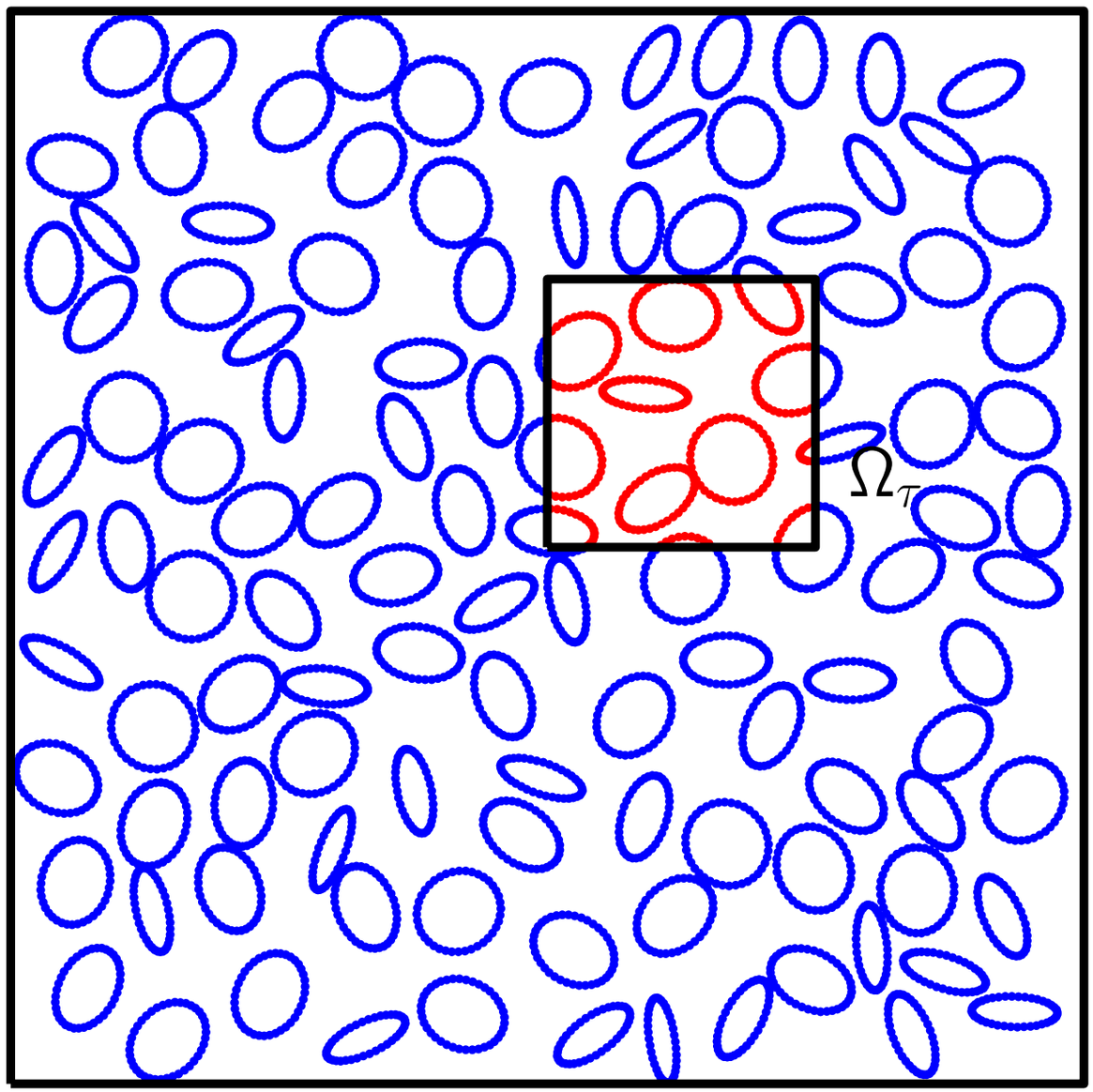
$$[Aq](\boldsymbol{x}) = q(\boldsymbol{x}) + \int_\Gamma \log|\boldsymbol{x} - \boldsymbol{y}|\, q(\boldsymbol{y})\, dA(\boldsymbol{y}), \qquad \boldsymbol{x} \in \Gamma,$$

where Γ is the collection of ellipses shown.

We must now use a binary tree based on *splitting in physical space* (as opposed to parameter space).



Compression stage: Finding $\tilde{I}_\tau$, $\mathbf{U}_\tau$, and $\mathbf{V}_\tau$, for a box τ works in principle the same as before, but the proxy surfaces are chosen a bit differently.



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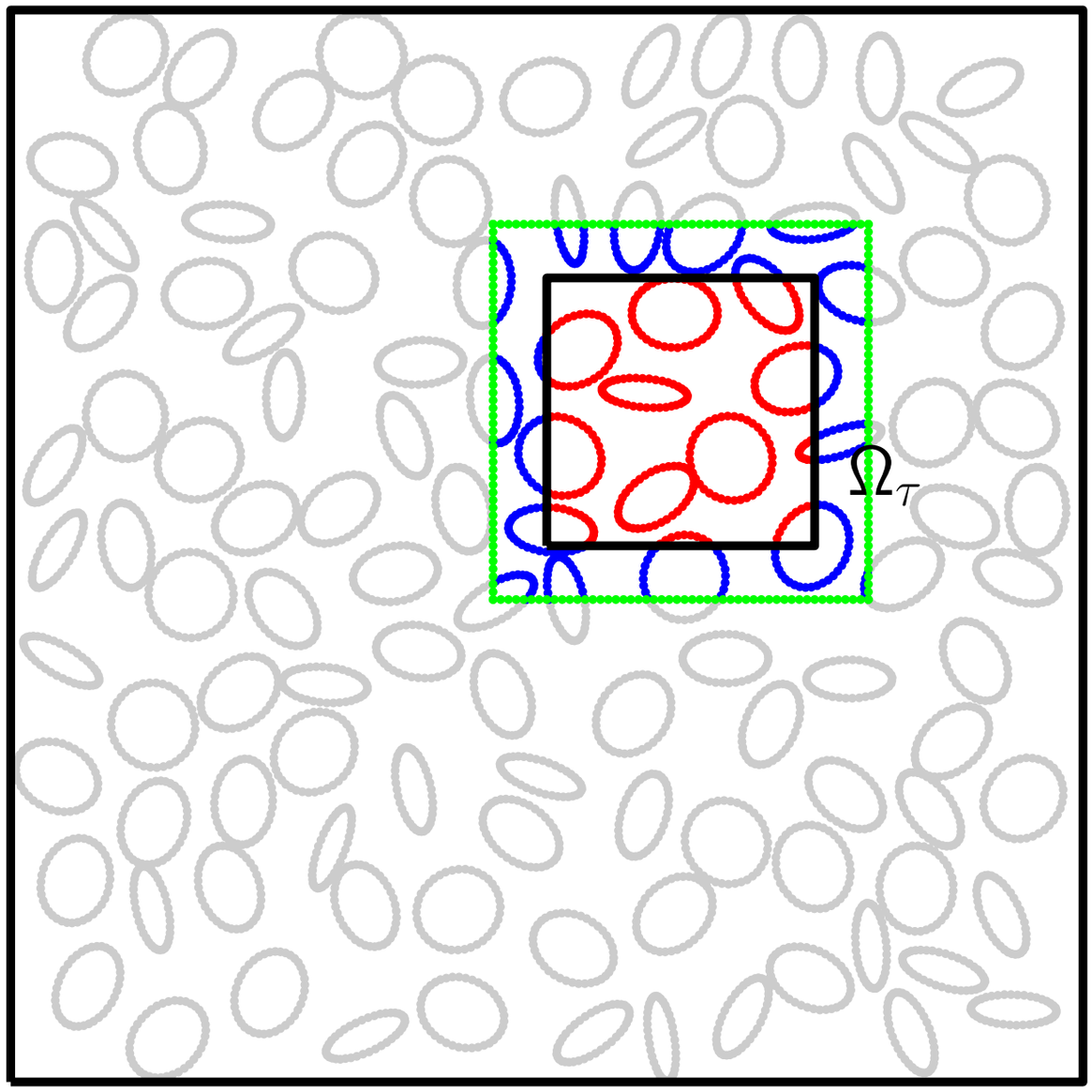

- Points in I_τ.
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(gray points are inactive)

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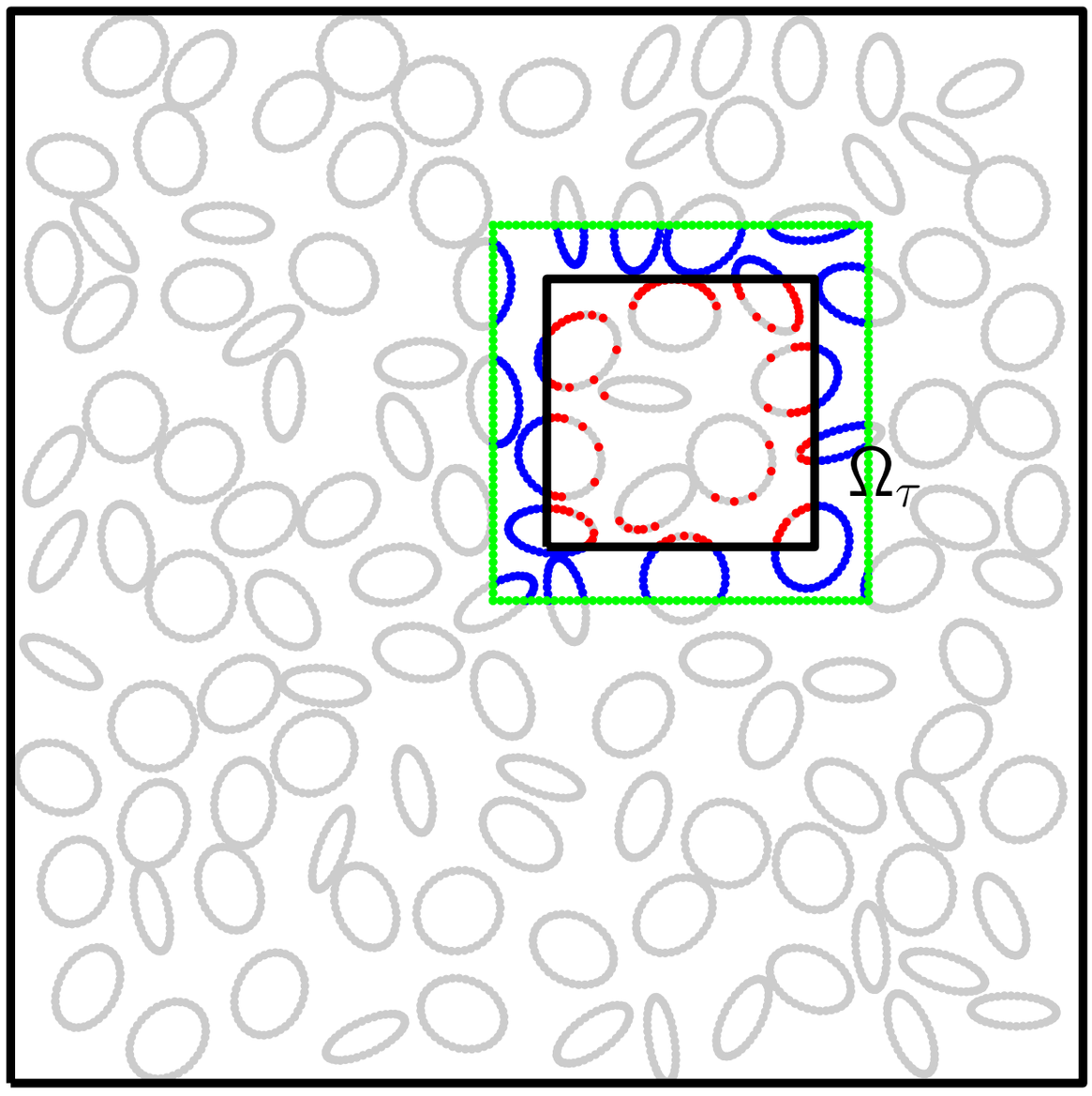

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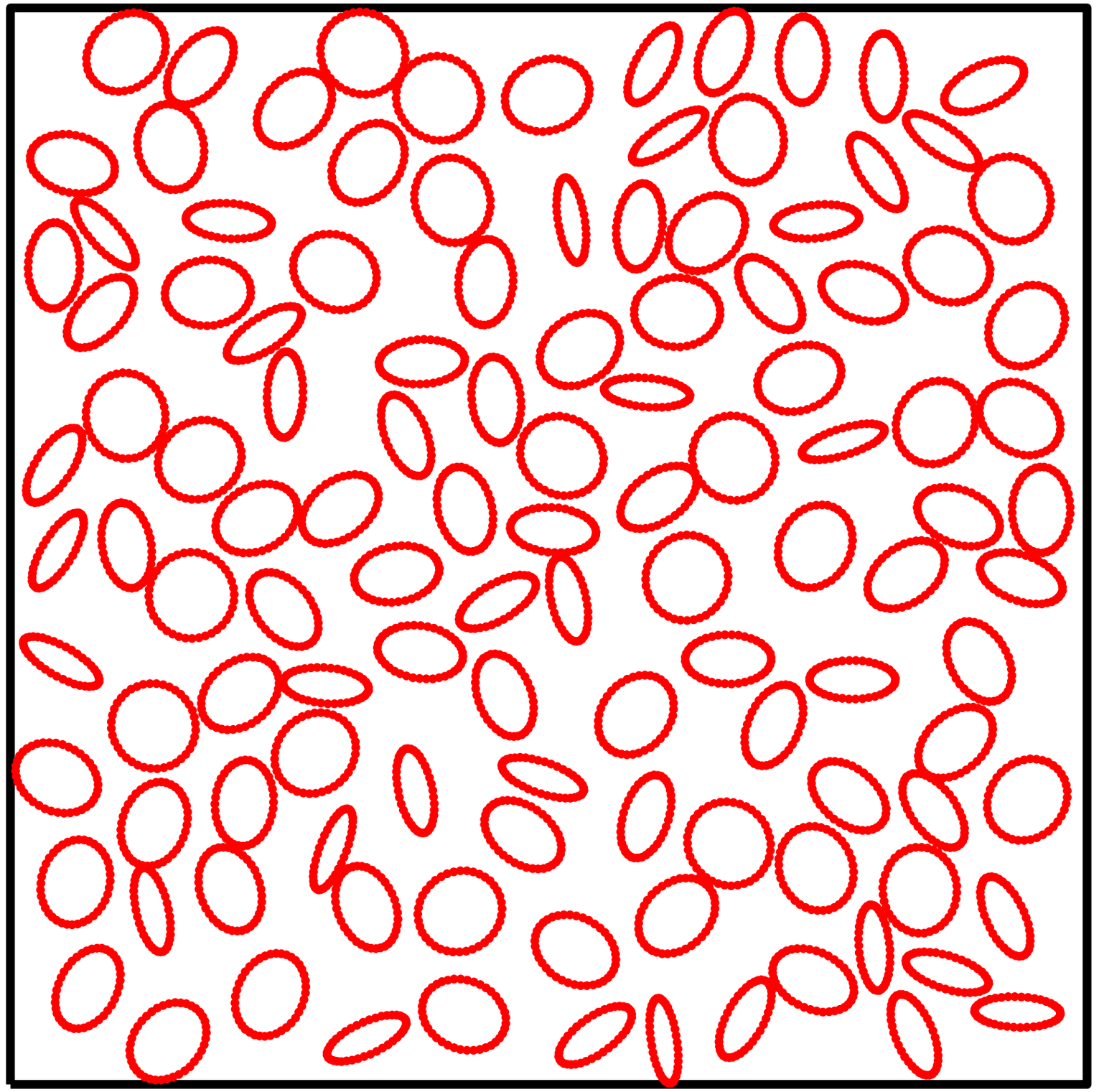
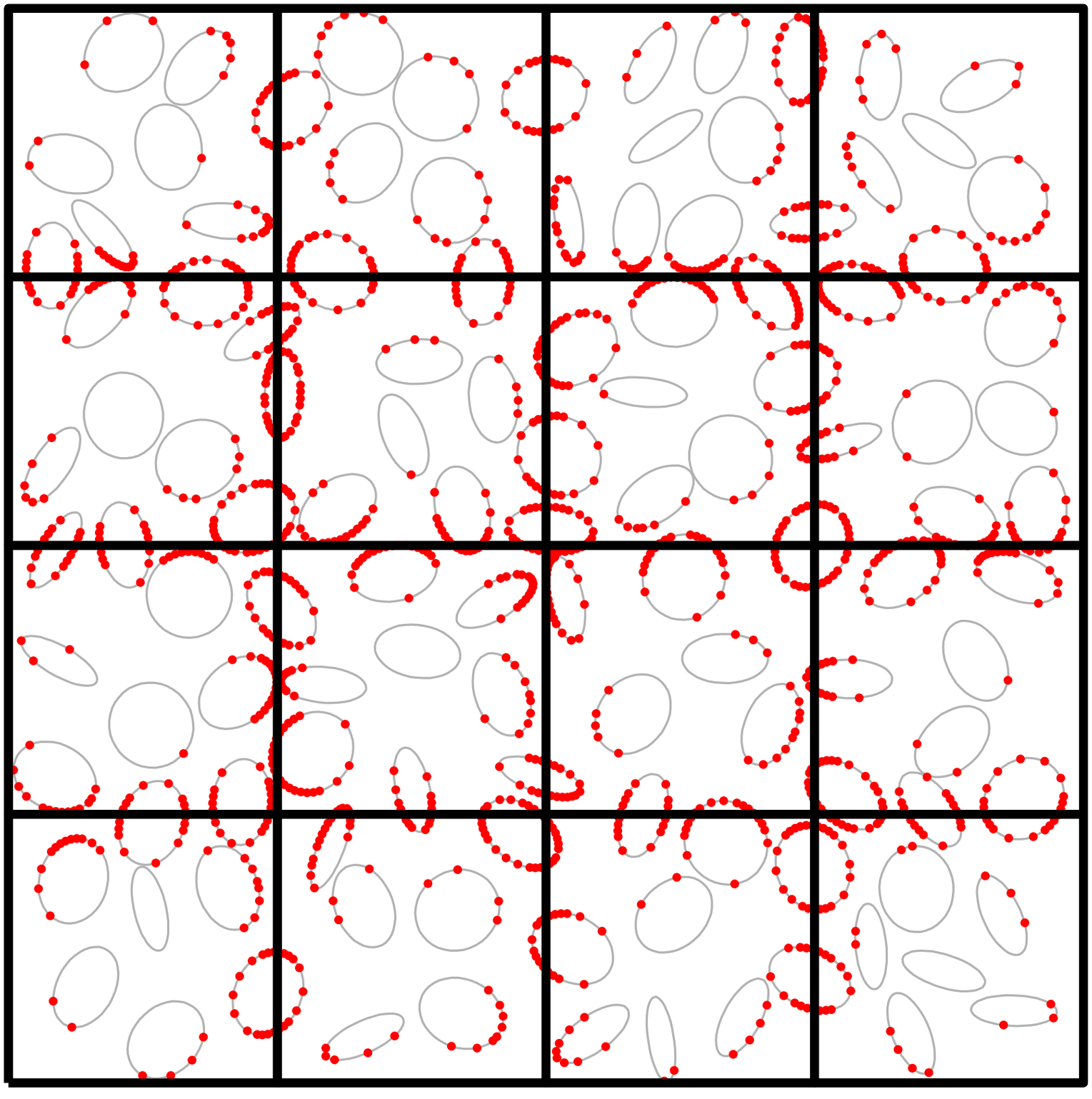
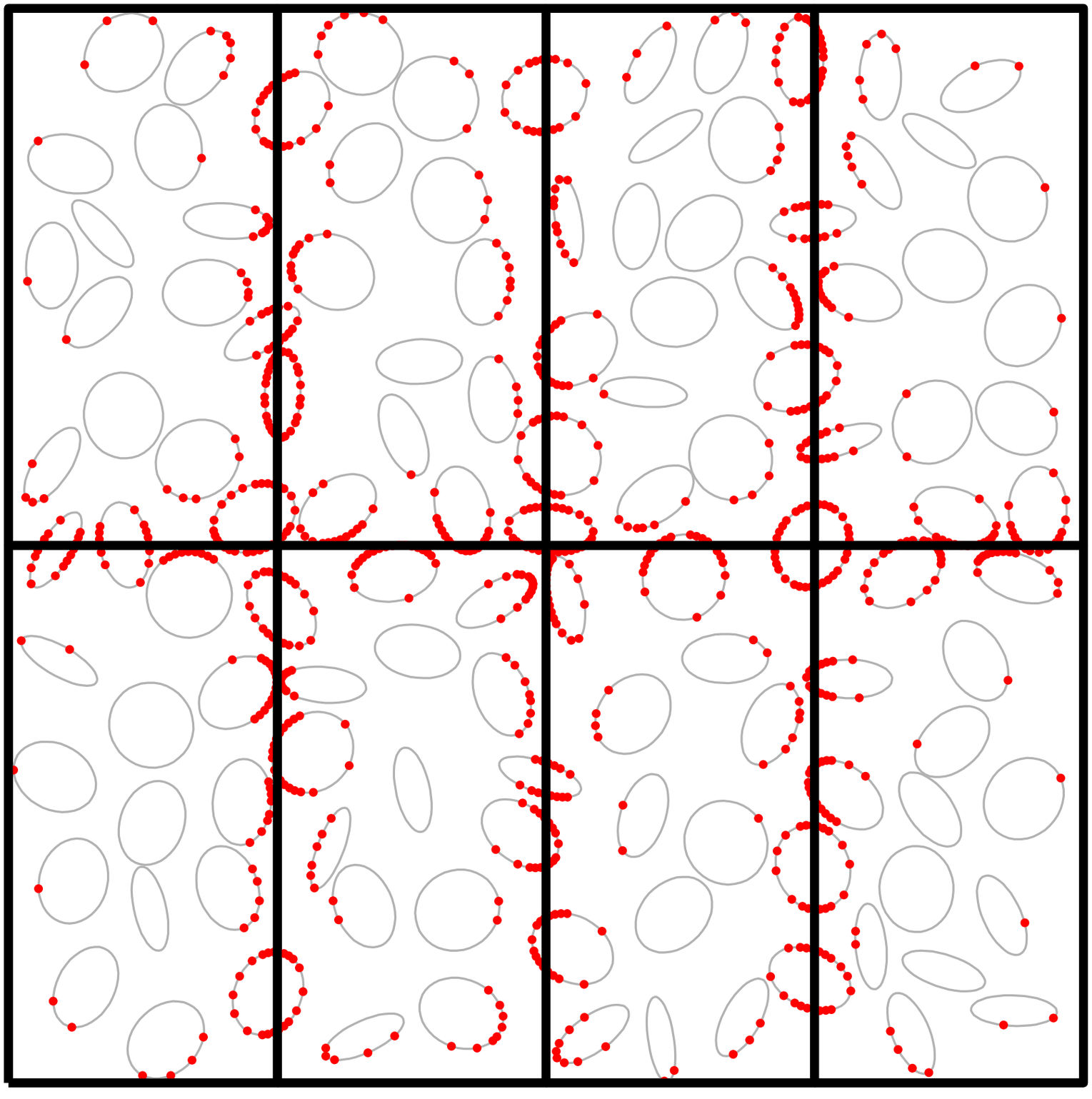
Original set of points



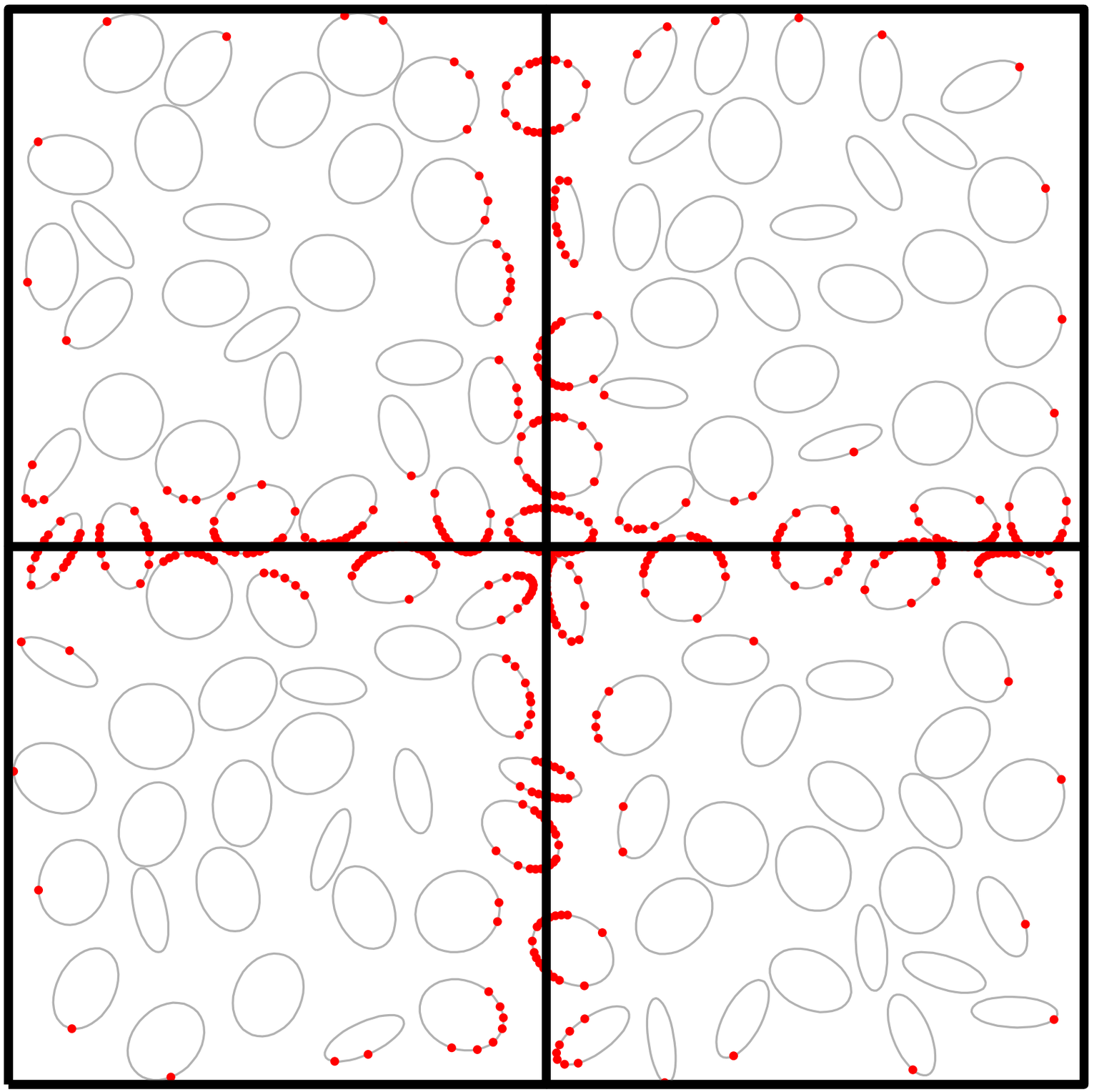
Skeleton points on level 4, acc = 1.000e−09



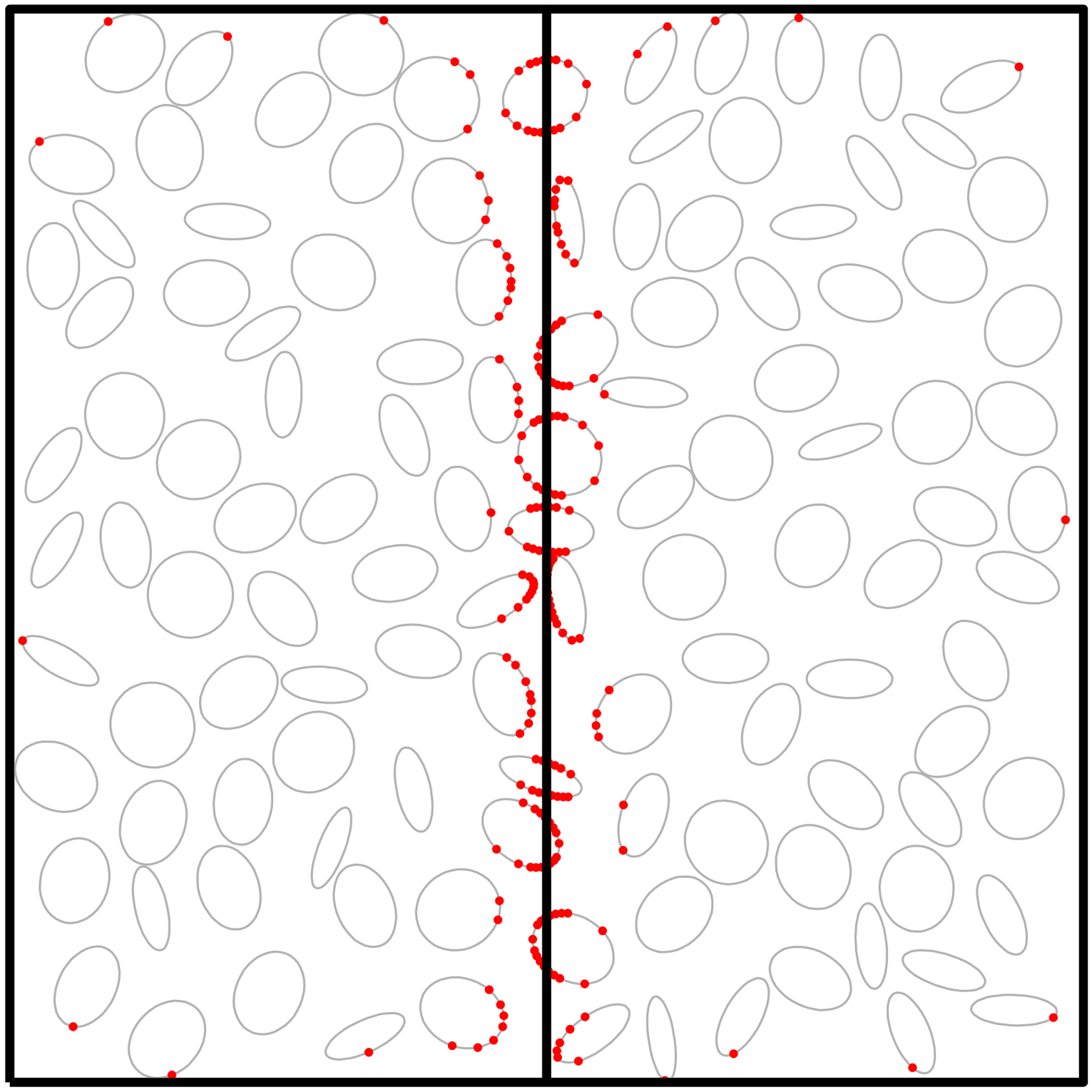
Skeleton points on level 3, acc = 1.000e−09



Skeleton points on level 2, acc = 1.000e−09



Skeleton points on level 1, acc = 1.000e−09



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Complexity analysis: For a box τ, define quantities:

N_τ	Number of discretization points in τ.
n	Number of points in the skeletons for the children of τ.
g	Number of points in the proxy contour.
k	Rank of interaction between τ and the outside world.

Then

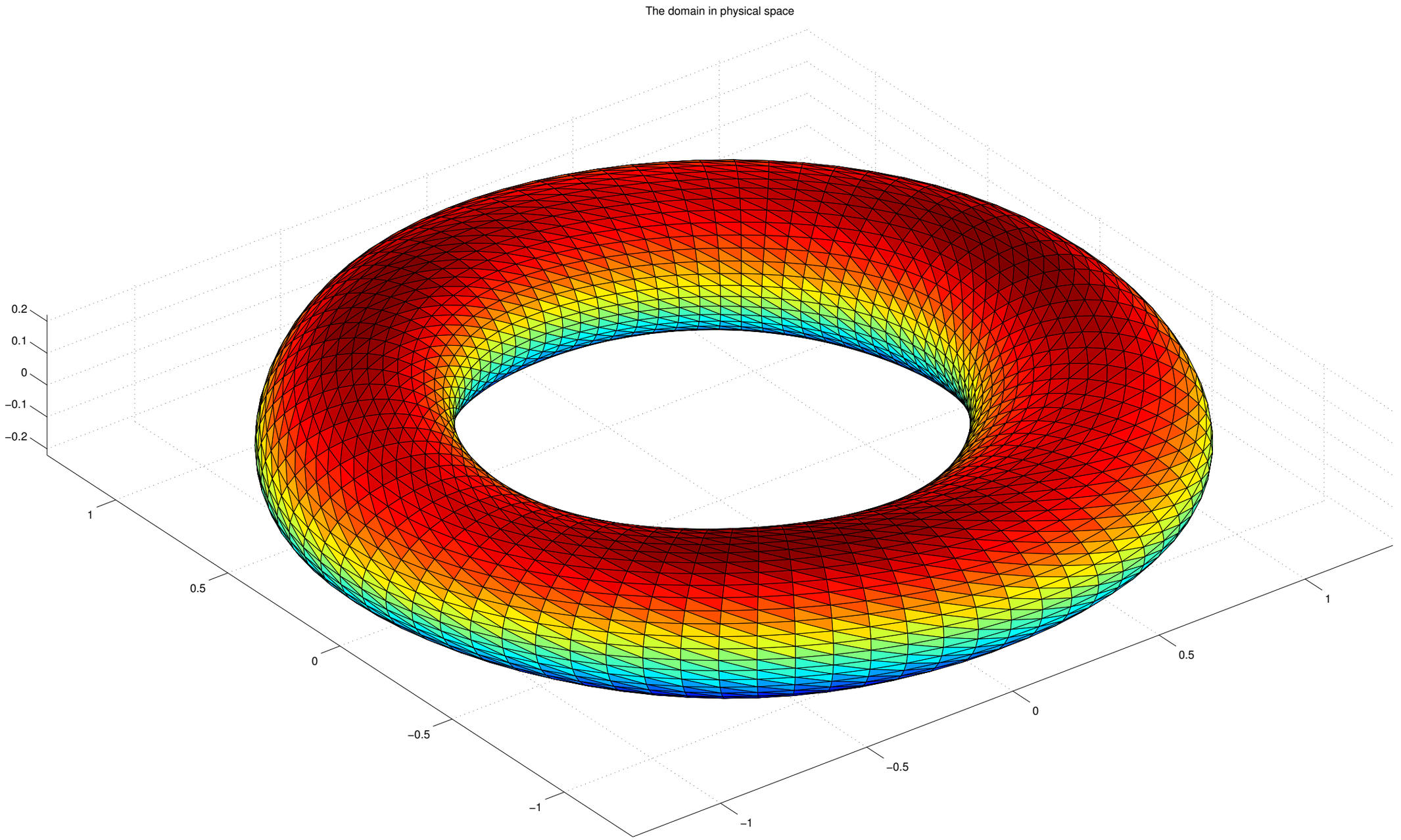
$$\begin{aligned} \text{Cost of compressing } \tau &\sim n\,g\,k \\ \text{Cost of building local operators } \tau &\sim n^3 \end{aligned}$$

Unfortunately, for a "volume filling" set of points, we have

$$n \sim \sqrt{N_\tau}, \qquad g \sim \sqrt{N_\tau}, \qquad k \sim \sqrt{N_\tau},$$

so the overall cost of the direct solver is $O(N^{3/2})$.

A surface in 3D: Now consider a surface in $\mathbb{R}^3$:



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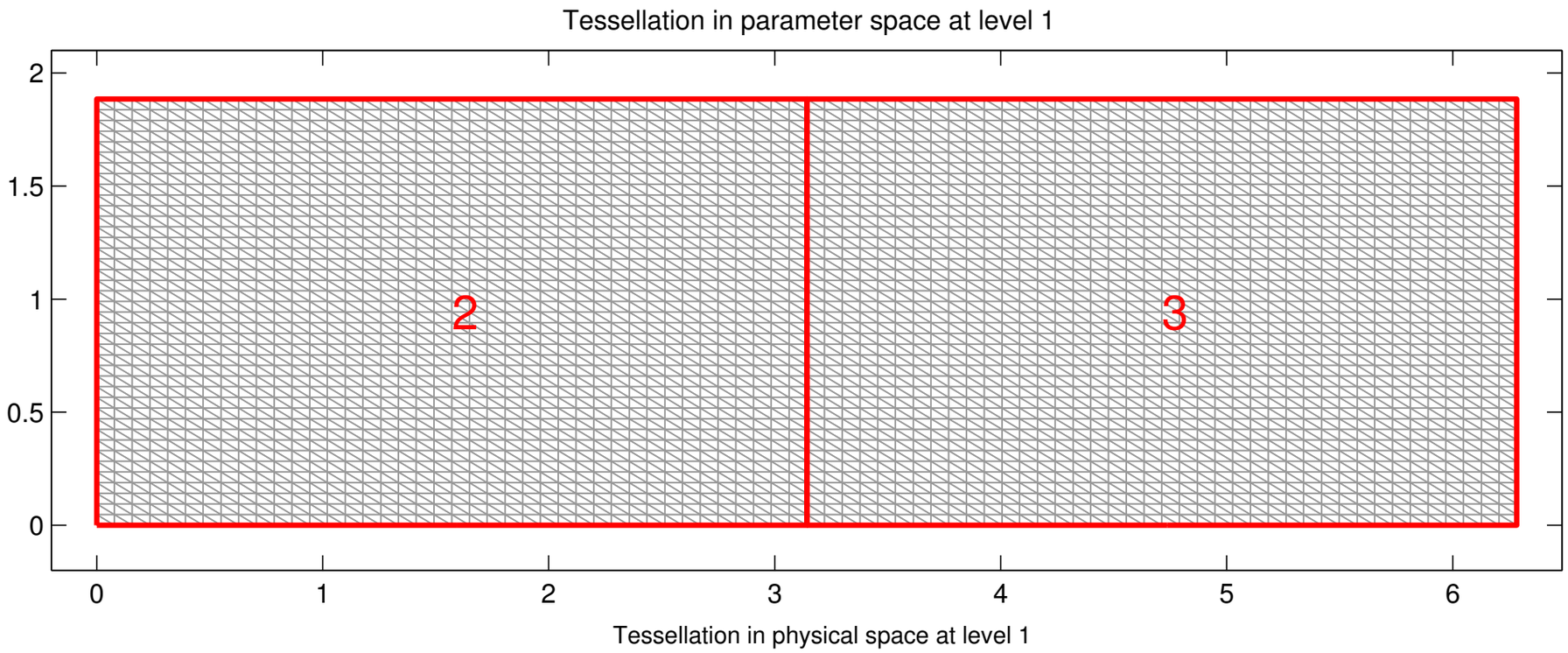
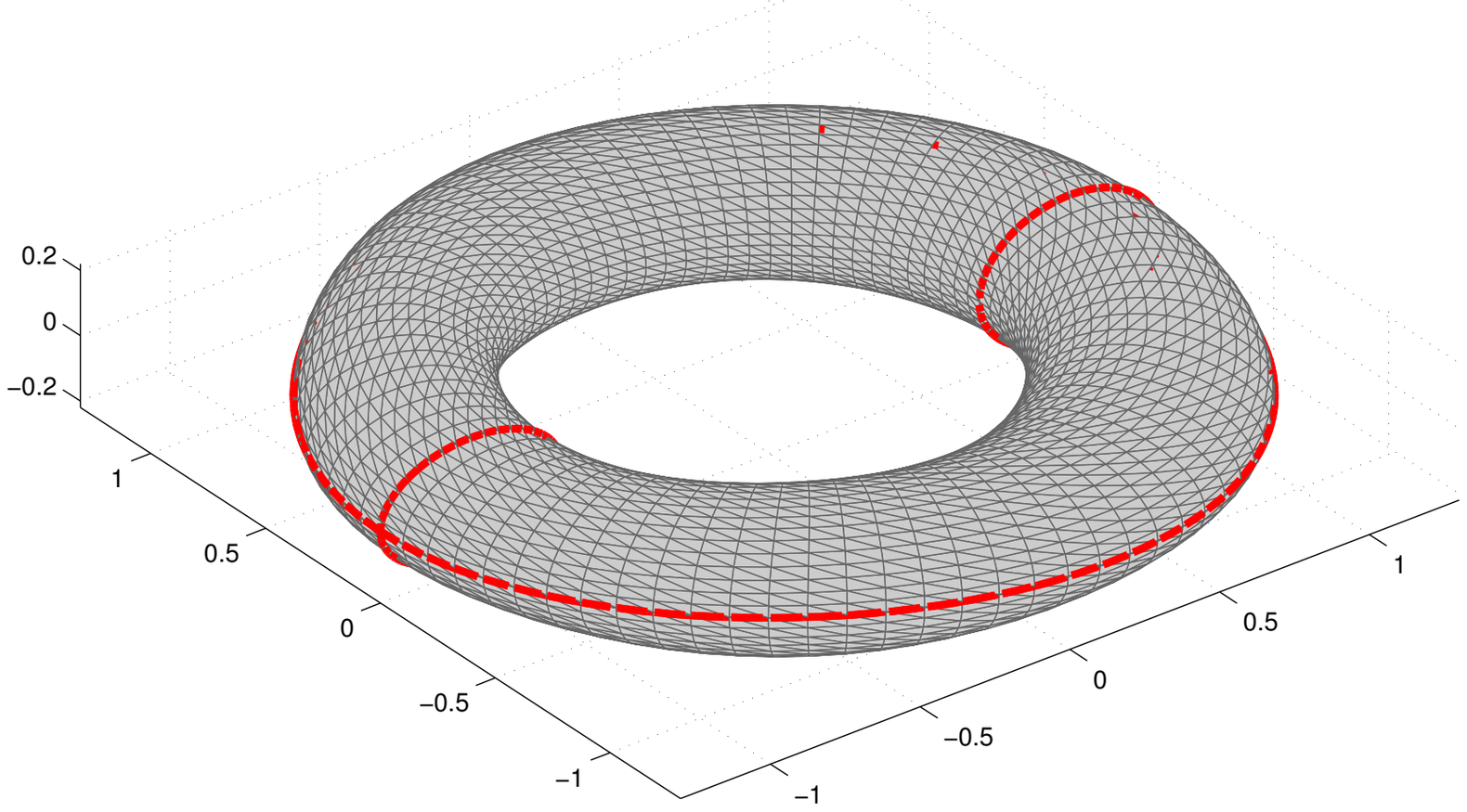
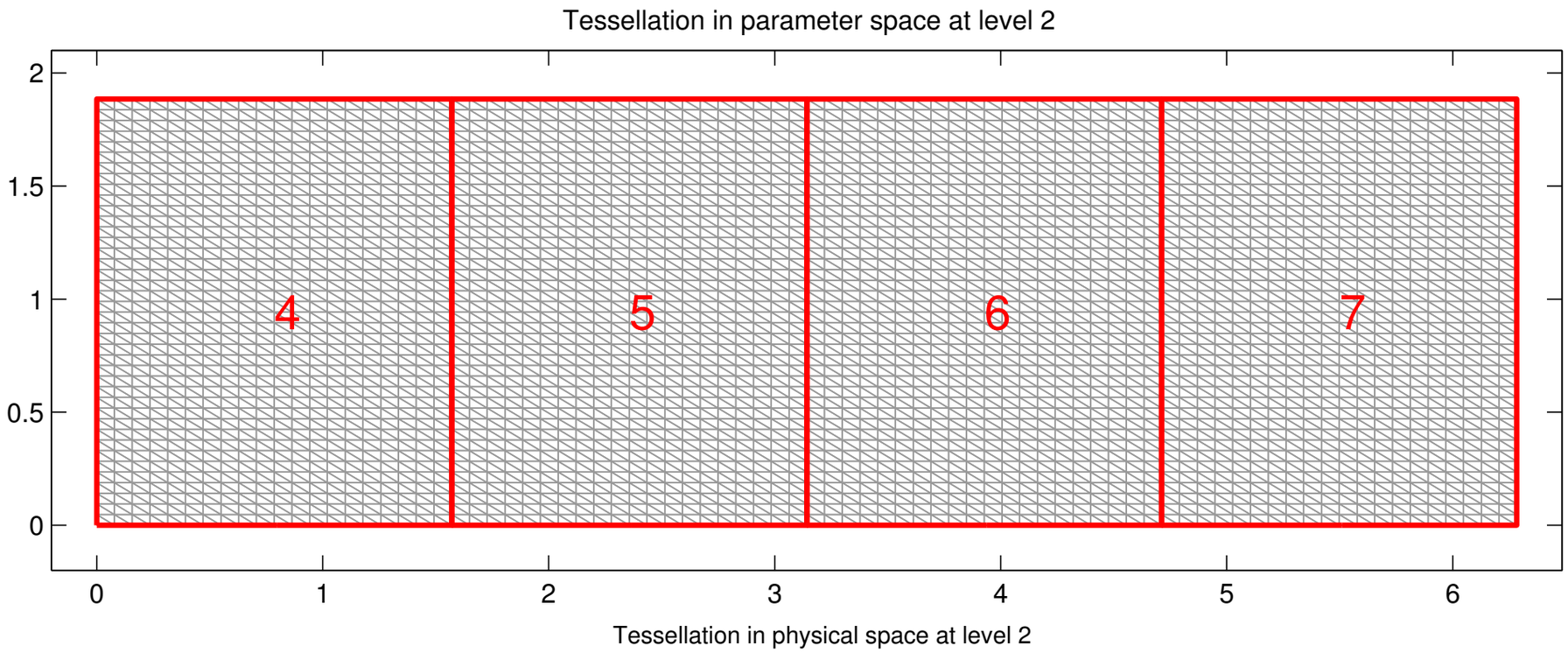
where Γ is the "torus-like" domain shown (it is deformed to avoid rotational symmetry).

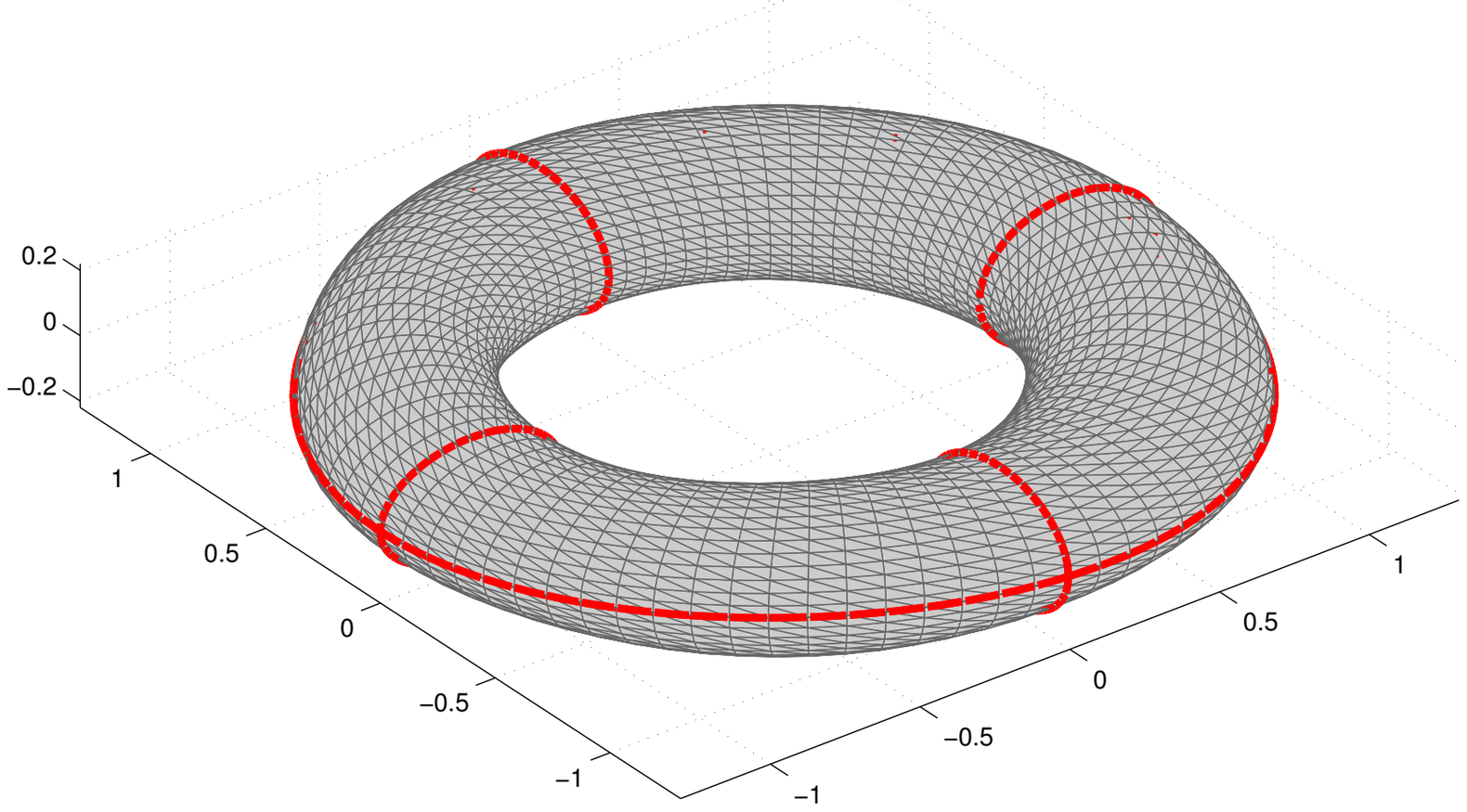
We construct a tree by bisecting *in parameter space* — level 1.





We construct a tree by bisecting *in parameter space* — level 2.





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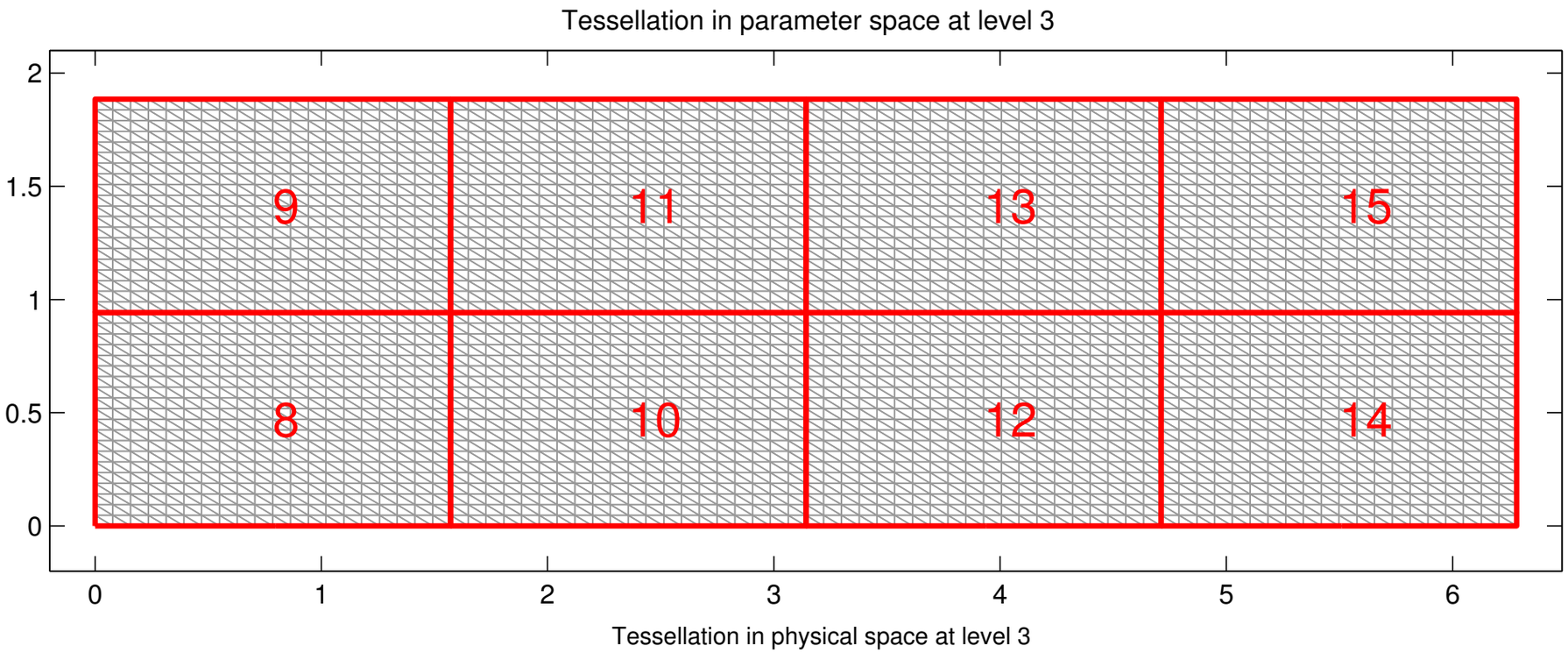
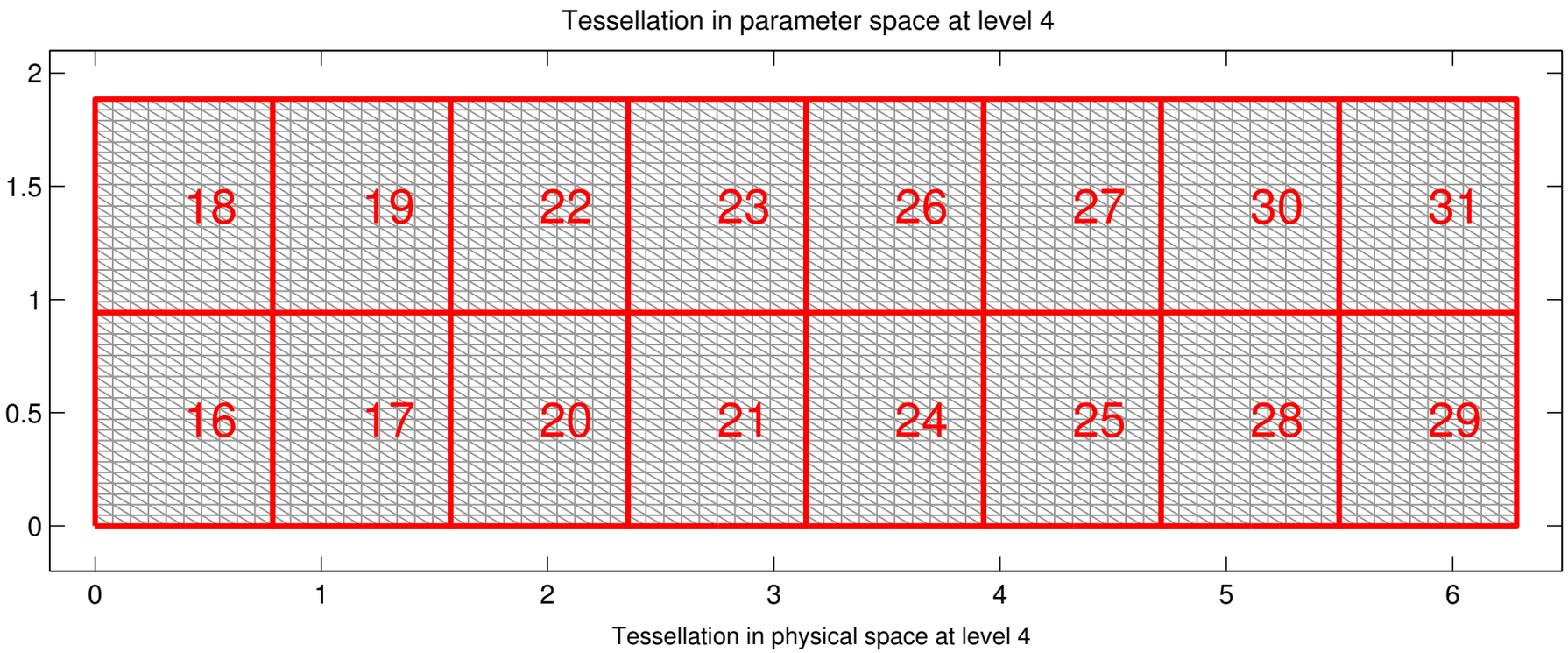


We construct a tree by bisecting *in parameter space* — level 4.



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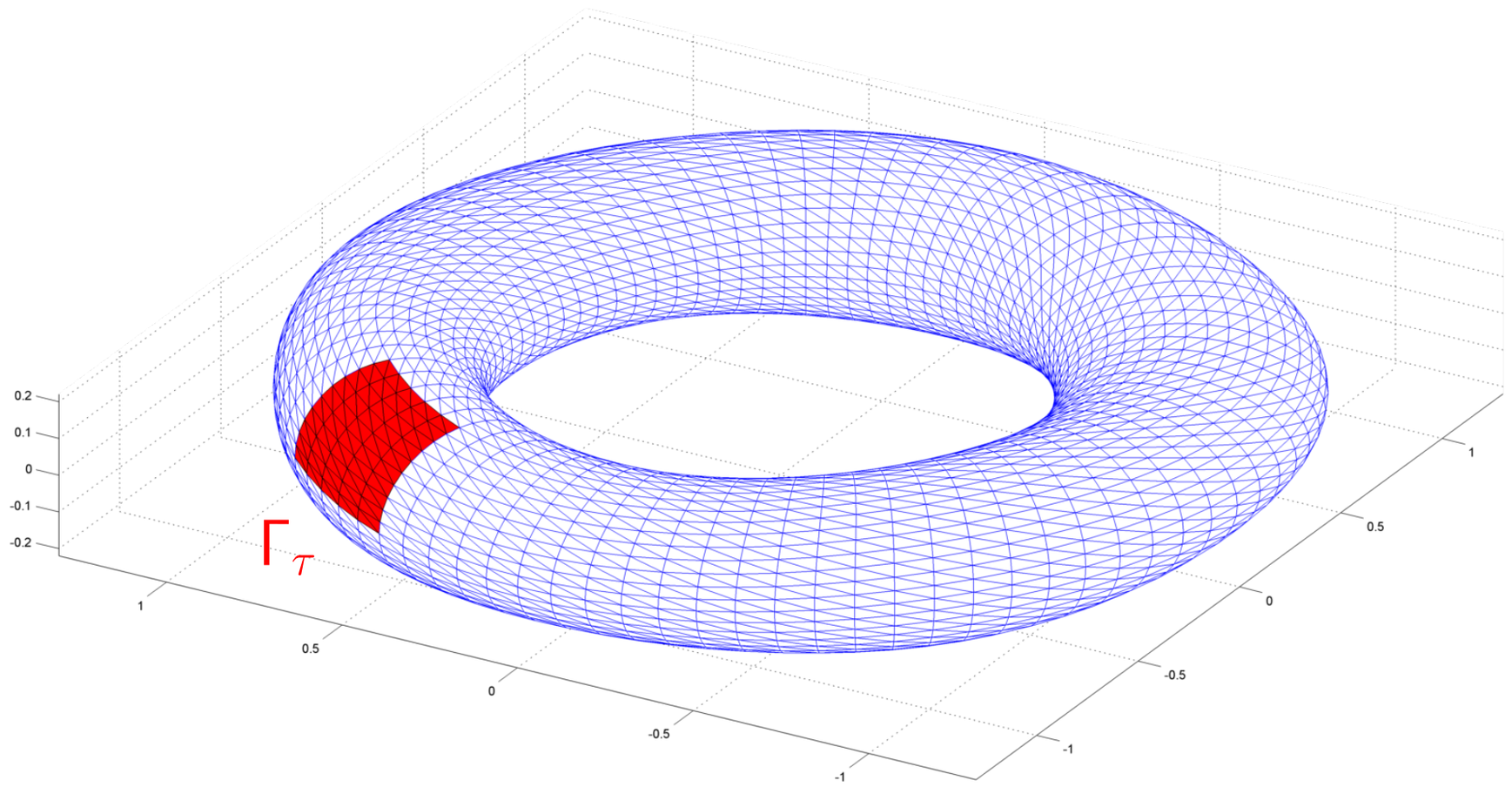

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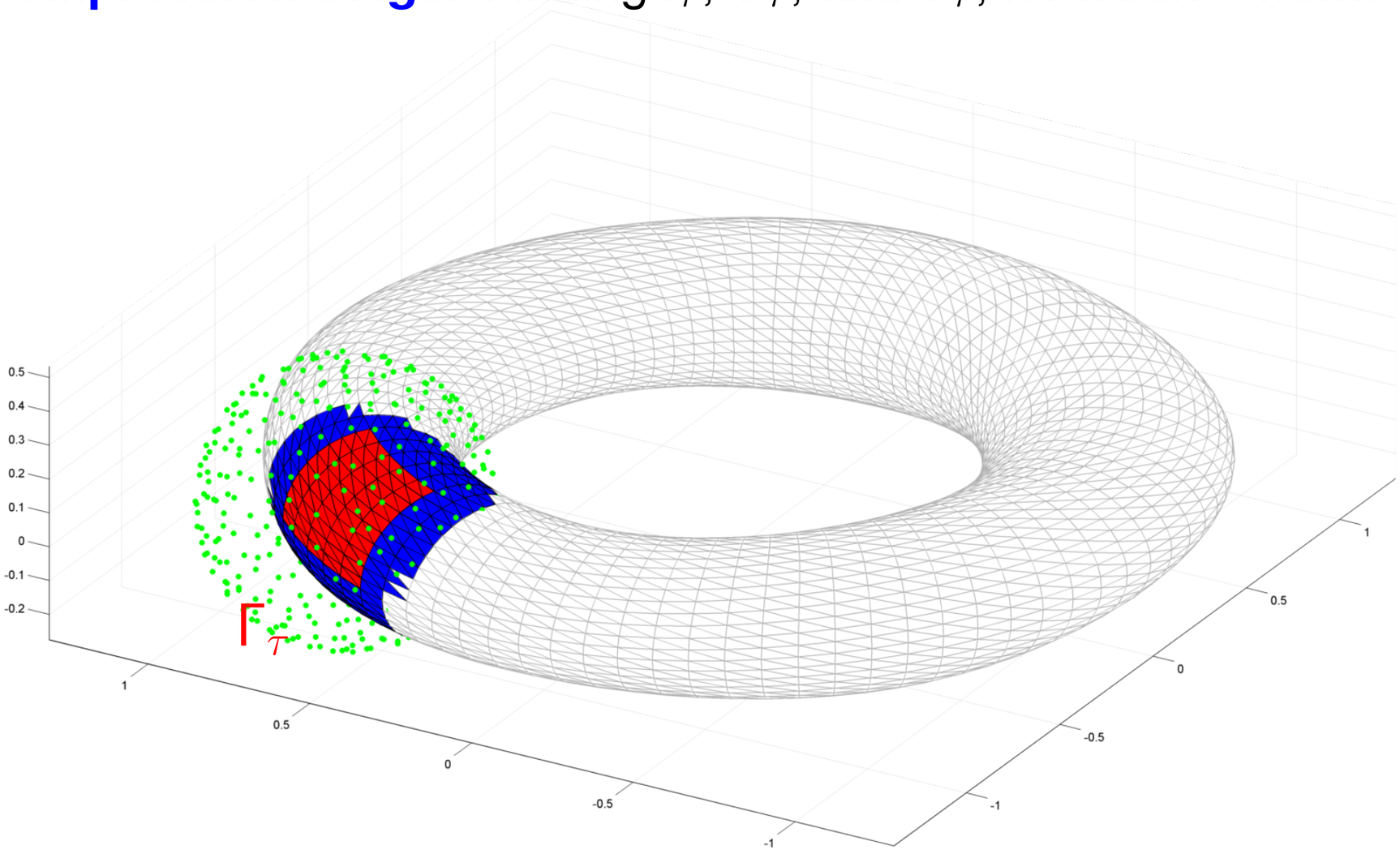

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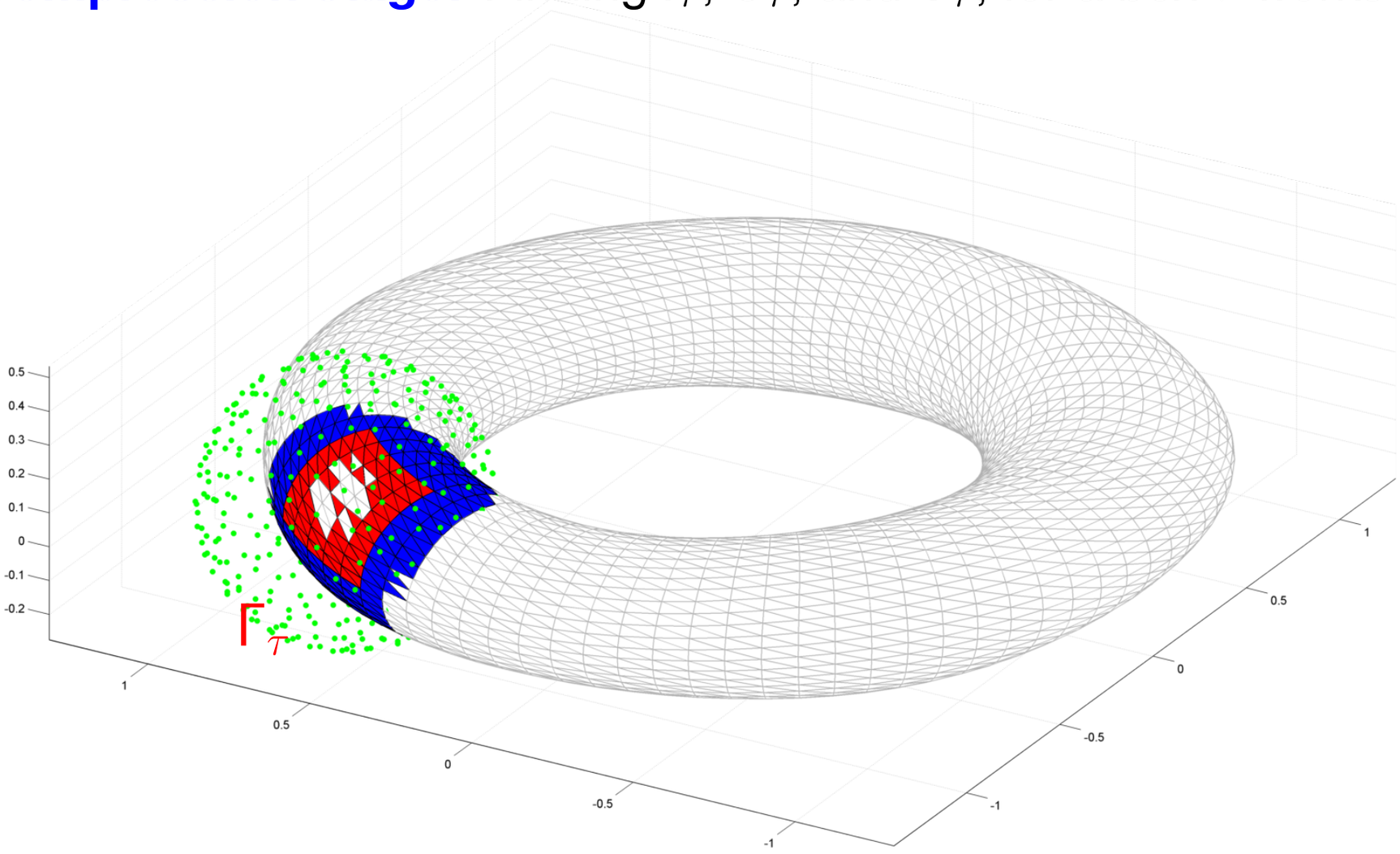

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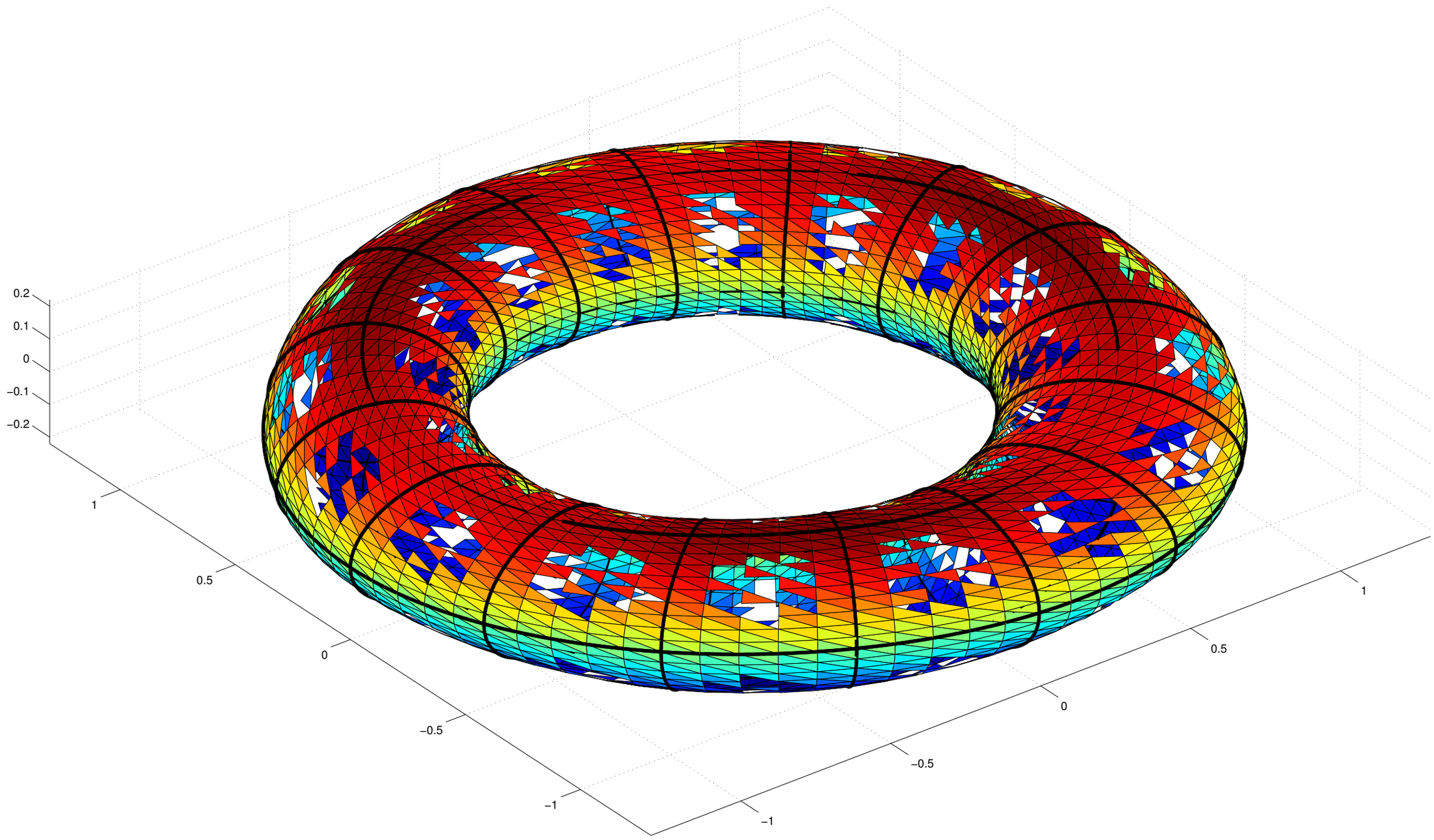
The domain in physical space



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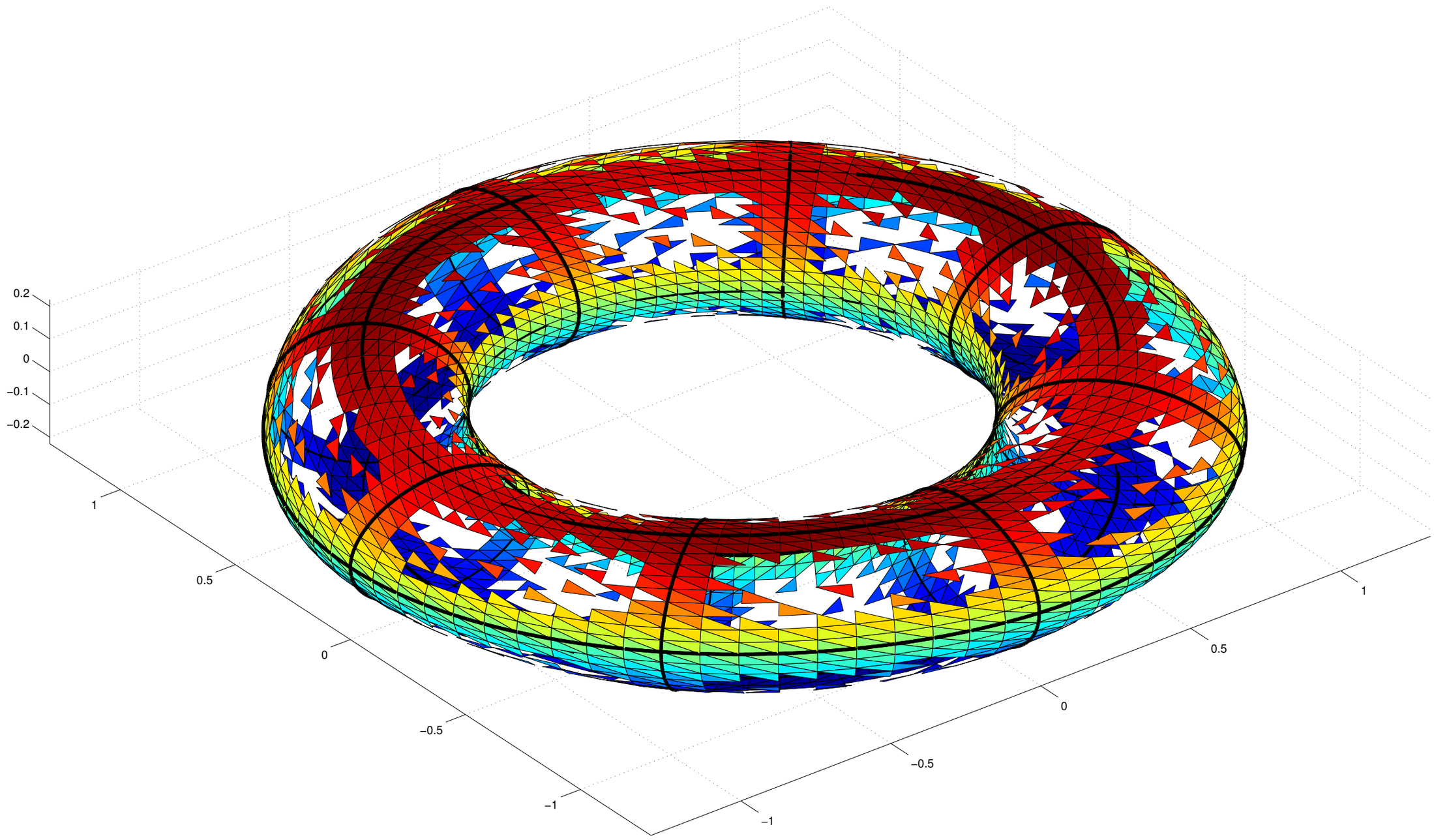

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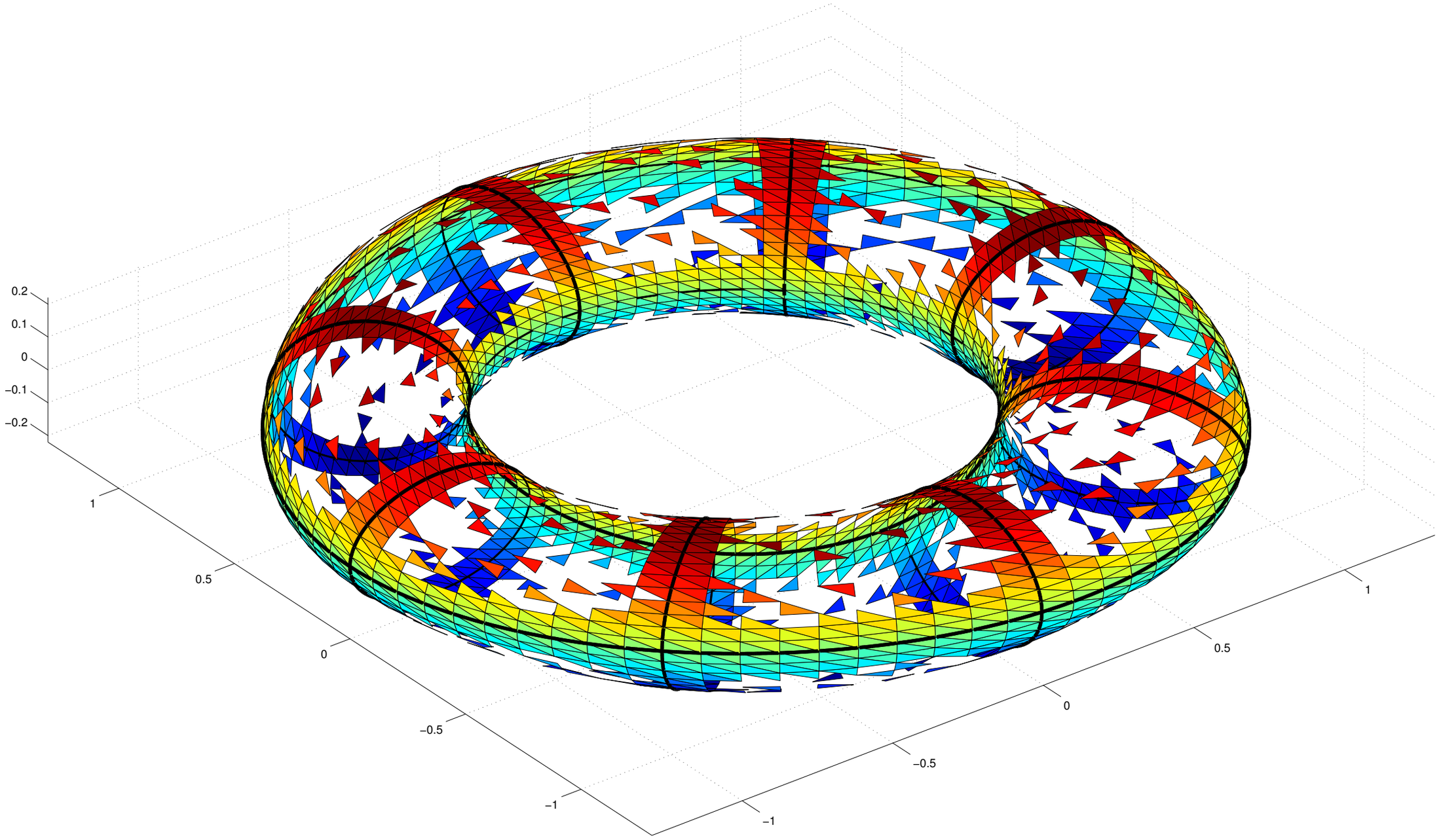

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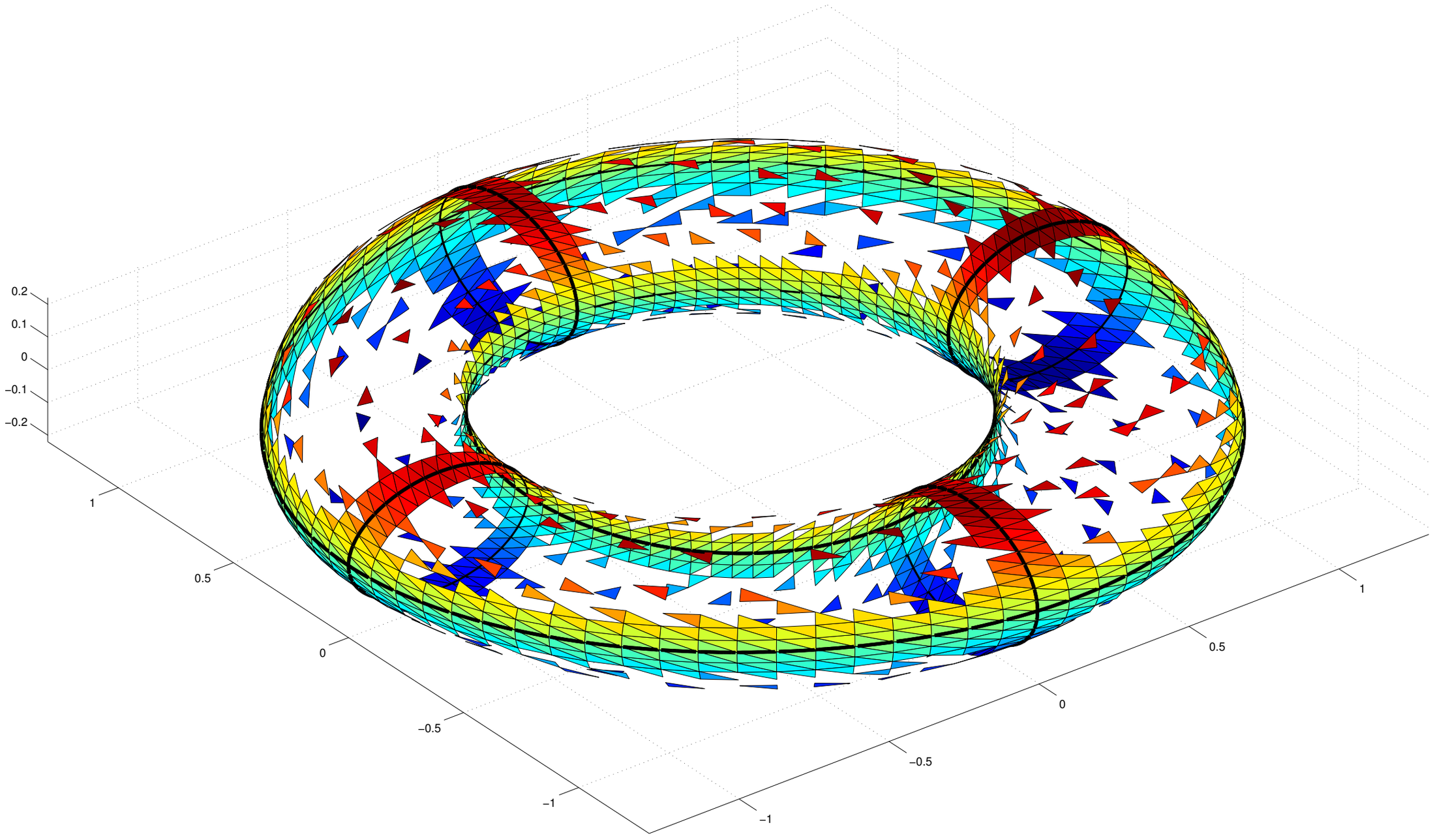

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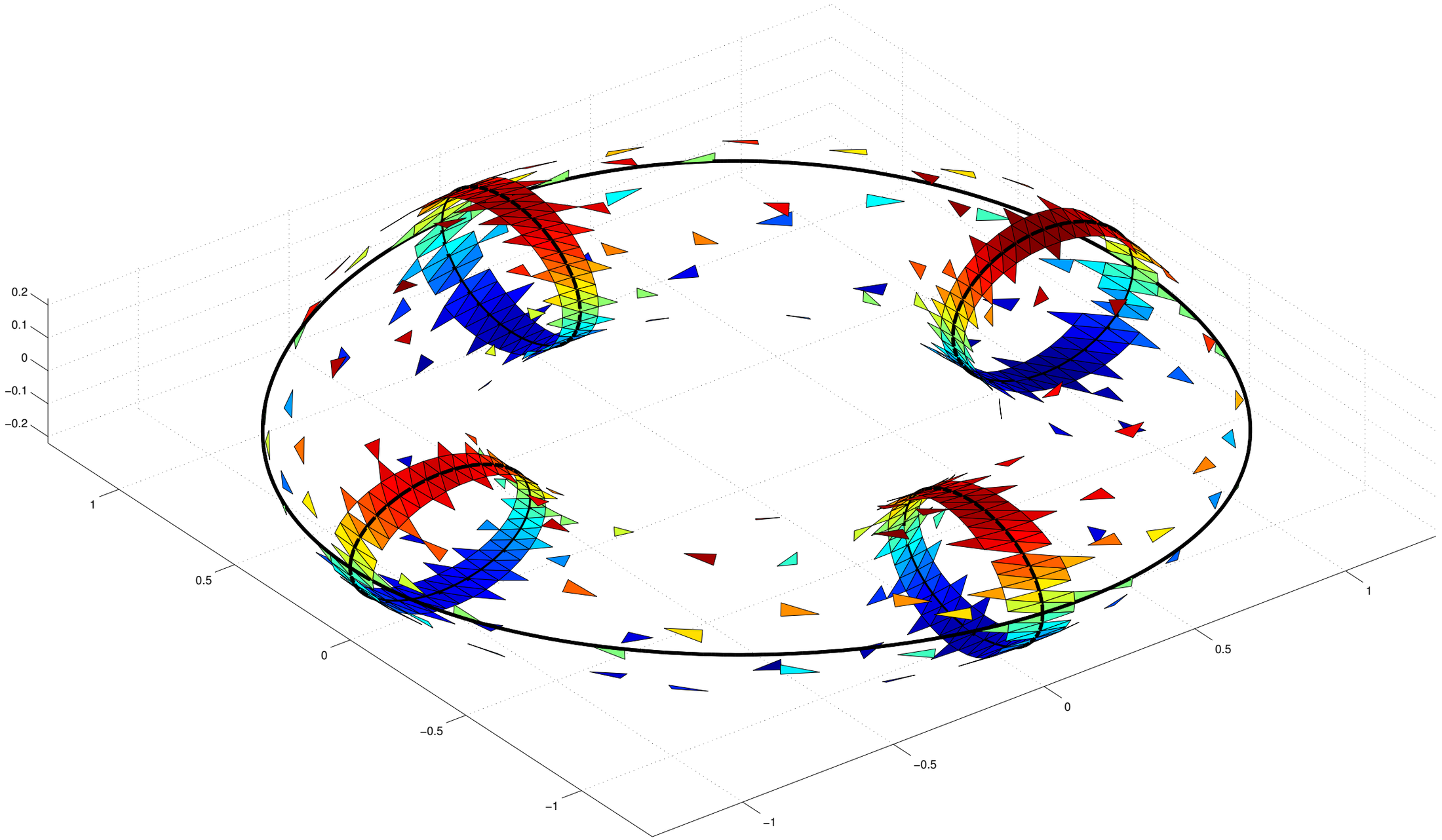

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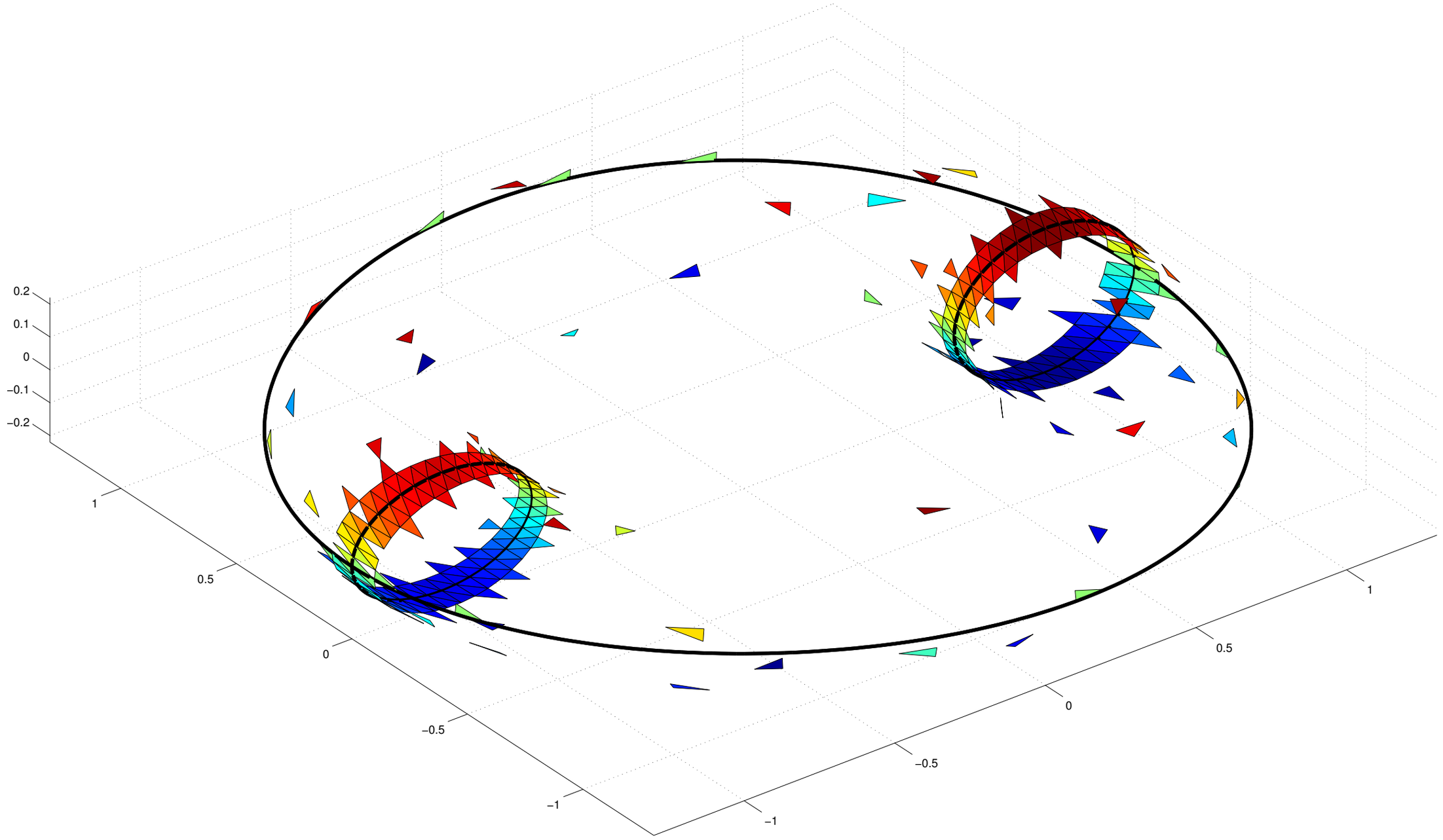

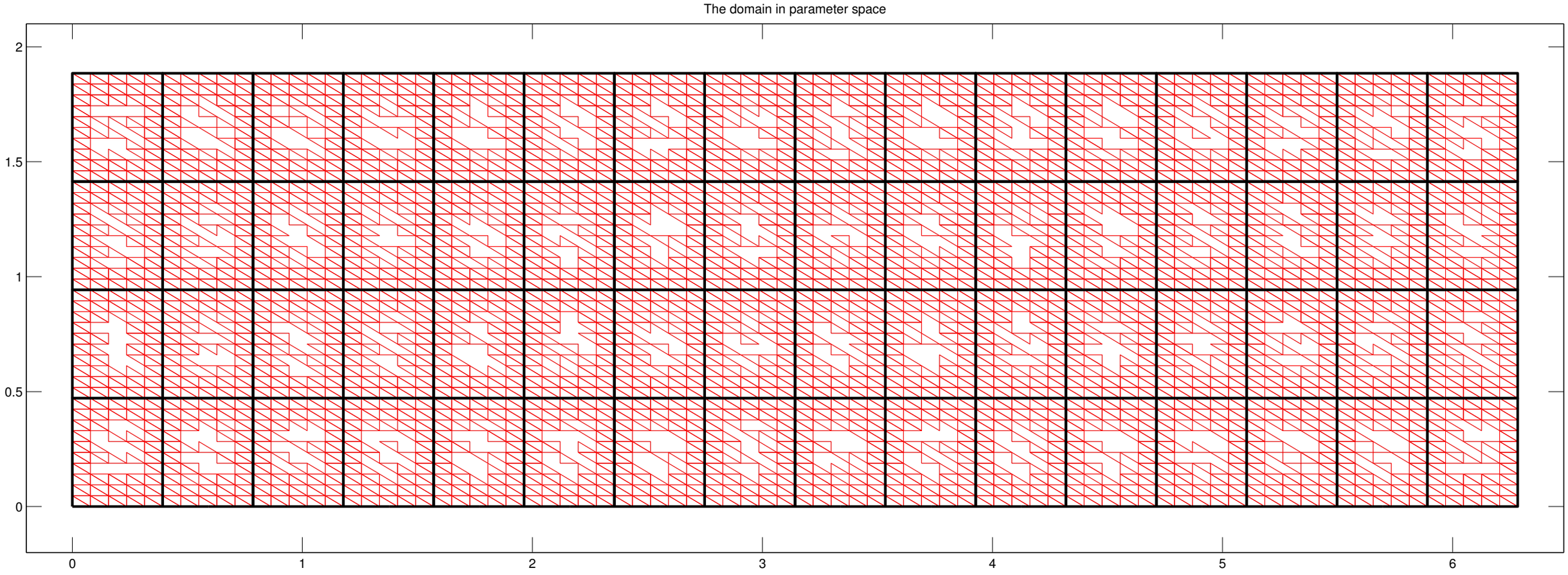
The domain in parameter space
2
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0
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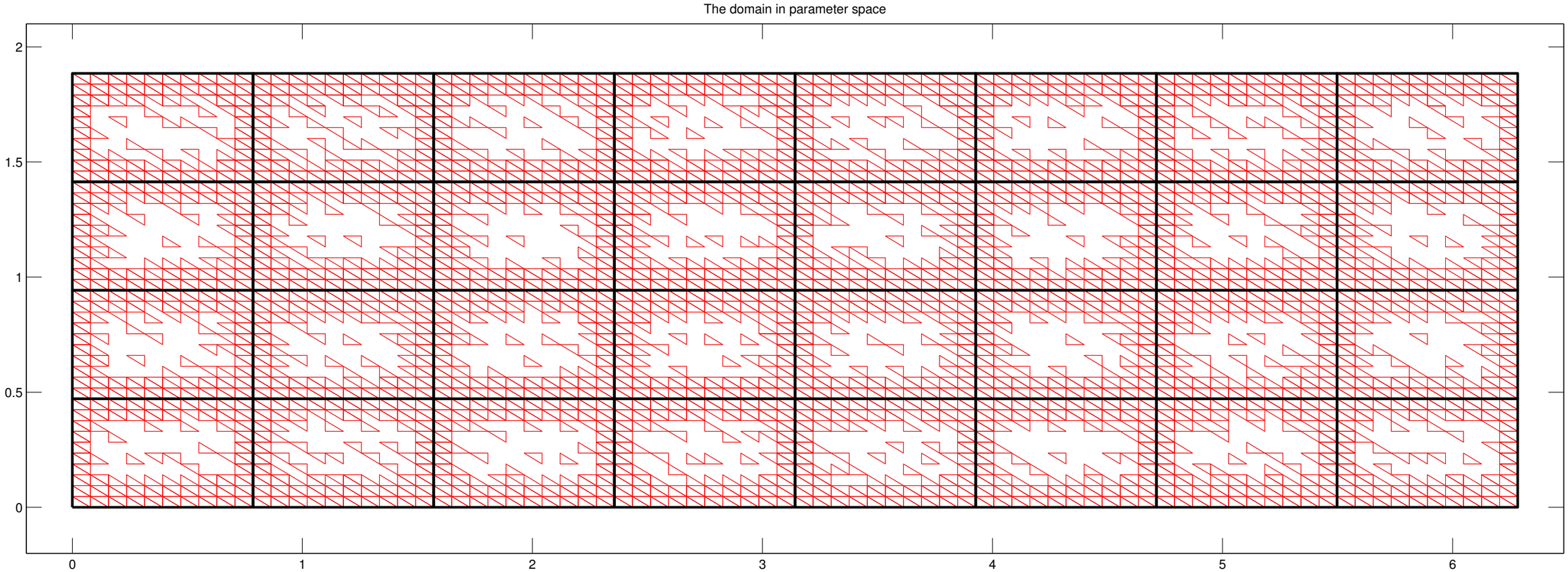
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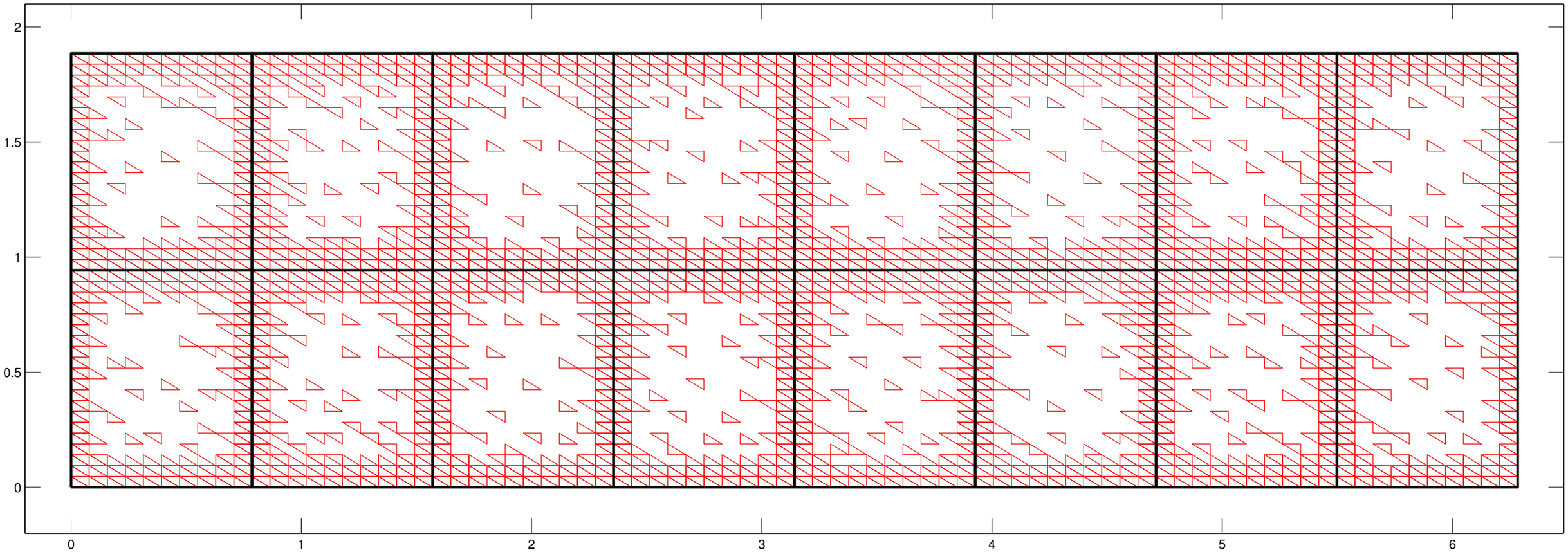

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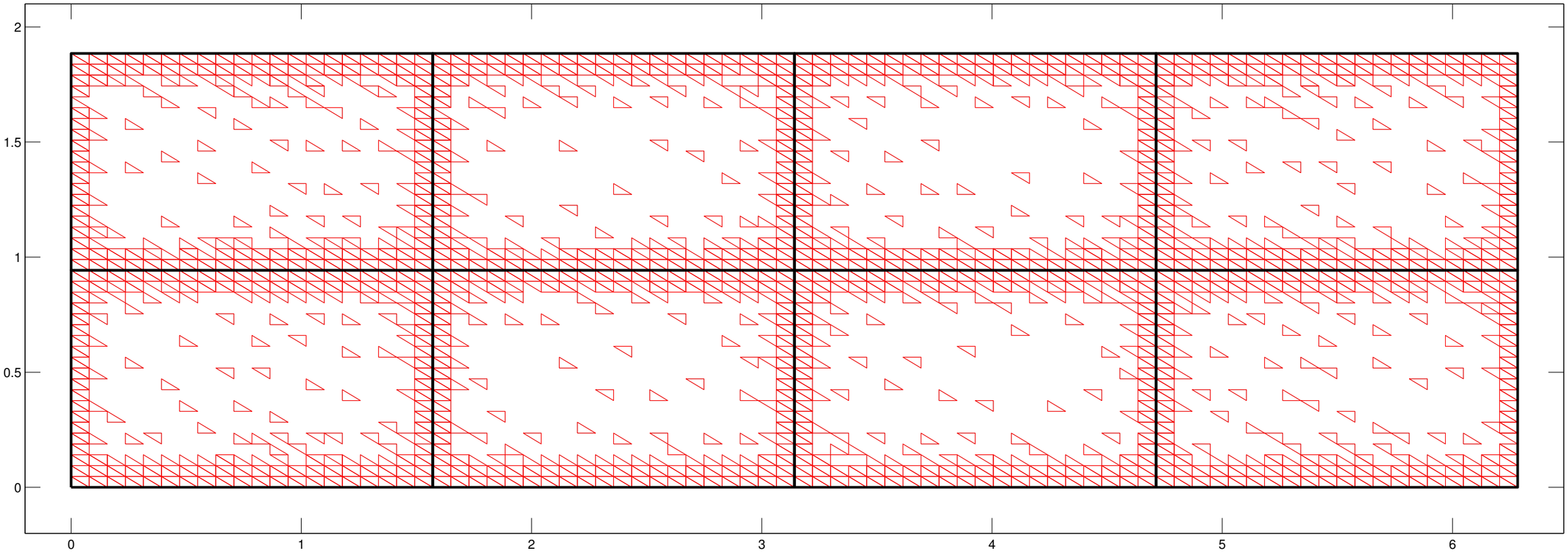

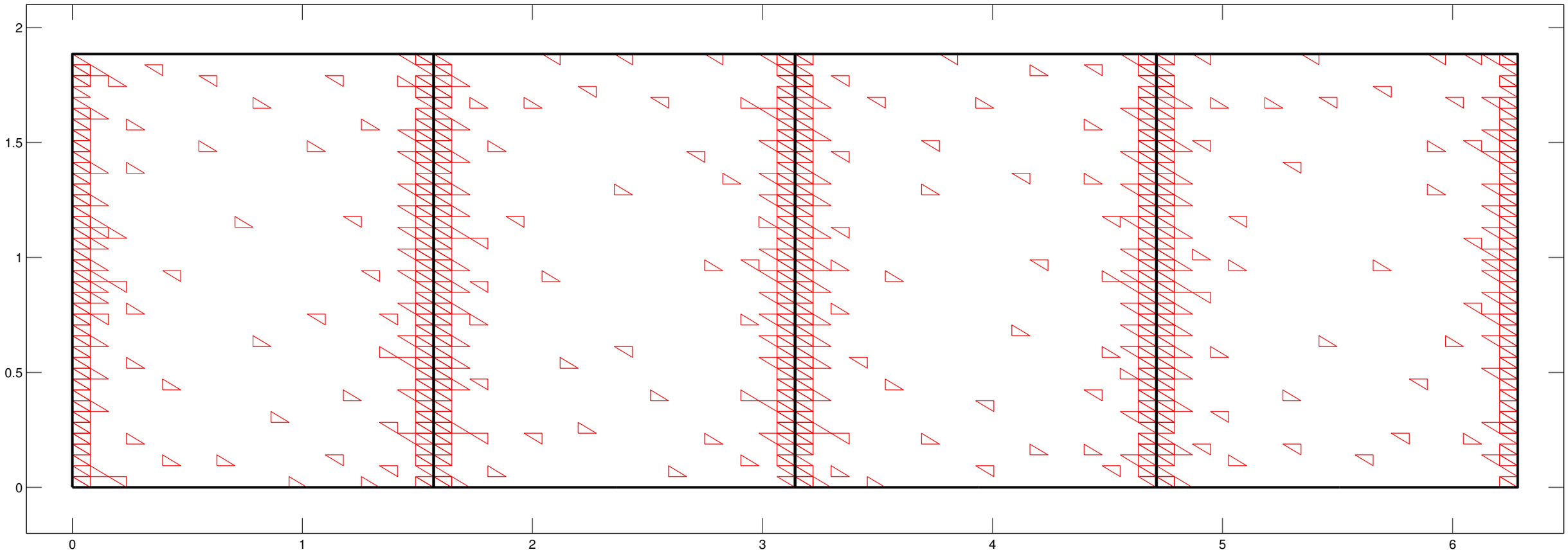
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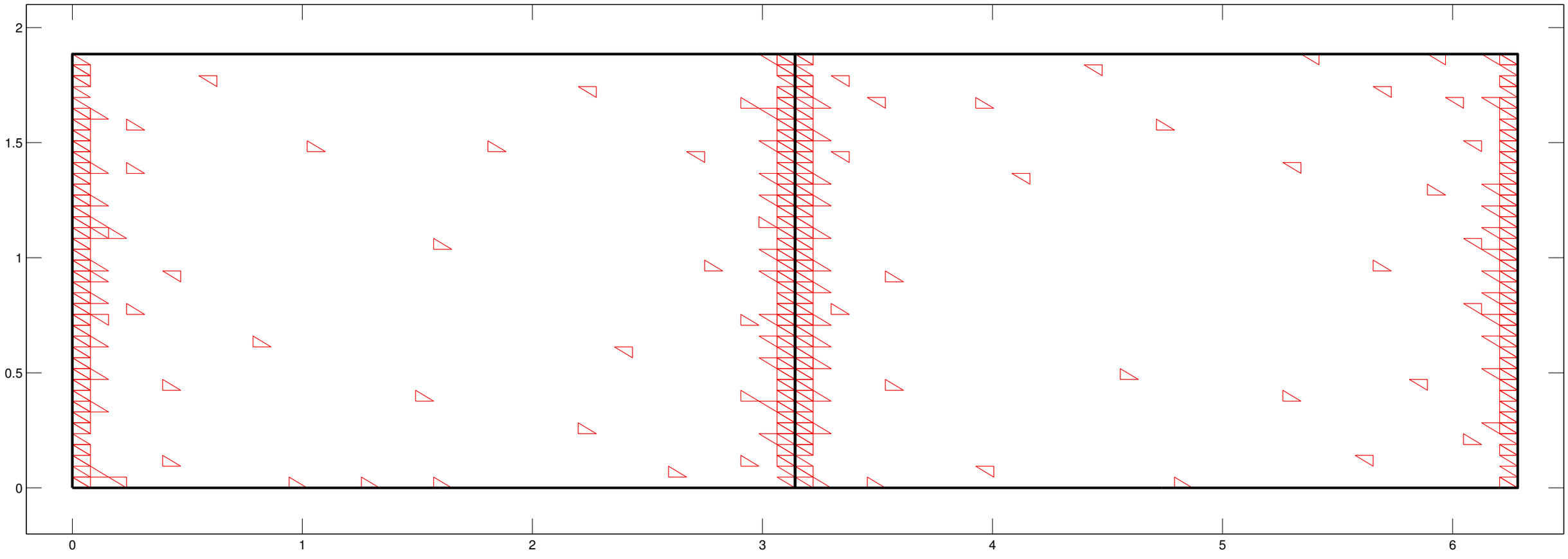
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2
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1
0.5
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2
3
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5
6

Example: Consider free space scattering from a domain with variable wave speed.

Given an "incoming wave" v, we seek to determine an "outgoing wave" u that solves

$$-\Delta u(\boldsymbol{x}) - k^2\,(1 - b(\boldsymbol{x}))\,u(\boldsymbol{x}) = -\,k^2\,b(\boldsymbol{x})\,v(\boldsymbol{x}) \qquad \boldsymbol{x} \in \mathbb{R}^2 \tag{2}$$

$$\lim_{|\boldsymbol{x}|\to\infty} \sqrt{|\boldsymbol{x}|}\big(\partial_{|\boldsymbol{x}|}u(\boldsymbol{x}) - ik\,u(\boldsymbol{x})\big) = 0 \tag{3}$$

We suppose that b is a smooth "scattering potential" whose support is contained to some rectangle Ω, $\text{support}(b) \subset \Omega$.

The scattering potential specifies the deviation of the local wave speed $v = v(\boldsymbol{x})$ from the free space wave speed v_{free}: $b(\boldsymbol{x}) = 1 - \left(\dfrac{v_{\text{free}}}{v(\boldsymbol{x})}\right)^2$.

We look for a solution of the form

$$u(\boldsymbol{x}) = [\phi_\kappa * q](\boldsymbol{x}) = \int_{\mathbb{R}^2} \phi_\kappa(\boldsymbol{x} - \boldsymbol{y})\,q(\boldsymbol{y})\,dA(\boldsymbol{y}). \tag{4}$$

where $\phi_\kappa(\boldsymbol{x}) = H_0^{(1)}(\kappa|\boldsymbol{x}|)$ is the free space fundamental solution. u satisfies (3) automatically, and (2) is satisfied if q satisfies the *Lippman-Schwinger integral equation*:

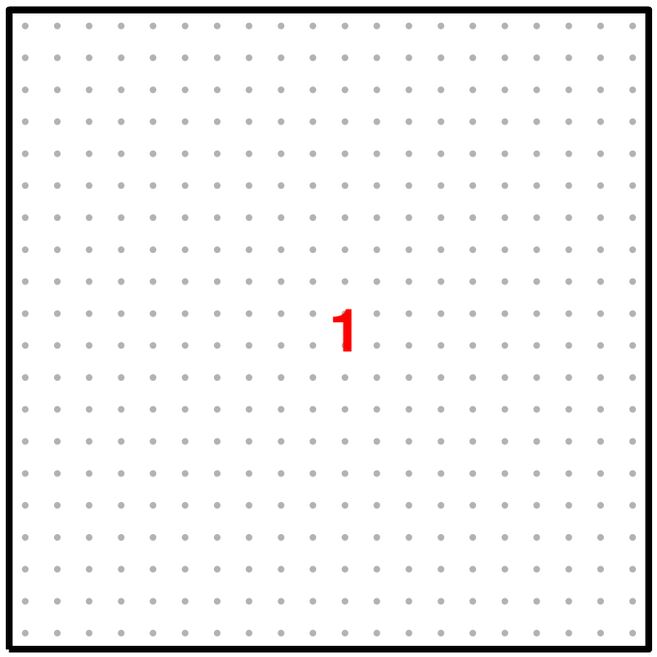
$$q(\boldsymbol{x}) + \kappa^2\,b(\boldsymbol{x}) \int_\Omega H_0^{(1)}(\kappa|\boldsymbol{x} - \boldsymbol{y}|)\,q(\boldsymbol{y})\,dA(\boldsymbol{y}) = -\kappa^2\,b(\boldsymbol{x})\,v(\boldsymbol{x}), \qquad \boldsymbol{x} \in \Omega. \tag{5}$$

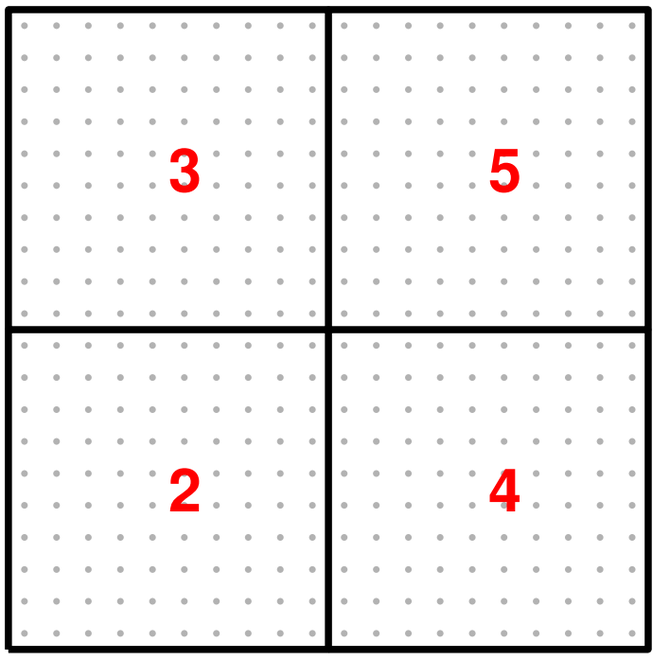
Observe that (5) is a *local equation* defined on the bounded set Ω.

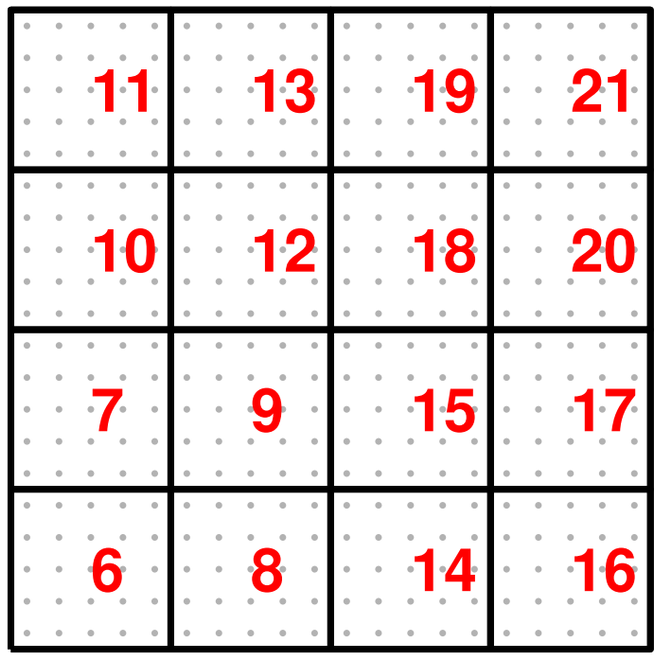
(It is also a second kind Fredholm equation, which is very nice.)

Recall: We seek to solve $q(\boldsymbol{x}) + \kappa^2 b(\boldsymbol{x}) \int_\Omega H_0^{(1)}(\kappa|\boldsymbol{x}-\boldsymbol{y}|)\, q(\boldsymbol{y})\, dA(\boldsymbol{y}) = -\kappa^2 b(\boldsymbol{x})\, v(\boldsymbol{x}),\ \boldsymbol{x} \in \Omega.$

We discretize Ω using a uniform grid, and then split the points into a quad-tree:







Now discretize the integral equation using Nyström with the trapezoidal rule.

A small number of elements "close to the diagonal" (in physical space) are modified since the kernel in the integral is singular, but most matrix elements are given by

$$\mathbf{A}(i,j) = \kappa^2 b(\boldsymbol{x}_i)\, H_0^{(1)}(\kappa|\boldsymbol{x}_i - \boldsymbol{x}_j|)\, \sqrt{w_i\, w_j}.$$

We will build a direct solver for $\mathbf{Aq} = \mathbf{f}$, where $\mathbf{f}(i) = -\kappa^2 b(\boldsymbol{x}_i)\, v(\boldsymbol{x}_i)\, \sqrt{w_i}$.

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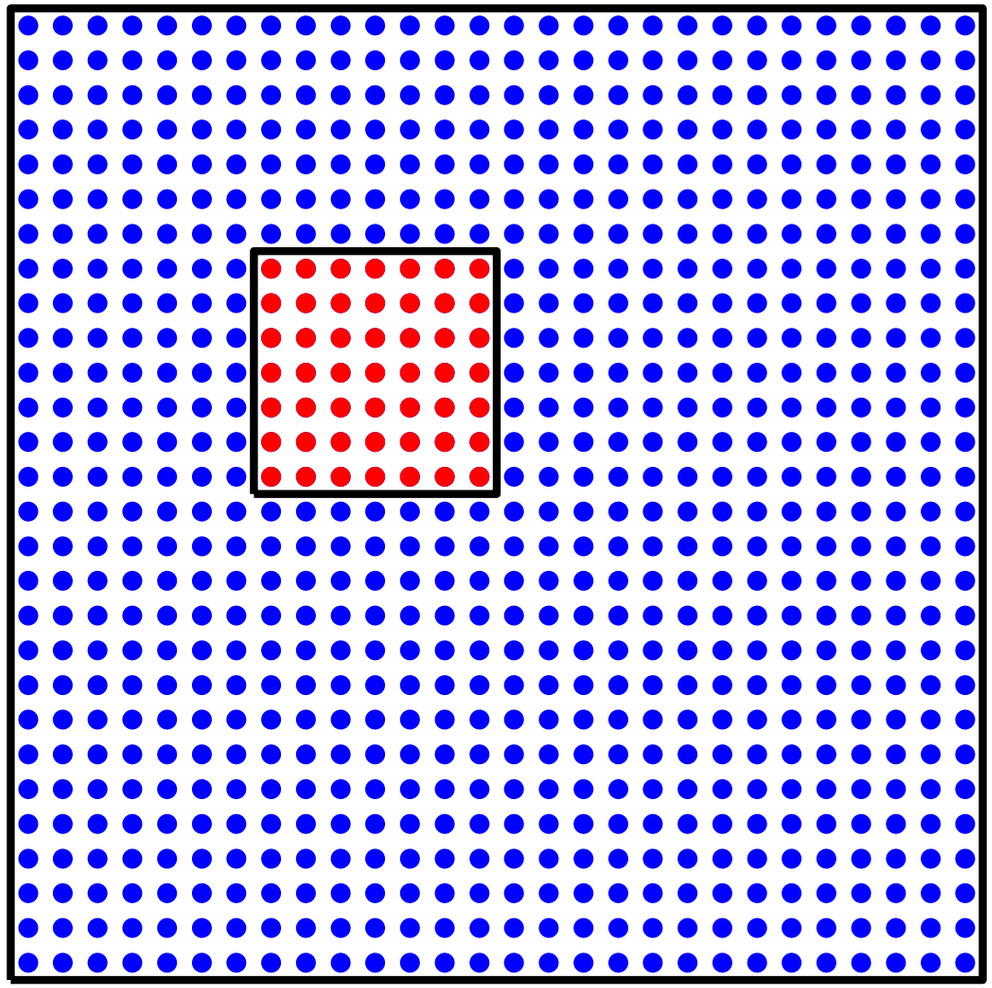

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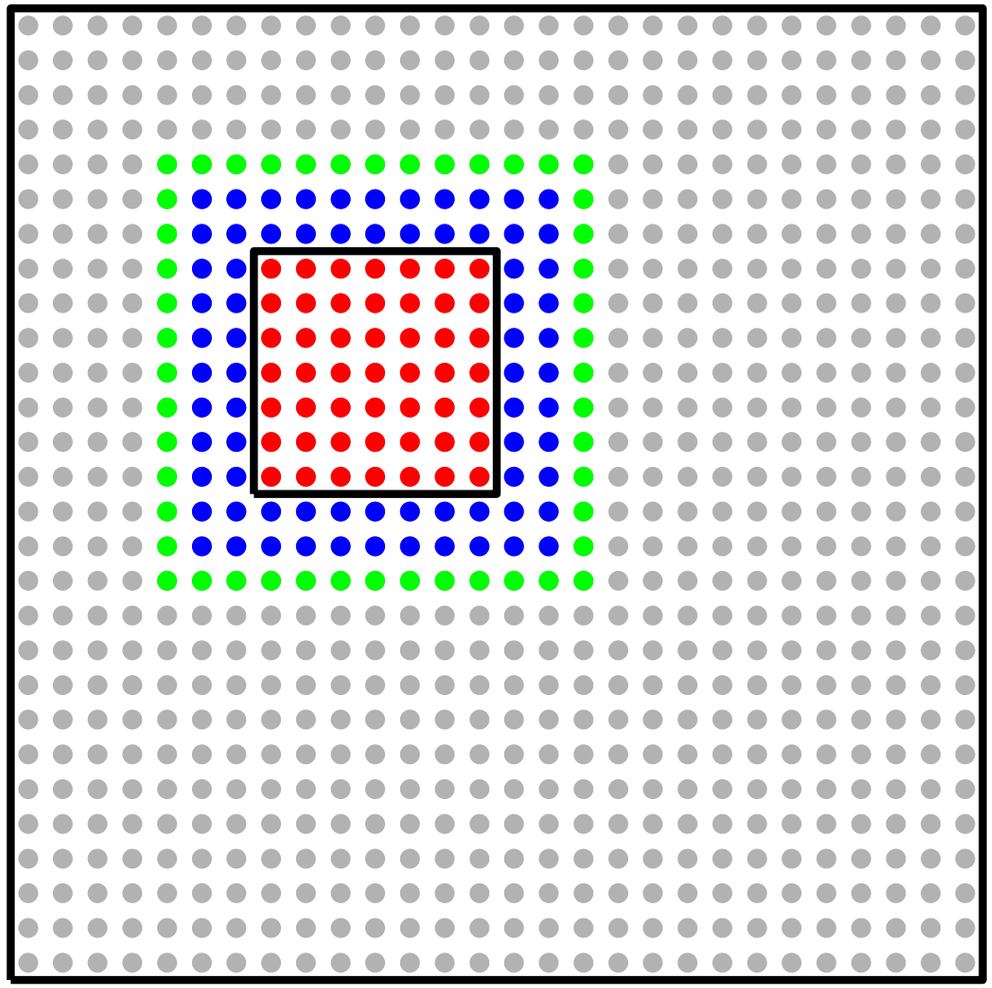

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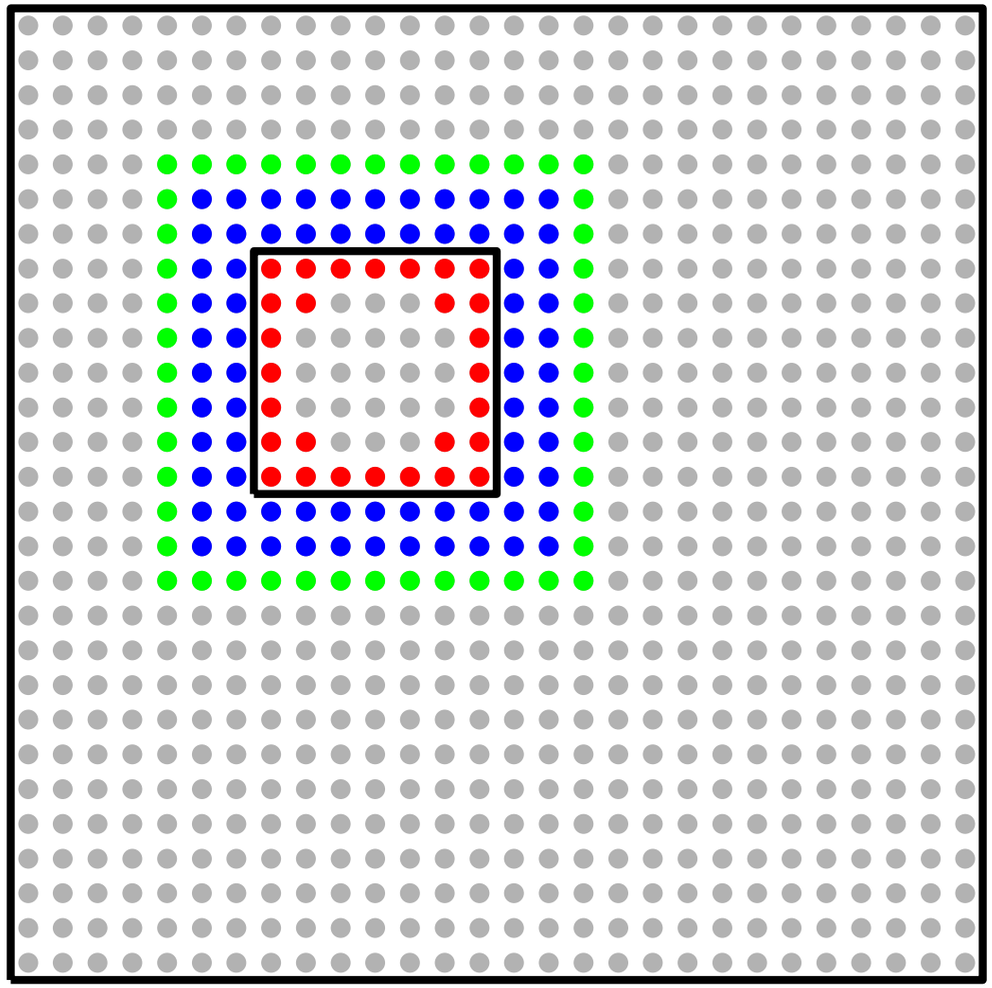

- Points in $\tilde{I}_\tau$.
- Points in $I_\tau^{(\mathrm{near})}$.
- Points in Γ_{proxy}.

At first, it seems like we need to perform an ID of the large matrix $\mathbf{A}(I_\tau, I_\tau^{\mathrm{c}})$.
But, using the *Green localization trick,* we only need to ID the matrix $[\mathbf{A}(I_\tau, I_\tau^{(\mathrm{near})})\ \mathbf{G}]$,
where **G** is the matrix of interaction with the proxy surface (green).

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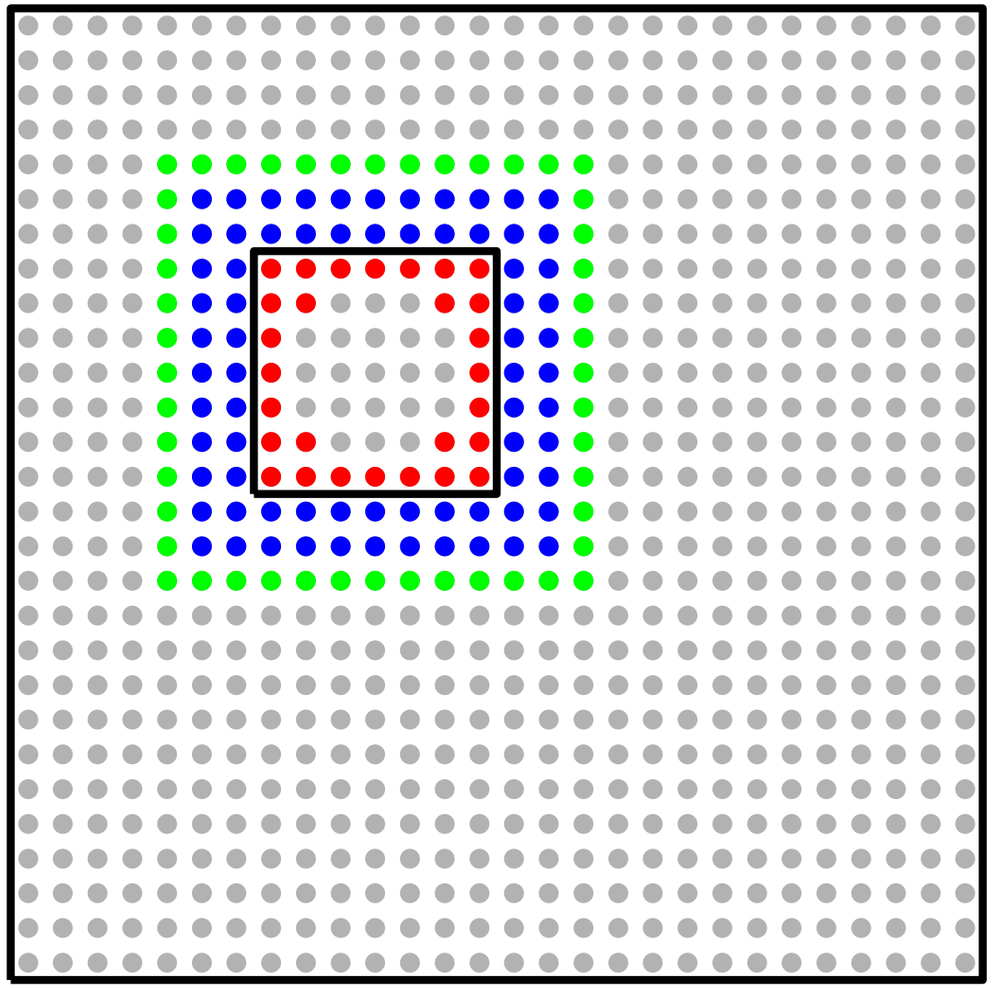

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Peculiarity of Lippman-Schwinger I: There is no need for a proxy surface in this case ...
Peculiarity of Lippman-Schwinger II: $\mathbf{A} = \mathbf{I} + \mathbf{BG}$ where $\mathbf{B}$ is diagonal, and $\mathbf{G}$ is translation invariant. This means we only need to compress one box per level.