Fast direct solvers

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Acknowledgements: Some of the work presented is joint work with Vladimir Rokhlin and Mark Tygert at Yale University.

In this talk, we will discuss numerical methods for solving the equation

$$\text{(BVP)} \qquad \begin{cases} A\,u(x) = g(x), & x \in \Omega, \\ B\,u(x) = f(x), & x \in \Gamma, \end{cases}$$

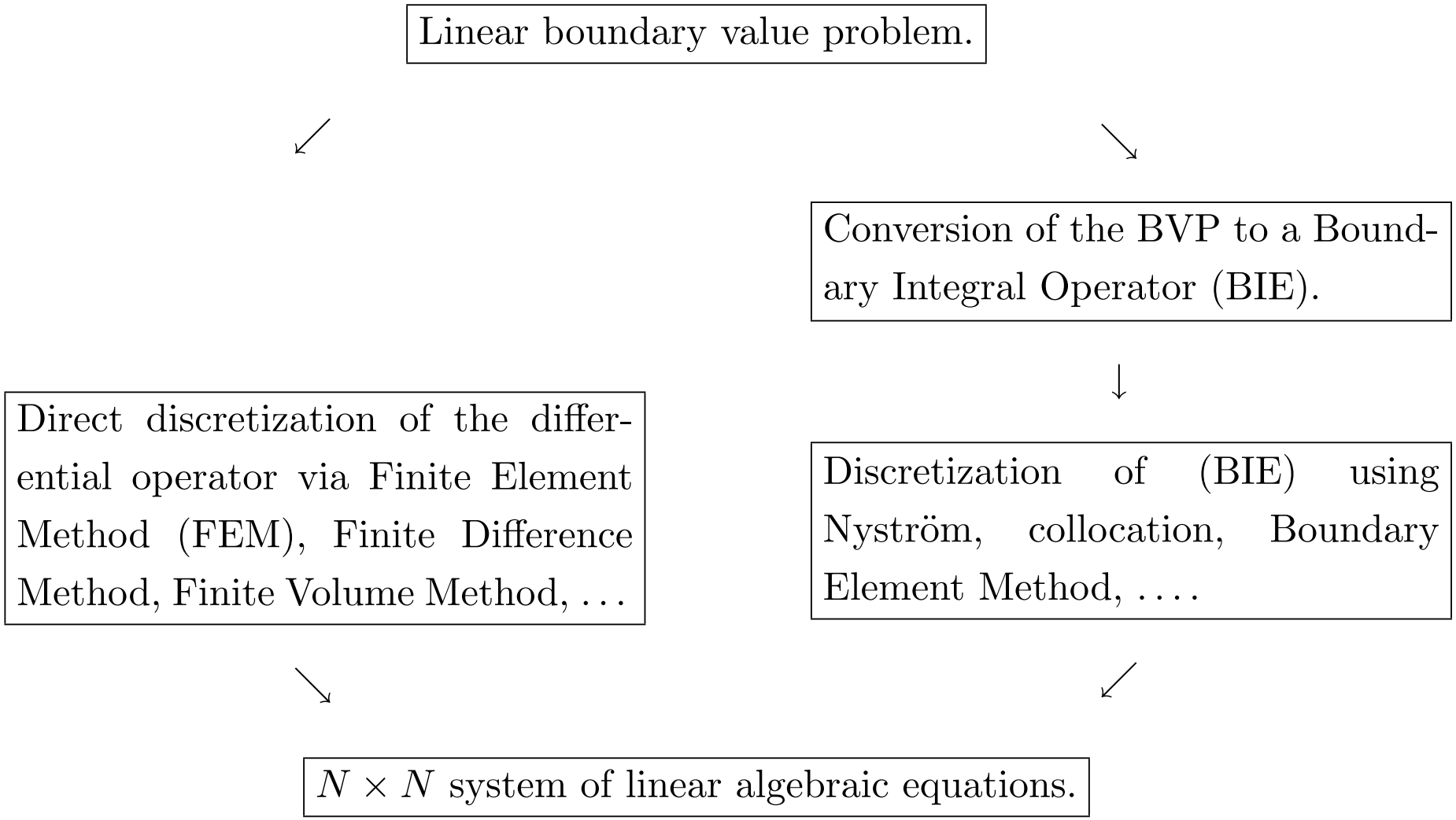
where A is a linear constant-coefficient partial differential operator, and B is some local linear boundary operator.

Examples include:

- Laplace's equation.
- Helmholtz' equation.
- Stokes' equation.
- The Yukawa equation.
- The equations of linear elasticity.

Specifically, we will be concerned with the fast solution of the system of linear equations obtained upon discretization of (BVP).

There are two standard techniques for obtaining the discretized system:



1 – Methods based on discretizing PDEs:

Discretize the differential operator directly; instead of

$$\text{(BVP)} \qquad \begin{cases} A\,u(x) = g(x), & x \in \Omega, \\ u(x) = f(x), & x \in \Gamma, \end{cases}$$

solve

$$\text{(BVP-DISC)} \qquad A_N\,u_N = h_N,$$

where u_N is a function in an N-dimensional function space, A_N is an $N \times N$ matrix discretizing the operator A (obtained via Finite Elements / Finite Differences / ...), and h_N is a vector of data derived from f and g.

Equation (BVP-DISC) is typically very large, and requires fast solvers.
Most such solvers are based on iterative methods.

Fundamental problem: A is an unbounded operator $\Rightarrow$
The matrix A_N is ill-conditioned $\Rightarrow$ The iterative solver converges slowly.

Pre-conditioners can help solving ill-conditioned linear systems.

A pre-conditioner is an operator P_N such that:

- It is cheap to apply P_N to a vector.
- The product $P_N\, A_N$ is well-conditioned.

Loosely speaking, $P_N \approx A_N^{-1}$.

The idea is to use an iterative solver to solve

$$P_N\, A_N\, u_N = P_N\, h_N.$$

The popular multigrid algorithm is a form of a pre-conditioner.

However, many problems related to ill-conditioning remain.

Would it be possible to directly compute A_N^{-1}?

2 – Methods based on discretizing integral equations:

Reformulate the BVP as an Integral Equation.

The idea is to convert a partial differential equation

$$\text{(BVP)} \qquad \begin{cases} A\,u(x) = g(x), & x \in \Omega, \\ B\,u(x) = f(x), & x \in \Gamma, \end{cases}$$

to an "equivalent" integral equation

$$\text{(BIE)} \qquad v(x) + \int_\Gamma k(x,y)\,v(y)\,ds(y) = h(x), \qquad x \in \Gamma.$$

- The kernel k is derived from the operator A.
- The data function h is derived from the data of (BVP).
- The conversion from (BVP) to (BIE) sometimes involves the evaluation of certain integrals over Γ and/or Ω.
- Sometimes the integral equation must be formulated on Ω.
- ...

Example:

Let us consider the equation

$$\text{(BVP)} \qquad \begin{cases} -\Delta u(x) = 0, & x \in \Omega, \\ u(x) = f(x), & x \in \Gamma, \end{cases}$$

We make the following Ansatz:

$$u(x) = \int_\Gamma \big(n(y) \cdot \nabla_y \log|x-y|\big) v(y)\, ds(y), \qquad x \in \Omega,$$

where $n(y)$ is the outward pointing unit normal of Γ at y. Then the boundary charge distribution u satisfies the Boundary Integral Equation

$$\text{(BIE)} \qquad v(x) + 2\int_\Gamma \big(n(y) \cdot \nabla_y \log|x-y|\big) v(y)\, ds(y) = 2f(x), \qquad x \in \Gamma.$$

- (BIE) and (BVP) are in a strong sense equivalent.
- (BIE) is appealing mathematically (2^{nd} kind Fredholm equation).

When integral equation formulations are available, there are compelling arguments in their favor, these include:

Conditioning:

When there exists an IE formulation that is a Fredholm equation of the second kind, the mathematical equation itself is well-conditioned.

Dimensionality:

Frequently, an IE can be defined on the boundary of the domain.

Integral operators are benign objects:

It is (relatively) easy to implement high order discretizations of integral operators. Relative accuracy of 10^{-10} or better is often achieved.

There is a fundamental difficulty with using integral operators in numerics:

Discretization of integral operators typically results in dense matrices.

In the 1950's when computers made numerical PDE solvers possible, researchers faced a grim choice:

PDE-based:	Ill-conditioned, N is too large, low accuracy.
Integral Equations:	Dense system.

The integral equations lost and were largely forgotten

— they were simply too expensive.

(Except in some scattering problems where there was no choice.)

The situation changed dramatically in the 1980's. It was discovered that while K_N (the discretized integral operator) is dense, it is possible to evaluate the matrix-vector product

$$v \mapsto K_N\, v$$

in $O(N)$ operations – to high accuracy and with a small constant.

A very succesful such algorithm is the Fast Multipole Method by Rokhlin and Greengard (circa 1985).

Combining such methods with iterative solvers (GMRES / conjugate gradient / ...) leads to very fast solvers for the integral equations, especially when second kind Fredholm formulations are used.

A prescription for rapidly solving BVPs:

(BVP)
$$\begin{cases} -\Delta v(x) = 0, & x \in \Omega, \\ v(x) = f(x), & x \in \Gamma. \end{cases}$$

Convert (BVP) to a second kind Fredholm equation:

(BIE)
$$u(x) + \int_\Gamma \big(n(y) \cdot \nabla_y \log|x-y|\big) u(y)\, ds(y) = f(x), \qquad x \in \Gamma.$$

Discretize (BIE) into the discrete equation

(DISC)
$$(I + K_N) u_N = f_N$$

where K_N is a (typically dense) $N \times N$ matrix.

Fast Multipole Method — Can multiply K_N by a vector in $O(N)$ time.

Iterative solver — Solves (DISC) using $\sqrt{\kappa}$ matrix-vector multiplies, where κ is the condition number of $(I + K_N)$.

Total complexity — $O(\sqrt{\kappa}\, N)$. (Recall that κ is small. Like 14.)

However, integral equation based methods are quite often not a choice:

Fundamental limitations: They require the existence of a fundamental solution to the (dominant part of the) partial difference operator. In practise, this means that the (dominant part of the) operator must be linear and constant-coefficient.

Practical limitations: Underdeveloped infra-structure; there does not exist a general framework for discretizing surfaces. Lack of engineering strength codes. Etc.

To summarize:

- There exist $O(N)$ (or $O(N \log^p N)$) algorithms for a wide range of BVPs.
- For some BVPs, the N in $O(N)$ can be the number of degrees of freedom required to discretize the boundary.
- Almost all existing $O(N)$ methods rely on *iterative* solvers.
- Regardless of how a BVP is discretized, there are complications in solving the resulting linear system.
  - Finite Element Methods: system is sparse but ill-conditioned.
  - Boundary Integral Methods: system is dense (and sometimes ill-conditioned, too).

In some environments, the linear solve presents a serious challenge:

1. Problems whose geometries require a very large number of unknowns:
   - Modeling of heterogeneous materials.
   - Radar scattering off of the ocean surface.

2. Applications that require a very large number of solves:
   - Molecular Dynamics.
   - Optimal design.

3. Problems that are inherently ill-conditioned:
   - Scattering problems at intermediate or high frequencies.
   - Ill-conditioning due to geometry (elongated domains, percolation, etc).

The inadequacy of existing methods in these environments stems from their reliance on iterative solvers. We need **direct** solvers.

What is a direct solver?

Recall that many BVPs can be cast in the following form:

$$\text{(BIE)} \qquad u(x) + \int_\Gamma g(x,y)u(y)\,ds(y) = f(x), \qquad x \in \Gamma.$$

Upon discretization, equation (BIE) turns into a discrete equation

$$\text{(DISC)} \qquad (I + K_N)u = f$$

where K_N is a (typically dense) $N \times N$ matrix.

A ***direct method*** computes a compressed representation for $(I + K_N)^{-1}$.

- Cost for pre-computing the inverse.
- Cost for applying the inverse to a vector.

In many environments, both of these costs can be made $O(N)$.

Direct methods are good for (1) ill-conditioned problems, (2) problems with multiple right-hand sides, (3) spectral decompositions, (4) updating, ...

Practical considerations:

Direct methods tend to be more **robust** than iterative ones.

This makes them more suitable for "black-box" implementations.

Commercial software developers appear to avoid implementing iterative solvers whenever possible. (Sometimes for good reasons.)

The effort to develop direct solvers should be viewed as a step towards getting a LAPACK-type environment for solving the basic linear boundary value problems of mathematical physics.

Sampling of related work:

1991 Sparse matrix algebra / wavelets, *Beylkin, Coifman, Rokhlin*,

1996 scattering problems, *E. Michielssen, A. Boag and W.C. Chew*,

1998 factorization of non-standard forms, *G. Beylkin, J. Dunn, D. Gines*,

1998 $\mathcal{H}$-matrix methods, *W. Hackbusch, et al*,

2002 $O(N^{3/2})$ inversion of Lippmann-Schwinger equations, *Y. Chen*,

2002 inversion of "Hierarchically semi-separable" matrices, *M. Gu, S. Chandrasekharan, et al*,

2004 $O(N)$ inversion of boundary integral equations in 2D, *Martinsson, Rokhlin*,

2007 $O(N \log N)$ inversion of 2D finite element matrices, *Martinsson*.

Current state of the research

The fast direct solvers currently being developed exploit the fact that off-diagonal blocks of the matrix to be inverted have low rank.

This restricts the range of application to non-oscillatory, or moderately oscillatory problems. In other words, such methods currently **can** handle:

- Laplace's equation, equations of elasticity, Yukawa's equation,...
- Helmholtz' and Maxwell's equations for low and intermediate frequencies. (In special cases, high frequency problem can also be solved.)

Holy grail: Fast inversion scheme for high-frequency problems.

How does the inversion scheme for 2D boundary integral equations work?

Consider the linear system

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ A_{21} & A_{22} & A_{23} & A_{24} \\ A_{31} & A_{32} & A_{33} & A_{34} \\ A_{41} & A_{42} & A_{43} & A_{44} \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \\ q_3 \\ q_4 \end{bmatrix} = \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{bmatrix}.$$

We suppose that for $i \neq j$, the blocks A_{ij} allow the factorization

$$\underbrace{A_{ij}}_{n_i \times n_j} = \underbrace{U_i}_{n_i \times k_i} \underbrace{\tilde{A}_{ij}}_{k_i \times k_j} \underbrace{U_j^{\mathrm{t}}}_{k_j \times n_j},$$

where the ranks k_i are significantly smaller than the block sizes n_i.

We then let

$$\underbrace{\tilde{q}_i}_{k_i \times 1} = U_i^{\mathrm{t}} \underbrace{q_i}_{n_i \times 1},$$

be the variables of the "reduced" system.

Recall: $A_{ij} = U_i \, \tilde{A}_{ij} \, U_j^{\mathrm{t}}$ and $\tilde{q}_i = U_i^{\mathrm{t}} \, q_i$.

The system $\sum_j A_{ij} \, q_j = v_i$ then takes the form

$$\left[\begin{array}{cccc|cccc} A_{11} & 0 & 0 & 0 & 0 & U_1\tilde{A}_{12} & U_1\tilde{A}_{13} & U_1\tilde{A}_{14} \\ 0 & A_{22} & 0 & 0 & U_2\tilde{A}_{21} & 0 & U_2\tilde{A}_{23} & U_2\tilde{A}_{24} \\ 0 & 0 & A_{33} & 0 & U_3\tilde{A}_{31} & U_3\tilde{A}_{32} & 0 & U_3\tilde{A}_{34} \\ 0 & 0 & 0 & A_{44} & U_4\tilde{A}_{41} & U_4\tilde{A}_{42} & U_4\tilde{A}_{43} & 0 \\ \hline -U_1^{\mathrm{t}} & 0 & 0 & 0 & I & 0 & 0 & 0 \\ 0 & -U_2^{\mathrm{t}} & 0 & 0 & 0 & I & 0 & 0 \\ 0 & 0 & -U_3^{\mathrm{t}} & 0 & 0 & 0 & I & 0 \\ 0 & 0 & 0 & -U_4^{\mathrm{t}} & 0 & 0 & 0 & I \end{array}\right] \left[\begin{array}{c} q_1 \\ q_2 \\ q_3 \\ q_4 \\ \tilde{q}_1 \\ \tilde{q}_2 \\ \tilde{q}_3 \\ \tilde{q}_4 \end{array}\right] = \left[\begin{array}{c} v_1 \\ v_2 \\ v_3 \\ v_4 \\ 0 \\ 0 \\ 0 \\ 0 \end{array}\right].$$

Now form the Schur complement to eliminate the q_j's.

After eliminating the "fine-scale" variables q_i, we obtain

$$\begin{bmatrix} I & U_1^{\mathrm{t}}\tilde{A}_{11}^{-1}U_1\tilde{A}_{12} & U_1^{\mathrm{t}}\tilde{A}_{11}^{-1}U_1\tilde{A}_{13} & U_1^{\mathrm{t}}\tilde{A}_{11}^{-1}U_1\tilde{A}_{14} \\ U_2^{\mathrm{t}}\tilde{A}_{22}^{-1}U_2\tilde{A}_{21} & I & U_2^{\mathrm{t}}\tilde{A}_{22}^{-1}U_2\tilde{A}_{23} & U_2^{\mathrm{t}}\tilde{A}_{22}^{-1}U_2\tilde{A}_{24} \\ U_3^{\mathrm{t}}\tilde{A}_{33}^{-1}U_3\tilde{A}_{31} & U_3^{\mathrm{t}}\tilde{A}_{33}^{-1}U_3\tilde{A}_{32} & I & U_3^{\mathrm{t}}\tilde{A}_{33}^{-1}U_3\tilde{A}_{34} \\ U_4^{\mathrm{t}}\tilde{A}_{44}^{-1}U_4\tilde{A}_{41} & U_4^{\mathrm{t}}\tilde{A}_{44}^{-1}U_4\tilde{A}_{42} & U_4^{\mathrm{t}}\tilde{A}_{44}^{-1}U_4\tilde{A}_{43} & I \end{bmatrix} \begin{bmatrix} \tilde{q}_1 \\ \tilde{q}_2 \\ \tilde{q}_3 \\ \tilde{q}_4 \end{bmatrix} = \begin{bmatrix} U_1^{\mathrm{t}}A_{11}^{-1}\,v_1 \\ U_2^{\mathrm{t}}A_{22}^{-1}\,v_2 \\ U_3^{\mathrm{t}}A_{33}^{-1}\,v_3 \\ U_4^{\mathrm{t}}A_{44}^{-1}\,v_4. \end{bmatrix}$$

We set

$$\tilde{A}_{ii} = \left(U_i^{\mathrm{t}}\,A_{ii}^{-1}\,U_i\right)^{-1},$$

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

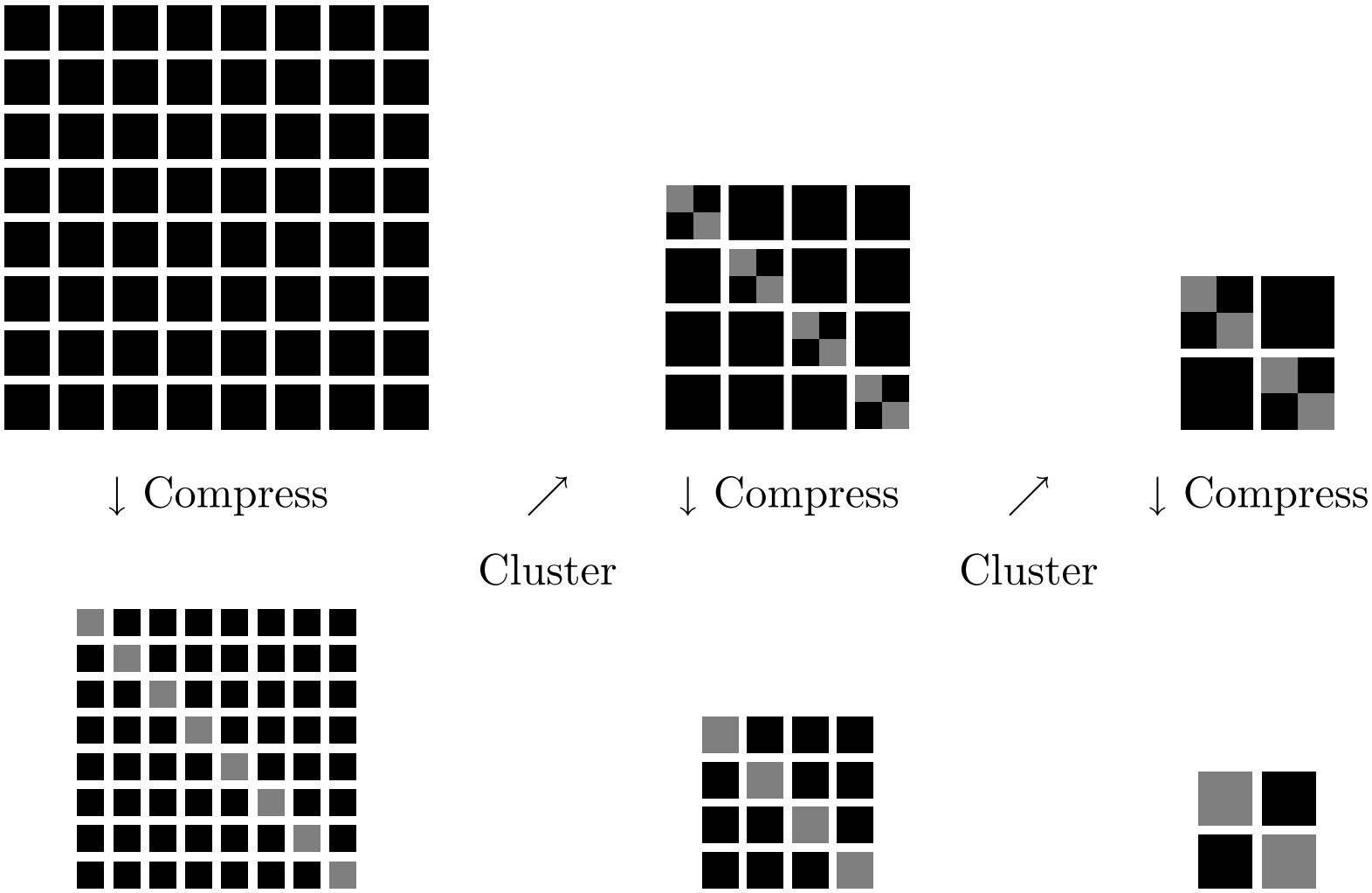
$$\begin{bmatrix} \tilde{A}_{11} & \tilde{A}_{12} & \tilde{A}_{13} & \tilde{A}_{14} \\ \tilde{A}_{21} & \tilde{A}_{22} & \tilde{A}_{23} & \tilde{A}_{24} \\ \tilde{A}_{31} & \tilde{A}_{32} & \tilde{A}_{33} & \tilde{A}_{34} \\ \tilde{A}_{41} & \tilde{A}_{42} & \tilde{A}_{43} & \tilde{A}_{44} \end{bmatrix} \begin{bmatrix} \tilde{q}_1 \\ \tilde{q}_2 \\ \tilde{q}_3 \\ \tilde{q}_4 \end{bmatrix} = \begin{bmatrix} \tilde{v}_1 \\ \tilde{v}_2 \\ \tilde{v}_3 \\ \tilde{v}_4 \end{bmatrix}.$$

where

$$\tilde{v}_i = \tilde{A}_{ii}\,U_i^{\mathrm{t}}\,A_{ii}^{-1}\,v_i.$$

(This derivation was pointed out by Leslie Greengard.)

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



The one-level coarse-graining involves the following steps:

- Compute U_i and $\tilde{A}_{ij}$ so that $A_{ij} = U_i \, \tilde{A}_{ij} \, U_j^{\mathrm{t}}$.

- Compute the new diagonal matrices

$$\tilde{A}_{ii} = \left(U_i^{\mathrm{t}} \, A_{ii}^{-1} \, U_i \right)^{-1},$$

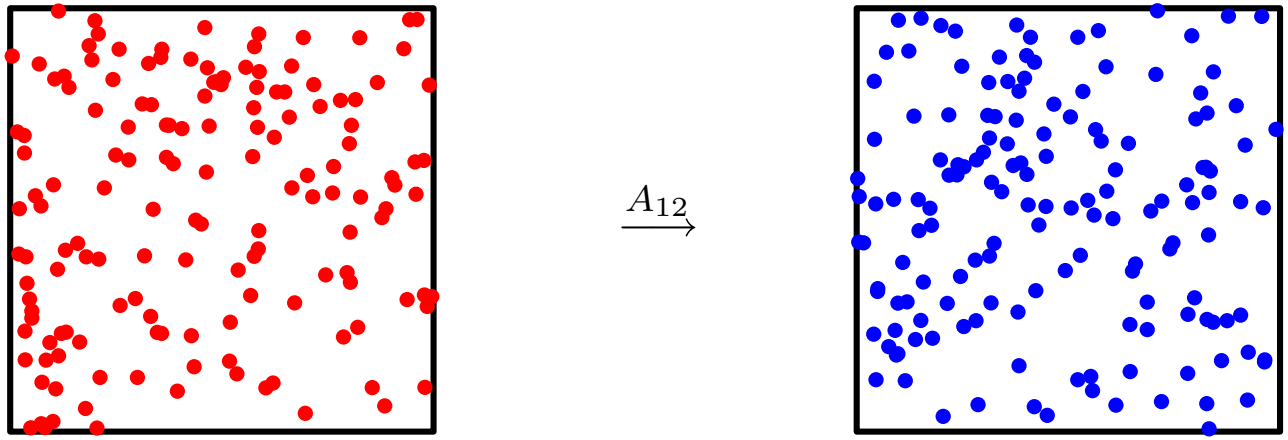
- Compute the new loads

$$\tilde{v}_i = \tilde{A}_{ii} \, U_i^{\mathrm{t}} \, A_{ii}^{-1} \, v_i.$$

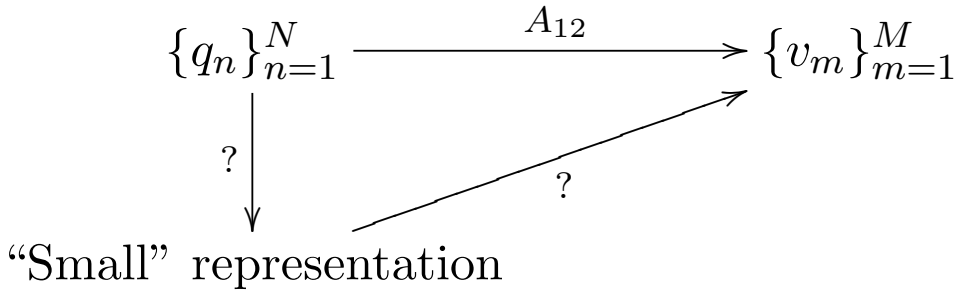
For the algorithm to be $O(N)$, it has to be able to carry out these steps *locally*.

To achieve this, we use interpolative representations.

$\tilde{A}_{ij}$ will be a submatrix of A_{ij}, so it will not need to be computed.

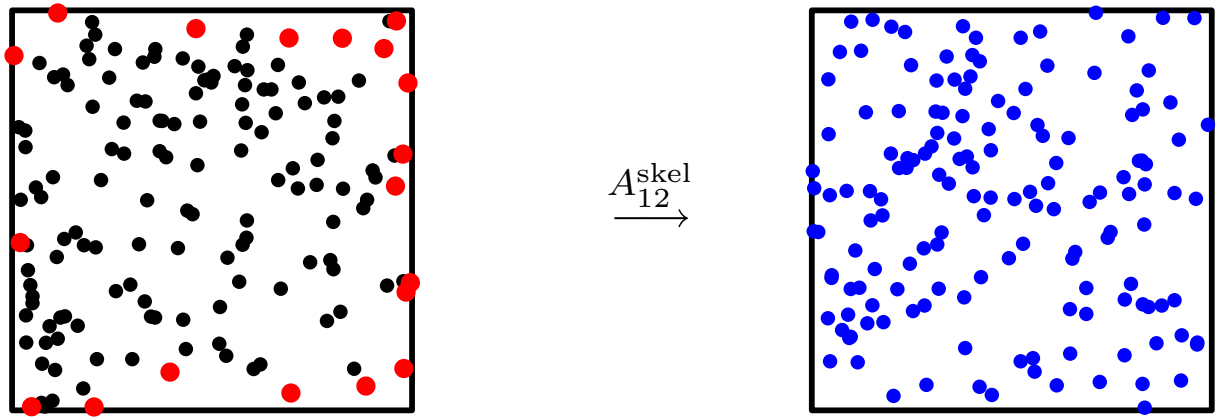


Sources $\{q_n\}_{n=1}^N$ Potentials $\{v_m\}_{m=1}^M$



The key observation is that $k = \text{rank}(A_{12}) < \min(M, N)$.

Skeletonization

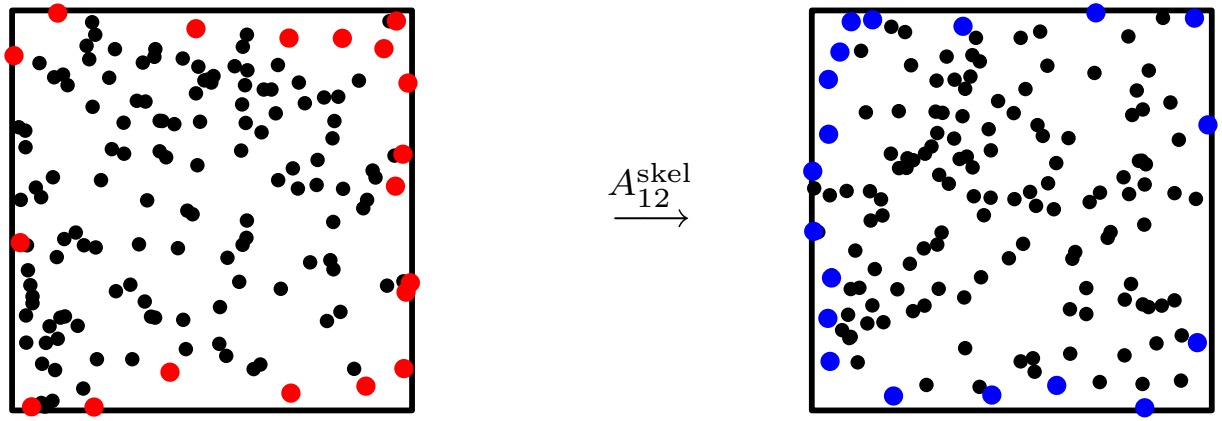


$$\begin{array}{ccc} \{q_n\}_{n=1}^{N} & \xrightarrow{\quad A_{12} \quad} & \{v_m\}_{m=1}^{M} \\ \Big\downarrow U_2^{\mathrm{t}} & \nearrow_{A_{12}^{\mathrm{skel}}} & \\ \{\tilde{q}_{n_j}\}_{j=1}^{k} & & \end{array}$$

We can pick k points in Ω_{S} with the property that any potential in Ω_{T} can be replicated by placing charges on these k points.

- The choice of points does not depend on $\{q_n\}_{n=1}^{N}$.
- A_{12}^{skel} is a submatrix of A_{12}.

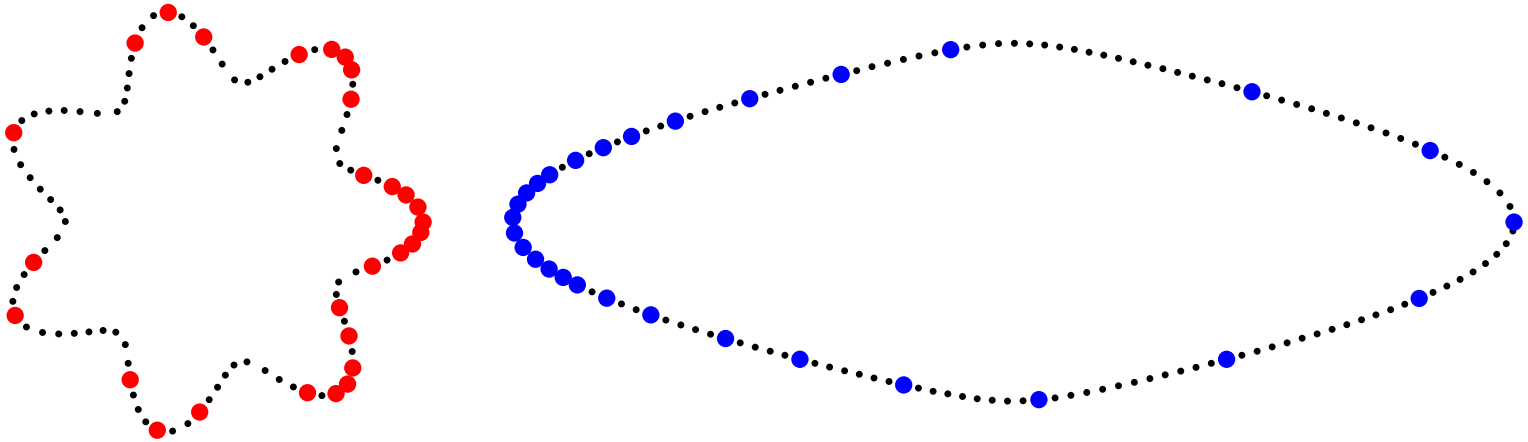
We can "skeletonize" both Ω_1 and Ω_2.



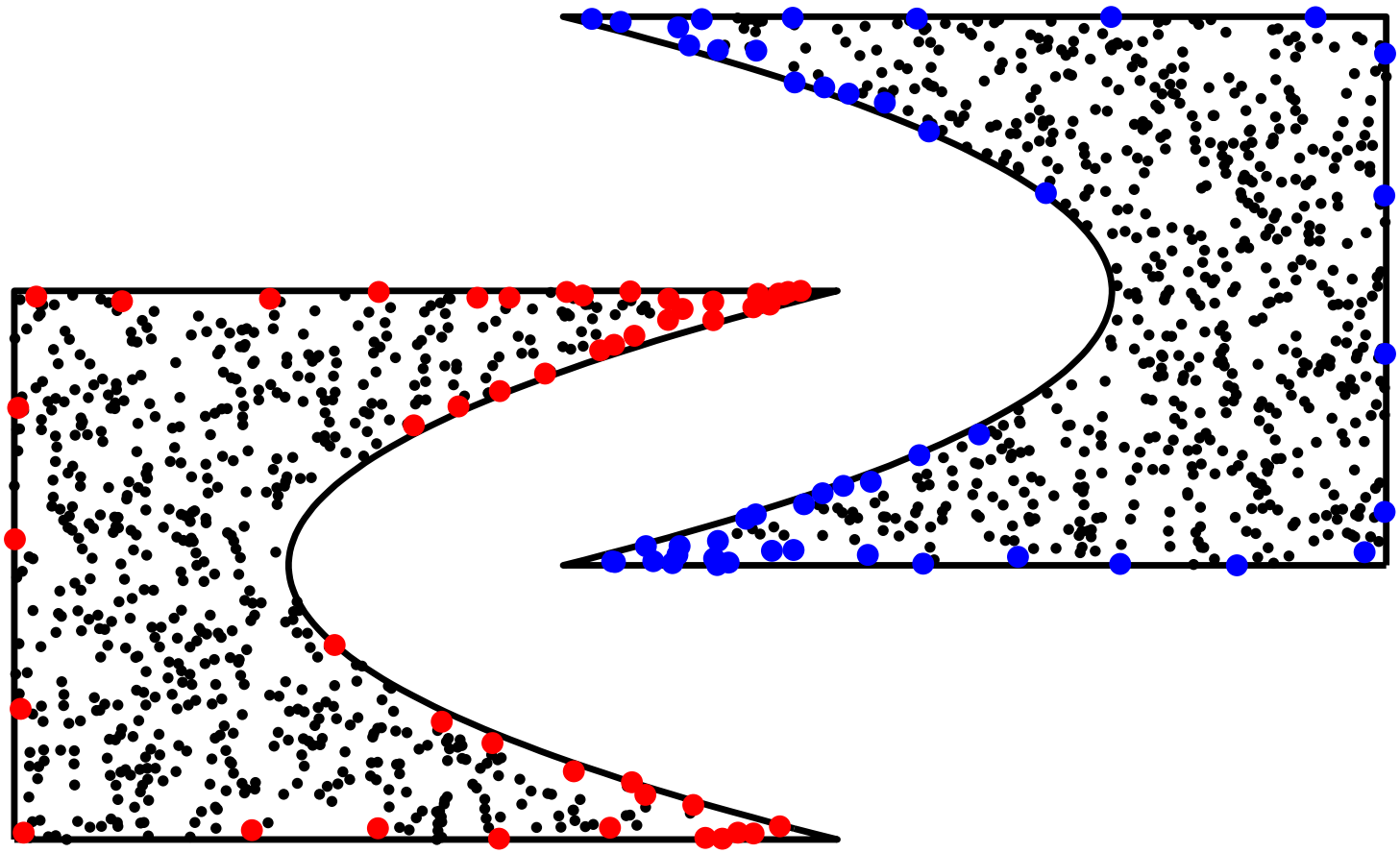
$$\begin{array}{ccc} \{q_n\}_{n=1}^{N} & \xrightarrow{\quad A_{12} \quad} & \{v_m\}_{m=1}^{M} \\ \Big\downarrow U_2^{\mathrm{t}} & & \Big\uparrow U_1 \\ \{\tilde{q}_{n_j}\}_{j=1}^{k} & \xrightarrow[\quad A_{12}^{\text{skel}} \quad]{} & \{v_{m_j}\}_{j=1}^{k} \end{array}$$

Rank $= 19$ at $\varepsilon = 10^{-10}$.

Skeletonization can be performed for Ω_{S} and Ω_{T} of various shapes.

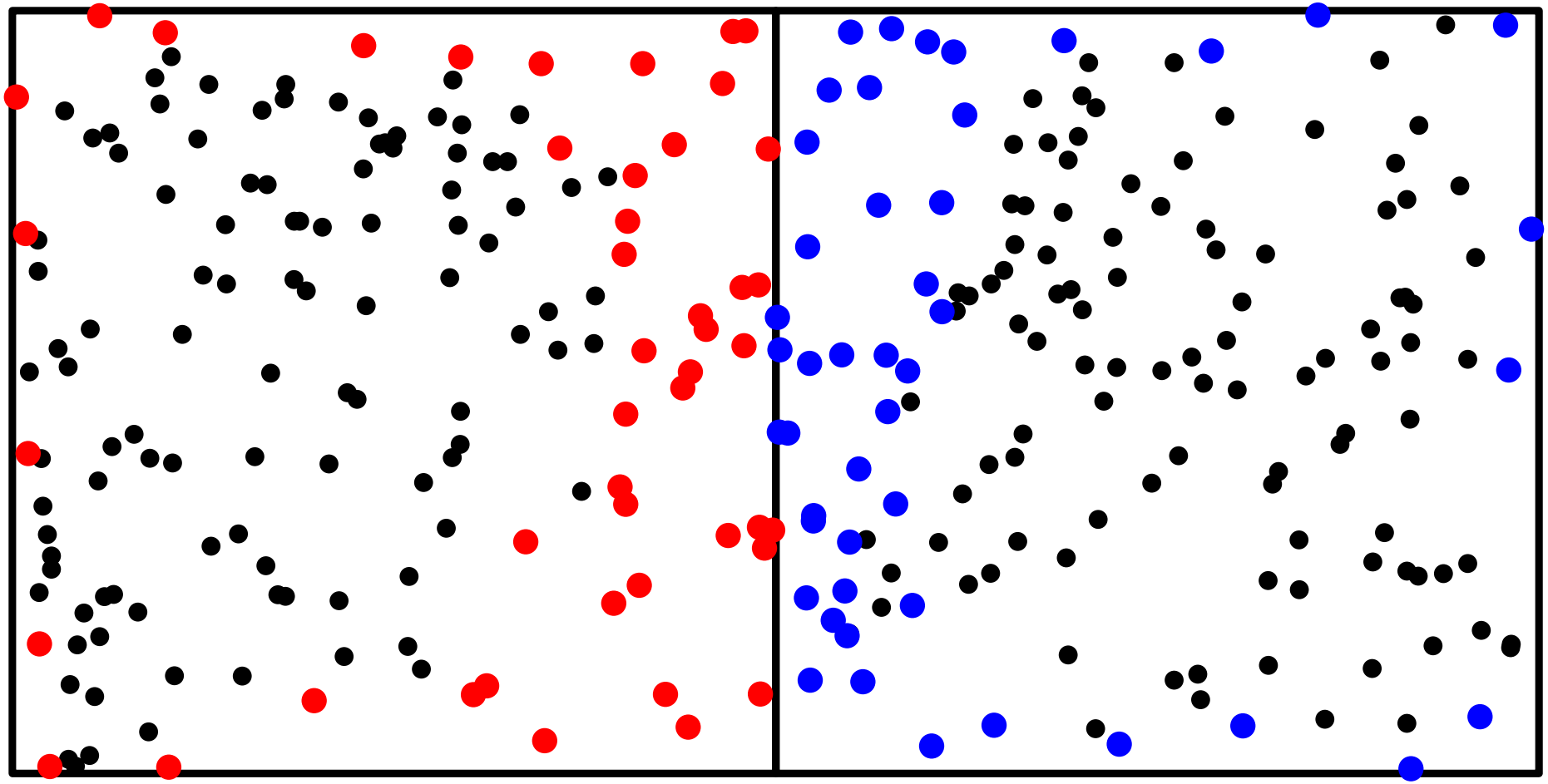


Rank $= 29$ at $\varepsilon = 10^{-10}$.

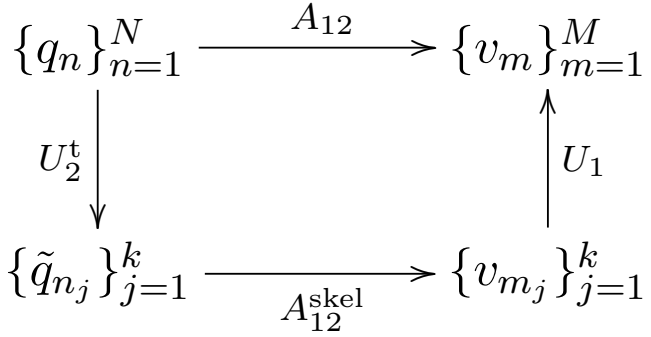


Rank $= 48$ at $\varepsilon = 10^{-10}$.

Adjacent boxes can be skeletonized.



Rank $= 46$ at $\varepsilon = 10^{-10}$.



Benefits:

- The rank is optimal.
- The projection and interpolation are cheap.
  U_1 and U_2 contain $k \times k$ identity matrices.
- The projection and interpolation are well-conditioned.
- Finding the k points is cheap.
- The map $\tilde{A}_{12}$ is simply a restriction of the original map A_{12}.
  (We can loosely say that "the physics of the problem is preserved".)
- Interaction between **adjacent** boxes can be compressed
  (no buffering is required).

Similar schemes have been proposed by many researchers:

1993 - C.R. Anderson

1995 - C.L. Berman

1996 - E. Michielssen, A. Boag

1999 - J. Makino

2004 - L. Ying, G. Biros, D. Zorin

A mathematical foundation:

1996 - M. Gu, S. Eisenstat

Let us return to the direct solver environment. Recall:

We convert the system

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ A_{21} & A_{22} & A_{23} & A_{24} \\ A_{31} & A_{32} & A_{33} & A_{34} \\ A_{41} & A_{42} & A_{43} & A_{44} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{bmatrix}.$$

to the reduced system

$$\begin{bmatrix} \tilde{A}_{11} & A_{12}^{\text{skel}} & A_{13}^{\text{skel}} & A_{14}^{\text{skel}} \\ A_{21}^{\text{skel}} & \tilde{A}_{22} & A_{23}^{\text{skel}} & A_{24}^{\text{skel}} \\ A_{31}^{\text{skel}} & A_{32}^{\text{skel}} & \tilde{A}_{33} & A_{34}^{\text{skel}} \\ A_{41}^{\text{skel}} & A_{42}^{\text{skel}} & A_{43}^{\text{skel}} & \tilde{A}_{44} \end{bmatrix} \begin{bmatrix} \tilde{x}_1 \\ \tilde{x}_2 \\ \tilde{x}_3 \\ \tilde{x}_4 \end{bmatrix} = \begin{bmatrix} \tilde{f}_1 \\ \tilde{f}_2 \\ \tilde{f}_3 \\ \tilde{f}_4 \end{bmatrix}.$$

We know that A_{ij}^{skel} is a submatrix of A_{ij} when $i \neq j$.

What is $\tilde{A}_{ii}$?

We recall that the new diagonal blocks are defined by

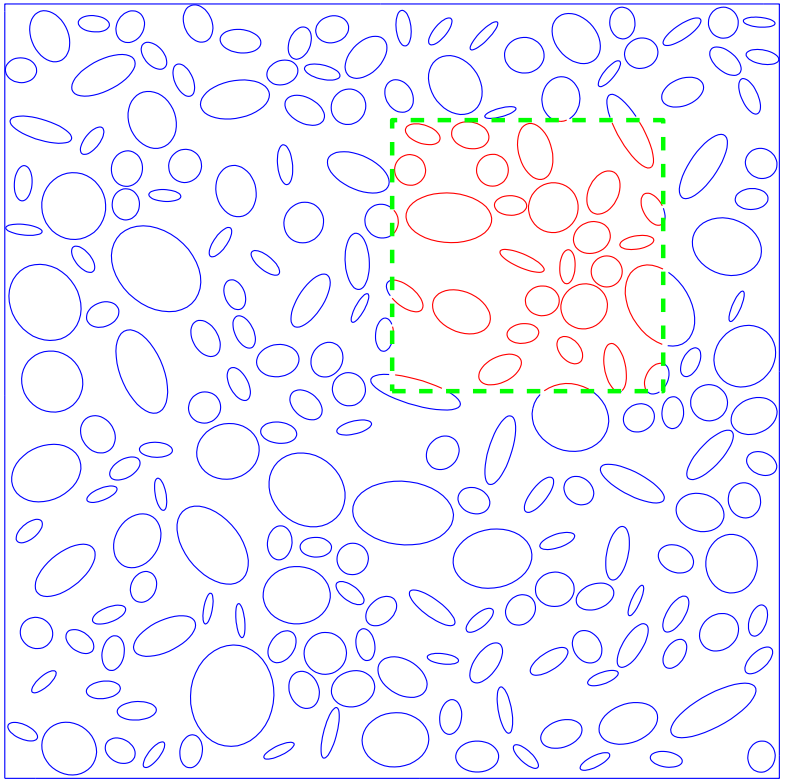
$$\underbrace{\tilde{A}_{ii}}_{k\times k} = \big(\underbrace{U_i^{\mathrm{t}}}_{k\times n}\ \underbrace{A_{ii}^{-1}}_{n\times n}\ \underbrace{U_i}_{n\times k}\big)^{-1}.$$

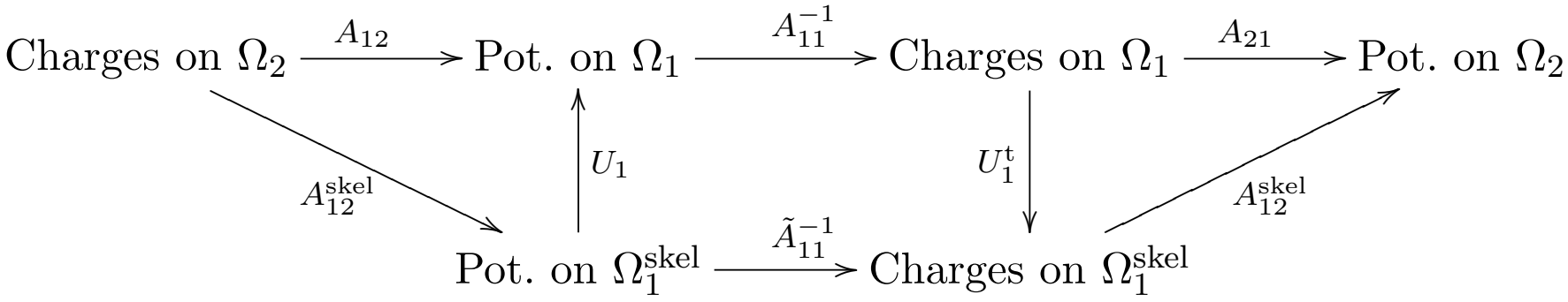
We call these blocks "proxy matrices".

What are they?

Let Ω_1 denote the block marked in red.

Let Ω_2 denote the rest of the domain.





$\tilde{A}_{11}$ contains *all the information the outside world needs to know about* Ω_1.

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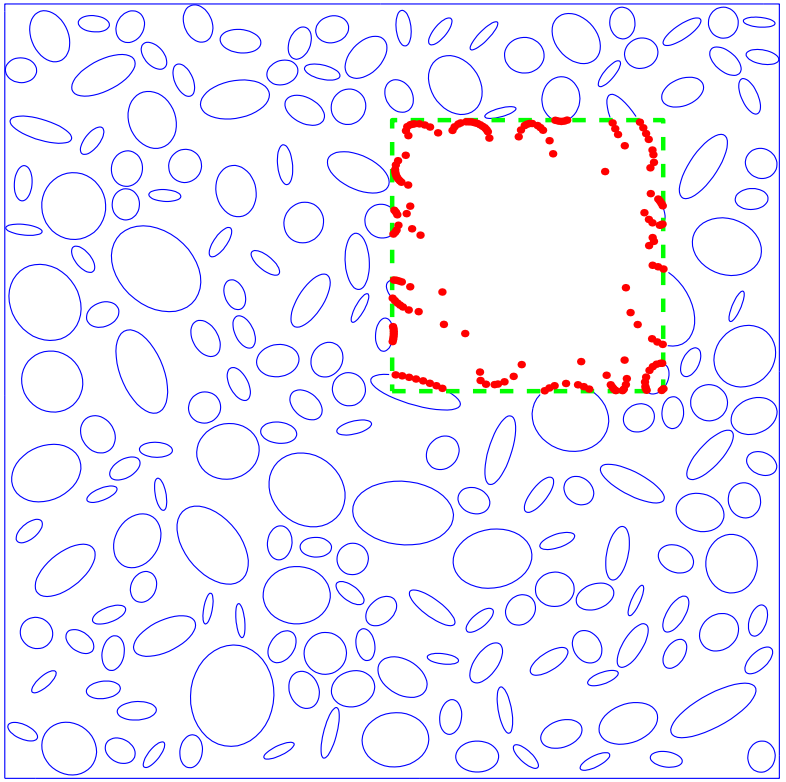
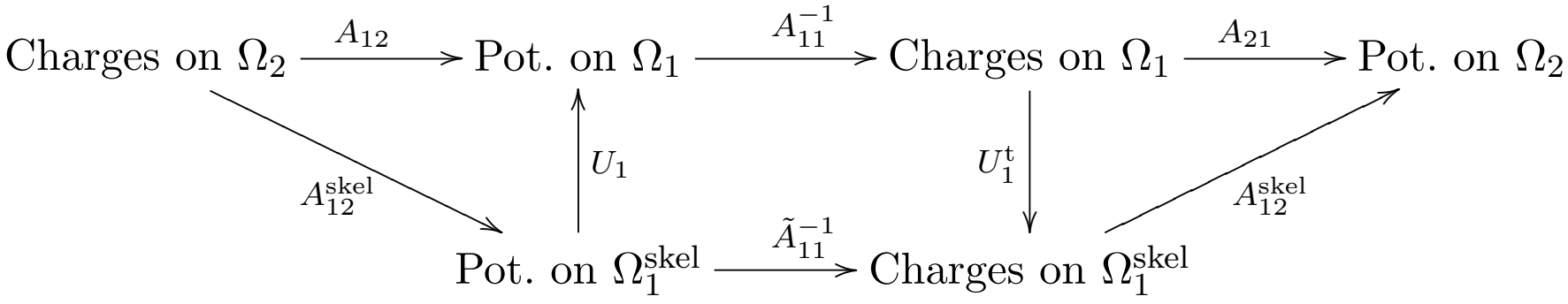
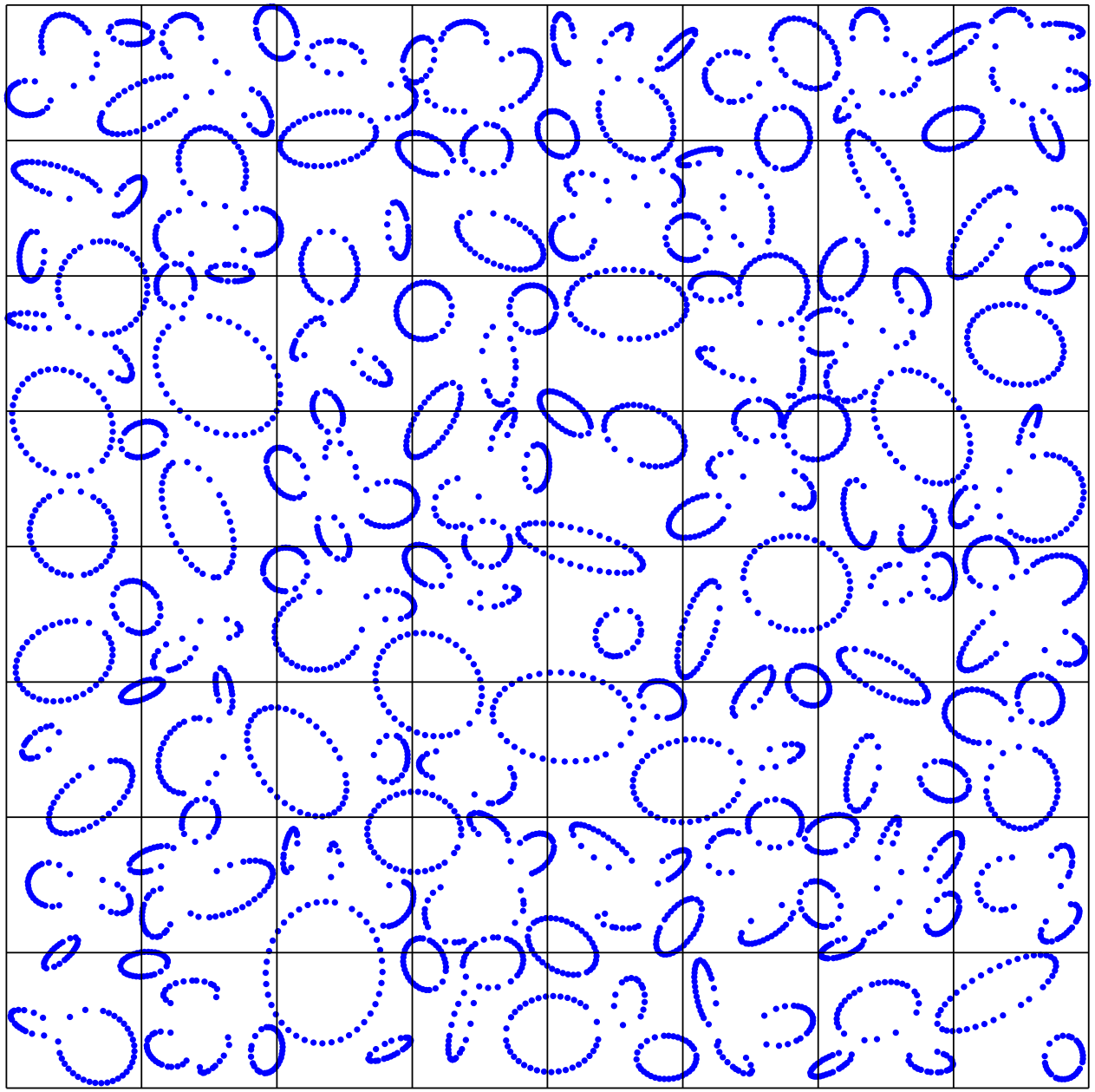
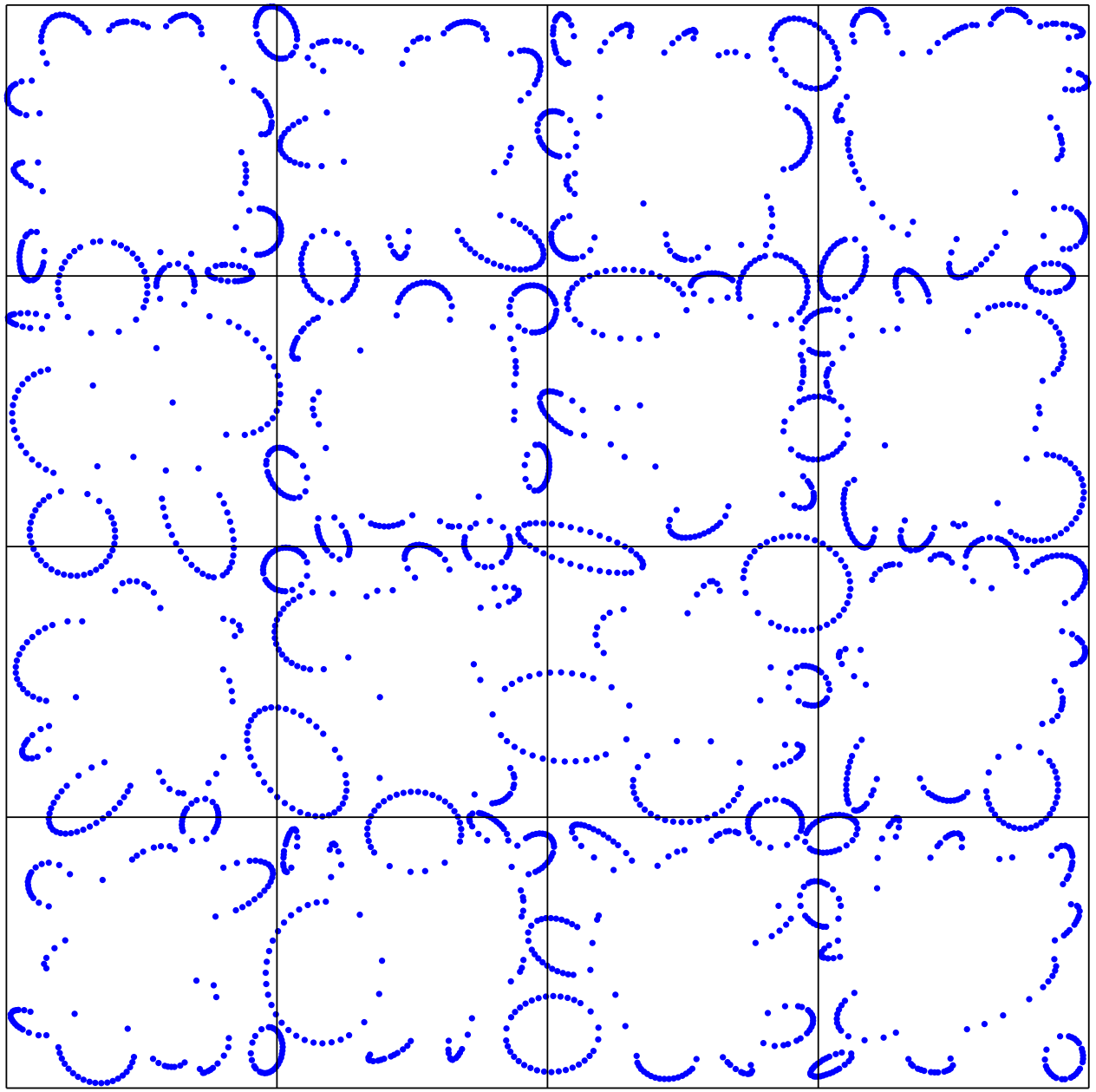


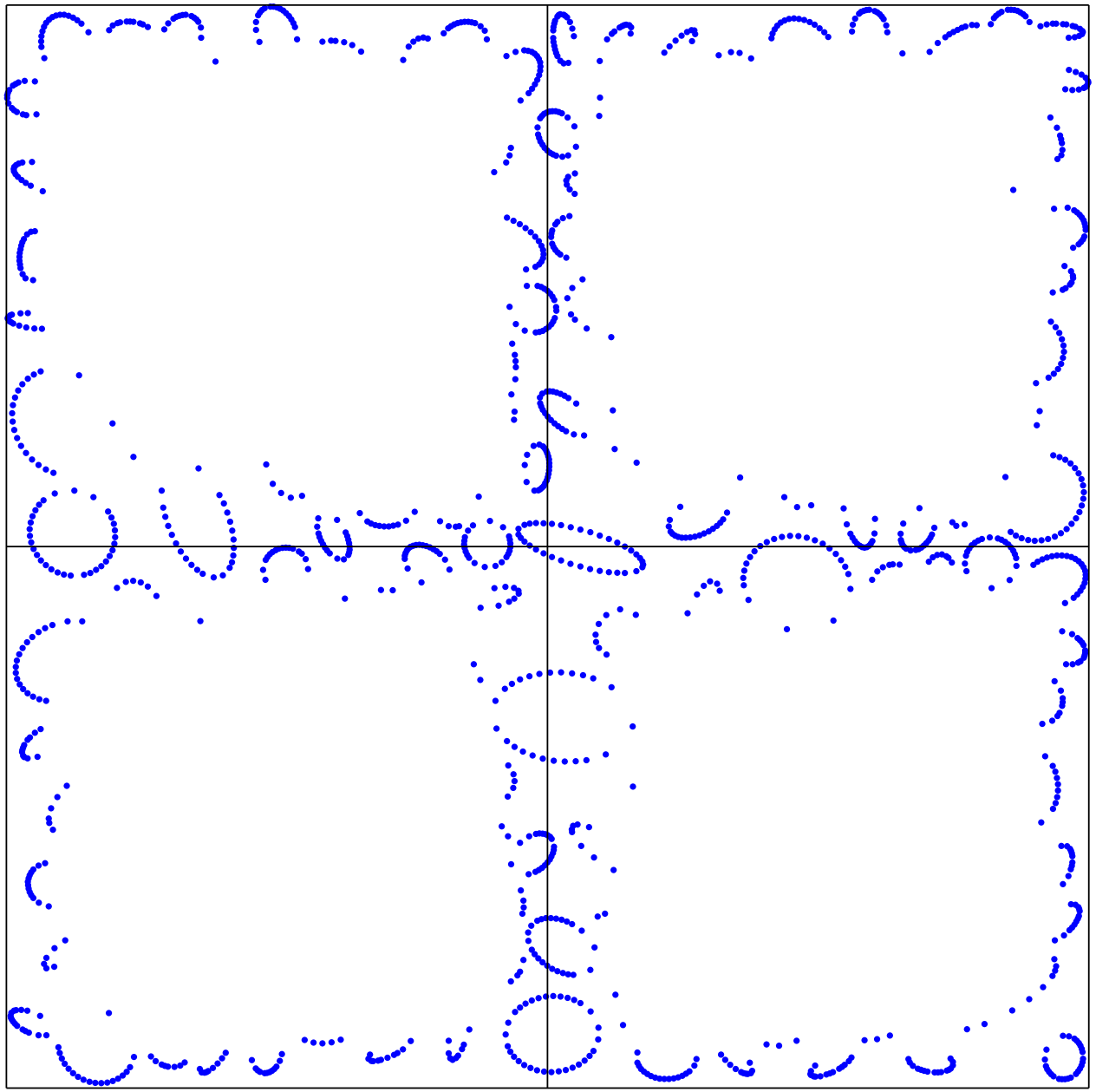


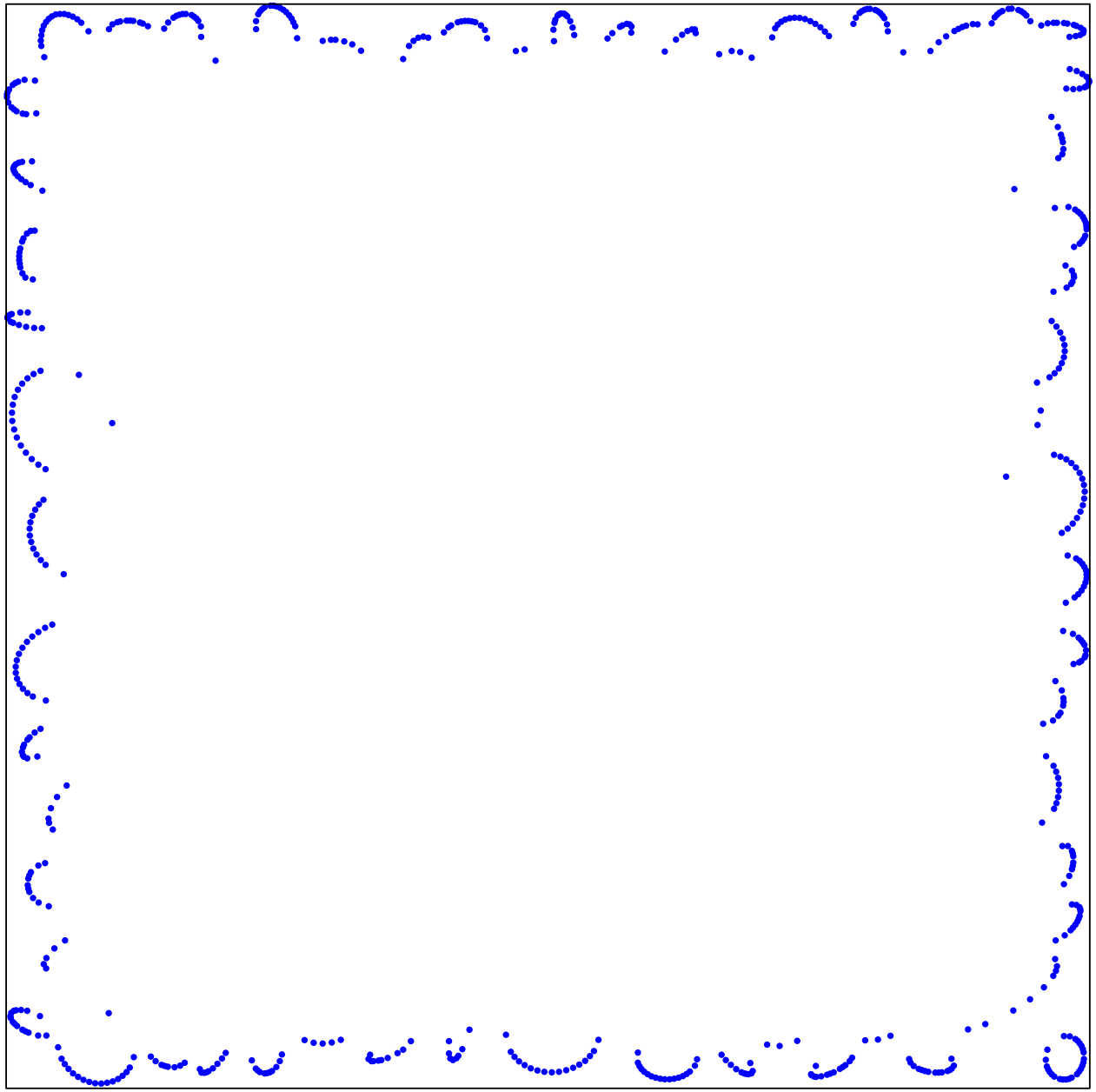
$\tilde{A}_{11}$ contains *all the information the outside world needs to know about* Ω_1.

To obtain a globally $O(N)$ scheme, we hierarchically merge proxy matrices.







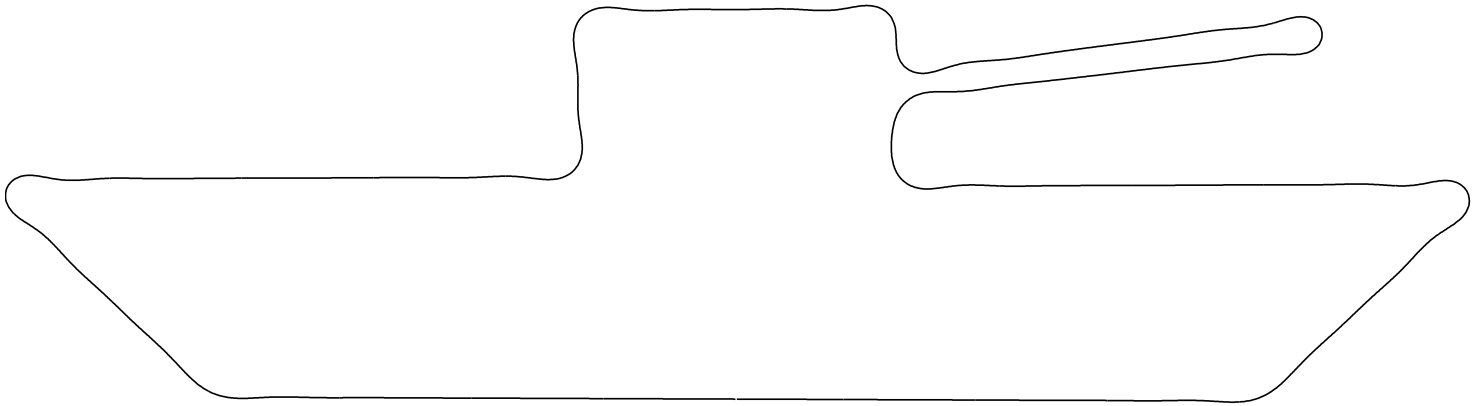


Numerical examples

In developing direct solvers, the "proof is in the pudding" — recall that from a theoretical point of view, the problem is already solved (by Hackbusch and others).

All computations were performed on standard laptops and desktop computers in the 2.0GHz - 2.8Ghz speed range, and with 512Mb of RAM.

An exterior Helmholtz Dirichlet problem



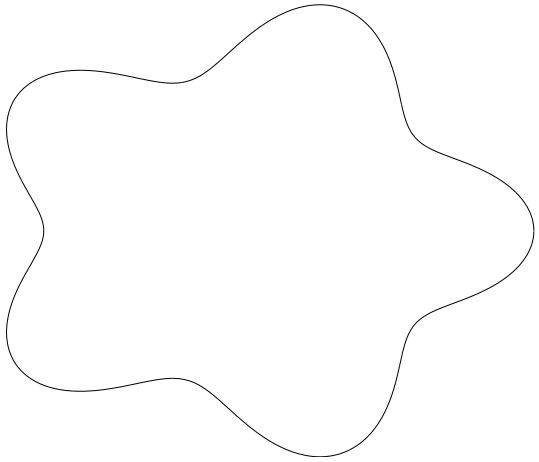
A smooth contour. Its length is roughly 15 and its horizontal width is 2.

k	N_{start}	N_{final}	t_{tot}	t_{solve}	E_{res}	E_{pot}	σ_{min}	M
21	800	435	1.5e+01	3.3e-02	9.7e-08	7.1e-07	6.5e-01	12758
40	1600	550	3.0e+01	6.7e-02	6.2e-08	4.0e-08	8.0e-01	25372
79	3200	683	5.3e+01	1.2e-01	5.3e-08	3.8e-08	3.4e-01	44993
158	6400	870	9.2e+01	2.0e-01	3.9e-08	2.9e-08	3.4e-01	81679
316	12800	1179	1.8e+02	3.9e-01	2.3e-08	2.0e-08	3.4e-01	160493
632	25600	1753	4.3e+02	8.0e-01	1.7e-08	1.4e-08	3.3e-01	350984

Computational results for an exterior Helmholtz Dirichlet problem discretized with 10^{th} order accurate quadrature. The Helmholtz parameter was chosen to keep the number of discretization points per wavelength constant at roughly 45 points per wavelength (resulting in a quadrature error about 10^{-12}).

Eventually ... the complexity is $O(n + k^3)$.

Example 2 - An interior Helmholtz Dirichlet problem

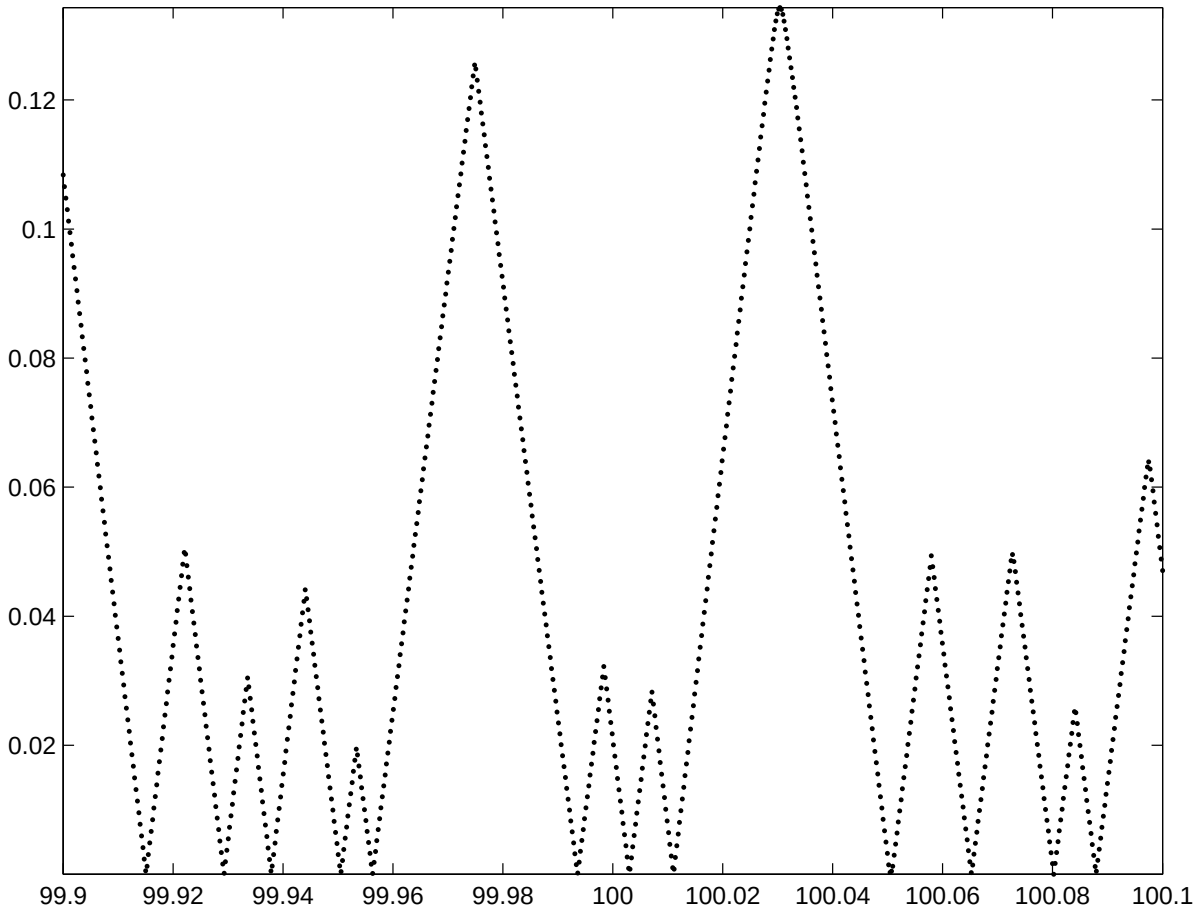


The diameter of the contour is about 2.5. An interior Helmholtz problem with Dirichlet boundary data was solved using $N = 6\,400$ discretization points, with a prescribed accuracy of 10^{-10}.

For $k = 100.011027569\cdots$, the smallest singular value of the boundary integral operator was $\sigma_{\min} = 0.00001366\cdots$.

Time for constructing the inverse: 0.7 seconds.

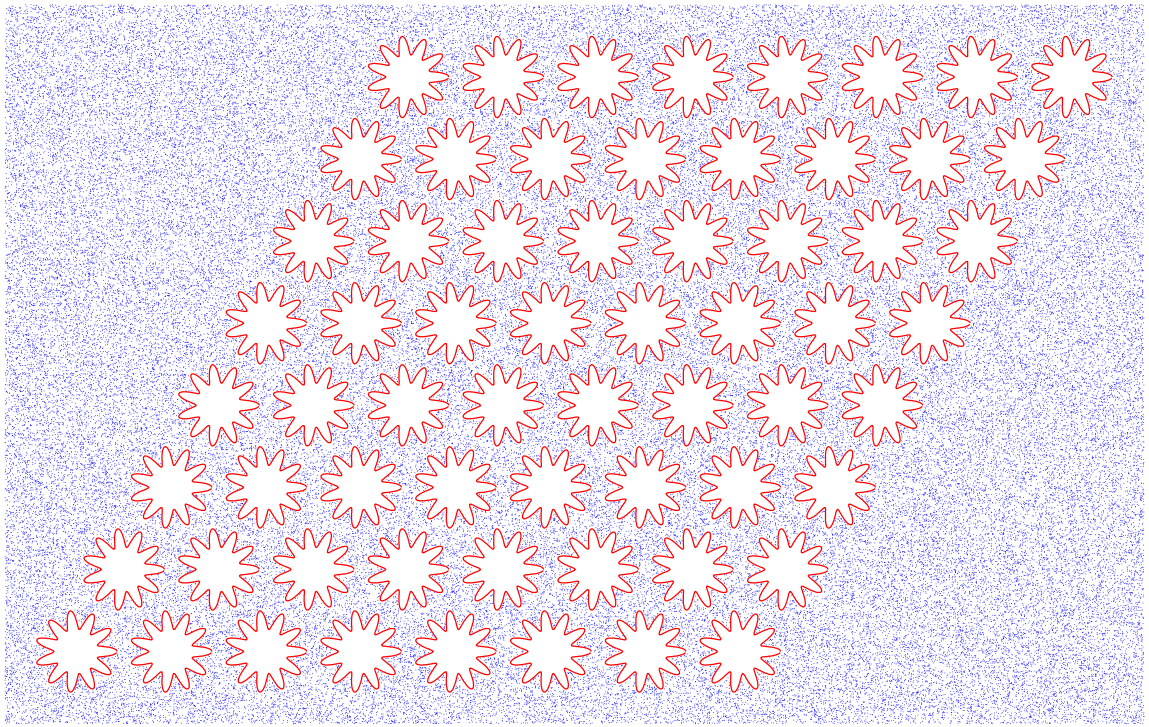
Error in the inverse: 10^{-5}.



Plot of $\sigma_{\min}$ versus k for an interior Helmholtz problem on the smooth pentagram. The values shown were computed using a matrix of size $N = 6400$. Each point in the graph required about $60s$ of CPU time.

Example 3:

An electrostatics problem in a dielectrically heterogeneous medium

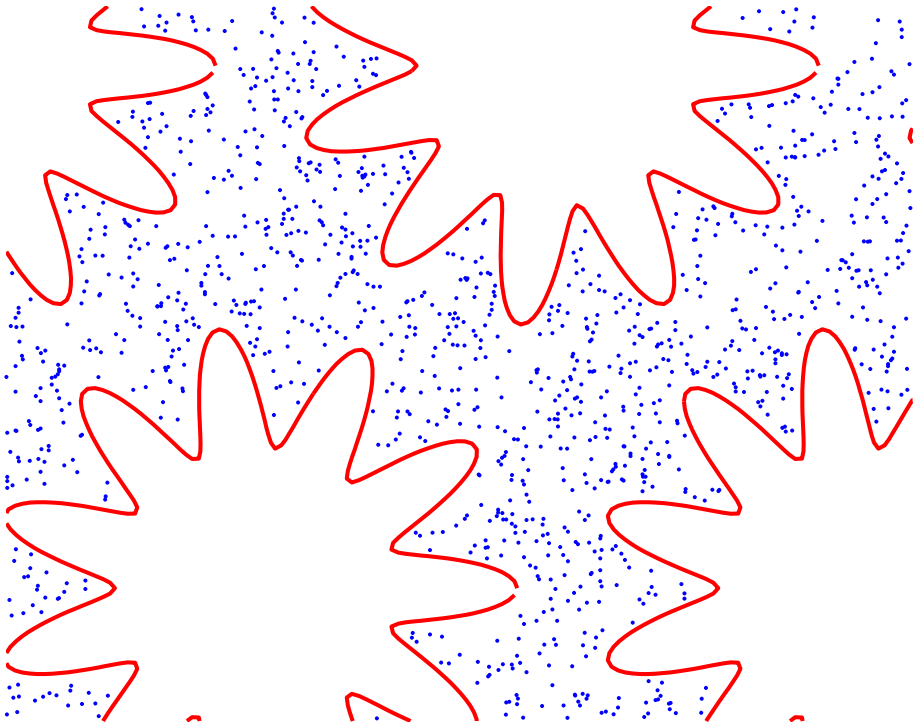


$\varepsilon = 10^{-5}$ $N_{\text{contour}} = 25\,600$ $N_{\text{particles}} = 100\,000$

Time to invert the boundary integral equation = 46sec.

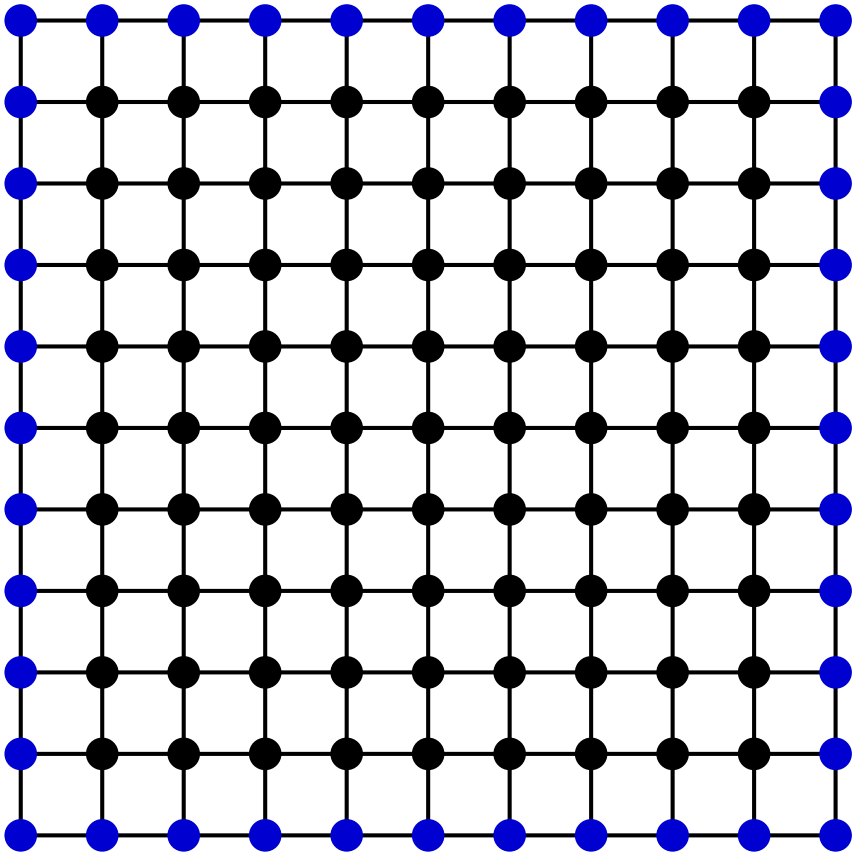
Time to compute the induced charges = 0.42sec.(2.5sec for the FMM)

Total time for the electro-statics problem = 3.8sec.



A close-up of the particle distribution.

Example 4: Inversion of a "Finite Element Matrix"



A grid conduction problem (the "five-point stencil").

The conductivity of each bar is a random number drawn from a uniform distribution on [1, 2].

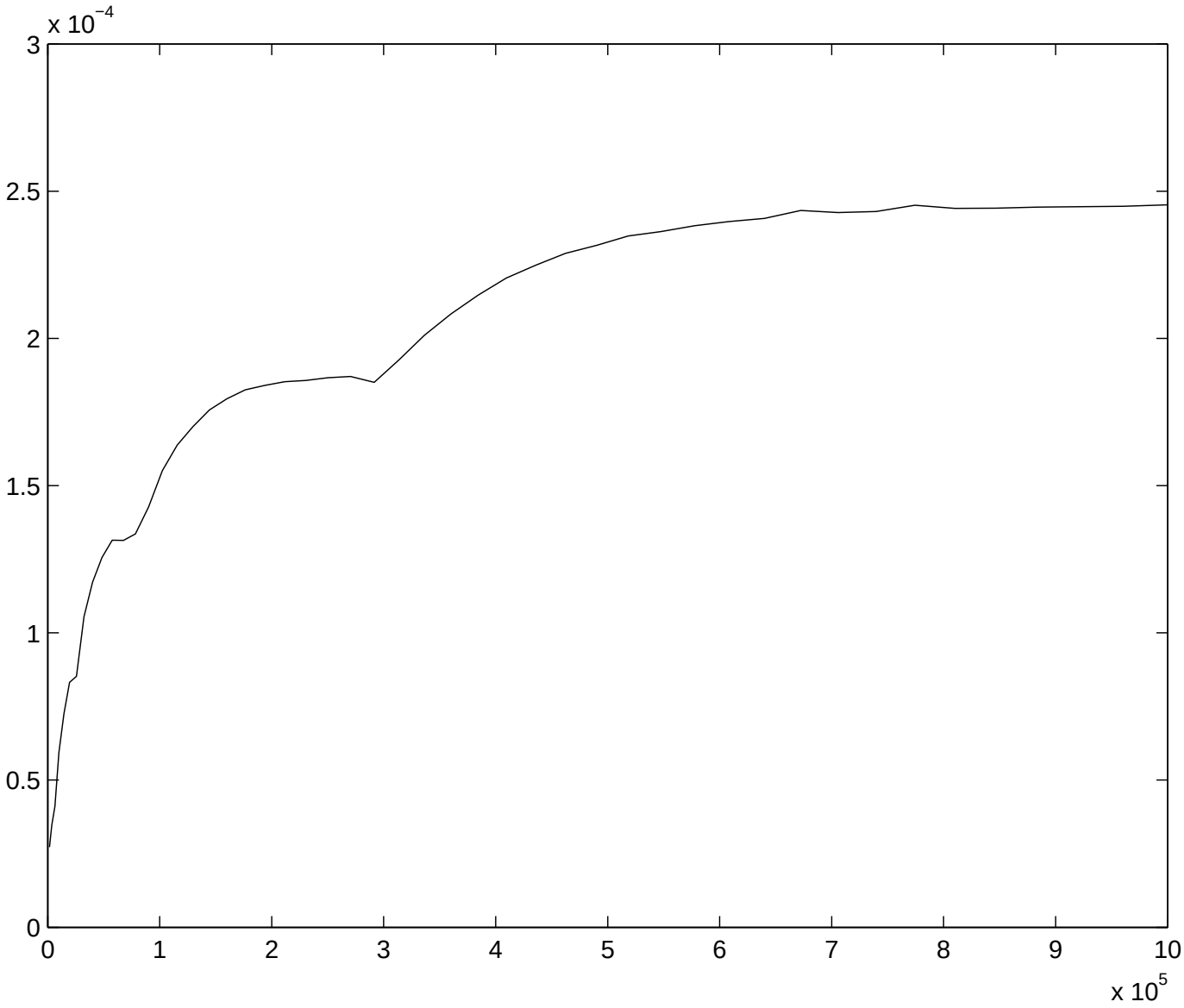
N	T_{invert} (seconds)	T_{apply} (seconds)	M (kB)	e_1	e_2	e_3	e_4
10 000	5.93e-1	2.82e-3	3.82e+2	1.29e-8	1.37e-7	2.61e-8	3.31e-8
40 000	4.69e+0	6.25e-3	9.19e+2	9.35e-9	8.74e-8	4.71e-8	6.47e-8
90 000	1.28e+1	1.27e-2	1.51e+3	—	—	7.98e-8	1.25e-7
160 000	2.87e+1	1.38e-2	2.15e+3	—	—	9.02e-8	1.84e-7
250 000	4.67e+1	1.52e-2	2.80e+3	—	—	1.02e-7	1.14e-7
360 000	7.50e+1	2.62e-2	3.55e+3	—	—	1.37e-7	1.57e-7
490 000	1.13e+2	2.78e-2	4.22e+3	—	—	—	—
640 000	1.54e+2	2.92e-2	5.45e+3	—	—	—	—
810 000	1.98e+2	3.09e-2	5.86e+3	—	—	—	—
1 000 000	2.45e+2	3.25e-2	6.66e+3	—	—	—	—

e_1 The largest error in any entry of $\tilde{A}_n^{-1}$

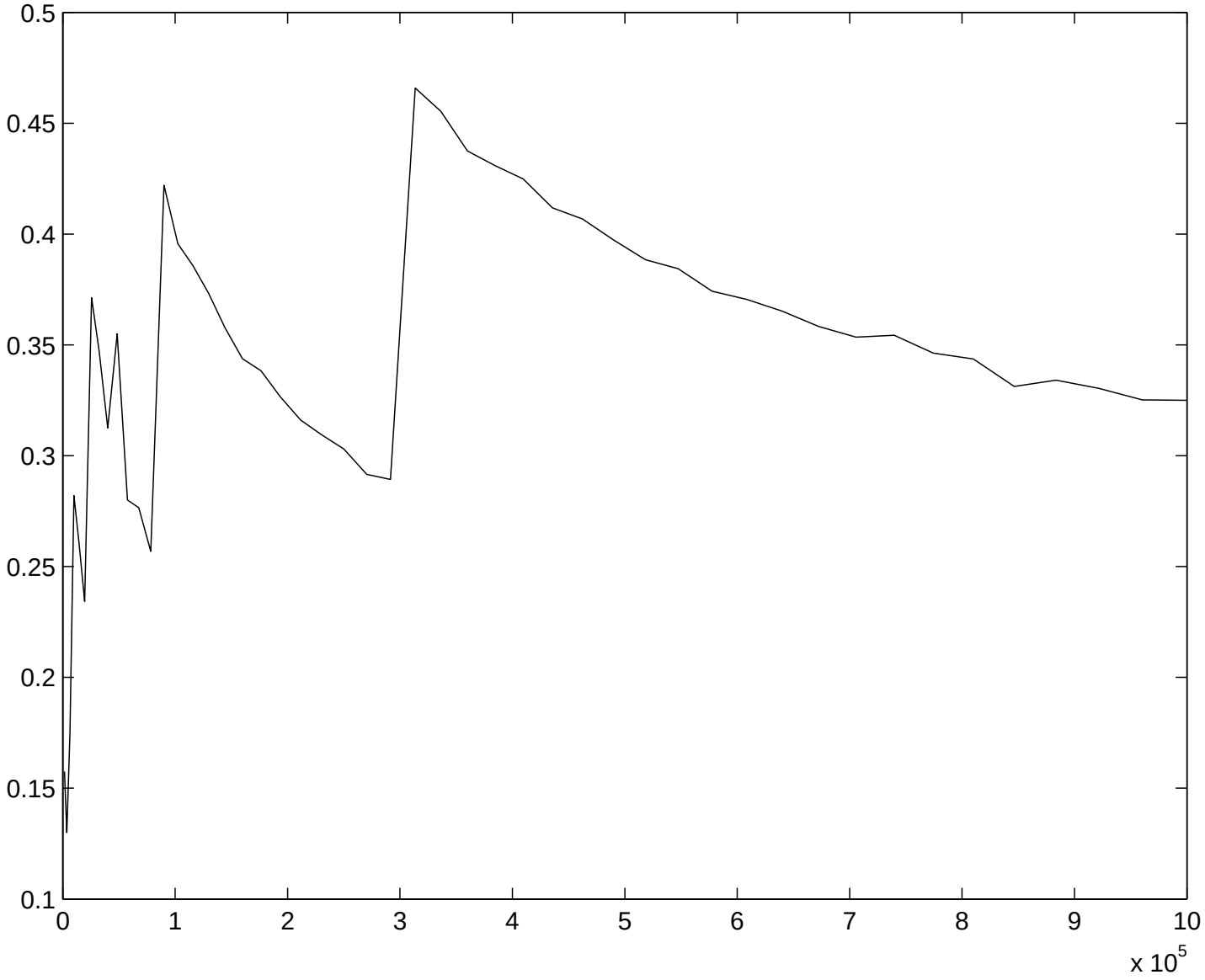
e_2 The error in l^2-operator norm of $\tilde{A}_n^{-1}$

e_3 The l^2-error in the vector $\tilde{A}_{nn}^{-1} r$ where r is a unit vector of random direction.

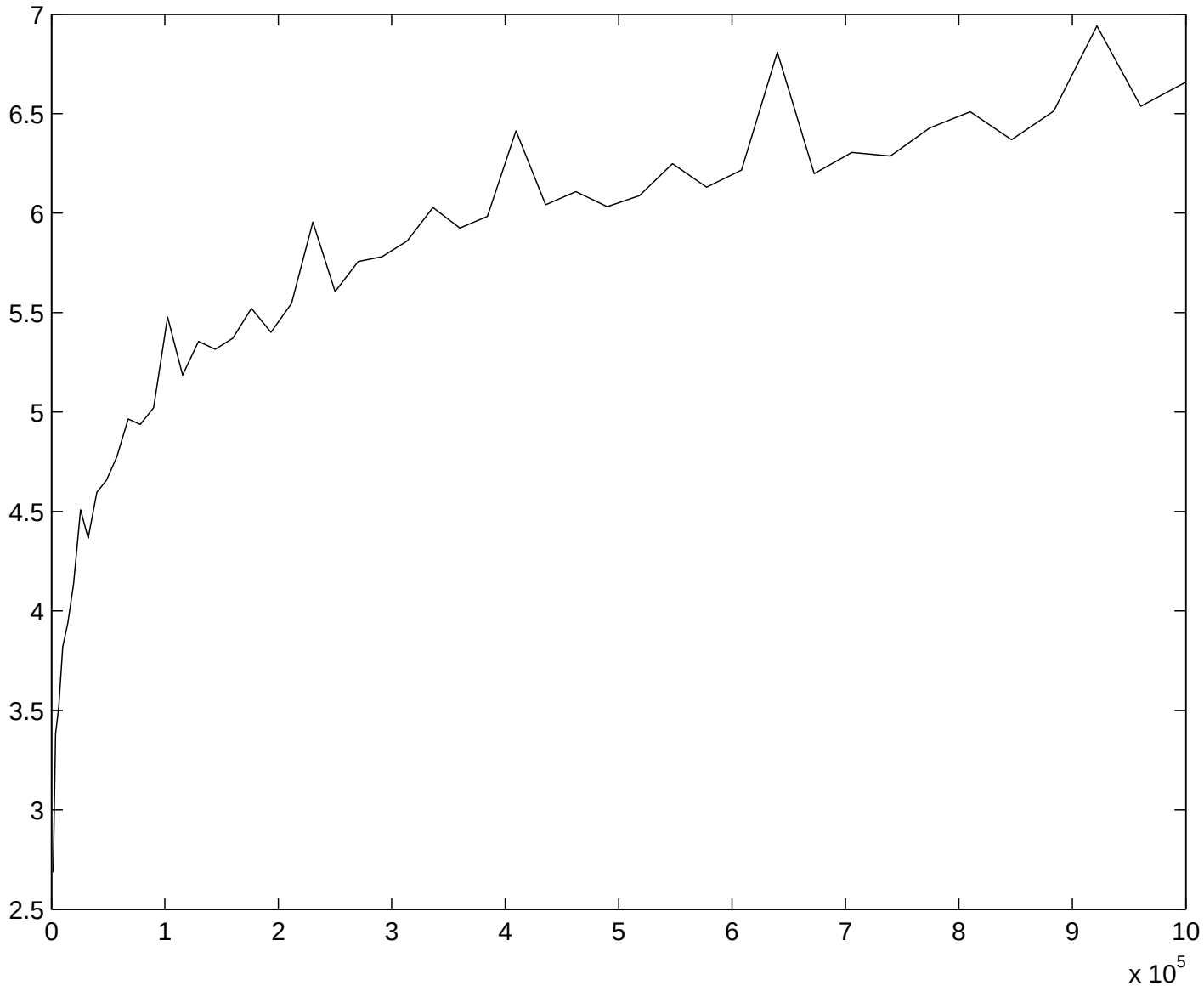
e_4 The l^2-error in the first column of $\tilde{A}_{nn}^{-1}$.



$$\frac{T_{\text{invert}}}{N} \text{ versus } N$$



$$\frac{T_{\text{apply}}}{\sqrt{N}} \quad \text{versus} \quad N$$



$\frac{M}{\sqrt{N}}$ versus N.

Existing fast direct solvers:

- 2D boundary integral equations. Very fast.
  Has proven capable of solving previously intractable problems.
- Certain 2D scattering problems.
- 2D finite element matrices.
  $1\,000\,000 \times 1\,000\,000$ matrix inverted in 4 minutes using 7Mb of memory, subsequent solves take 0.03 seconds.

In development:

- Fast inversion schemes for 2D volume integral equations.
- 3D boundary integral equations.
- Applications to biochemical modelling.
- Applications to multiscale modelling.