Code Development for Large-Scale Eigenvalue Calculations

TECHNISCHE UNIVERSITÄT DARMSTADT

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Status Meeting
November 15, 2018
DESY, Hamburg

Outline

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- Motivation
- Computational model
  - Numerical problem formulation
- Numerical examples
  - Spherical cavity (lossless / lossy)
    Properties of the system matrix
  - 1.3 GHz structure (single cavity)
    Evaluation of promising preconditioner and related linear solvers
- Summary / Outlook

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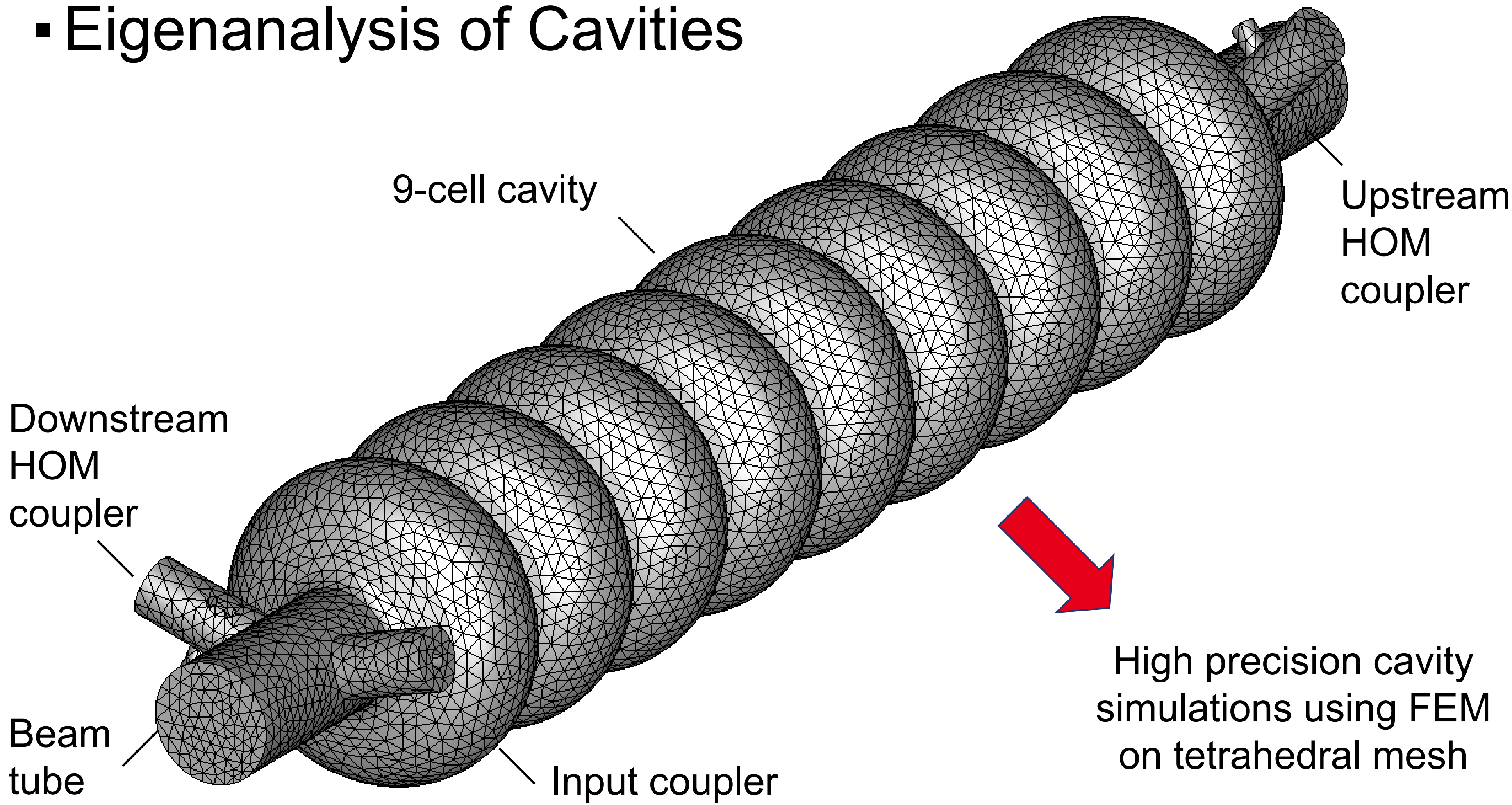
Motivation

- Eigenanalysis of Cavities



High precision cavity simulations using FEM on tetrahedral mesh

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Computational Model

- Numerical Eigenanalysis for Resonant Structures
  - Algebraic problem definition

$$A(\lambda)\,x = \lambda\,B\,x$$

  - Generally available solver types
    - Krylov-type solver methods with linearization
    - Rational Krylov-type methods with linearization
    - MOR-type solver methods
    - Contour integral methods
    - Jacobi-Davidson with fixed-point iteration → Critical step: Subspace expansion

Computational Model

- Jacobi-Davidson method $M = A - \lambda_\tau B$
  - Important properties
    - Direct solution difficult because of dense matrix in correction equation.
    - Iterative solution not immediately applicable because vectors $\Delta\vec{x}$ with $\Delta\vec{x} \in R\{(V_B)_\perp\}$ are not mapped back onto $R\{(V_B)_\perp\}$ again.
  - Preconditioning
    - The JD - preconditioner

$$\begin{aligned} PC &= \{I - M^{-1}V_B[(M^{-1}V_B)^T V_B]^{-1} V_B^T\} M^{-1} \\ &= M^{-1} - M^{-1}V_B[(M^{-1}V_B)^T V_B]^{-1} V_B^T M^{-1} \end{aligned}$$

retains the property $\Delta\vec{x} \in R\{(V_B)_\perp\}$ for any preconditioner M^{-1}.

Simplest case: $M^{-1} = I \quad \hookrightarrow \quad PC = I - VV_B^T = P$

Computational Model

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- Numerical formulation
  - Implementation

$$a_{ij} = \iiint_\Omega 1/\mu_\mathrm{r} \, \mathrm{curl}\vec{w}_i \cdot \mathrm{curl}\vec{w}_j \, \mathrm{d}\Omega$$

$$b_{ij} = \iiint_\Omega \varepsilon_\mathrm{r} \, \vec{w}_i \cdot \vec{w}_j \, \mathrm{d}\Omega$$

Mathematica

Edge basis elements

- Matrix A

```
(* Element matrix calculation *)
fktA2[i_Integer, j_Integer] :=
  Integrate[(curlW[i].curlW[j]) * jacobi,
   {u1, 0, 1}, {u2, 0, 1 - u1}, {u3, 0, 1 - u1 - u2}];
matA2 = Array[fktA2, {nEdges, nEdges}];
TableForm[Flatten[matA2]]
```

- Matrix B

```
(* Element matrix calculation *)
fktB2[i_Integer, j_Integer] :=
  Integrate[(W[i].W[j]) * jacobi, {u1, 0, 1},
   {u2, 0, 1 - u1}, {u3, 0, 1 - u1 - u2}];
matB2 = Array[fktB2, {nEdges, nEdges}];
TableForm[Flatten[matB2]]
```

→ contribution of element-matrices ready availabe

Computational Model

- Numerical formulation
  - Function definition

FEM06: lowest order approximation (edge elements, Nédélec)

	Space	Basis functions	Assoc.
scalar	$\tilde{\mathcal{V}}_1$	ϕ_i	$\{i\}$
	$\tilde{\mathcal{V}}_2$	$\phi_i\phi_j$	$\{ij\}$
	$\tilde{\mathcal{V}}_3$	$\phi_i\phi_j(\phi_i - \phi_j)$,	$\{ij\}$
		$\phi_i\phi_j\phi_k$	$\{ijk\}$
vector	$\tilde{\mathcal{A}}_1$	$\phi_i\nabla\phi_j - \phi_j\nabla\phi_i$	$\{ij\}$
	$\tilde{\mathcal{A}}_2$	$3\phi_j\phi_k\nabla\phi_i - \nabla(\phi_i\phi_j\phi_k)$,	$\{ijk\}$
		$3\phi_k\phi_i\nabla\phi_j - \nabla(\phi_i\phi_j\phi_k)$	$\{ijk\}$
	$\tilde{\mathcal{A}}_3$	$4\phi_j\phi_k(\phi_j - \phi_k)\nabla\phi_i - \nabla(\phi_i\phi_j\phi_k(\phi_j - \phi_k))$,	$\{ijk\}$
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Pär Ingelström,
A New Set of H(curl)-Conforming Hierarchical Basis Functions for Tetrahedral Meshes,
IEEE TRANSACTIONS ON MICROWAVE THEORY AND TECHNIQUES, VOL. 54, NO. 1, JANUARY 2006

Computational Model

TECHNISCHE UNIVERSITÄT DARMSTADT

- Numerical formulation
  - Function definition

FEM12: higher order approximation

Space	Basis functions	Assoc.
$\tilde{\mathcal{V}}_1$	ϕ_i	$\{i\}$
$\tilde{\mathcal{V}}_2$	$\phi_i\phi_j$	$\{ij\}$
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scalar ($\tilde{\mathcal{V}}_1$–$\tilde{\mathcal{V}}_3$), vector ($\tilde{\mathcal{A}}_1$–$\tilde{\mathcal{A}}_3$)

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Computational Model

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- Numerical formulation
  - Function definition

FEM20: higher order approximation

	Space	Basis functions	Assoc.
scalar	$\tilde{\mathcal{V}}_1$	ϕ_i	$\{i\}$
	$\tilde{\mathcal{V}}_2$	$\phi_i\phi_j$	$\{ij\}$
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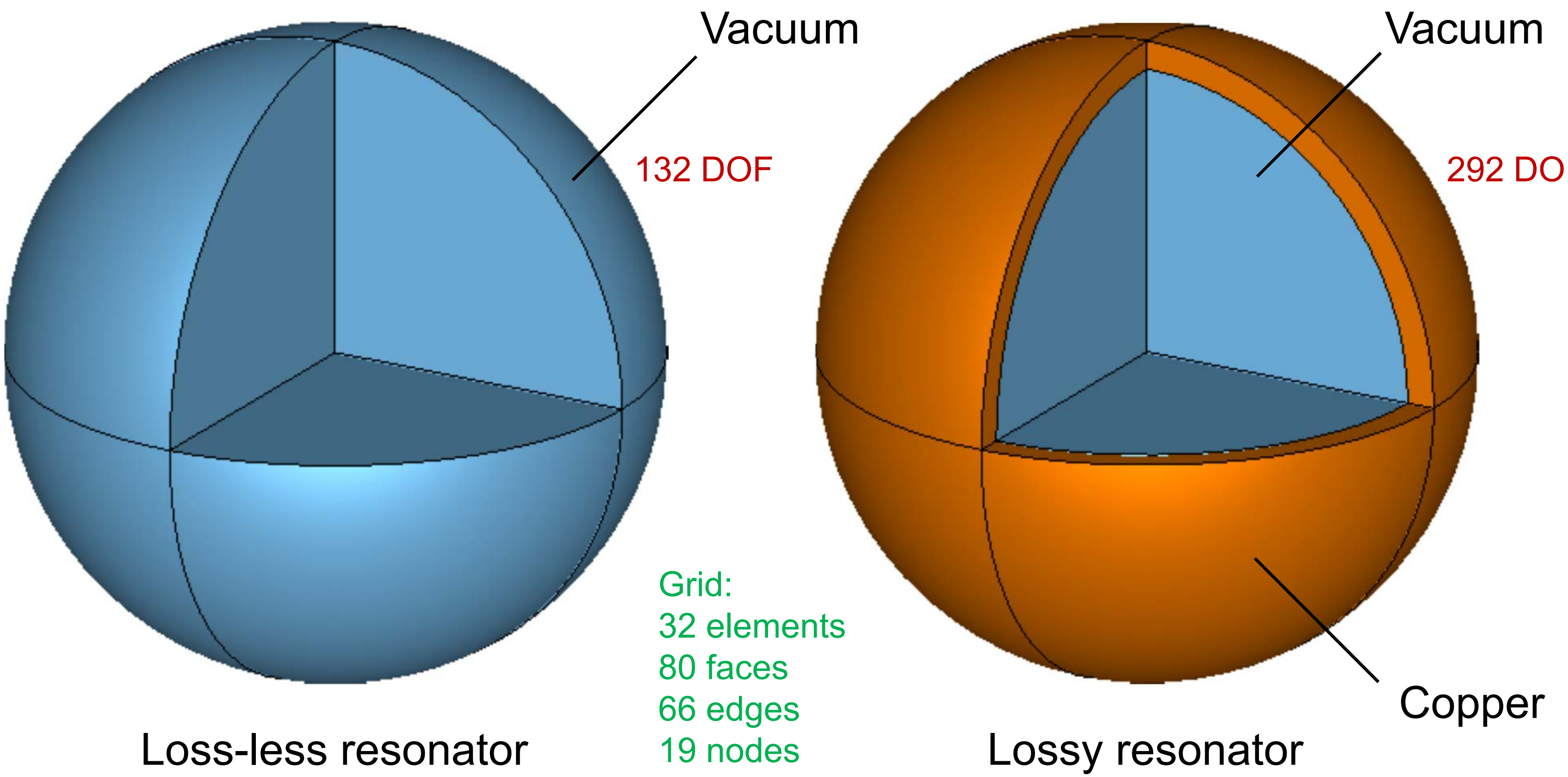
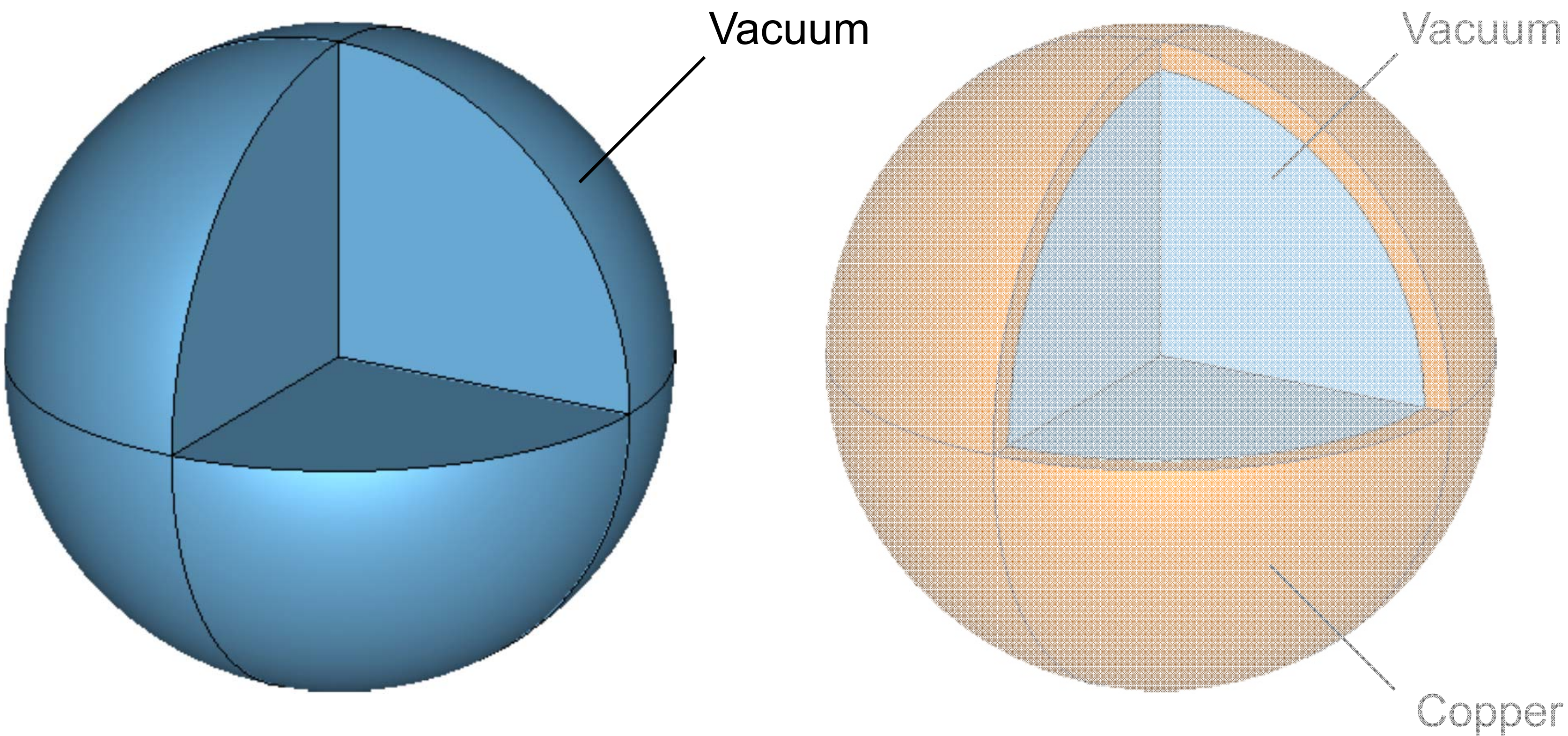
Numerical Examples

- Spherical Resonators



Numerical Examples

- Spherical Resonators



Loss-less resonator

Lossy resonator

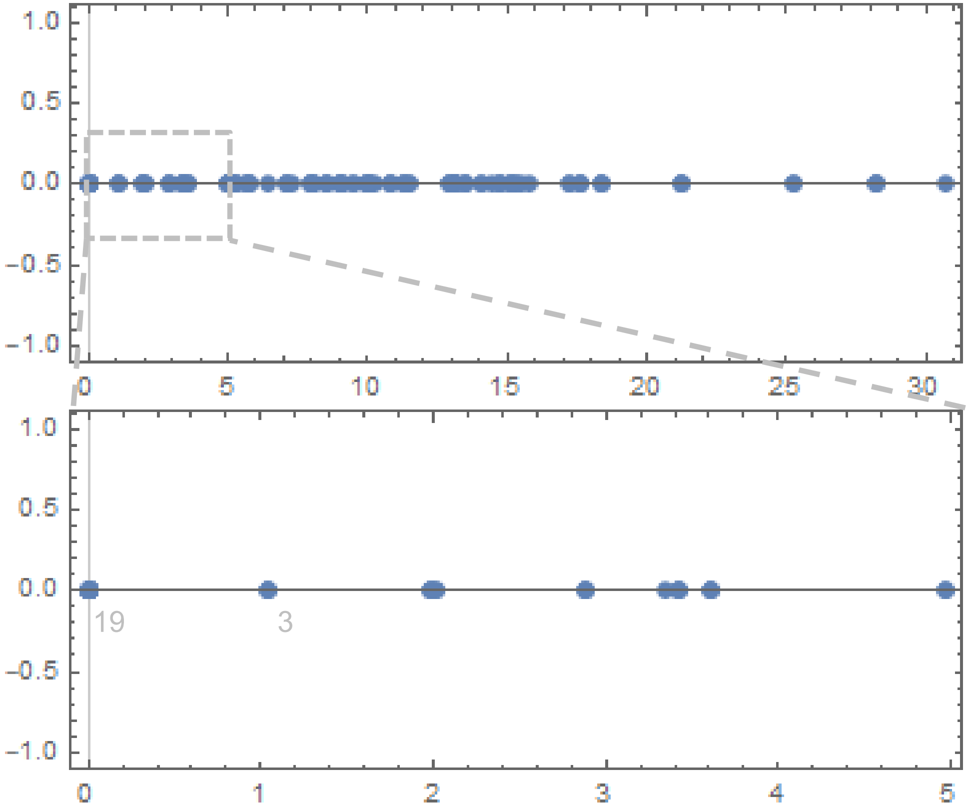
- Properties of the Matrix Pencil
  - Eigenvalue distribution

$$A' \, x = \lambda' \, B' \, x$$

$$\underbrace{\frac{A'}{s}}_{A} \, x = \underbrace{\frac{\lambda'}{s^2}}_{\lambda} \, \underbrace{s B'}_{B} \, x$$

$$A \, x = \lambda \, B \, x$$

Choose scaling such that $\lambda_\tau = 1$

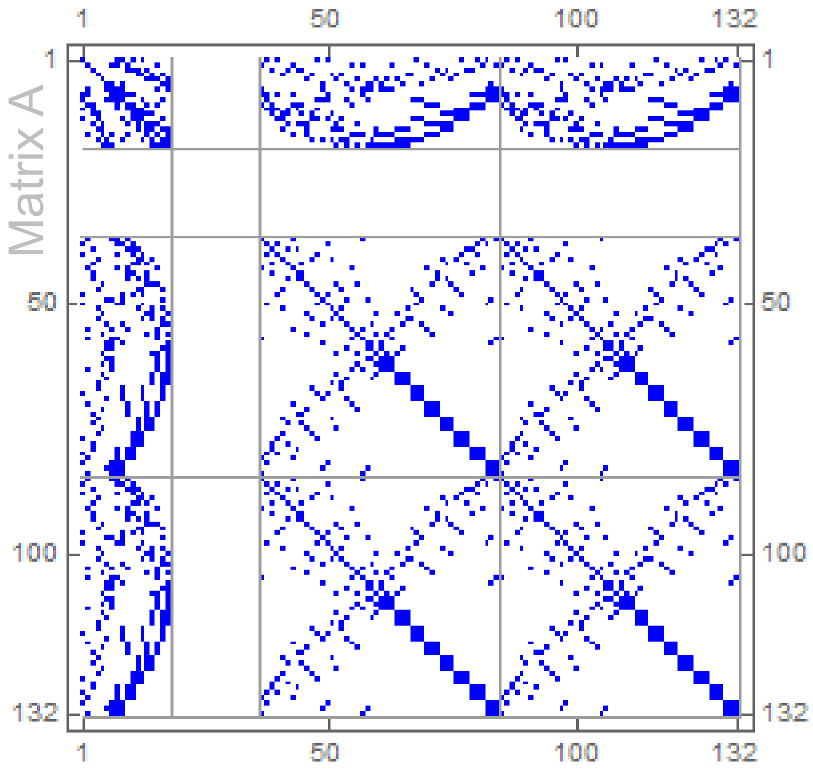


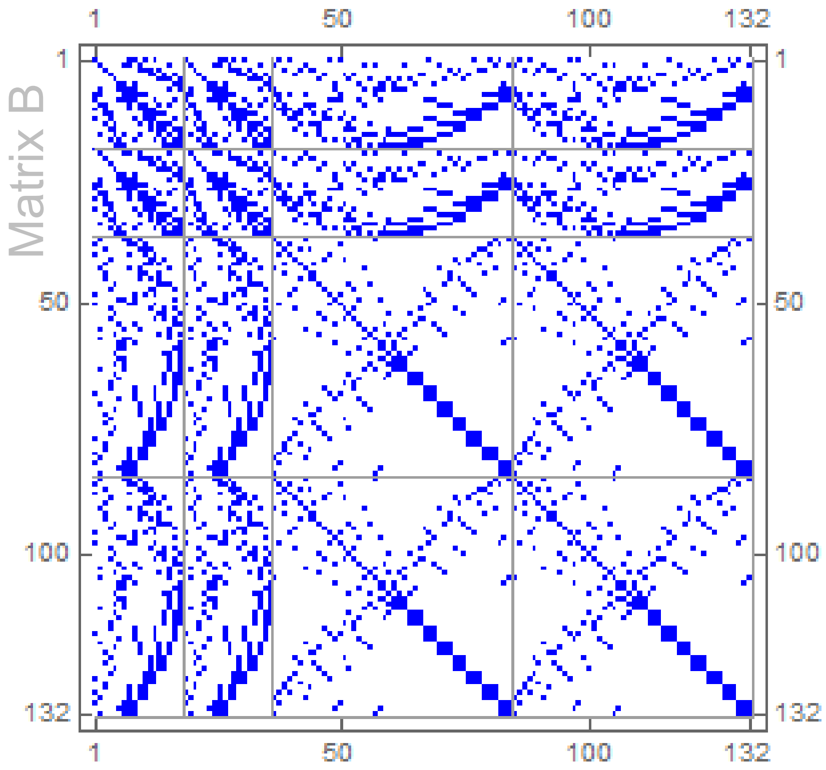
Numerical Examples

- Properties of the Matrix Pencil

$$A\,x = \lambda\,B\,x$$

  - Population pattern for the loss-less case



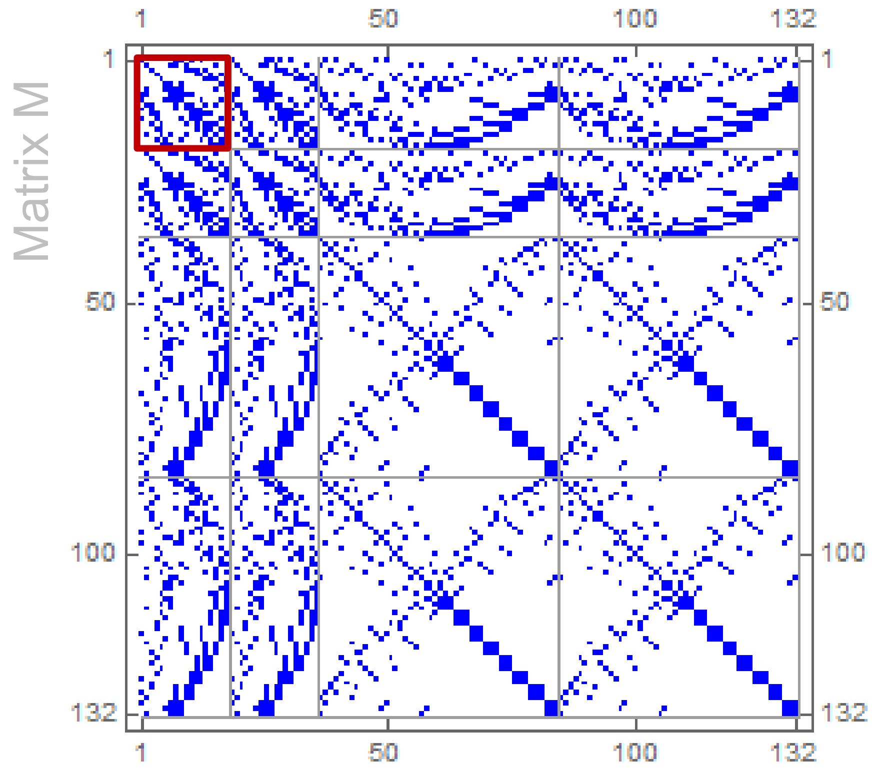


Numerical Examples

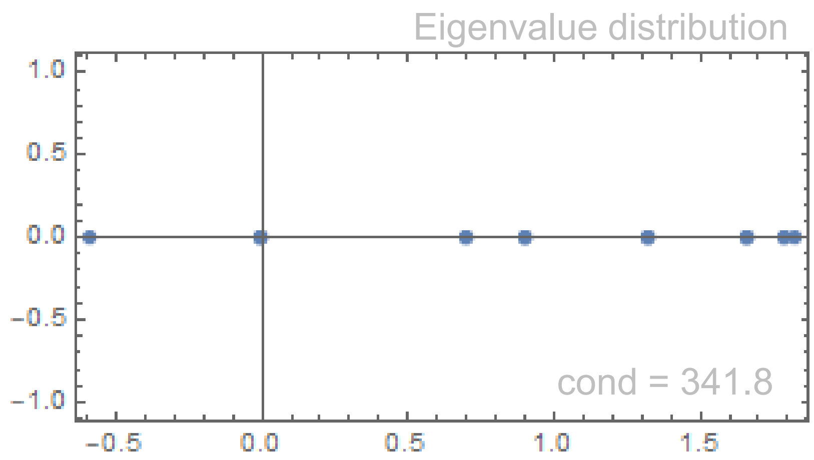
- Properties of the System Matrix

$$\underbrace{(A - \lambda_\tau B)}_{M}\, x = r$$

  - Population pattern for the loss-less case



M_{11} indefinite



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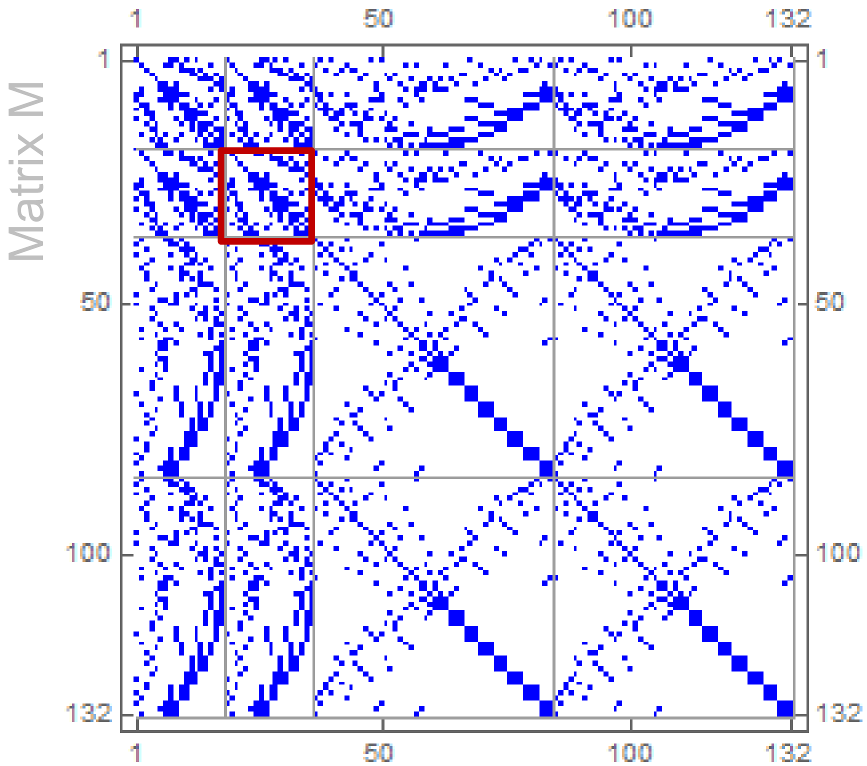
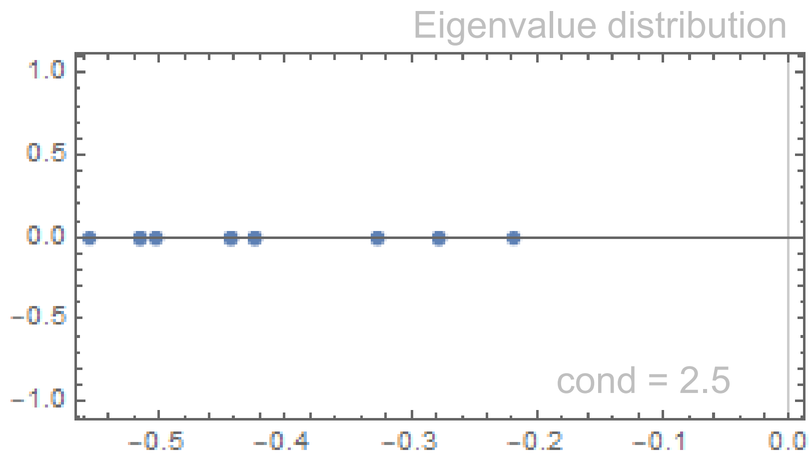


M_{22} negative definite



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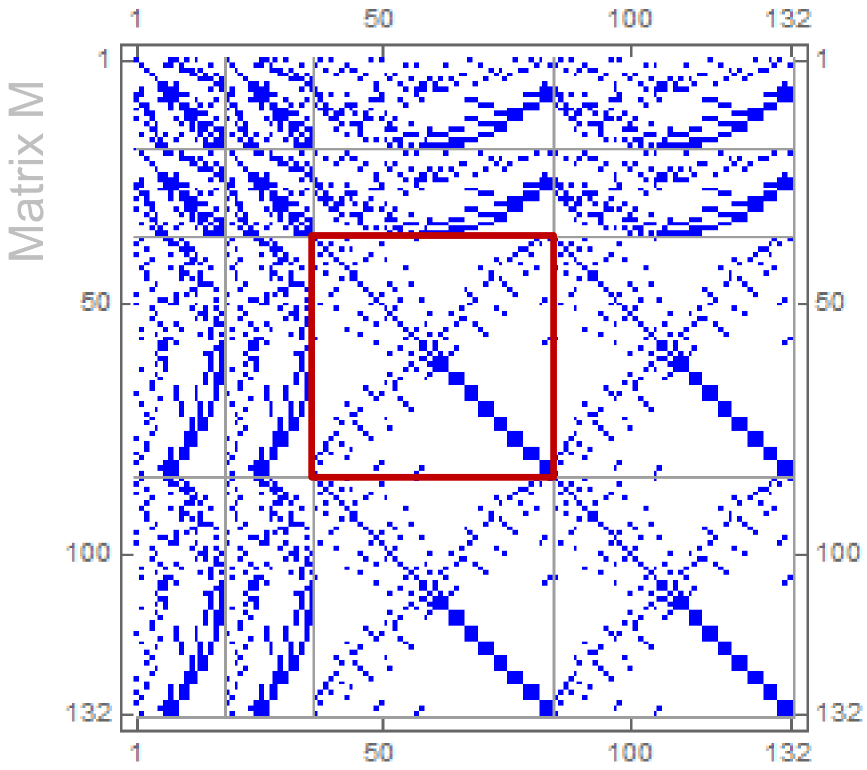
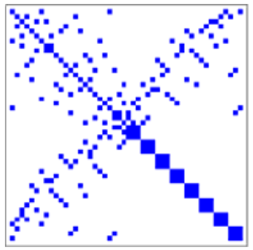
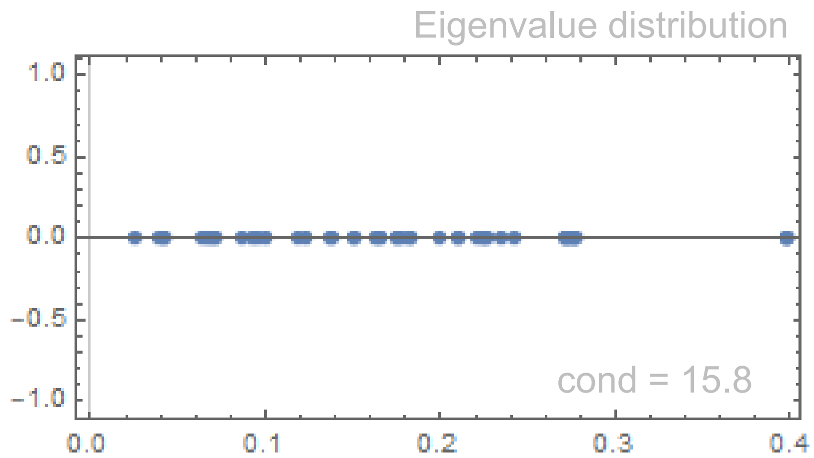




M_{33} positive definite



Numerical Examples

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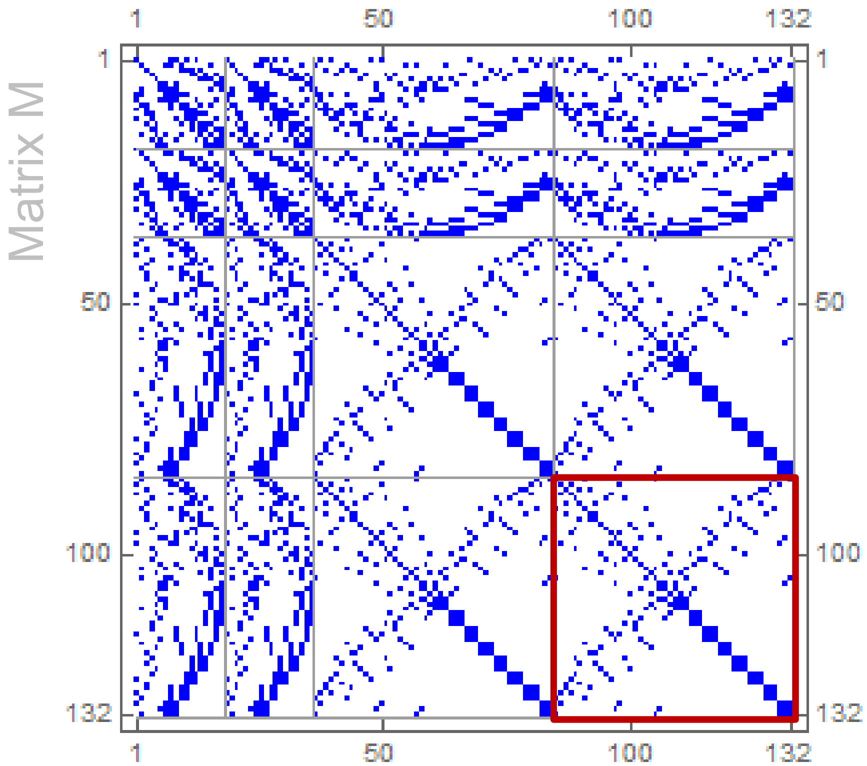
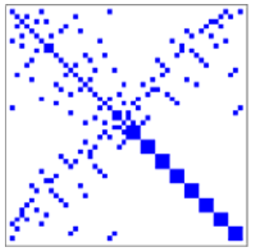
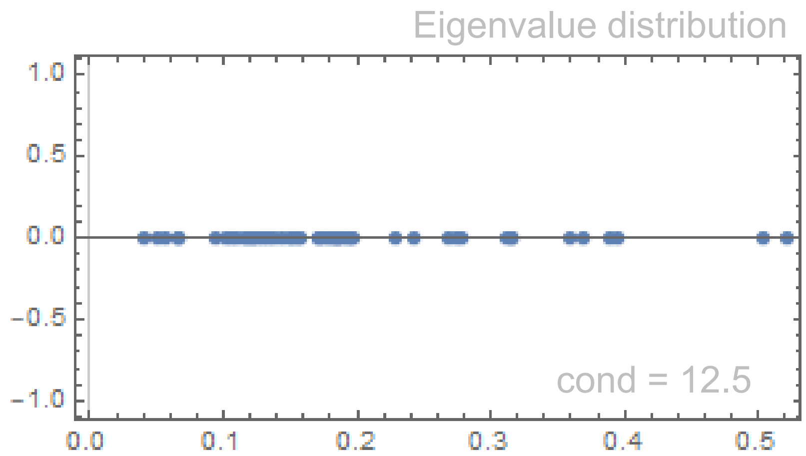
$$\underbrace{(A - \lambda_\tau B)}_{M}\, x = r$$





M_{44} positive definite



Numerical Examples

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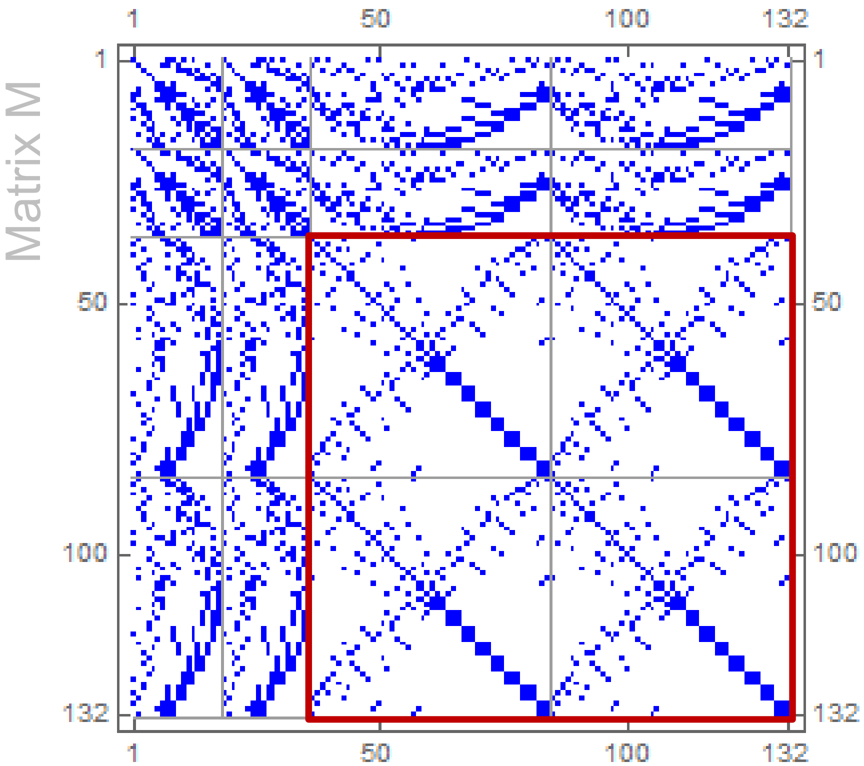
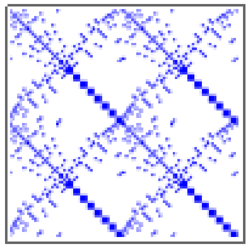
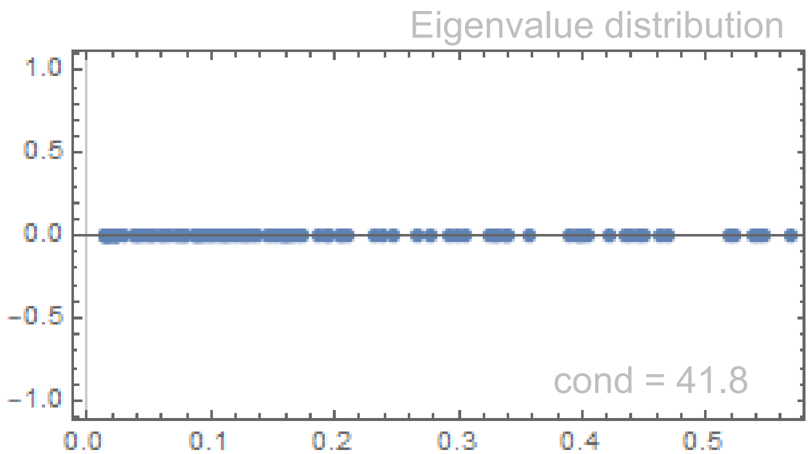
- Properties of the System Matrix
  - Population pattern for the loss-less case

$$\underbrace{(A - \lambda_\tau B)}_{M}\, x = r$$





M positive definite



Numerical Examples

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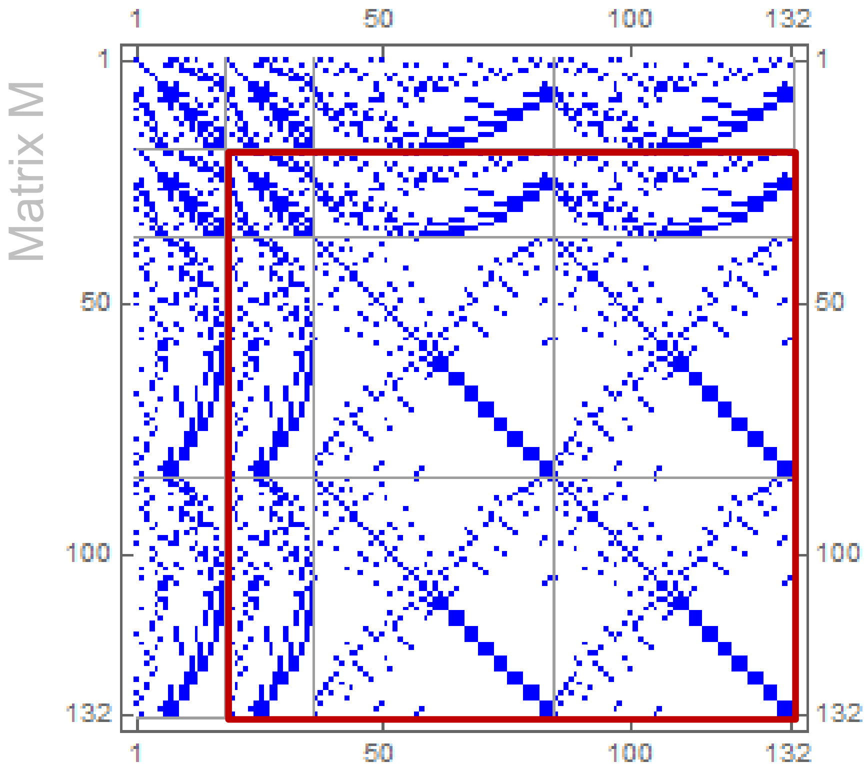
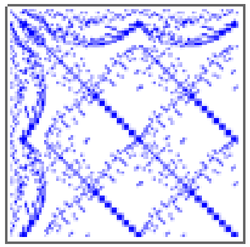
$$\underbrace{(A - \lambda_\tau B)}_{M}\, x = r$$





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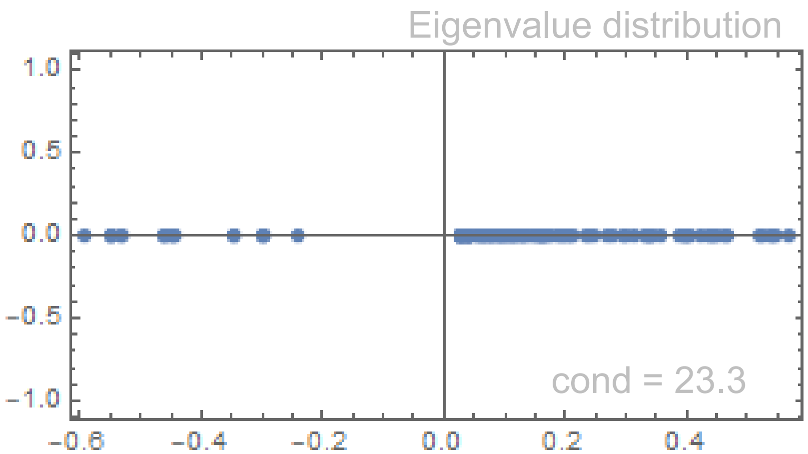

Numerical Examples

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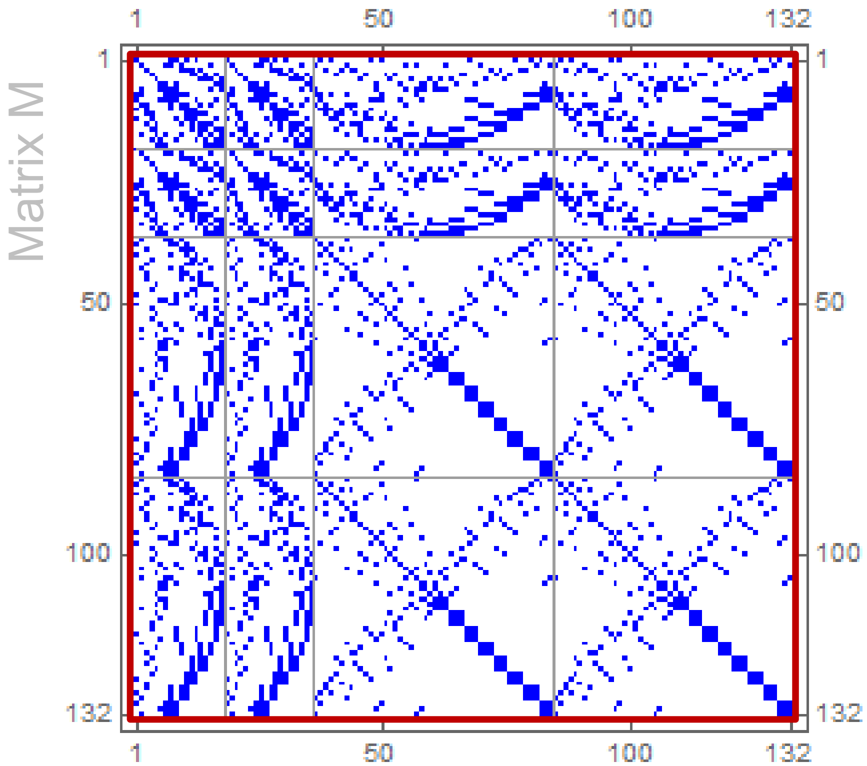

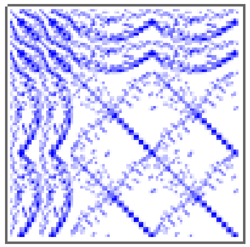

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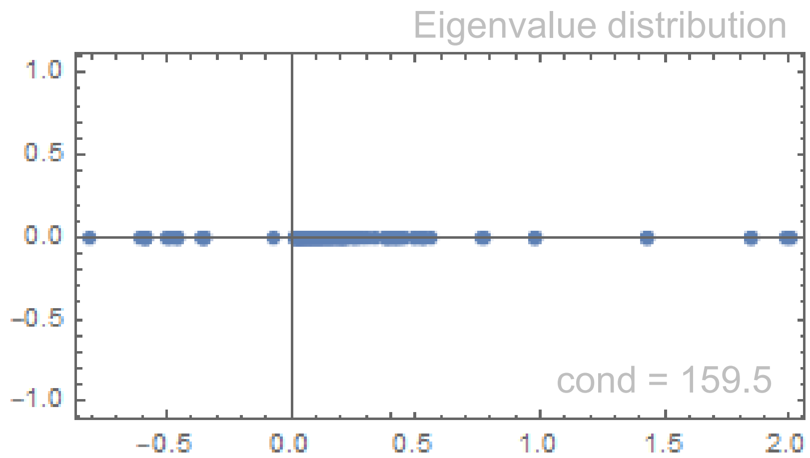

Numerical Examples

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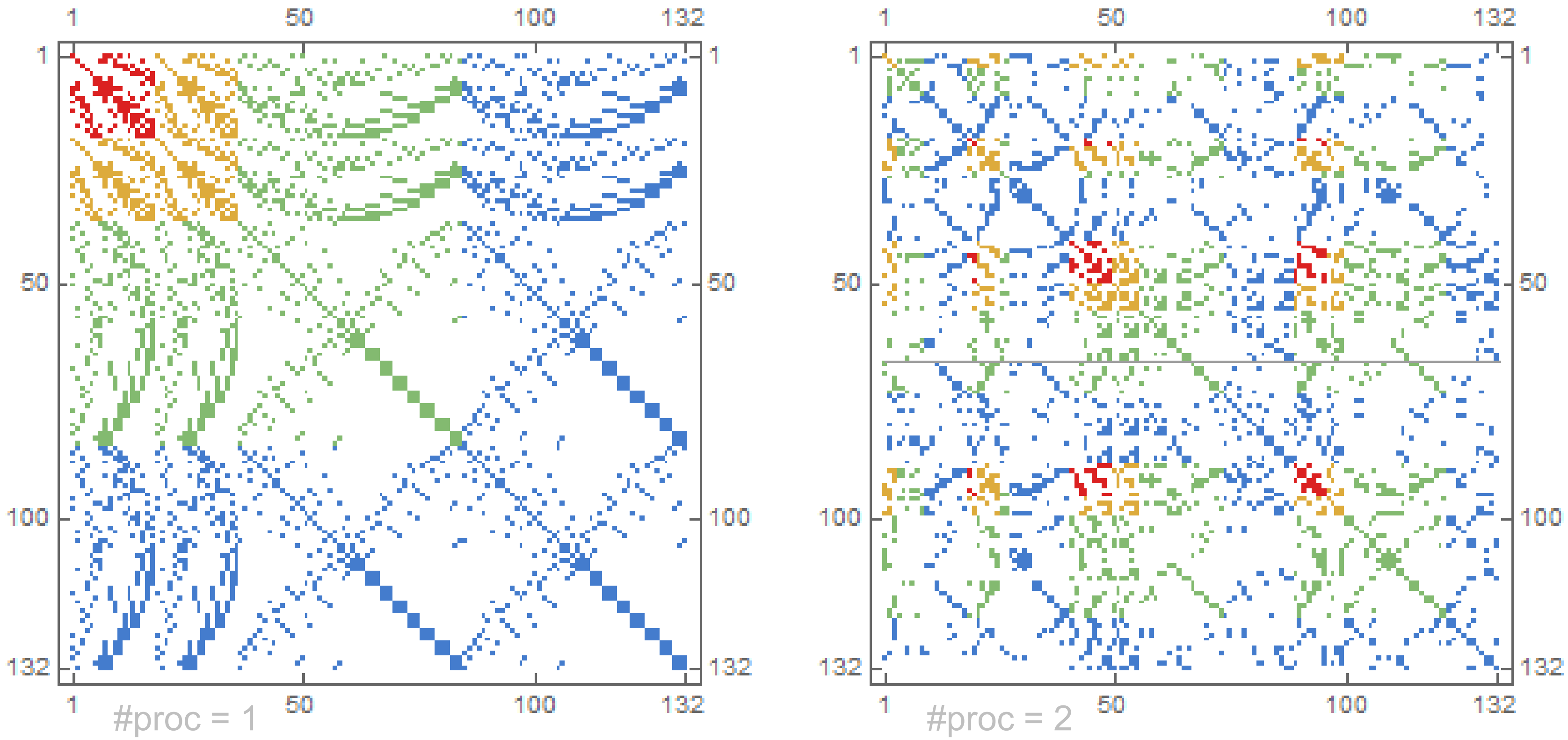

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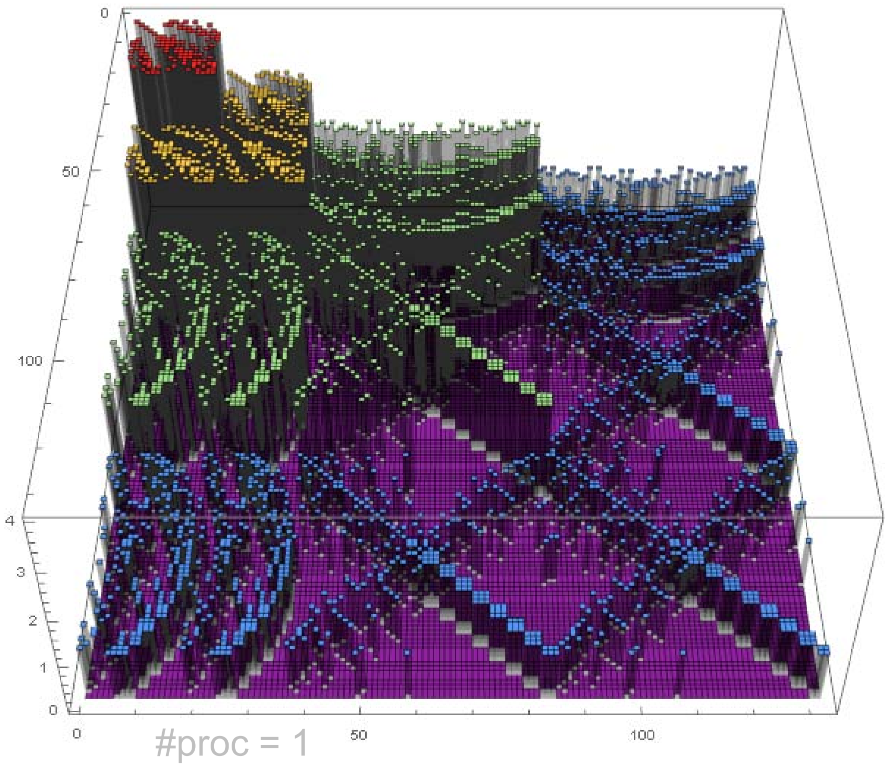
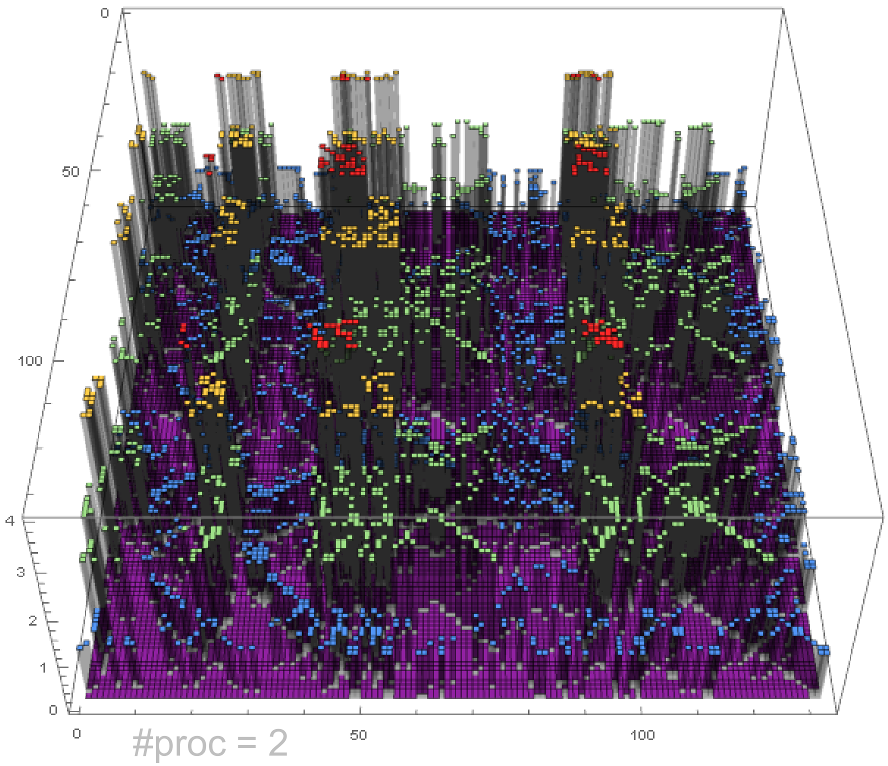
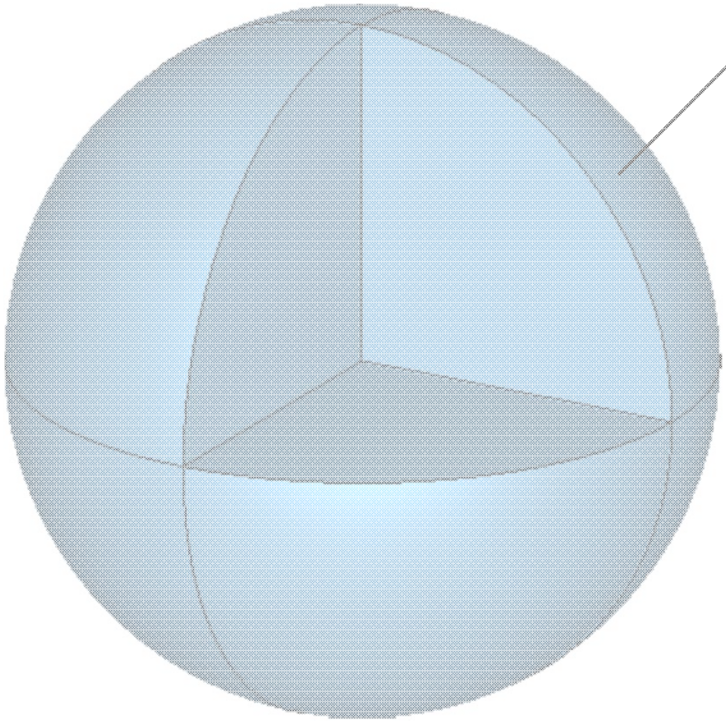
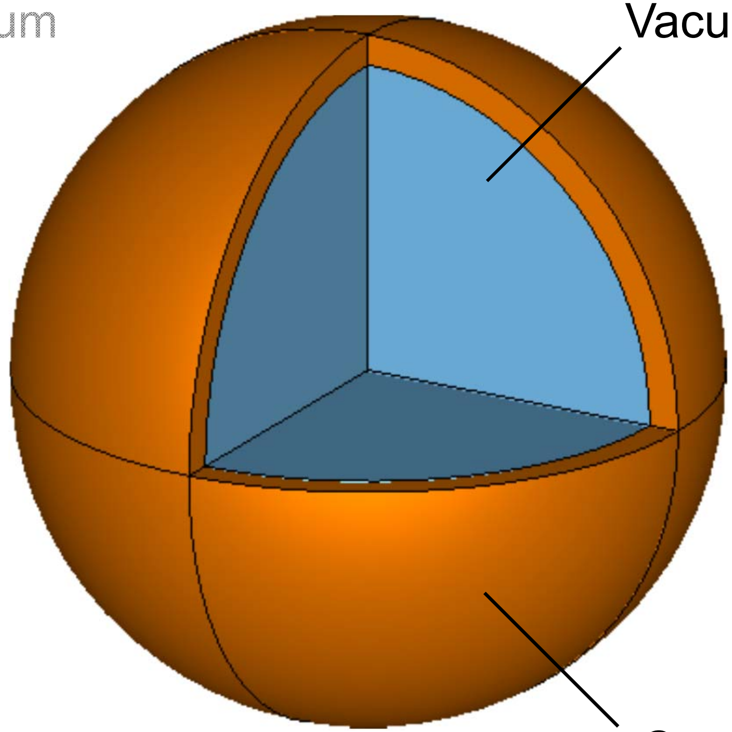




Numerical Examples

- Spherical Resonators





Numerical Examples

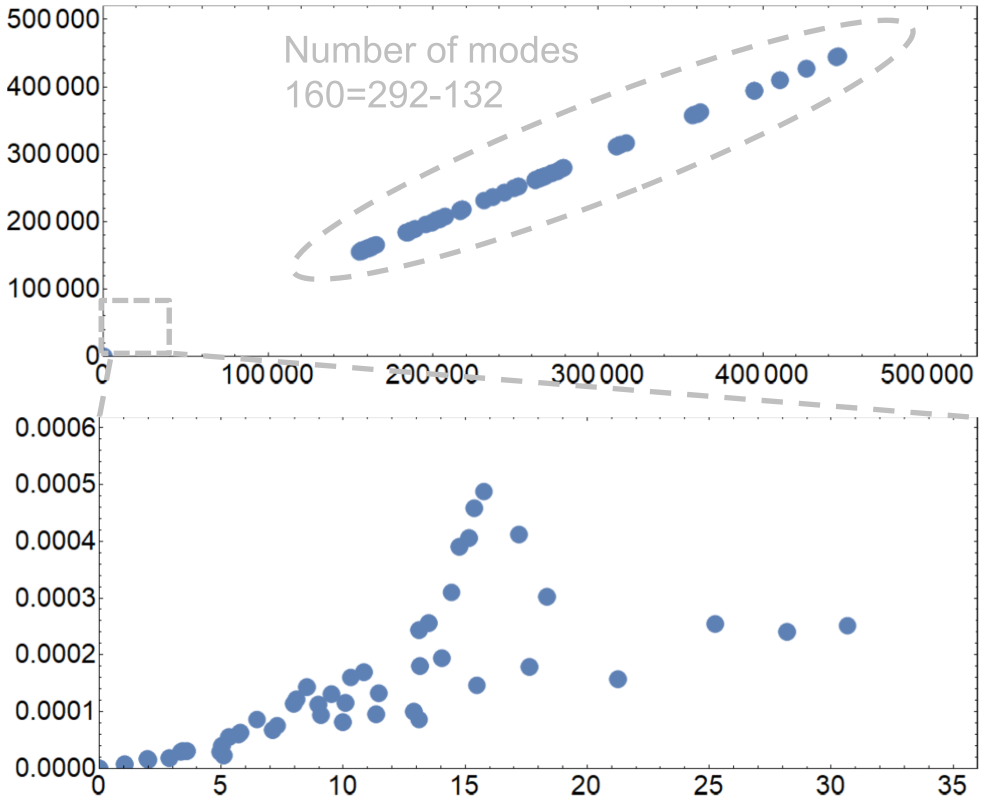
- Properties of the Matrix Pencil
  - Eigenvalue distribution

$$A'\,x = \lambda'\,B'\,x$$

$$\underbrace{\frac{A'}{s}}_{A}\,x = \underbrace{\frac{\lambda'}{s^2}}_{\lambda}\,\underbrace{sB'}_{B}\,x$$

$$A\,x = \lambda\,B\,x$$

Choose scaling such that $\lambda_\tau = 1$



Numerical Examples

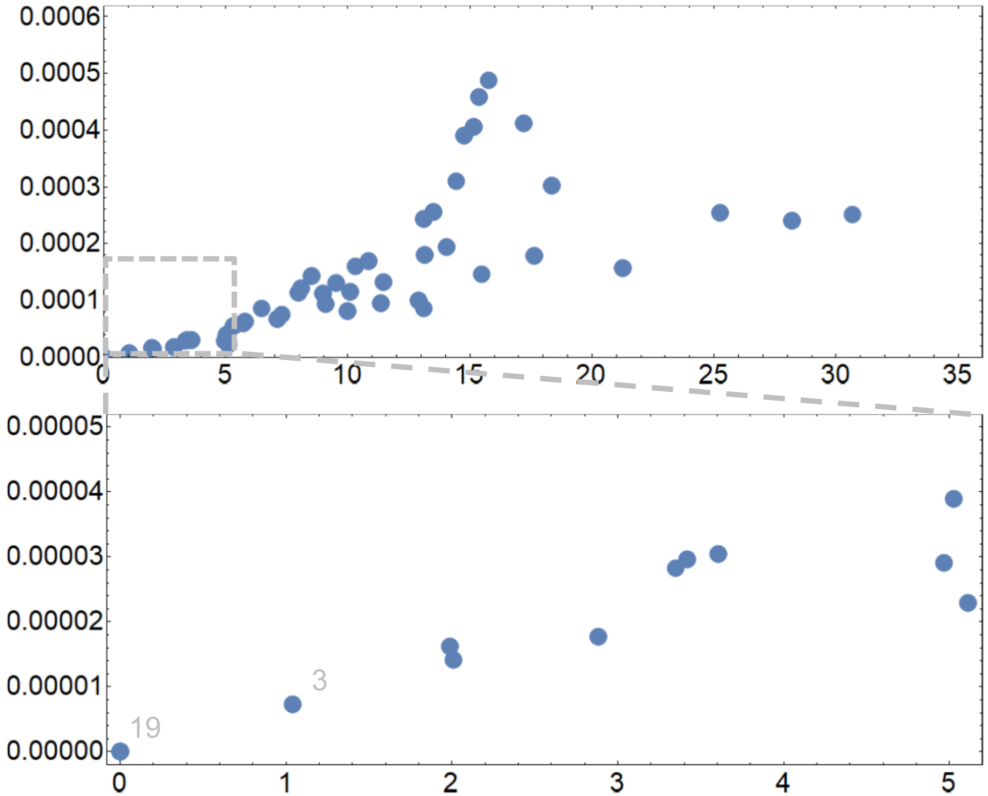
- Properties of the Matrix Pencil
  - Eigenvalue distribution

$$A' x = \lambda' B' x$$

$$\underbrace{\frac{A'}{s}}_{A} x = \underbrace{\frac{\lambda'}{s^2}}_{\lambda} \underbrace{sB'}_{B} x$$

$$A x = \lambda B x$$

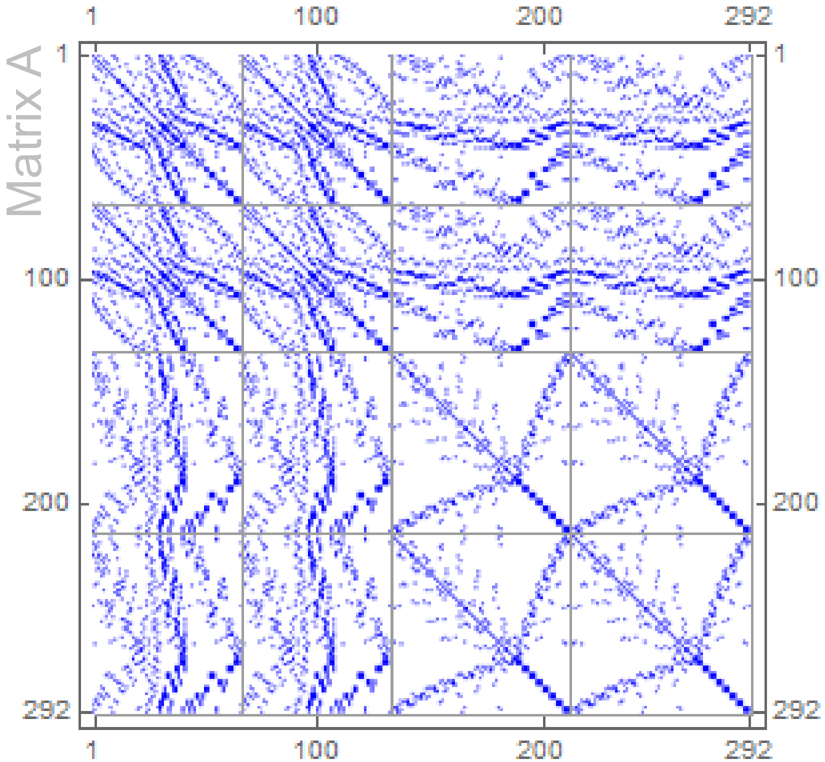
Choose scaling such that $\lambda_\tau = 1$

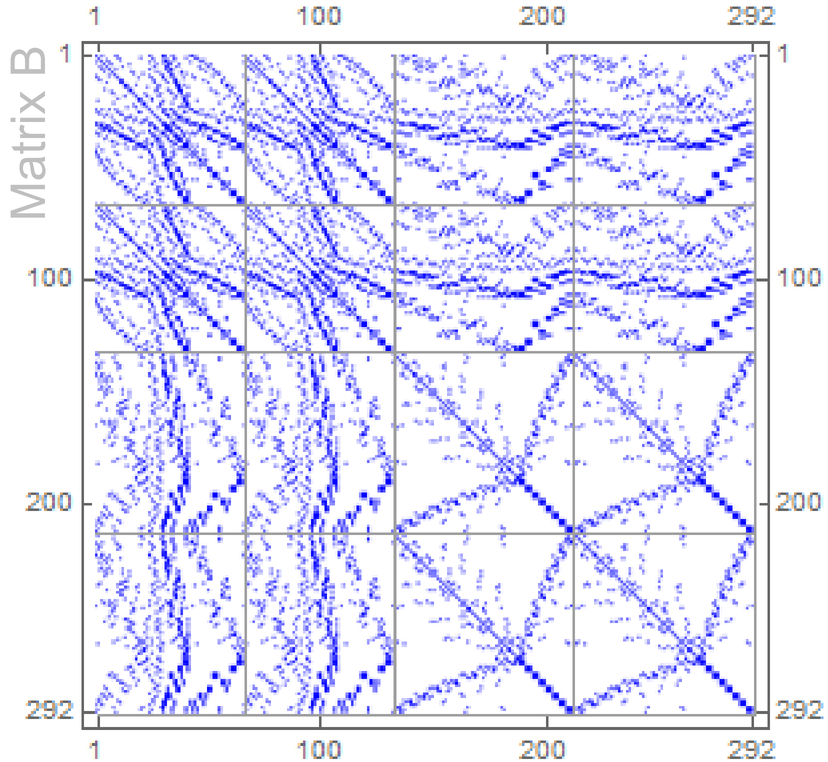


Numerical Examples

- Properties of the Matrix Pencil
  - Population pattern for the lossy case

$$A\,x = \lambda\,B\,x$$





Numerical Examples

- Properties of the System Matrix
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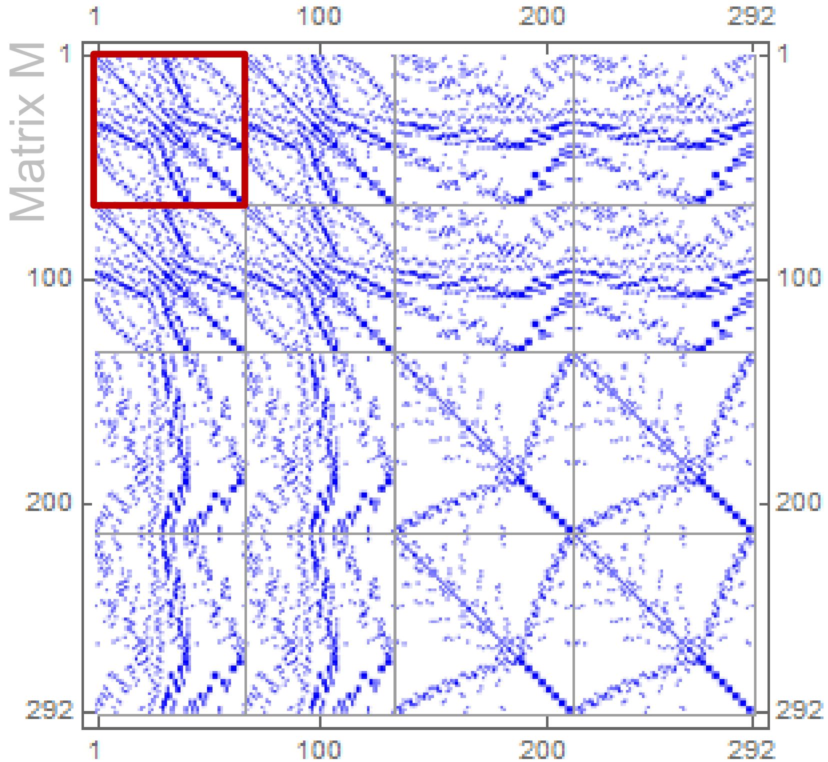
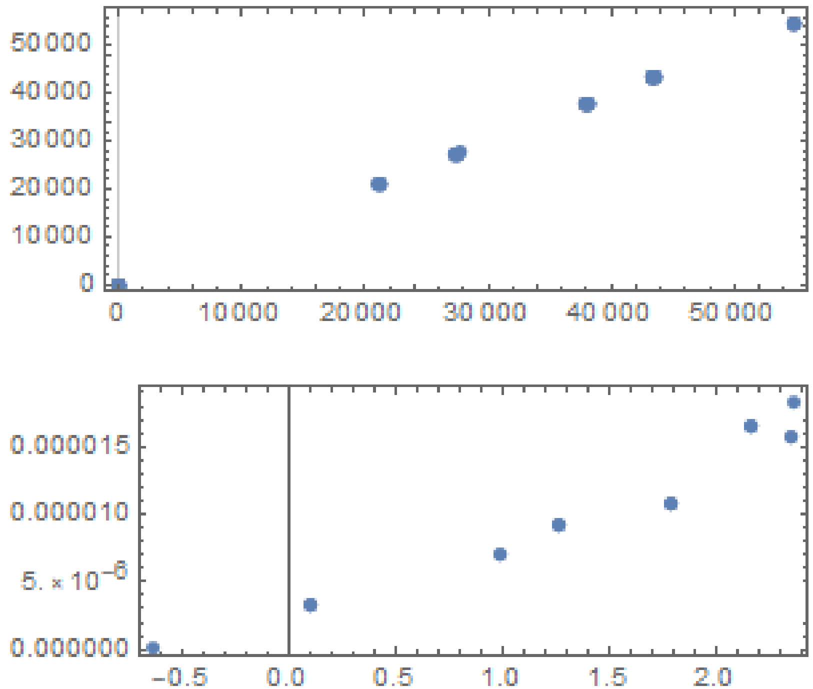
$$\underbrace{(A - \lambda_\tau B)}_{M}\, x = r$$



Eigenvalue distribution



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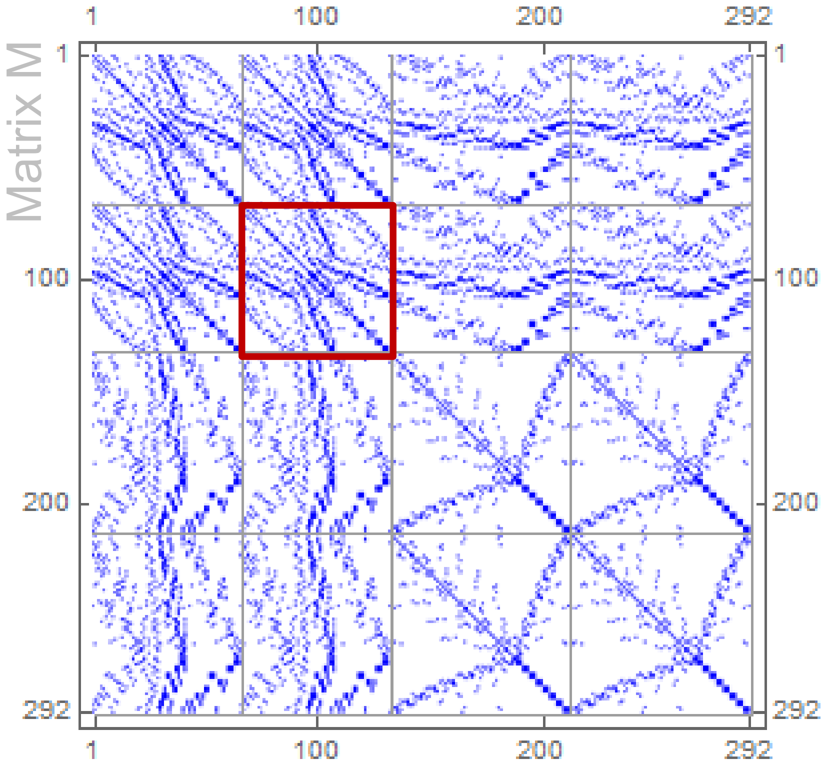
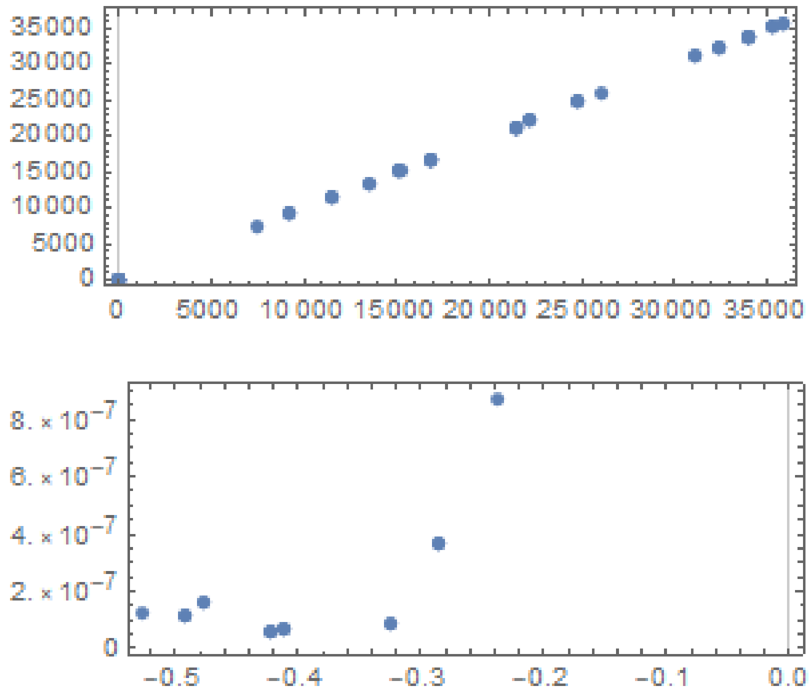


Eigenvalue distribution

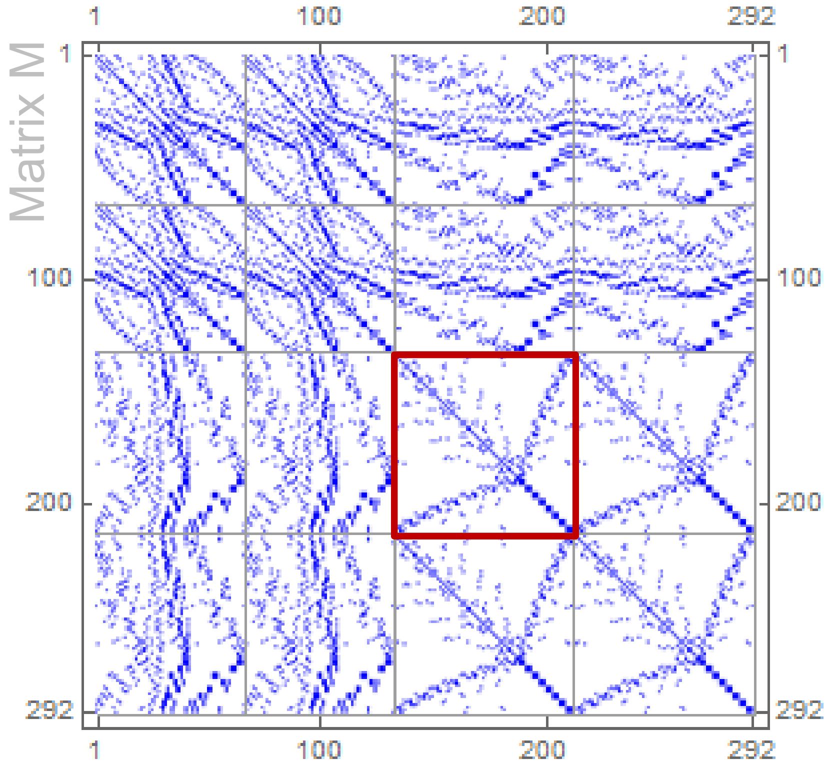


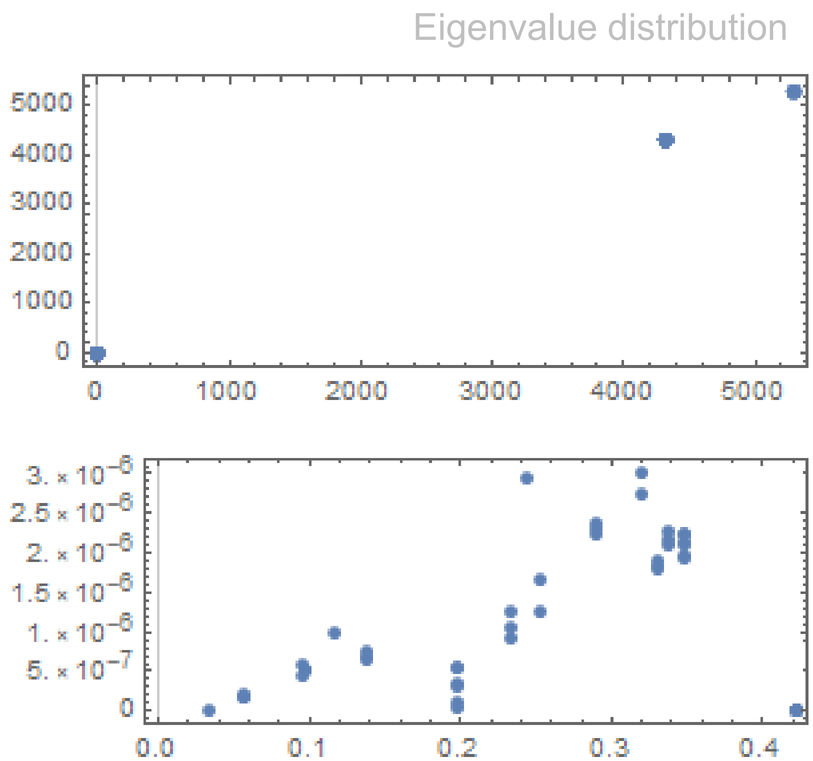
Numerical Examples

- Properties of the System Matrix

$$\underbrace{(A - \lambda_\tau B)}_{M} x = r$$

  - Population pattern for the lossy case





Numerical Examples

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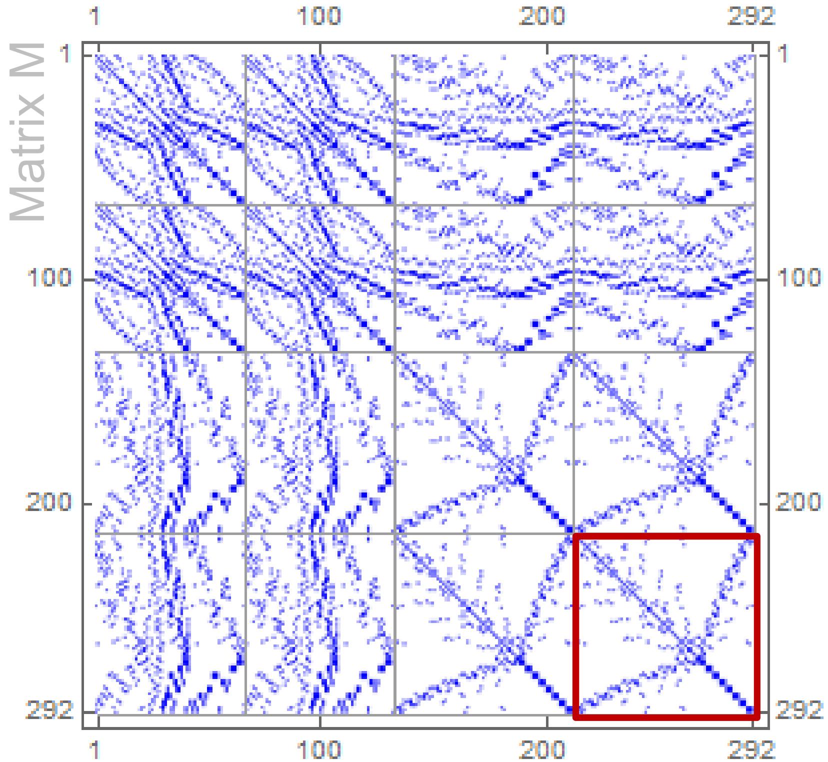

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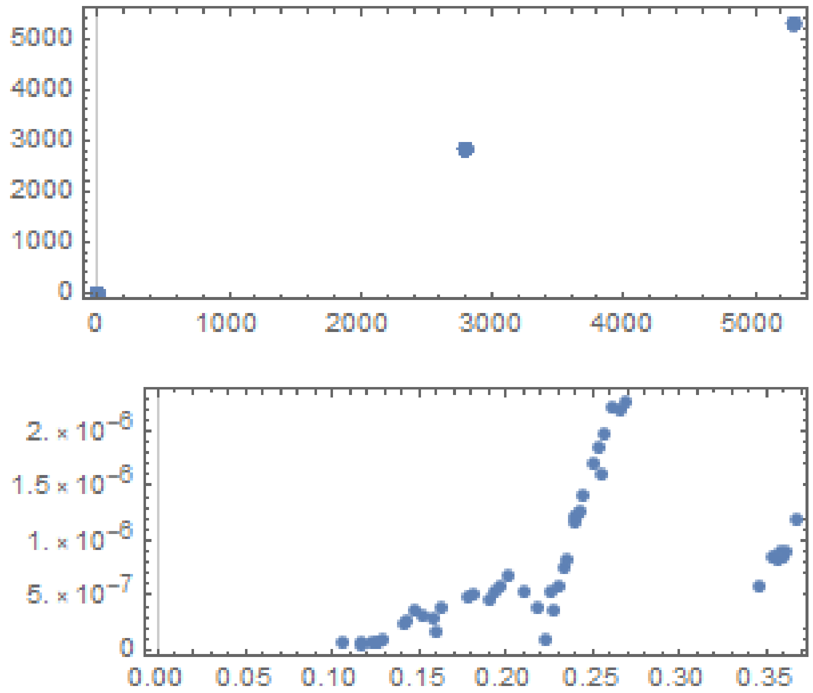

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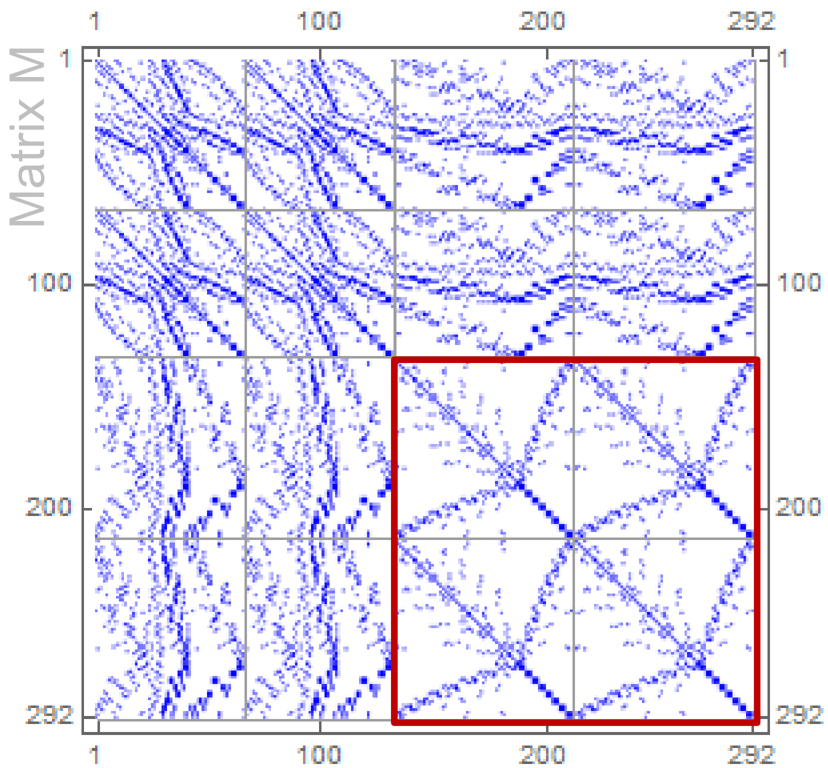

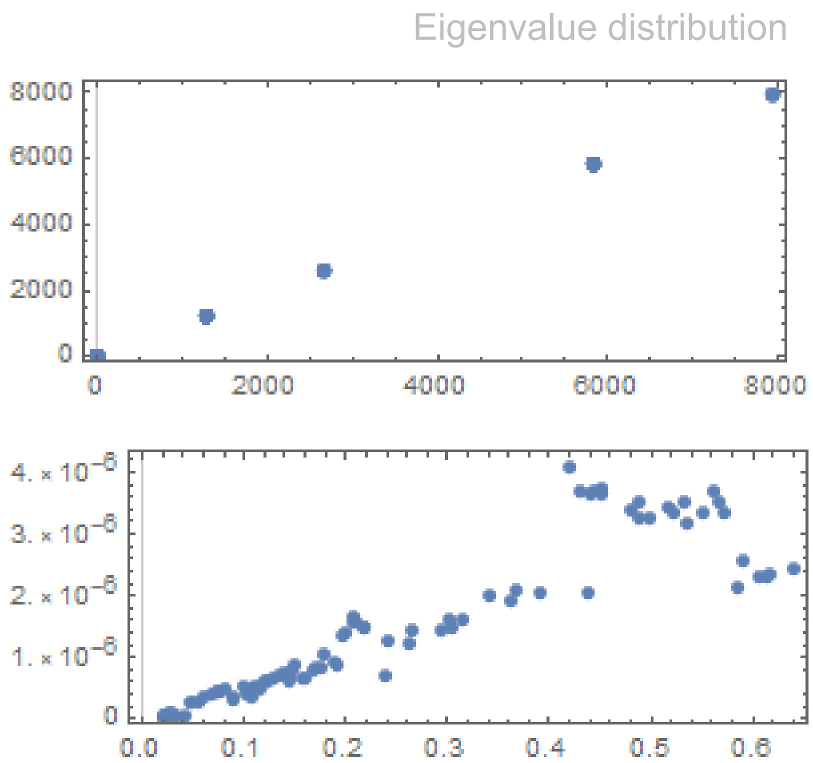

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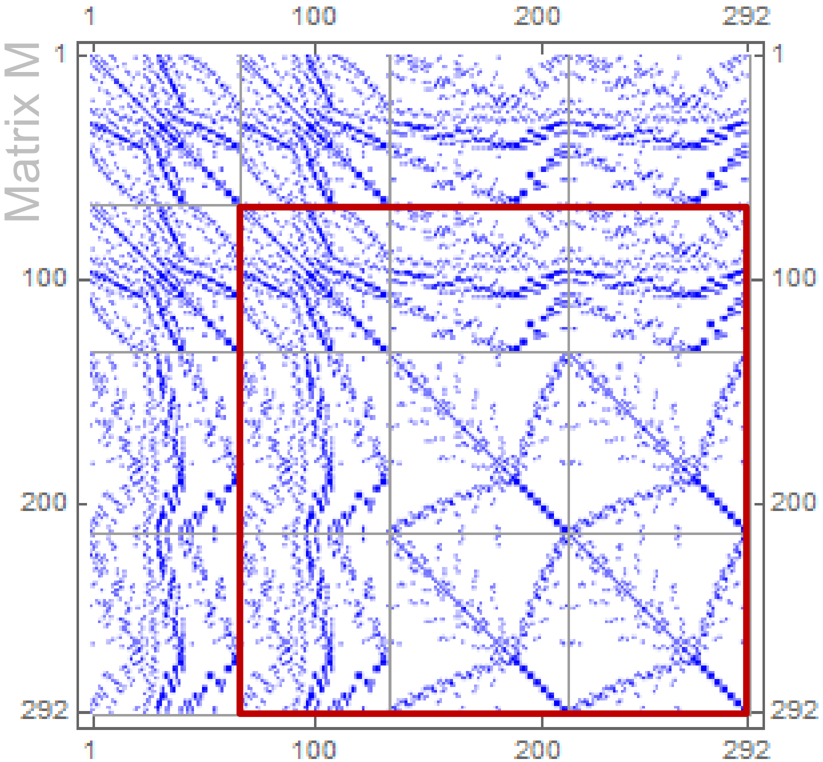

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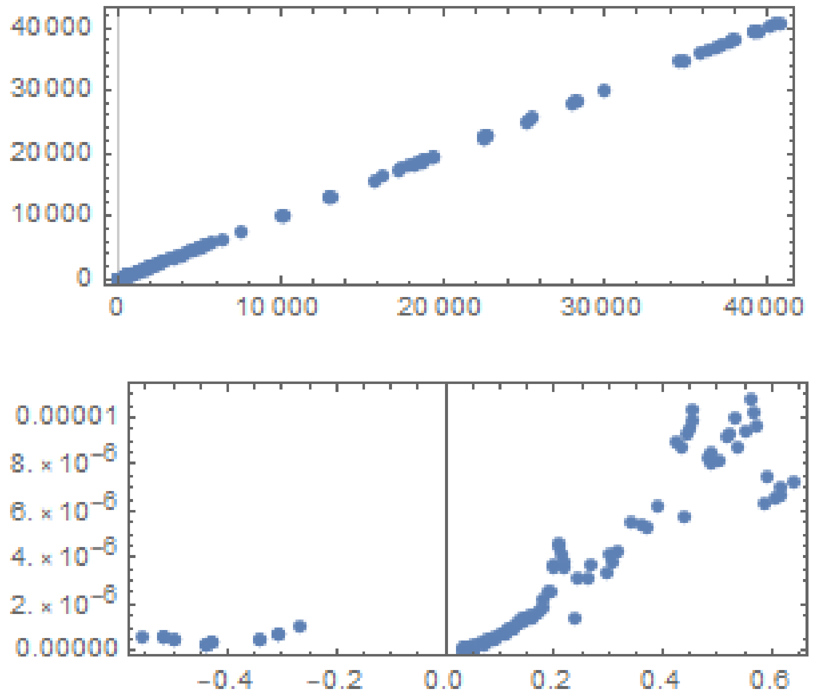

Numerical Examples

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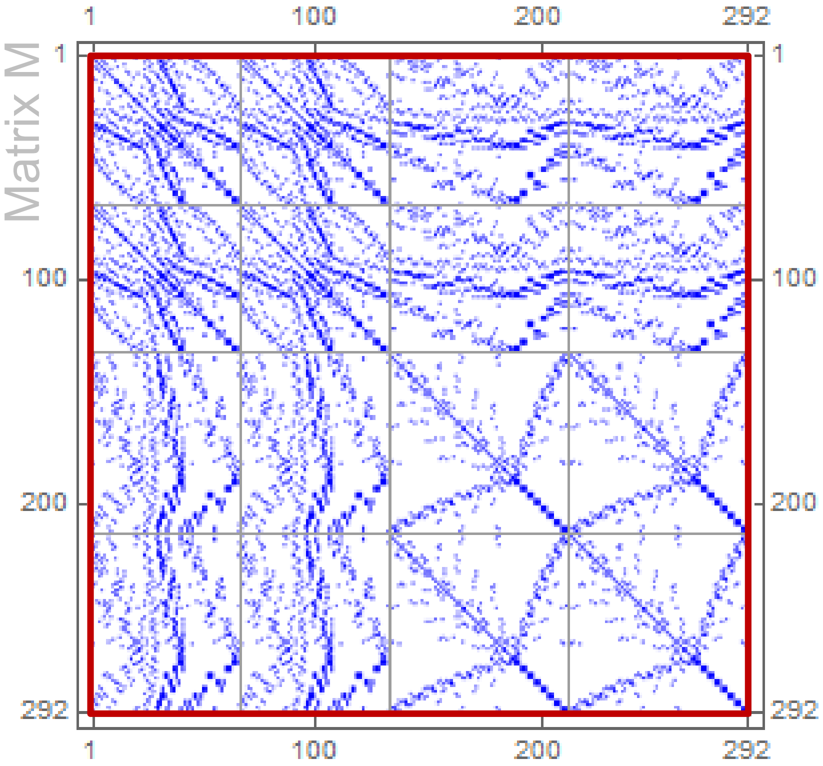

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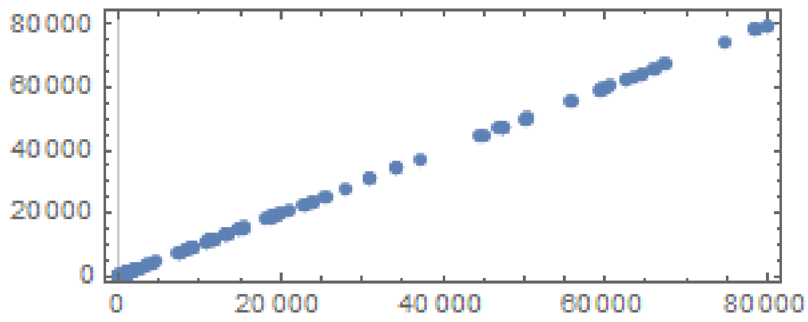
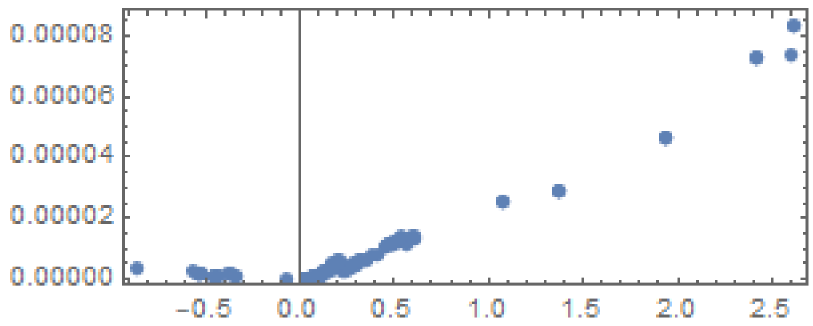
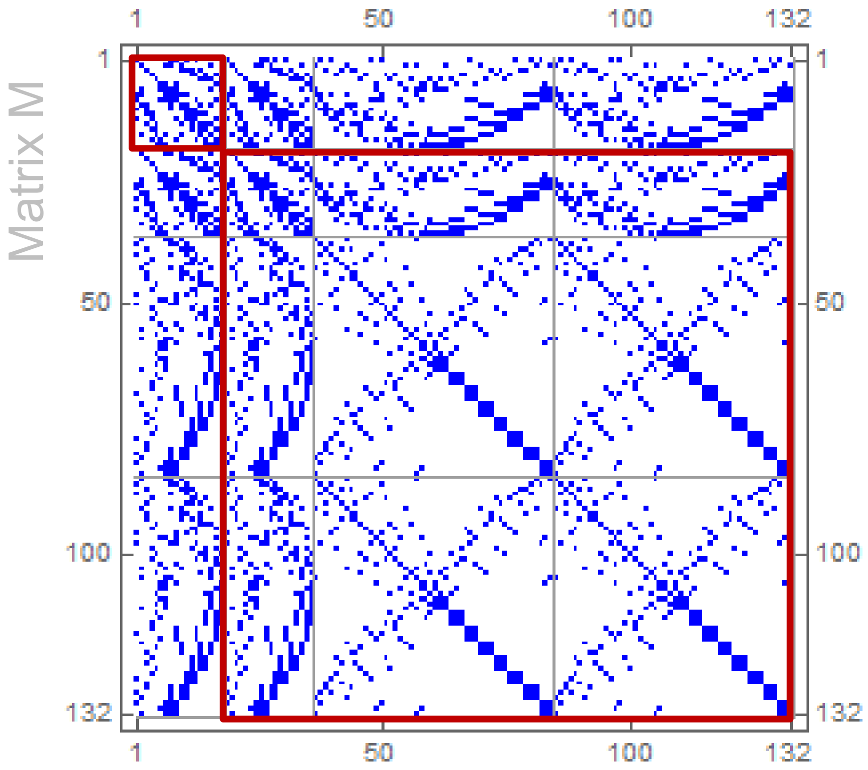




Numerical Examples

- Selection of an Efficient Preconditioner
  - Two-Level Approach for higher-order field approximation



System matrix

$$\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

Preconditioner (left)

$$\begin{pmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{pmatrix} \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

Numerical Examples

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- Selection of Available Preconditioner (PETSc)
  - Block Jacobi

$$\begin{pmatrix} M_{11}^{-1} & 0 \\ 0 & M_{22}^{-1} \end{pmatrix}$$

  - Block Gauss-Seidel

$$\begin{pmatrix} I & 0 \\ 0 & M_{22}^{-1} \end{pmatrix} \begin{pmatrix} I & 0 \\ -A_{21} & I \end{pmatrix} \begin{pmatrix} M_{11}^{-1} & 0 \\ 0 & I \end{pmatrix}$$

  - Symmetric block Gauss-Seidel

$$\begin{pmatrix} M_{11}^{-1} & 0 \\ 0 & I \end{pmatrix} \begin{pmatrix} I & -A_{12} \\ 0 & I \end{pmatrix} \begin{pmatrix} M_{11} & 0 \\ 0 & M_{22}^{-1} \end{pmatrix} \begin{pmatrix} I & 0 \\ -A_{21} & I \end{pmatrix} \begin{pmatrix} M_{11}^{-1} & 0 \\ 0 & I \end{pmatrix}$$

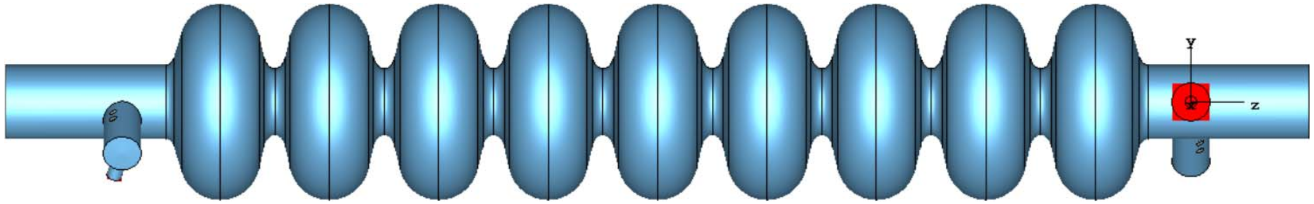
Reference: PETSc Users Manual

Outline

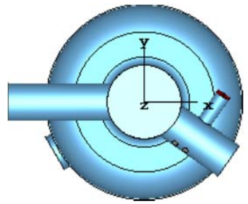
- Motivation
- Computational model
  - Numerical problem formulation
- Numerical examples
  - Spherical cavity (lossless / lossy)
    Properties of the system matrix
  - 1.3 GHz structure (single cavity)
    Evaluation of promising preconditioner and related linear solvers
- Summary / Outlook

Numerical Examples

- Eigenanalysis of a single TESLA Cavity
  - Concentration on the fundamental mode



side view



front view

  - JD Eigenvalue Solver, subspace expansion
    - SuperLU (direct solver for large sparse systems of linear equations)
    - Symmetric block Gauss-Seidel (two level strategy)
      - M_{11}: Direct solver "Super LU" as preconditioner
      - M_{22}: Diagonal preconditioner

Numerical Examples

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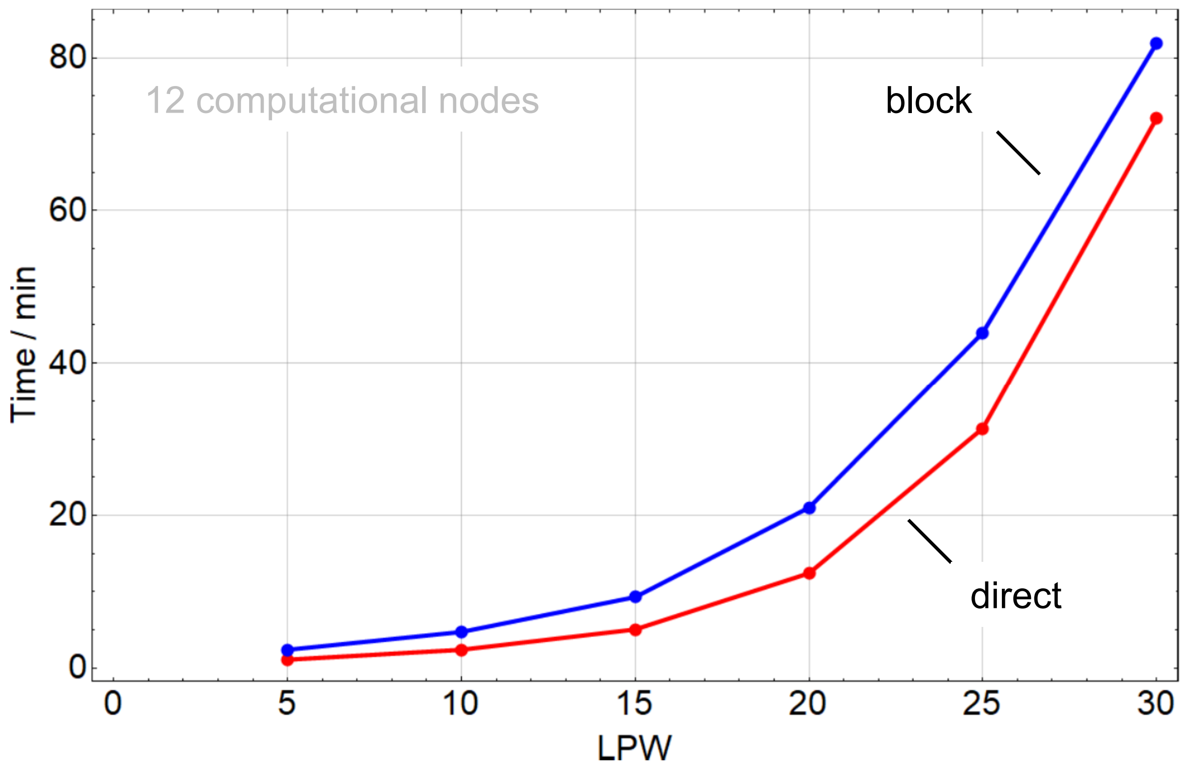
- Eigenanalysis of a single TESLA Cavity
  - Jacobi-Davidson Eigenvalue-Solver Statistics



f_{max}=1.5 GHz

Numerical Examples

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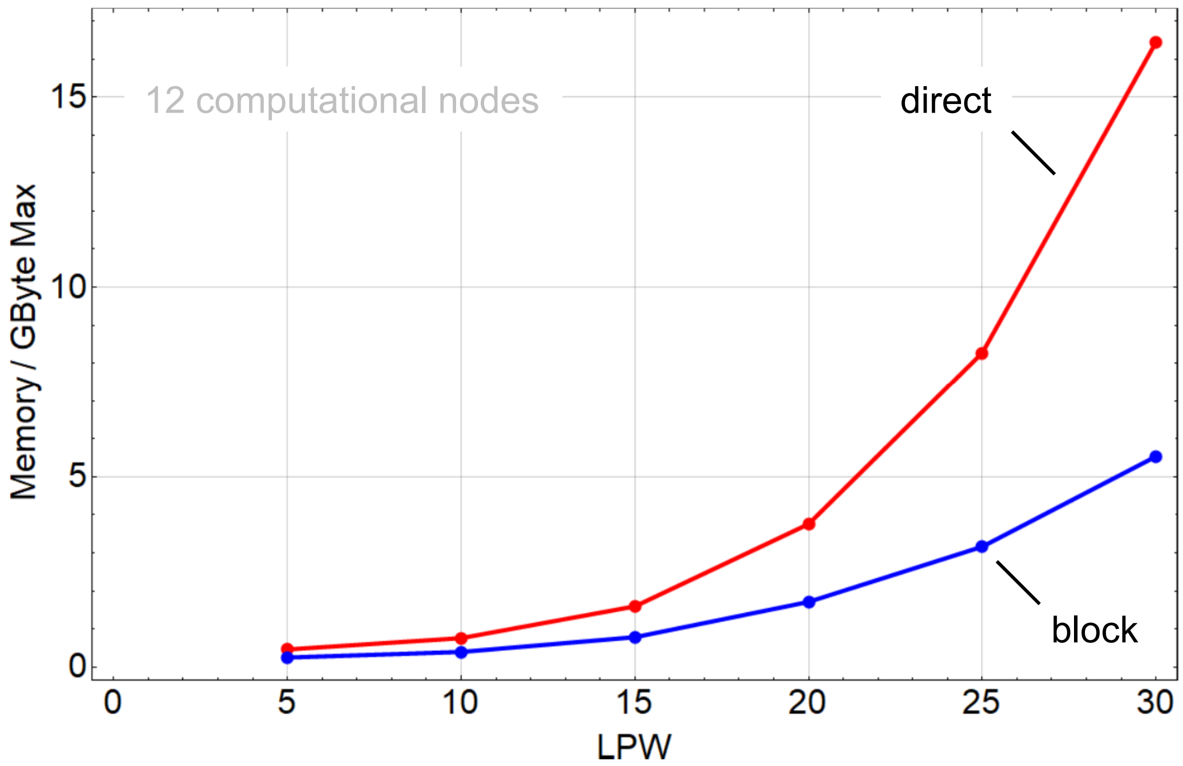

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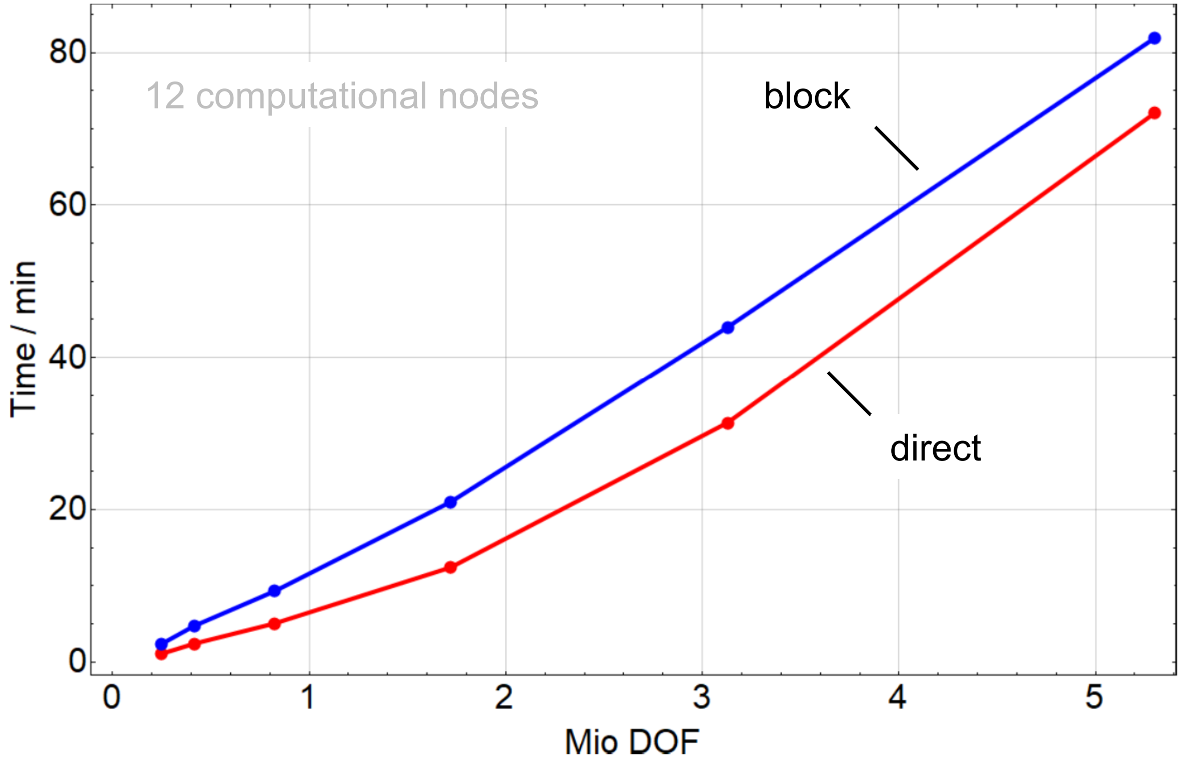

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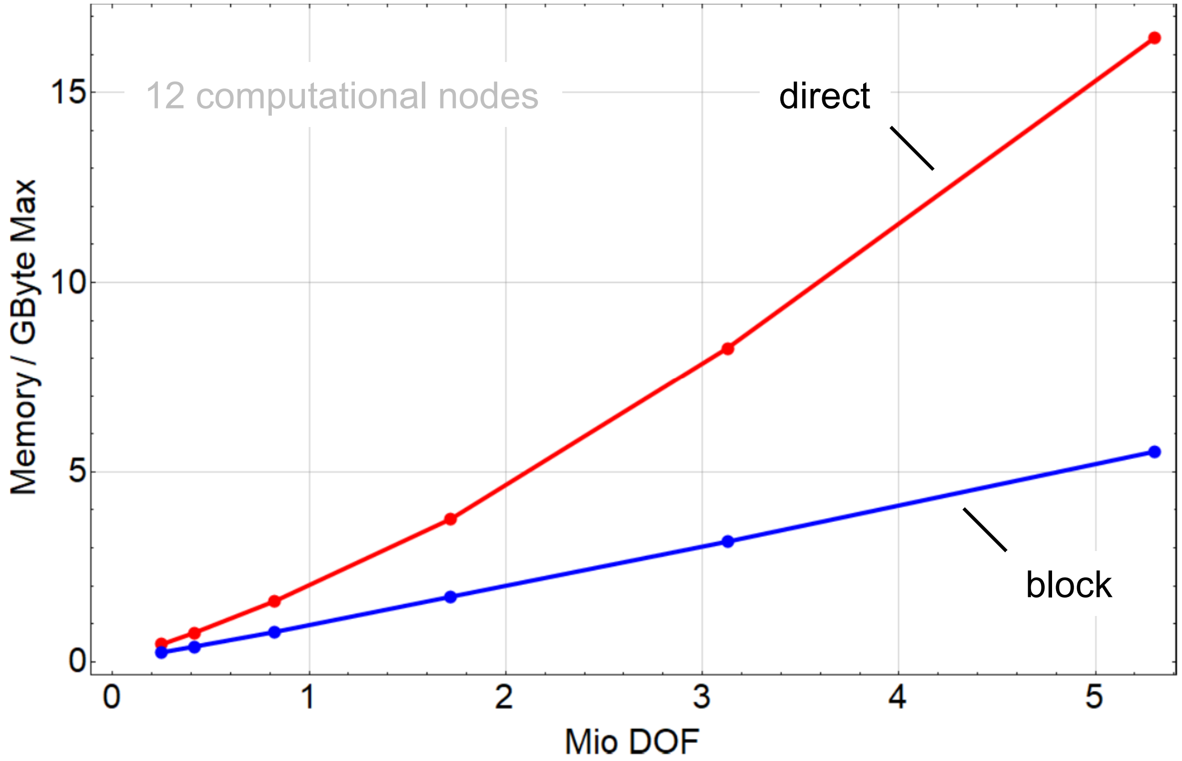

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TECHNISCHE UNIVERSITÄT DARMSTADT

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Summary / Outlook

- Summary
  - Implementation of a block preconditioner into a nonlinear Jacobi-Davidson eigenvalue solver (PETSc index sets)
  - Block structure is motivated by the hierarchical setup of the underlying FEM basis functions
  - Flexible selection of individual block solver from the command line without recompiling the code (PETSc feature)
  - Usage of block solver can reduce total memory consumption
- Outlook
  - Implementation of periodic boundary condition started