Contour Integral Method for the Simulation of Accelerator Cavities

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TECHNISCHE UNIVERSITÄT DARMSTADT

DESY meeting (14.11.2017)

Outline of the Talk

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- Motivation
  - Iterative methods
  - Contour integral methods
- Formulation
  - Mathematical model
  - Eigenvalue algorithms
  - Contour integral methods
  - Multigrid method as a preconditioner
- Implementation
- Preliminary Results
- Possible Improvements

Presentation Outline

Motivation

Problem statement

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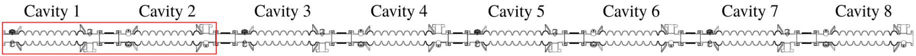
- the problem is large and sparse;
- the number of eigenvalues is large;

Figure: Chain of cavities (from [1])



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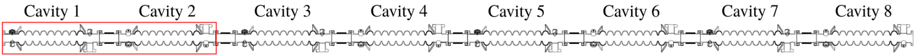

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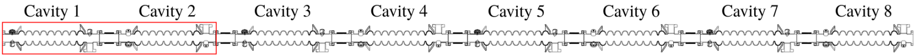

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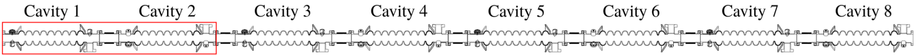

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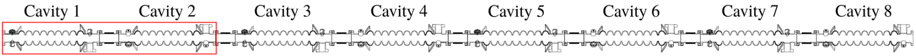

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- Iterative methods: Jacobi-Davidson [2], Arnoldi, Lanczos, etc.
- Contour integral methods: Beyn methods [3], resolvent sampling based Rayleigh-Ritz method (RSRR) [4], etc.

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Lossless accelerator cavity: eigenvalues are on real axis

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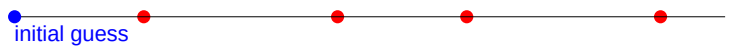

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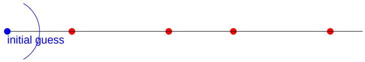

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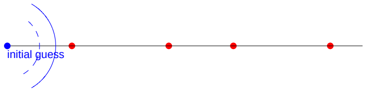

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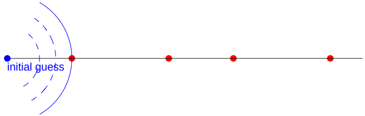

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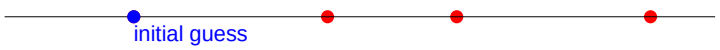

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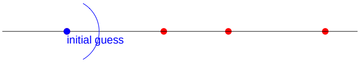

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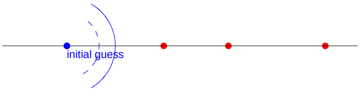

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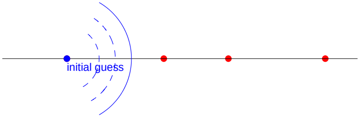

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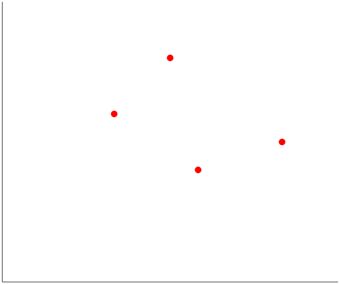

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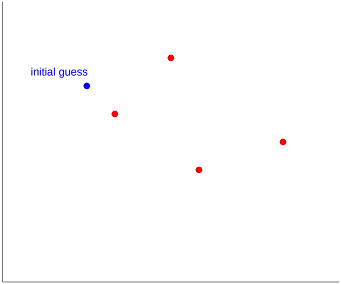

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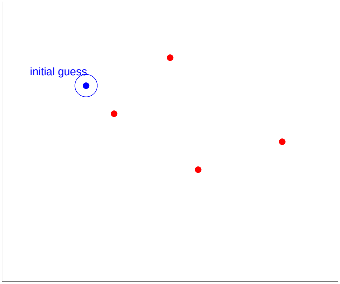

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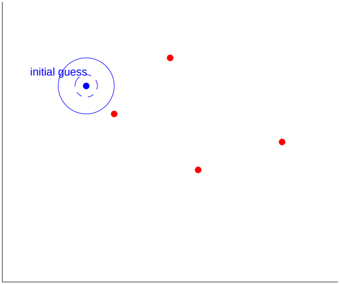

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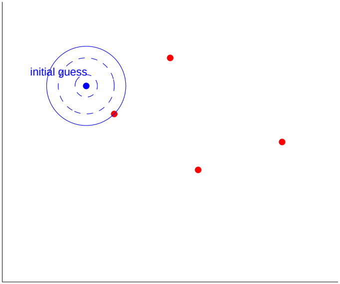

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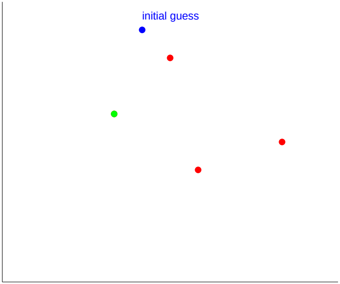

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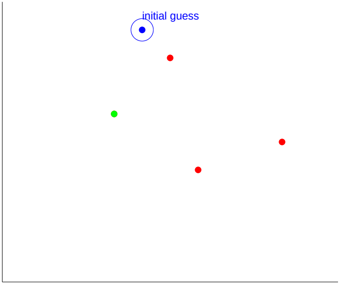

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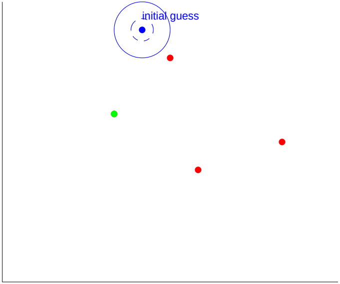

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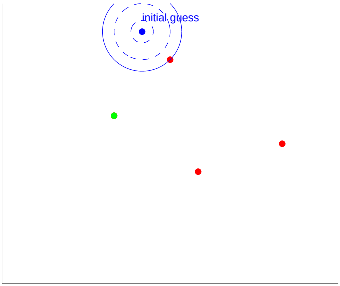

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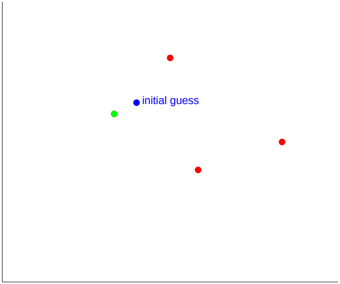

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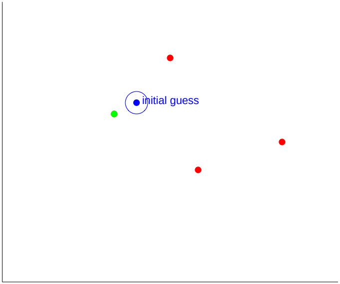

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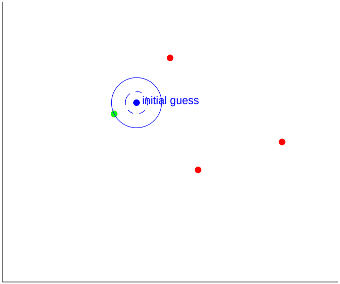

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- a previously determined eigenvalue!!!!!

Presentation Outline

Motivation

Contour integral methods

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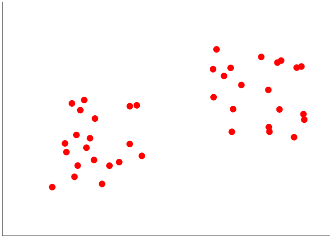
An accurate computation of eigenpairs inside a region enclosed by a non-self-intersecting curve.



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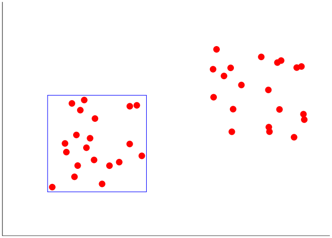

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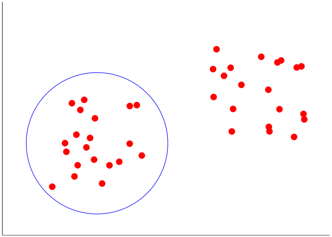

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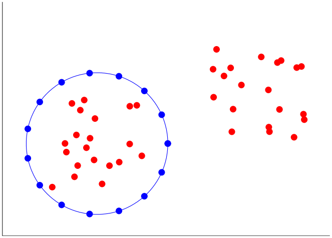

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- most computation is spent to solve linear equation systems at different interpolation points which can be parallelized.

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Formulation
Mathematical model

The combination of Maxwell-Ampère equation and the Maxwell-Faraday equation results in the double-curl equation

$$\nabla \times \frac{1}{\mu} \nabla \times \vec{E} - j\omega\sigma\vec{E} = \varepsilon\omega^2\vec{E} \tag{1}$$

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Applying the Galerkin's approach to discretize (1) results in an eigenvalue problem

$$A^{3D}\vec{x} + j\omega\mu_0 C^{3D}\vec{x} - \omega^2\mu_0\varepsilon_0 B^{3D}\vec{x} = 0 \qquad (2)$$

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$$\boxed{P(\omega)\vec{x} = 0} \quad (3)$$

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obtain matrix Q

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Eigenvalue algorithms

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↓

Project the original NEP to a reduced NEP — using Rayleigh-Ritz procedure:
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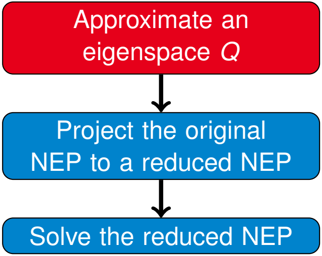

obtain matrix Q

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↓ Project the original NEP to a reduced NEP	using Rayleigh-Ritz procedure: $P_Q(z) = Q^H P(z) Q$
↓ Solve the reduced NEP	solve $P_Q(z)g = 0$ for eigenvalues z and eigenvectors g
↓ Compute eigenpairs of the original NEP	same eigenvalues as for the reduced problem; eigenvectors $x = Qg$

Formulation
Eigenvalue algorithms

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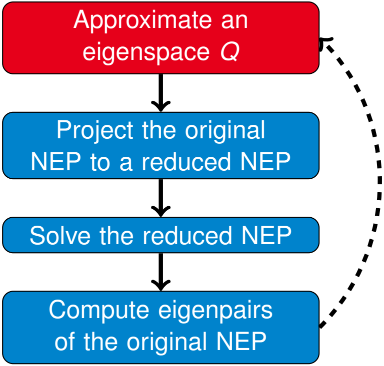

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Some basic spectral theory

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The resolvent $P(z)^{-1}$ reveals the existence of eigenvalues, indicates where eigenvalues are located, and show how sensitive these eigenvalues are to pertubation.

As explained in [3], from Keldysh's theorem, we know that the resolvent function $P(z)^{-1}$ can be written (for simple eigenvalues λ_i) as

$$P(z)^{-1} = \sum_i v_i w_i^H \frac{1}{z - \lambda_i} + R(z) \tag{4}$$

where

- v_i and w_i are suitably scaled right and left eigenvectors, respectively, corresponding to the (simple) eigenvalue λ_i
- $R(z)$ and $P(z)$ are analytic functions

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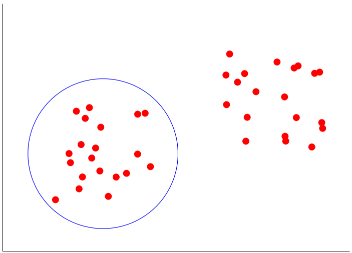

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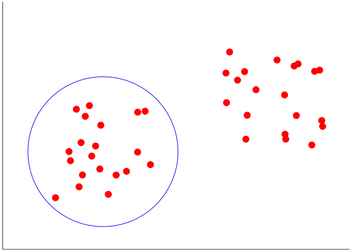
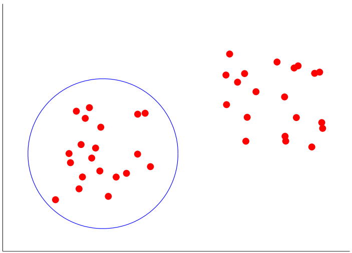


$Q = (q_1, q_2, ..., q_k)$



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$\text{span}\{q_1, q_2, ..., q_k\} \supseteq \text{span}\{v_1, v_2, ..., v_{n(\Gamma)}\}$

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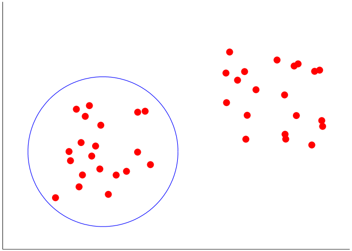

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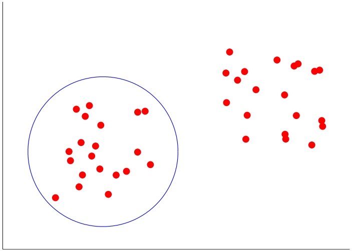
$$P(z)^{-1} = \sum_i v_i w_i^H \frac{1}{z - \lambda_i} + R(z)$$

Applying Cauchy's integral formula

$$\frac{1}{2\pi i} \oint_\Gamma f(z) P(z)^{-1} dz = \sum_{i=1}^{n(\Gamma)} f(\lambda_i) v_i w_i^H$$



$Q = (q_1, q_2, ..., q_k)$

$\text{span}\{q_1, q_2, ..., q_k\} \supseteq \text{span}\{v_1, v_2, ..., v_{n(\Gamma)}\}$

Formulation

Contour integral methods

Some basic spectral theory

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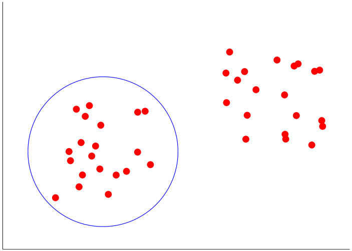
$$P(z)^{-1} = \sum_i v_i w_i^H \frac{1}{z - \lambda_i} + R(z)$$



Applying Cauchy's integral formula

$$\frac{1}{2\pi i} \oint_\Gamma f(z) P(z)^{-1} dz = \sum_{i=1}^{n(\Gamma)} f(\lambda_i) v_i w_i^H$$

In practice, we evaluate the integral

$$\frac{1}{2\pi i} \oint_\Gamma f(z) P(z)^{-1} \hat{V} dz$$

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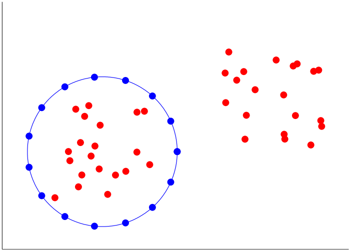

$$P(z)^{-1} = \sum_i v_i w_i^H \frac{1}{z - \lambda_i} + R(z)$$

Applying Cauchy's integral formula

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In practice, we evaluate the integral

$$\frac{1}{2\pi i} \oint_\Gamma f(z) P(z)^{-1} \hat{V} dz$$

Using interpolation, we obtain

$$\frac{1}{2\pi i} \oint_\Gamma f(z) P(z)^{-1} \hat{V} dz = \sum_{i=1}^{n_{int}} \xi_i f(z_i) P(z_i)^{-1} \hat{V}$$

$Q = (q_1, q_2, ..., q_k)$

$\text{span}\{q_1, q_2, ..., q_k\} \supseteq \text{span}\{v_1, v_2, ..., v_{n(\Gamma)}\}$

Presentation Outline

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Formulation

Multigrid method as a preconditioner

The most expensive operation is to compute

$$X = P^{-1}(z_i)V \tag{5}$$

equivalent to solving the linear system

$$P(z_i)X = V \tag{6}$$

- Direct inverse becomes prohibitively expensive for large problems.

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- For large-scale problems, iterative methods are preferable.
- Linear systems generated by Maxwell's equations are extremely ill-conditioned.
- Krylov iterative solvers with simple preconditioners often stagnate or diverge as when applied to these linear systems.
- Suitable preconditioners/iterative solvers should be applied to improve the convergence of the iterative solvers.

Formulation

Multigrid method as a preconditioner

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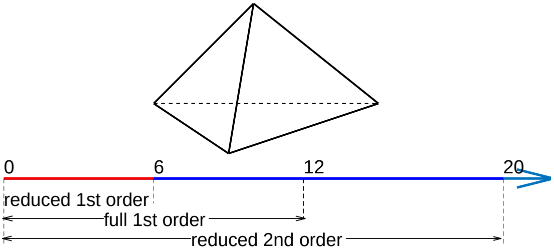
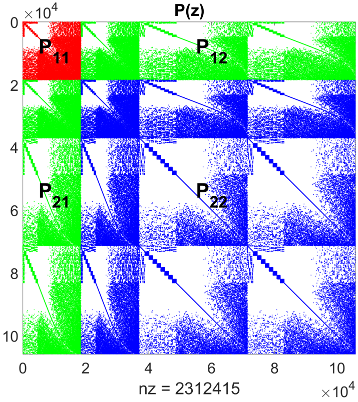
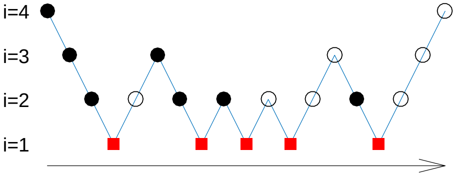


Pär Ingelström, "A New Set of H(curl) Conforming Hierarchical Basis Functions for Tetrahedral Meshes, IEEE Transactions on Microwave Theory and Techniques, vol. 54, no. 1, Jan. 2006.



Formulation

Multigrid method as a preconditioner



W-cycle

Pär Ingelström et al., "Comparison of Hierarchical Basis Functions for Efficient Multilevel Solvers", IET Science, Measurement and Technology, vol. 1, no. 1, Jan. 2007.

$$M^{-1}b = e \tag{7}$$

This equation is repeatedly computed at each iteration where M is the preconditioner, b is the input and e is the output. The output is computed by solving systems of the type

$$P_{ii}e_i = b_i - \sum_{i \neq j} P_{ij}e_j \tag{8}$$

where i and j refer to the order of the trial and test functions.

Presentation Outline

Motivation

- Iterative methods
- Contour integral methods

Formulation

- Mathematical model
- Eigenvalue algorithms
- Contour integral methods
- Multigrid method as a preconditioner

Implementation

Preliminary Results

Possible Improvements

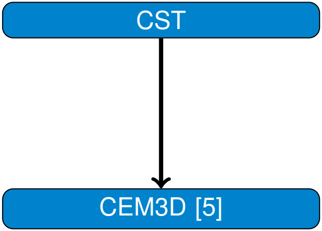
Implementation

Nonlinear Eigenvalue Solver for Accelerator Cavities (NES4AC)

CST — cavity design, FEM discretization

Implementation

Nonlinear Eigenvalue Solver for Accelerator Cavities (NES4AC)



cavity design, FEM discretization

generate matrices $P(z_i)$

Implementation

Nonlinear Eigenvalue Solver for Accelerator Cavities (NES4AC)

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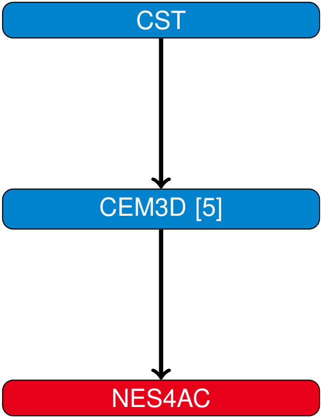


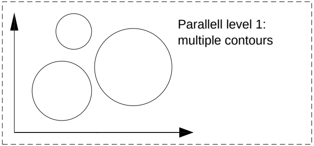
cavity design, FEM discretization

generate matrices $P(z_i)$

Solve nonlinear eigenvalue problem

Implementation

Nonlinear Eigenvalue Solver for Accelerator Cavities (NES4AC)



Implementation

Nonlinear Eigenvalue Solver for Accelerator Cavities (NES4AC)

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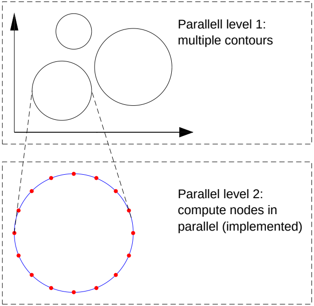
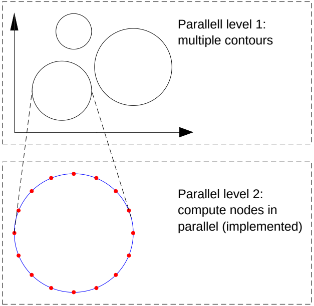
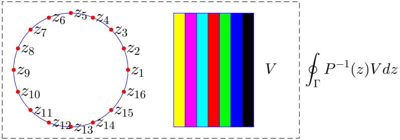


Implementation

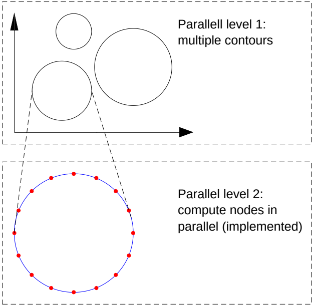
Nonlinear Eigenvalue Solver for Accelerator Cavities (NES4AC)

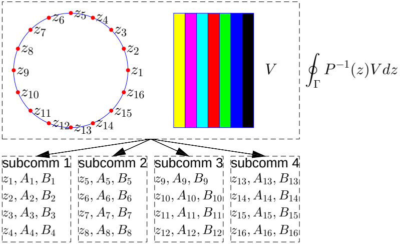




Implementation

Nonlinear Eigenvalue Solver for Accelerator Cavities (NES4AC)





Implementation

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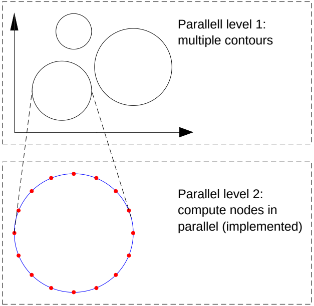

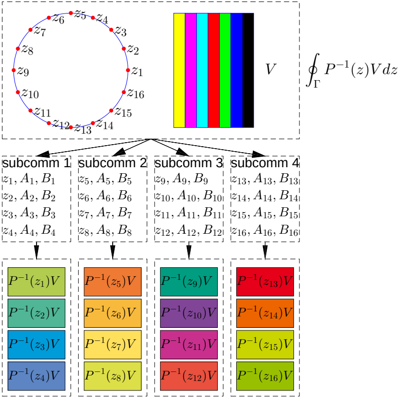

Implementation

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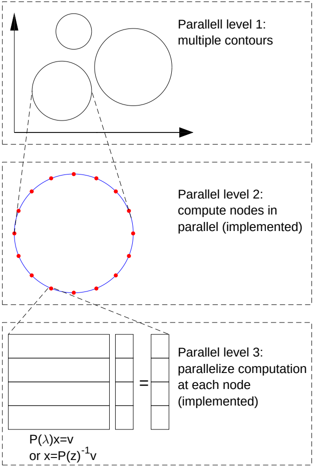
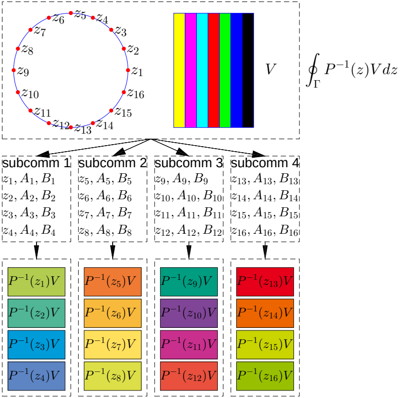
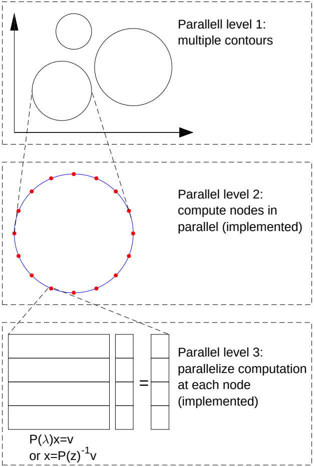
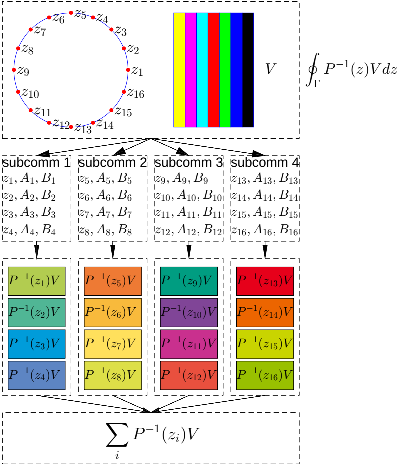




Implementation

Nonlinear Eigenvalue Solver for Accelerator Cavities (NES4AC)





Implementation

Nonlinear Eigenvalue Solver for Accelerator Cavities (NES4AC)

NES4AC highlights:

- extends the functionality of CEM3D [5].
- parallelized and developed in C++.
- based on PETSc (Portable, Extensible Toolkit for Scientific Computation) v3.3.0 and LAPACK.
- adopts the parallel scheme of the contour integral method from SLEPc (Scalable Library for Eigenvalue Problem Computations).
- uses the superLU_DIST for the computation of LU decompositions.
- including three contour integral algorithms for eigenvalue solution: Beyn1 (for a few eigenvalues), Beyn2 (for many eigenvalues) and RSRR.
- with two types of closed contour: ellipse and rectangle.

Presentation Outline

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Motivation
- Iterative methods
- Contour integral methods

Formulation
- Mathematical model
- Eigenvalue algorithms
- Contour integral methods
- Multigrid method as a preconditioner

Implementation

Preliminary Results

Possible Improvements

Preliminary Results

Nonlinear Eigenvalues Problems in [6]

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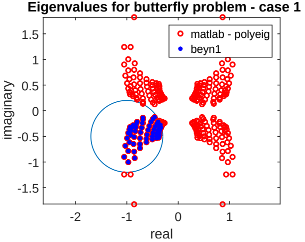
Butterfly Problem

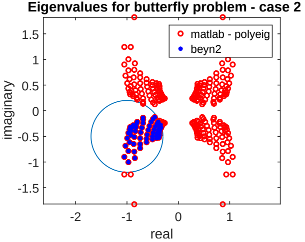
- Name: butterfly (Quartic matrix polynomial with T-even structure)
- $P(\lambda) = \lambda^4 A_4 + \lambda^3 A_3 + \lambda^2 A_2 + \lambda A_1 + A_0$
- Size: 64
- Region: circle(-1.0,-0.5,0.7)
- Number of eigenvalues: 55
- Algorithm parameters:
  - N = 60 (number of integration points)
  - L = 100:2:200 (number of columns of the random matrix)
  - K = 2 (for BEYN2)
  - Lorg = 20 (for RSRR)
  - Lred = 100 (for RSRR)
  - Nred = 30 (for RSRR)
  - Kred = 2 (for RSRR)
  - Rank tolerance = 1.0×10^{-12}

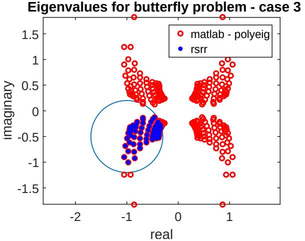
Preliminary Results

Nonlinear Eigenvalues Problems in [6]

Butterfly Problem







	beyn1	beyn2	rsrr
Min. residual	4.9×10^{-5}	2.05×10^{-14}	4.05×10^{-12}
Max. residual	0.0015	1.72×10^{-13}	4.38×10^{-9}

$$\epsilon = \frac{\|P(\lambda)x\|}{\|P(\lambda)\|\,\|x\|}$$

Preliminary Results

Nonlinear Eigenvalues Problems in [6]

Schrödinger

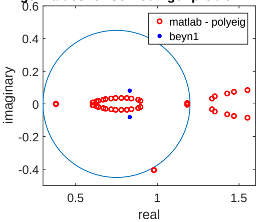
- Name: Schrödinger (QEP from Schrödinger operator)
- $P(\lambda) = K - 2\lambda C + \lambda^2 B$
- Size: 1998
- Region: circle(0.75,0.0,0.45)
- Number of eigenvalues: 30
- Algorithm parameters:
  - N = 20 (number of integration points)
  - L = 50:2:100 (number of columns of the random matrix)
  - K = 2 (for BEYN2)
  - Lorg = 20 (for RSRR)
  - Lred = 50 (for RSRR)
  - Nred = 30 (for RSRR)
  - Kred = 2 (for RSRR)
  - Rank tolerance = 1.0×10^{-12}

Preliminary Results

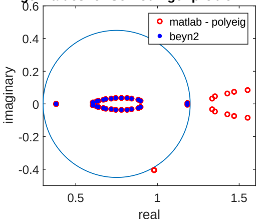
Nonlinear Eigenvalues Problems in [6]

Schrödinger

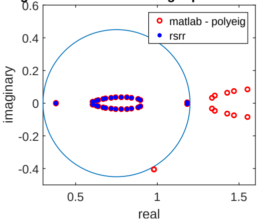
Eigenvalues for Schrödinger problem - case 1



Eigenvalues for Schrödinger problem - case 2



Eigenvalues for Schrödinger problem - case 3



	beyn1	beyn2	rsrr
Min. residual	n/a	1.08×10^{-15}	1.97×10^{-17}
Max. residual	n/a	1.73×10^{-14}	2.52×10^{-17}

Preliminary Results

Spherical Cavity

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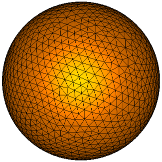
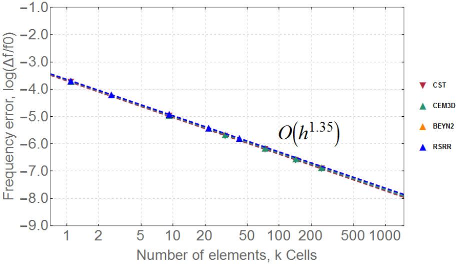
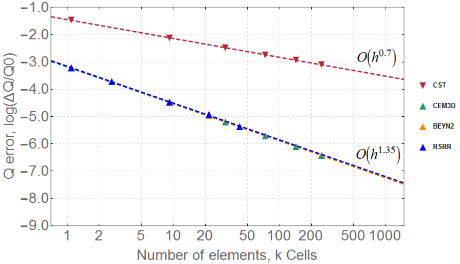


- Name: spherical cavity
- Electrical conductivity: 58×10^6 Ohm/sq
- Radius: 1m
- Size: 7614/17830/61106/143354/278138
- Target frequency: 125MHz
- Number of eigenvalues: 3
- Algorithm parameters:
  - Region: rectangle(1.0, 1.5, 1.0×10^{-15}, 0.05)
  - N = 20 (number of integration points)
  - L = 40:10:100 (number of columns of the random matrix)
  - K = 2 (for BEYN2)
  - Lorg = 20 / Lred = 20 / Nred = 20 / Kred = 2 (for RSRR)
  - Rank tolerance = 1.0×10^{-8}

Preliminary Results

Spherical Cavity



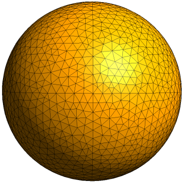


$$\epsilon_f = \frac{\| f - f_{analytical} \|}{\| f_{analytical} \|}$$

$$\epsilon_Q = \frac{\| Q - Q_{analytical} \|}{\| Q_{analytical} \|}$$

Preliminary Results

Multigrid preconditioner - Spherical Cavity



	# elements	# dofs	# dofs (1st order)
Dis. 1	342	1,652	250
Dis. 2	1,256	6,640	1,078
Dis. 3	2,918	16,300	2,755
Dis. 4	18,062	105,828	18,487

Table: Mesh refinement of a spherical cavity

	Dis. 1	Dis. 2	Dis. 3	Dis. 4
mg-GMRES	17	21	23	23
GMRES	500 (1.0e-5)	500 (1.0e-2)	500 (1.0e-2)	500 (5.0e-2)

Table: Number of iterations required to achieve a residual of 1.0e-8

Preliminary Results

Multigrid preconditioner - Tesla Cavity

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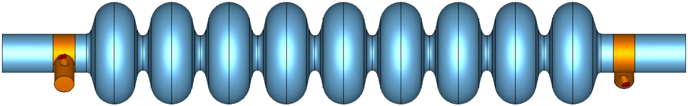


	# elements	# dofs	# dofs (1st order)
Dis. 1	48,819	286,026	50,067
Dis. 2	57,394	339,664	59,864
Dis. 3	76,113	373,812	80,552

Table: Mesh refinement of a Tesla cavity

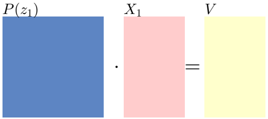
	Dis. 1	Dis. 2	Dis. 3
mg-GMRES	30	25	24
GMRES	500 (0.2)	500 (0.15)	500 (0.2)

Table: Number of iterations required to achieve a residual of 1.0e-8

Presentation Outline

Possible Improvements
Recycling Krylov subspace methods

$$X_i = P^{-1}(z_i)V$$
$$P(z_i)X_i = V$$



Possible Improvements
Recycling Krylov subspace methods

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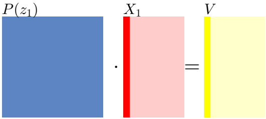

- Iterative method is repeatedly applied for different RHS.

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Recycling Krylov subspace methods

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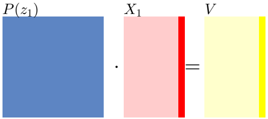

- Iterative method is repeatedly applied for different RHS.
- The matrix is unchanged.

Possible Improvements

Recycling Krylov subspace methods

$$X_i = P^{-1}(z_i)V$$
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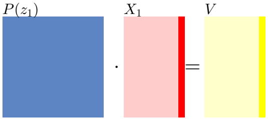

- Iterative method is repeatedly applied for different RHS.
- The matrix is unchanged.
- Opportunity for applying recycling Krylov subspace methods or block Krylov subspace methods.

Possible Improvements

Recycling Krylov subspace methods

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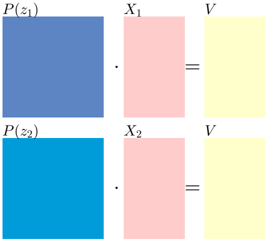

- Iterative method is repeatedly applied for different RHS.
- The matrix is unchanged.
- Opportunity for applying recycling Krylov subspace methods or block Krylov subspace methods.
- The system-matrices are slightly changed for different interpolation points

Possible Improvements

Recycling Krylov subspace methods

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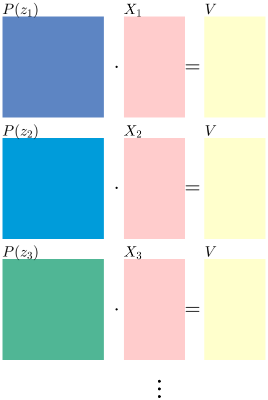
$$P(z_i)X_i = V$$



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Thank you for your attention

References I

[1] T. Flisgen, J. Heller, T. Galek, L. Shi, N. Joshi, N. Baboi, R. M. Jones, and U. van Rienen, “Eigenmode Compendium of The Third Harmonic Module of the European X-Ray Free Electron Laser,” *Physical Review Accelerators and Beams*, vol. 20, p. 042002, Apr 2017.

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Define the matrices A_0 and $A_1 \in \mathbb{C}^{n\times k}$

$$A_0 = \frac{1}{2\pi i}\oint_\Gamma P(z)^{-1}\hat{V}dz \qquad (9)$$

$$A_1 = \frac{1}{2\pi i}\oint_\Gamma zP(z)^{-1}\hat{V}dz \qquad (10)$$

Then $A_0 = VW^H\hat{V}$ and $A_1 = V\Lambda W^H\hat{V}$ where

- $\Lambda = \text{diag}(\lambda_1, ..., \lambda_{n(\Gamma)})$
- $V = \begin{bmatrix} v_1 & \cdots & v_{n(\Gamma)} \end{bmatrix}$
- $W = \begin{bmatrix} w_1 & \cdots & w_{n(\Gamma)} \end{bmatrix}$

$\hat{V}$ is a random matrix $\hat{V} \in \mathbb{C}^{n\times L}$. L is smaller than n and equal or greater and k

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Beyn's method is based on the singular value decomposition of A_0

$$A_0 = V_0 \Sigma_0 W_0^H \tag{11}$$

Beyn has shown that the matrix

$$B = V_0^H A_1 W_0^H \Sigma_0^{-1} \tag{12}$$

is diagonalizable. Its eigenvalues are the eigenvalues of P inside the contour and its eigenvectors lead to the corresponding eigenvectors of P.

Define the matrices $A_p \in \mathbb{C}^{n\times k}$

$$A_p = \frac{1}{2\pi i} \oint_{\Gamma} z^p P(z)^{-1} \hat{V} dz \qquad (13)$$

Then $A_p = V\Lambda^p W^H \hat{V}$. The matrices B_0 and B_1 are defined as follows

$$B_0 = \begin{pmatrix} A_0 & \cdots & A_{K-1} \\ \vdots & & \vdots \\ A_{K-1} & \cdots & A_{2K-2} \end{pmatrix} \quad ; \quad B_1 = \begin{pmatrix} A_1 & \cdots & A_K \\ \vdots & & \vdots \\ A_K & \cdots & A_{2K-1} \end{pmatrix} \qquad (14)$$

Performing the singular value decomposition of B_0

$$B_0 = V_0 \Sigma_0 W_0^H \tag{15}$$

Beyn has shown that the matrix

$$D = V_0^H B_1 W_0^H \Sigma_0^{-1} \tag{16}$$

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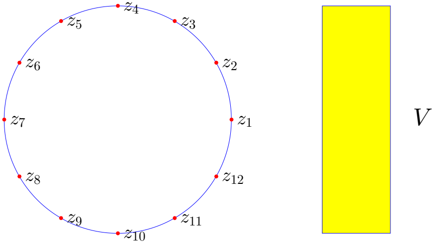
Appendix

Contour integral methods

Resolvent Sampling based Rayleigh-Ritz method



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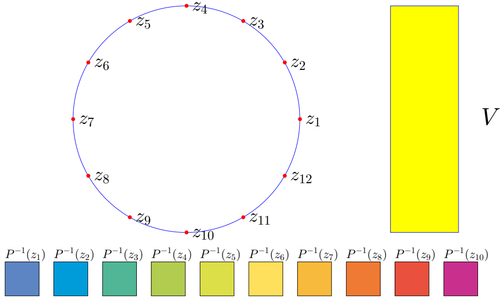

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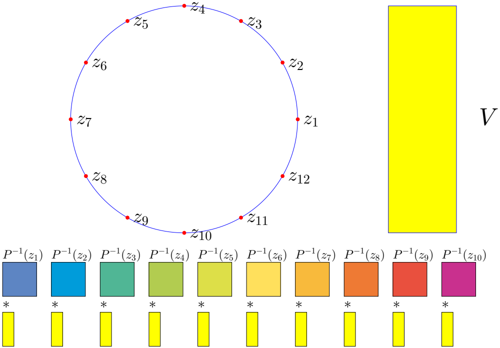

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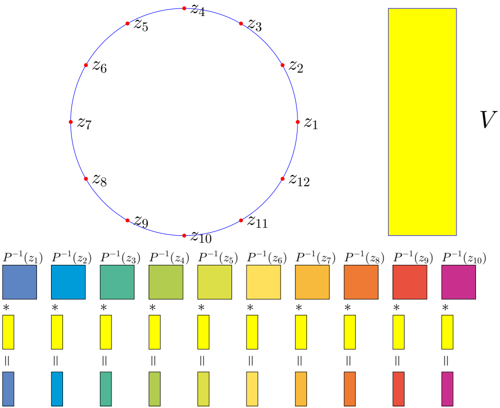

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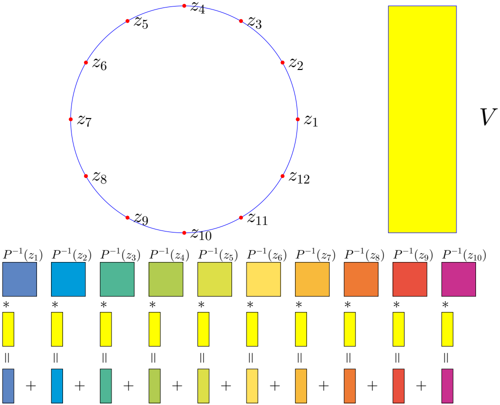

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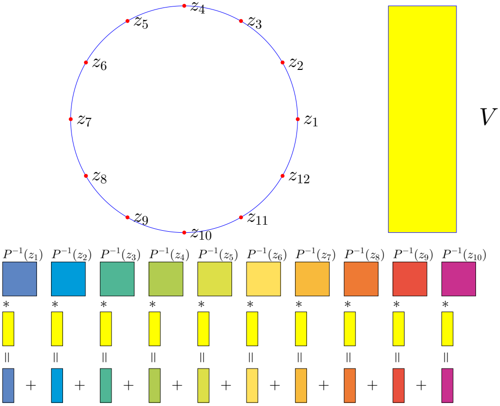

The Beyn2 algorithm is robust and accurate if a large L but a small K are used.

However, for large-scale problems, a small L is essential to reduce the computational burden.

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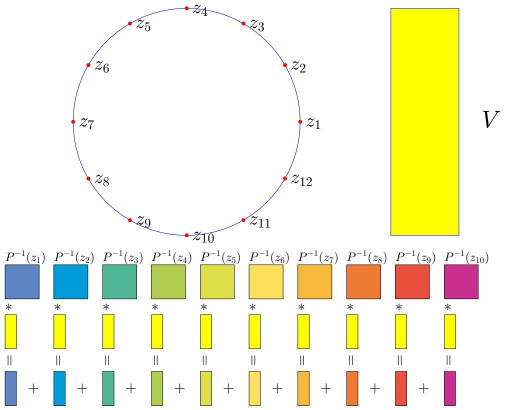

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Decrease L and increase K make the algorithm unstable and inaccurate.

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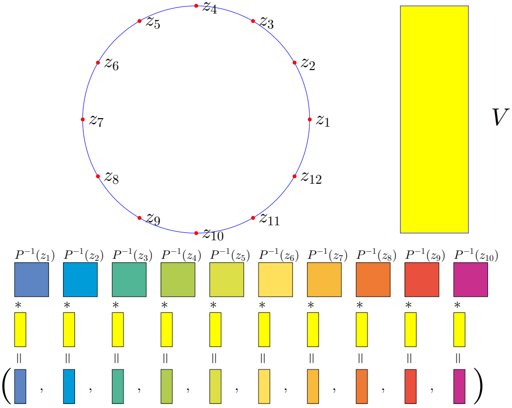

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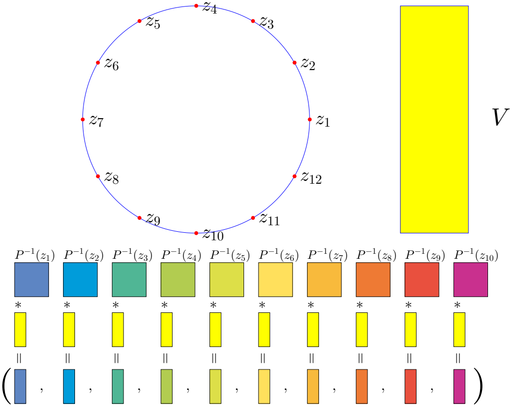

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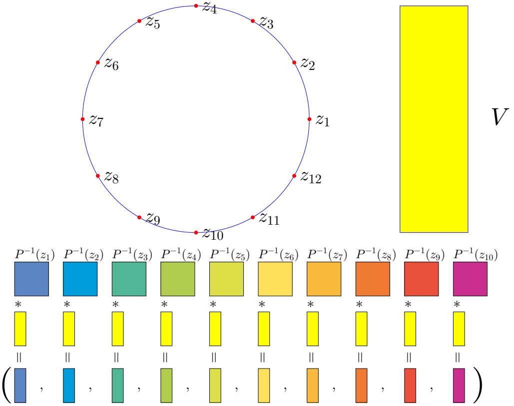

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Let $Q \in \mathbb{C}^{n\times k}$ be an orthogonal basis of search space, then the original NEP can be converted to the following reduced NEP

$$P_Q(z)g = 0$$

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(1) Initialization: Fix the contour Γ, the number N and the sampling points z_i. Fix the number L and generate a $n \times L$ random matrix U

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(3) Form S as follows

$$S = \left[P(z_0)^{-1}U, \quad P(z_1)^{-1}U, \quad \cdots, \quad P(z_{N-1})^{-1}U\right] \in \mathbb{C}^{n \times N \cdot L} \tag{17}$$

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(6) Compute the eigenpairs of the original NEP via the eigenpairs of the reduced NEP.