Contour Integral Method for the Computation of Eigenmodes of the Tesla Cavity

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Outline of the Talk

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Introduction
- Iterative methods
- Contour integral methods

Formulation

Results
- 9 monopole modes in the 1st passband
- 36 dipole modes in the 1st and 2nd passband
- Comparison between different linear solvers in the contour integral method

Conclusion

Presentation Outline

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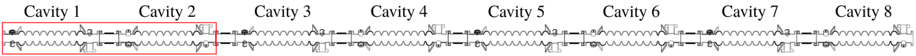
Introduction
Problem statement

Problem statement: we have to solve **a nonlinear eigenvalue problem (NEP)** where

- the problem is large and sparse;
- the number of eigenvalues is large;
- prior information about eigenvalues is available;
- in several applications, one is only interested in a few eigenvalues within a certain range.

Figure: Chain of cavities (from [1])



Available methods:

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

Contour Integral Method for the Computation of Eigenmodes of the Tesla Cavity

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Lossless accelerator cavity: eigenvalues are on real axis

Introduction
Iterative methods (Jacobi-Davidson)

Lossless accelerator cavity: eigenvalues are on real axis

choose an initial guess

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Lossless accelerator cavity: eigenvalues are on real axis

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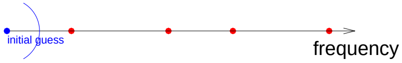
expand the search space ...



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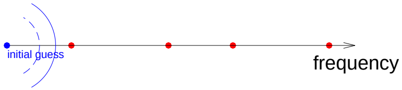

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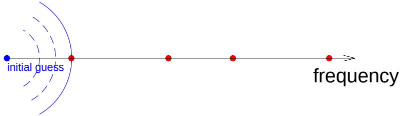

choose an initial guess

expand the search space ...

until an approximate solution is found

Lossless accelerator cavity: eigenvalues are on real axis

- choose an initial guess
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- until an approximate solution is found
- the solution becomes the new initial guess

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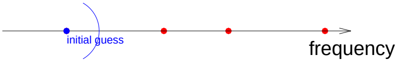

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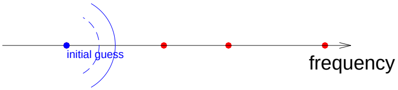

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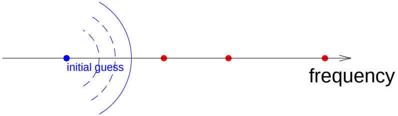

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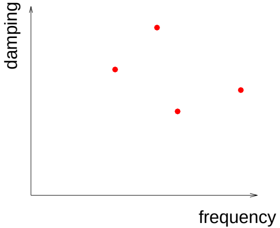
Lossy accelerator cavity: eigenvalues are in the complex plane



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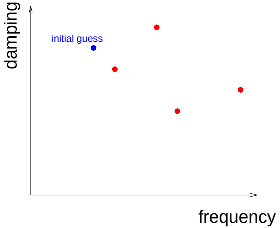

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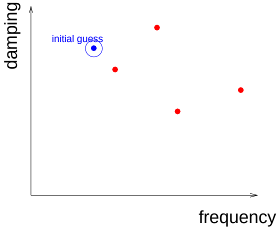

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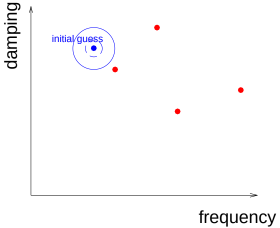

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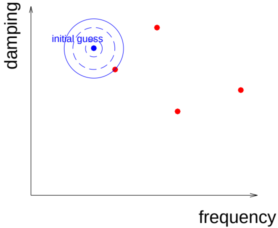

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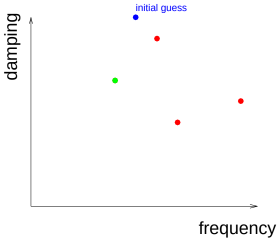

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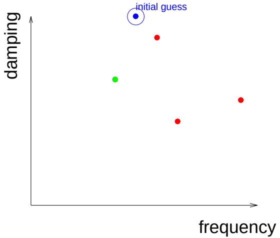

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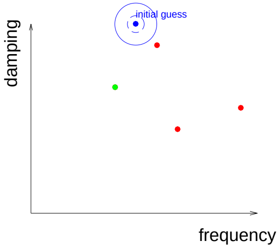

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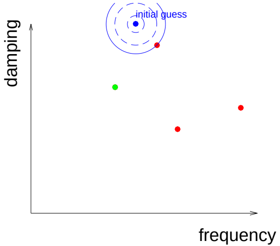

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find another approximate solution

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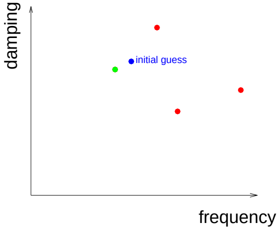

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if we choose an unsuitable initial guess

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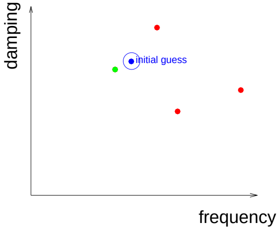

choose an initial guess

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until an approximate solution is found

if we choose an unsuitable initial guess

the algorithm will converge to ...

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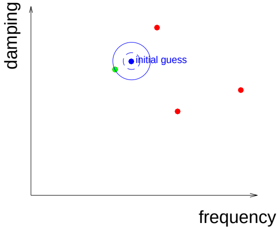

choose an initial guess

expand the search space ...

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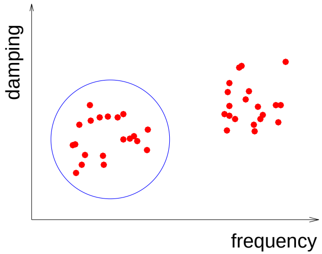
if we choose an unsuitable initial guess

the algorithm will converge to ...

an already determined eigenvalue!!!!!

Introduction
Contour integral methods

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



choose a region to look for eigenvalues

the region can be of any shape, e.g rectangle, circle/ellipse.

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Contour integral methods

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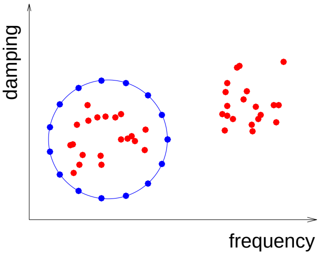
An accurate computation of eigenpairs inside a region enclosed by a non-self-intersecting curve.



- choose a region to look for eigenvalues
- the region can be of any shape, e.g rectangle, circle/ellipse.
- most computation is spent to solve linear equation systems at different interpolation points, which can be parallelized.

Formulation

Contour integral methods

To solve $P(z)x = 0$ most of the standard eigenvalue algorithms exploit a projection procedure in order to extract approximate eigenvectors from a given subspace.

Construct an approximate eigenspace Q — obtain matrix Q

↓

Project the original NEP to a reduced NEP — using Rayleigh-Ritz procedure:
$P_Q(z) = Q^H P(z) Q$

↓

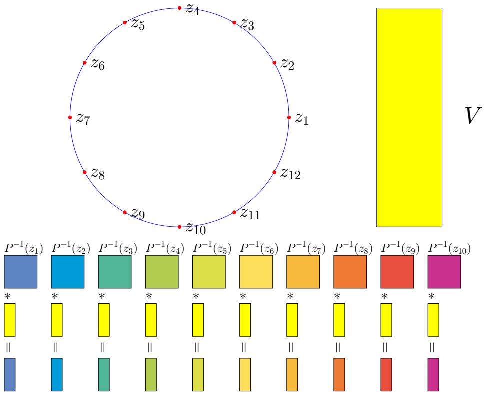
Solve the reduced NEP — solve $P_Q(z)g = 0$
for eigenvalues z and eigenvectors g

↓

Compute eigenpairs of the original NEP — same eigenvalues as for the reduced problem;
eigenvectors $x = Qg$

Formulation

Contour integral methods



The evaluation of Q requires the computation of

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

where $P(z_n)$ is the matrix system at an integration point z_n and V is a random matrix.
The most expensive operation is to compute

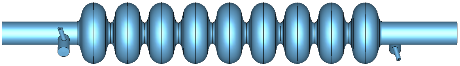
$$X = P^{-1}(z_i) V \qquad (2)$$

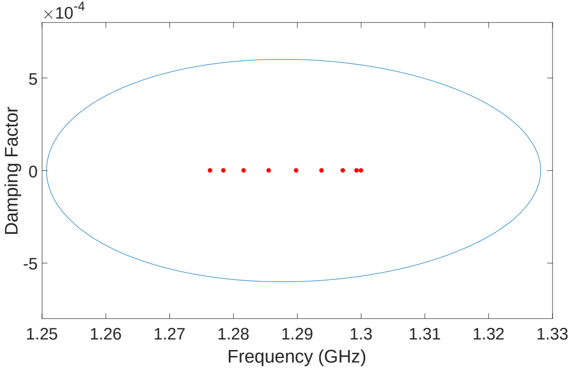
Contour Integral Method for the Computation of Eigenmodes of the Tesla Cavity

Results

Lossless Tesla Cavity

9 Monopole Modes in the 1st Passband





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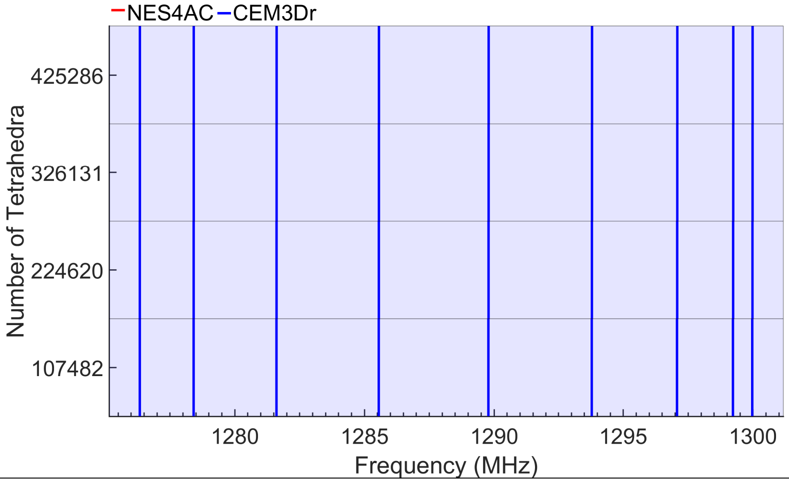

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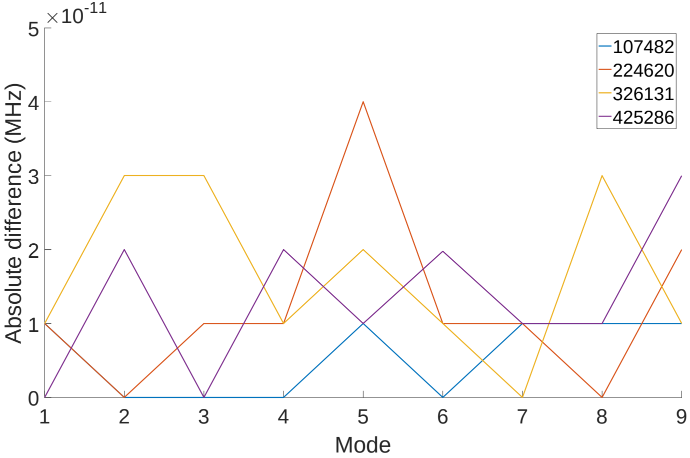

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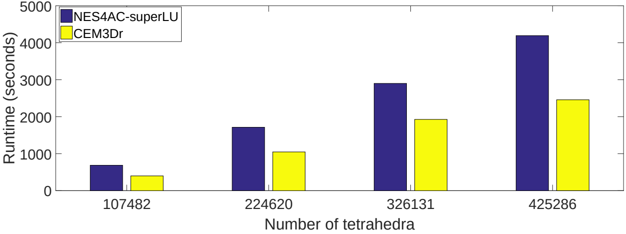

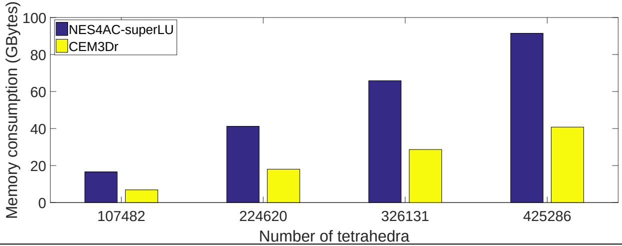

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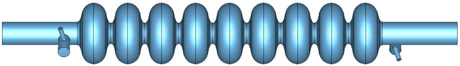
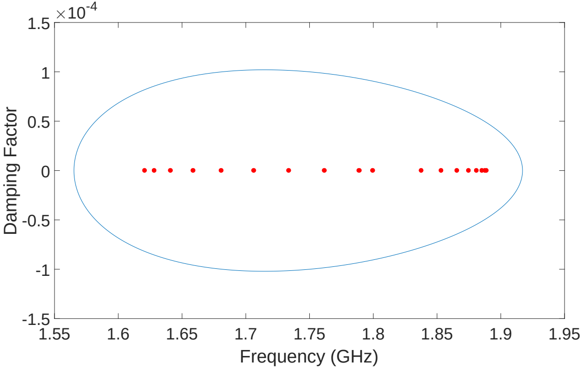
36 Dipole Modes in the 1st and 2nd Passband





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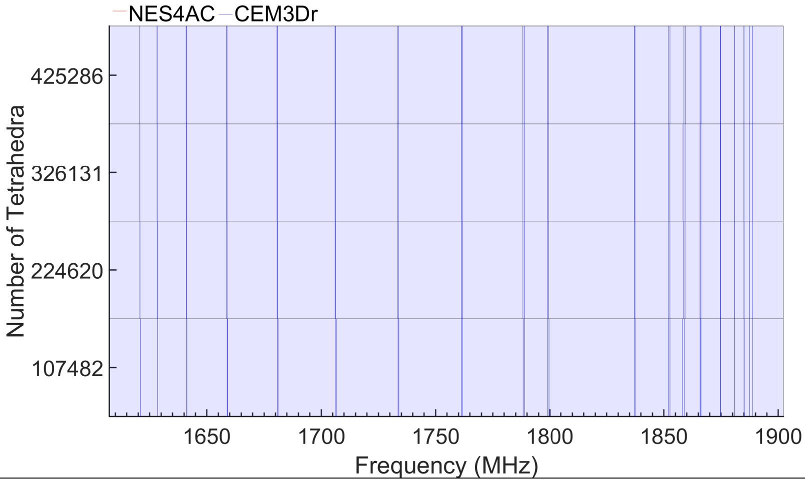

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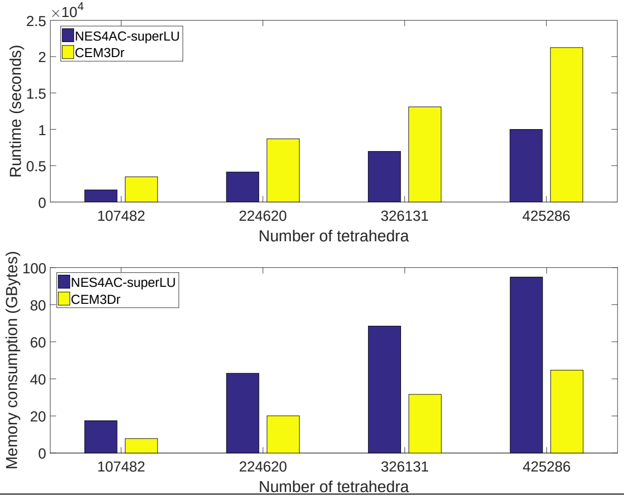
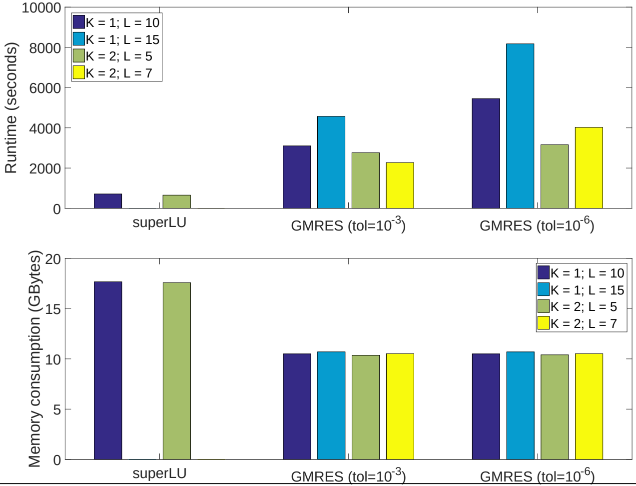


Results

Lossless Tesla Cavity

Comparison between Different Linear Solvers



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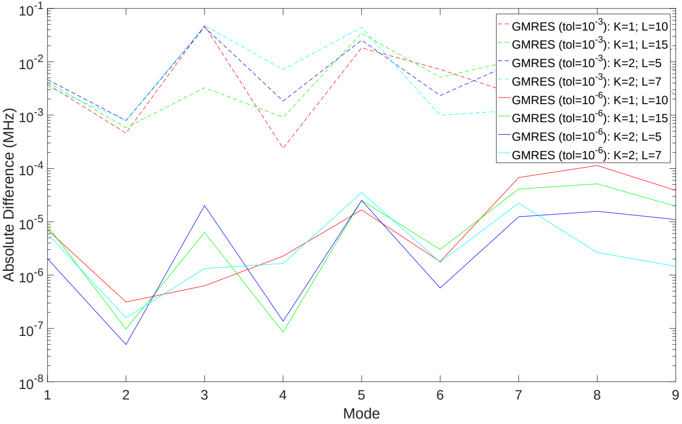

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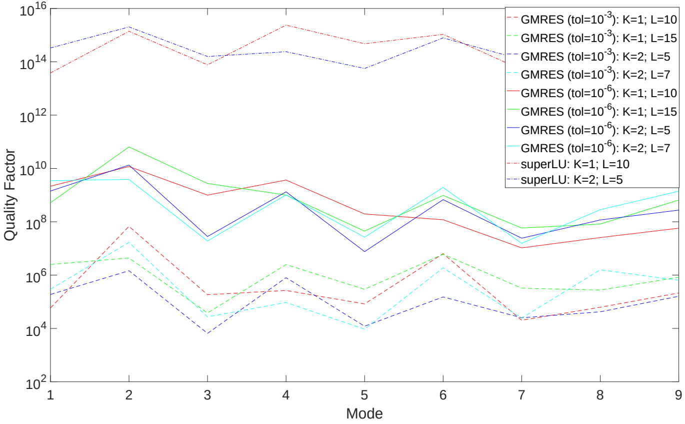

Contour Integral Method for the Computation of Eigenmodes of the Tesla Cavity

Conclusion

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- Good agreement between NES4AC and CEM3Dr.
- NES4AC requires memory twice as much as CEM3Dr.
- NES4AC is efficient for computing multiple modes.
- Direct solver is more robust but requires more memory than iterative solver.
- The accuracy of the solution significantly depends on the number of interpolation points and the tolerance of the linear solvers.

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Thank you for your attention

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[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.

[2] H. Voss, "A Jacobi-Davidson Method for Nonlinear and Nonsymmetric Eigenproblems," *Computers and Structures*, vol. 85, no. 17-18, pp. 1284–1292, 2007.

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[4] J. Xiao, C. Zhang, T. M. Huang, and T. Sakurai, "Solving Large-Scale Nonlinear Eigenvalue Problems by Rational Interpolation and Resolvent Sampling Based Rayleigh-Ritz Method," *International Journal for Numerical Methods in Engineering*, vol. 110, no. 8, pp. 776–800, 2017.

[5] T. Banova, W. Ackermann, and T. Weiland, "Accurate Determination of Thousands of Eigenvalues for Large-Scale Eigenvalue Problems," *IEEE Transactions on Magnetics*, vol. 50, pp. 481–484, Feb. 2014.

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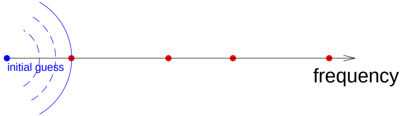
Lossless accelerator cavity: eigenvalues are on real axis



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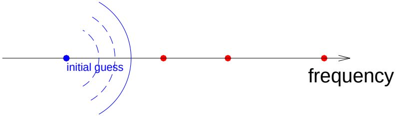

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- continue expanding the search space ...

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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

$$P(z)^{-1} = \sum_i v_i w_i^H \frac{1}{z - \lambda_i} + R(z) \tag{3}$$

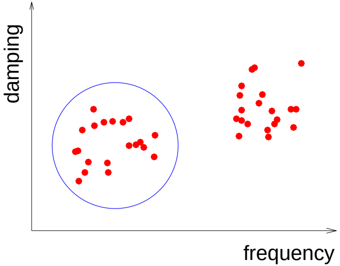
where

- 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

Appendix

Contour integral methods

Some basic spectral theory



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

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

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

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

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

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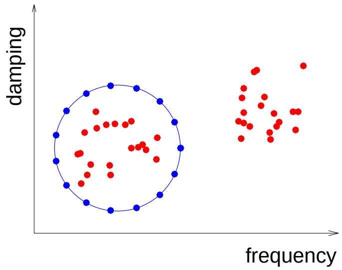

$$P(z)^{-1} = \sum_i \color{red}{v_i} w_i^H \frac{1}{z-\lambda_i} + R(z)$$

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In practice, we evaluate the integral

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Using interpolation, we obtain

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

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

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

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

$$A_0 = \frac{1}{2\pi i} \oint_\Gamma P(z)^{-1} \hat{V} dz \tag{4}$$

$$A_1 = \frac{1}{2\pi i} \oint_\Gamma z P(z)^{-1} \hat{V} dz \tag{5}$$

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

$$A_0 = V_0 \Sigma_0 W_0^H \tag{6}$$

Beyn has shown that the matrix

$$B = V_0^H A_1 W_0^H \Sigma_0^{-1} \tag{7}$$

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

$$A_p = \frac{1}{2\pi i} \oint_{\Gamma} z^p P(z)^{-1} \hat{V} dz \tag{8}$$

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

$$B_0 = \begin{pmatrix} A_0 & \cdots & A_{K-1} \\ \vdots & & \vdots \\ A_{K-1} & \cdots & A_{2K-2} \end{pmatrix} \quad ; \quad B_1 = \begin{pmatrix} A_1 & \cdots & A_K \\ \vdots & & \vdots \\ A_K & \cdots & A_{2K-1} \end{pmatrix} \tag{9}$$

Performing the singular value decomposition of B_0

$$B_0 = V_0 \Sigma_0 W_0^H \tag{10}$$

Beyn has shown that the matrix

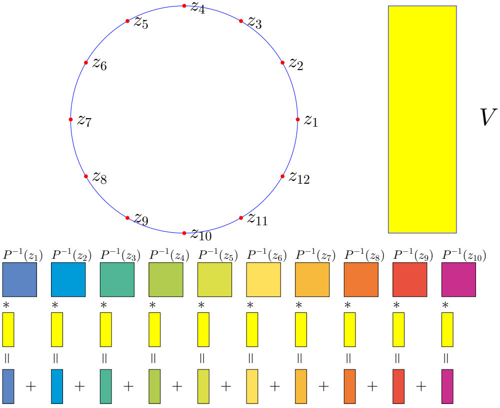
$$D = V_0^H B_1 W_0^H \Sigma_0^{-1} \tag{11}$$

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

Appendix

Contour integral methods

Resolvent Sampling based Rayleigh-Ritz method

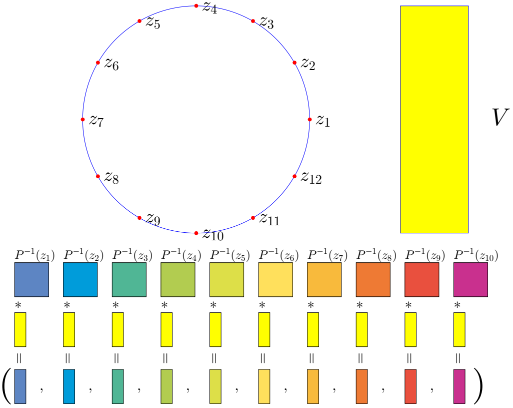


The Beyn2 algorithm is robust and accurate if a large L but a small K are used.

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

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

Resolvent Sampling based Rayleigh-Ritz method



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.

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

RSRR reduce the number of columns of V.

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

$$P_Q(z)g = 0$$

(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

(2) Compute $P(z_i)^{-1}U$ for $i = 0, 1, ..., N-1$

(3) Form S as follows

$$S = \left[P(z_0)^{-1}U, \quad P(z_1)^{-1}U, \quad \cdots, \quad P(z_{N-1})^{-1}U \right] \in \mathbb{C}^{n \times N \cdot L} \tag{12}$$

(4) Generate the matrix Q via the truncated singular value decomposition $S \approx Q\Sigma V^H$.

(5) Compute $P_Q(z) = Q^H P(z) Q$, and solve the projected NEP $P_Q(\lambda)g = 0$ using the SS-FULL algorithm to obtain $n(\Gamma)$ eigenapairs (g_j, λ_j).

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

Appendix

Nonlinear Eigenvalue Solver for Accelerator Cavities (NES4AC)

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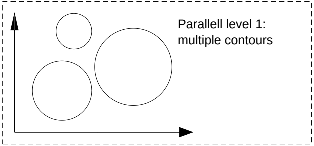
CST	cavity design, FEM discretization
↓	
CEM3D [5]	generate matrices $P(z_i)$
↓	
NES4AC	Solve nonlinear eigenvalue problem

Appendix
Nonlinear Eigenvalue Solver for Accelerator Cavities (NES4AC)



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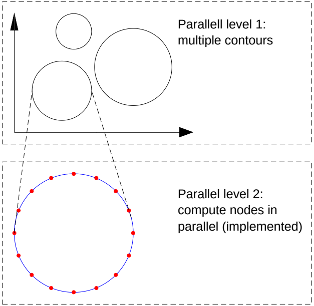
Nonlinear Eigenvalue Solver for Accelerator Cavities (NES4AC)



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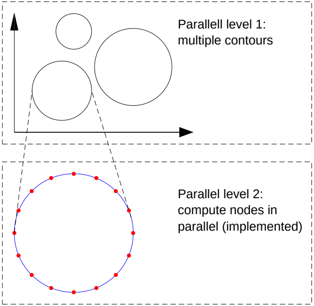
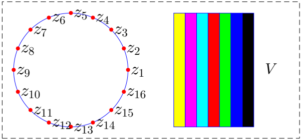
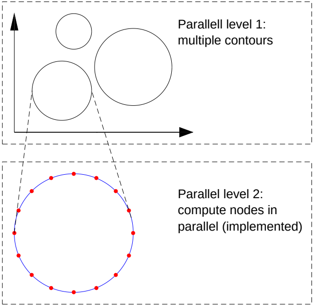
Nonlinear Eigenvalue Solver for Accelerator Cavities (NES4AC)

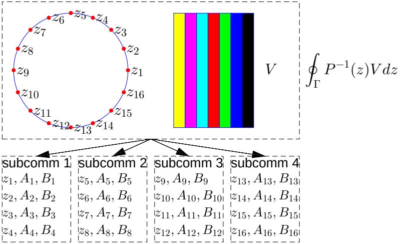




$$\oint_\Gamma P^{-1}(z)V\,dz$$

Appendix
Nonlinear Eigenvalue Solver for Accelerator Cavities (NES4AC)





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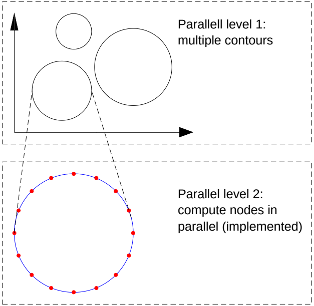

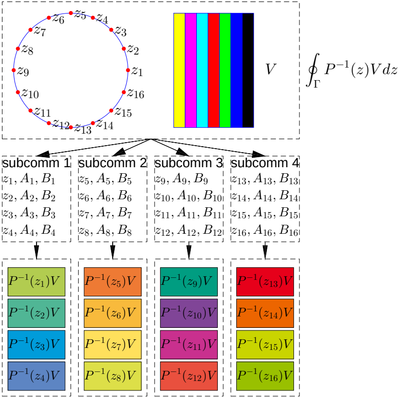

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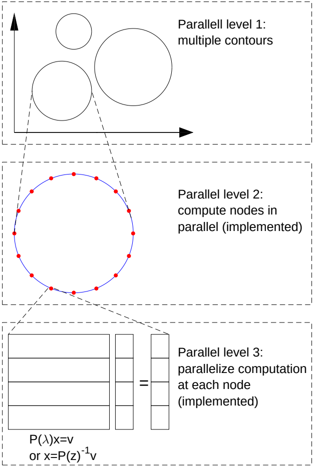

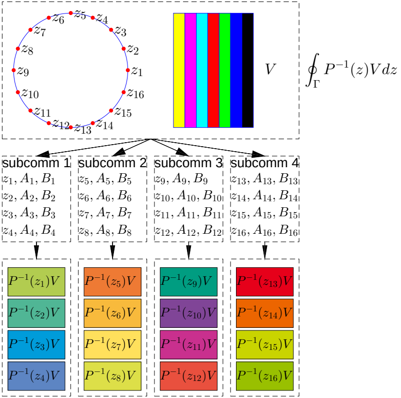

Appendix

Nonlinear Eigenvalue Solver for Accelerator Cavities (NES4AC)

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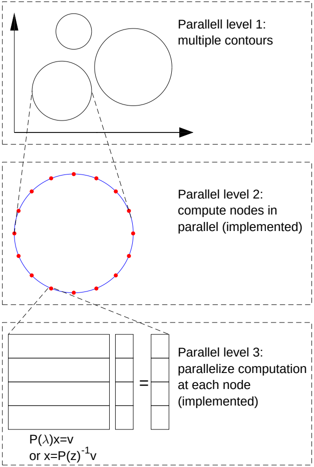

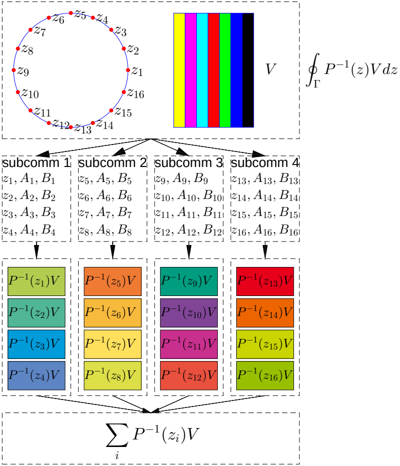

Appendix

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.

Appendix

Target frequency in CEM3D

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

$$\nabla \times \frac{1}{\mu} \nabla \times \vec{E} + j\omega\sigma\vec{E} = \varepsilon\omega^2\vec{E} \tag{13}$$

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

$$A^{3D}x + j\omega\mu_0 C^{3D}x = \omega^2\mu_0\varepsilon_0 B^{3D}x \tag{14}$$

where

$$A_{ij}^{3D} = \iiint_{\Omega} \frac{1}{\mu_r} \nabla \times \vec{w}_i \cdot \nabla \times \vec{w}_j d\Omega \tag{15}$$

$$B_{ij}^{3D} = \iiint_{\Omega} \varepsilon_r \vec{w}_i \cdot \vec{w}_j d\Omega \tag{16}$$

$$C_{ij}^{3D} = \iiint_{\Omega} \sigma \vec{w}_i \cdot \vec{w}_j d\Omega \tag{17}$$

Appendix

Target frequency in CEM3D

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Equation 14 can be rewritten as follows

$$(A^{3D} + j\omega\mu_0 C^{3D})x = (\frac{\omega}{c_0})^2 B^{3D} x \tag{18}$$

$$s(A^{3D} + j\omega\mu_0 C^{3D})x = s^2(\frac{\omega}{c_0})^2 \frac{B^{3D}}{s} x \tag{19}$$

$$A^{CEM3D} x = \lambda B^{CEM3D} x \tag{20}$$

where

$$s = \frac{c_0}{2\pi f_T} \tag{21}$$