

Calculation of Eigenmodes for Accelerator Cavities with Losses using CIM

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Outline of the Talk

Motivation

- Iterative methods
- Contour integral methods

Formulation

- Mathematical model
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- Multigrid method as a preconditioner
- Block Krylov methods and recycling Krylov methods

Numerical Results

Possible Improvements



Presentation Outline



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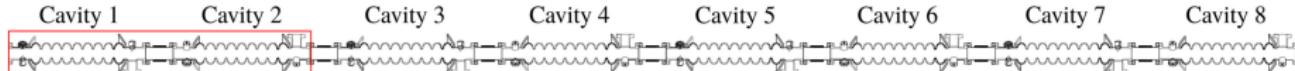
Problem statement



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.

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Iterative methods (Jacobi-Davidson)

Lossy accelerator cavity: eigenvalues are in **the complex plane**



- choose an initial guess
- expand the search space ...
- until an approximate solution is found

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Iterative methods (Jacobi-Davidson)

Lossy accelerator cavity: eigenvalues are in **the complex plane**



- choose an initial guess
- expand the search space ...
- until an approximate solution is found
- choose another initial guess
- continue expanding the search space ...
- find another approximate solution

Motivation

Iterative methods (Jacobi-Davidson)

Lossy accelerator cavity: eigenvalues are in **the complex plane**



- choose an initial guess
- expand the search space ...
- until an approximate solution is found

- if we choose unsuitable initial guess
- the algorithm will converge to ...
- **a previously determined eigenvalue!!!!**

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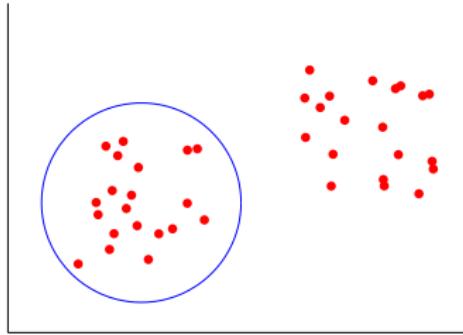


Motivation

Contour integral methods

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

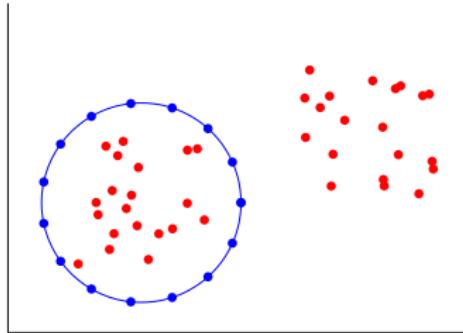
- choose a region to look for eigenvalues
- the region can be of any shape, e.g rectangle, circle/ellipse.



Motivation

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

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

$$\nabla \times \frac{1}{\mu} \nabla \times \vec{E} + j\omega\sigma\vec{E} = \varepsilon\omega^2\vec{E} \quad (1)$$

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

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

which includes only losses from volumetric lossy material. Special treatment is carried out to incorporate 2D losses at port interfaces into (2), resulting in a nonlinear eigenvalue problem (NEP)

$$P(z)x = 0 \quad (3)$$

where $z = (\frac{\omega}{2\pi f_r})^2$

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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

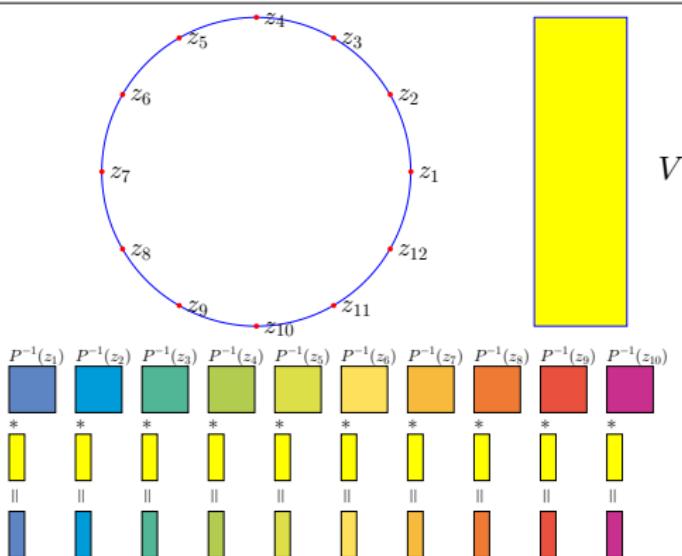
solve $P_Q(z)g = 0$
for eigenvalues z and eigenvectors g

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

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

$P(z_n)$ is the matrix system at an integration point z_n . V is a random matrix.

The most expensive operation is to compute

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

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Formulation

Multigrid method as a preconditioner

The most expensive operation is to compute

$$X = P^{-1}(z_i) V \quad (6)$$

equivalent to solving the linear system

$$P(z_i)X = V \quad (7)$$

- Direct inverse becomes prohibitively expensive for large problems.
- 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 when applied to such linear systems.
- **Suitable preconditioners/iterative solvers** should be applied to improve the convergence of the iterative solvers.

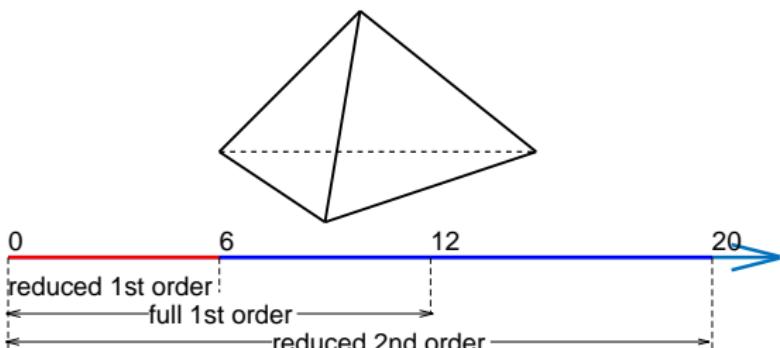
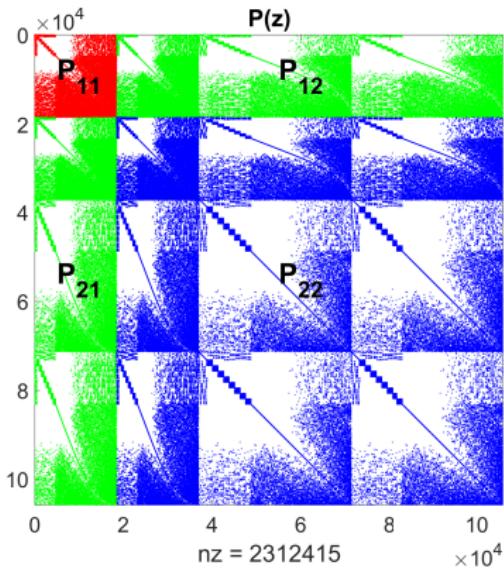


Formulation

Multigrid method as a preconditioner



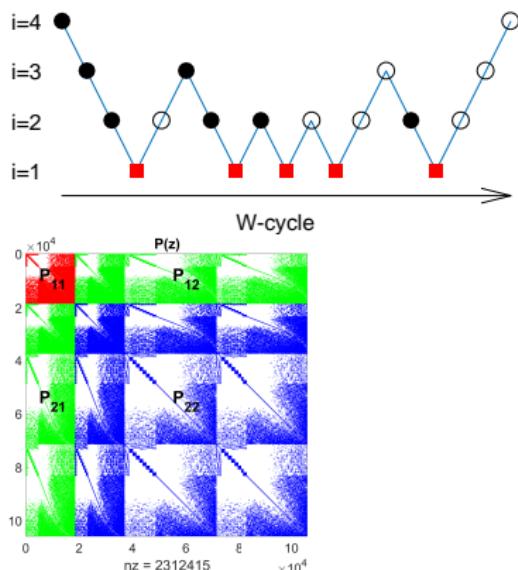
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Pär Ingelström, "A New Set of $H(\text{curl})$ Conforming Hierarchical Basis Functions for Tetrahedral Meshes, IEEE Transactions on Microwave Theory and Techniques, vol. 54, no. 1, Jan. 2006.

Formulation

Multigrid method as a preconditioner



$$M^{-1}b = e \quad (8)$$

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

$$P_{ii}e_i = b_i - \sum_{i \neq j} P_{ij}e_j \quad (9)$$

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

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

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Block Krylov methods

$$P(z) \cdot X = V$$

At each integration point, we need to solve a system with multiple right-hand-sides (RHSs)



Formulation

Block Krylov methods

$$P(z) \cdot X = V$$

At each integration point, we need to solve a system with multiple right-hand-sides (RHSs)

We sequentially solve for each RHS. Each solution is approximated from a Krylov space $x_i \in \mathcal{K}(P, v_i)$



Formulation

Block Krylov methods

$$P(z) \cdot X = V$$

At each integration point, we need to solve a system with multiple right-hand-sides (RHSs)

We sequentially solve for each RHS. Each solution is approximated from a Krylov space $x_i \in \mathcal{K}(P, v_i)$



Formulation

Block Krylov methods



$$P(z) \cdot X = V$$

At each integration point, we need to solve a system with multiple right-hand-sides (RHSs)

We sequentially solve for each RHS. Each solution is approximated from a Krylov space $x_i \in \mathcal{K}(P, v_i)$

$$P(z) \cdot X = V$$

The block Krylov methods solve for all RHSs at once. Each solution is approximated from a larger subspace

$$\mathcal{B} = \mathcal{K}(P, v_1) + \dots + \mathcal{K}(P, v_n)$$

Formulation

Recycling Krylov methods

$$P(z) \cdot X = V$$

Approximate the first solution from $\mathcal{K}(P, v_1)$



Formulation

Recycling Krylov methods



$$P(z) \cdot X = V$$

Approximate the first solution from $\mathcal{K}(P, v_1)$

$$P(z) \cdot X = V$$

Approximate the second solution from
 $\mathcal{R}^{(1)} + \mathcal{K}(P, v_2)$

Formulation

Recycling Krylov methods



$$P(z)$$

$$\cdot$$

$$X$$

$$=$$

$$V$$

Approximate the first solution from $\mathcal{K}(P, v_1)$

$$P(z)$$

$$\cdot$$

$$X$$

$$=$$

$$V$$

Approximate the second solution from
 $\mathcal{R}^{(1)} + \mathcal{K}(P, v_2)$

$$P(z)$$

$$\cdot$$

$$X$$

$$=$$

$$V$$

Approximate the third solution from
 $\mathcal{R}^{(2)} + \mathcal{K}(P, v_3)$

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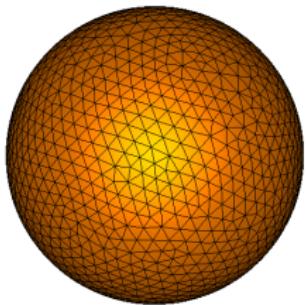
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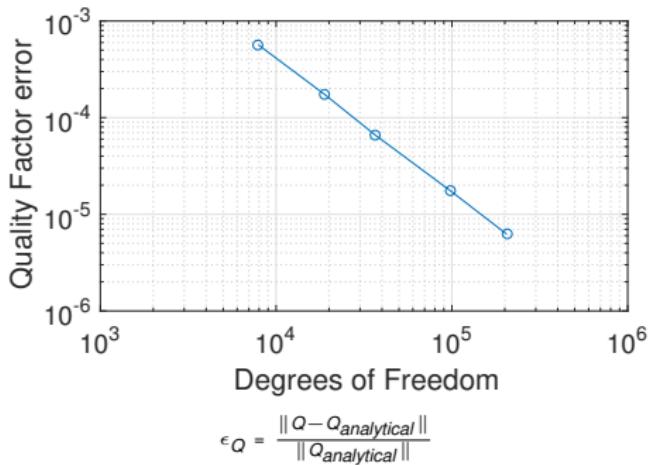
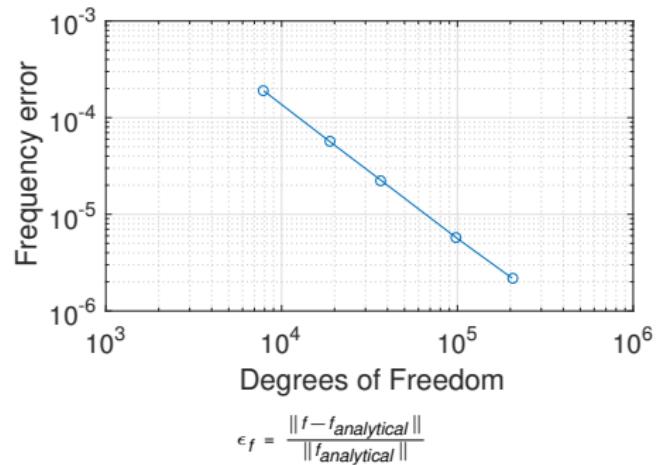
Accuracy Validation

- Name: spherical cavity
- Electrical conductivity: 62×10^6 S/m
- Radius: 1m
- Degrees of freedom : 7914/18728/36730/98244/205056
- Target frequency: 125MHz
- Number of eigenvalues: 3
- Algorithm parameters:
 - Region: $\text{rectangle}(1.0, 1.5, 1.0 \times 10^{-15}, 0.05)$
 - $N = 20$ (number of integration points)
 - $L = 20:10:100$ (number of columns of the random matrix)
 - $K = 2$ (for BEYN2)
 - Rank tolerance = 1.0×10^{-10}



Numerical Results

Accuracy Validation



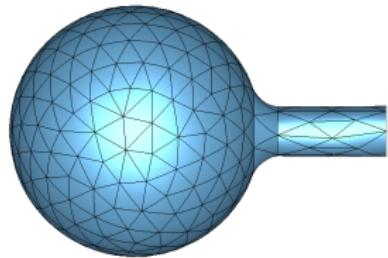
Numerical Results

Incorporating losses from ports



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- Name: spherical cavity with a coupler
- Radius: 1m
- Degrees of freedom : 3294/6158/10854/17880
- 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 = 20:10:100 (number of columns of the random matrix)
 - K = 2 (for BEYN2)
 - Rank tolerance = 1.0×10^{-10}



Numerical Results

Incorporating losses from ports

DOF	3294	6158	10854	17880
Freq. 1 (MHz)	130.641496	130.579307	130.543168	130.561674
Freq. 2 (MHz)	130.810936	130.756186	130.706348	130.698581
Freq. 3 (MHz)	130.821949	130.760146	130.724020	130.699990
Qual. 1	$2.771\ 842 \times 10^2$	$2.469\ 505 \times 10^2$	$2.787\ 006 \times 10^2$	$2.871\ 997 \times 10^2$
Qual. 2	$2.716\ 048 \times 10^5$	$2.875\ 342 \times 10^6$	$2.192\ 351 \times 10^6$	$1.114\ 248 \times 10^8$
Qual. 3	$2.109\ 400 \times 10^6$	$2.836\ 039 \times 10^7$	$7.579\ 235 \times 10^6$	$1.663\ 706 \times 10^7$

Table: Resonant frequencies and quality factors of spherical cavity with a coupler for different mesh sizes

Numerical Results

Recycling Subspace Methods

Using recycling subspace methods provided by a framework for high-performance domain decomposition methods (HPDDM) [5]

- Name: spherical cavity with a coupler
- Radius: 1m
- Degrees of freedom : 17880
- Number of RHSs: 20
- Tolerance: 10×10^{-9}

Krylov Methods	GMRES	GCRODR-5	GCRODR-10	GCRODR-20	BGMRES	BGCRODR
average # of iterations	29	25.2	25.1	24.3	24	24
runtime (s)	18.4	22.5	20.5	20.5	19	23.8

Table: Number of iterations and runtime for different Krylov methods

Numerical Results

Recycling Subspace Methods



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Using recycling subspace methods provided by a framework for high-performance domain decomposition methods (HPDDM) [5]

- Name: Tesla cavity with a main coupler
- Degrees of freedom : 60970
- Number of RHSs: 20
- Tolerance: 10×10^{-9}

Krylov Methods	GMRES	GCRODR-5	GCRODR-10	GCRODR-20	BGMRES	BGCRODR
average # of iterations	31.7	26.4	26.3	25.9	25	25
runtime (s)	69	63.3	76.8	61.2	89.2	78.9

Table: Number of iterations and runtime for different Krylov methods

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Possible Improvements

- Improve the speed of exporting system matrices.



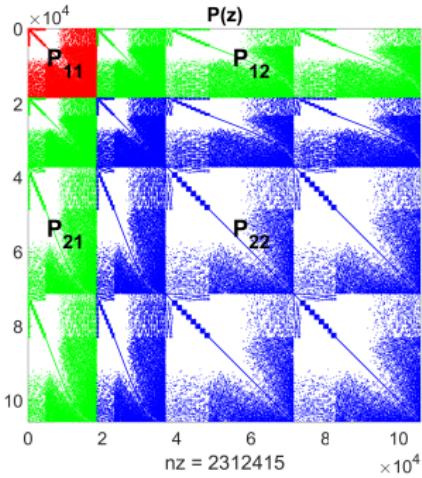
Possible Improvements

- Improve the speed of exporting system matrices.
- Improve the efficiency in using block iterative methods.



Possible Improvements

- Improve the speed of exporting system matrices.
- Improve the efficiency in using block iterative methods.
- Apply the Auxiliary Space Preconditioning [6, 7, 8] to reduce the cost in solving iterative problems



Thank you for your attention



References I



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- [3] W.-J. Beyn, “An Integral Method for Solving Nonlinear Eigenvalue Problems,” *Linear Algebra and its Applications*, vol. 436, no. 10, pp. 3839 – 3863, 2012.



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- [9] 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.

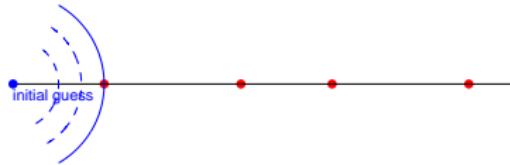


Appendix

Iterative methods (Jacobi-Davidson)

Lossless accelerator cavity: eigenvalues are on **real axis**

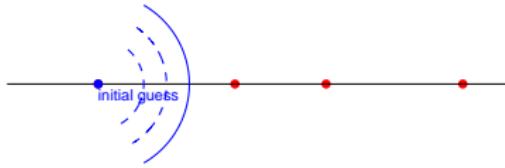
- choose an initial guess
- expand the search space ...
- until an approximate solution is found



Appendix

Iterative methods (Jacobi-Davidson)

Lossless accelerator cavity: eigenvalues are on **real axis**



- choose an initial guess
- expand the search space ...
- until an approximate solution is found
- the solution becomes the new initial guess
- continue expanding the search space ...

Appendix

Contour integral methods

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 perturbation.

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

$$P(z)^{-1} = \sum_i v_i w_i^H \frac{1}{z - \lambda_i} + R(z) \quad (10)$$

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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Contour integral methods

Some basic spectral theory



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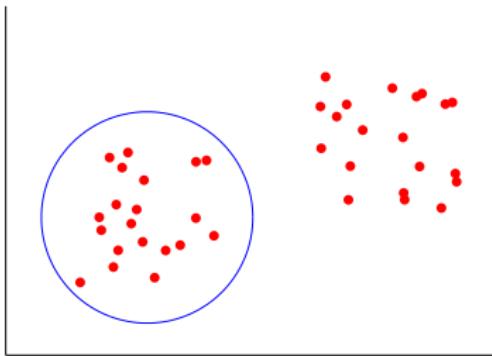
$$P(z)^{-1} = \sum_i \textcolor{red}{v}_i w_i^H \frac{1}{z - \lambda_i} + R(z)$$

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

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



$$Q = (q_1, q_2, \dots, q_k)$$

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

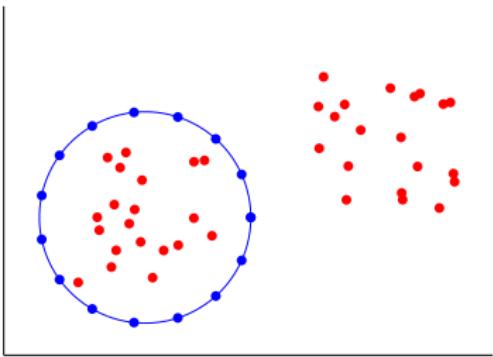
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Contour integral methods

Some basic spectral theory



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$$Q = (q_1, q_2, \dots, q_k)$$

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

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

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

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

Appendix

Contour integral methods

Beyn1 (for a few eigenvalues)



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

$$A_0 = \frac{1}{2\pi i} \oint_{\Gamma} P(z)^{-1} \hat{V} dz \quad (11)$$

$$A_1 = \frac{1}{2\pi i} \oint_{\Gamma} z P(z)^{-1} \hat{V} dz \quad (12)$$

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

- $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_{n(\Gamma)})$
- $V = [v_1 \quad \cdots \quad v_{n(\Gamma)}]$
- $W = [w_1 \quad \cdots \quad w_{n(\Gamma)}]$

\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

Appendix

Contour integral methods

Beyn1 (for a few eigenvalues)



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

$$A_0 = V_0 \Sigma_0 W_0^H \quad (13)$$

Beyn has shown that the matrix

$$B = V_0^H A_1 W_0^H \Sigma_0^{-1} \quad (14)$$

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

Beyn2 (for many eigenvalues)



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

$$A_p = \frac{1}{2\pi i} \oint_{\Gamma} z^p P(z)^{-1} \hat{V} dz \quad (15)$$

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

$$B_0 = \begin{pmatrix} A_0 & \cdots & A_{K-1} \\ \vdots & & \vdots \\ A_{K-1} & \cdots & A_{2K-2} \end{pmatrix} \quad ; \quad B_1 = \begin{pmatrix} A_1 & \cdots & A_K \\ \vdots & & \vdots \\ A_K & \cdots & A_{2K-1} \end{pmatrix} \quad (16)$$

Appendix

Contour integral methods

Beyn2 (for many eigenvalues)



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Performing the singular value decomposition of B_0

$$B_0 = V_0 \Sigma_0 W_0^H \quad (17)$$

Beyn has shown that the matrix

$$D = V_0^H B_1 W_0^H \Sigma_0^{-1} \quad (18)$$

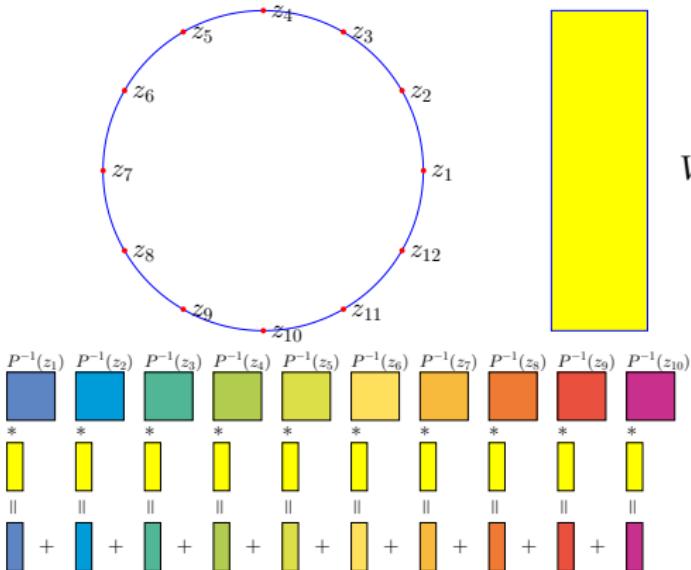
is diagonalizable. Its eigenvalues are the eigenvalues of P inside the contour and its eigenvectors lead to the corresponding eigenvectors of P .



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.

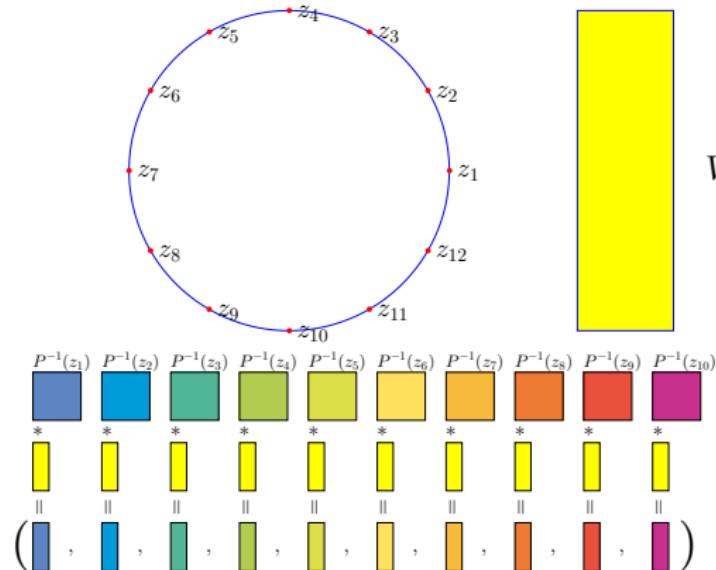
However, for large-scale problems, a small L is essential to reduce the computational burden.

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

Appendix

Contour integral methods

Resolvent Sampling based Rayleigh-Ritz method



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

$$P_Q(z)g = 0$$

Appendix

Contour integral methods



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Resolvent Sampling based Rayleigh-Ritz method

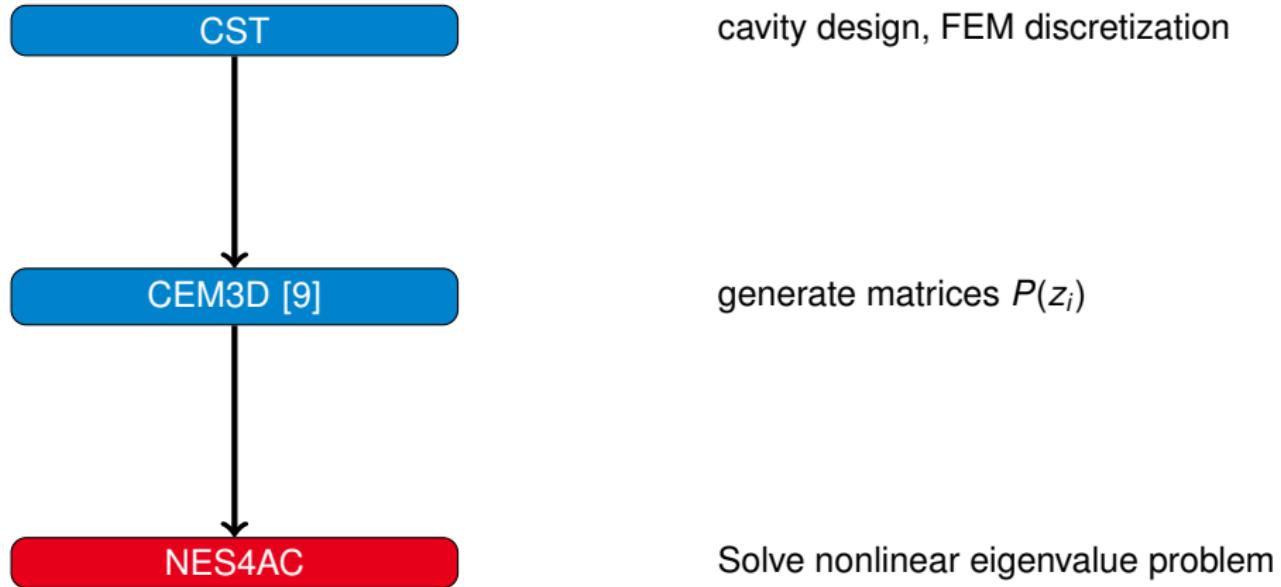
- (1) Initialization: Fix the contour Γ , the number N and the sampling points z_i . Fix the number L and generate a $n \times L$ random matrix U
- (2) Compute $P(z_i)^{-1}U$ for $i = 0, 1, \dots, N - 1$
- (3) Form S as follows

$$S = [P(z_0)^{-1}U, \quad P(z_1)^{-1}U, \quad \dots, \quad P(z_{N-1})^{-1}U] \in \mathbb{C}^{n \times N \cdot L} \quad (19)$$

- (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 $n(\Gamma)$ eigenpairs (g_j, λ_j) .
- (6) Compute the eigenpairs of the original NEP via the eigenpairs of the reduced NEP.

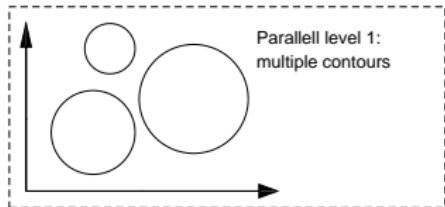
Appendix

Nonlinear Eigenvalue Solver for Accelerator Cavities (NES4AC)



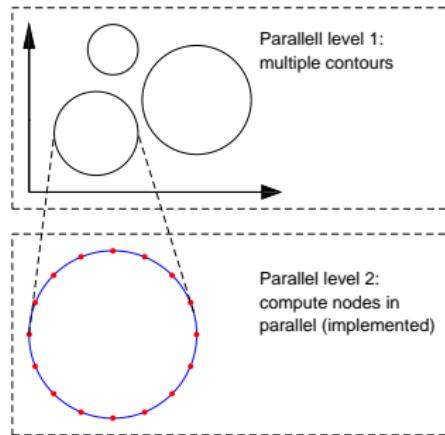
Appendix

Nonlinear Eigenvalue Solver for Accelerator Cavities (NES4AC)



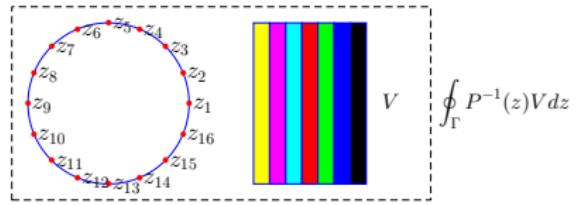
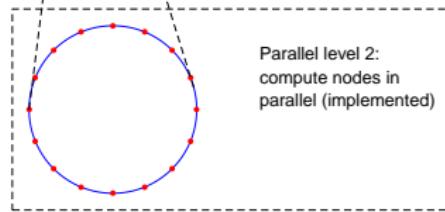
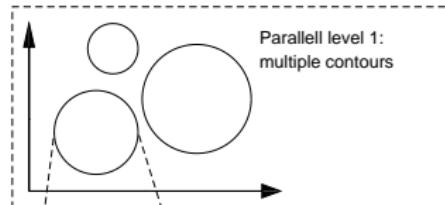
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Nonlinear Eigenvalue Solver for Accelerator Cavities (NES4AC)



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Nonlinear Eigenvalue Solver for Accelerator Cavities (NES4AC)

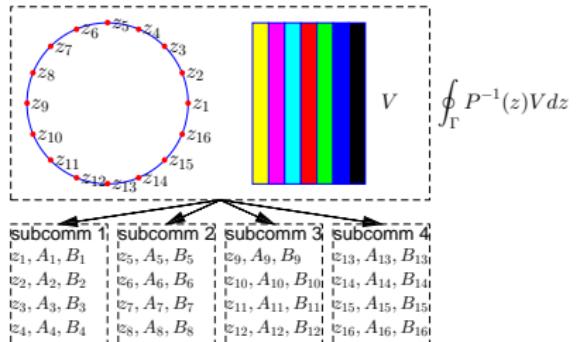
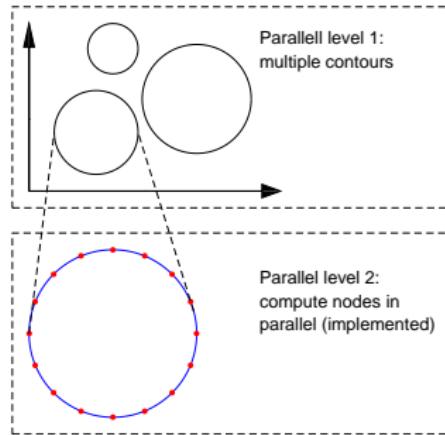


Appendix

Nonlinear Eigenvalue Solver for Accelerator Cavities (NES4AC)

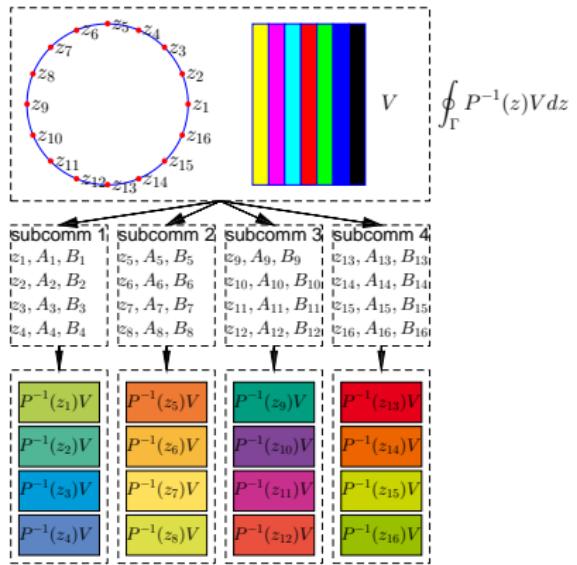
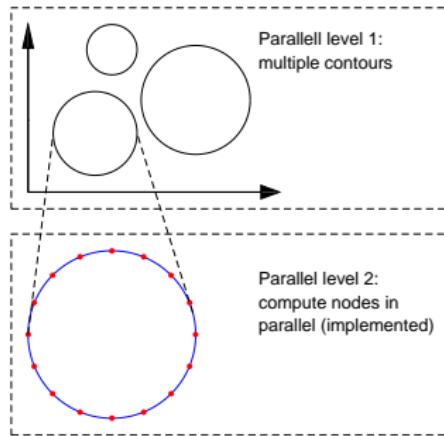


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Nonlinear Eigenvalue Solver for Accelerator Cavities (NES4AC)

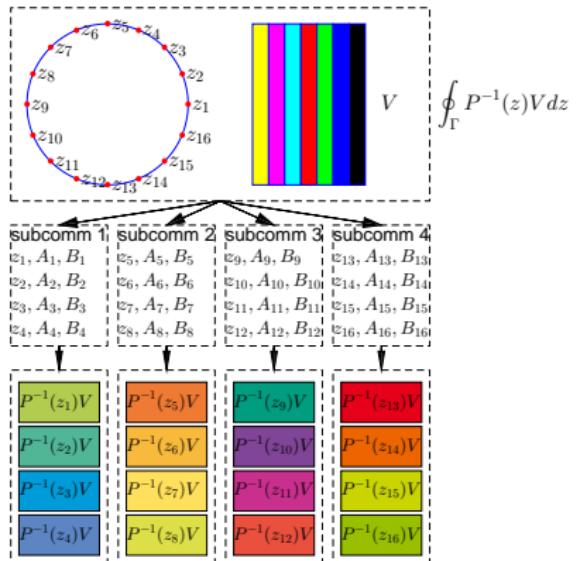
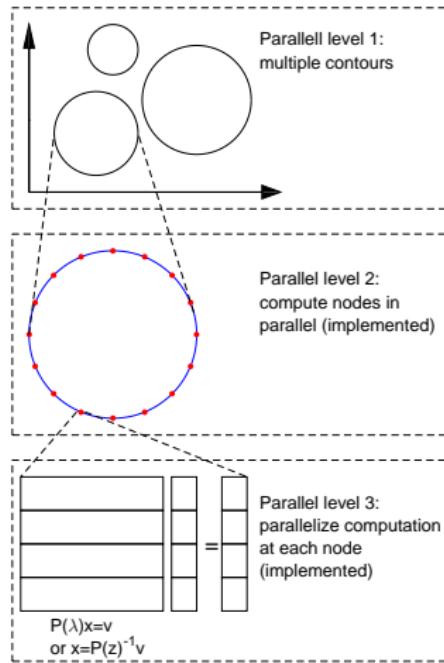


Appendix

Nonlinear Eigenvalue Solver for Accelerator Cavities (NES4AC)



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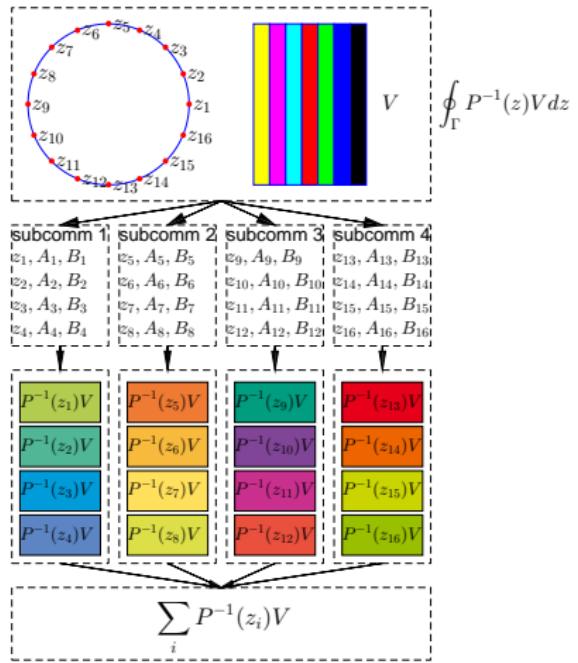
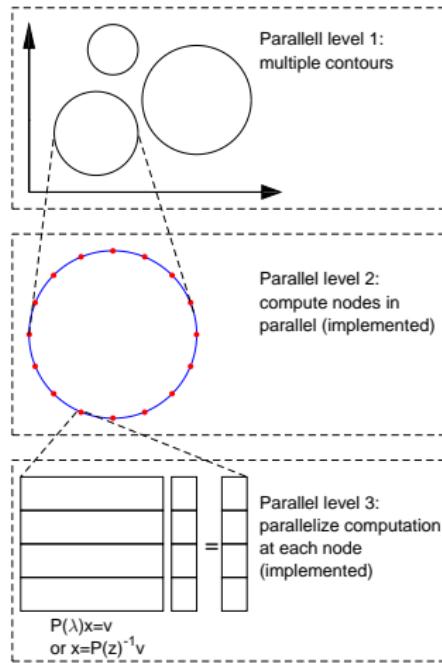


Appendix

Nonlinear Eigenvalue Solver for Accelerator Cavities (NES4AC)



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Appendix

Nonlinear Eigenvalue Solver for Accelerator Cavities (NES4AC)



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NES4AC highlights:

- extends the functionality of CEM3D [9].
- 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

$$\nabla \times \frac{1}{\mu} \nabla \times \vec{E} + j\omega\sigma\vec{E} = \varepsilon\omega^2\vec{E} \quad (20)$$

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

$$A^{3D}x + j\omega\mu_0 C^{3D}x = \omega^2\mu_0\varepsilon_0 B^{3D}x \quad (21)$$



Appendix

Target frequency in CEM3D

where

$$A_{ij}^{3D} = \iiint_{\Omega} \frac{1}{\mu_r} \nabla \times \vec{w}_i \cdot \nabla \times \vec{w}_j d\Omega \quad (22)$$

$$B_{ij}^{3D} = \iiint_{\Omega} \varepsilon_r \vec{w}_i \cdot \vec{w}_j d\Omega \quad (23)$$

$$C_{ij}^{3D} = \iiint_{\Omega} \sigma \vec{w}_i \cdot \vec{w}_j d\Omega \quad (24)$$



Appendix

Target frequency in CEM3D



Equation 21 can be rewritten as follows

$$(A^{3D} + j\omega\mu_0 C^{3D})x = \left(\frac{\omega}{c_0}\right)^2 B^{3D}x \quad (25)$$

$$s(A^{3D} + j\omega\mu_0 C^{3D})x = s^2 \left(\frac{\omega}{c_0}\right)^2 \frac{B^{3D}}{s} x \quad (26)$$

$$A^{CEM3D}x = \lambda B^{CEM3D}x \quad (27)$$

where

$$s = \frac{c_0}{2\pi f_\tau} \quad (28)$$