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Parallel Algorithms for solving Nonlinear Eigenvalue Problems in Accelerator Cavity Simulations

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Joint work with O. Marques (LBNL), E.G. Ng (LBNL), C. Yang (LBNL), Z. Bai (UC Davis), L. Ge (SLAC), O. Kononenko (SLAC), Z. Li (SLAC), C.-K. Ng (SLAC), L. Xiao (SLAC)

ICAP'18 – Key West, FL – October 23, 2018

Motivation: Nonlinear boundary conditions

Maxwell's equations

$$\nabla \times \left(\frac{1}{\mu} \nabla \times E \right) - \lambda \varepsilon E = 0$$

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particular freq.

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Eigenvalue problem

- eigenvalue $\rightarrow$ complex frequency
- eigenvector $\rightarrow$ electric field

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Option 1:

- closed cavity
- no volumetric losses
- no surface loss

$\Longrightarrow$ Real symmetric **linear** eigenvalue problem

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- eigenvalue $\rightarrow$ complex frequency
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Option 1:

- closed cavity
- no volumetric losses
- no surface loss

$\Longrightarrow$ Real symmetric **linear** eigenvalue problem

Option 2:

- cavity with waveguides
- to couple external power sources
- to damp high order modes

$\Longrightarrow$ **Nonlinear** eigenvalue problem

Motivation: Nonlinear boundary conditions

Terminate propagation of E

$\rightarrow$ (nonlinear) boundary conditions

Accelerator cavity nonlinear eigenvalue problem

$$\left(K - \lambda M + \mathrm{i}\sqrt{\lambda}\, W^{\mathrm{TEM}} + \mathrm{i}\sum_m \sqrt{\lambda - \kappa_m}\, W_m^{\mathrm{TE}} + \mathrm{i}\sum_m \frac{\lambda}{\sqrt{\lambda - \kappa_m}} W_m^{\mathrm{TM}}\right) x = 0$$

- $\lambda = k^2$
- $\kappa_m = (k_m^c)^2$ cutoff values of mth waveguide mode

Outline

1. Solving Nonlinear Eigenvalue Problems
   - Approximation
   - Linearization pencils
   - Solving linear eigenvalue problem

2. Numerical Experiments
   - Pillbox cavity
   - TESLA SRF cavity cryomodule

Nonlinear eigenvalue problem (NLEP)

NLEP

The nonlinear eigenvalue problem:

$$F(\lambda)x = 0$$

where

- $\lambda \in \Omega \subseteq \mathbb{C}$: eigenvalue
- $x \in \mathbb{C}^n \backslash \{0\}$: eigenvector
- $F : \Omega \to \mathbb{C}^{n \times n}$: matrix-valued function

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Note that the NLEP is

$\rightsquigarrow$ nonlinear in eigenvalue λ,

$\rightsquigarrow$ linear in eigenvector x.

Nonlinear eigenvalue problem (NLEP)

NLEP

The nonlinear eigenvalue problem:

$$F(\lambda)x = \left(\sum_{i=1}^{k} B_i f_i(\lambda)\right) x = 0$$

where

- $\lambda \in \Omega \subseteq \mathbb{C}$: eigenvalue
- $x \in \mathbb{C}^n \backslash \{0\}$: eigenvector
- $F : \Omega \to \mathbb{C}^{n \times n}$: matrix-valued function

Solving NLEPs

NLEP
$F(\lambda)x = 0$

$\Downarrow$ ❶ approximation via interpolation

PEP
$P_d(\lambda)x = 0$

$\Downarrow$ ❷ linearization

GEP
$\mathbf{L}(\lambda)\mathbf{x} = 0$

$\Downarrow$ ❸ solving linear eigenvalue problem

Solution

Approximation

NLEP

$F(\lambda)x = 0$

$\Downarrow$

PEP

$P_d(\lambda)x = 0$

$\Downarrow$

GEP

$\mathbf{L}(\lambda)\mathbf{x} = 0$

$\Downarrow$

Solution

Step 1: Polynomial interpolation

$$F(\lambda) \approx P_d(\lambda) = A_0 + A_1\lambda + A_2\lambda^2 + \cdots + A_d\lambda^d$$

Approximation

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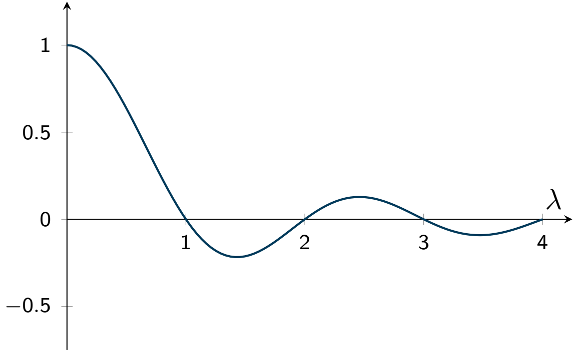

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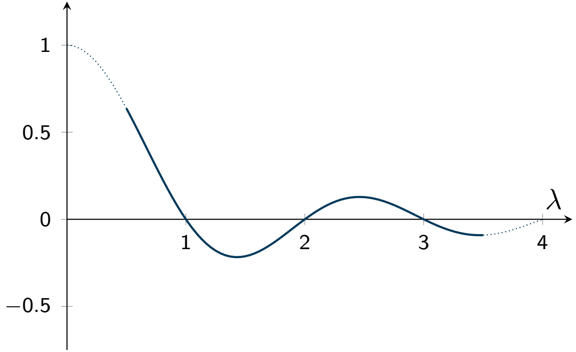

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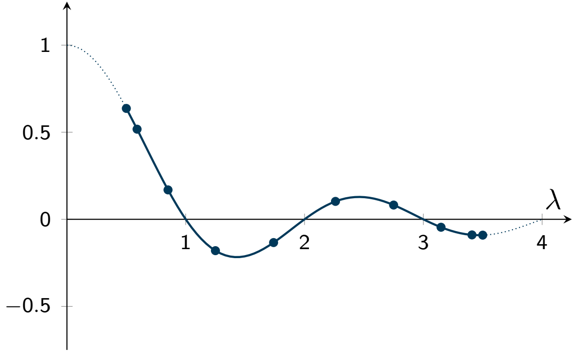

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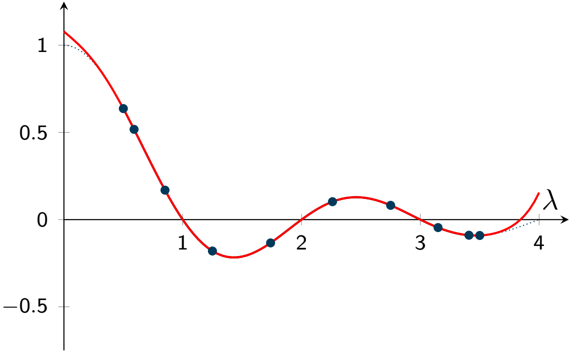
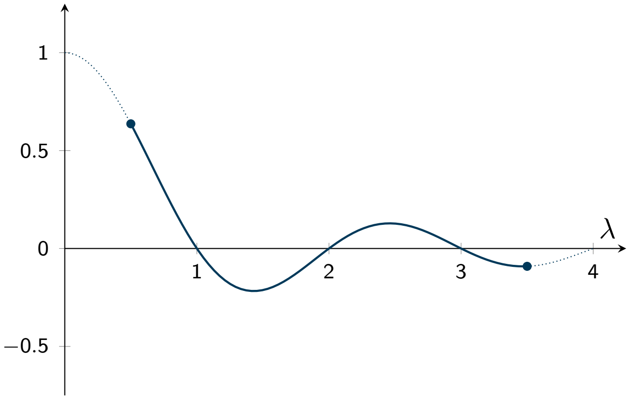


Approximation: Newton interpolation

Dynamic polynomial interpolation (Newton)

$$F(\lambda) \approx A_0 n_0(\lambda) + A_1 n_1(\lambda)$$



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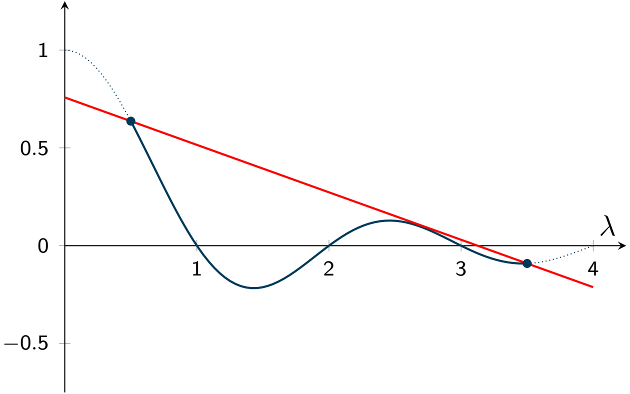

Approximation: Newton interpolation

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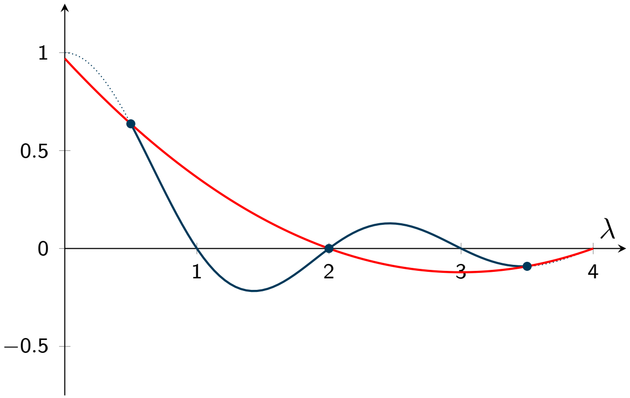
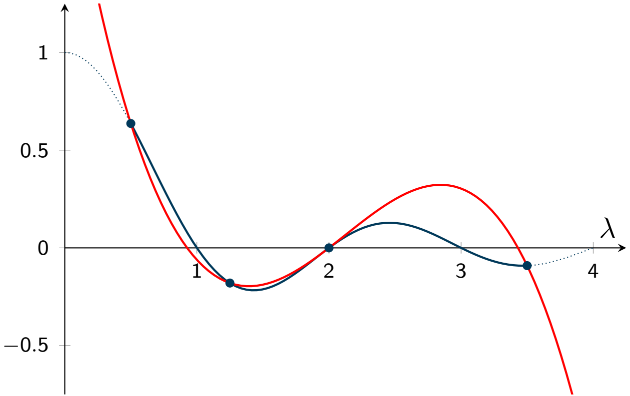


Approximation: Newton interpolation

Dynamic polynomial interpolation (Newton)

$$F(\lambda) \approx A_0 n_0(\lambda) + A_1 n_1(\lambda) + \cdots + A_3 n_3(\lambda)$$



Approximation: Newton interpolation

Dynamic polynomial interpolation (Newton)

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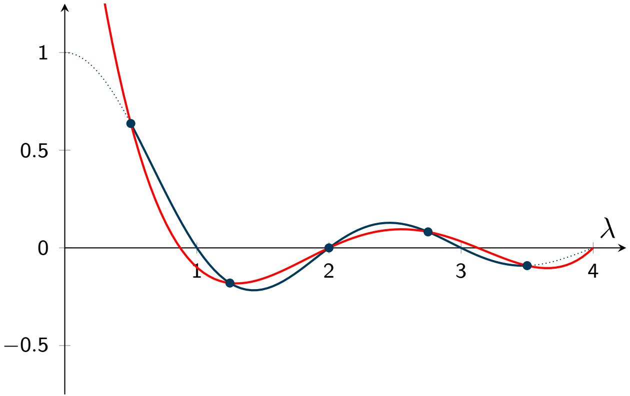

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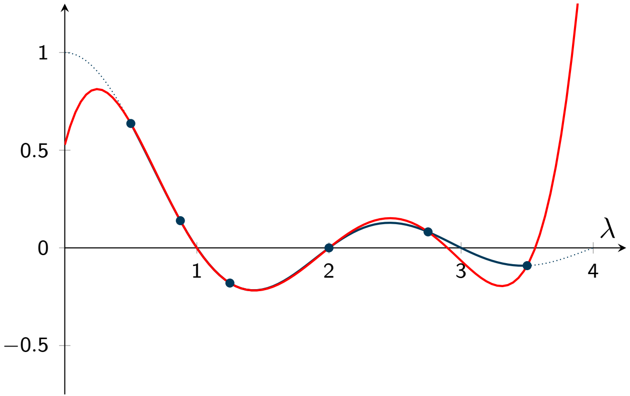

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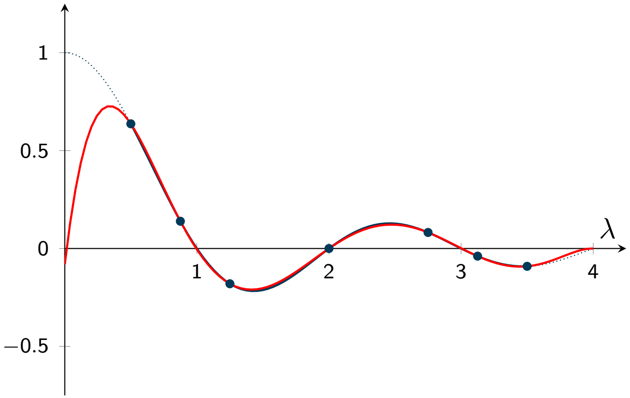

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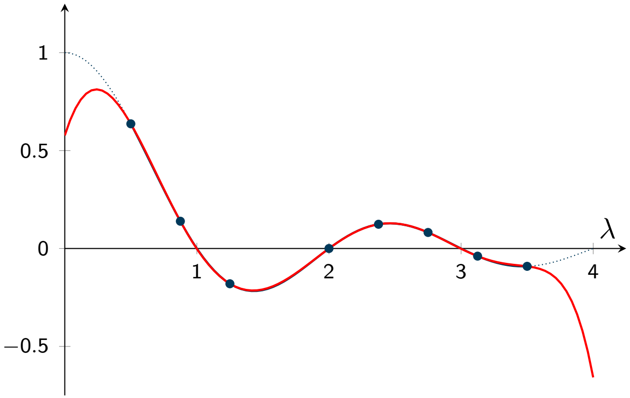

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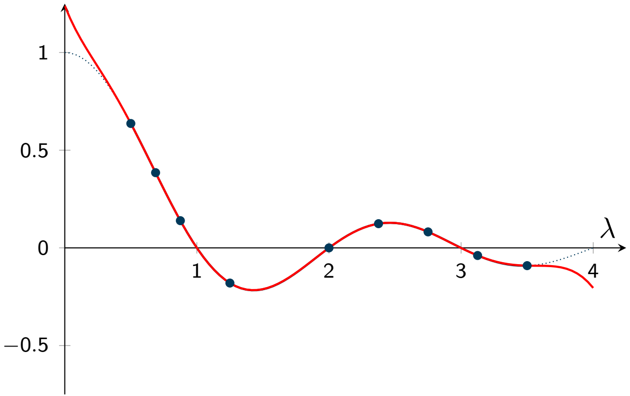

Approximation: Newton interpolation

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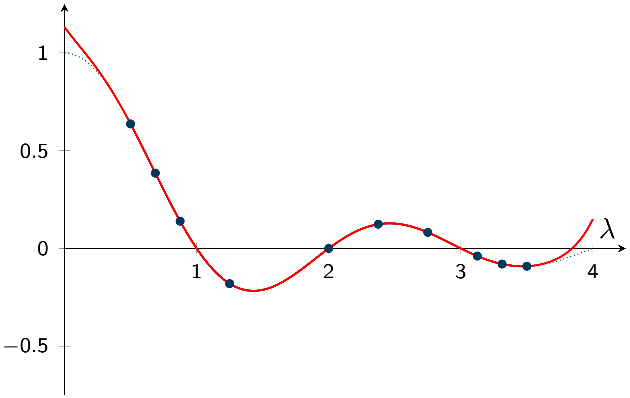
$$F(\lambda) \approx A_0 n_0(\lambda) + A_1 n_1(\lambda) + \cdots + A_9 n_9(\lambda)$$

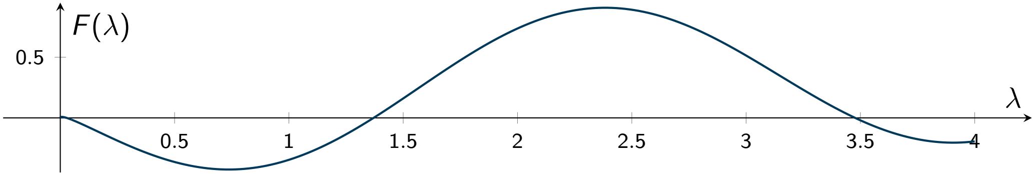


Approximation: Polynomial versus Rational

Scalar nonlinear function:

$$F(\lambda) = 0.2\sqrt{\lambda} - 0.6\sin(2\lambda) = 0$$

with target set: $\Sigma = [0.01, 4]$



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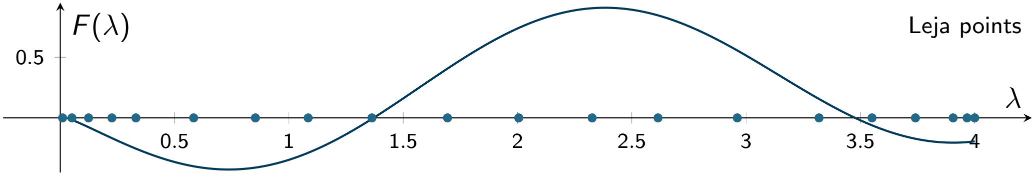

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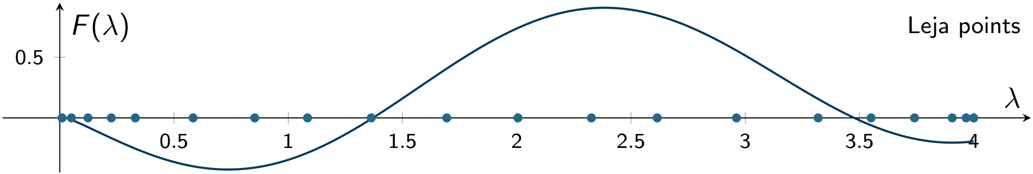

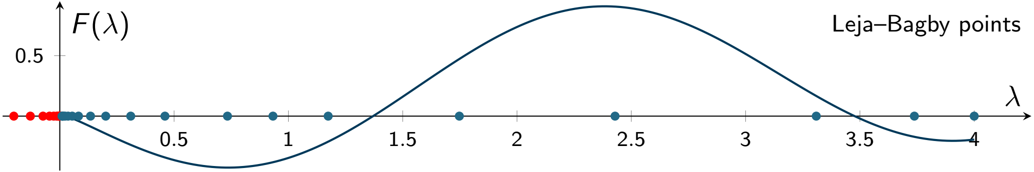

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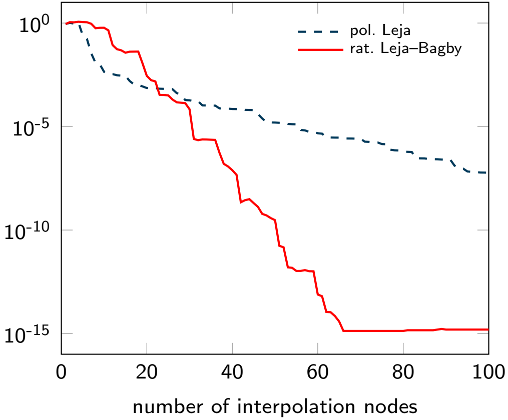
interpolation error



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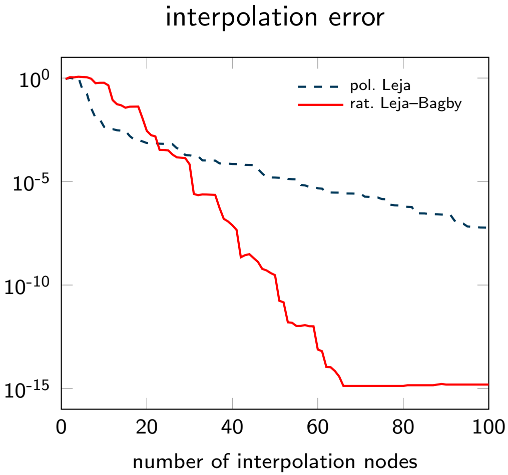
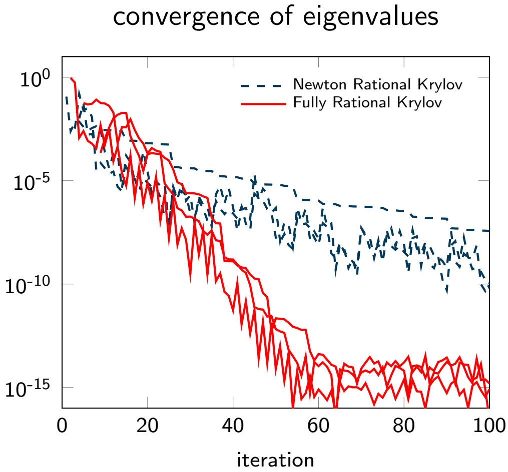




Linearization pencils

NLEP

$F(\lambda)x = 0$

$\Downarrow$

PEP

$P_d(\lambda)x = 0$

$\Downarrow$

GEP

$\mathbf{L}(\lambda)\mathbf{x} = 0$

$\Downarrow$

Solution

Step 2: Linearization

$$P_d(\lambda)x = 0$$

$$\Downarrow$$

$$\mathbf{L}(\lambda)\mathbf{x} = (\mathbf{A} - \lambda\mathbf{B})\mathbf{x} = 0$$

Linearization pencils

Linearization: idea

Second order ODE

$$M\ddot{q} + C\dot{q} + Kq = 0$$

System of first order ODEs

$$\begin{cases} \dot{q}_1 = q_2 \\ M\dot{q}_2 = -Cq_2 - Kq_1 \end{cases}$$

$$\begin{bmatrix} I & 0 \\ 0 & M \end{bmatrix} \begin{bmatrix} \dot{q}_1 \\ \dot{q}_2 \end{bmatrix} = \begin{bmatrix} 0 & I \\ -K & -C \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \end{bmatrix}$$

Linearization pencils

Linearization: idea

Second order ODE

$$M\ddot{q} + C\dot{q} + Kq = 0$$

Quadratic eigenvalue problem

$$\left(M\lambda^2 + C\lambda + K\right)x = 0$$

System of first order ODEs

$$\begin{cases} \dot{q}_1 = q_2 \\ M\dot{q}_2 = -Cq_2 - Kq_1 \end{cases}$$

$$\begin{bmatrix} I & 0 \\ 0 & M \end{bmatrix} \begin{bmatrix} \dot{q}_1 \\ \dot{q}_2 \end{bmatrix} = \begin{bmatrix} 0 & I \\ -K & -C \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \end{bmatrix}$$

Linear eigenvalue problem

$$\lambda \begin{bmatrix} I & 0 \\ 0 & M \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 & I \\ -K & -C \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

Linearization pencils

Step 2: Companion linearization

PEP

$P_d(\lambda)x = 0$

$\Rightarrow$

GEP

$\mathbf{L}(\lambda)\mathbf{x} = (\mathbf{A} - \lambda\mathbf{B})\mathbf{x} = 0$

$$P_d(\lambda)x = \left(A_0 + A_1\lambda + A_2\lambda^2 + \cdots + A_d\lambda^d\right)x = 0$$

$$\underbrace{\begin{bmatrix} A_0 & A_1 & A_2 & \cdots & A_{d-1} \\ & I & & & \\ & & I & & \\ & & & \ddots & \\ & & & & I \end{bmatrix}}_{\mathbf{A}} \underbrace{\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_d \end{bmatrix}}_{\mathbf{x}} = \lambda \underbrace{\begin{bmatrix} 0 & 0 & \cdots & 0 & -A_d \\ I & 0 & & & \\ & \ddots & \ddots & & \\ & & I & 0 & \\ & & & I & 0 \end{bmatrix}}_{\mathbf{B}} \underbrace{\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_d \end{bmatrix}}_{\mathbf{x}}$$

Linearization pencils: Uniform representation

$$\mathbf{L}(\lambda) = \underbrace{\left[\begin{array}{cccc} A_0 & A_1 & \cdots & A_{d-1} \\ \hline \multicolumn{4}{c}{M \otimes I_n} \end{array}\right]}_{\mathbf{A}} - \lambda \underbrace{\left[\begin{array}{cccc} B_0 & B_1 & \cdots & B_{d-1} \\ \hline \multicolumn{4}{c}{N \otimes I_n} \end{array}\right]}_{\mathbf{B}}$$

- Monomial basis [Mackey, Mackey, Mehl, Mehrmann 2006]
- Chebyshev basis [Effenberger, Kressner 2012]
- Lagrange basis [VB, Michiels, Meerbergen 2015]
- Newton/Hermite basis [Amiraslani, Corless, Lancaster 2009]
- Rational monomial basis [Nakatsukasa, Tisseur 2014]
- Rational Newton basis [Güttel, VB, Meerbergen, Michiels 2014]
- Spectral discretization [Jarlebring, Meerbergen, Michiels 2010]
- ...

Linearization pencils: Structured eigenvectors

Suppose λ is an eigenvalue of

$$L(\lambda) = \left[\begin{array}{cccc} A_0 & A_1 & \cdots & A_{d-1} \\ \hline \multicolumn{4}{c}{M \otimes I_n} \end{array}\right] - \lambda \left[\begin{array}{cccc} B_0 & B_1 & \cdots & B_{d-1} \\ \hline \multicolumn{4}{c}{N \otimes I_n} \end{array}\right]$$

with corresponding structured eigenvector

$$\mathbf{x} = a \otimes x$$

where $a \in \mathbb{C}^d$.

Solving linear eigenvalue problem

NLEP

$F(\lambda)x = 0$

$\Downarrow$

PEP

$P_d(\lambda)x = 0$

$\Downarrow$

GEP

$\mathbf{L}(\lambda)\mathbf{x} = 0$

$\Downarrow$

Solution

Step 3: Solve generalized linear eigenvalue problem

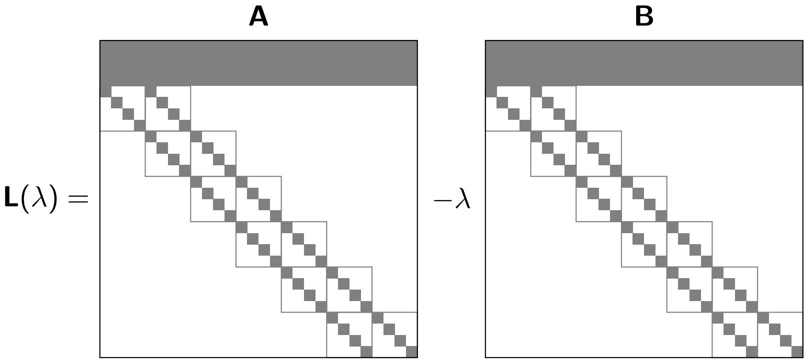
$$\mathbf{L}(\lambda)\mathbf{x} = (\mathbf{A} - \lambda\mathbf{B})\mathbf{x} = 0$$

by the rational Krylov method.

Solving NLEPs

$$F(\lambda)\, x = 0 \quad \Longrightarrow \quad \mathbf{L}(\lambda)\, \mathbf{x} = 0$$

Compact Rational Krylov (CORK) framework



- full exploitation of structure
- reduction in memory cost
- reduction in computation cost

Rational Krylov method

GEP

$$Ax = \lambda Bx$$

Arnoldi method:

- one shift σ
- shift-and-invert step:

$$w := (A - \sigma B)^{-1} B v_j$$

- recurrence relation:

$$B^{-1} A V = V \underline{H}$$

Rational Krylov method

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Rational Krylov method [Ruhe 1984]*:*

- multiple shifts $\sigma_1, \sigma_2, \ldots$
- shift-and-invert step:

$$w := (A - \sigma_j B)^{-1} B v_j$$

- recurrence relation:

$$A V \underline{H} = B V \underline{K}$$

CORK method

Compact Rational Krylov (CORK) method

Rational Krylov method with:

1. linearization matrices **A** and **B**

$$\left[\begin{array}{cccc} A_0 & A_1 & \cdots & A_{d-1} \\ \hline & M \otimes I_n & & \end{array}\right], \quad \left[\begin{array}{cccc} B_0 & B_1 & \cdots & B_{d-1} \\ \hline & N \otimes I_n & & \end{array}\right].$$

2. compact representation of subspace

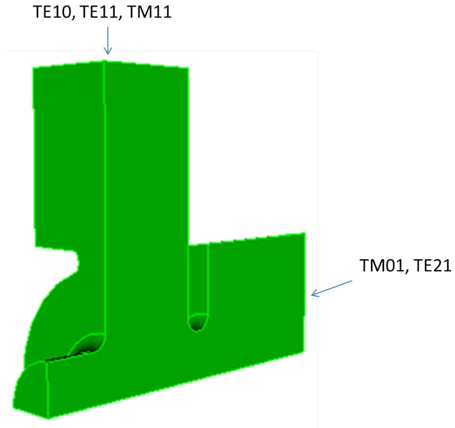
$$\mathbf{V} = (I_d \otimes Q)\mathbf{U}.$$

Simplified RF gun cavity (LCLS)

Nonlinear eigenvalue problem

$$F(\lambda)x = 0$$

target frequency window [1.0 GHz, 2.2 GHz]



Simplified RF gun cavity (LCLS)

Nonlinear eigenvalue problem

$$F(\lambda)x = 0$$

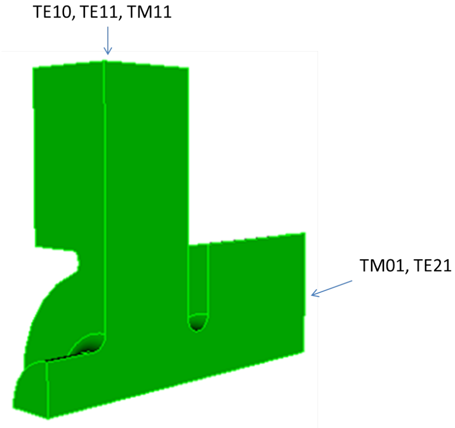
where

$$\begin{aligned} F(\lambda) = K - \lambda M &+ \mathrm{i}\sqrt{\lambda - \kappa_1}\, W_{10}^{\mathrm{TE}} \\ &+ \mathrm{i}\frac{\lambda}{\sqrt{\lambda - \kappa_2}} W_{01}^{\mathrm{TM}} + \mathrm{i}\sqrt{\lambda - \kappa_3}\, W_{21}^{\mathrm{TE}} \\ &+ \mathrm{i}\sqrt{\lambda - \kappa_4}\, W_{11}^{\mathrm{TE}} + \mathrm{i}\frac{\lambda}{\sqrt{\lambda - \kappa_4}} W_{11}^{\mathrm{TM}} \end{aligned}$$

and

$$f_1^c = 0.908\,\mathrm{GHz} \qquad f_2^c = 1.043\,\mathrm{GHz}$$
$$f_3^c = 1.325\,\mathrm{GHz} \qquad f_4^c = 1.897\,\mathrm{GHz}$$

target frequency window [1.0 GHz, 2.2 GHz]



Simplified RF gun cavity (LCLS)

$$\left(K - \lambda M + \mathrm{i}\sqrt{\lambda - \kappa_1}\, W_{10}^{\mathsf{TE}} + \mathrm{i}\frac{\lambda}{\sqrt{\lambda - \kappa_2}} W_{01}^{\mathsf{TM}} + \mathrm{i}\sqrt{\lambda - \kappa_3}\, W_{21}^{\mathsf{TE}} + \mathrm{i}\sqrt{\lambda - \kappa_4}\, W_{11}^{\mathsf{TE}} + \mathrm{i}\frac{\lambda}{\sqrt{\lambda - \kappa_4}} W_{11}^{\mathsf{TM}}\right) x = 0$$

Problem parameters:

- adaptive unstructured mesh with 27,384 quadratic tetrahedral elements
- second order basis functions
- total degrees of freedom $n = 170,562$

Simplified RF gun cavity (LCLS)

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Problem parameters:

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- second order basis functions
- total degrees of freedom $n = 170,562$

Solution:

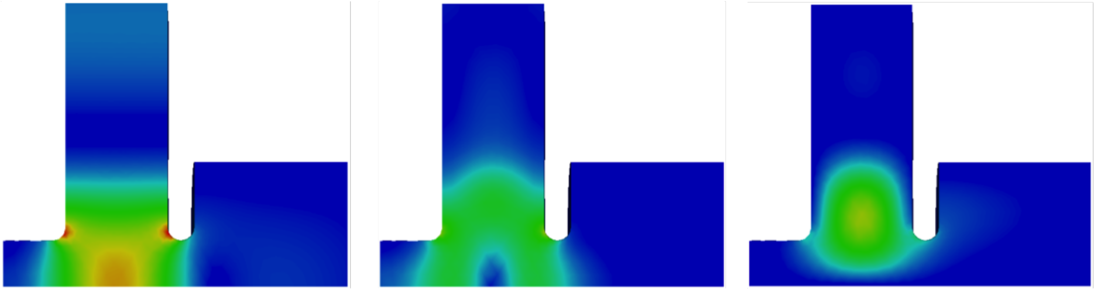
- 64 cores on NERSC Cori
- less than 3 minutes for all resonant modes in [1.0 GHz, 2.2 GHz]

Simplified RF gun cavity (LCLS)

Eigenvalue λ:

- resonant mode frequency: $\mathrm{Re}(\lambda)$
- damping factor $Q = \frac{1}{2}\frac{\mathrm{Re}(\lambda)}{\mathrm{Im}(\lambda)}$

$f_1 = 1.1762\,\mathrm{GHz}$	$f_2 = 1.1762\,\mathrm{GHz}$	$f_3 = 1.1762\,\mathrm{GHz}$
$Q_1 = 271$	$Q_2 = 739$	$Q_3 = 693$



Omega3P (CORK) vs S3P

Omega3P (CORK)

Solving NLEP directly

S3P

1. response calculations
2. Lorentzian fitting

Omega3P (CORK) vs S3P

Omega3P (CORK)

Solving NLEP directly

S3P

1. response calculations
2. Lorentzian fitting

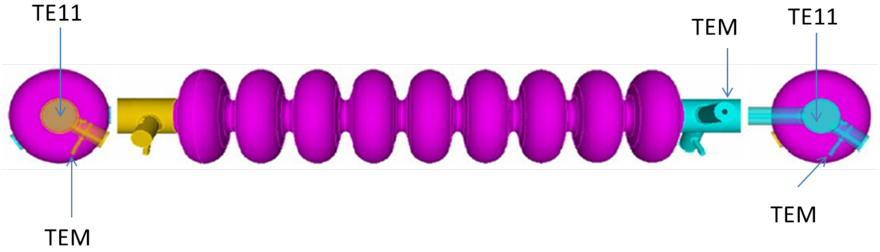
Mode	Omega3P (CORK)			S3P	
	f [GHz]	Q	rel. error	f [GHz]	Q
1	1.1762	271	1.2827e−14	1.1762	270
2	2.0567	739	2.1098e−14	2.0567	760
3	2.1960	693	4.5892e−15	2.1965	780

TESLA SRF cavity cryomodule (LCLS-II)

LCLS-II cryomodule consisting of 8 TESLA cavities

$$\left(K - \lambda M + \mathrm{i}\sqrt{\lambda}\, W^{\mathsf{TEM}} + \mathrm{i}\sqrt{\lambda - \kappa}\, W_{11}^{\mathsf{TE}}\right) x = 0$$

where $\kappa = (2\pi f_c/c)^2$ with $f_c = 2.253\,\mathrm{GHz}$ the beampipe cutoff frequency



TESLA SRF cavity cryomodule (LCLS-II)

$$\left(K - \lambda M + \mathrm{i}\sqrt{\lambda}\, W^{\mathsf{TEM}} + \mathrm{i}\sqrt{\lambda - \kappa}\, W_{11}^{\mathsf{TE}}\right) x = 0$$

Problem parameters:

- adaptive unstructured mesh with 2,877,955 quadratic tetrahedral elements
- second order basis functions
- total degrees of freedom $n = 17,273,664$

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Problem parameters:

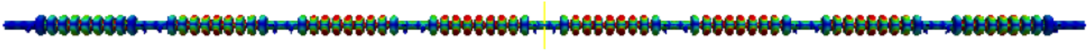
- adaptive unstructured mesh with 2,877,955 quadratic tetrahedral elements
- second order basis functions
- total degrees of freedom $n = 17,273,664$

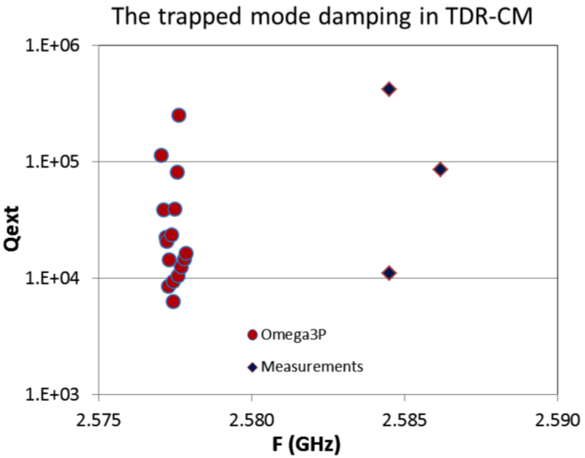
Solution:

- 960 cores on NERSC Edison
- less than 10 minutes to compute 16 trapped modes

TESLA SRF cavity cryomodule (LCLS-II)

Electric field amplitude profile for the highest external Q mode





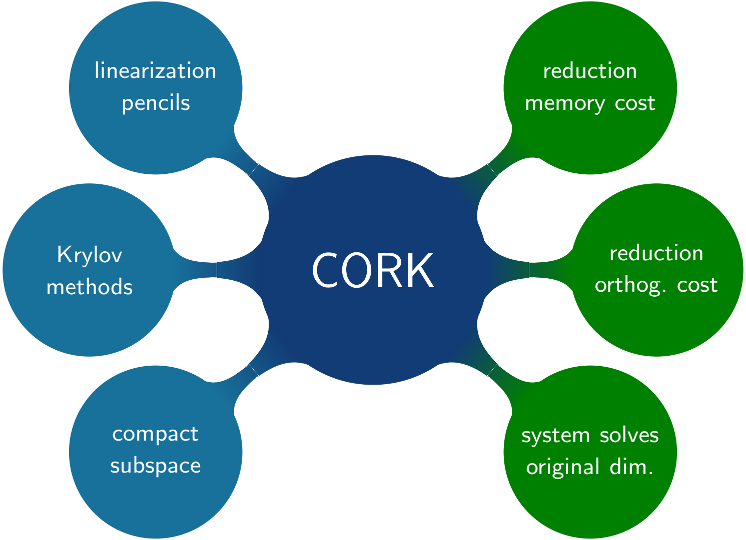
Conclusions

How to solve NLEP's

$$F(\lambda)x = 0$$

1. Approximation via interpolation
2. Linearization
3. Solve linear eigenvalue problem

Compact Rational Krylov (CORK) framework



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CORK software available on my homepage:
`http://www.roelvanbeeumen.be`