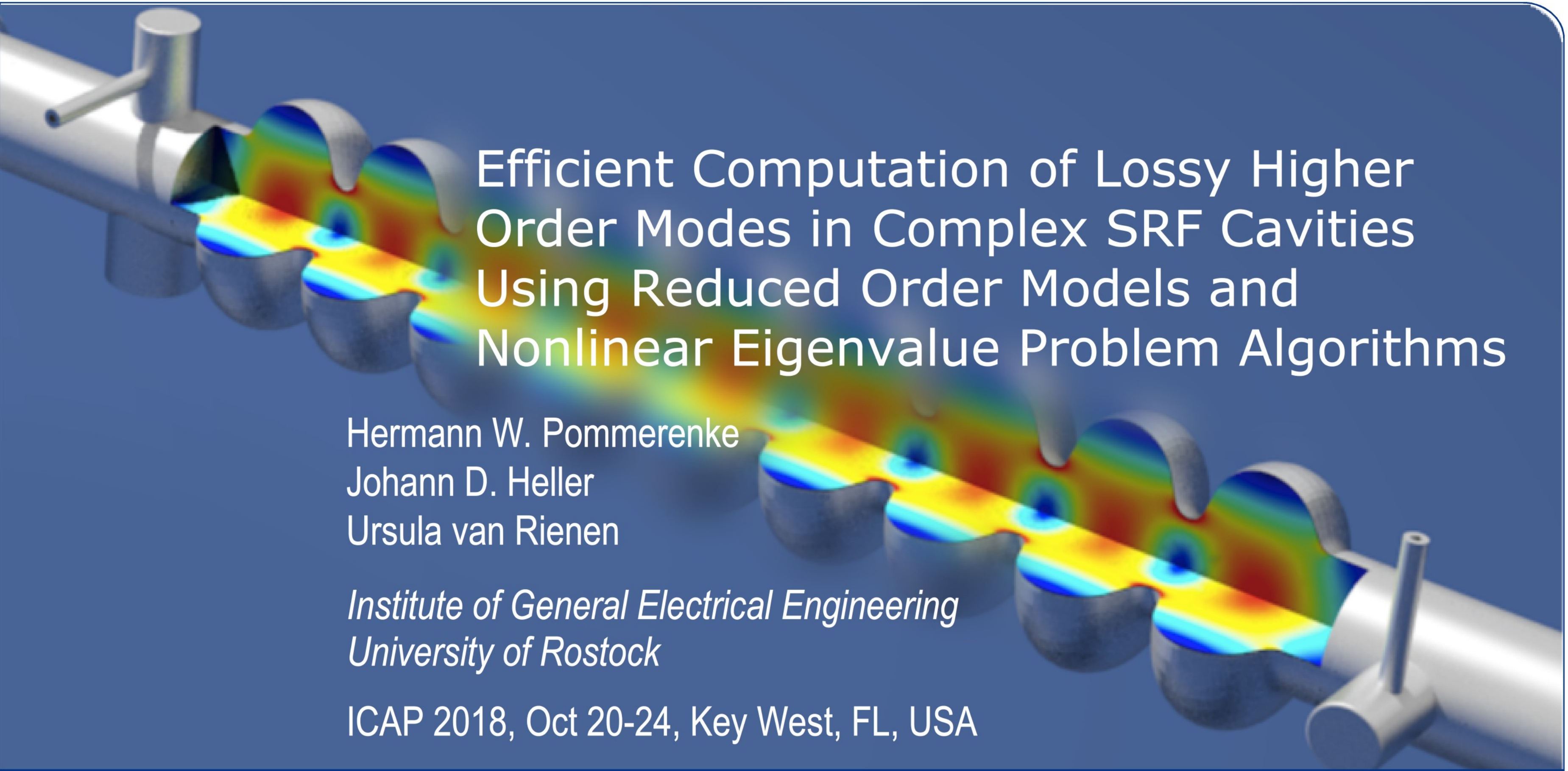

Efficient Computation of Lossy Higher Order Modes in Complex SRF Cavities Using Reduced Order Models and Nonlinear Eigenvalue Problem Algorithms

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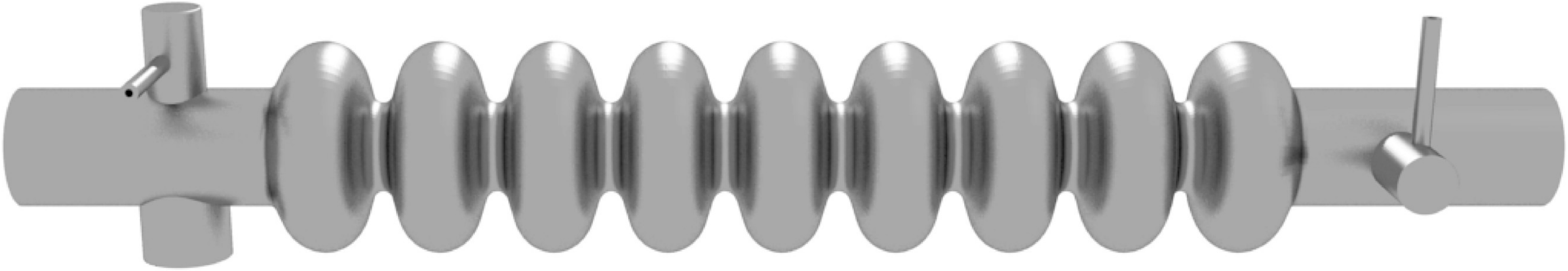
Introduction

- Superconducting radio frequency (SRF) cavities essential to modern particle accelerators, provide resonant EM fields for acceleration
- precise knowledge of resonant frequencies *f*, power losses *P* and field distributions required



FLASH Third Harmonic Module Cavity, figure taken from [Heller '18]

Introduction

- Power losses: dielectric, magnetic, surface/ohmic, **external**

  generally dominant in SRF cavities

- Q factor

$$Q = 2\pi f W / P$$

frequency (f), stored energy (W), power loss (P)

- External losses particularly important for Higher Order Modes (HOM)
- HOMs excited by beam current, may lower beam quality by deviation, emittance growth…
- damp HOMs using cavity “openings”: beam pipe, input & HOM couplers

Introduction

- Design done by numerical methods due to complex shape
  - Finite Integration Technique (FIT) [Weiland '77, van Rienen '12]
  - Finite Element Method (FEM) [e.g. Bondeson '05]
  - etc.

- lossless structures → linear eigenvalue problem

  $(\boldsymbol{A} - \lambda \boldsymbol{I})\boldsymbol{x} = \boldsymbol{0}$

- Structure with external losses → **nonlinear eigenvalue problem** (NLEVP)

  $\boldsymbol{T}(\lambda)\boldsymbol{x} = \boldsymbol{0}$

- Solutions: „eigenmodes“

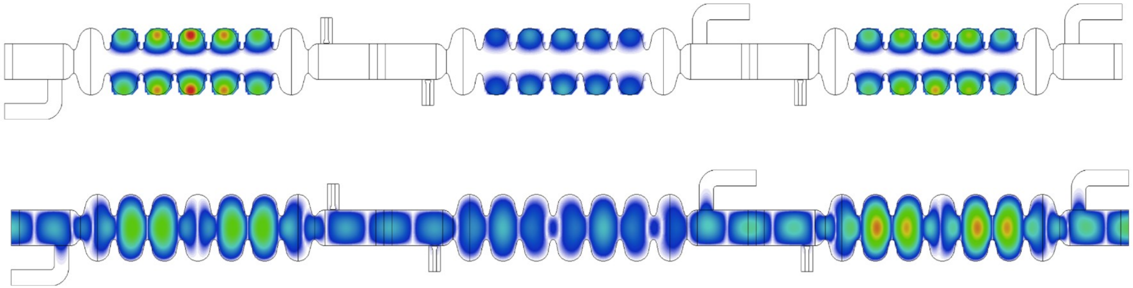
  eigenvalue → f, Q eigenvector → field distribution

Introduction

- Numerical methods scale disadvantageously with size/complexity of structure, large number of DOF necessary for accurate results

Solution approaches

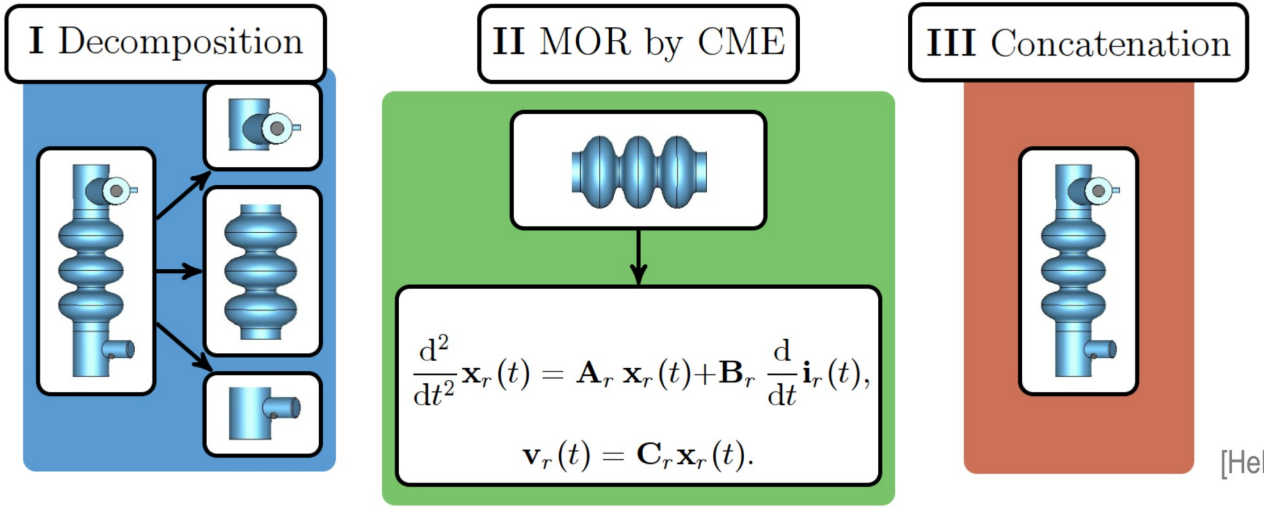
- Brute force
- Simulate only parts of the structure
  works for constrained modes like this →
  but not multi-cavity modes like this →
- Model Order Reduction



BERLinPro HOMs, figure taken from [Heller '18]

State-Space Concatenation (SSC)

- scheme suggested by [Flisgen '13, '15] to solve Maxwell's equations for large complex SRF structures
- combination of domain decomposition and model order reduction (MOR)



[Heller '15]

State-Space Concatenation (SSC)

- decompose structure into segments
- each segment: Correct Modal Expansion [Wittig '04] into N_{3D} 3D eigenmodes
  - incomplete eigendecomposition in domain of interest
  - expand orthogonal base from frequency response snapshots
- cutting planes treated as waveguide ports: N_{2D} 2D port modes

State-Space Concatenation (SSC)

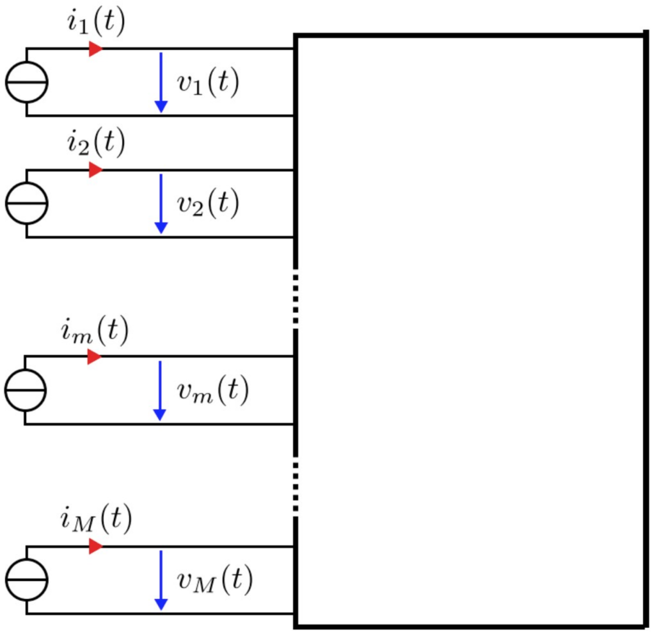
internal states ***x***

3D eigenmodes

modal currents ***i***

and voltages ***v***

2D port modes



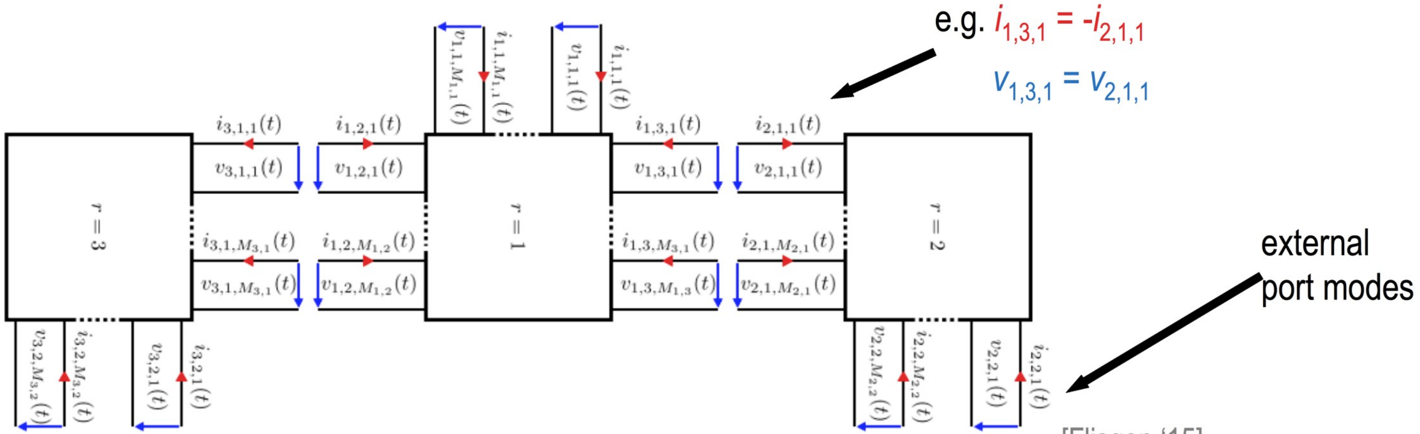
[Flisgen '15]

1st order state space model (SSM)

$$s\boldsymbol{x}(s) = \boldsymbol{A}\boldsymbol{x}(s) + \boldsymbol{B}\boldsymbol{i}(s)$$
$$\boldsymbol{v}(s) = \boldsymbol{C}\boldsymbol{x}(s),$$

State-Space Concatenation (SSC)

- concatenation of segments by eliminating redundant modal currents/voltages at connected waveguide ports using Kirchhoff's laws



[Flisgen '15]

- apply MOR by CME to concatenated structure
- assign excitation or boundary conditions to external port modes

State-Space Concatenation (SSC)

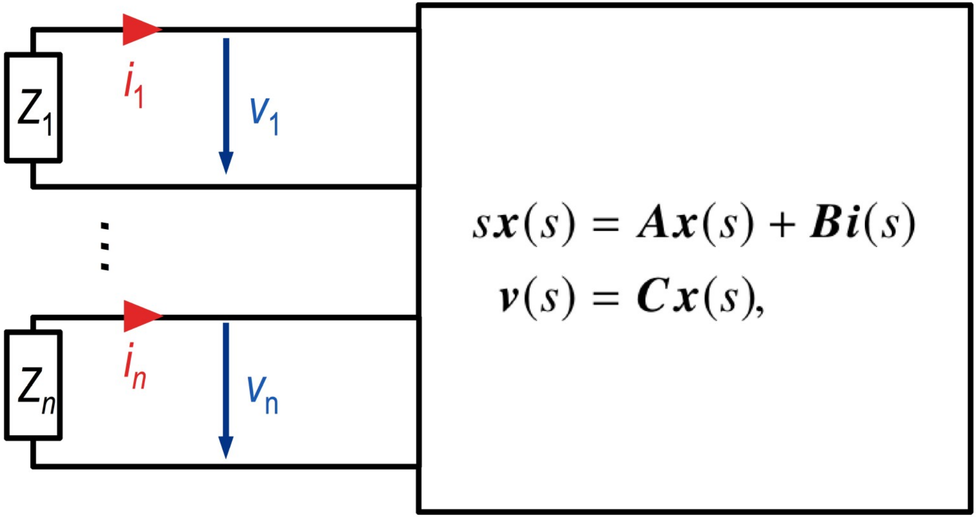
- SSC advantages compared to other domain decomposition techniques [Heller '18]

	Circuit Model	Generalized Scattering Matrix (GSM)	Coupled S-parameter Calculation (CSC)	Mode Matching	State-Space Concatenation (SSC)
	[e.g. Wittig '04]	[eg. Shinton '08, Jones '16]	[e.g. Glock '02, Rothemund '00]	[e.g. van Rienen '93, Weiland '99, Cooke '08]	
Time domain	o	✓	o	✓	✓
Freq. domain	o	✓	✓	✓	✓
MOR	✓	X	X	X	✓
3D fields	o	o	o	✓	✓

✓ available o partially/with great effort X not available

External Losses in SRF Cavities

- model cavity with infinitely long waveguides attached to ports → reflection-free
- impedance matching: port mode termination = wave impedance [Flisgen '14]



$$s\boldsymbol{x}(s) = \boldsymbol{A}\boldsymbol{x}(s) + \boldsymbol{B}\boldsymbol{i}(s)$$
$$\boldsymbol{v}(s) = \boldsymbol{C}\boldsymbol{x}(s),$$

$$Z_{\text{wave}}^{\text{TE}}(\lambda) = Z_0 \frac{\lambda}{\sqrt{\lambda^2 + \omega_{\text{co}}^2}}$$

$$Z_{\text{wave}}^{\text{TM}}(\lambda) = Z_0 \frac{\sqrt{\lambda^2 + \omega_{\text{co}}^2}}{\lambda}$$

$$Z_{\text{wave}}^{\text{TEM}} = 50\,\Omega.$$

TE, TM impedances nonlinear in frequency $\lambda = j\omega$

External Losses in SRF Cavities

- perturbation ansatz: each eigenmode of lossy structure described as weighted sum of eigenmodes (internal states) of lossless structure
- resulting nonlinear eigenvalue problem (NLEVP) [Flisgen '14, Heller '18]

$$\boldsymbol{T}(\lambda)\boldsymbol{x} = \left(\boldsymbol{A} - \boldsymbol{B}\boldsymbol{G}(\lambda)\boldsymbol{B}^{\mathrm{T}} - \lambda\boldsymbol{I}\right)\boldsymbol{x} = \boldsymbol{0}$$

eigenvalue

diagonal matrix with reciprocal wave impedances (nonlinearity)

eigenvector (amplitudes of lossless modes)

$$f = \frac{\Im\{\lambda\}}{2\pi} \qquad Q = -\frac{\Im\{\lambda\}}{2\Re\{\lambda\}}$$

Solving the Nonlinear Eigenvalue Problem

- NLEVP solution much more intricate than linear eigenvalue problems

- variety of solution approaches exists, overview in [e.g. Bai ‘00, Güttel ’17]
  - **Newton**-type methods [e.g. Anselone ‘68, Effenberger ‘13]
  - **contour integrals** [Sakurai/Sugiura ‘03, Beyn ‘12]
  - generalized QR decompositions [Kublanovskaja ‘69]
  - Rayleigh functionals [Duffin ‘55, Hadeler ‘67]
  - etc

- general approach: map NLEVP onto several linear problems

Solving the NLEVP with Newton Iteration

- find roots in (N+1)-dimensional search space (eigenvalue, eigenvector)
- formulation of Newton's method to solve [e.g. Ruhe '73, Voss '13]

$$\boldsymbol{P}\begin{pmatrix}\boldsymbol{x}\\ \lambda\end{pmatrix} = \begin{pmatrix}\boldsymbol{T}(\lambda)\boldsymbol{x}\\ \boldsymbol{v}^{\mathrm{H}}\boldsymbol{x} - 1\end{pmatrix} = \boldsymbol{0}$$

normalization vector

- apply iteration rule

$$\begin{pmatrix}\boldsymbol{x}_{\nu+1}\\ \lambda_{\nu+1}\end{pmatrix} = \begin{pmatrix}\boldsymbol{x}_{\nu}\\ \lambda_{\nu}\end{pmatrix} - \left(\boldsymbol{P}'\begin{pmatrix}\boldsymbol{x}_{\nu}\\ \lambda_{\nu}\end{pmatrix}\right)^{-1}\boldsymbol{P}\begin{pmatrix}\boldsymbol{x}_{\nu}\\ \lambda_{\nu}\end{pmatrix}$$

(***P'*** : Frechet derivative of ***P*** w.r.t $(\boldsymbol{x}, \lambda)^{\mathrm{T}}$

Solving the NLEVP with Newton Iteration

- more convenient implementation: introduce auxiliary search direction ***u***

$$\boldsymbol{u}_{\nu+1} = \boldsymbol{T}^{-1}(\lambda_\nu)\frac{\partial \boldsymbol{T}}{\partial \lambda}(\lambda_\nu)\boldsymbol{x}_\nu$$

$$\boldsymbol{x}_{\nu+1} = c_{\nu+1}\boldsymbol{u}_{\nu+1}$$

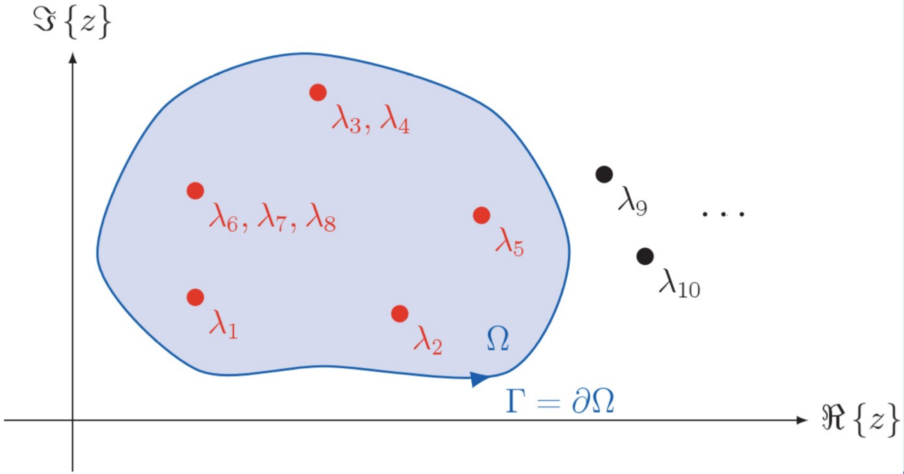
$$\lambda_{\nu+1} = \lambda_\nu - \frac{\boldsymbol{v}^{\mathrm{H}}\boldsymbol{x}_\nu}{\boldsymbol{v}^{\mathrm{H}}\boldsymbol{u}_{\nu+1}},$$

- initial eigenpair from linearized problem $\boldsymbol{T}(z_0)\boldsymbol{x} = \boldsymbol{\lambda x}$, grid / Monte-Carlo sampling etc.
- employ deflation techniques to avoid converging against already found solutions
  e.g. choose ***v*** orthogonal to all previously computed eigenvectors
- successfully employed by [Heller '18] to solve the SRF cavity NLEVP

Solving the NLEVP with Beyn's Algorithm

- Problem with Newton iteration: no guarantee for completeness
  (but very important to find all resonant modes within specified domain!)

- Contour integral algorithm
  suggested by [Beyn '12] computes
  complete NLEVP solution within
  finite enclosed subdomain
  of complex plane



Solving the NLEVP with Beyn's Algorithm

- theory: NLEVP operator inverse can be expressed as Laurent series in vicinity of eigenvalues [Keldysh '51]

$$\boldsymbol{T}^{-1}(z) = \sum_{j=1}^{k} \frac{1}{z-\lambda_j} \boldsymbol{x}_j \boldsymbol{y}_j + (\text{holomorphic part})$$

- compute contour integrals

$$\boldsymbol{L}_p = \frac{1}{2\pi \mathrm{j}} \oint_{\Gamma} z^p \boldsymbol{T}^{-1}(z) \boldsymbol{\Psi} \mathrm{d}z \quad , \quad p = 0, 1$$

  in practice: solve $\boldsymbol{T}^{-1}(z)\boldsymbol{\Psi}$ at each discrete quadrature point

eigenvalues

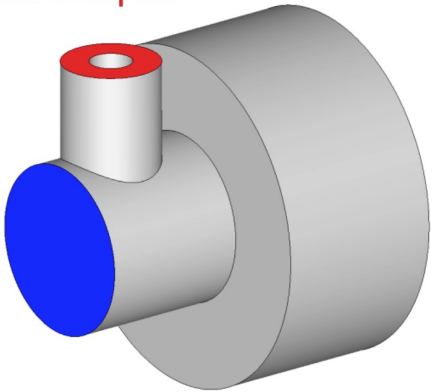
right/left eigenvectors

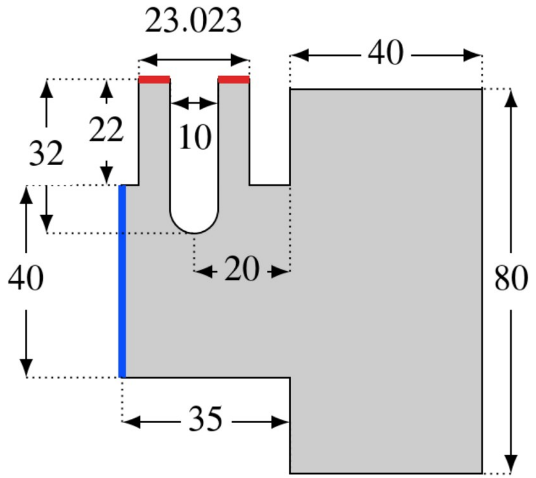
- by Cauchy's integral formula: (extract using SVD, LEVP)

$$\boldsymbol{L}_0 = \boldsymbol{X}\boldsymbol{Y}\boldsymbol{\Psi} \text{ and } \boldsymbol{L}_1 = \boldsymbol{X}\boldsymbol{\Lambda}\boldsymbol{Y}\boldsymbol{\Psi}$$

Example: Minimalistic Resonator

- hypothetical SRF cavity with

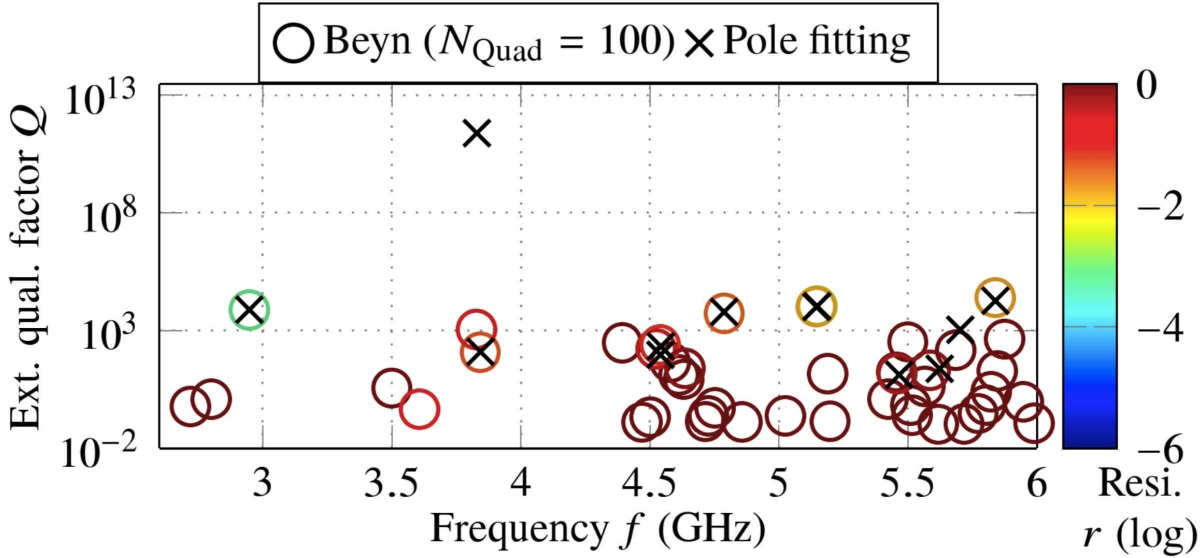




- initial FIT mesh: 233,000 cells; NLEVP after MOR of order N = 178

Minimalistic Resonator: Beyn's Algorithm

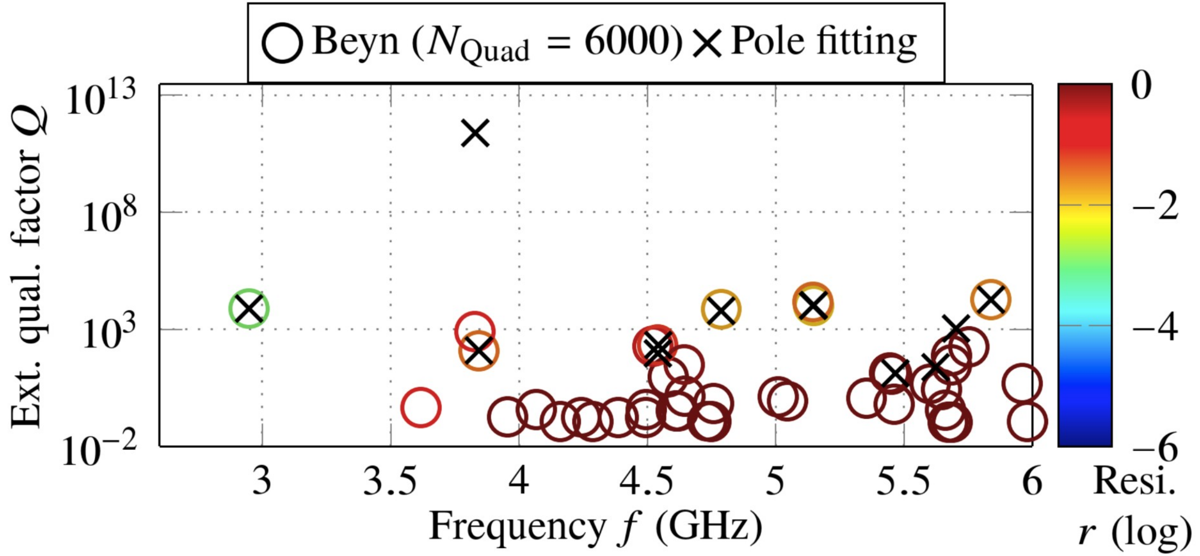
- with 100 quadrature points (100 linear systems solved)



- reference solutions by pole fitting [Gustavsen '06, Galek '12]

Minimalistic Resonator: Beyn's Algorithm

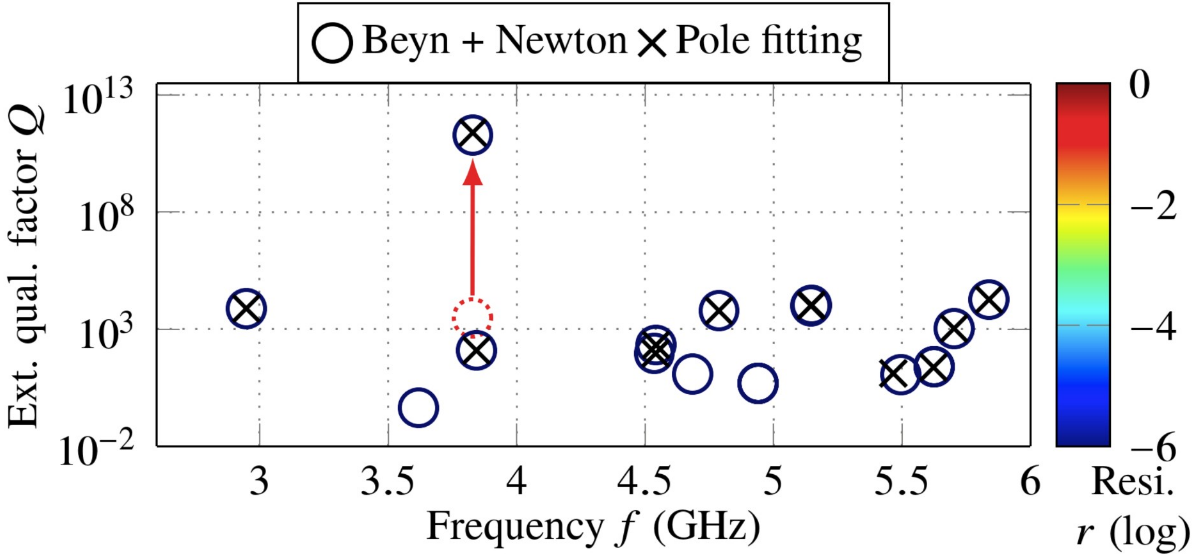
- with 6000 quadrature points



- practically no improvement in convergence!

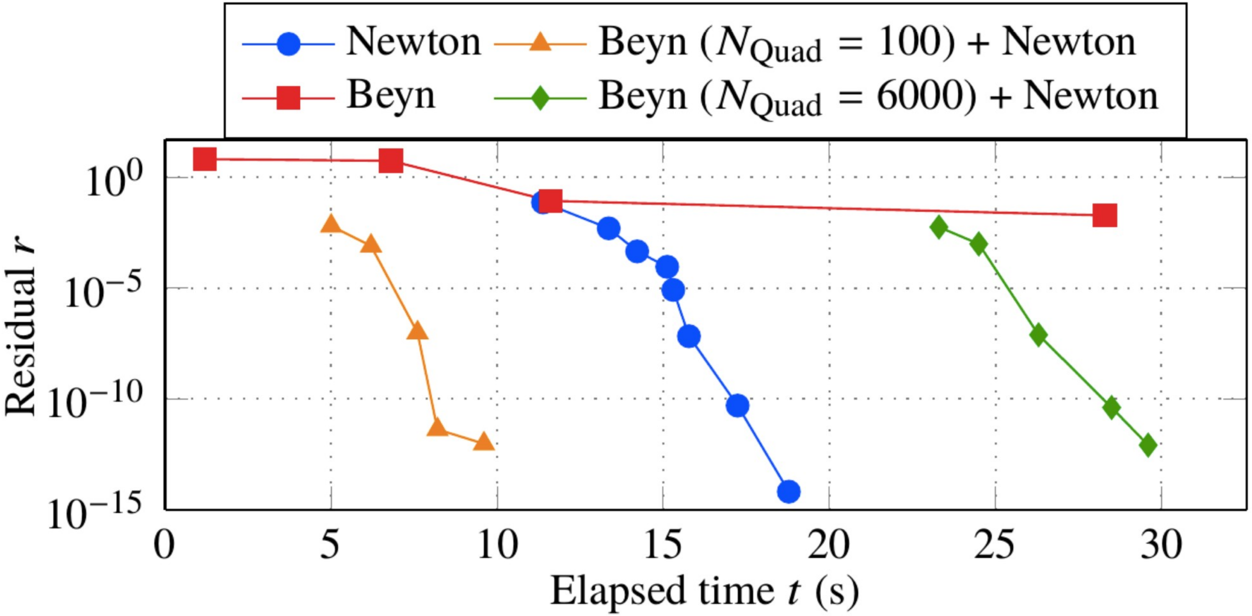
Minimalistic Resonator: Beyn’s Alg. + Newton Iteration

- 100 quadrature points, solutions from Beyn as Newton starting pair



- residual improved significantly with only a few iterations

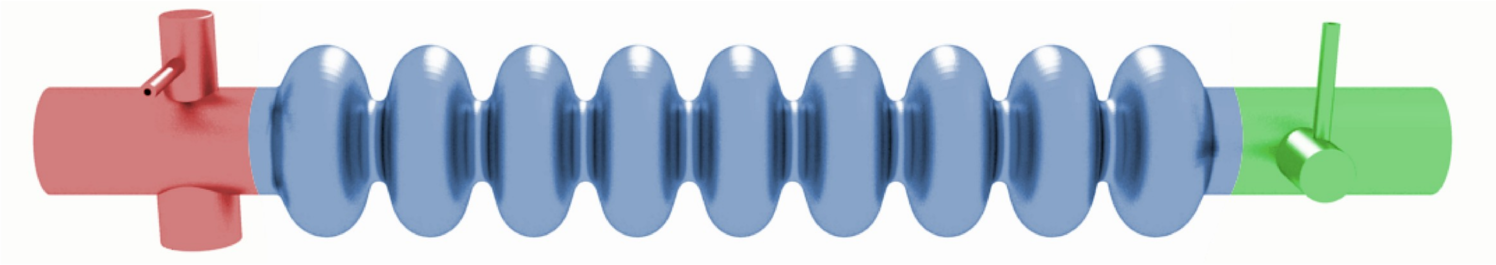
Minimalistic Resonator: Solution Time



- most efficient combination: Beyn' algorithm with few quadrature points and consecutive Newton iteration

Example: FLASH Cavity

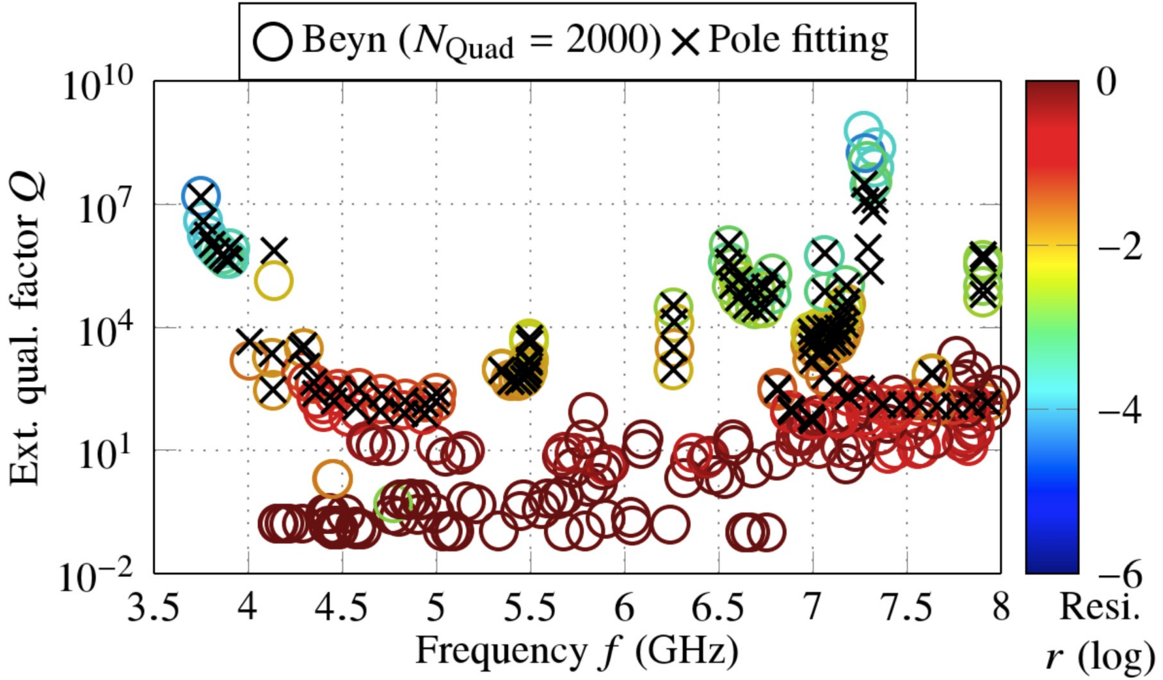
- real life example: TESLA-type cavity from Third Harmonic Module of FLASH at DESY, e.g. [Sekutowicz '02, Solyak '03]



- five external waveguide ports: 2x beam pipe, input coupler, 2x HOM coupler
- NLEVP after MOR by SSC is of order $N = 780$

FLASH Cavity: Beyn's Algorithm

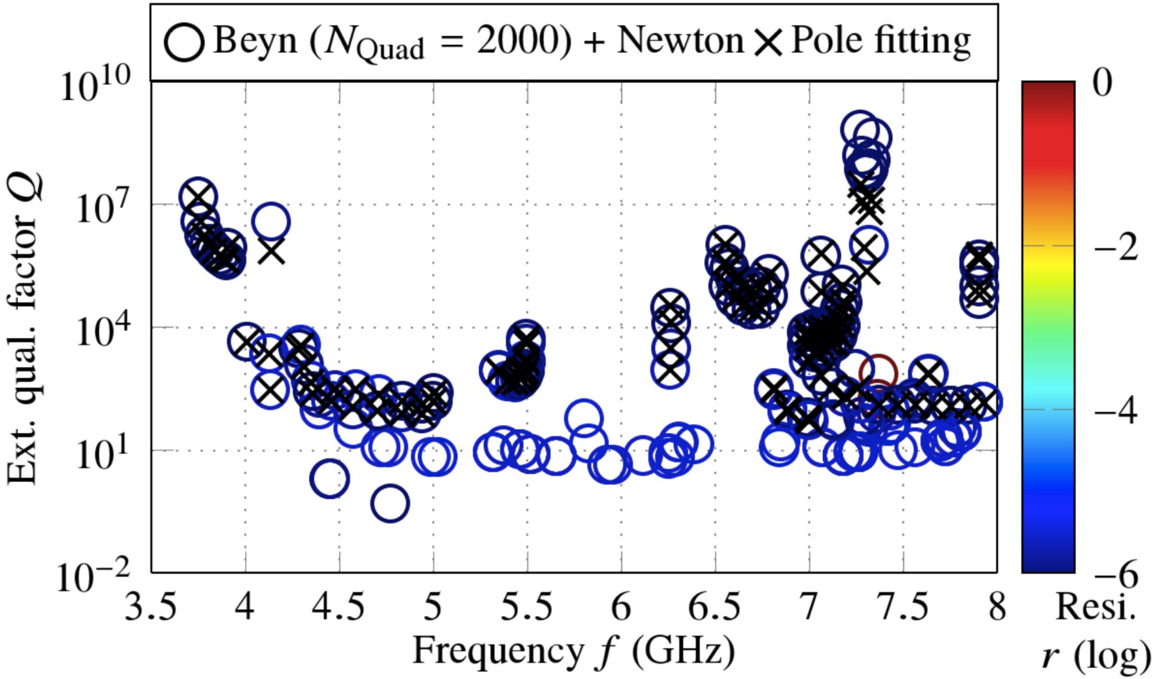
- with 2000 quadrature points



- residuals do not improve significantly for higher number of quadrature points

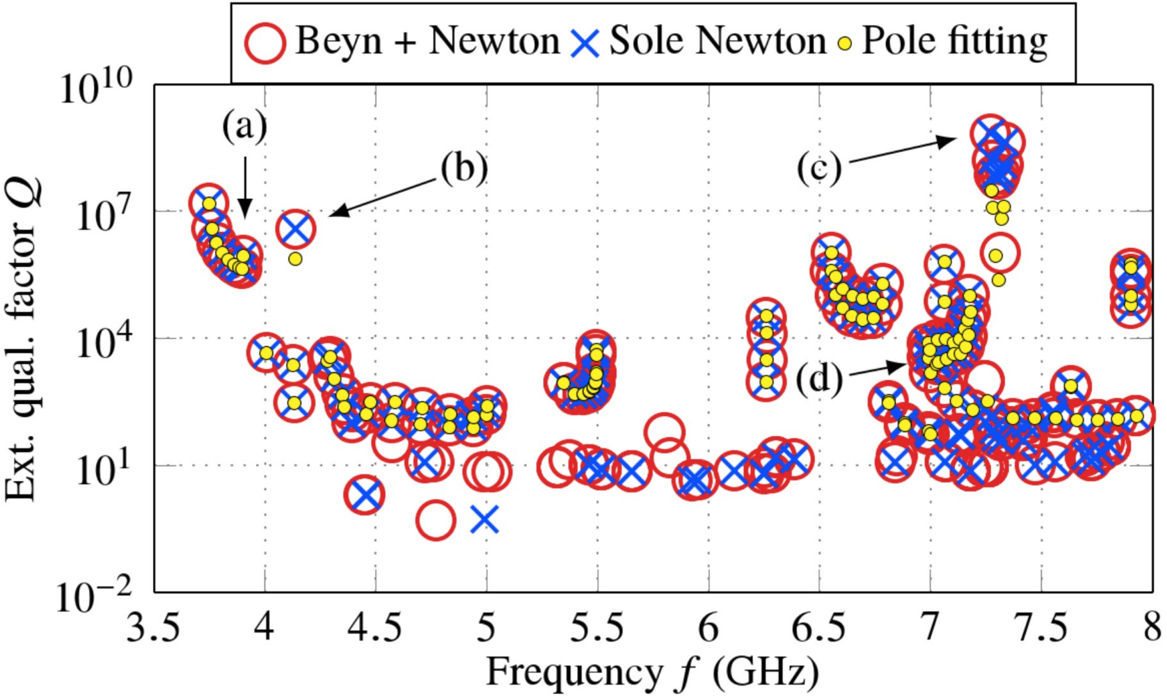
FLASH Cavity: Beyn's Algorithm + Newton iteration

- 2000 quadrature points and refinement by Newton



- convergence can again be improved by Newton iteration

FLASH Cavity: Comparison



more solutions in lower-Q range found by combining both algorithms

MOR by SSC Time
7 h

NLEVP Solution Time	
Beyn + Newton	Sole Newton
10 min	7 min

* on a workstation PC!

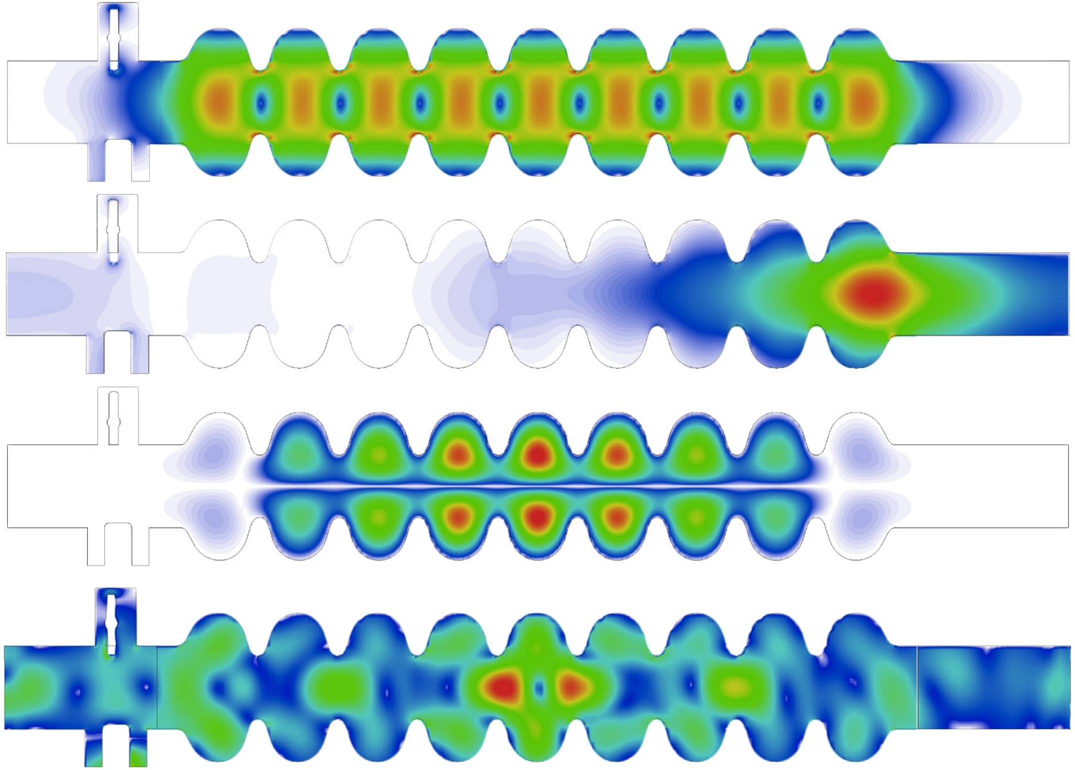
FLASH Cavity: Fields

(a) π-mode @ 3.90 GHz

(b) high-Q trapped mode @ 4.14 GHz and non-zero R/Q

(c) mode with highest Q @ 7.27 GHz but R/Q = 0

(d) low-Q mode @ 7.10 GHz



Summary

- MOR by SSC yields compact description of complex SRF structures incl. resonant frequencies, Q factors, 3D fields
- Perturbation approach with nonlinear boundary conditions leads to NLEVP to describe external losses
- NLEVP can be solved efficiently by Newton‘s method
- Convergence of Beyn’s algorithm limited for this type of NLEVP
- Promising results when using contour integrals to compute starting pairs for consecutive Newton iteration: higher completeness, insignificantly slower


Thank you!