Propagating Higher Order Mode Simulations in SRF Multi-Cavity Cryomodules Using ACE3P

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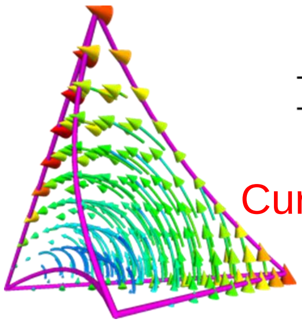
OUTLOOK

- ACE3P and Omega3P
- Nonlinear Eigensolver CORK in Omega3P
- Benchmark of CORK Eigensolver
- 3rd dipole band trapped mode simulations in TDR CM using Omega3P
- Summary

ACE3P

ACE3P is a comprehensive set of parallel multi-physics codes

- Based on *high-order curved finite elements* for high-fidelity modeling
- Implemented on *massively parallel computers* for increased problem size and speed



$$\mathbf{E} = \sum_i x_i \mathbf{N}_i$$

Curved finite element

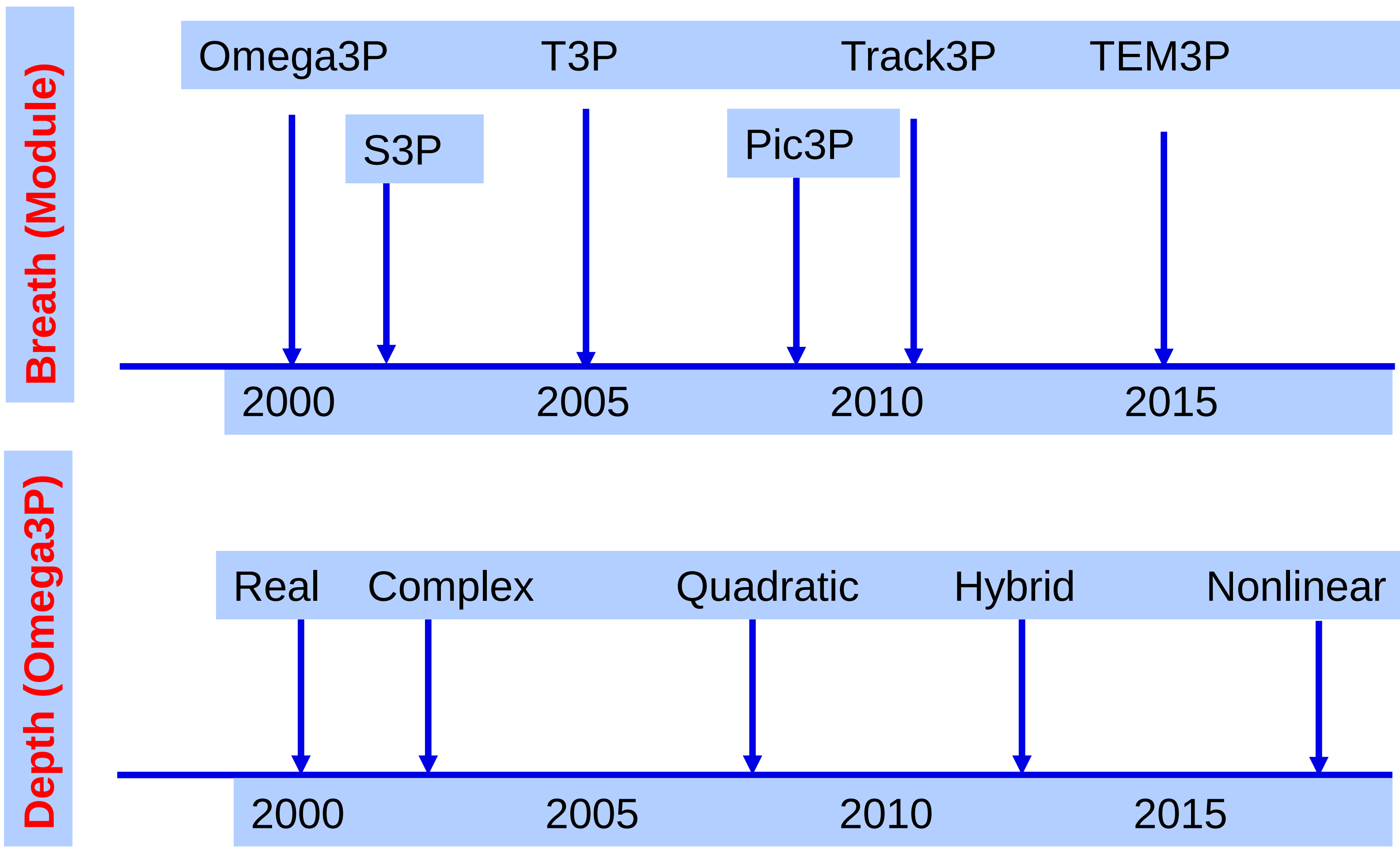
NERSC Cori: Cray XC40

- 632,672 compute cores
- 1 PB of memory
- peak performance of 27.9 Pflops/sec

ACE3P (Advanced Computational Electromagnetics 3P)

Frequency Domain:	**Omega3P**	**– Eigensolver (damping)**
	S3P	**– S-Parameter**
Time Domain:	**T3P**	**– Wakefields and Transients**
Particle Tracking:	**Track3P**	**– Multipacting and Dark Current**
EM Particle-in-cell:	**Pic3P**	**– RF guns & space charge effects**
Multi-physics:	**TEM3P**	**– EM, Thermal & Mechanical analysis**

ACE3P Development



RF Eigenmode Analysis in Omega3P

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Maxwell's Equations in Frequency Domain in the E-formulation

$$\nabla \times \left(\frac{1}{\mu}\nabla \times \vec{\mathbf{E}}\right) - k^2\epsilon\vec{\mathbf{E}} = 0 \ on \ \Omega$$

$$\vec{\mathrm{n}} \times \vec{\mathbf{E}} = 0 \ on \ \Gamma_E$$ PEC

$$\vec{\mathrm{n}} \times \frac{1}{\mu}\nabla \times \vec{\mathbf{E}} = 0 \ on \ \Gamma_M$$ PMC

$$\vec{\mathrm{n}} \times \frac{1}{\mu}\nabla \times \vec{\mathbf{E}} + i\sqrt{k^2 - k_{c_1}^2}\,\vec{\mathrm{n}} \times \vec{\mathrm{n}} \times \vec{\mathbf{E}} = 0 \quad on \ \Gamma_{wg}$$ WG (eg. TE mode)

Discretizing electric field using high-order Nedelec type basis functions N_i

$$\mathbf{E} = \sum_i x_i \mathbf{N}_i$$

Eigenvalue problem

$F(\lambda)x = 0$, λ (= k^2) the eigenvalue, x the eigenvector

$$k_{\mathrm{real}} = \frac{2\pi f}{c}, Q = \frac{K_{real}}{2Kim_{ag}}$$

Omega3P Capabilities

$F(\lambda)x = 0,$

Lossless Cavity

Cavity w/ Lossy Materials

$$Kx = k^2 Mx$$

Real/Complex eigenvalue problem

Cavity w/ SIBC

Cavity w/ WG ports (one cutoff)

$$Kx + ikWx = k^2 Mx$$

$$Kx + i\sqrt{k^2 - k_c{}^2}\,Wx = k^2 Mx$$

Quadratic eigenvalue problem

Cavity w/ WG ports (multi-modes) → Nonlinear eigenvalue problem

Lie-Quan Lee, et al., “Omega3P: A Parallel Finite-Element Eigenmode Analysis Code for Accelerator Cavities”, SLAC-PUB-13529

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Nonlinear RF Eigenvalue Problem

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- When waveguide ports have different cutoff frequency modes, the RF system is a nonlinear eigensolver problem;

$$Kx + i\sqrt{k^2 - \left(k^c\right)^2}\, W^{TEM} x + i\sum_m \sqrt{k^2 - \left(k_m^c\right)^2}\, W_m^{TE} x + i\sum_m \frac{k^2}{\sqrt{k^2 - \left(k_m^c\right)^2}} W_m^{TM} x = k^2 M x$$

$$K = \int_\Omega (\nabla \times N_i) \cdot \frac{1}{\mu} (\nabla \times N_j)\, d\Omega$$

$$M = \int_\Omega N_i \cdot \varepsilon N_j\, d\Omega$$

$$W^{TEM} = \int e_0^{TEM} \cdot \vec{N}_i\, ds \int e_0^{TEM} \cdot \vec{N}_j\, ds$$

$$W^{TE} = \int e_0^{TE} \cdot \vec{N}_i\, ds \int e_0^{TE} \cdot \vec{N}_j\, ds$$

$$W^{TM} = \int e_0^{TM} \cdot \vec{N}_i\, ds \int e_0^{TM} \cdot \vec{N}_j\, ds$$

M: the mass matrix, K: the stiffness matrix, e_0: the normalized waveguide mode

Compact Rational Krylov for Nonlinear Eigenvalue Problem

- The development of a *nonlinear eigensolver CORK* with LBNL has been integrated in Omega3P;

Three steps for solving NLEPs using CORK:

1. Approximation of the scalar nonlinear functions by interpolating rational functions, yielding a rational eigenvalue problem;

$$\boldsymbol{F}(\boldsymbol{\lambda}) = \mathbf{0} \ \rightarrow \mathbf{max}\|\boldsymbol{F}(\boldsymbol{\lambda}) - \boldsymbol{R}(\boldsymbol{\lambda})\| < \boldsymbol{\varepsilon}_{\boldsymbol{approx}}$$

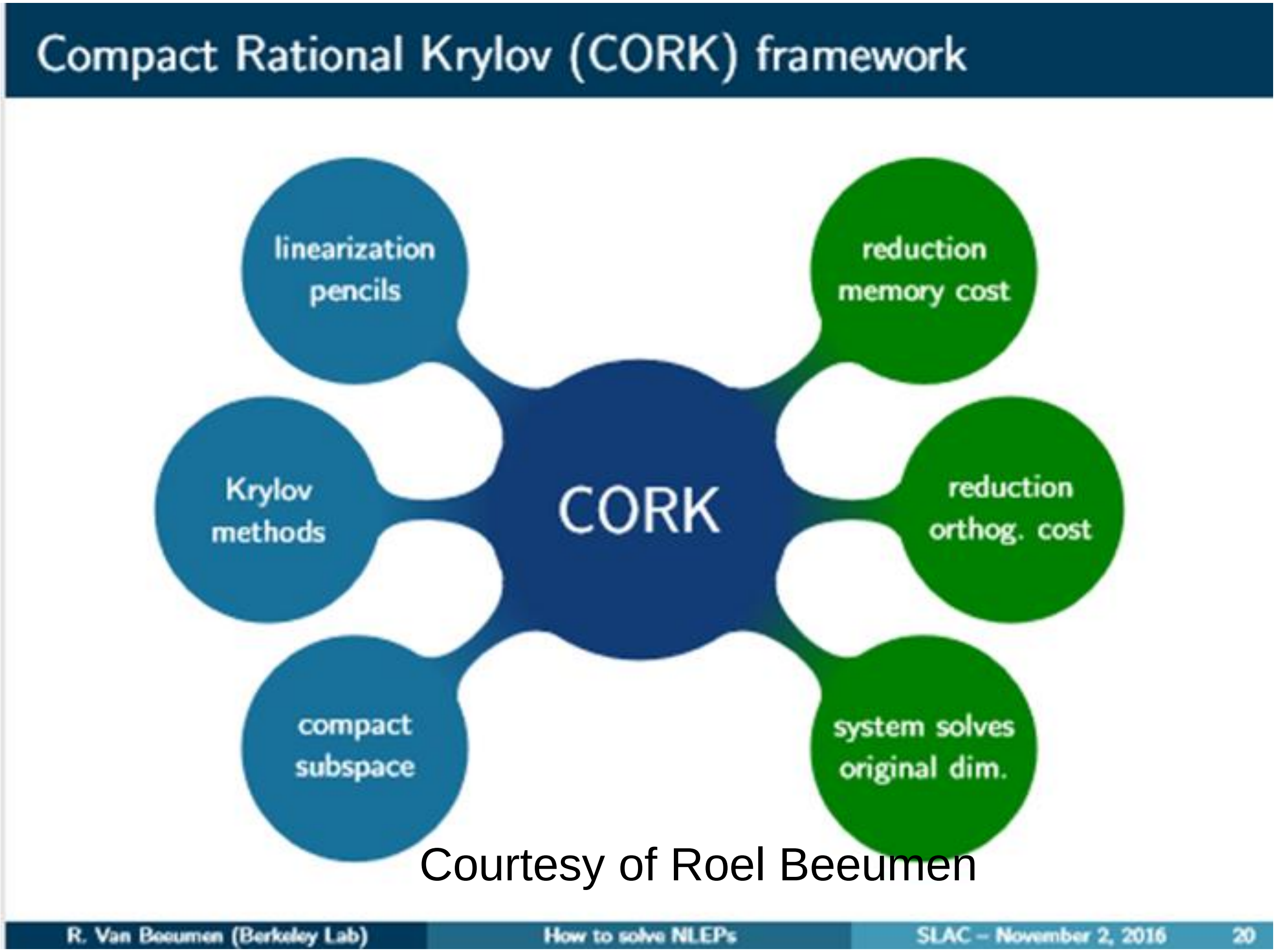
2. Linearization of the resulting rational eigenvalue problem, i.e., a reformulation of the rational eigenvalue problem as a generalized (linear) eigenvalue problem with the same eigenvalues but much larger in problem size;

$$\mathbf{R_d(\lambda) = A_0 + A_1\lambda + A_2\lambda^2 + \cdots + A_d\lambda^d}$$

3. Solving the generalized eigenvalue problem by a CORK method.

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

Compact Rational Krylov Framework



Courtesy of Roel Beeumen

Roel Van Beeumen, et al, "Computing Resonant Modes of Accelerator Cavities by Solving Nonlinear Eigenvalue Problems via Rational Approximation", Journal of Computational Physics, Aug. 2018

- ACE3P and Omega3P
- Nonlinear Eigensolver CORK in Omega3P code
- **Benchmark of CORK Eigensolver**
- 3^{rd} dipole band trapped mode simulations in TDR CM using Omega3P
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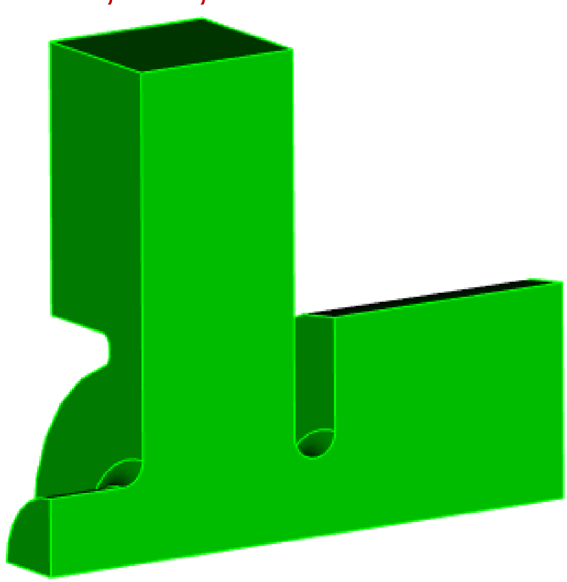
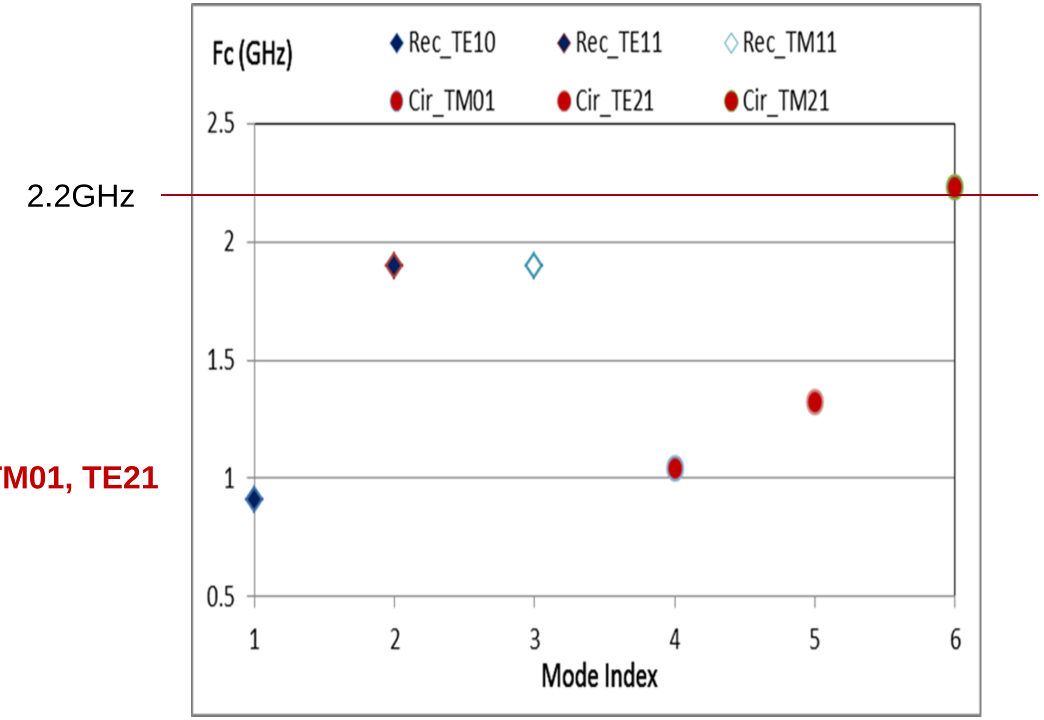
Benchmark of CORK Eigensolver

- Using a pillbox with circular & rectangular waveguides for the solver benchmark;
- It is a nonlinear eigenvalue problem, which can be solved using S3P or Omega3P.



Two sym. Planes: PMC
Beampipe End: PEC (f<fc)



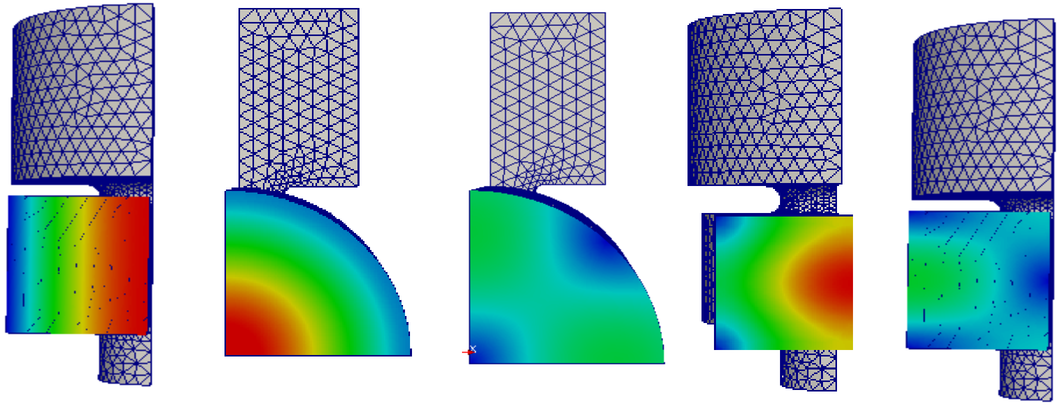
The lowest 6 eigenmodes fc in the couplers

Nonlinear RF Eigenvalue Problem

- The eigenmodes in the RF cavity under 2.2GHz can couple to three rectangular & two circular waveguide modes;
- This configuration yields the nonlinear eigenvalue problem F(λ)x=0, where

$$F(\lambda) = K - \lambda M + i\sqrt{\lambda - k_1^2}\,W_{10}^{TE} + i\lambda/\sqrt{\lambda - k_2^2}\,W_{01}^{TM} + i\sqrt{\lambda - k_3^2}\,W_{21}^{TE} + i\sqrt{\lambda - k_4^2}\,W_{11}^{TE} + i\lambda/\sqrt{\lambda - k_5^2}\,W_{11}^{TM}$$

$$k_i = 2\pi f_{ci}/c$$



TE10
Fc1=0.908GHz

TM01
Fc2=1.043GHz

TE21
Fc3=1.325GHz

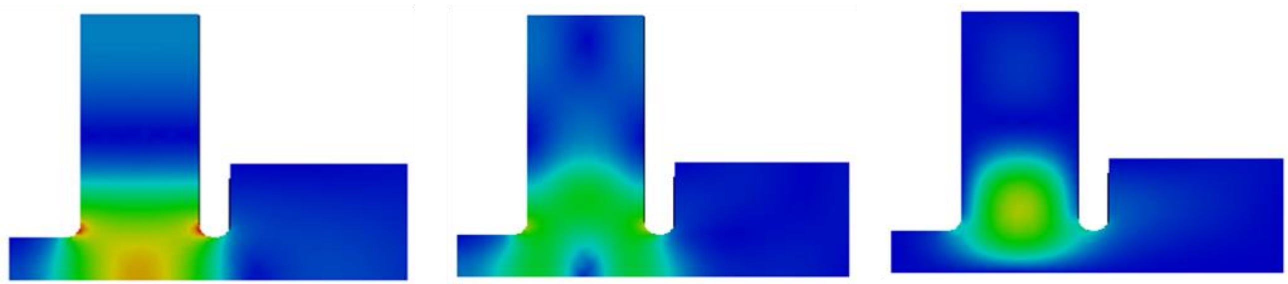
TE11
Fc4=1.897GHz

TM11
Fc5=1.897GHz

2D port modes from Omega3P

Eigenmode Solutions from Omega3P

- CORK solver integrated into Omega3P allows correct calculation of mode damping with different cutoff frequencies at waveguide ports.
- There are three eigenmodes below beampipe cutoff (2.2GHz) from Omega3P.



Eigenmodes from Omega3P

Error parameter

$$E(\lambda, x) = \frac{\|F(\lambda)x\|_2/\|x\|_2}{\alpha(\lambda)}$$

$$\alpha(\lambda) = \|K\|_2 + |\lambda|\|M\|_1 + \sqrt{|\lambda - k^2{}_1|}\|W_{10}{}^{TE}\|_1 + \frac{|\lambda|}{\sqrt{|\lambda - k^2{}_2|}}\|W_{01}{}^{TM}\|_1 + \sqrt{|\lambda - k^2{}_3|}\|W_{21}{}^{TE}\|_1 + \sqrt{|\lambda - k^2{}_4|}\|W_{11}{}^{TE}\|_1 + \frac{|\lambda|}{\sqrt{|\lambda - k^2{}_5|}}\|W_{11}{}^{TM}\|_1$$

Omega3p-CORK			
Mode	**F (GHz)**	**Qext**	**E(λ, x)**
1	1.1762	271	1.2827e-14
2	2.0567	739	2.1098e-14
3	2.1960	693	4.5892e-15

Eigenmode Solutions from S3P

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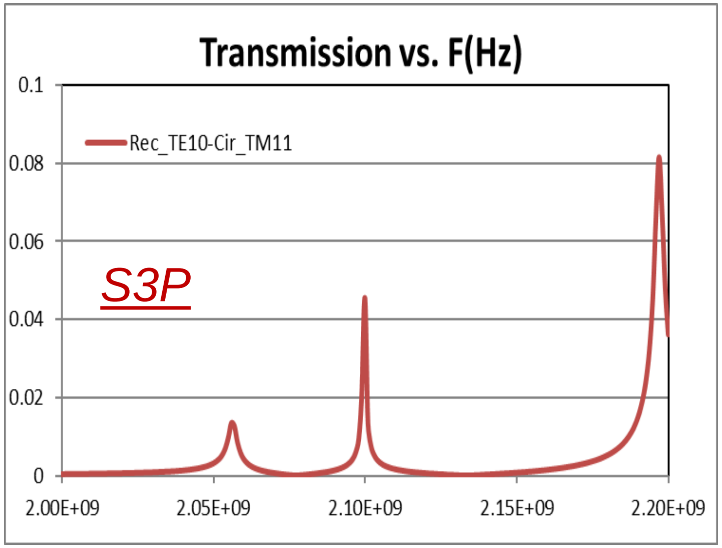
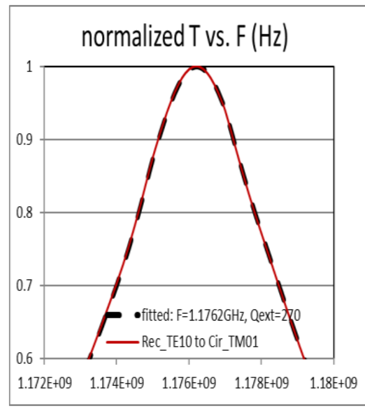
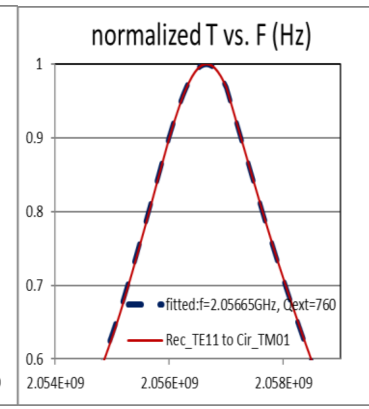
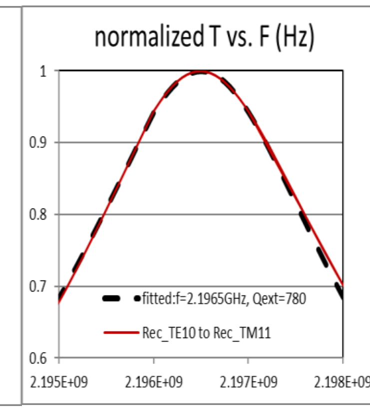
- Searching for the eigenmodes below beampipe cutoff (2.2GHz) using S3P;
- Getting eigenmode f_0 and Q_{ext} through fitting the transmission coefficients.



$$T^2 = \frac{1}{1+Q_{ext}^{\;2}\left(\frac{f}{f_0}-\frac{f_0}{f}\right)^2}$$







- The cavity eigenmode results from Omega3P and S3P agree well;
- Omega3P provides a direct way to compute the eigenmode parameters;
- Omega3P can solve the eigenmodes with strong damping accurately, which S3P cannot.

	Omega3P		S3P	
Mode	F (GHz)	Qext	F (GHz)	Qext
1	1.1762	271	1.1762	270
2	2.0567	739	2.0566	760
3	2.1960	693	2.1965	780

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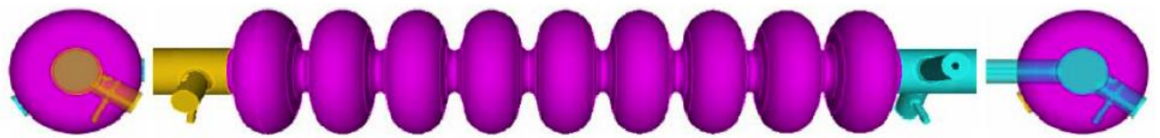
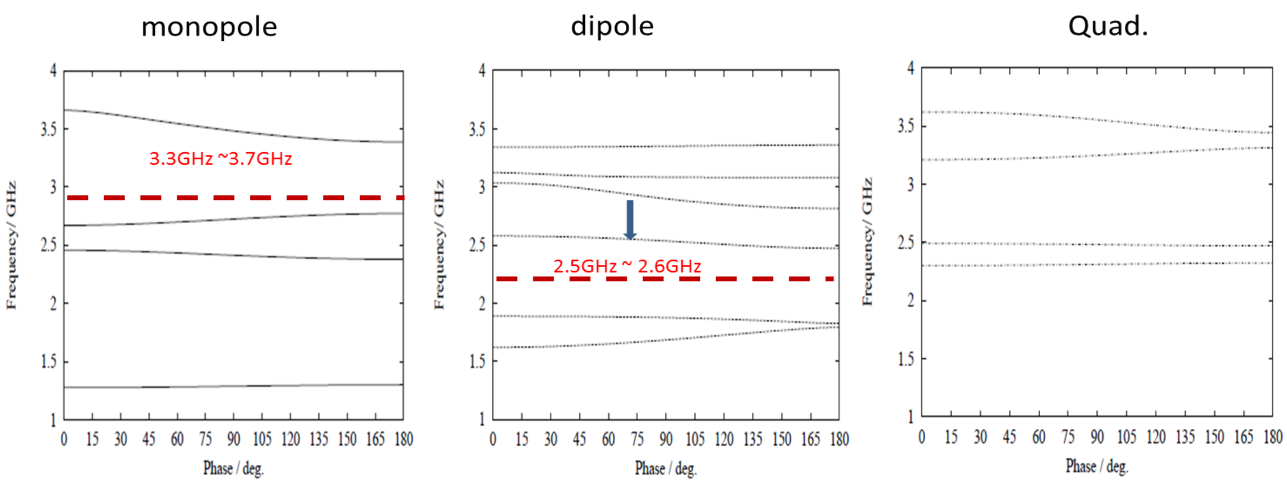
8-Cavity TESLA TDR Cryomodule

- TESLA cavity has been adopted by XFEL and LCLS-II as well as proposed in ILC;
- The higher-order modes need to be damped properly for reliable operation of the machines;
- The lower monopole and dipole band modes below the beampipe cutoff have been well studied in a single TESLA cavity;
- The HOMs above the beampipe cutoff need to be studied in a whole CM.

TESLA Cavity



R_beampipe=39mm, Fc(dipole)=2.2GHz, Fc(mono)=2.9GHz



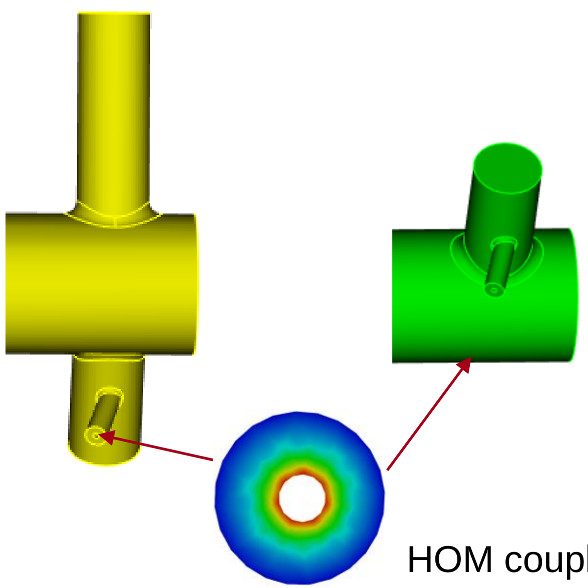
HOMs under 4GHz

8-Cavity CM for LCLS-II

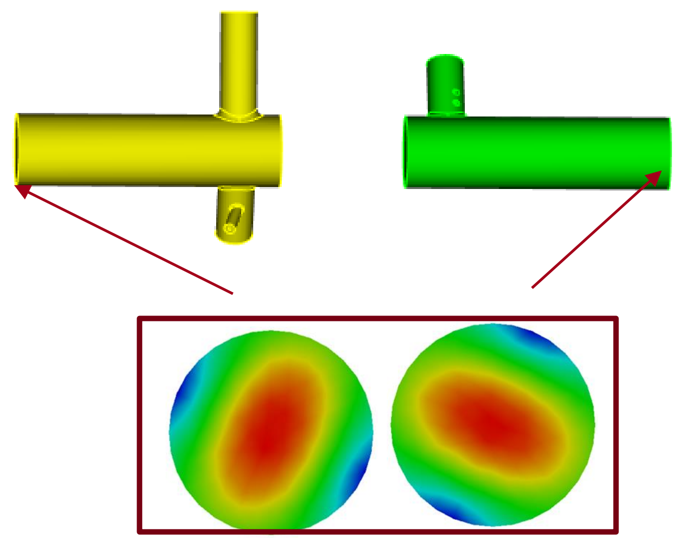
Nonlinear RF Eigenvalue Problem for 3rd Dipole Band Modes

- It was found that there were trapped modes (~2.58GHz) in TDR CM;
- The trapped modes can propagate through the cavities to the beampipe absorber;
- Determining the propagating 3rd dipole band mode damping needs to solve a nonlinear eigenvalue problem.

$$F(\lambda) = K - \lambda M + i\lambda W^{TEM} + i\sqrt{\lambda - k_1{}^2}\, W_{11}{}^{TE} + i\sqrt{\lambda - k_2{}^2}\, W_{11}{}^{TE}$$



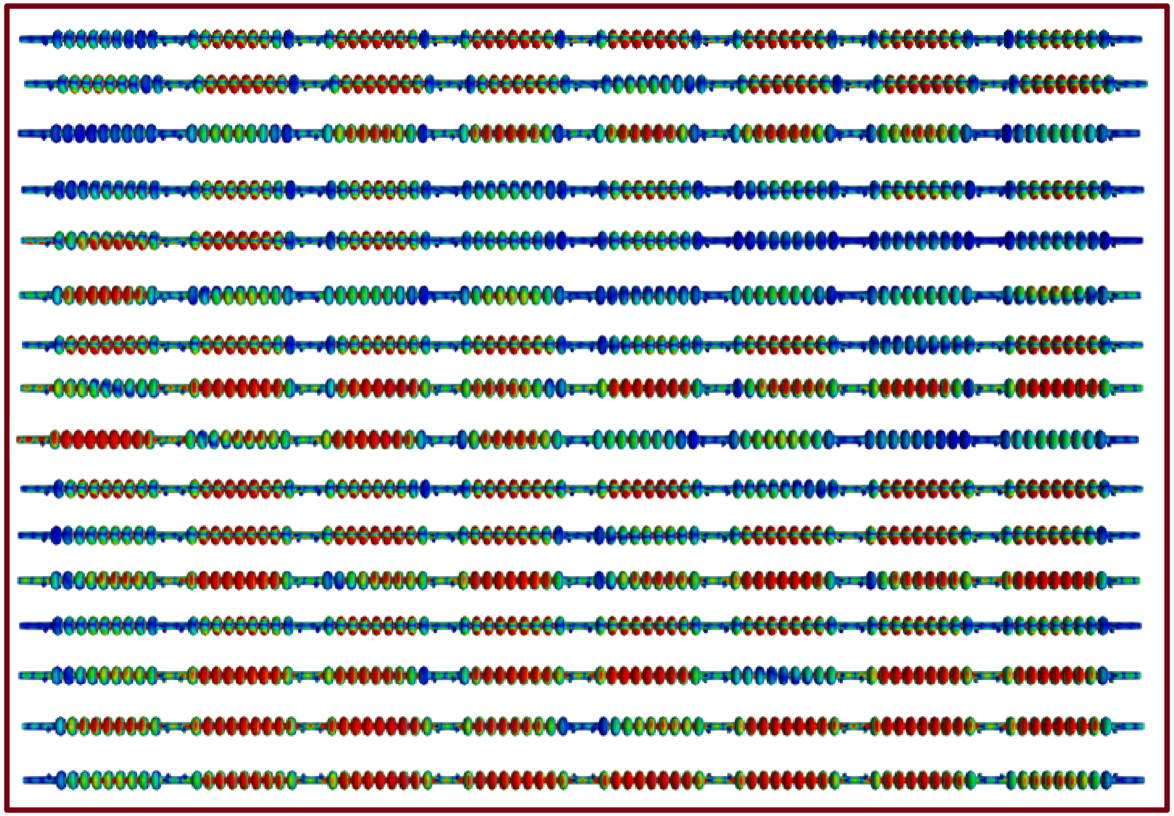
HOM coupler ports:
TEM, Fc=0



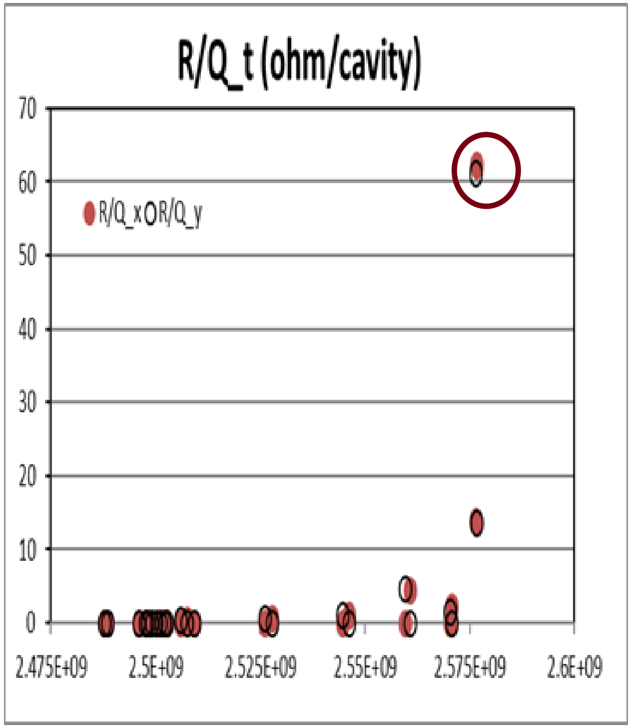
Beampipe ports:
TE11 Fc1=Fc2=2.2525GHz

The Last Mode of the 3rd Dipole Band in TDR CM

- Searching for the trapped modes in the 3rd dipole band in TDR CM;



3rd dipole band in a single cavity



Omega3P simulation parameters –
~ 3 million curved element mesh, ~ 20 million DOFs,
960 cores, 1.8 TB of memory on NERSC Edison, 1min per mode

The Trapped Mode Damping Results

- The trapped mode damping factors calculated using Omega3P agree well with measurements at DESY, and the simulated frequencies are shifted to lower values due to cavity imperfection;
- Furthermore, cavity imperfection should be taken into account to study the propagating HOMs damping.

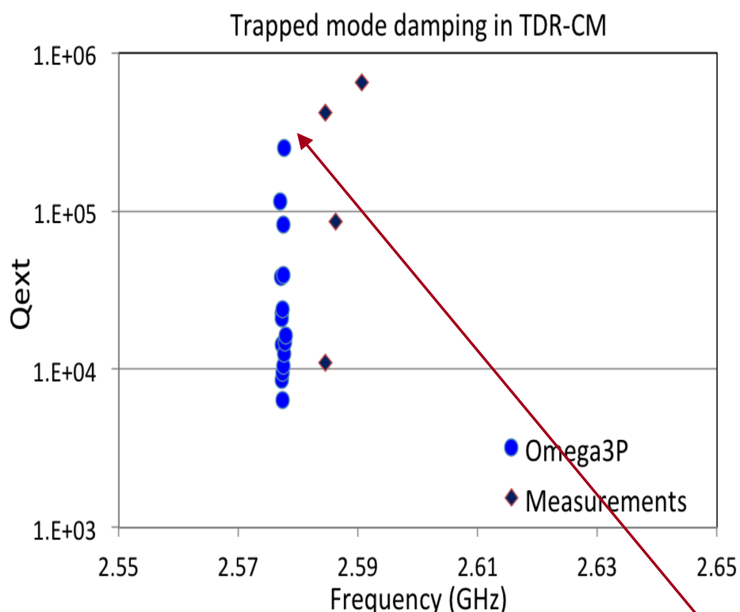
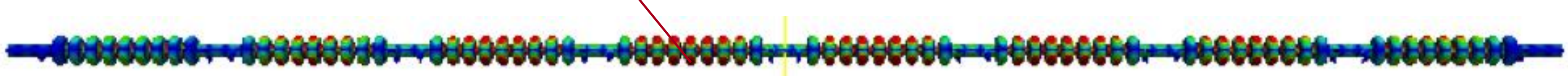


Table 1. Results of HOM investigations for the last mode of the 3rd dipole passband (R/Q = 15 Ω/cm²)

Cavity nr./module	Freq. [GHz]	Q
#3 (S10) / 1	2.5845	$1.1 \cdot 10^4$
#6 (S11) / 1	2.5862	$8.6 \cdot 10^4$
#5 (A15) / 2	2.5845	$4.2 \cdot 10^5$
#7 (S28) / 3	2.5906	$6.5 \cdot 10^5$

Courtesy of Nicoleta-Ionela Baboi



3rd dipole band trapped mode in TDR CM

Summary

- Recently developed CORK algorithm in Omega3P can solve a nonlinear eigenvalue problem in accelerator RF cavities arising from waveguide boundary conditions;
- Omega3P nonlinear eigensolver has been benchmarked against S3P;
- The simulated damping factors of the propagating 3rd dipole band trapped modes in TDR 8-cavity CM using Omega3P agree well with measurements at DESY;
- Omega3P parallel computation enables a direct method to calculate propagating modes in large scale problems.

Learn more on modeling capabilities of ACE3P at
ACE3P CW18 Accelerator Code Workshop, Nov. 5 to 9, 2018

https://conf.slac.stanford.edu/cw18/