Characterisation of HOMs in coupled 8-cavity chain of 3H module on EXFEL using GSM simulations

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Outline

- ❑ Introduction to E-XFEL and 3.9 GHz accelerating module.
- ❑ Motivation for application of Generalised Scattering Matrix (GSM) method.
- ❑ Principle of GSM technique, advantages and features of the developed code package.
- ❑ Reconstruction of single cavity structure.
- ❑ Reconstruction of 8-cavity chain for E-XFEL.
- ❑ Calculation of Q-values for single cavity and 8-cavity chain.
- ❑ Fabrication error study
- ❑ Experimental measurements and comparison to simulation.
- ❑ Summary and discussion.

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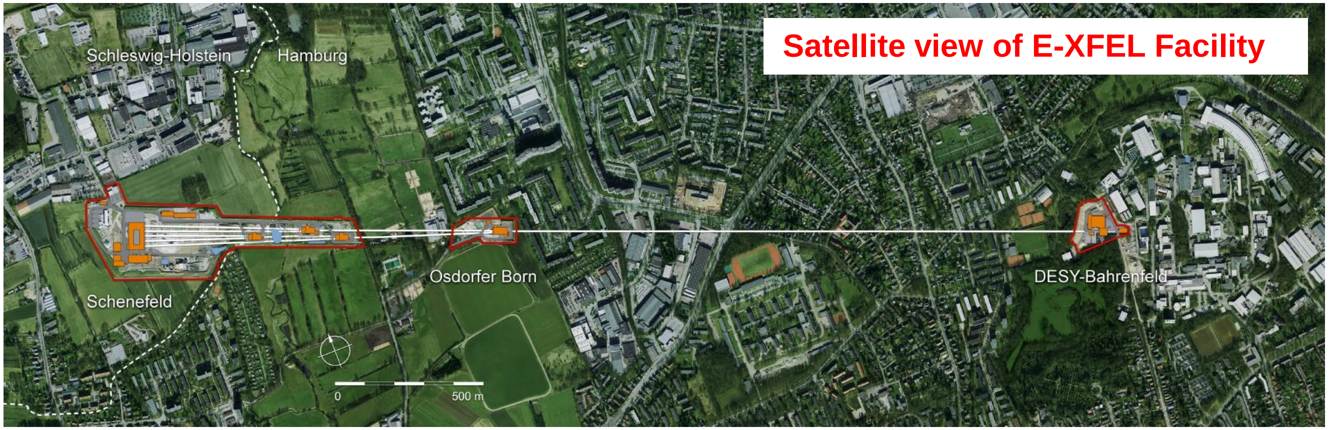
European X-ray Free Electron Laser

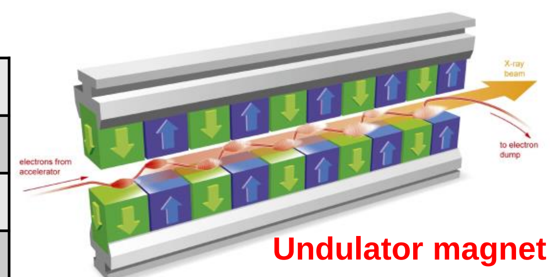


Accelerator Parameter	Value
Length of accelerator	2.1 km (Total 3.4 km)
Electron energy	17.5 GeV
SC RF cavities Fundamental Acceleration	23.6 MV/m, 1.3GHz 800 cavities in 100 modules
SC RF cavities Third harmonic correction	8 cavities (1 or 3 modules)
Peak Current	2 - 5 kA

It is based on Self Amplified Stimulated Emission (SASE) effect to generate coherent X-ray pulses by passing electron bunch through Undulator magnets

$$\lambda_r = \frac{\lambda_u}{2\gamma^2}(1+K^2)$$

X-Ray Laser Parameter	Value	Benefit
Flashes per second	27000	
Wavelength λ_r	0.05 - 4.7 nm	Small λ can examine atomic details
Brilliance Pulse length	5×10^{33} /s/mm^2/mrad^2 2 – 47 fs	Fast short pulses of high brightness can fast film formation on molecules

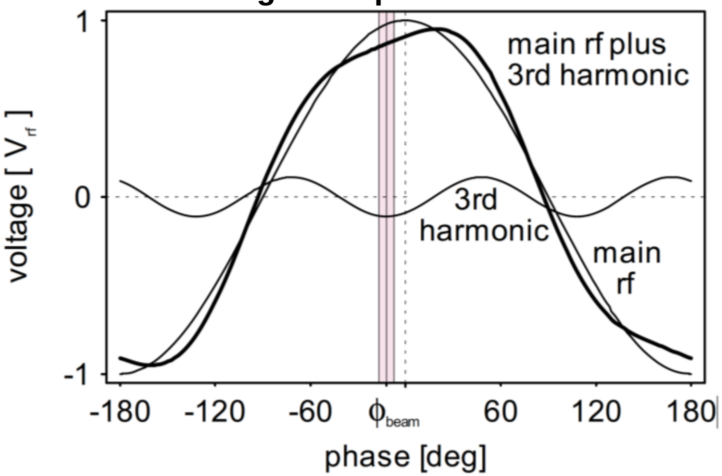


Third Harmonic Acceleration module: Energy spread correction on FLASH/XFEL

$$v_{rf}(f) = V_{funda}\left(\cos(f) + \frac{V_{3rd}}{V_{funda}}\cos 3(f - f_{3rd})\right)$$

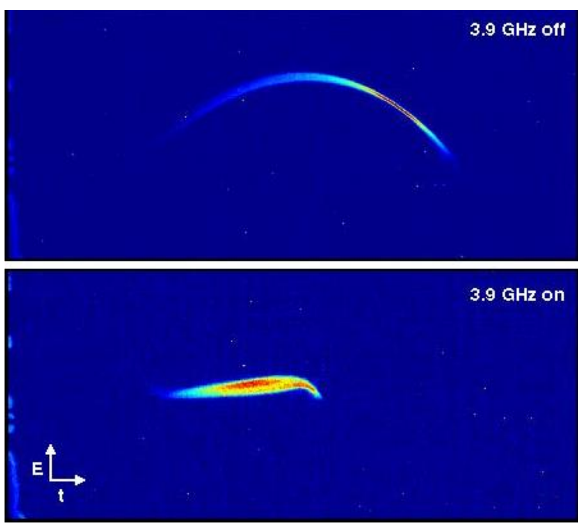
$$f_{3rd} = 180° + f_{beam} \qquad v_{3rd}(f) » \frac{1}{9} V_{funda}$$

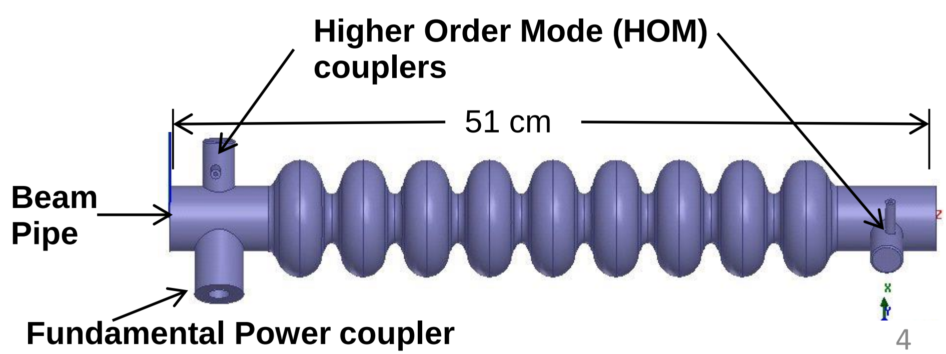
Working Principle



Third Harmonic module parameters	Value
Number of cavities in a module	8
Number of cells in a cavity	9
Monopole Power and frequency (π - mode)	14 / 20 MV/m at 3.9 GHz
Q_0	6 – 8 x 10^8
R/Q (monopole)	750 Ω
First dipole frequency band	4.2- 5.2 GHz
Beam-pipe radius (and cutoff frequency)	20 mm
Beam pipe cutoff frequency (TE_{11})	4.392 GHz

Energy spread on FLASH, Elmar Vogel et al. DESY.



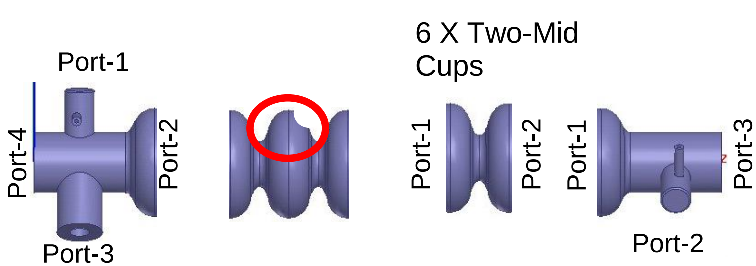


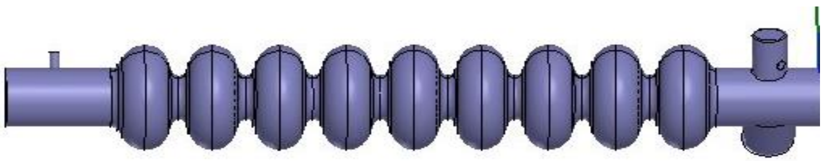
Motivation: The sheer size of simulation

- FLASH and Eu-XFEL use third harmonic accelerating modules with eight 9-cell cavities connected in chain.
- EM simulation of a cavity, and the whole module, is a very large computational problem, which takes lot of time and requires larger computational facility.
- A cascading technique is developed, in which the large structure is divided in smaller building blocks. S-parameters of each block is simulated separately, and cascaded to reconstruct the large structure.

Advantages of Cascading technique:

- To study the effect of structural change in any part of the large structure, only that building block needs to be re-simulated, not the whole large structure.
- Smaller structure can be simulated with higher accuracy and in shorter time duration, improving turn around time.
- Performance of the whole structure can be realised using normal workstation computer, without requiring larger special purpose high performance computational facility.



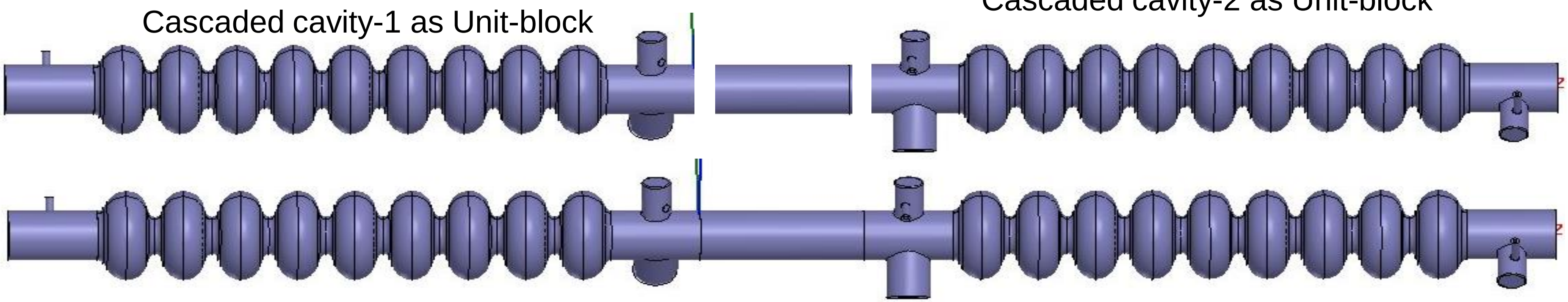


Cavity-1 with 9 cells

Multi-layer cascading

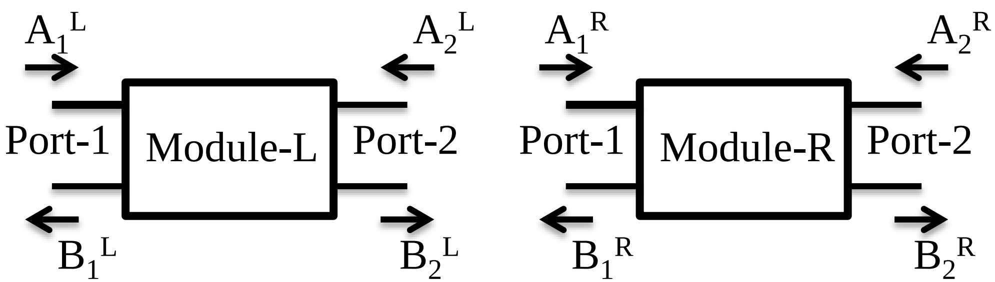
Cascaded cavity-1 as Unit-block

Cascaded cavity-2 as Unit-block



Cascaded pair of Cavity-1 and Cavity-2 as a new unit-block

Generalized Scattering Matrix: principle



$$S_{11}^{L} = \frac{B_{1L}}{A_{1L}} \qquad S_{21}^{L} = \frac{B_{2L}}{A_{1L}} \qquad S_{22}^{L} = \frac{B_{2L}}{A_{2L}}$$

$$S_{11}^{LR} = S_{11}^{L} + S_{12}^{L}\left(I - S_{11}^{R} S_{22}^{L}\right)^{-1} S_{11}^{R} S_{21}^{L}$$

$$S_{21}^{LR} = S_{21}^{R}\left(I - S_{22}^{L} S_{11}^{R}\right)^{-1} S_{21}^{L}$$

- S-parameters of two compatible modules can be cascaded to calculate the resultant S-parameters of the whole module.
- A cascading code is developed in Python, which reads S-parameters of unit-modules exported from HFSS or CST, and cascaded them to recreate larger structures
- If more than one modes are calculated at ports, then each S value in the equation will be a matrix of all modes.
- Possible problem of matrix blow up can arise in the inversion terms.

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GSM code: Features and capabilities

- **Multiple input files**: The code can read multiple input files, and combine them to recreate a single frequency sweep.
- **Frequency range selection:** The user can choose only specific frequency range of interest from the possible large frequency range in input files. This is very helpful in limiting the memory requirement for a single cascading operation.
- **Dynamic port generation:** The code generates ports dynamically, based on unit blocks, and tracks port references using a port-map.
- **Specific mode selection:** The user can specify which modes to consider in cascading. If the power is not coupled into all modes, limiting the cascading to only specific modes increases its speed and reduces the memory requirement.
- **Multi-layer cascading:** It can cascade two cascaded objects. Reusing the already cascaded object, reduces the number of matrix inversion operations, and increases the overall cascading speed drastically.
- **Result dump:** The code also saves result in an efficient format, which can be read back quickly., and it works with all functions for further data processing.
- **Data processing and plotting:** The package also has functions to find specific S-parameters, plot them for further analysis, calculation of power conservation etc..

Reconstruction of single cavity

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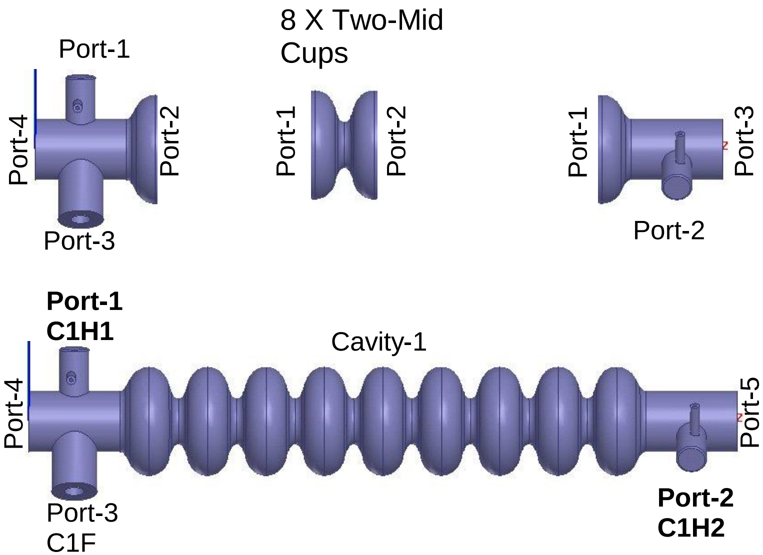
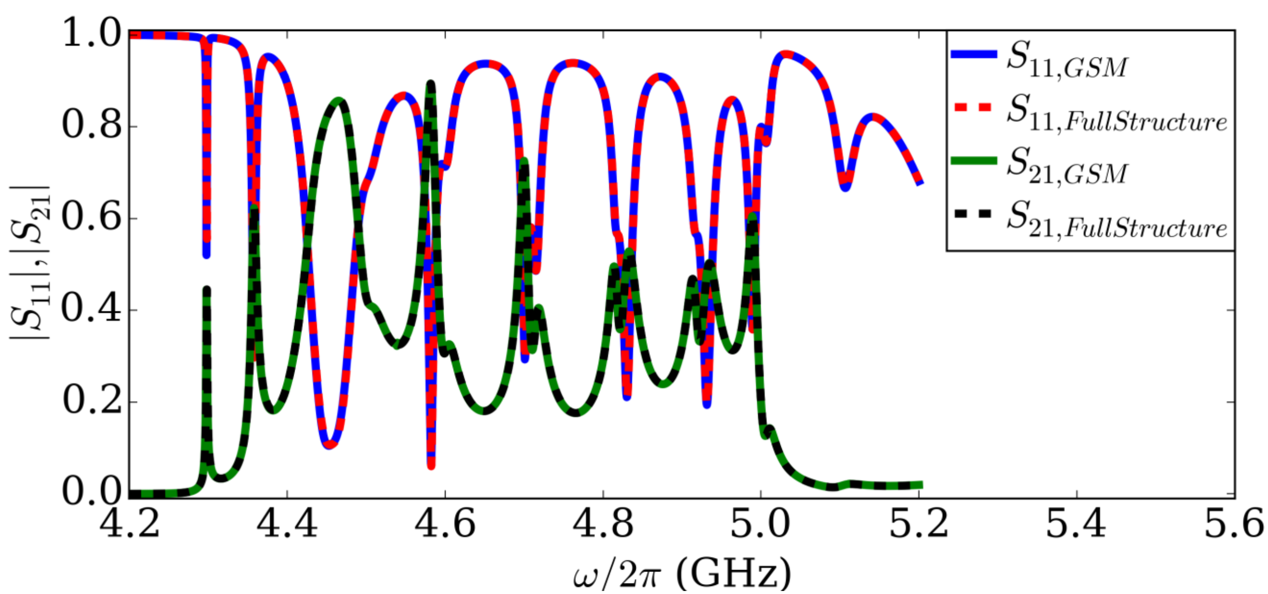


Structure	HFSS Version-15 (Trial)	
	Mesh (tets)	Time (Hours)
Start coupler	73019	41
Mid cups	31320	28
End coupler	60958	33
Full Cavity-1	234,175	204 (9days)

- **Cascading unit cells on a laptop computer took less than 2 minutes, for 2000 frequency steps.**
- **Cascading is 50% faster even for even a single cavity structure**



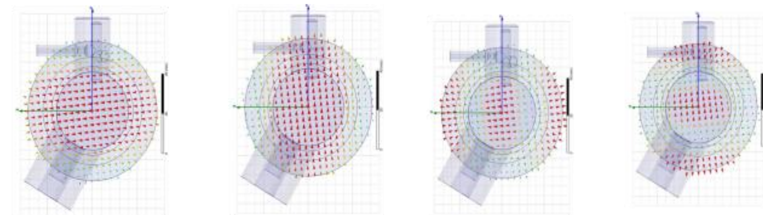
Effect of number of equator modes

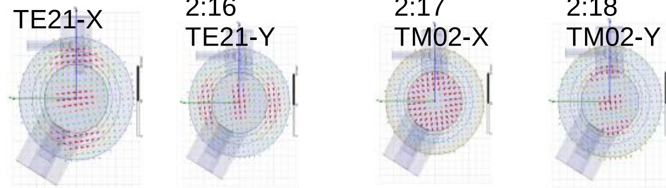
FLASH Cavity-1 Up-stream coupler:
Min/Max(S-magnitude(over whole frequency range))

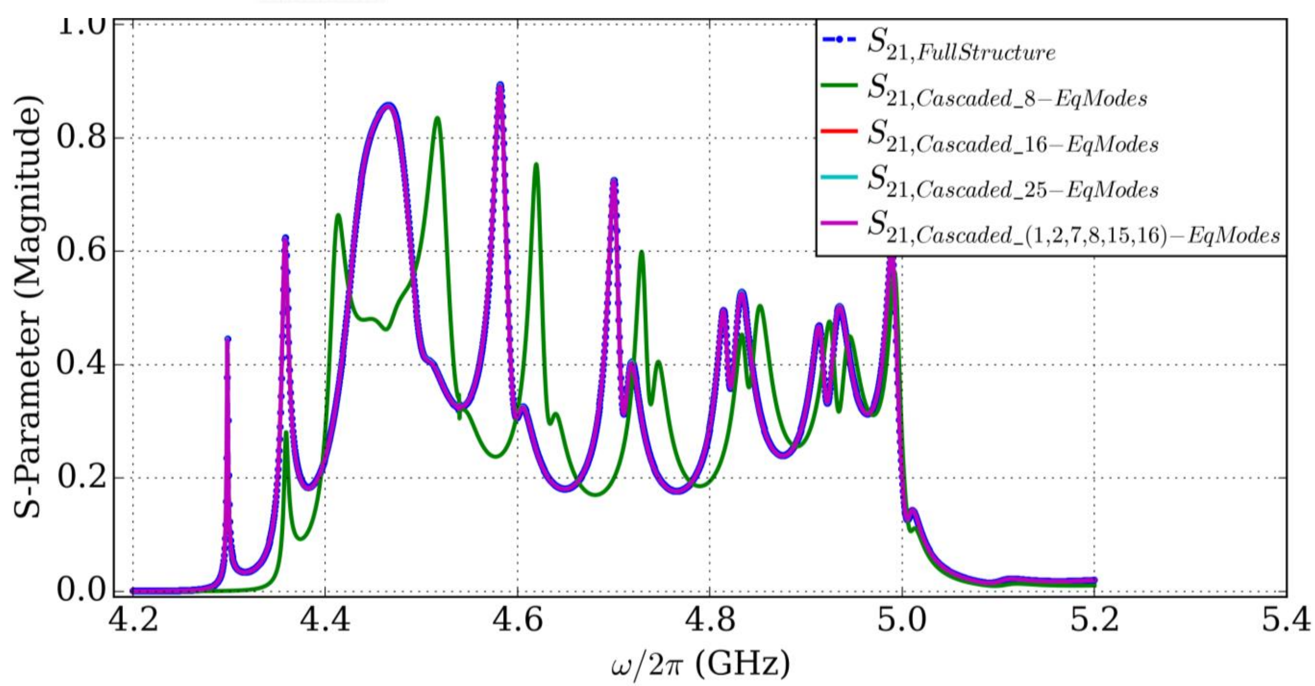
HIGHLY COUPLED MODES:
Reflection <0.2 or Transmission>0.8
(S(1:1,1:1)) [] = -0.18220

MEDIUM COUPLED MODES:
0.2<Reflection<0.6 or
0.8>Transmission>0.4
(S(2:1,1:1)) [] = 0.52545
(S(2:2,1:1)) [] = 0.47118
(S(2:7,1:1)) [] = 0.49276
(S(2:8,1:1)) [] = 0.43153
(S(3:2,1:1)) [] = 0.45775

LOW COUPLED MODES:
0.6<Reflection <0.99 or
0.4>Transmission>0.01
(S(2:3,1:1)) [] = 0.03989
(S(2:15,1:1)) [] = 0.03836







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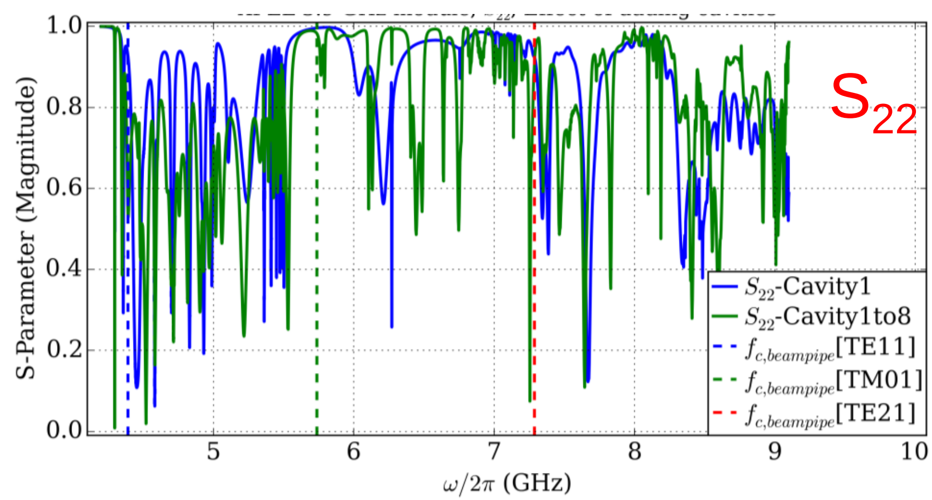
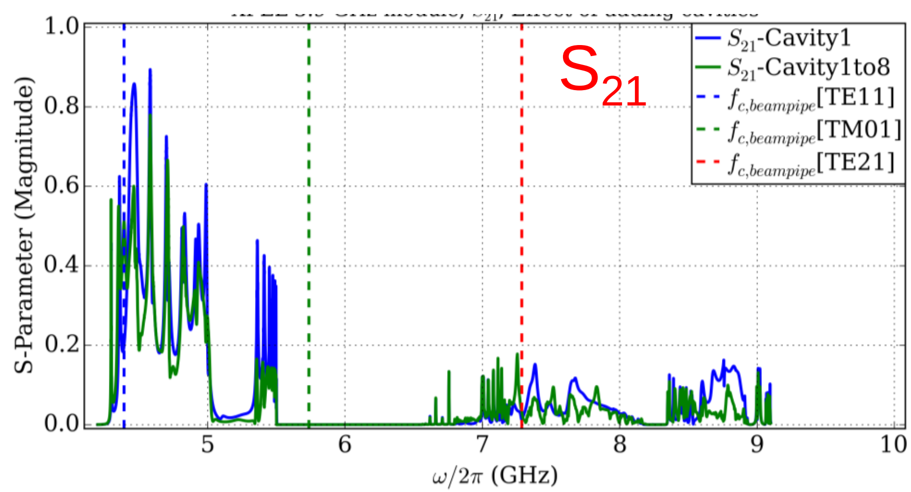
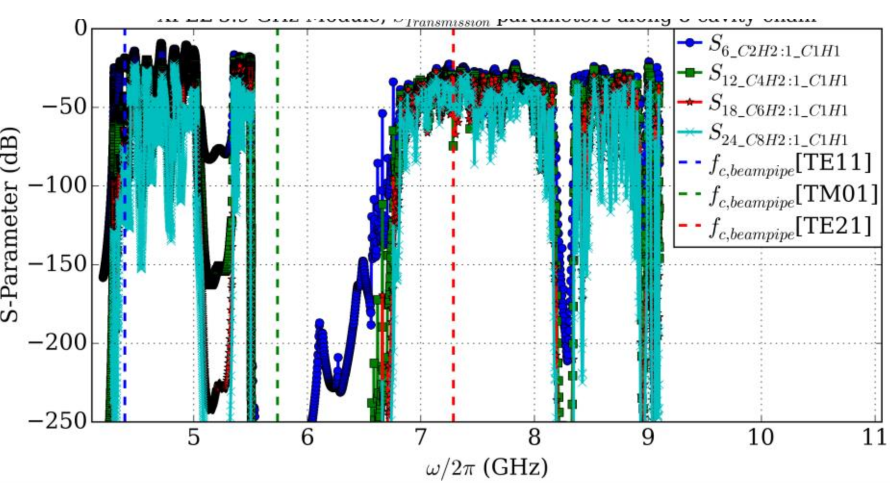
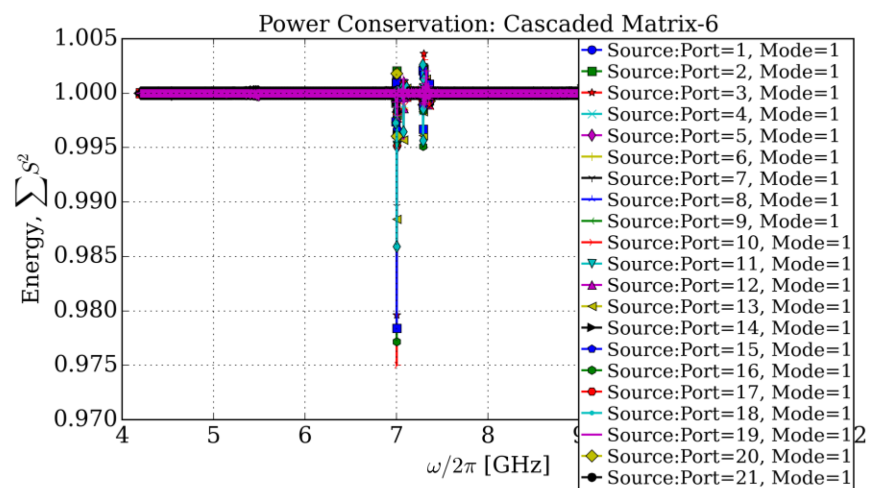
Cascading complete 8-Cavity chain on XFEL

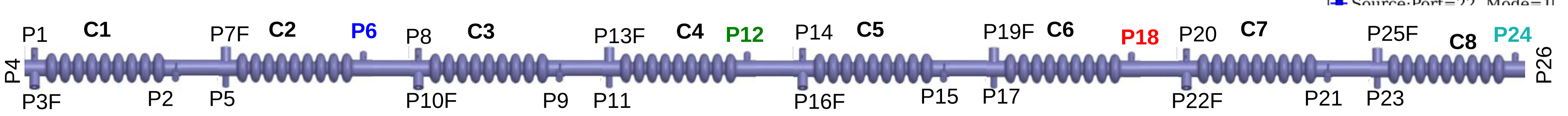
- Cascading all 8 cavities from 6 unit modules, over a frequency band (2000 frequency steps), on a laptop computer took only 3m:30s (2:00 load module files + 1:30 cascade).











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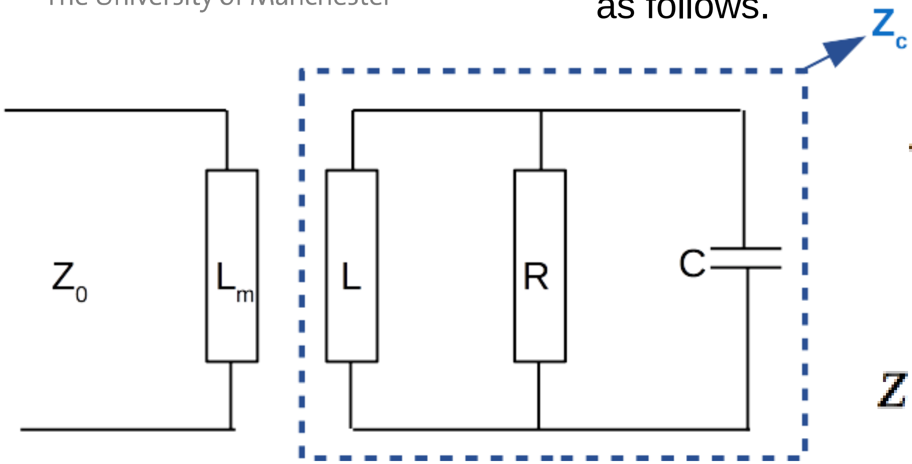
Q calculation: circuit analog of cavity

- Reflection parameter for the cavity can be calculated from circuit analogy as follows.



$$Z_c = \frac{R}{1 + j\frac{R}{\omega L}\left(\frac{\omega^2}{\omega_0^2} - 1\right)} = \frac{R}{1 + jQ_0\rho}$$

$$Z = \frac{L_m}{L} Z_c = \frac{\beta Z_0}{1 + jQ_0\rho} \qquad Coupling\ \beta = \frac{R L_m}{Z_0 L}$$

$$S_{11} = \frac{Z - Z_0}{Z + Z_0} = \frac{b - 1 - jQ_0 r}{b + 1 + jQ_0 r} \quad \text{Where,} \quad r = \left(\frac{w}{w_0} - \frac{w_0}{w}\right)$$

At resonance, $S_{11,peak} = \dfrac{b-1}{b+1}$

$$S_{11}^2 = \frac{(b-1)^2 + Q_0^2 r^2}{(b+1)^2 + Q_0^2 r^2} = \frac{\left(\frac{b-1}{b+1}\right)^2 + \frac{Q_0^2}{(b+1)^2} r^2}{1 + \frac{Q_0^2}{(b+1)^2} r^2} = \frac{S_{11,peak}^2 + Q_l^2 r^2}{1 + Q_l^2 r^2}$$

Where as the S21 can be fitted using Lorentzian function

$$S_{21}^2 = \frac{S_{21,peak}^2}{1 + Q_l^2 r^2}$$

Q calculation: comparison of Q_l from reflection and transmission curves

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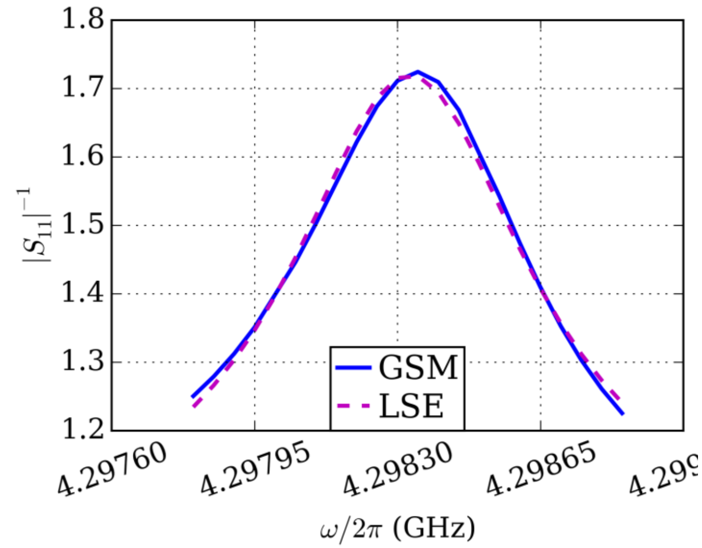
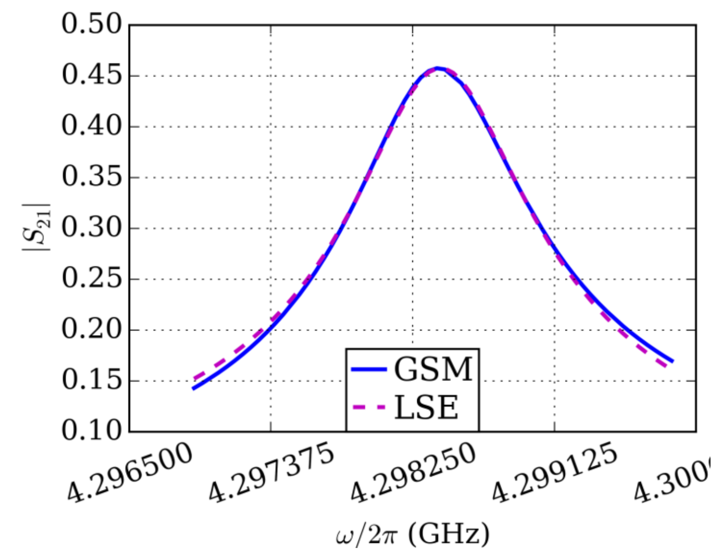
In case of S11, the formula to calculate Q, using half power bandwidth method modifies to

$$Q_{l,refl\,3dB} = \frac{S_{11,peak,linear}}{\sqrt{1-2S_{11,peak,linear}^2}} \frac{\omega}{\Delta\omega_{3dB}}$$

Peak *f* (GHz)	**Q_l from S_{21}**	**Q_l from S_{11}**
4.2983	3907	4194
4.3578	665	653
4.4460	60	34
4.5817	330	269
4.7002	435	369
4.8148	316	315
4.9142	271	273
4.9886	412	372





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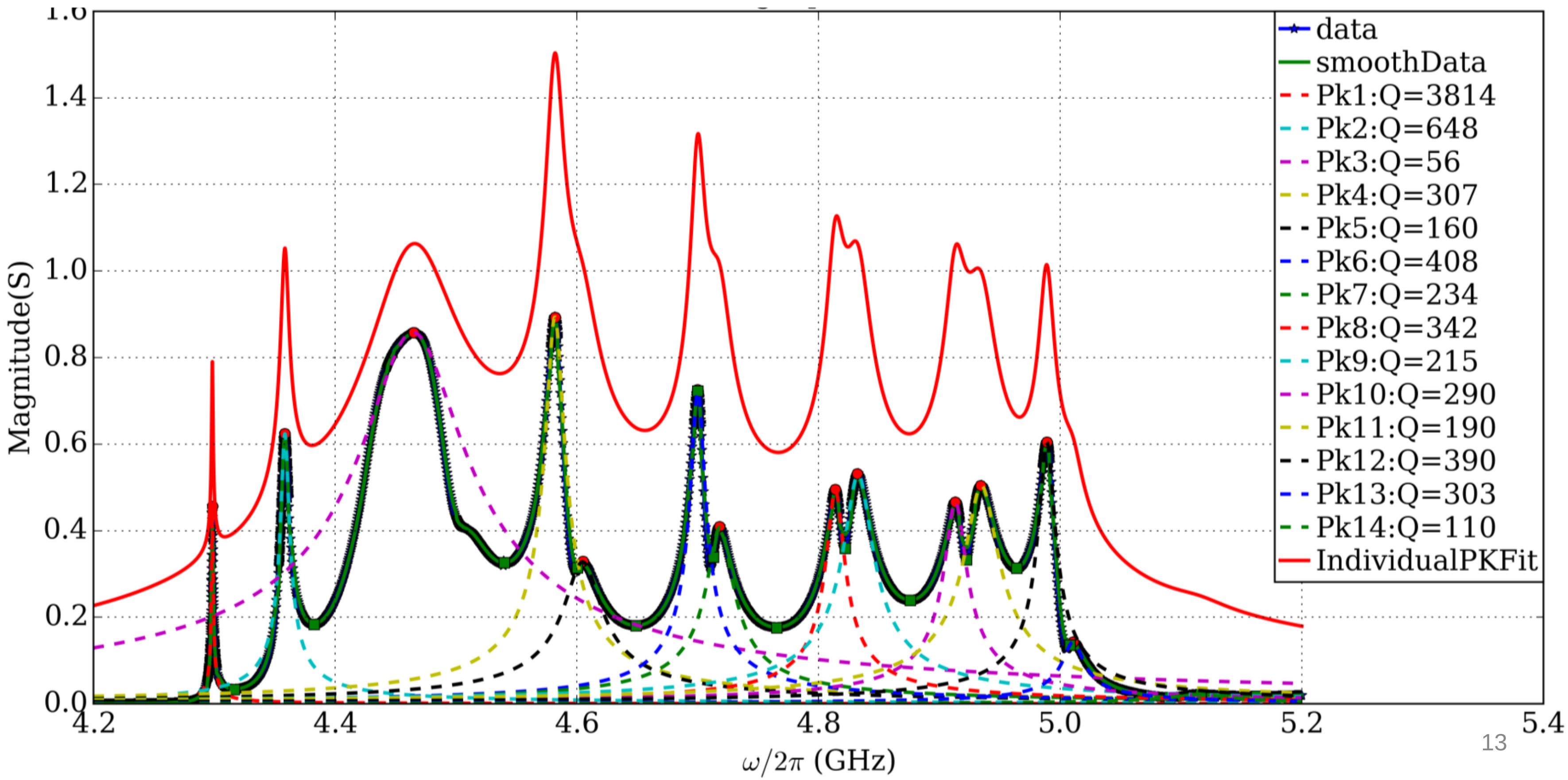
Q calculation: Fitting peaks individually

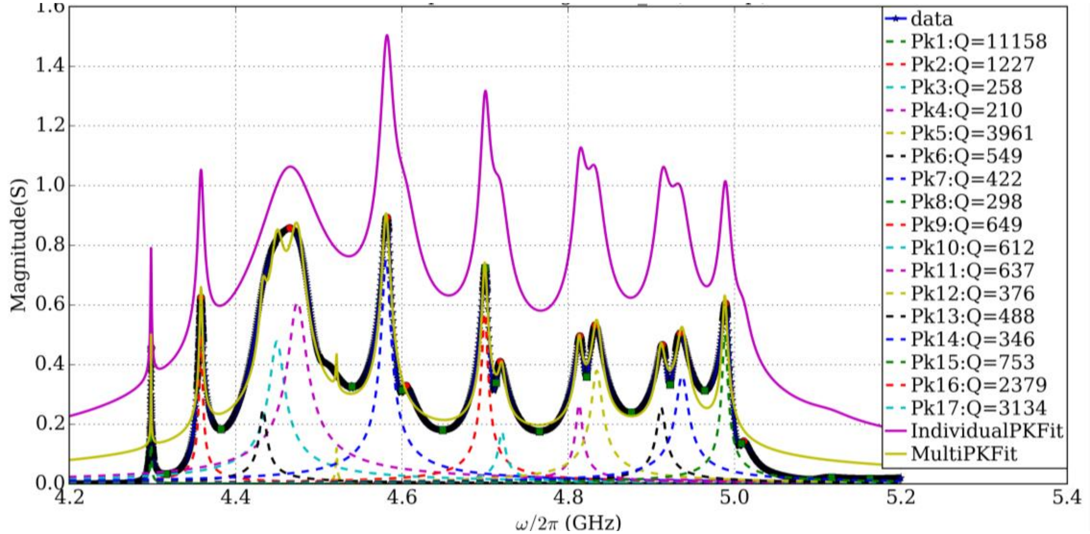
$$S_{21}^2 = \frac{S_{21,peak}^2}{1+Q_l^2 r^2}$$

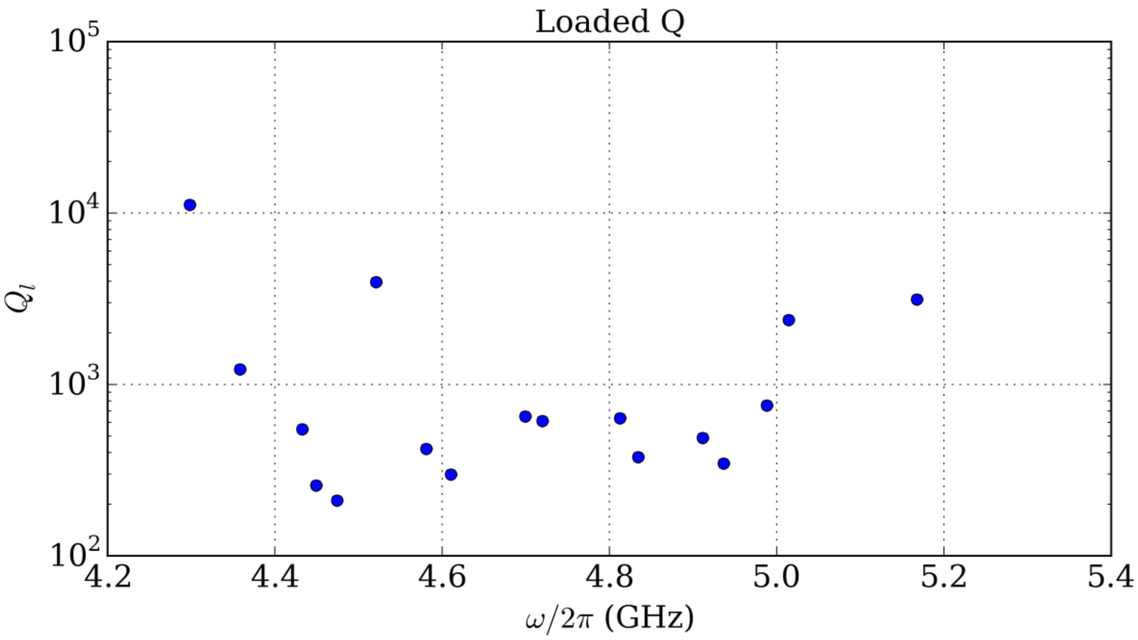
- Using resonant circuit analogy, following equations can be derived to fit the reflection and transmission S-parameter curves.
- The code automatically detect peaks, and individual peak is fitted separately, and are summed to create total S_{21} , which does not agree with the simulated plot.
- The modes are degenerated due to asymmetric orientation of HOM couplers. All the peaks has to be fitted, simultaneously for accurate Q-calculation.



Q calculation: Fitting peaks simultaneously, Single cavity

- Peak frequencies from S11 and S22 are used as an initial guess for fitting.
- Peak-3 has been degenerated in to 4 peaks to re-create non-lorentzian shape.
- Total of 17 peaks used to reconstruct the first dipole band of
- Minimising the multiple peaks together, reduces the error considerably.
- Minimization is sensitive to initial guess value, and will be optimized further for best result.





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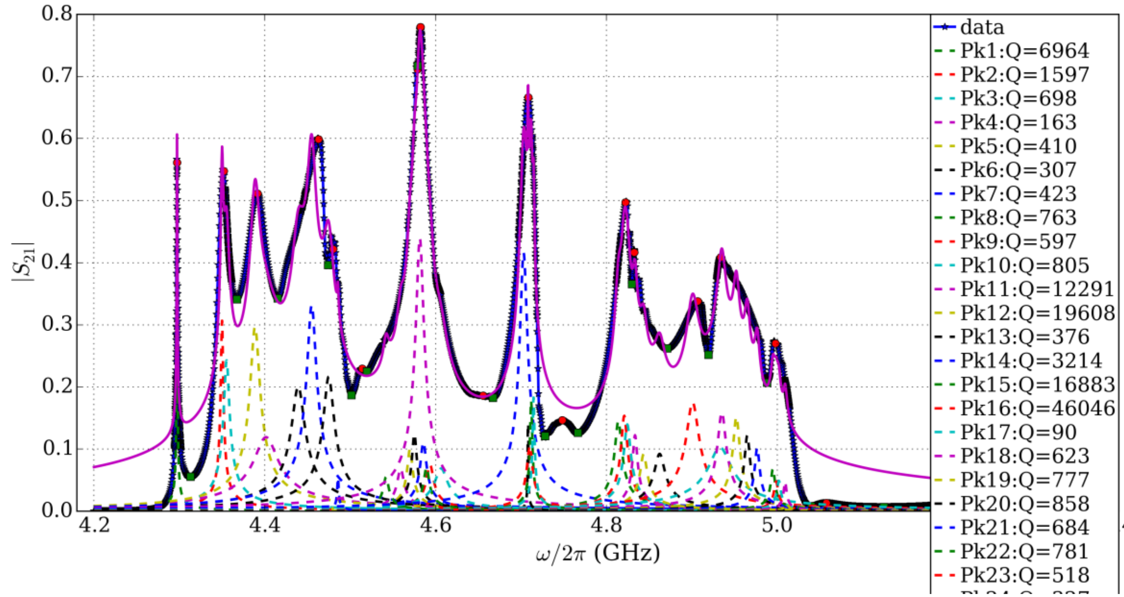
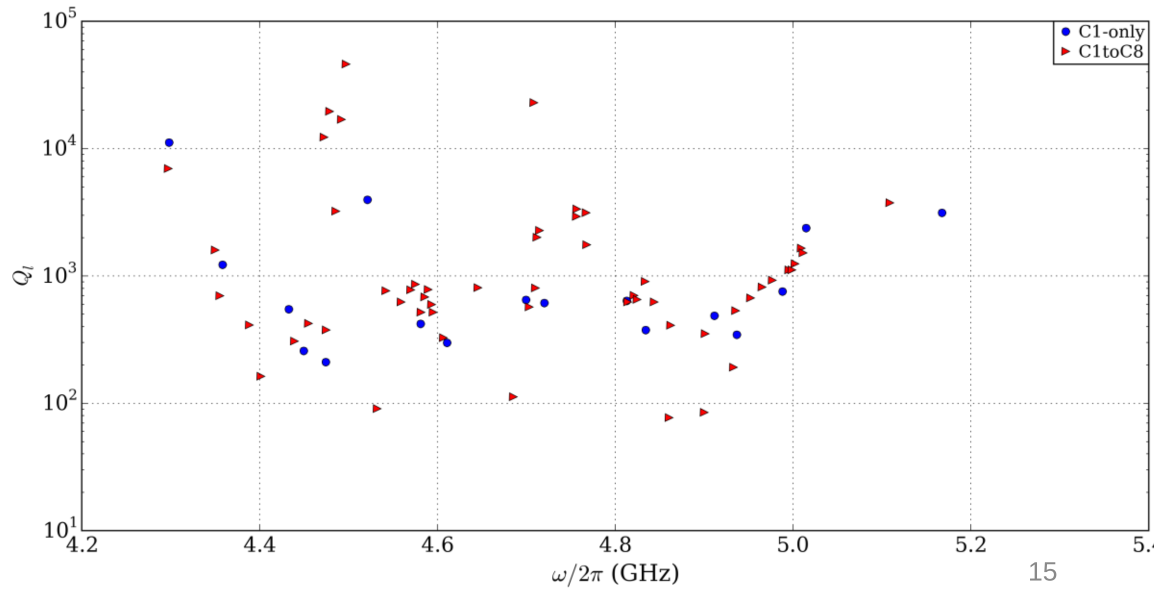
Q calculation: 8-cavity chain, 1st dipole band

- The whole dipole band fitted with 56 peaks.
- The peaks observed in the S_{21} curves were used as an initial values.
- All peaks are minimized simultaneously.
- The Q-values are in range from 10^2 to 10^4.





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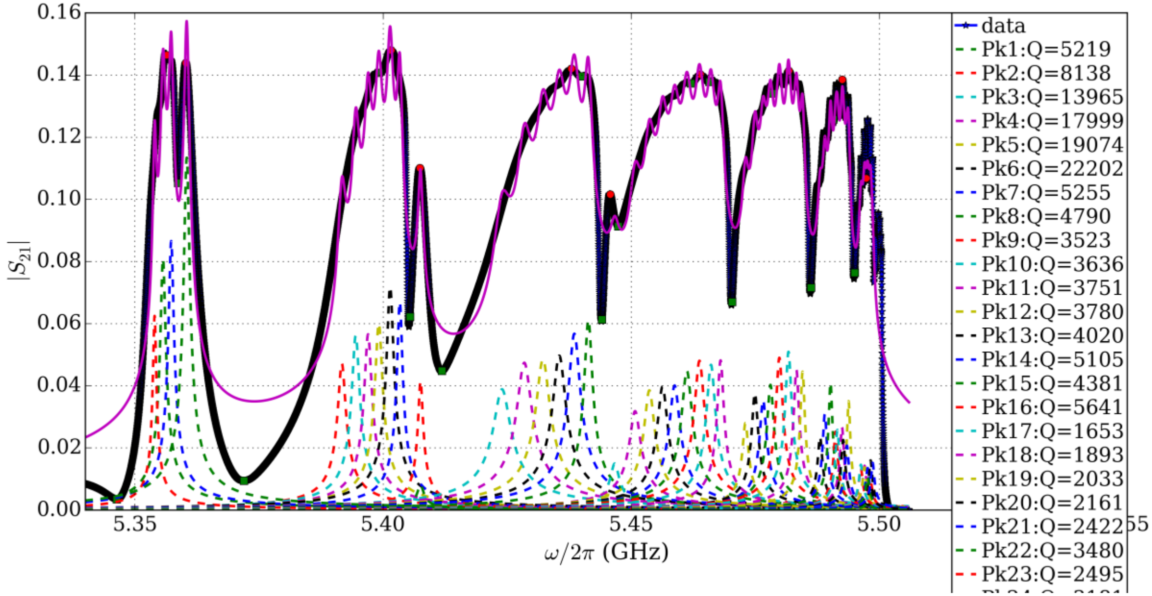
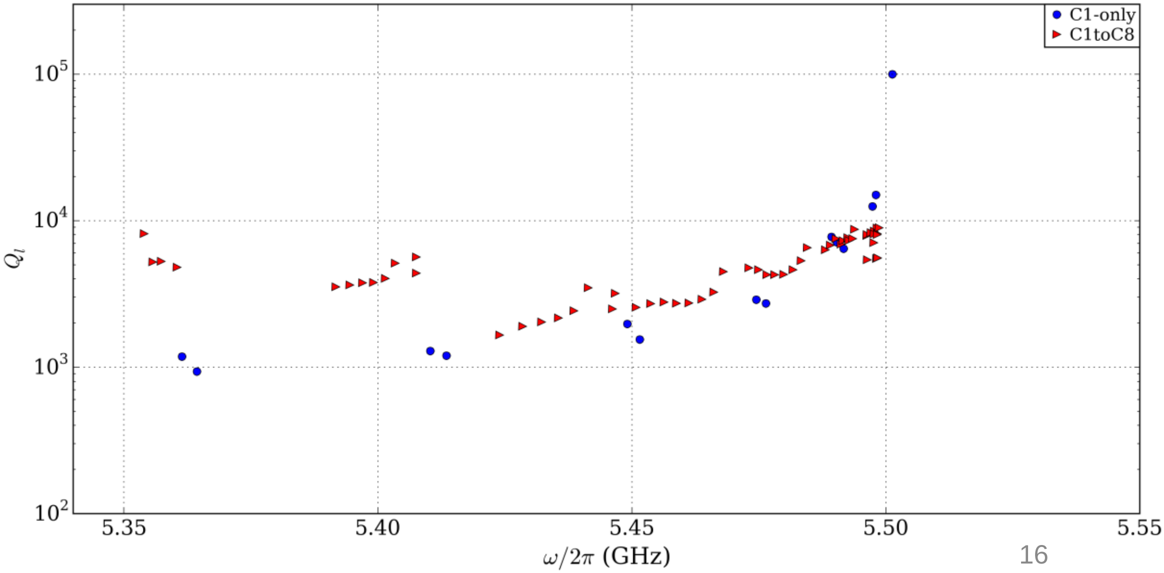
Q calculation: 8-cavity chain, 2nd dipole band

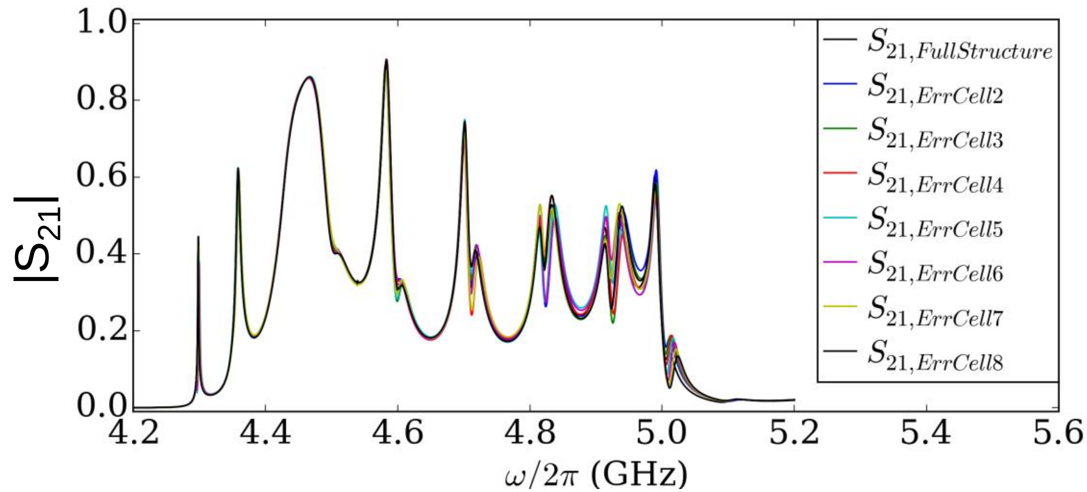
- The whole dipole band fitted with 64 peaks.
- The peaks observed in the S_{21} curves were used as an initial values.
- All peaks are minimized simultaneously.
- The Q-values are in range from 10^3.

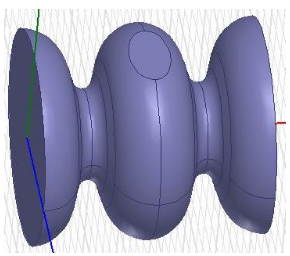


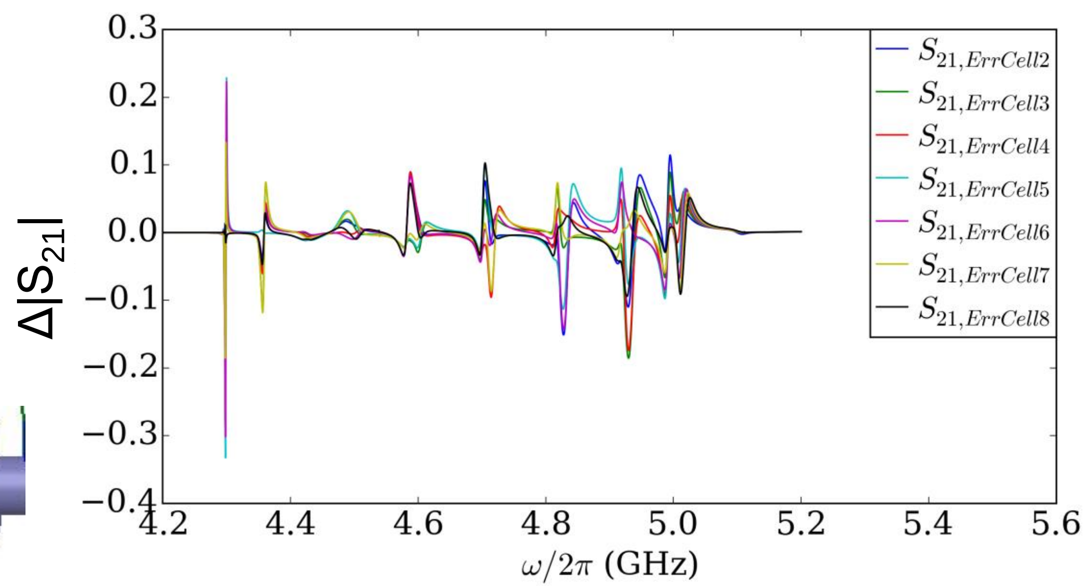


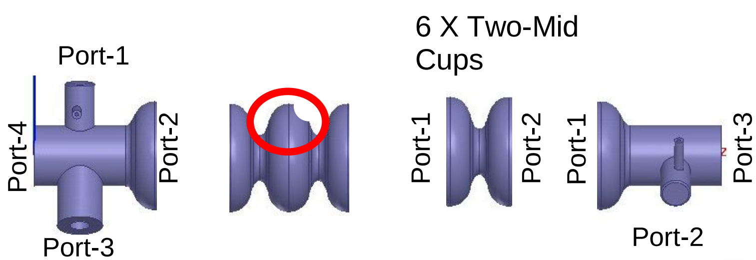
Fabrication Error in mid-cells

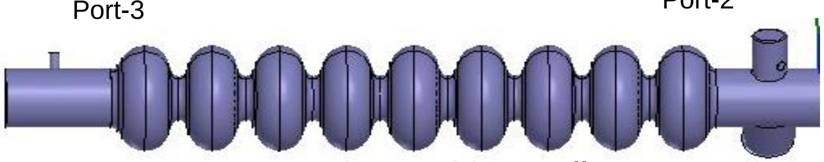
- A dent was introduced in mid-cell along X or Y axes, and S-parameter response of the unit cell was simulated using HFSS.
- Once simulated, the same error cell is cascaded at different positions to recreate error in different mid-cells instantaneously.
- In this study the error was cascaded only once, but different set of errors can be combined to carry extensive study.











Cavity-1 with 9 cells

Comparison with Experimental measurements on 8-cavity chain

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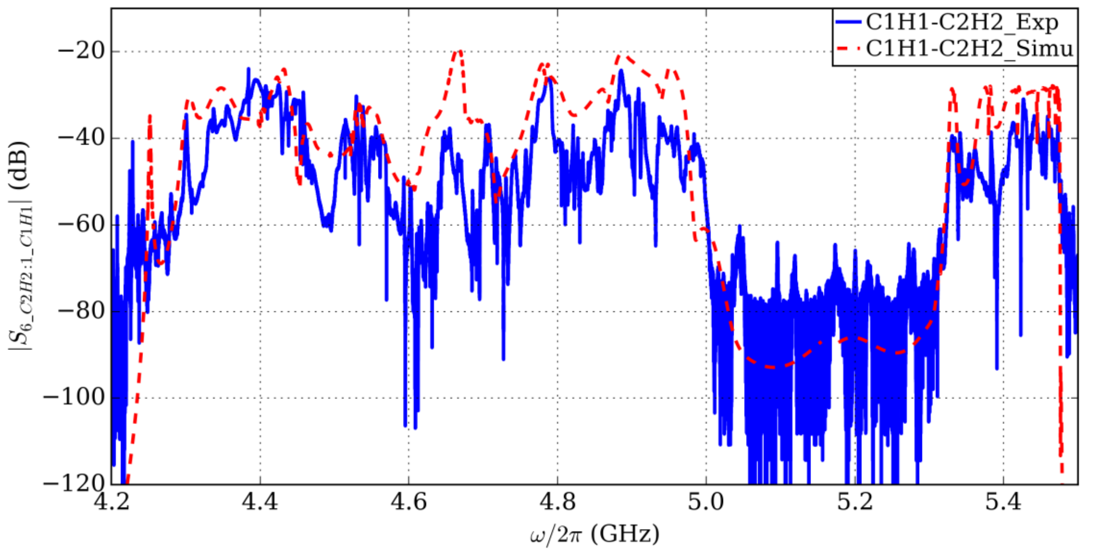
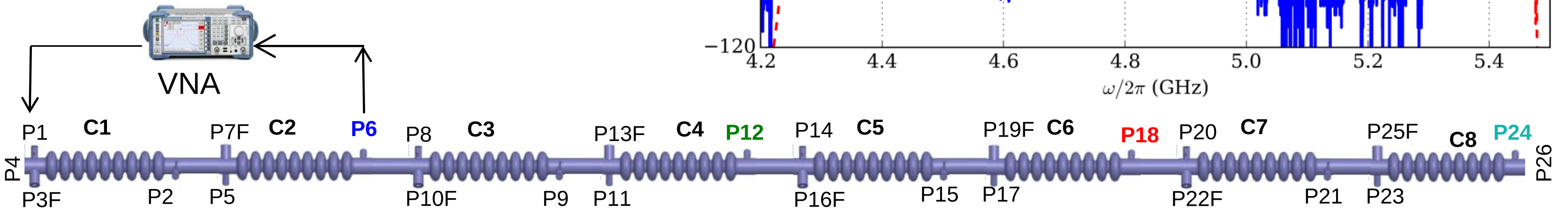
- S-parameters measured on 8-cavity chain module installed in the injector section, in superconducting state.
- Input port: HOM-1 port on first cavity
- Output measured at HOM-2 ports of Cavity-1 to Cavity-8.
- Frequency step size 5kHz (Experiment), 500 kHz (simulation, 50kHz in narrow peak regions.)
- Additional amplitude loss of 10 dB observed in experiment, attributed to additional cable loss in experimental setup.
- The simulated first dipole band was shifted left by 45 MHz, and second band was shifted by 25 MHz.

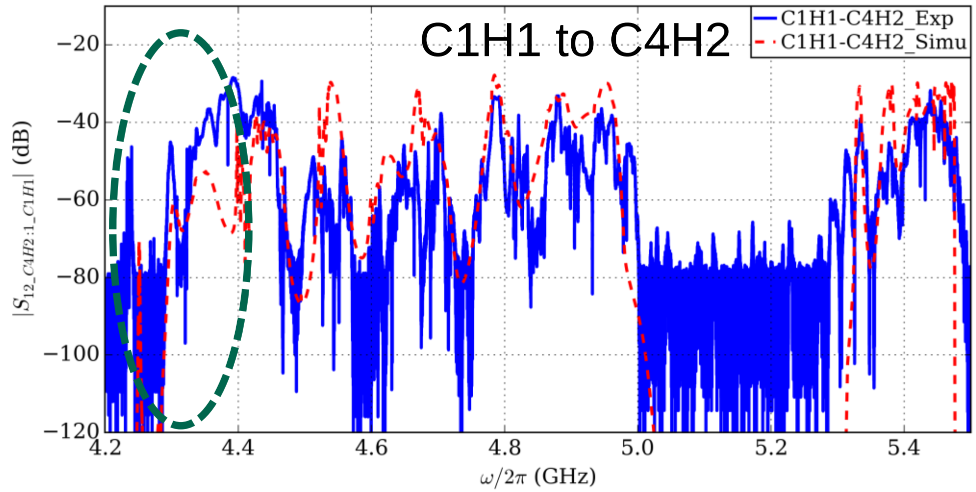


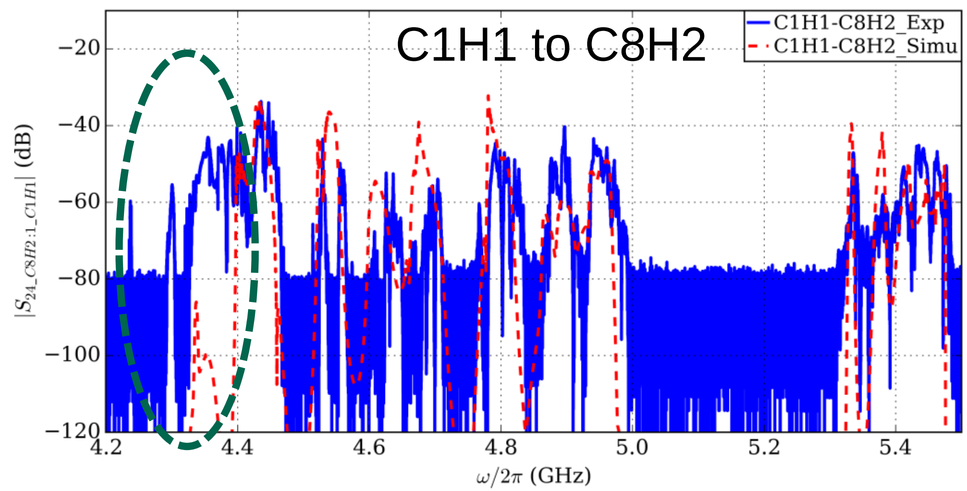


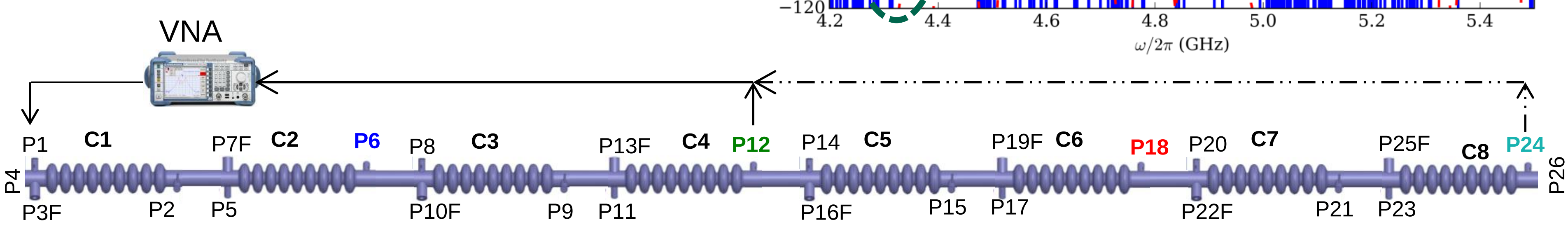
Comparison with Experimental measurements on 8-cavity chain

- Input port: HOM-1 port on first cavity
- Output measured at HOM-2 ports of Cavity-4 and Cavity-8.
- The cylindrical beam pipe connecting cavity has fundamental mode cutoff frequency of 4.39 GHz. The power received below the cutoff decreases considerably when moved away along the cavity chain.

- The beam pipes at ends of the cavity chain are terminated with ports, but the actual module is installed on beam line, allowing power to reflect back into structure.







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Summary and Future work

- A GSM based code has been developed to cascade the S-Matrices of unit blocks, to reconstruct larger structure response.
- Cascaded S-matrix results for a single cavity structure agreed very well with simulation of a whole structure.
- The mode spectrum of the complete 8-cavity chain has been reconstructed, and simulation showed considerable coupling between the cavity.
- Quality factors in the first two dipole bands were calculated from transmission curve and are in range from 10^2 to 10^4.
- A set of fabrication error in mid-cells is studied using cascading to determine sensitivity of different modes/frequencies to the error in different cell positions.
- The transmission spectrum along the cavity chain has been measured and compared to the GSM simulation, which agrees to each other.

- Further fabrication errors in end-cell geometry and power couplers will be studied if time and resources will allow.

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Thank you