RF Modeling

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SLAC NATIONAL ACCELERATOR LABORATORY
Stanford University | U.S. DEPARTMENT OF ENERGY

Outline

- Advanced RF modeling needs (P5 report)
- ACE3P updates
- S-Band distributed coupling structure RF design and tuning
- Conclusion

Acknowledgement: C.-K. Ng, L. Li, L. Xiao, Z. Li, D. Bizzozero, E. Nanni, A. Dhar, A. Haase, M. Bei, S. Tantawi

DOE HEP GARD, SLAC LDRD, US-Japan collaboration
Collaboration: KEK, LBNL, LANL

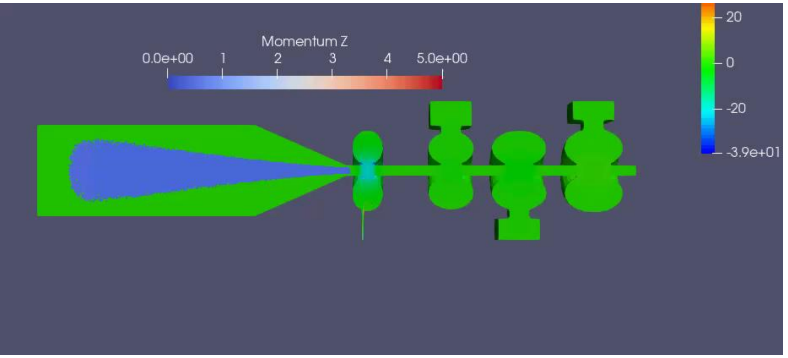
Modeling & Simulation for Advanced RF Accelerators and Sources

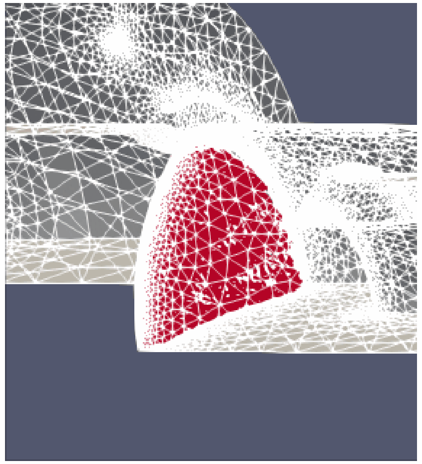
- **Novel RF structures present a challenge in terms of modeling and performance perdiction**
- **Multi-scale problems, spatiotemporal**
- **Diverse R&D approach includes full rf structure optimization**

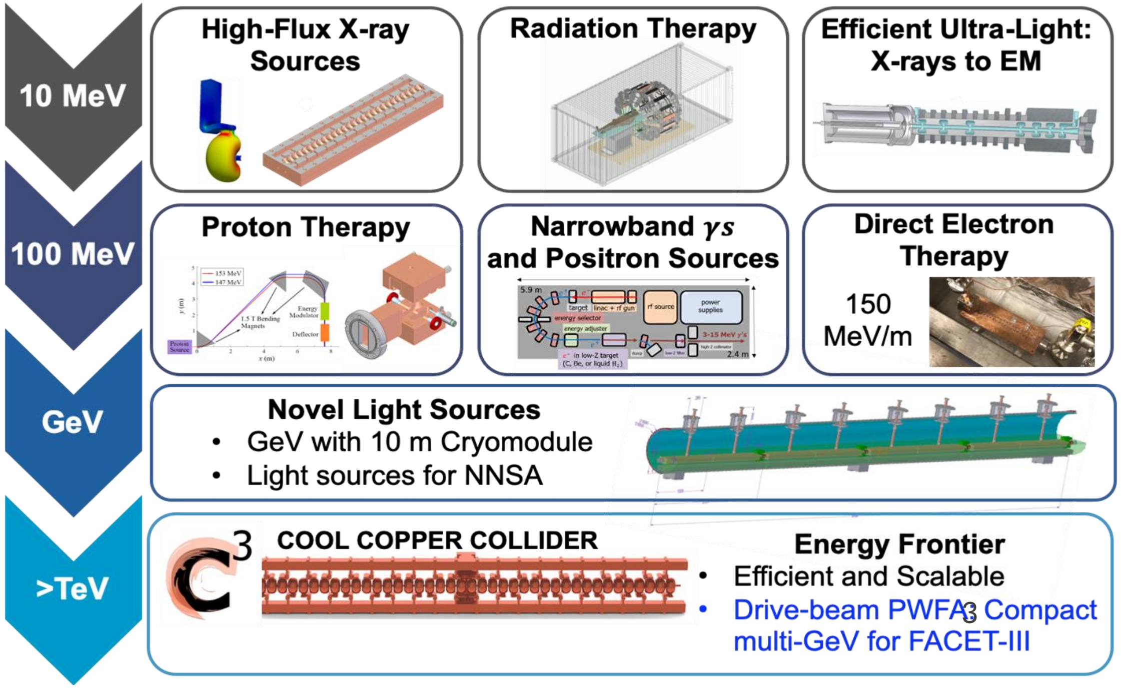
- Relativistic beam
- Space charge
- Fields generated by beam act back on beam
- Exotic materials

nonlinear, parametric behavior

- Virtual prototyping → need diverse portfolio of supported codes
- Shorten wait time to solution + robust optimization → need HPC infrastructure







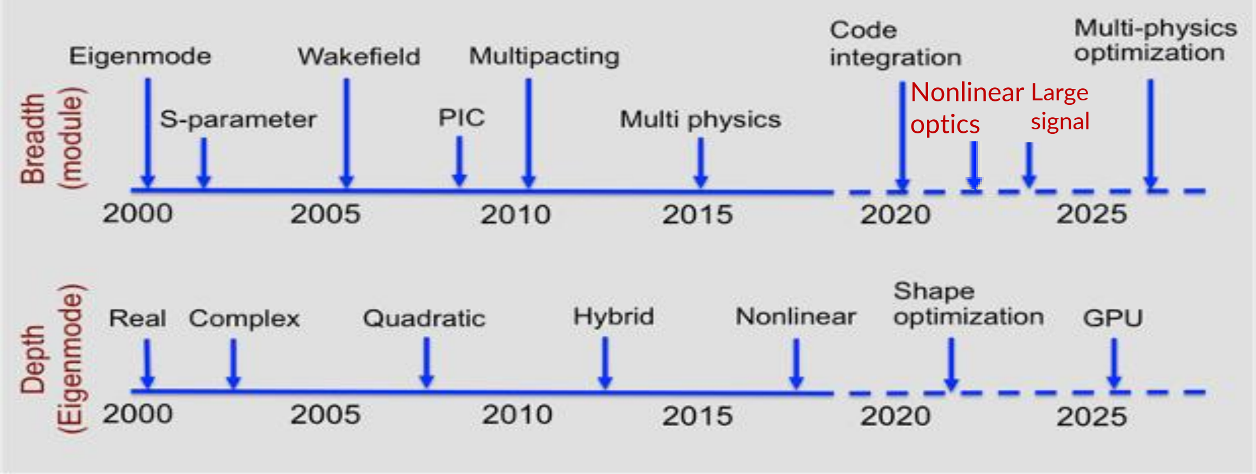
Multi-Physics Modeling Capabilities of RF Accelerators

- **ACE3P** is a parallel multi-physics code suite including electromagnetic (EM), thermal and mechanical simulations for virtual prototyping of accelerator and RF components
  - Based on *curved high-order finite elements* for high-fidelity modeling
  - Implemented on *massively parallel computers* for increased problem size and speed
  - C++ & MPI based

- **Capabilities to match CCC R&D needs (add more…)**

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**
Static Particle-in-cell:	**Gun3P**	– **DC guns & space charge effects**
Optimization:	**Opt3P**	– **Cavity shape optimization**



- ***"ACE3P is the advanced EM code available to the community and the result of thousands of person-hours over the past several decades. Maintaining broad access to this code while providing continual improvements will be a challenge."***

P5 Recommendations Relevant to Advanced Computing efforts

Recommendation 4: Support a comprehensive effort toward yield revolutionary accelerator designs that chart a realistic path to a 10 TeV pCM collider.

Recommendation 16: Resources for national initiatives in AI/ML, quantum, computing, and microprocessors should be leveraged and incorporated into research and R&D efforts to maximize the physics reach of the program.

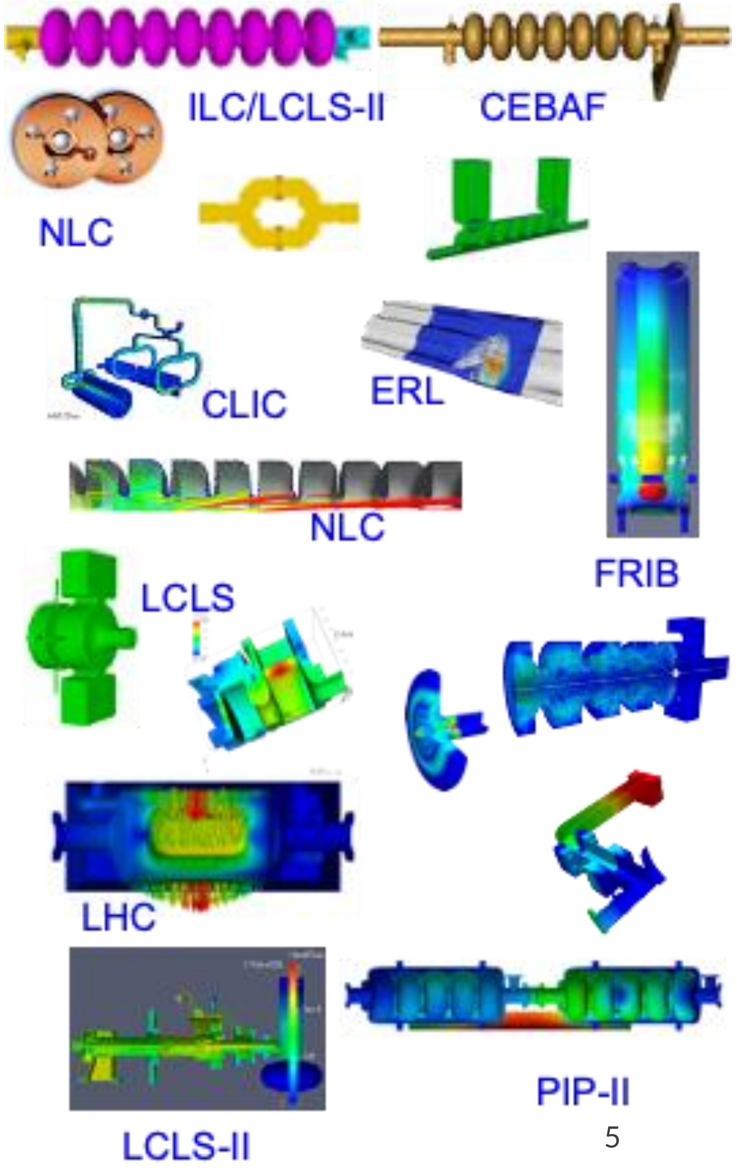
Exploring the Quantum Universe

Report of the 2023 Particle Physics Project Prioritization Panel

Recommendation 17: Add support for a sustained R&D effort at the level of $9M per year in 2023 dollars to adapt software and computing systems to emerging hardware -GARD

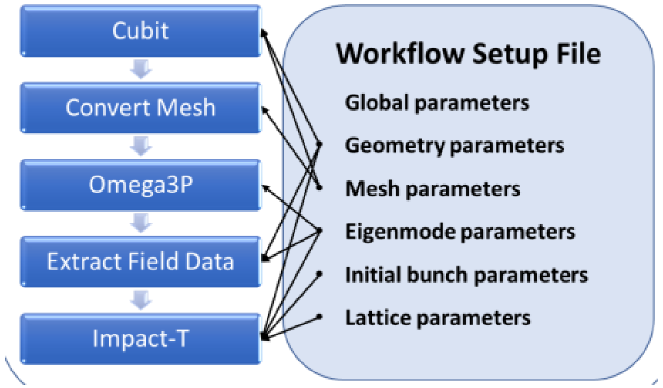
Recommendation 19: Research software engineers and other professionals at universities and labs are key to realizing the vision of the field and are critical for maintaining a technologically advanced workforce.

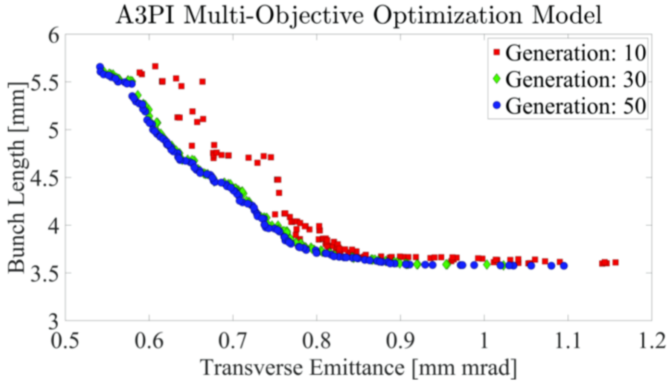
>>Targeted increases in support for theory, general accelerator R&D (GARD), instrumentation, and computing will bolster areas where US leadership has begun to erode.



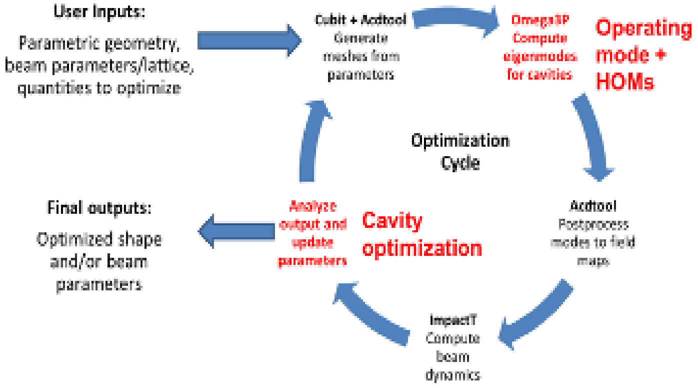
EM-Beam Optimization for Accelerator System Optimization

- Integrated Electromagnetics and Beam Dynamics Optimization
- Integration of ACE3P with particle dynamics solver
- Multi objective optimization and AL/ML techniques

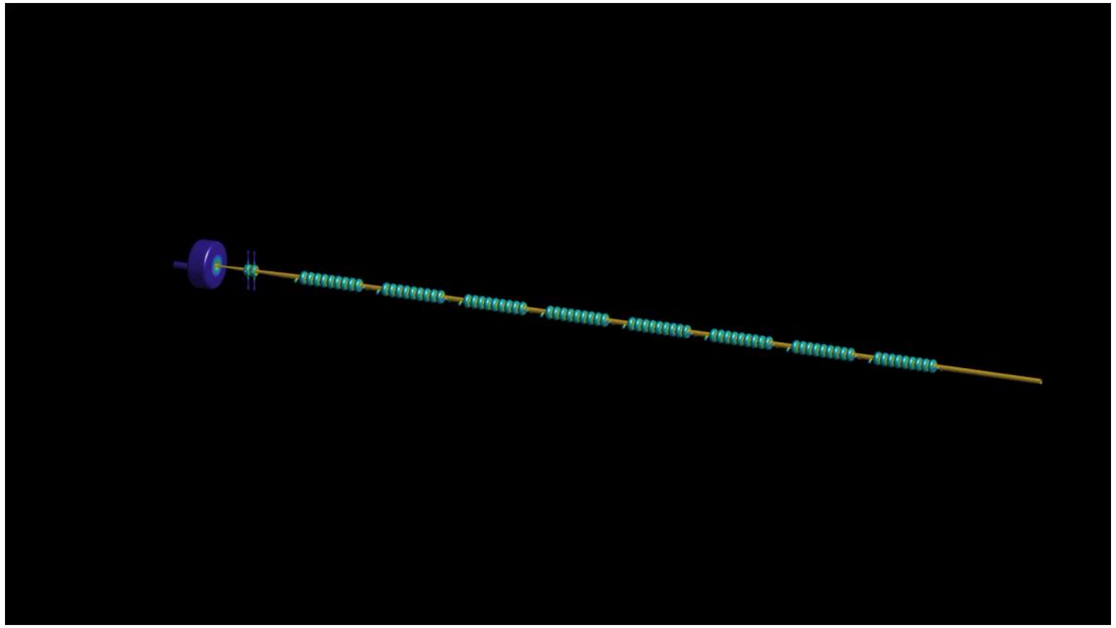




•Implemented optimization procedure in the integrated simulation workflow for combined beam dynamics and electromagnetics simulation.
•Applied simulation workflow to evaluate HOM effects on beam dynamics in LCLS-II injector.
•Started development of coupled optimization of cavity shape and beam dynamics for SRF gun.

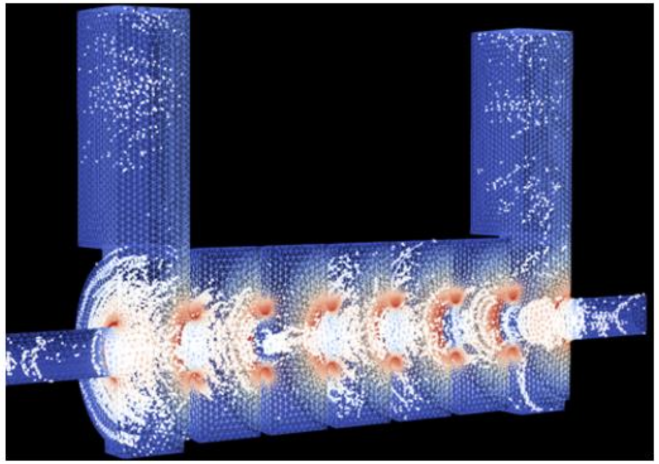


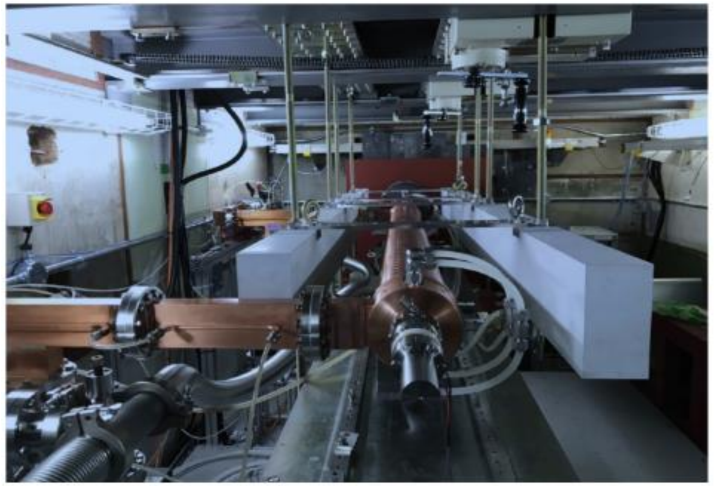
Simulation workflow for ACE3P and IMPACT optimization

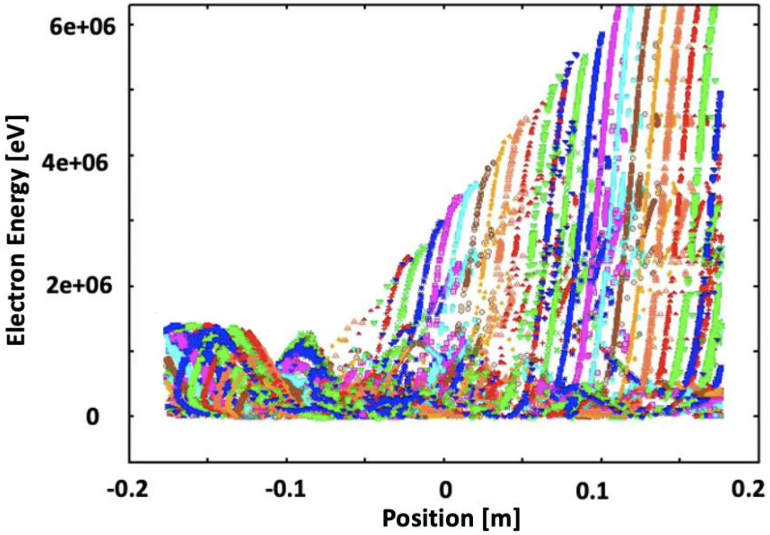


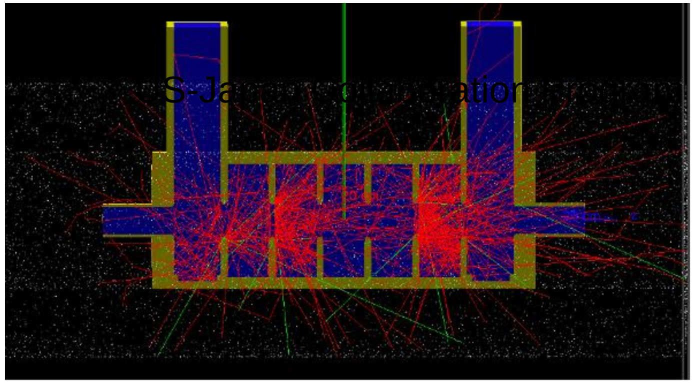
Integrated EM-Beam and radiation for Accelerator Facilities

- ACE3P-Geant4 integration
  - tracking of field-emitted e⁻ in cavity using ACE3P
  - radiation transport in cavity enclosure using Geant4
  - particle data transfer and CAD models for integrated tool
  - applied to evaluating dark current radiation effects





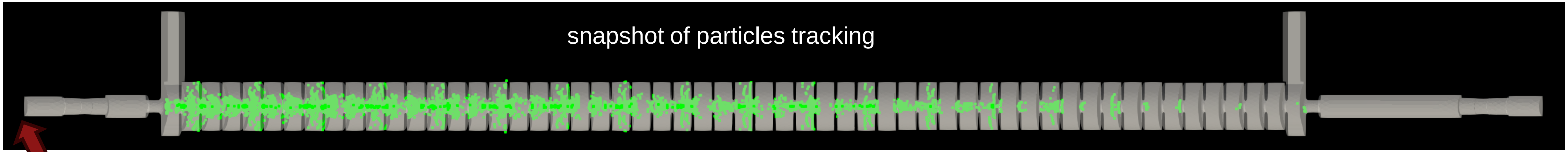




Particle trajectories in accelerator structure using Geant4

KEK 56 Cells Dark Current Simulation by Track3P

- Particles emission: Fowler Nordheim Law
- 30 RF cycles for particles fly through
- Particles collected while hitting the wall

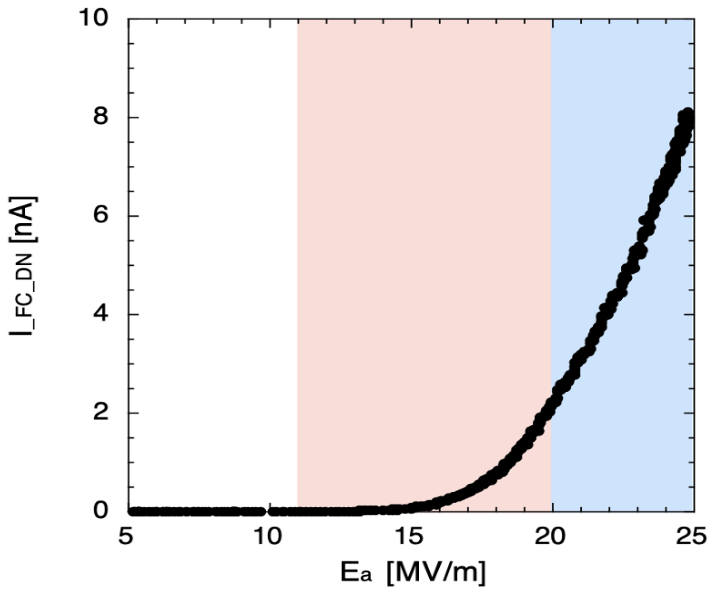


Faraday Cup Up-stream

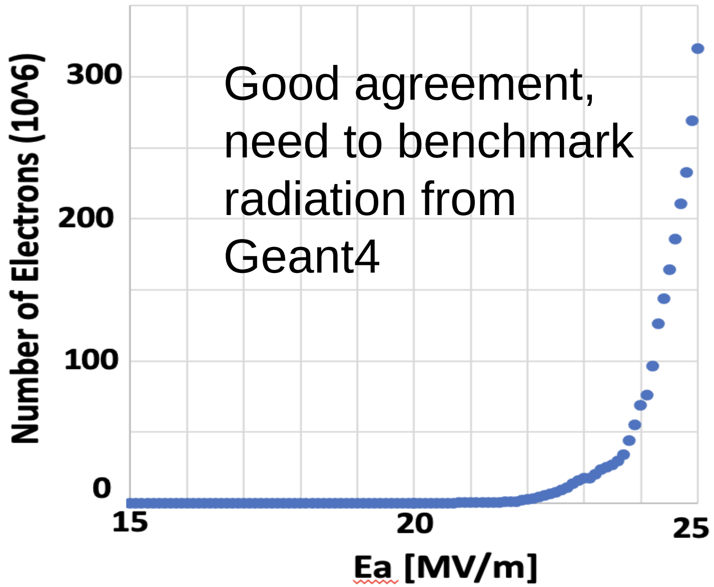
Faraday Cup Down-stream

Dark current validation

Measurement by KEK



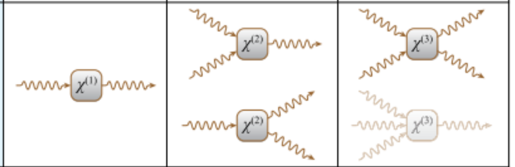
Simulation through Track3P

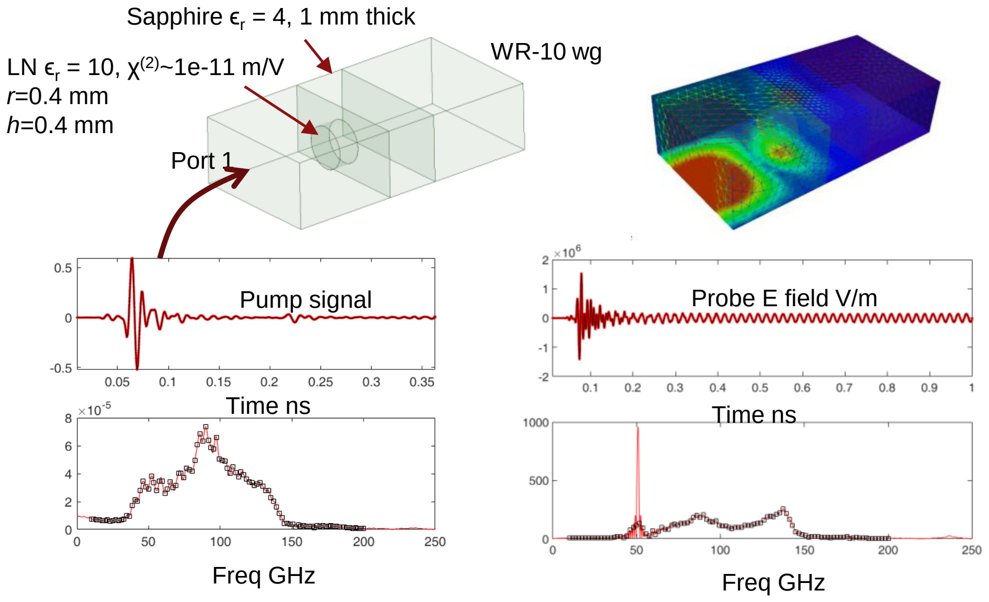


Development of Nonlinear Material Solvers

$$P = \varepsilon_0\left(\chi^{(1)}E + \chi^{(2)}E^2 + \chi^{(3)}E^3 + \cdots\right)$$

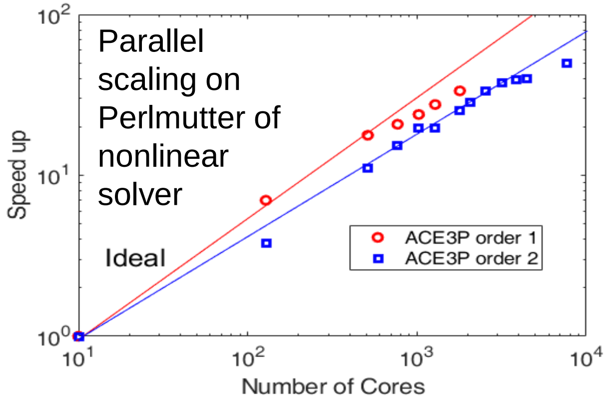
- Nonlinear dielectric materials
  - higher-order susceptibilities
  - applicable to THz accelerators and optical devices for QIS
  - supported by LDRD

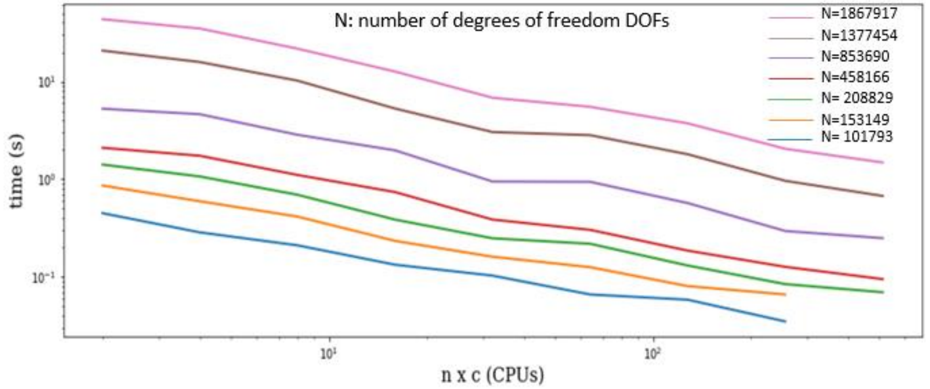
	$\chi^{(1)}$ process	$\chi^{(2)}$ process	$\chi^{(3)}$ process
Hamiltonian	$(m_1 + m_1^\dagger)(m_2 + m_2^\dagger)$	$m_1^\dagger m_1 (m_2 + m_2^\dagger)$	$m_1^\dagger m_2^\dagger m_3 m_4 + m_1 m_2 m_3^\dagger m_4^\dagger$
Processes			
Examples	Piezoelectric Effect	Electro-optic Effect Electromechanical Effect Optomechanical Effect	Four-wave Mixing



Developed a robust simulation platform with efficient numerical techniques for virtual prototyping of nonlinear comments, superconducting devices.

- HPC on NERSC supercomputer
  - ACE3P on Perlmutter CPU nodes with linkage to software libraries
  - significant speedup achieved using the new architecture
  - Using PETSc solver for massive scalability

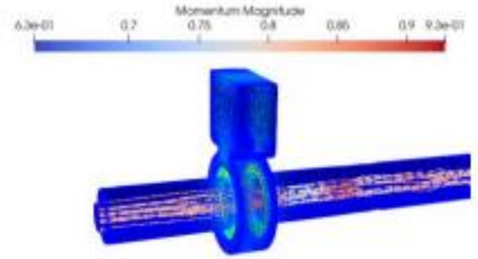


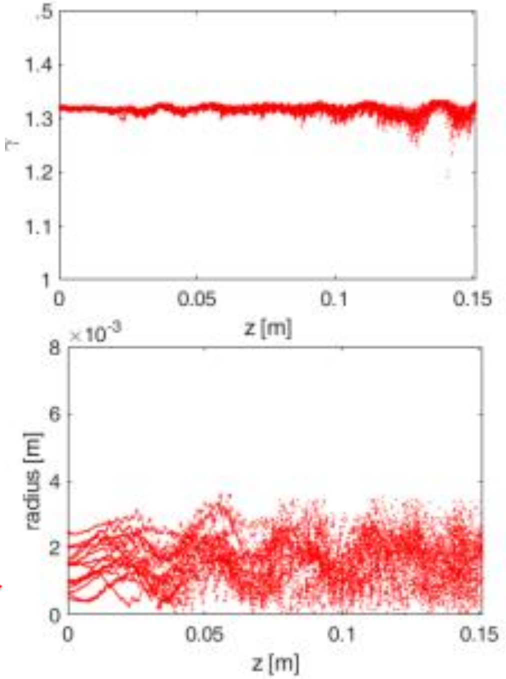


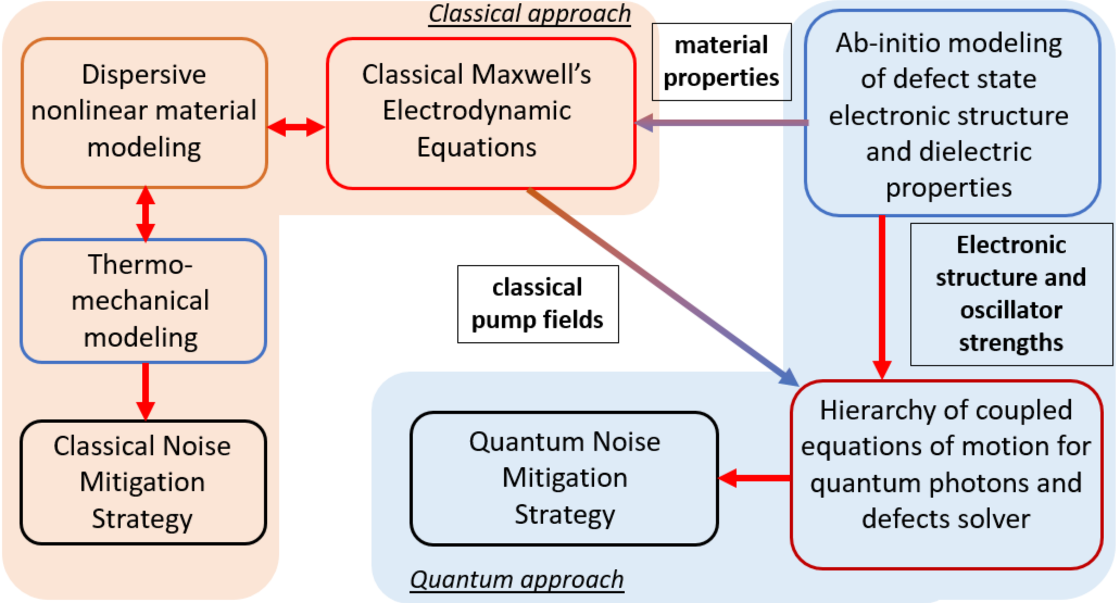
General ACE3P updates

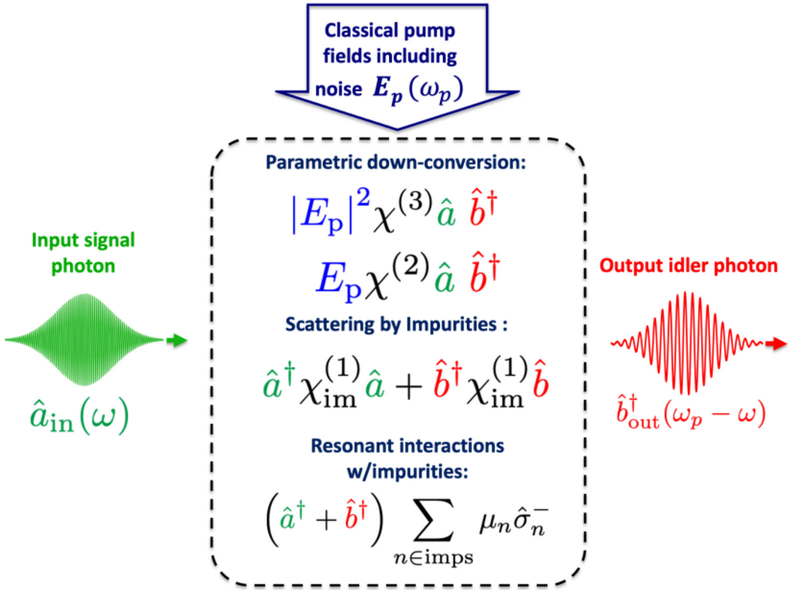
- Upgrade GUI with Kitware Inc.
- Prepare code documentation
- Convert ACE3P compilation from boost build to Makefile
- Improve PETSc GPU performance in T3P
- Offload data to GPU for parallel kernels in Track3P using OpenMP

- Apply PIC3P to klystron simulations
- Investigate quantum phenomena (integration with DFT)





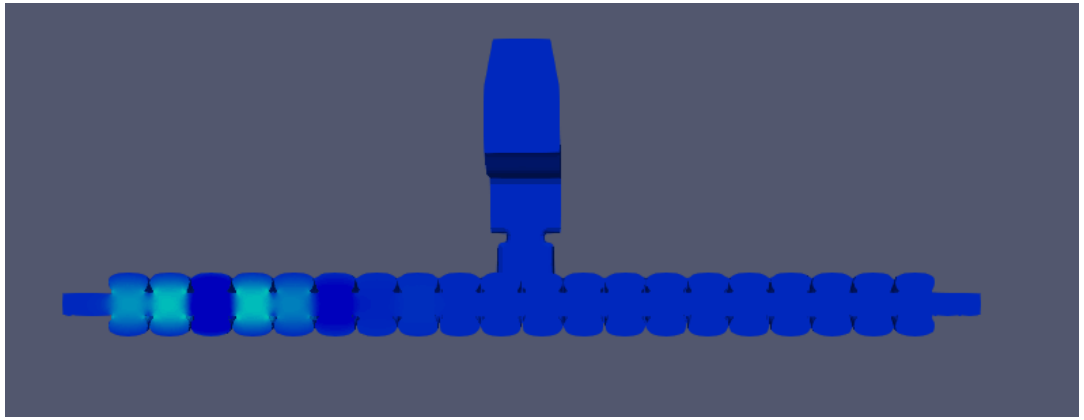


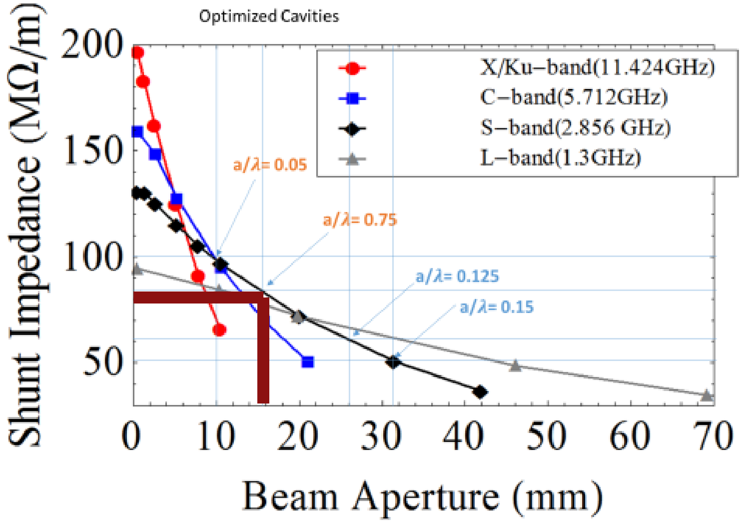


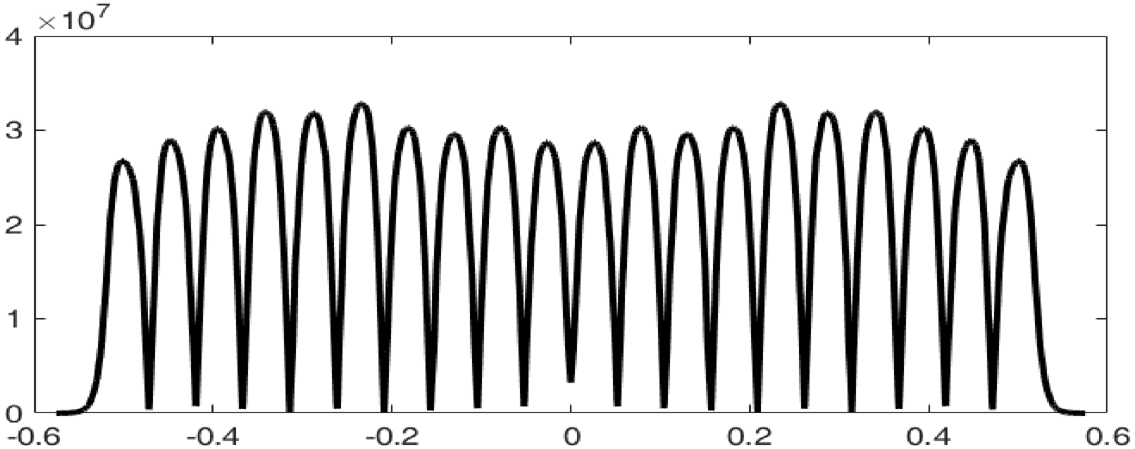
Distributed Coupling Accelerators Structures

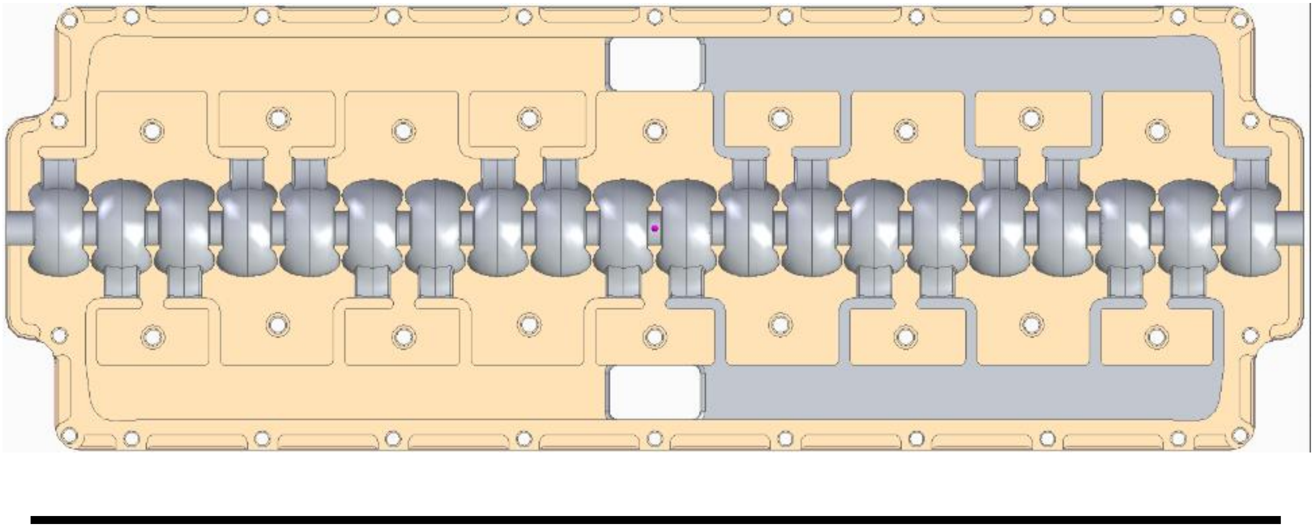
Design balances shunt impedance with aperture size

- S-band cavities designed with aperture a=14.71 mm
- At the π- mode there is no power transfer between cells
- However, frequency of individual cell is influenced by neighboring cells





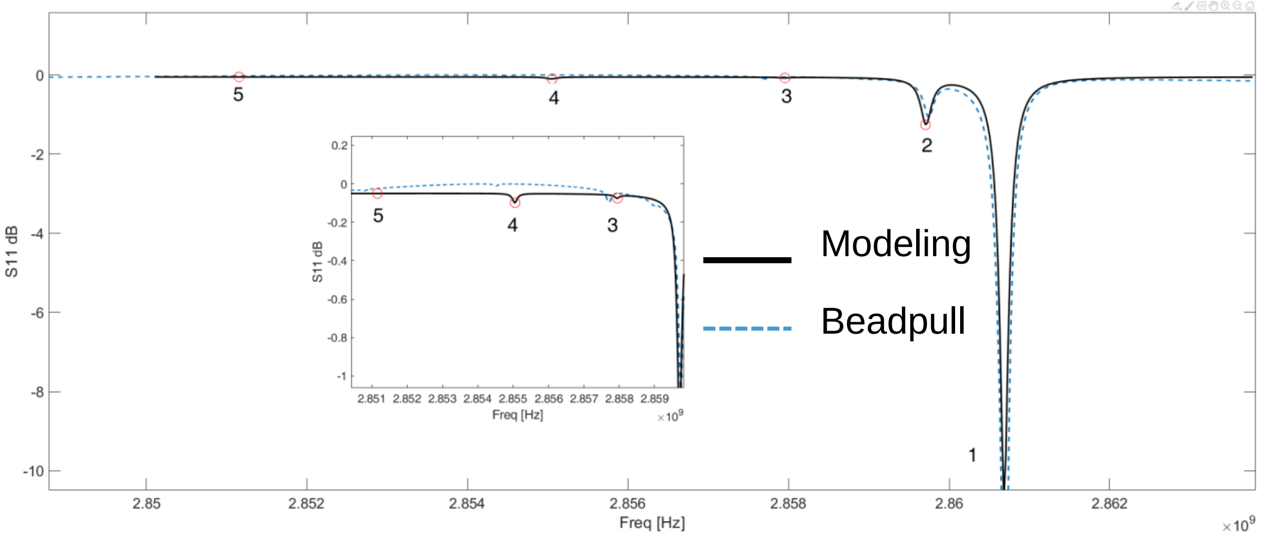




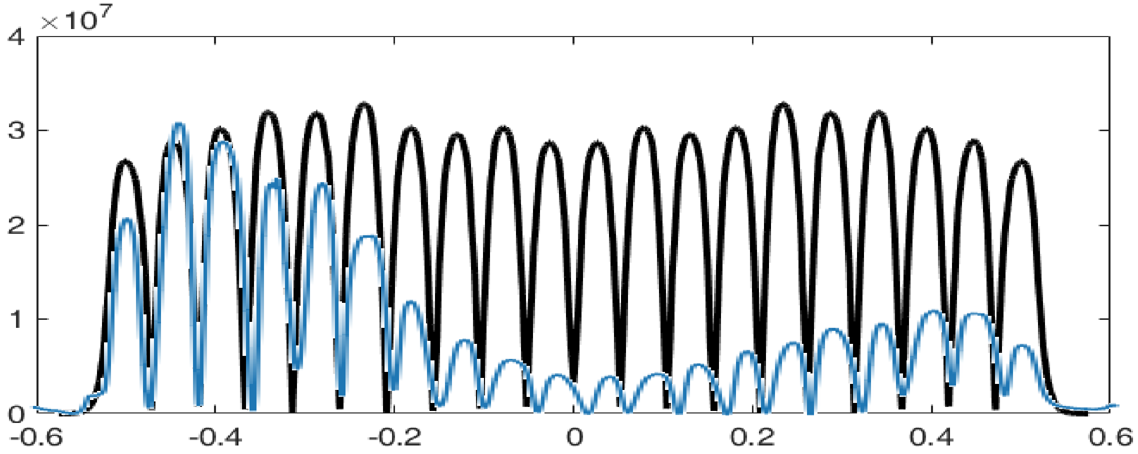
1 meter

Structure Fabrication and Tuning

- Fabricated structure showed ~4 MHz frequency shift in pi-mode
- However, each individual cell was tuned so collectively the pi-mode shape was different



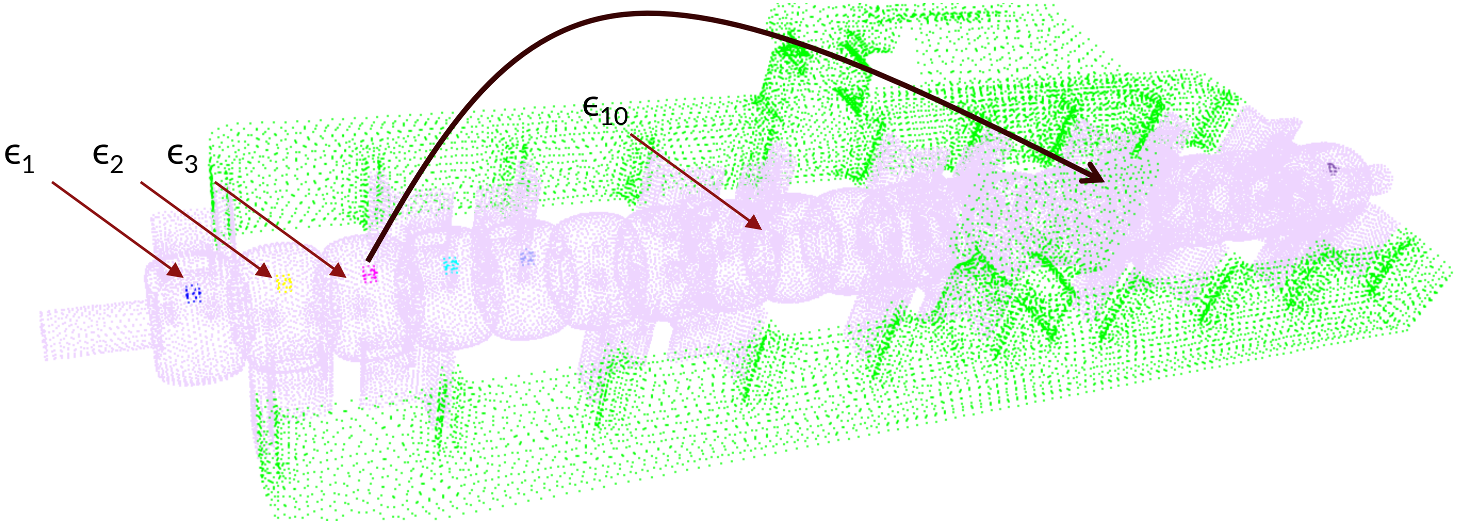
Data	Mode 5 GHz	Δ MHz	Mode 4 GHz	Δ MHz	Mode 3 GHz	Δ MHz	Mode 2 GHz	Δ MHz	Mode 1 (pi mode)
Original Design simulation	2.8437	3.6	2.8473	3.3	2.85060	2.8	2.85340	2.5	2.85590
Cold test	2.85076	3.74800	2.85451	3.2000	2.85771	2.0360	2.85974	0.9480	2.86069
Retuned Simulation	2.85115	3.900	2.85505	2.900	2.85795	1.7500	2.85970	0.975	2.86068



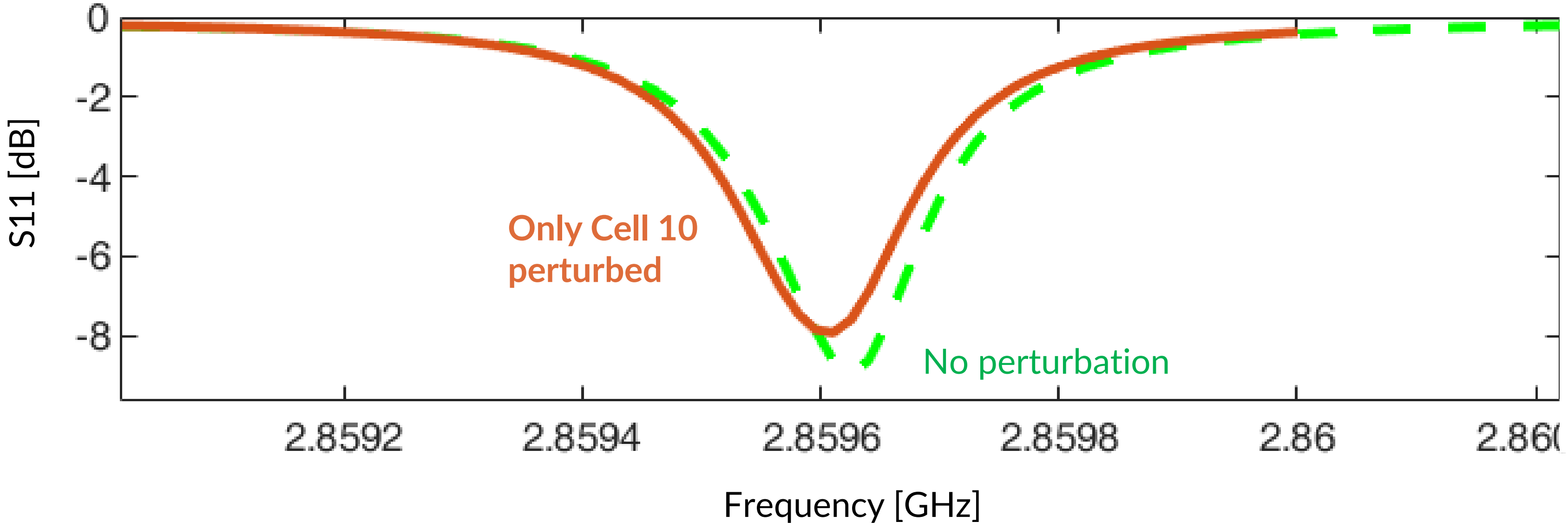
Virtual RF Tuning

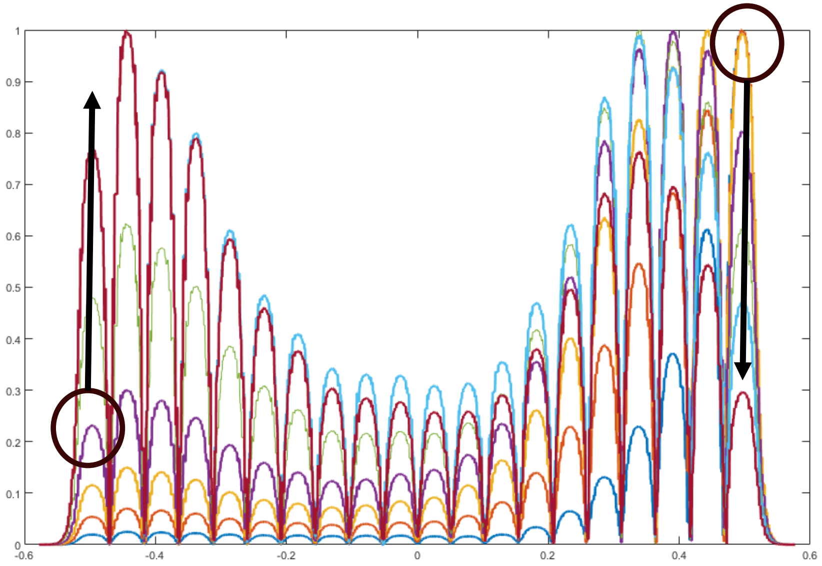
Virtual beam pull

- Each cavity has a dielectric bead with a relative permittivity to induce tuning
- Each bead can be turned ON or OFF in simulation



$\epsilon_{i=1,2,..,20, i\neq 10} = 1$, $\epsilon_{10} = 3.5$ → Overall pi mode shift of -15 kHz





Tuning Distributed Coupling S-Band LINAC

$|\frac{\partial E_{mi}}{\partial f_{mi}}|$ unit is MV/m / GHz with 1 W input power

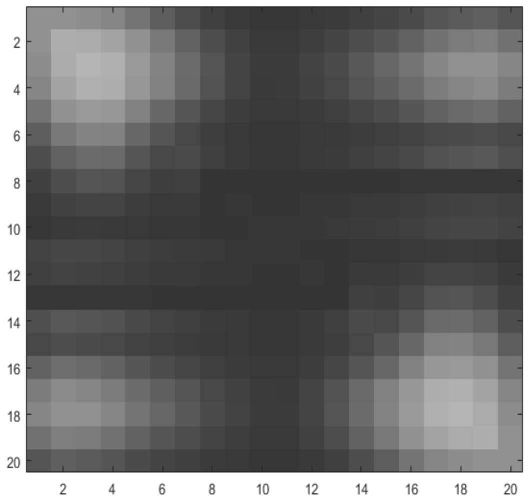
- First, calculate derivatives of pi mode frequency of each cell versus perturbation ε_i

$$f_m = \frac{\partial f_m}{\partial \varepsilon_m}, m = 1,2,\ldots,20$$

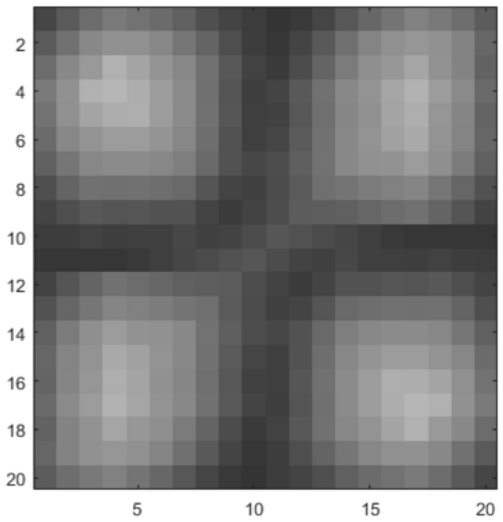
- Gradient perturbation in each cell

$$E'_{mn} = \frac{\partial E_m}{\partial \varepsilon_n} \times \left(\frac{\partial f_n}{\partial \varepsilon_n}\right)^{-1} = \frac{\partial E_m}{\partial f_n}, m,n = 1,2,\ldots,20$$

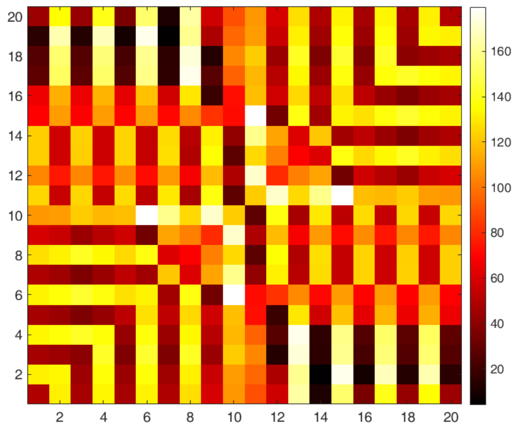
Modeling



Measurement



$\arg\left(\frac{\partial E_{mi}}{\partial f_{mi}}\right)$ unit is degree



- In general good agreement, some discrepancies due to accuracy of frequency measurement s (100 kHz)

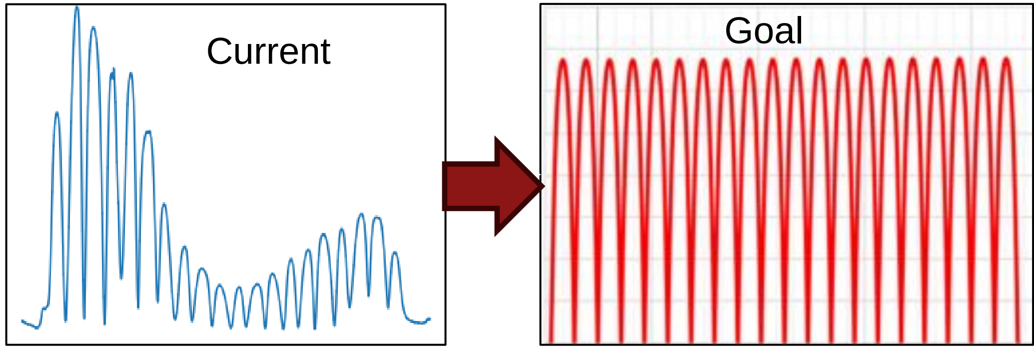
- Cavities in the middle are less sensitive to tuning, need collective tuning

Target Optimal Frequencies Based on Perturbative Method

- The resulting field in the cell j after iteration i $E_{m,i} = E_{m,i-1} + df_{m,i-1}\frac{\partial E_{m,i-1}}{\partial f_{m,i-1}} + \dots$

- Target normalized fields are given by the following

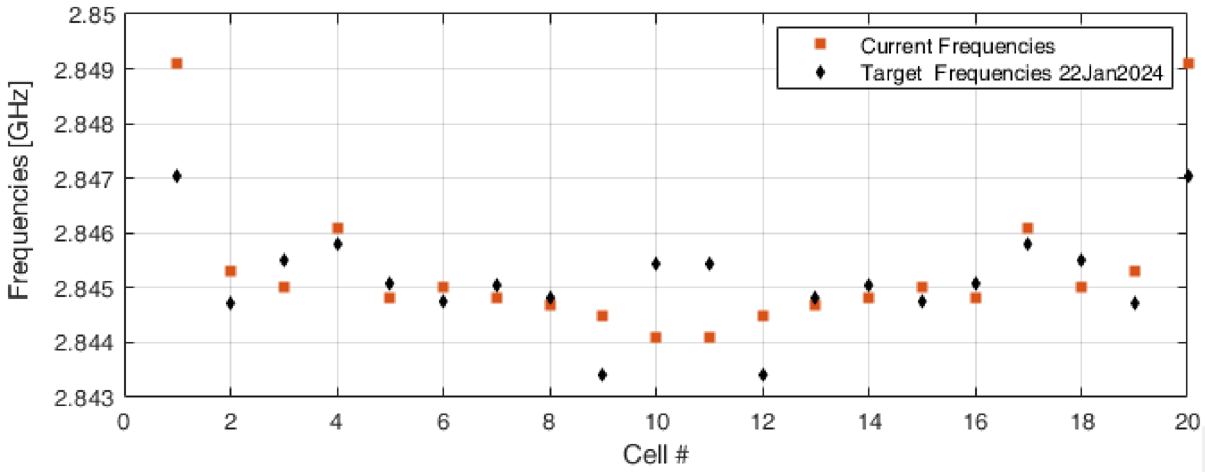
$$E_{im} = 1e^{jm\pi}$$



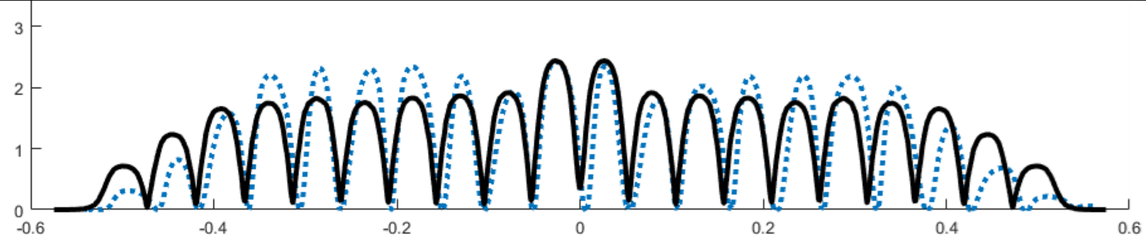
- Target frequencies are given by $f_{m,i} = f_{m,i-1} - df_{m,i}$

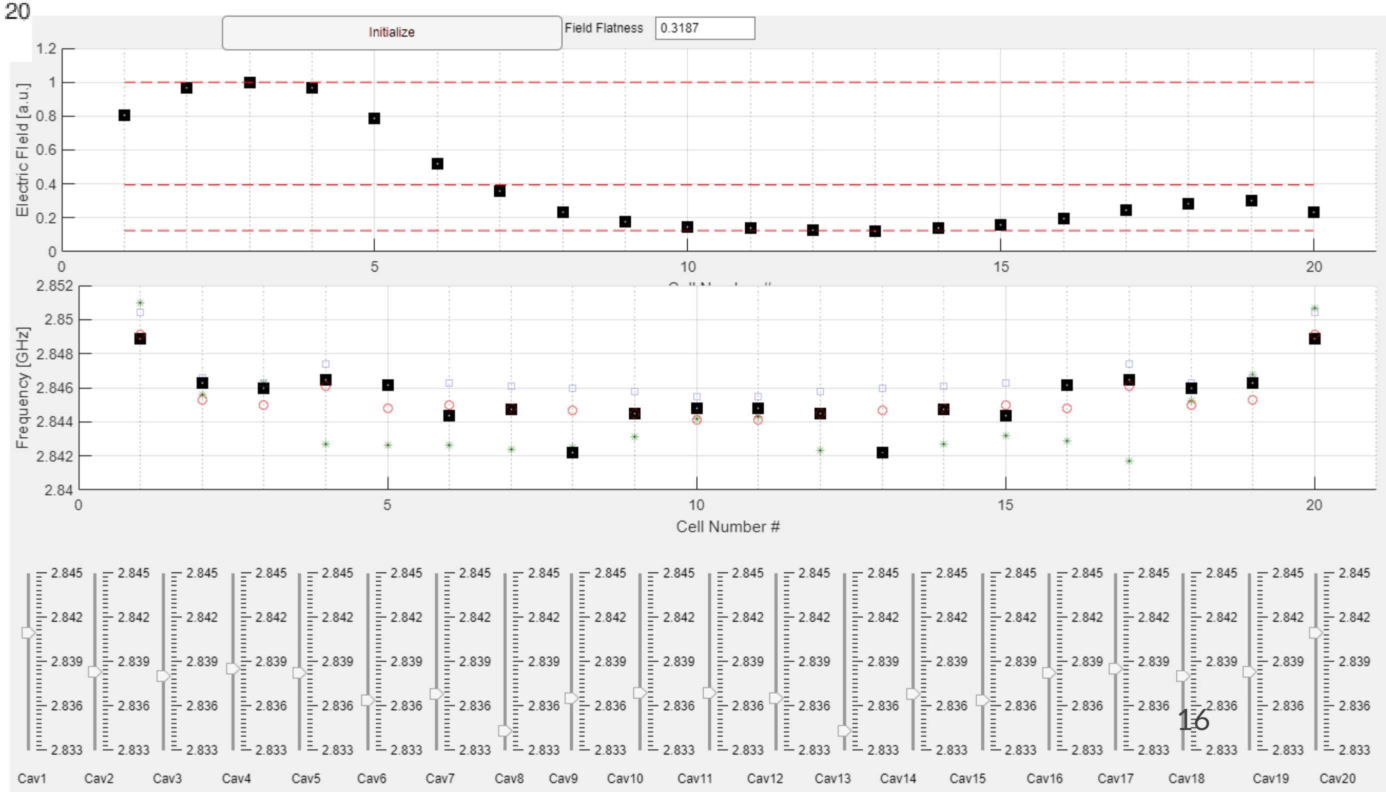
$$f_{m,i} = f_{m,i-1} - \left(\frac{\partial E_{m,i-1}}{\partial f_{m,i-1}}\right)^{-1}\left(1e^{jm\pi} - E_{m,i-1}\right)$$

Tuning



$$f_{m,1} = f_{m,0} - \left(\frac{\partial E_{m0}}{\partial f_{m0}}\right)^{-1} \left(1e^{jm\pi} - E_{m,0}\right)$$





- First iteration of tuning has been successful in retrieving symmetry and improve coupling to cells
- Developed tool for using machine learning to train a model for adaptive control and muti-objective optimization

Conclusion

- Efforts in advanced RF modeling and virtual prototyping are crucial for CCC

- Development of ACE3P is ongoing with more features, add-on and use cases

- Tuning S-Band injector realizes heavily on virtual prototyping