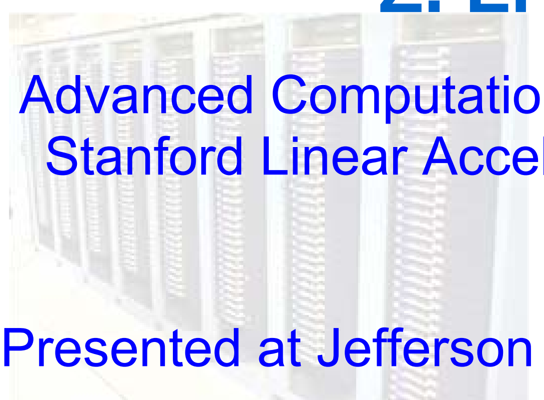
Accelerator Modeling Through High Performance Computing



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Outline

- DOE SciDAC Program
- Parallel Code Development under SciDAC
- Applications to DOE Accelerator Projects
- Collaborations in Computational Science Research

SciDAC Program

SciDAC: Scientific Discovery through Advanced Computing

- DOE Office of Science (SC) Simulation Initiative
- Promotes application of High Performance Computing to SC programs across BES/NP/HEP Offices
- Multi-disciplinary approach – computational scientists (CS & AM) work alongside application scientists
- Accelerator project started as *Accelerator Simulation and Technology (AST)* in SciDAC1, and continues as *Community Petascale Project for Accelerator Science and Simulation (COMPASS)* in SciDAC2

Goal – To develop next generation simulation tools to improve the performance of present accelerators and optimize the design of future machines using flagship supercomputers at NERSC (LBNL) and NLCF (ORNL)

SLAC SciDAC Activities

- Parallel code development in electromagnetics and beam dynamics for accelerator design, optimization and analysis
- Application to accelerator projects across HEP/BES/NP such as ILC, LHC, LCLS, SNS, etc…
- Petascale simulations under SciDAC2 on DOE's supercomputers - currently 3 allocation awards at NERSC (Seaborg, Bassi, Jacquard) and NCCS (Phoenix)
- Computational science research through collaborations with SciDAC CET/Institutes' computer scientists and applied mathematicians

SLAC Parallel Codes under SciDAC1

- Electromagnetic codes in production mode:

Omega3P – frequency domain eigensolver for mode and damping calculations

S3P – frequency domain S-parameter computations

T3P – time domain solver for transient effects and wakefield computations with beam excitation

Track3P – particle tracking for dark current and multipacting simulations

V3D – visualization of meshes, fields and particles

SLAC Parallel Codes under SciDAC2

Codes under development:

- *Electromagnetics*

  Gun3P – 3D electron trajectory code for beam formation and transport

  Pic3P – self-consistent particle-in-cell code for RF gun and klystron (LSBK) simulations

  TEM3P – integrated EM/thermal/mechanical analysis for cavity design

- *Beam dynamics*

  Nimzovich – particle-in-cell strong-strong beam-beam simulation

SciDAC Tools for Accelerator Applications

ILC

- *Accelerating Cavity (DESY, KEK, JLab)*
  - *TDR, Low-loss, ICHIRO & cryomodule designs*
- *Input Coupler (SLAC, LLNL) – TTFIII multipacting studies*
- *Crab Crossing (FNAL/UK) - Deflecting cavity design*
- *Damping Ring (LBNL) – Impedance calculations*
- *L-Band Sheet Beam Klystron – Gun and window modeling*

LHC

- *Beam-beam simulations*

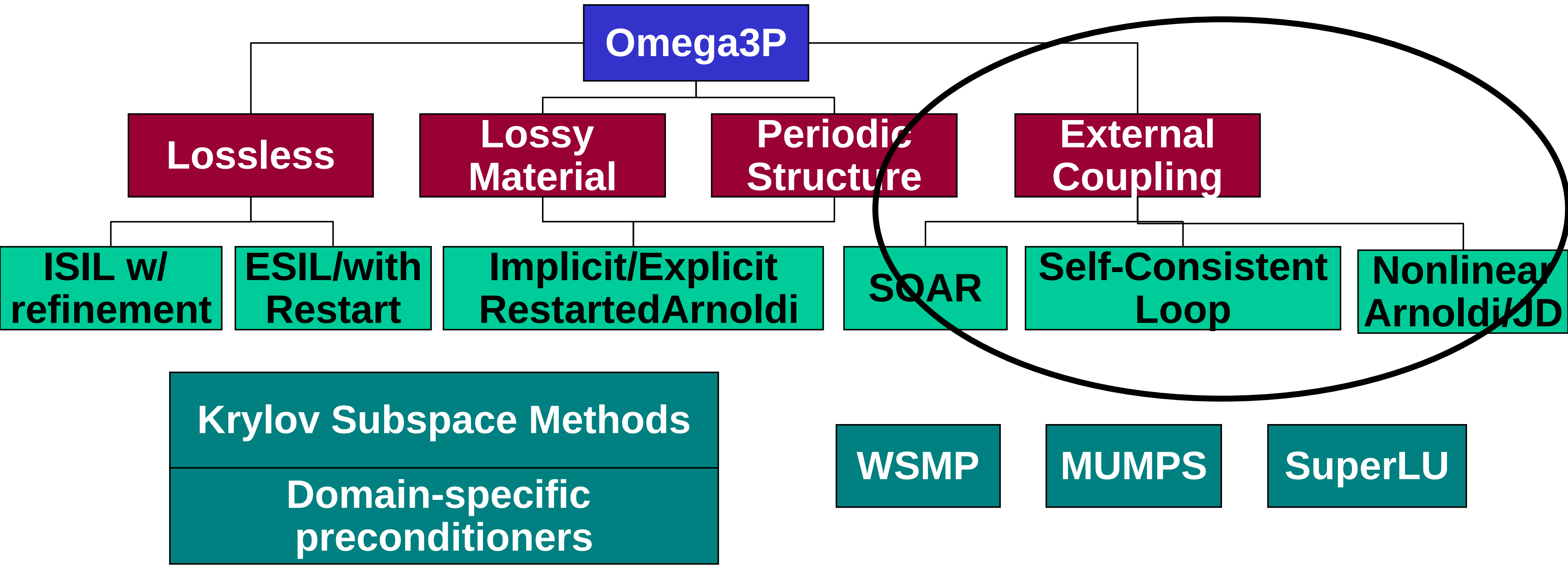
LCLS

- *RF gun – emittance calculations using PIC codes*

SNS

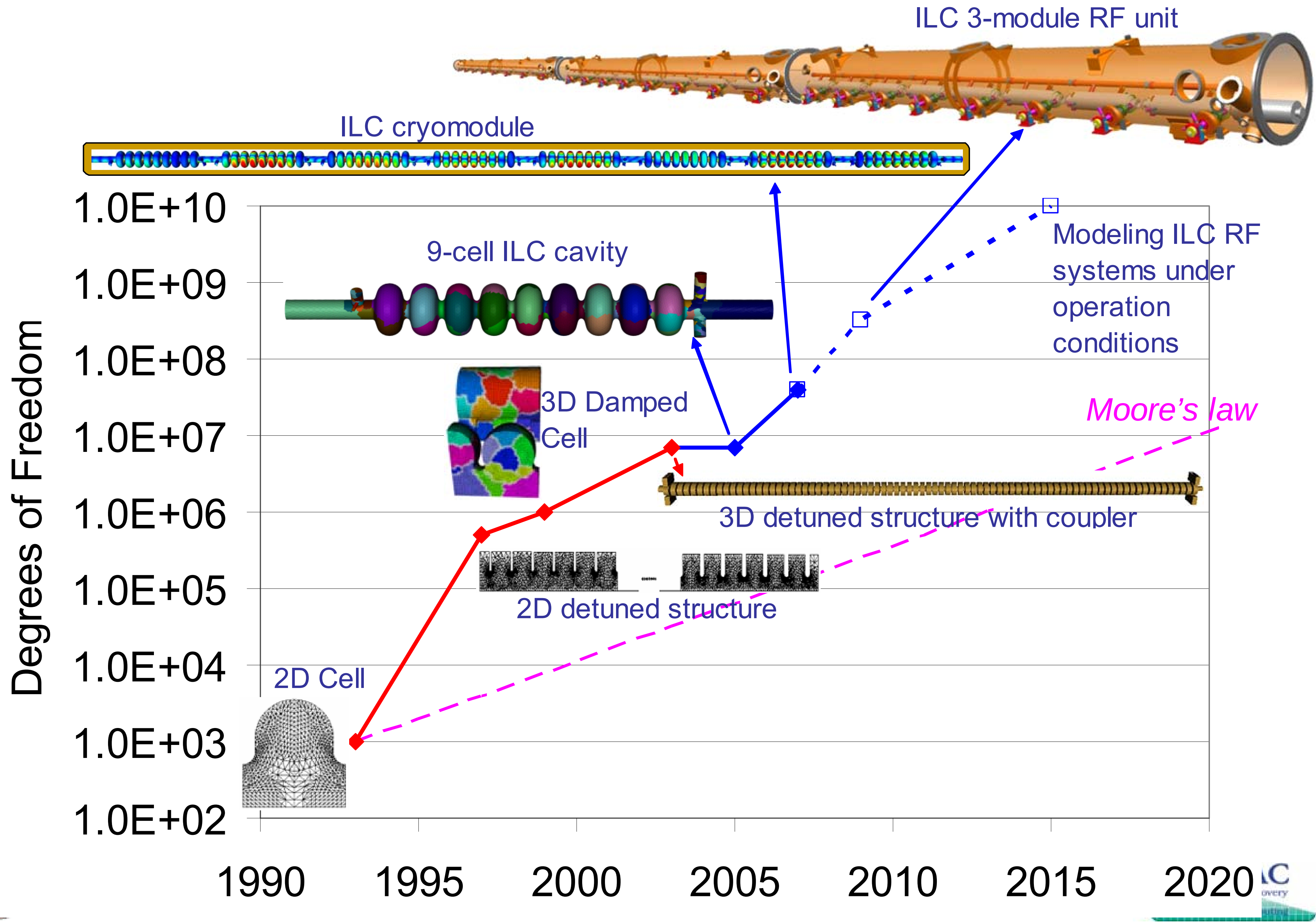
- *Beta 0.81 cavity – end-group heating and multipacting*

Problems and Solver Options



- *Calculating HOM damping in the ILC cavities requires a nonlinear eigensolver when modeling the coupling to external waveguides (FP & HOM couplers) to obtain the complex mode frequencies as a result of power outflow*

Advances In Accelerator Simulation

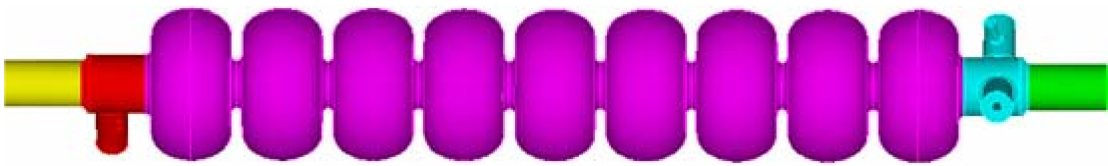


End Group Design – HOM Damping

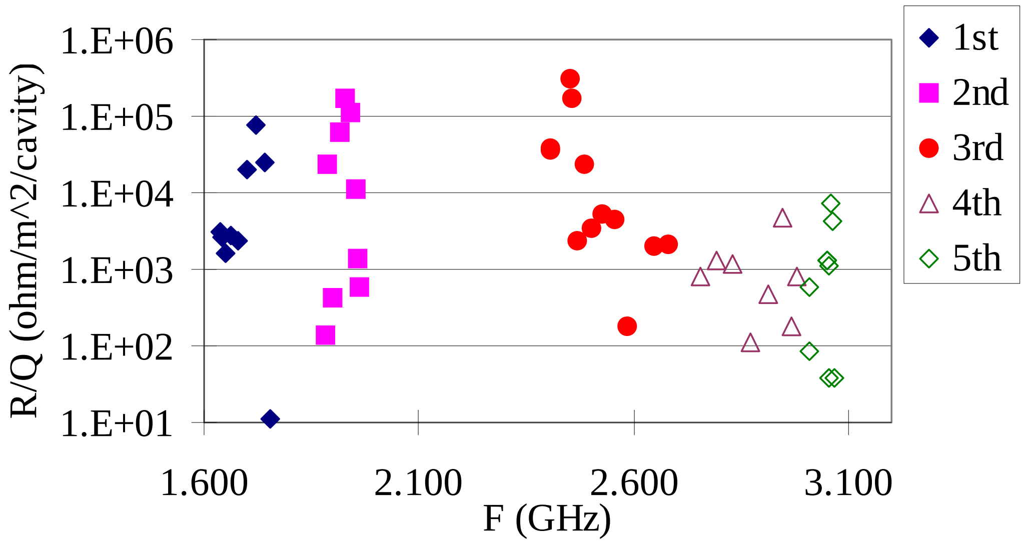
LL Cavity End-group Design

LL Shape

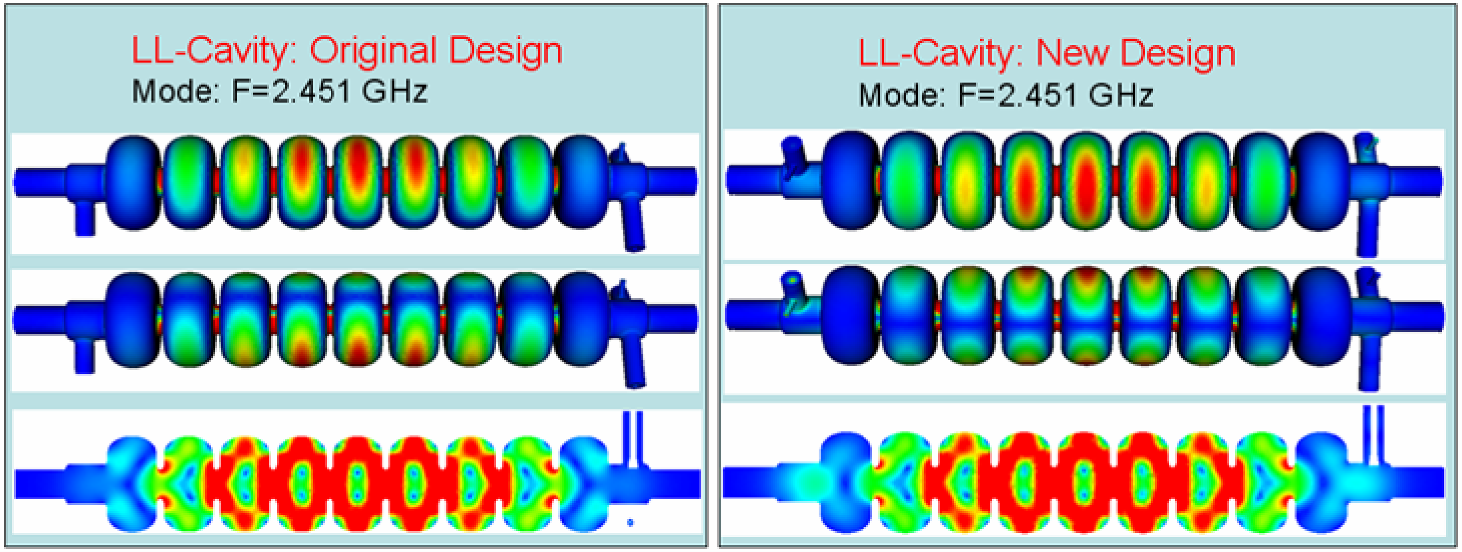
- >15% higher R/Q (1177 ohm/cavity)
- >12% lower Bpeak/Eacc ratio
- 20% lower cryogenic heating



- Most important modes are 0-mode in the 3rd band
- High R/Q in the 1st&2nd bands are up to 1/3 of the 3rd band
- Beam pipe tapers down to 30-mm, 3rd band damped locally by HOM couplers
- Damping criteria: 3rd band mode Qext<10^5 (?)



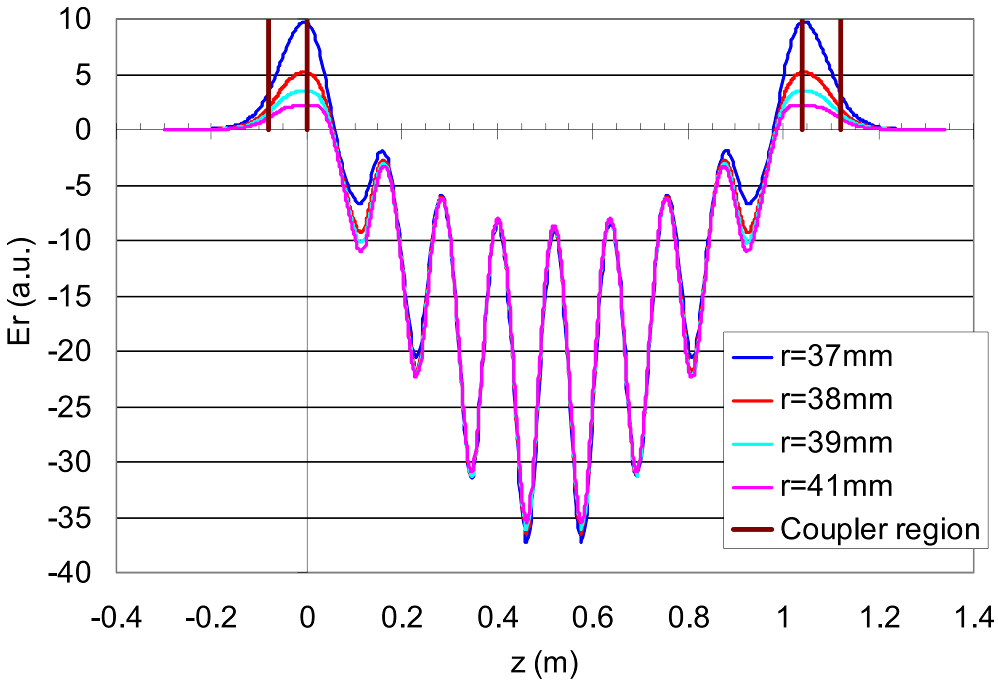
High R/Q 3rd Band Modes



Qext=4.6×10^5

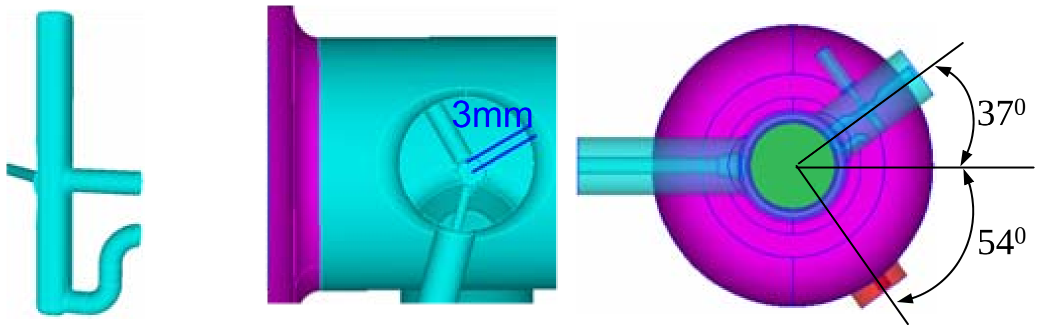
Qext=1.4×10^4

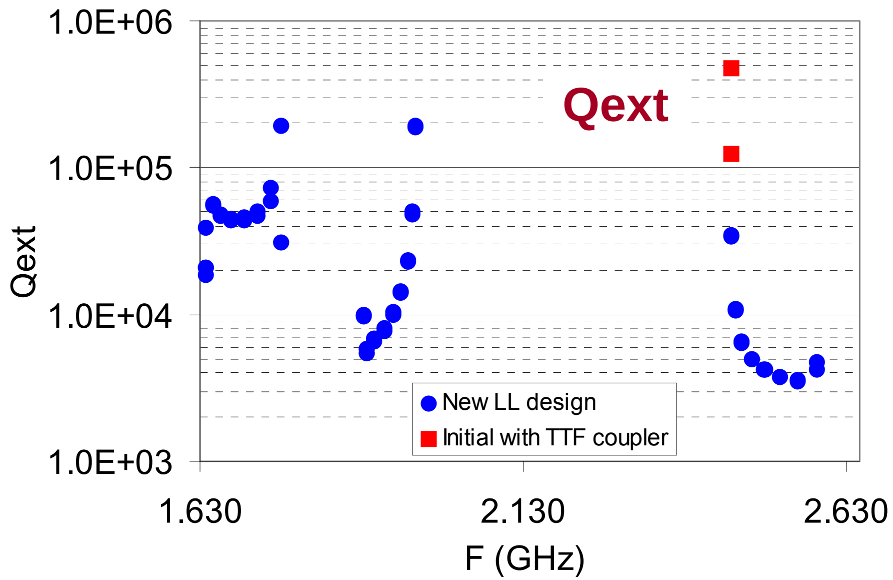
- 41mm end pipe radius
- Low field in the coupler region

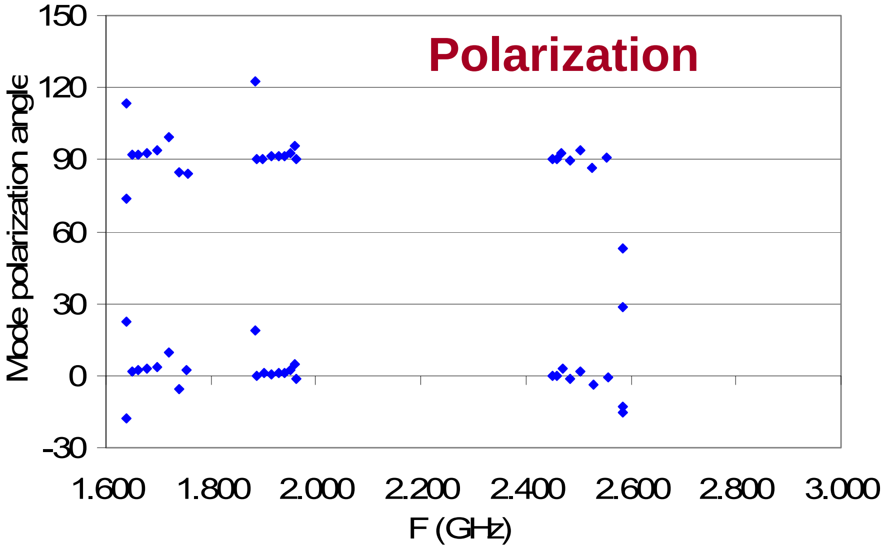


- 38mm pipe radius
- Field significantly improved
- End-group modified to enhance damping

LL Cavity End-group







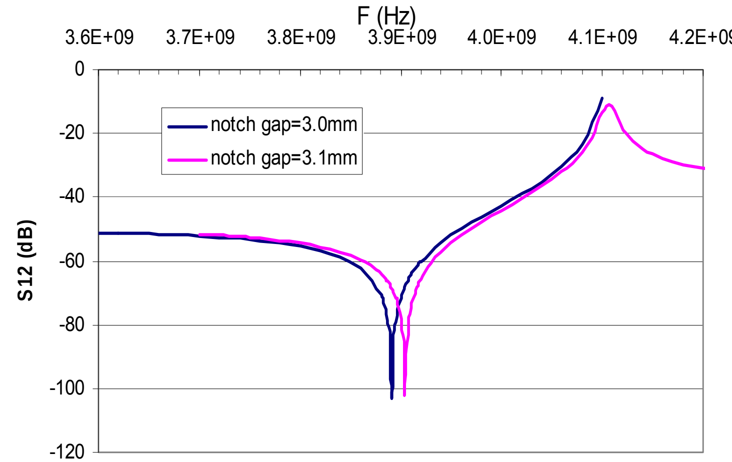
Effective damping achieved by optimizing:

- End-group geometry to increase fields in coupler region
- Loop shape and orientation to enhance coupling
- Optimized azimuthal coupler orientation for x-y mode polarization

Crab Cavity Design for ILC BDS

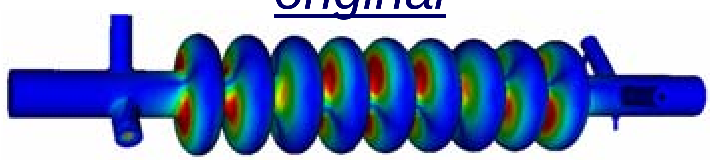
Improved FNAL design

- *better HOM, LOM and SOM damping*
- *reduced HOM notch gap sensitivity (to 0.1 MHz/μm from original 1.6 MHz/μm)*
- *eliminates LOM notch filter*
- *avoids x-y SOM coupling*



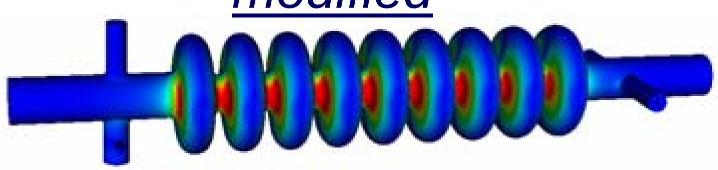
Notch gap sensitivity

original



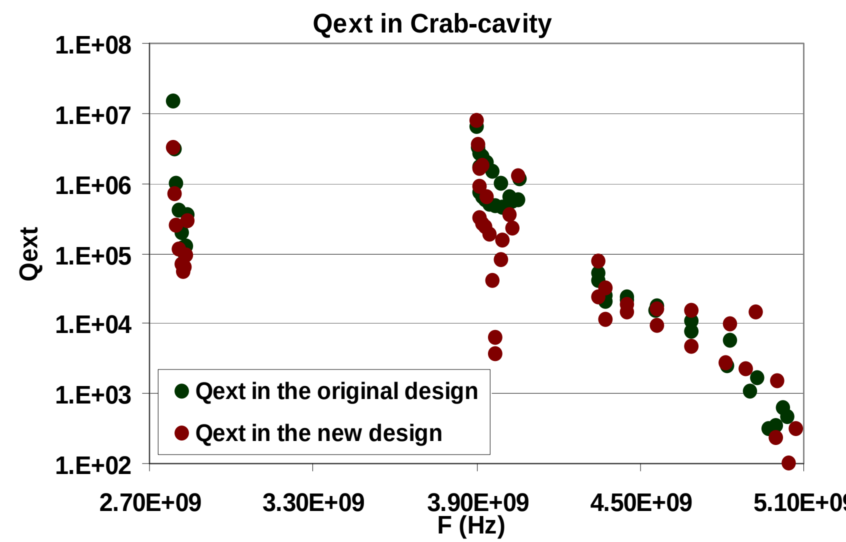
Original Design

modified



New Design

SOM x-y coupling



Omega3P damping calculation

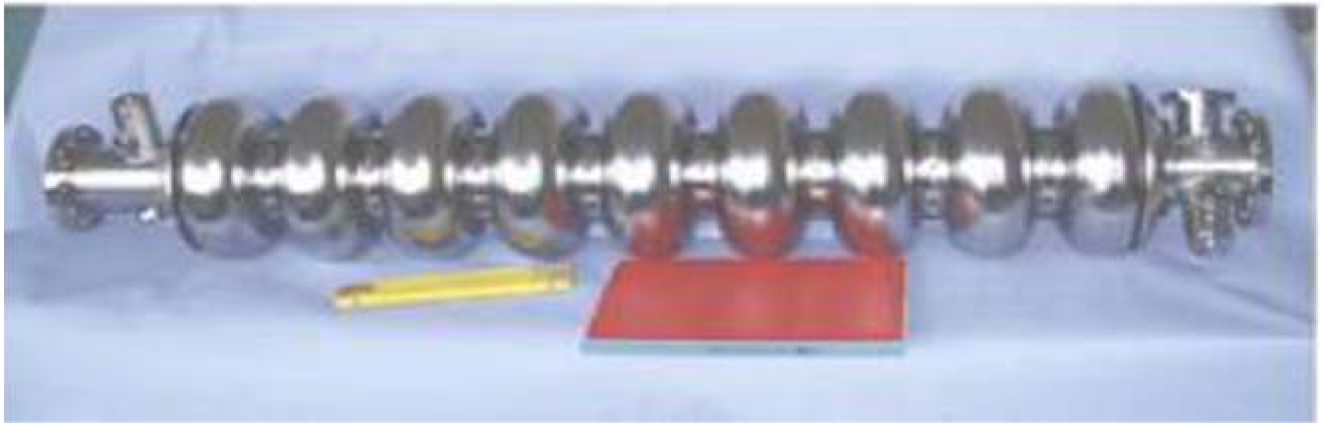
A copper model is being built in UK lab based on this design.

Cavity Imperfection

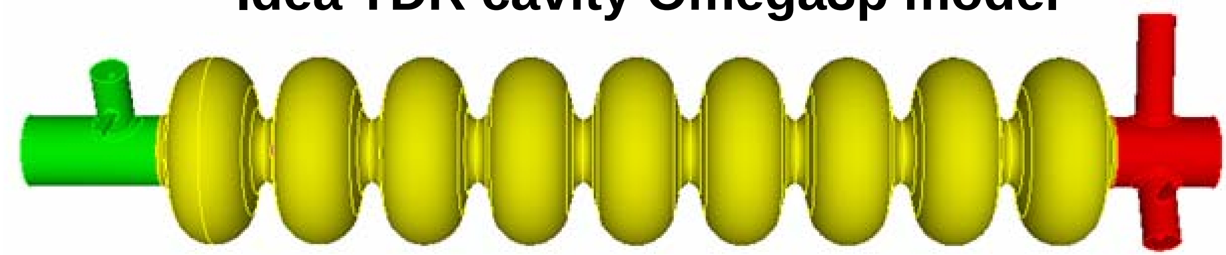
- HOM damping
- X-Y coupling
- Effects on beam emittance

TESLA cavity imperfection study

TDR prototype cavity



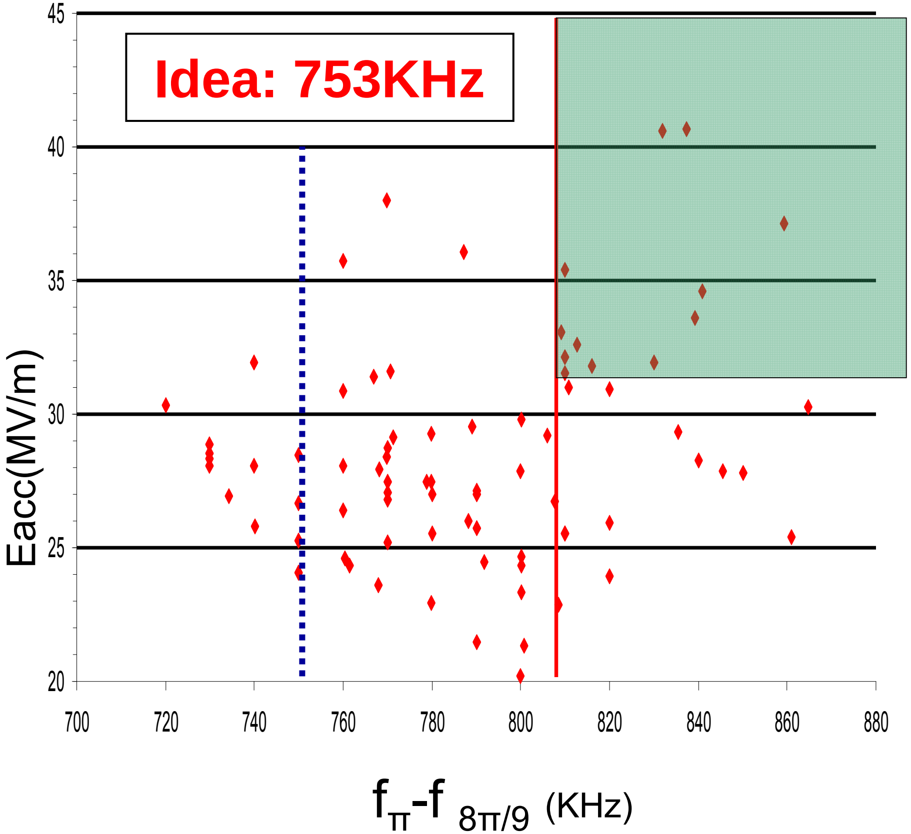
Idea TDR cavity Omega3p model



The actual cell shape of the TESLA cavities differ from the idea due to *fabrication errors*, the addition of *stiffening rings* and the *frequency tuning process*.

TESLA cavity Measurement Data Study

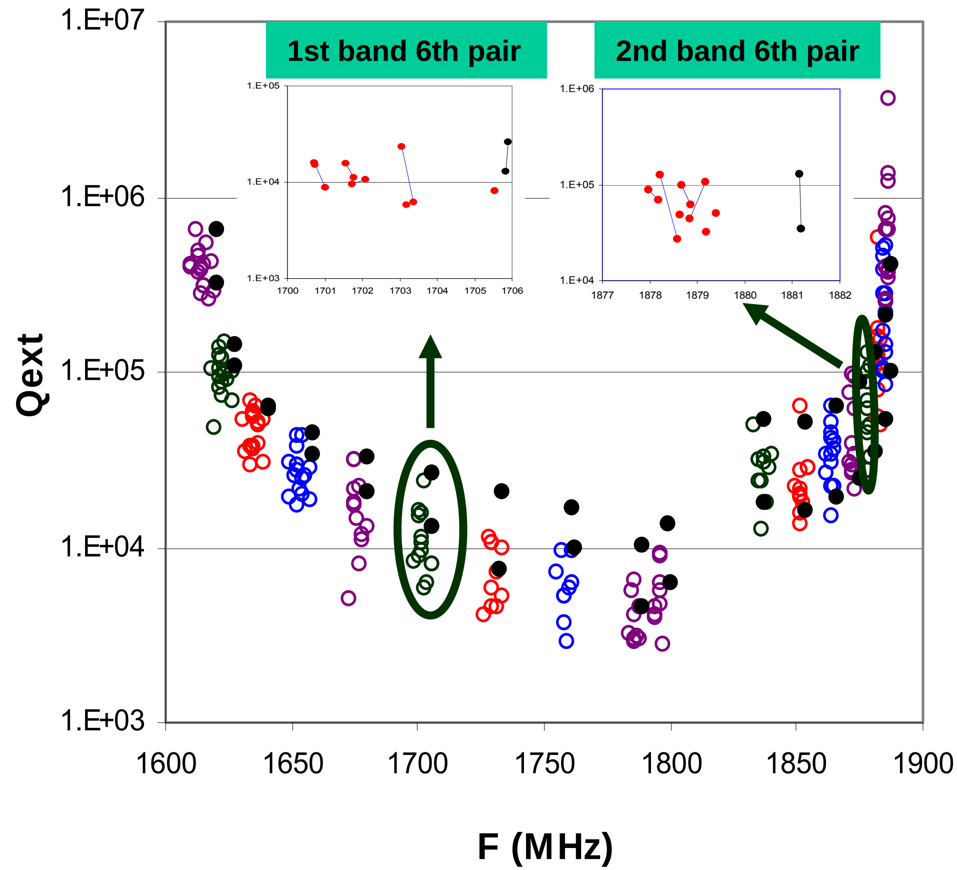
TDR cavity: operating mode from 80 cavities



(Neubauer, Michael L.)

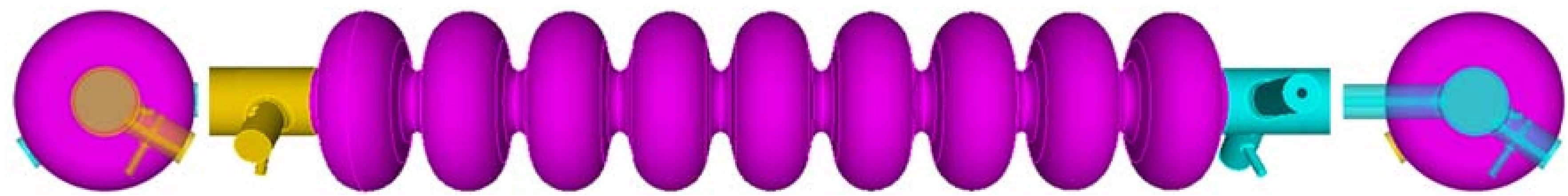
The mode spacing increases.

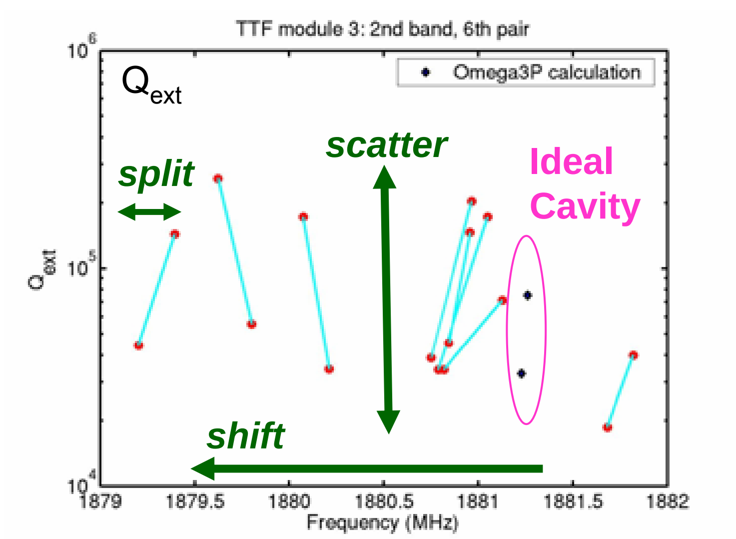
TTF module 5: 1st/2nd dipole band

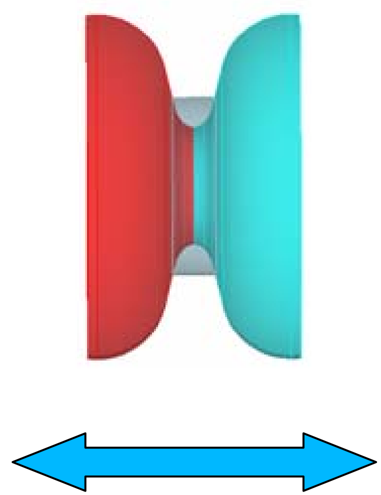


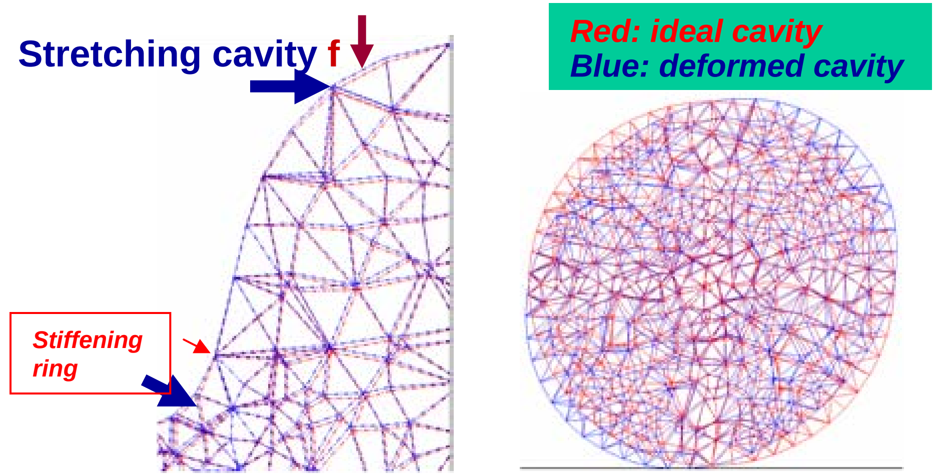
Dipole mode frequencies shift and Qext scatter.

Modeling Imperfection Of ILC TDR Cavity









Welding stiffening ring deforms disk f

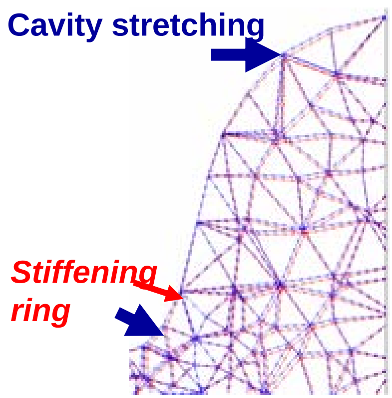
Cell elliptically deformed

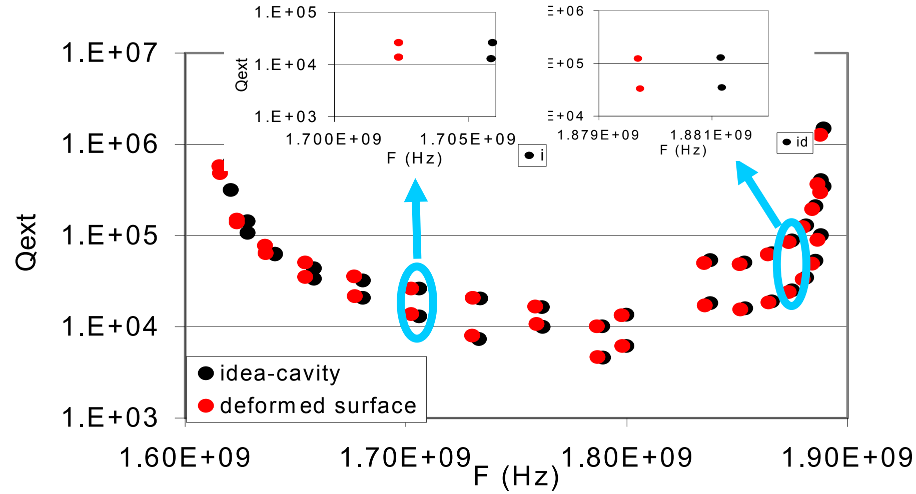
- Determine shape deformation from measured cavity data, inverse and forward methods
- Important to understand effect on Qext and x-y coupling of beam dynamics
- Actual deformation? – geometry measurement data will be very helpful

Cylindrical Symmetric Deformation (*200micro on top/607micro on disk*)

- cause frequency shift

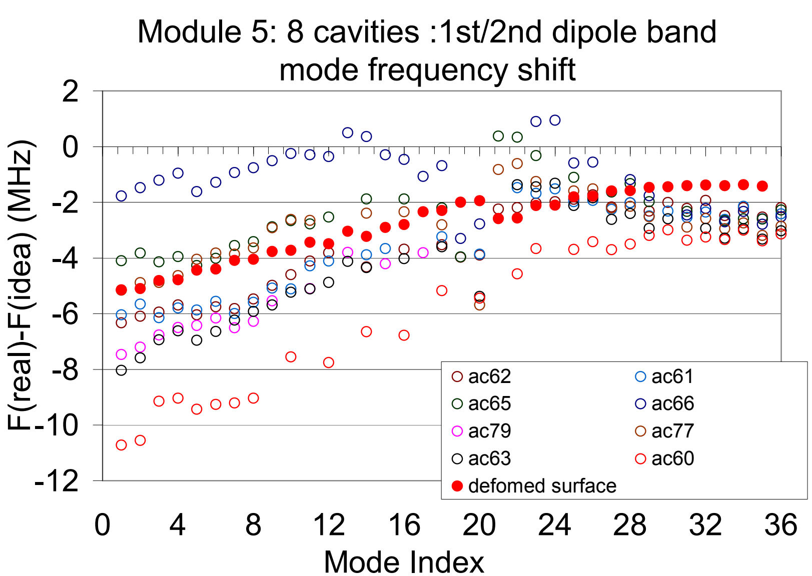
Ideal v.s. deformed

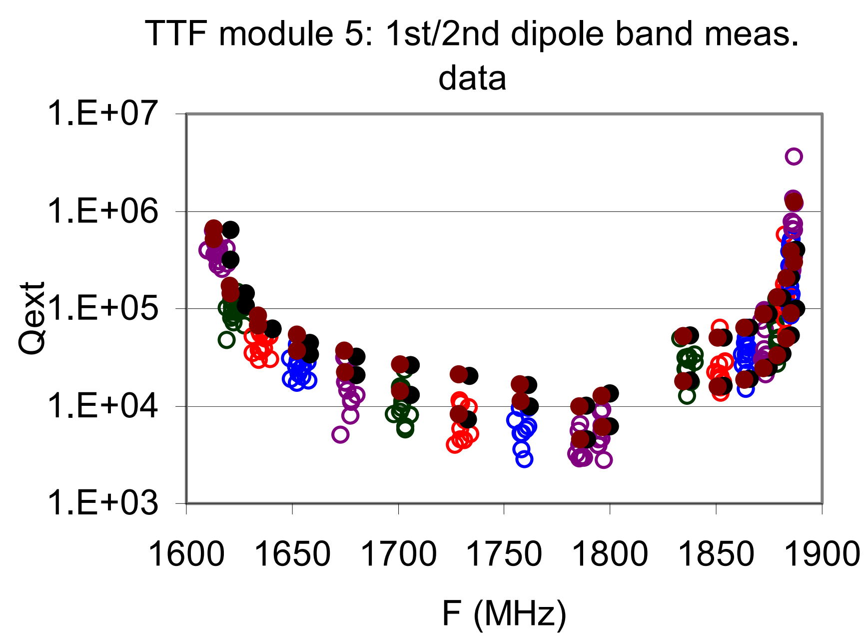




fπ-f8π/9=772KHz within meas. Range. 1st/2nd dipole band mode freq. shift roughly fit measurement data.

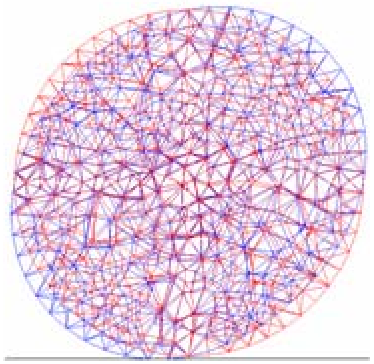
8-cavity measurement v.s. simulation





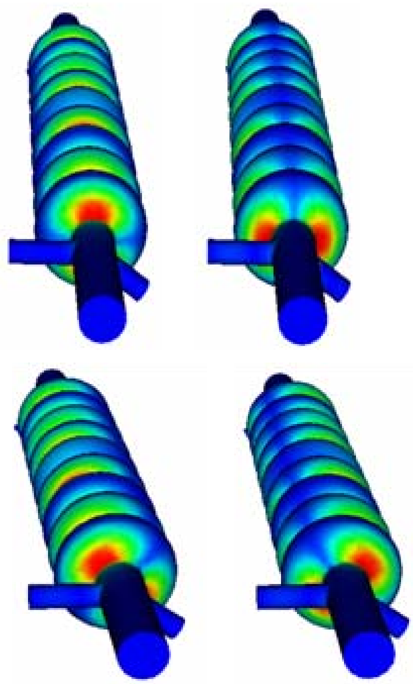
Cell elliptical deformation (dr=250micro)

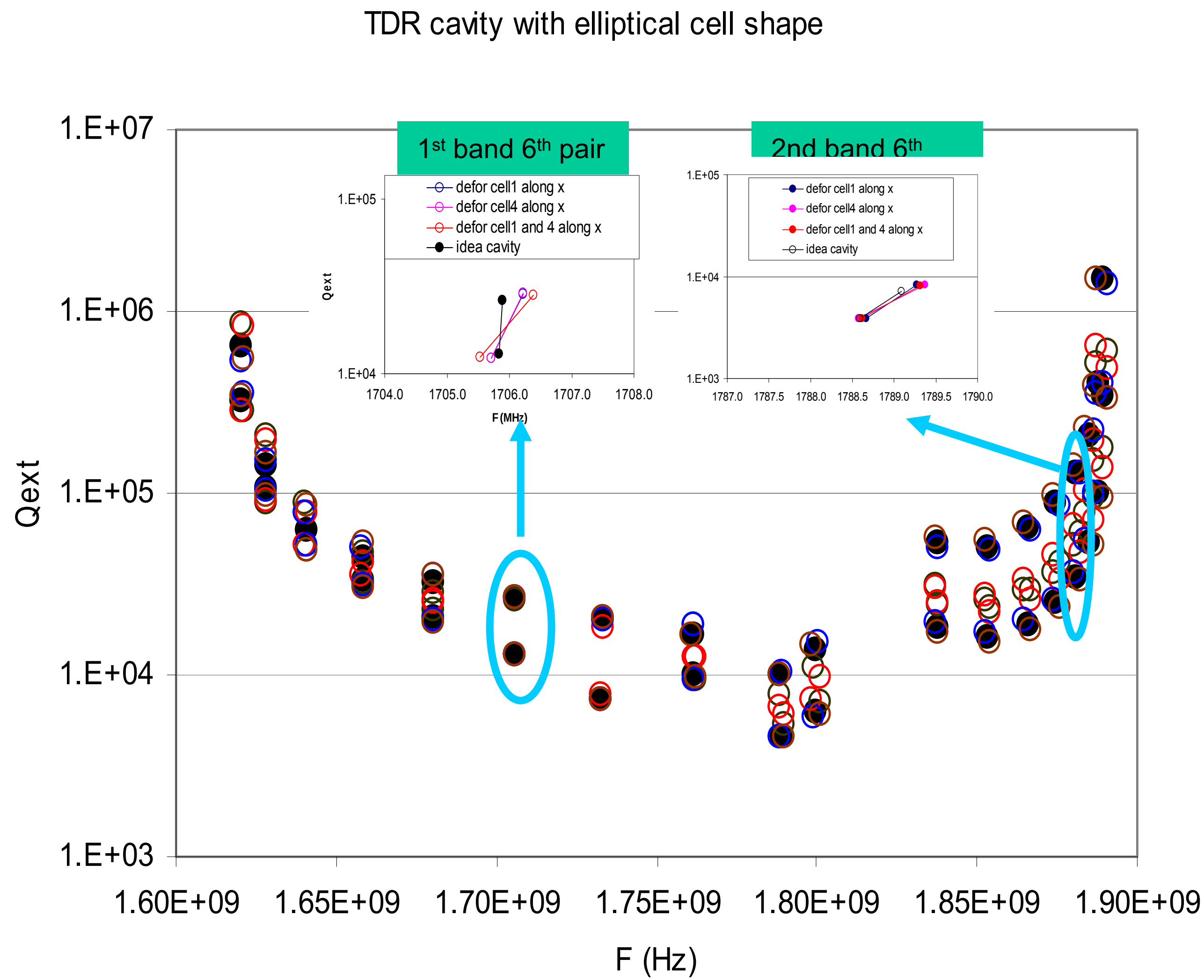
- cause mode Mode x-y coupling& Qext scattering



ideal cavity

elliptically deformed cavity

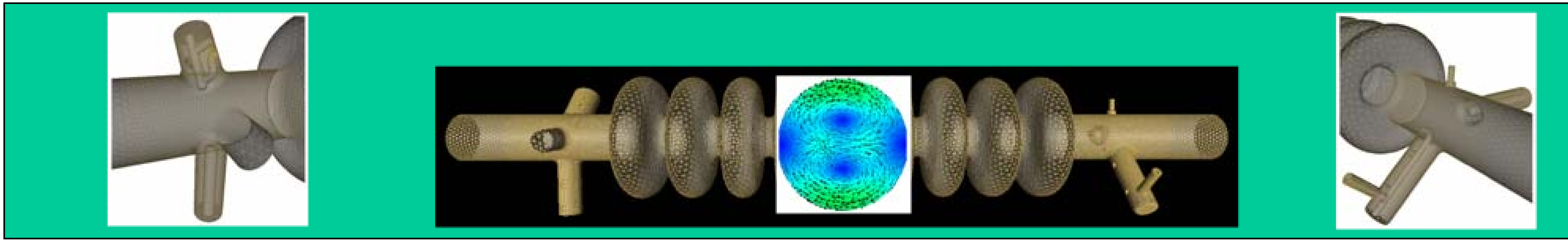




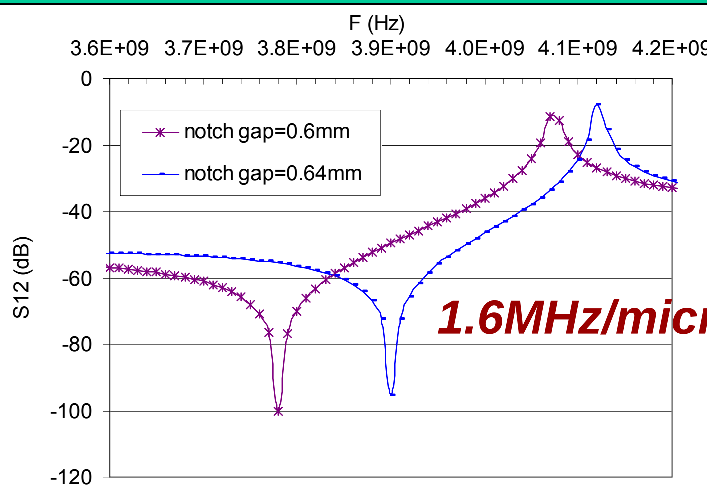
End Group RF Study

- Notch filter
- Peak surface field
- Multipacting

Crab Cavity: HOM Notch Filter Sensitivity

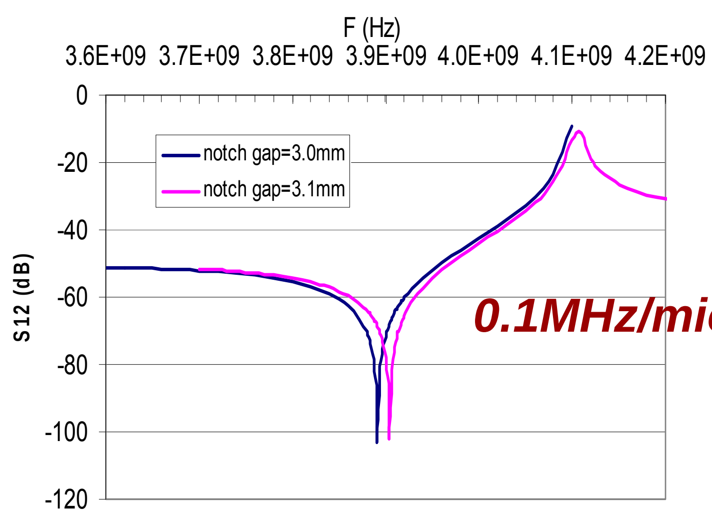


Original Design



1.6MHz/micron

New Design

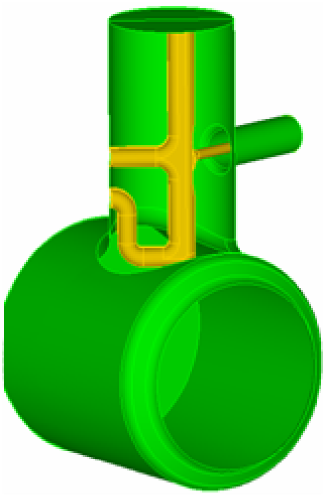


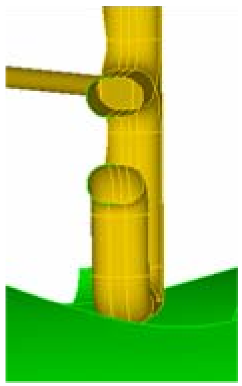
0.1MHz/micron

- Very sensitive tuning was found in the original design
  - 1.6MHz/micron
  - 0.1MHz/micron for TESLA TDR
- Resonator geometry was modified to improve the tunability
  - 0.1MHz/micron achieved

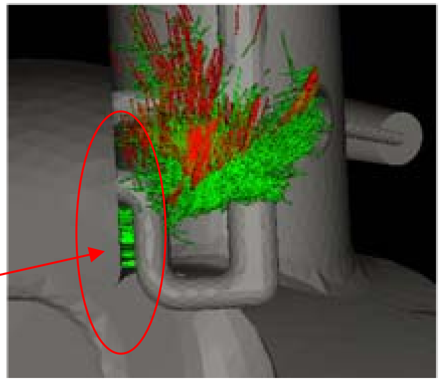
SLAC-PUB-12409

Multipacting in HOM Coupler

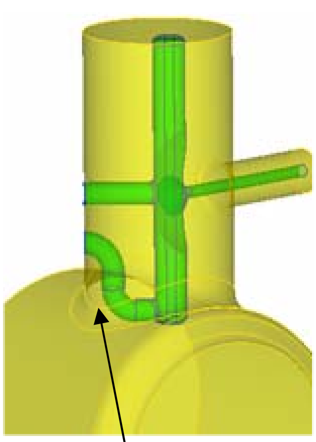




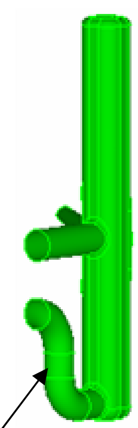
MP trajectories at 15-MV/m.



Initial optimized design: multipacting in the gap between the flat surface and outer cylinder at field levels starting from 10-MV/m and up.



larger gap

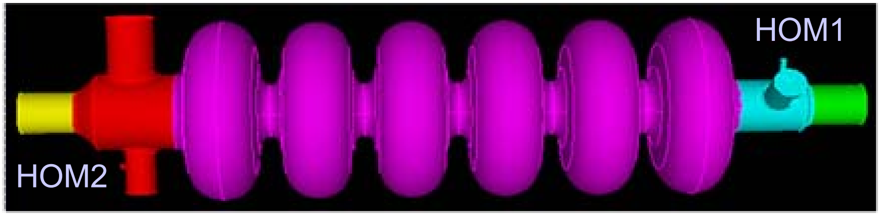


round surfaces

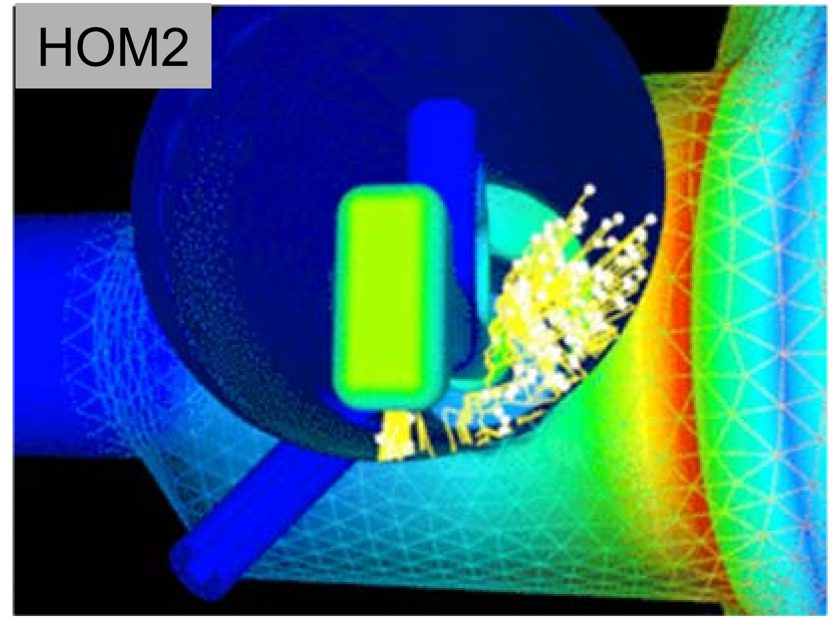
Re-optimized loop: with round surfaces and a larger gap.

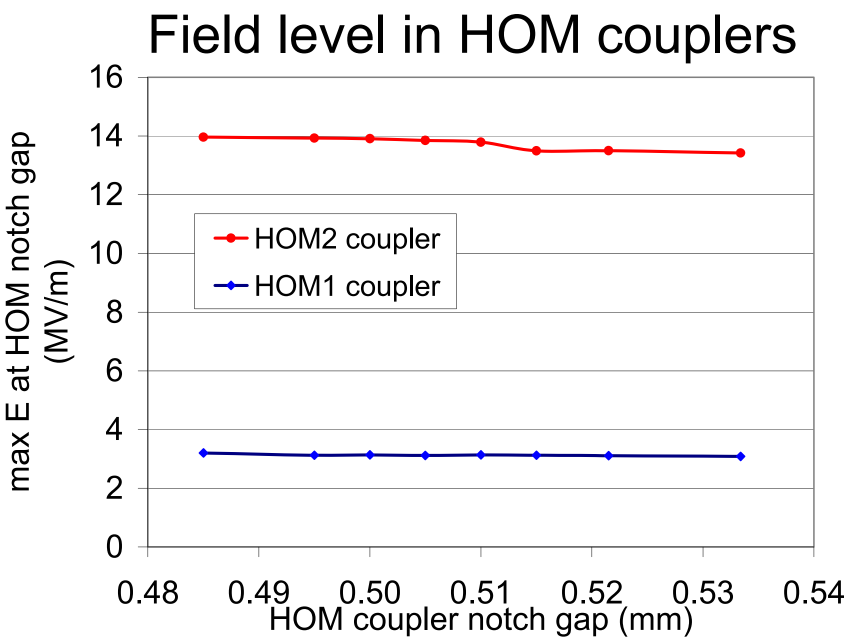
- No multipacting up to 50MV/m.
- Qext for the 3rd band mode is 3.4×10^4

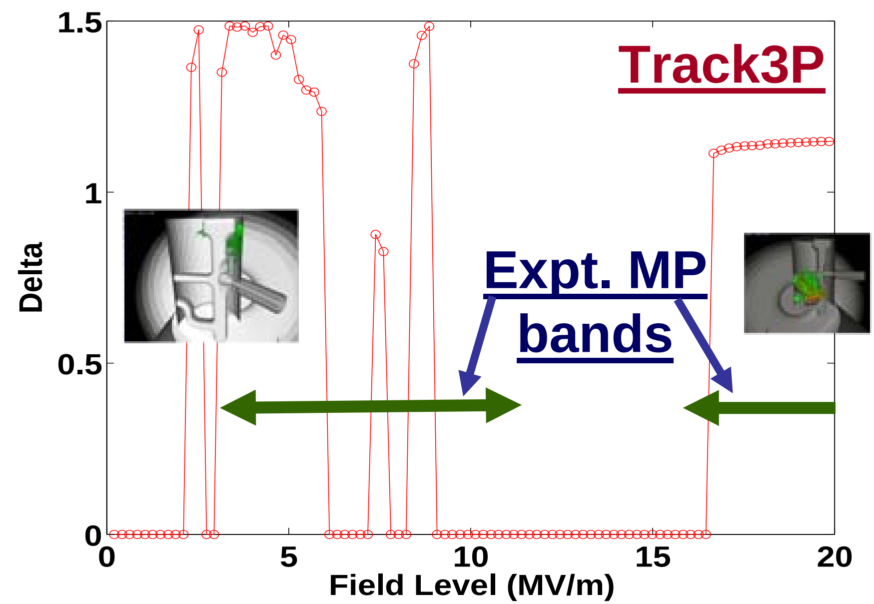
Multipacting in SNS HOM Coupler



- SNS SCRF cavity experienced RF heating at HOM coupler
- 3D MP simulations showed MP barriers closed to measurements
- Similar analysis are carried out for ILC ICHIRO and crab cavity







Multipacting Simulation – Track3P

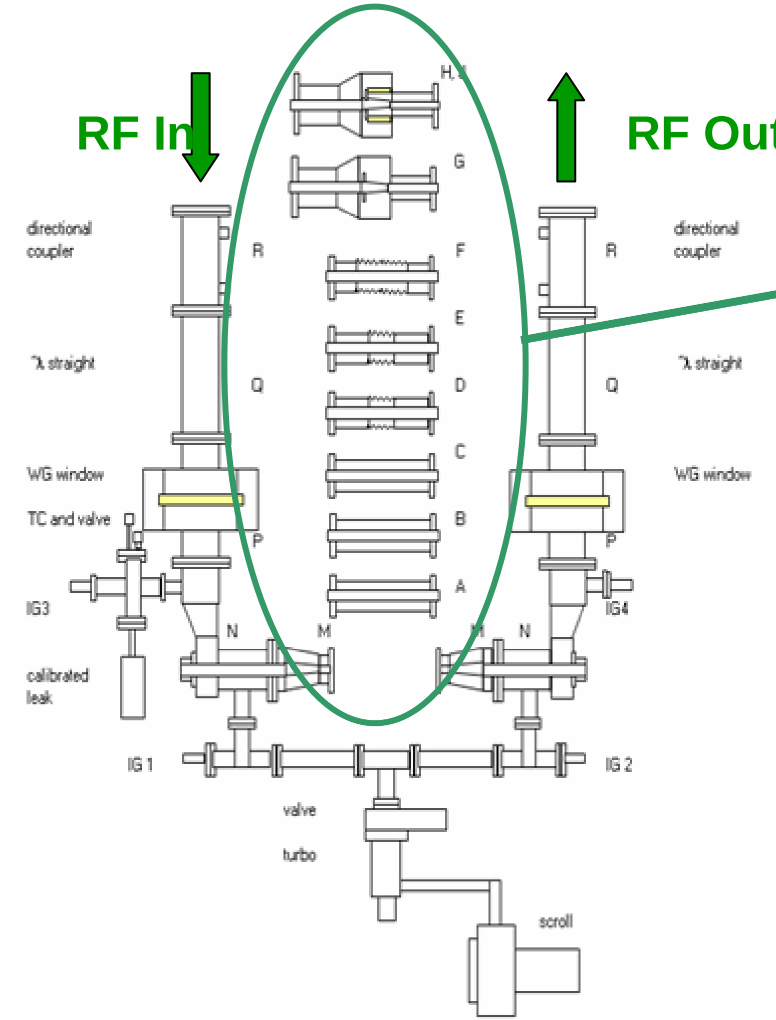
- 3D parallel high-order finite-element particle tracking code for dark current and multipacting simulations (developed under SciDAC)

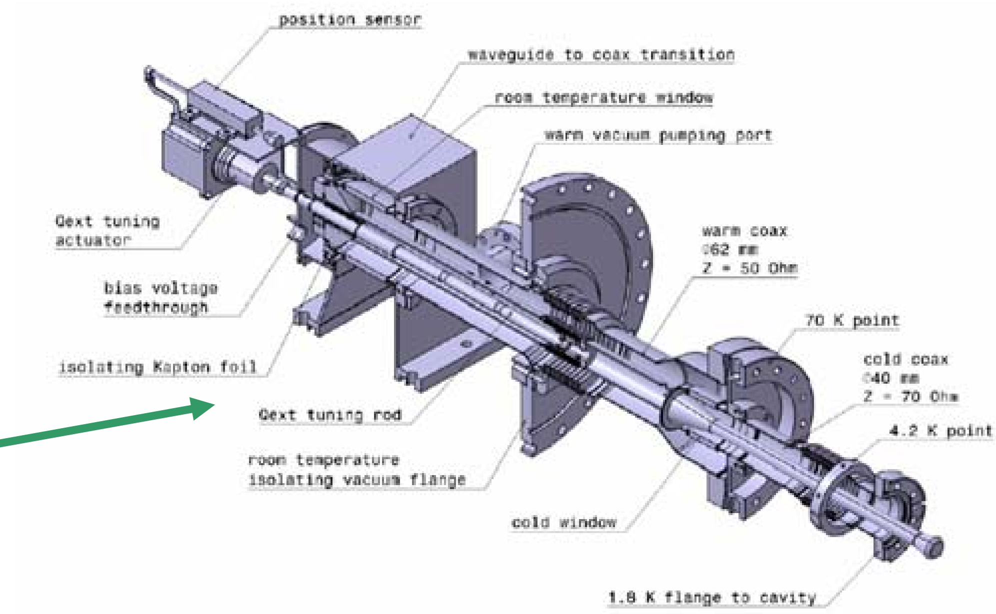
- Track3P
  - traces particles in resonant modes, steady state or transient fields
  - accommodates several emission models: thermal, field and secondary

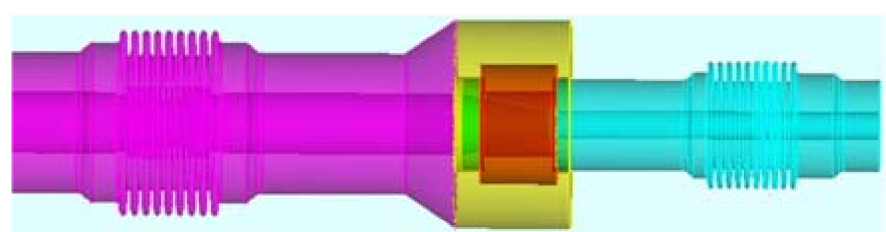
- MP simulation procedure
  - Launch electrons on specified surfaces with different RF phase, energy and emission angle
  - Record impact position, energy and RF phase; generate secondary electrons based on SEY according to impact energy
  - Determine “resonant” trajectories by consecutive impact phase and position
  - Calculate MP order (#RF cycles/impact) and MP type (#impacts /MP cycle)
- Track3P benchmarked extensively
  - Rise time effects on dark current for an X-band 30-cell structure
  - Prediction of MP barriers in the KEK ICHIRO cavity

TTFIII Coupler – Multipacting Analysis

MP simulations are carried out in support of ILC test stand at SLAC (LLNL) to study the cause of the TTFIII coupler's long processing time



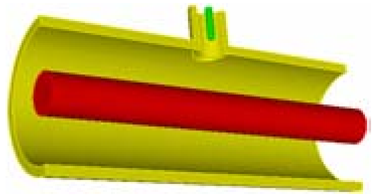




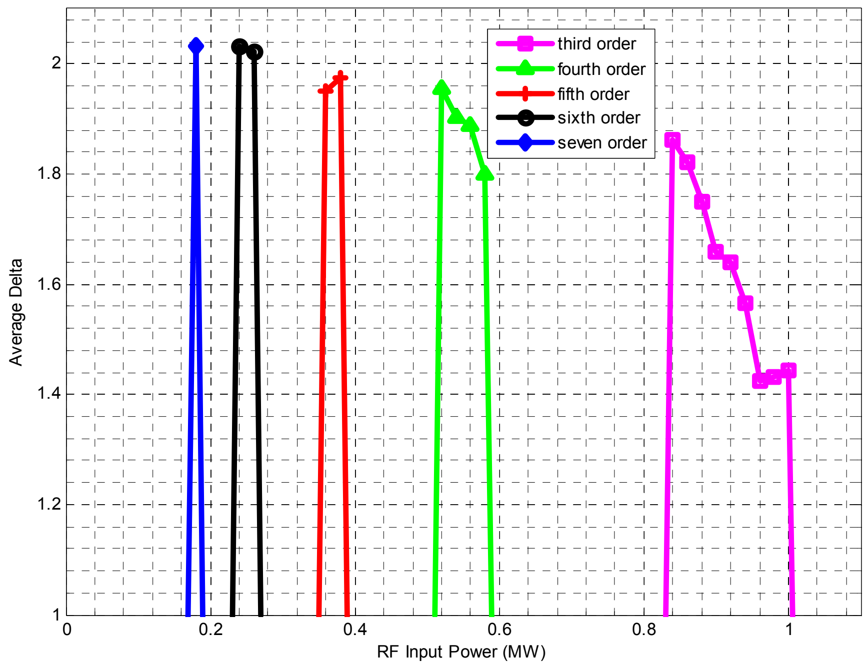
Track3P model

Mulitpacting in Coax of TTFIII Coupler

Cold coax

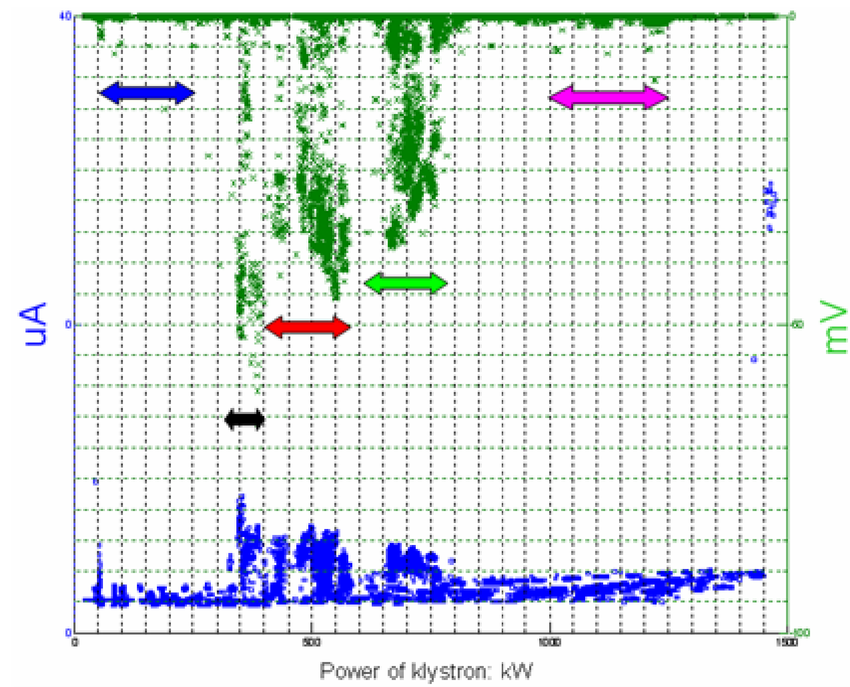


Track3P simulation



(F. Wang, C. Adolphsen, et. al)

After high power processing



Simulated power (kW)	170~190	230~270	350~390	510~590	830~1000
Power in Coupler (kW)	43~170	280~340	340~490	530~660	850~1020
klystron power (kW)	50~200	330~400	400~580	620~780	1000~1200

Parallel Finite Element Particle-In-Cell Code for Simulations of Space-Charge Dominated Beam-Cavity Interactions

Arno Candel

Andreas Kabel, Liequan Lee, Zenghai Li, Cho Ng,
Ernesto Prudencio, Greg Schussman, Ravi Uplenchwar and Kwok Ko

ACD, Stanford Linear Accelerator Center

Cecile Limborg

LCLS, Stanford Linear Accelerator Center

PAC07, Albuquerque, Jun 25-29, 2007

* Work supported by U.S. DOE ASCR & HEP Divisions under contract DE-AC02-76SF00515

SLAC

SciDAC
Scientific Discovery through Advanced Computing

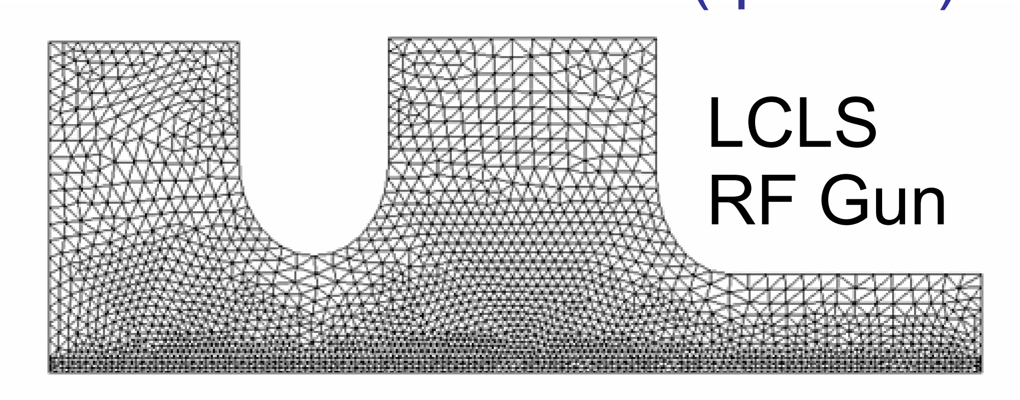
Parallel Finite Element Time-Domain

Maxwell's Wave Equation in Time-Domain:

$$\frac{1}{c^2}\frac{\partial^2 \mathbf{E}}{\partial t^2} + \nabla \times \nabla \times \mathbf{E} = -\mu \frac{\partial \mathbf{J}}{\partial t}$$

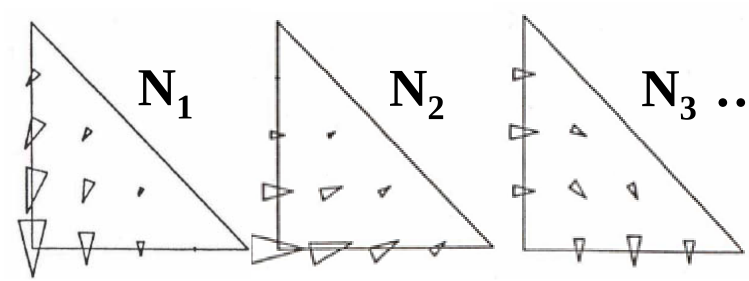
- ***Spatial discretization*** -

Conformal, unstructured grid with curved surfaces (q=1…2)



Higher-order (p=1…6) Whitney basis functions:

$$\mathbf{E}(\mathbf{x}, t) = \sum_i e_i(t) \cdot \mathbf{N_i}(\mathbf{x})$$



- ***Time integration*** - Unconditionally stable implicit Newmark scheme (to do: solve Ax=b)
- ***Parallelization*** - MPI on distributed memory platforms

SciDAC Codes – Pic3P/Pic2P

- ***Pic3P*** – **Parallel 3D FE PIC Code**
- ***Pic2P*** – **Parallel 2.5D FE PIC Code**

1) Compute particle current $\mathbf{J} = \rho\mathbf{v}$

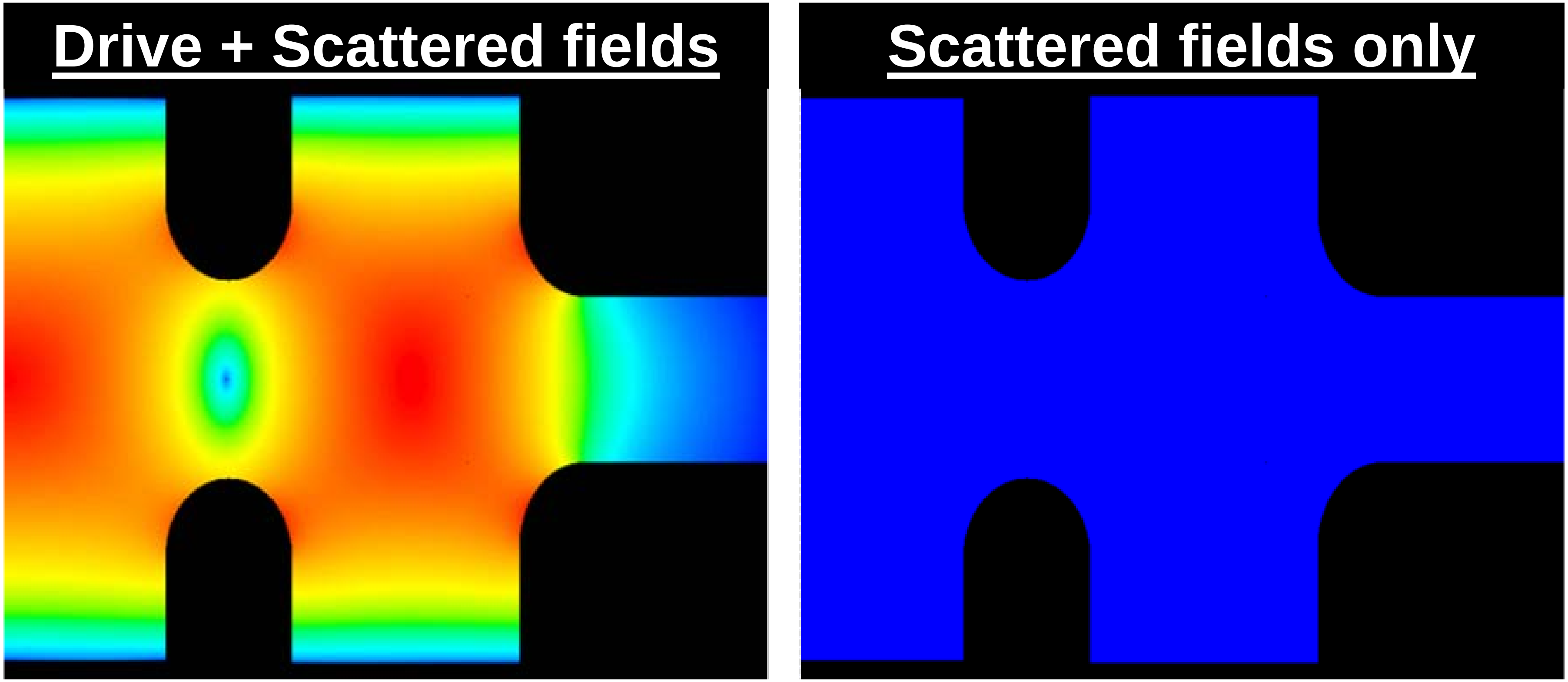
2) Calculate EM fields from Maxwell's Eqs.

3) Push particles $\frac{d\mathbf{p}}{dt} = q(\mathbf{E} + \mathbf{v} \wedge \mathbf{B})$

} *Higher-order particle-field coupling, no interpolation required*

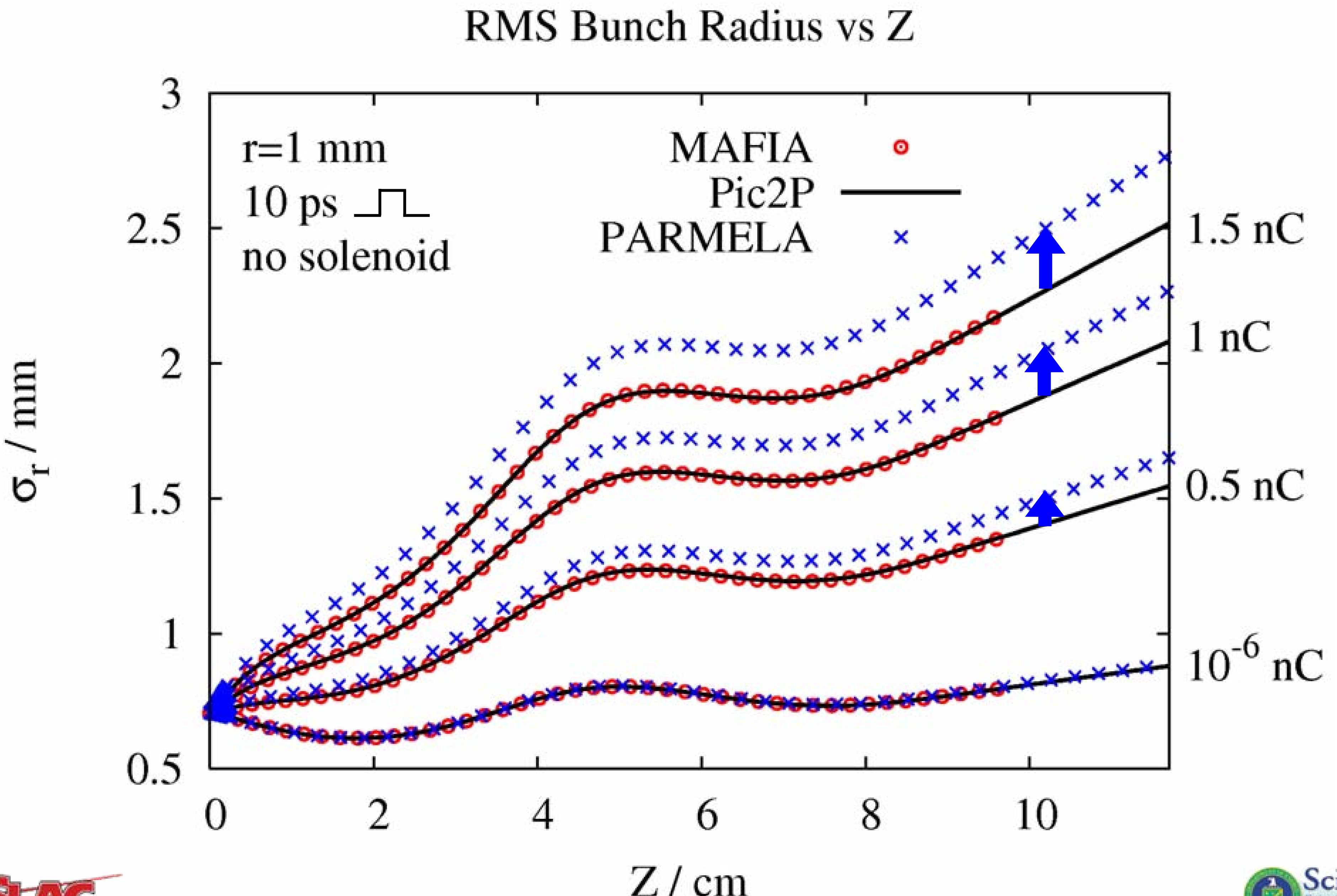
1st successful implementation of self-consistent, charge-conserving PIC code with conformal Whitney elements on unstructured FE grid

Pic2P Simulation of LCLS RF Gun

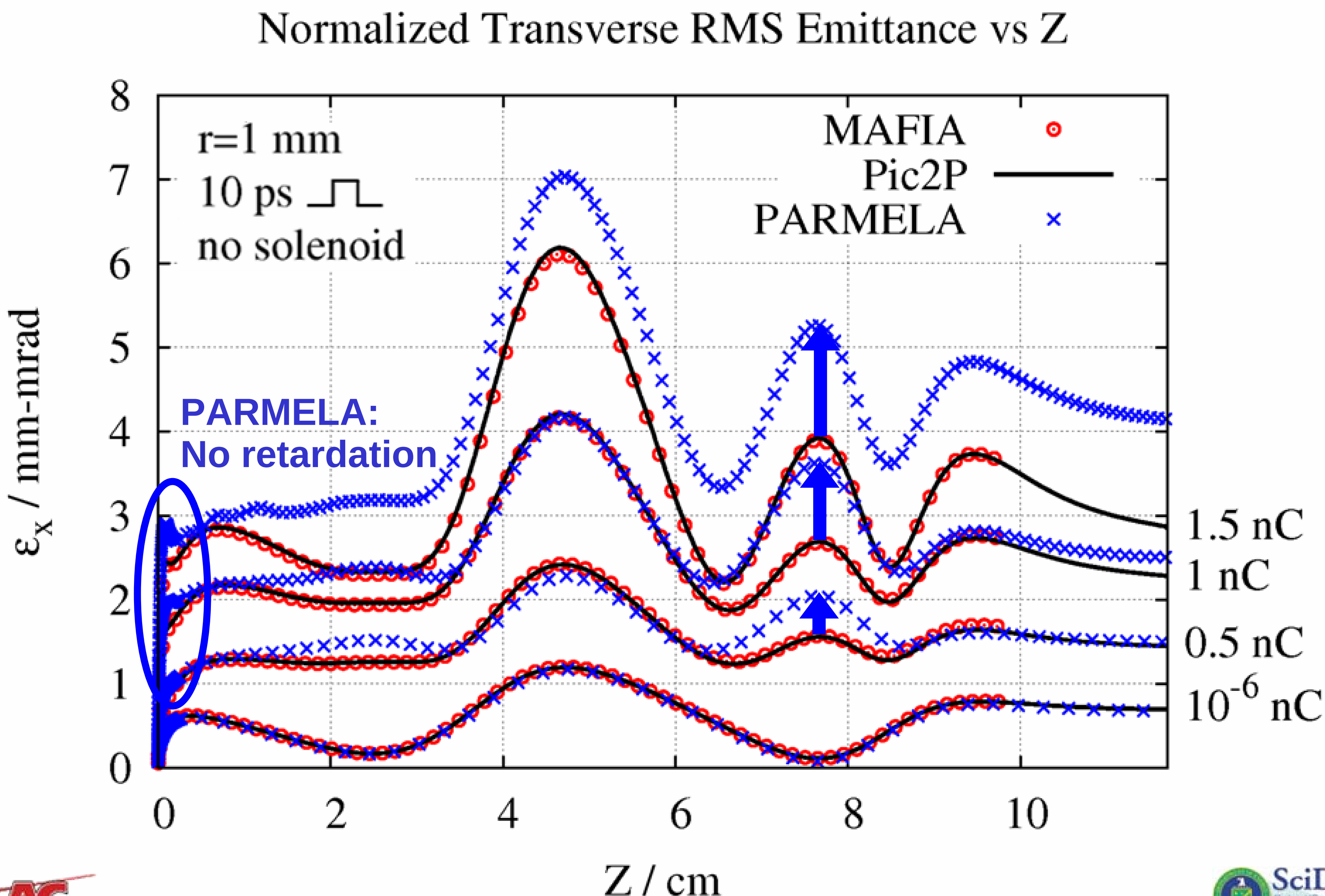


- ***Pic2P*** *– Code from 1st principles, accurately includes effects of* **space charge, retardation, and wakefields**
- *Uses conformal grid, higher-order particle-field coupling and parallel computing for large, fast and accurate simulations*

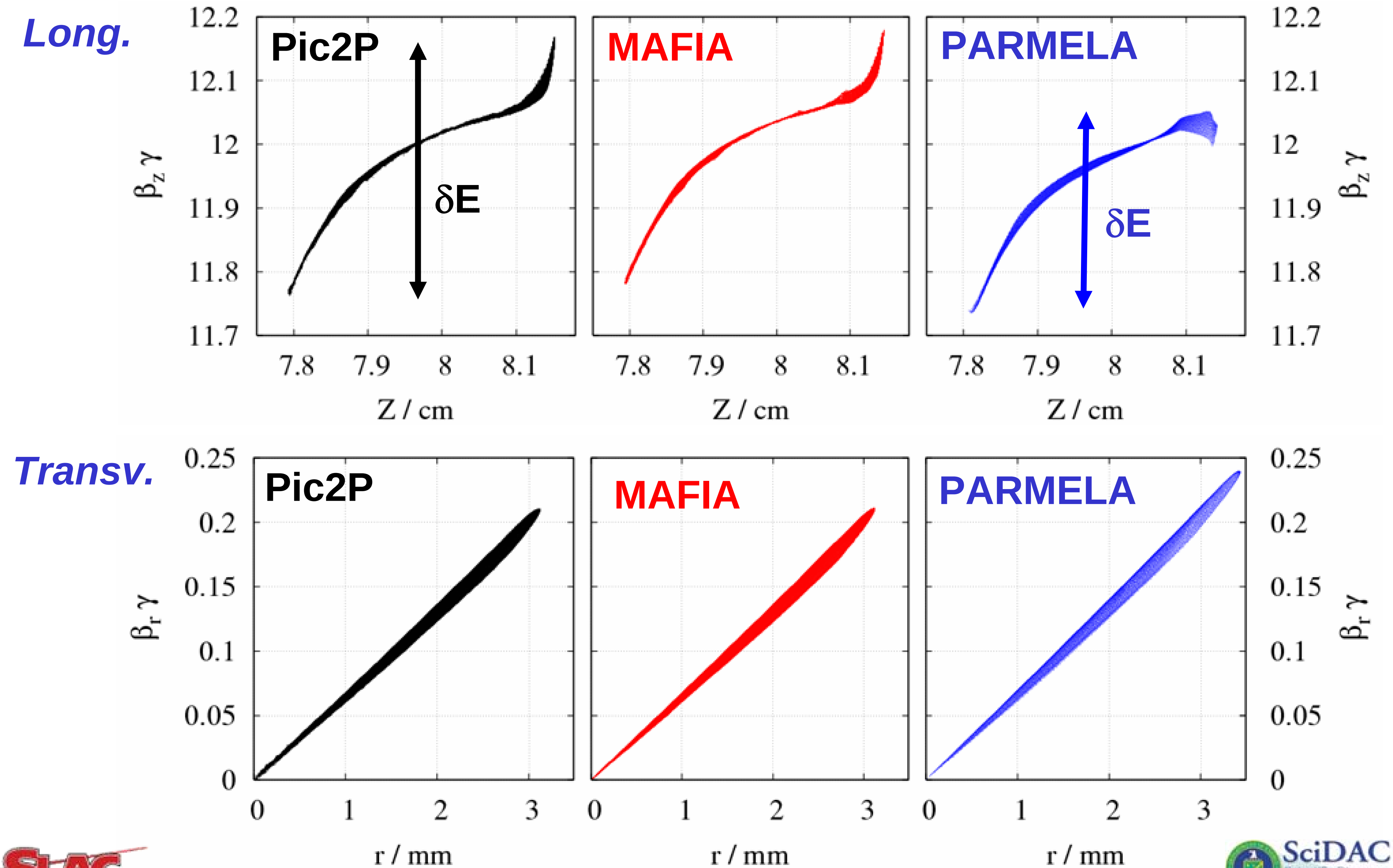
LCLS RF Gun Bunch Radius



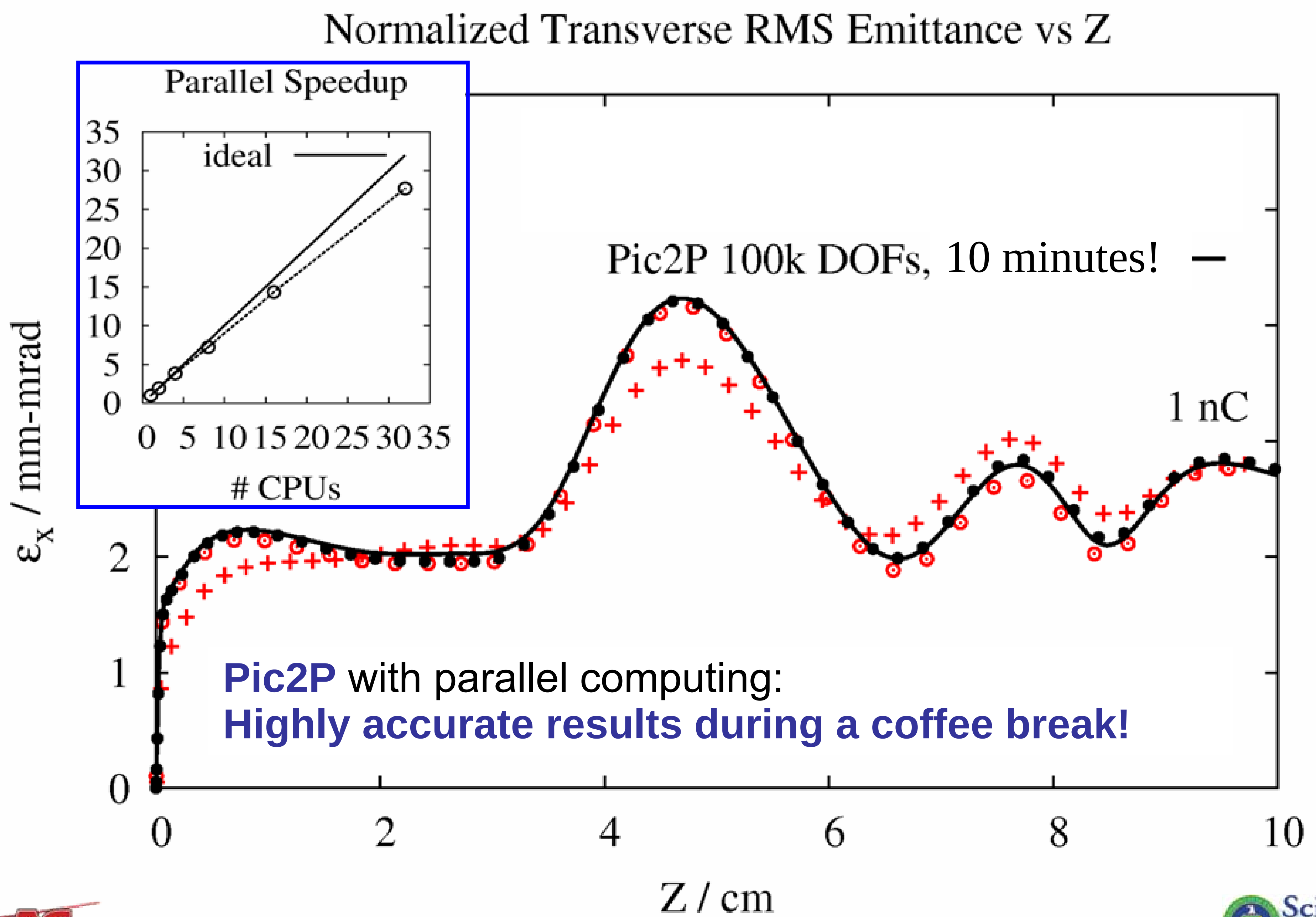
LCLS RF Gun Emittance



LCLS RF Gun Phasespace (1.5 nC)

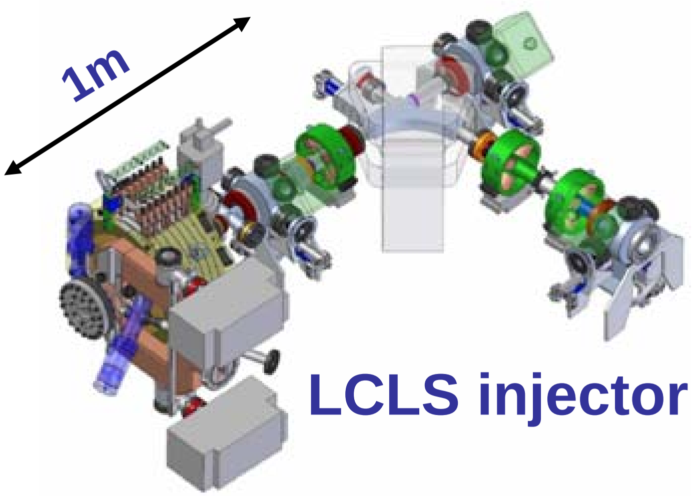


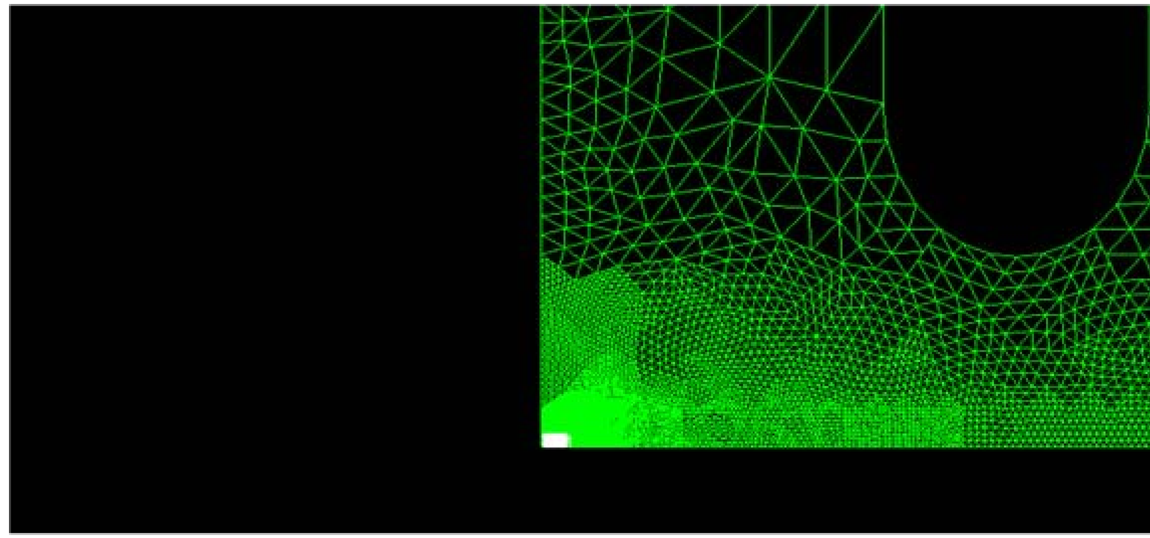
Pic2P - Performance



LCLS Injector Modeling

- ***PIC in long structures*** – Klystrons, injectors, … Active research

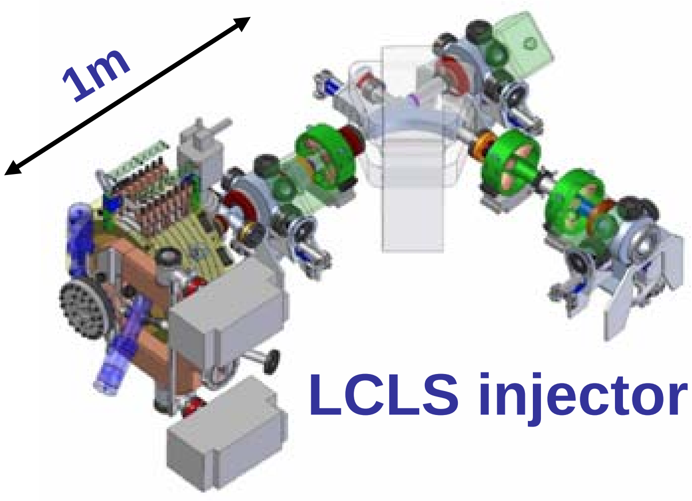


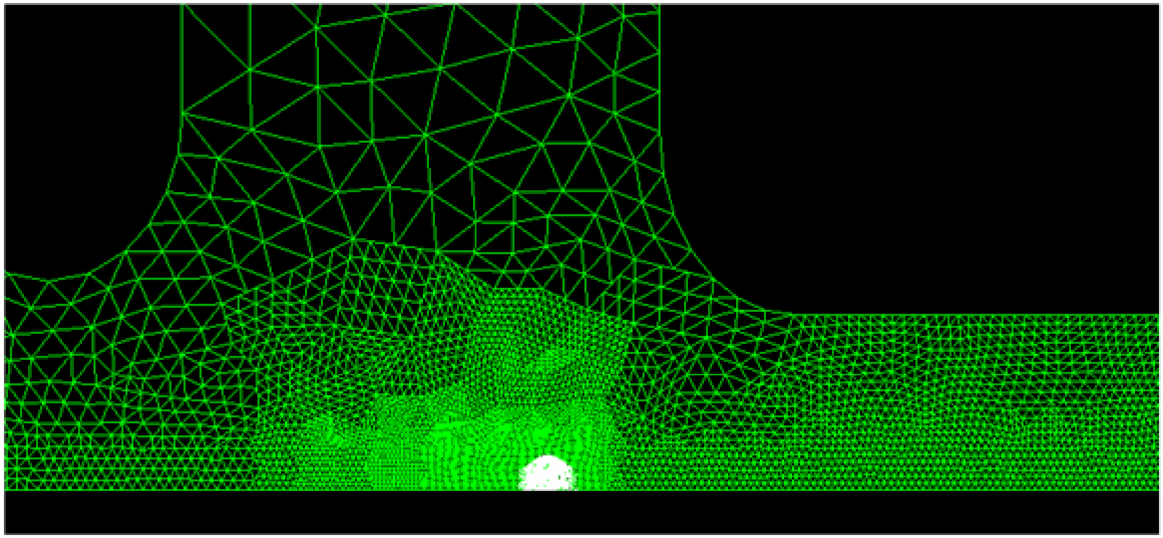


- ***Adaptive refinement*** – Efficient simulations of long structures

LCLS Injector Modeling

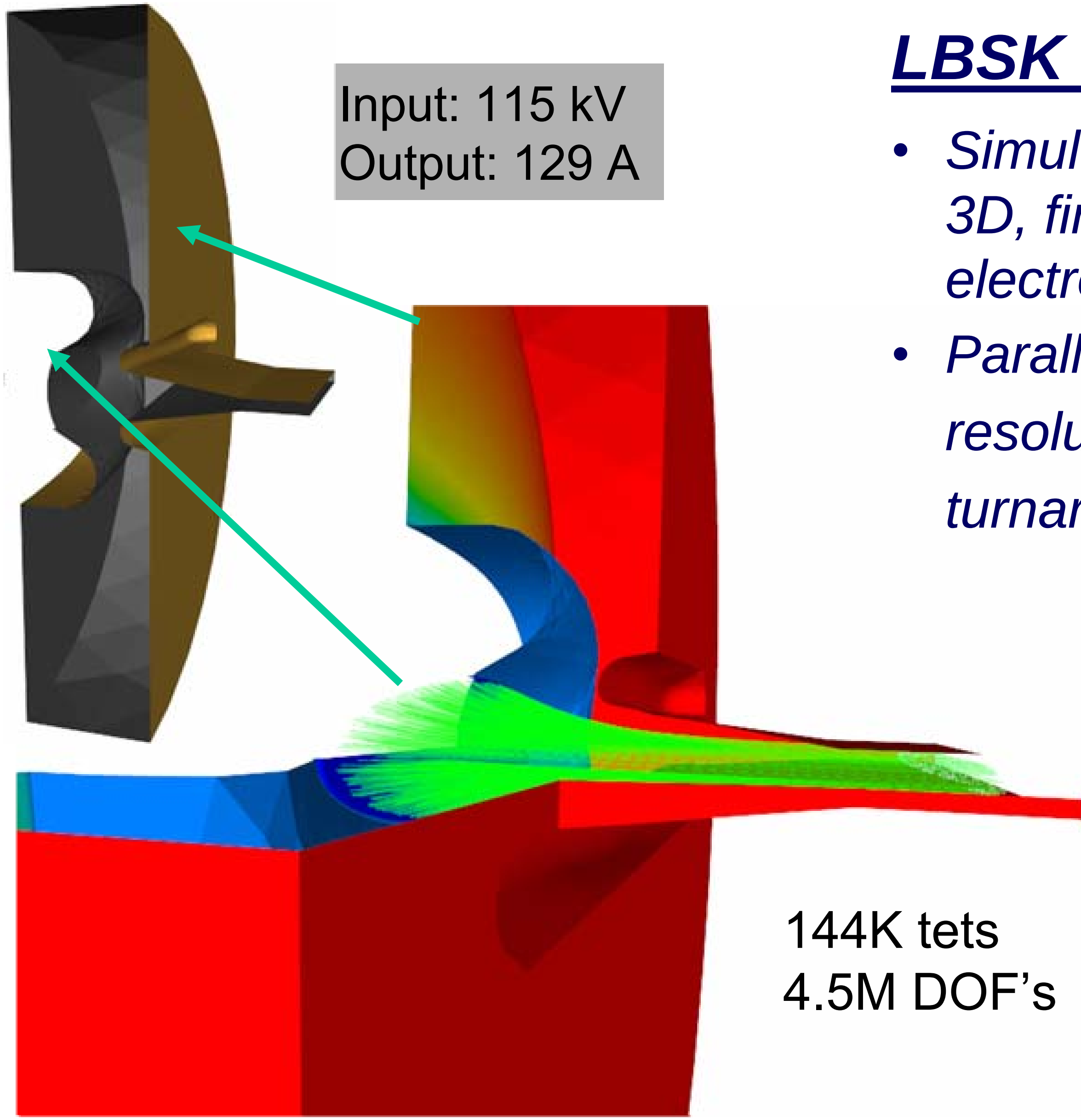
- ***PIC in long structures*** – Klystrons, injectors, … Active research





- ***Adaptive refinement*** – Efficient simulations of long structures

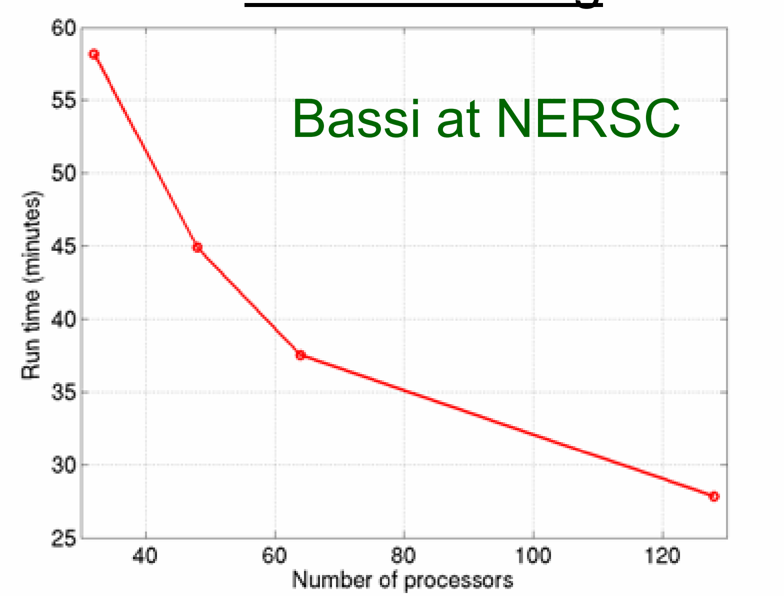
L-Band Sheet Beam Klystron



***LBSK gun* –**

- *Simulated using GUN3P, a parallel, 3D, finite-element (up to 4th order) electron trajectory code*
- *Parallel computation allows high resolution simulation with fast turnaround time*

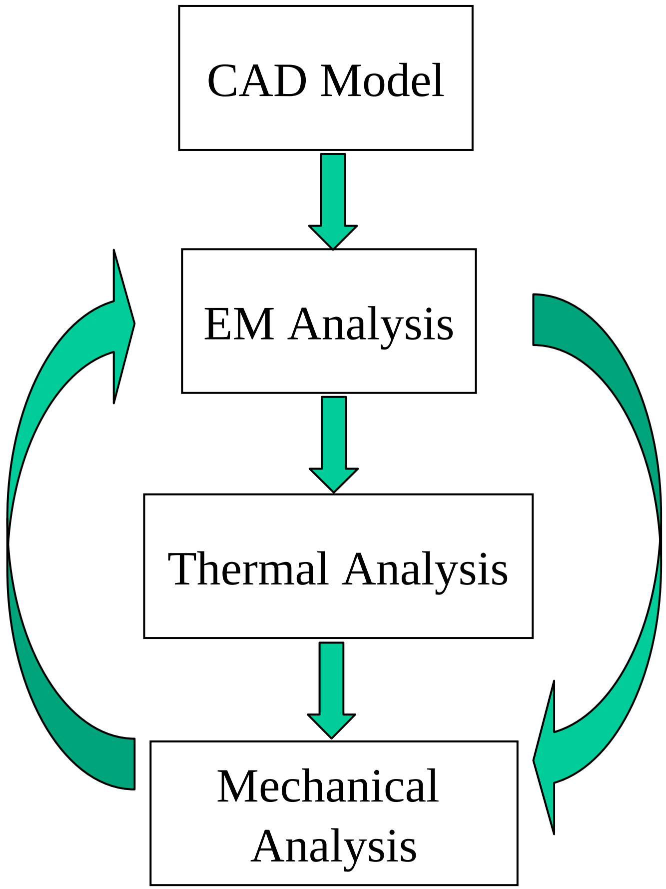
Parallel scaling



Multi-physics Analysis for Accelerator Components

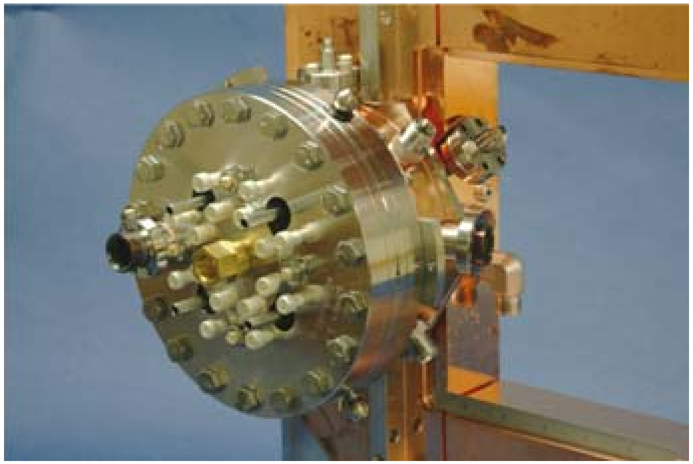
- Virtual prototyping through computing
  - RF design
  - RF heating
  - Thermal radiation
  - Lorentz force detuning
  - Mechanical stress
  - Optimization
- Large-scale parallel computing enables:
  - Large system optimization
  - Accurate and reliable multi-physics analysis
  - Fast turn around time
- TEM3P – integrated parallel multi-physics tools

TEM3P: Multi-Physics Analysis

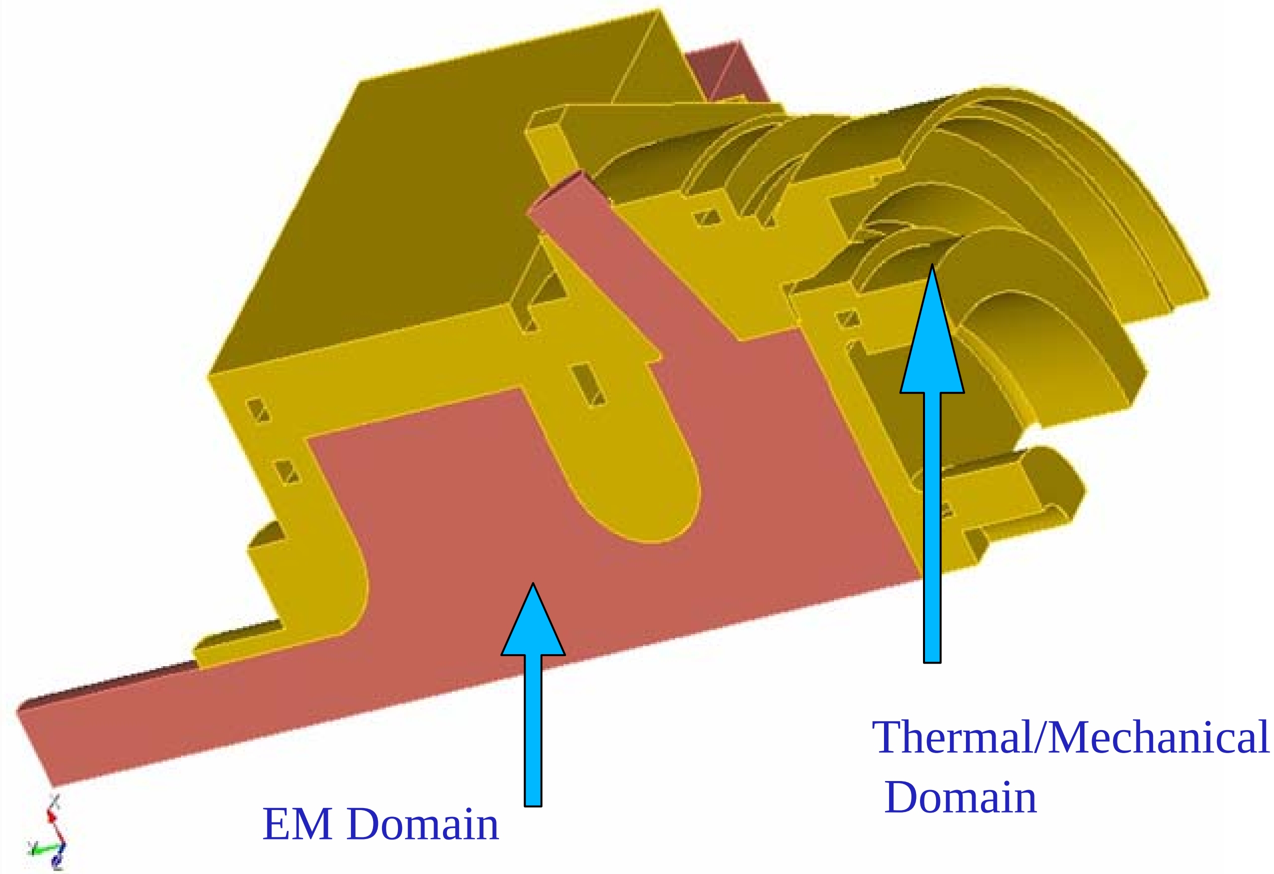


- Finite element based with high-order basis functions
  - Natural choice: FEM originated from structural analysis!
- Use the same software infrastructure as Omega3P
  - Reuse solvers framework
  - Mesh data structures and format
- Parallel

TEM3P for LCLS RF Gun

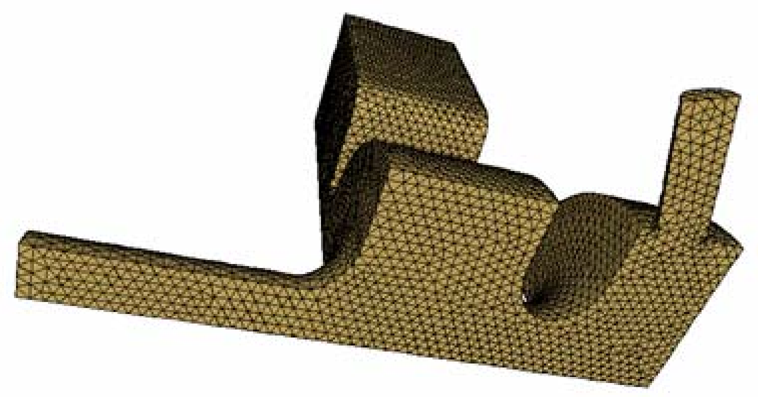


CAD Model (courtesy of Eric Jongewaard)

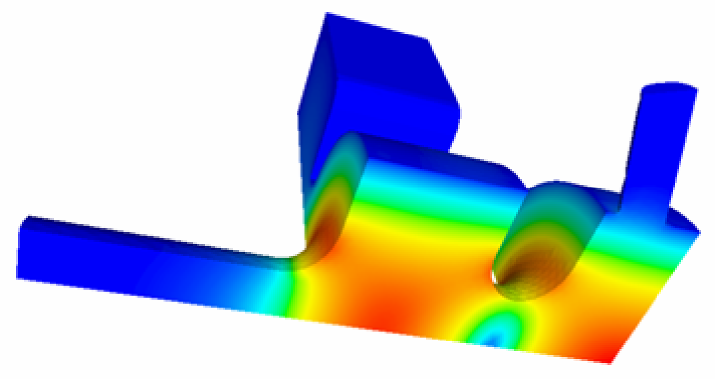


Benchmark TEM3P against ANSYS

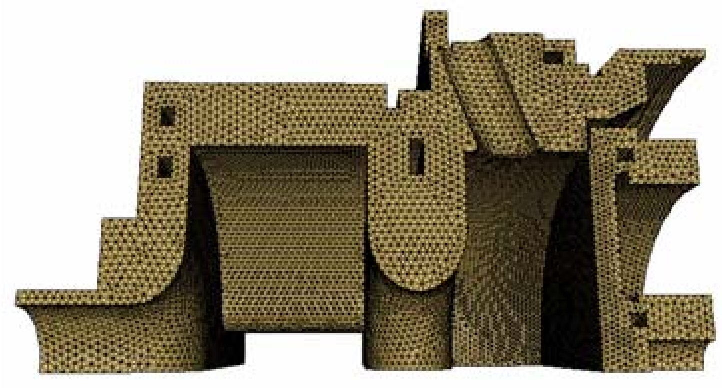
RF Gun EM Thermal/Mechanical Analysis



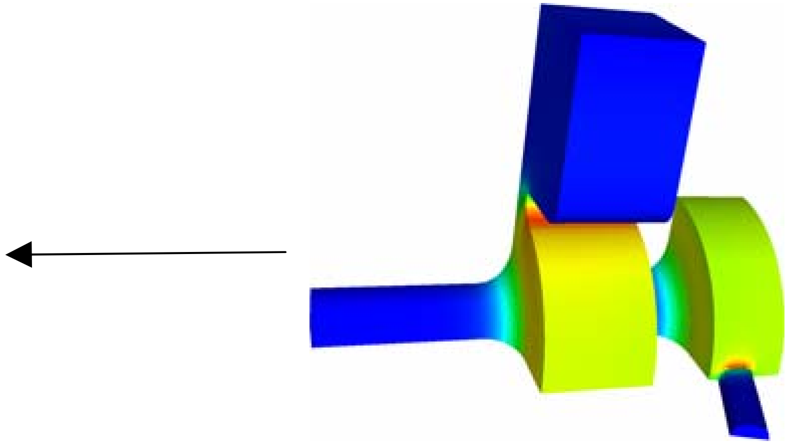
Mesh for RF analysis



Operating mode: 2.856GHz



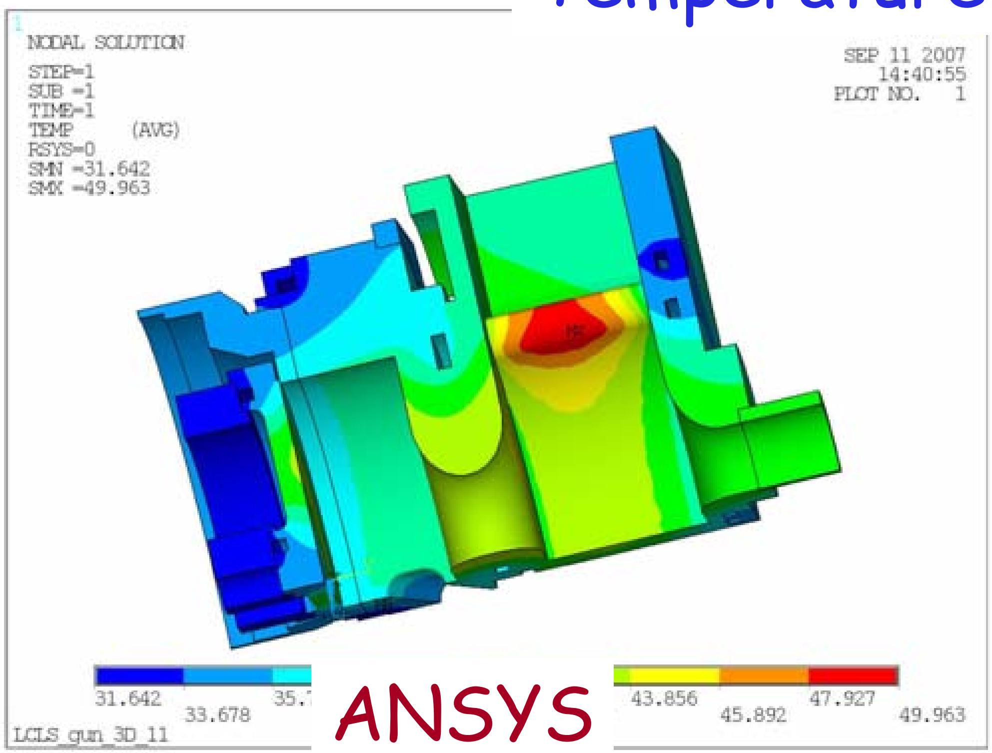
Mesh for Thermal/Mechanical analysis
Mesh: 0.6 million nodes.
Materials: Copper + Stainless steel
Thermal analysis: 7 cooling channels



Magnetic field on the cavity inner surface generates RF heat load

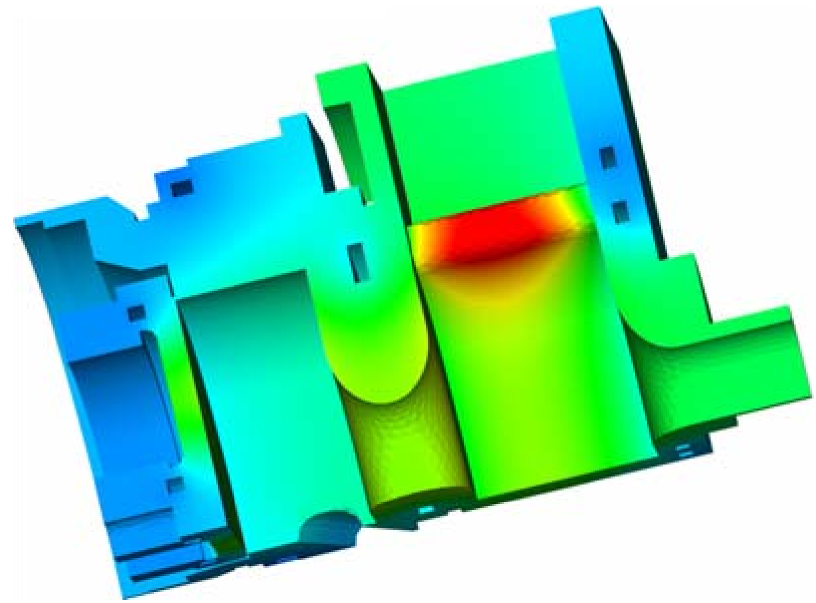
Thermal Analysis Benchmarked With ANSYS

Temperature Distribution



ANSYS

Maximal Temperature 49.96 C

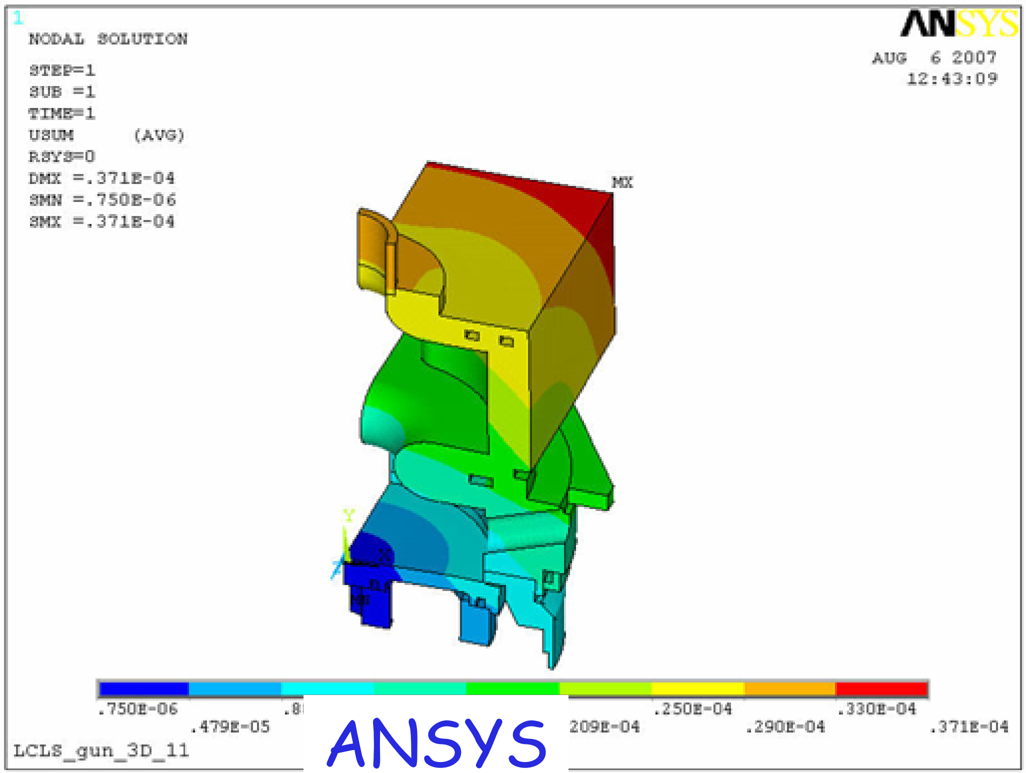


TEM3P

Maximal Temperature 49.82 C

RF heat load: 4000 Watt
Cooling channels: with given temperature, Robin BC
Thermal conductivity: copper 391; stainless steel 16.2

Mechanical Analysis With Thermal Load



ANSYS

Maximal displacement: 37.1 μm

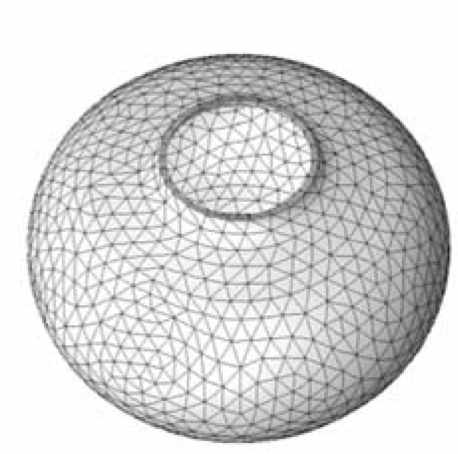
TEM3P

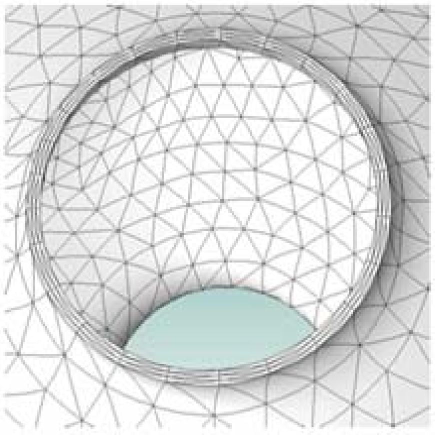
Maximal displacement: 36.99 μm

- Future work: compute stress and drift frequency

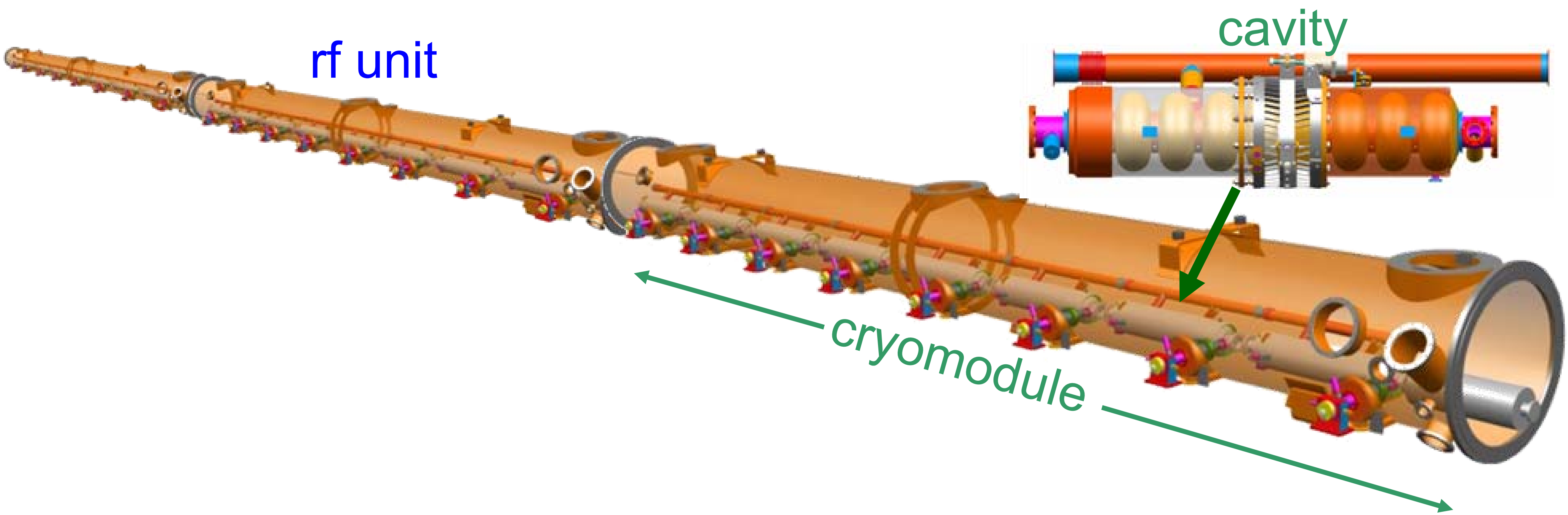
Multi-physics Analysis for SRF Cavities and Cryomodules

- Thermal behaviors are highly nonlinear
- Meshing thin shell geometry
  - Anisotropic high-order mesh will reduce significant amount of computing
  - Working with RPI/ITAPS





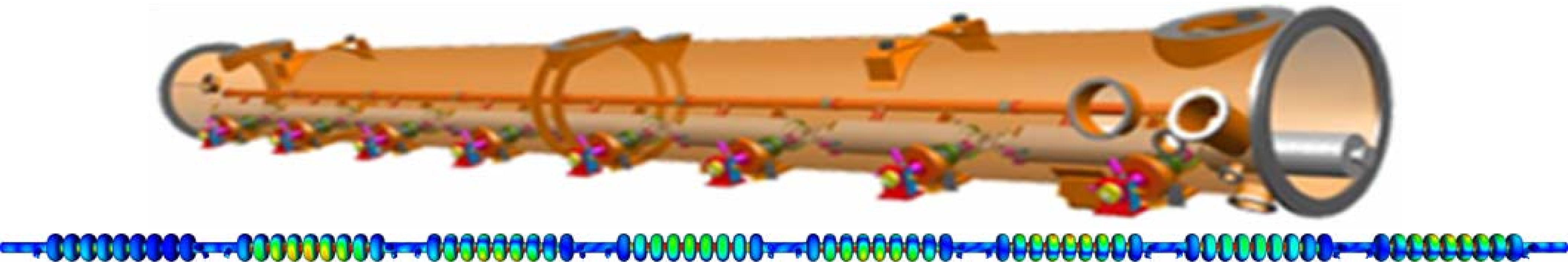
Modeling ILC Cryomodule & RF Unit



Physics Goal: *Calculate wakefield effects in the 3-cryomodule RF unit with realistic 3D dimensions and misalignments*

- *Trapped mode and damping*
- *Cavity imperfection effects on HOM damping*
- *Wakefield effect on beam dynamics*
- *Effectiveness of beam line aborsorber*

ILC 8-Cavity Module



A dipole mode in 8-cavity cryomodule at 3^{rd} band

First ever calculation of a 8 cavity cryomodule

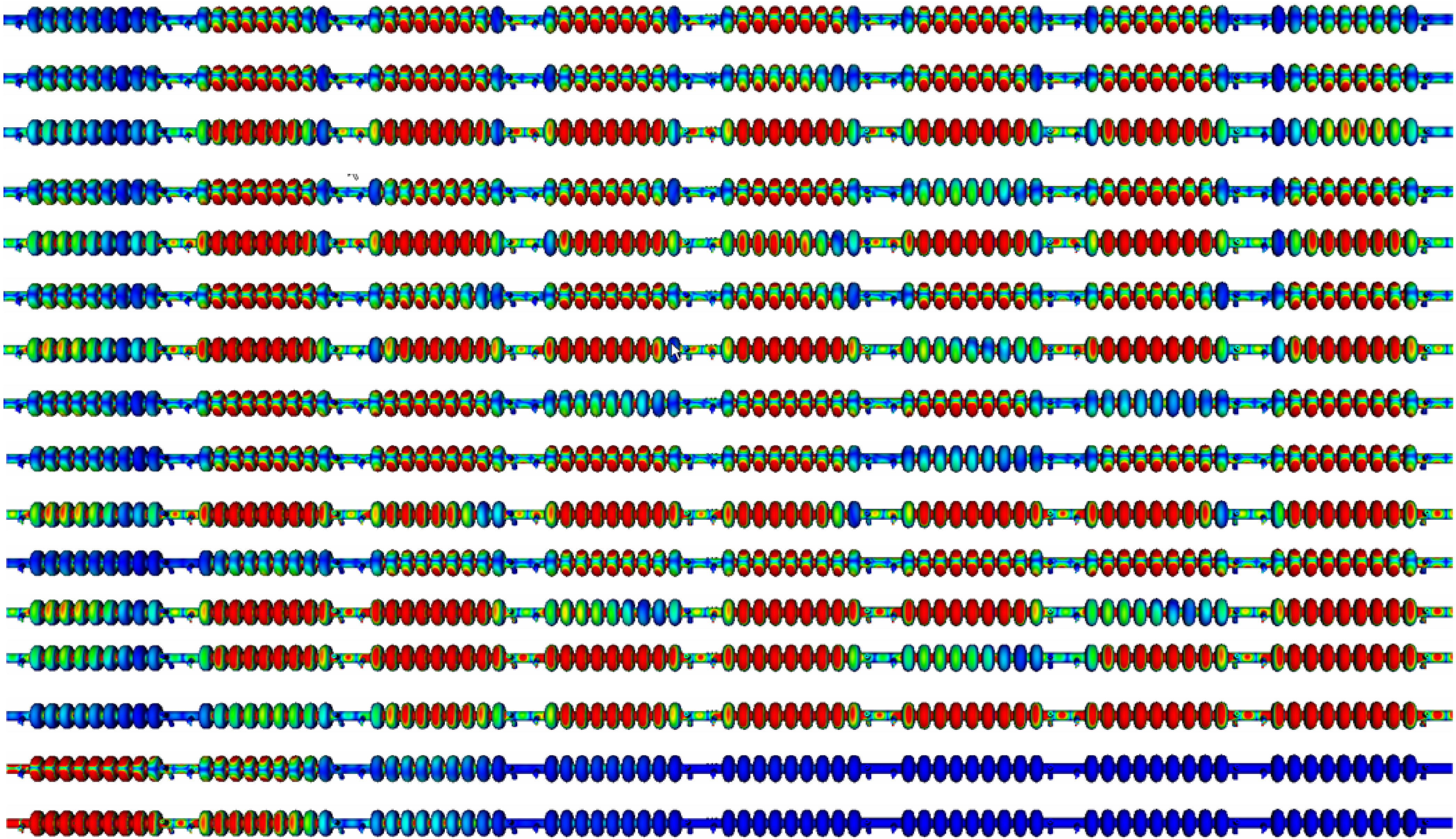
- *~ 20 M DOFs*
- *~ 1 hour per mode on 1024 CPUs for the cryomodule*

To model a 3-module RF unit would require

- *>200 M DOFs*
- *Advances in algorithm and solvers*
- *Petascale computing resources*

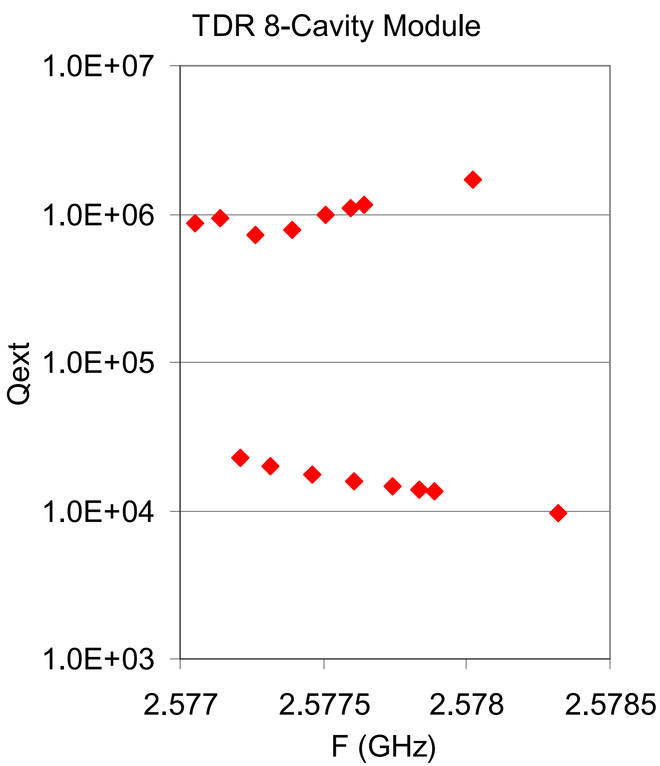
TDR 8-Cavity Module 3rd Band Modes From Omega3P Calculation

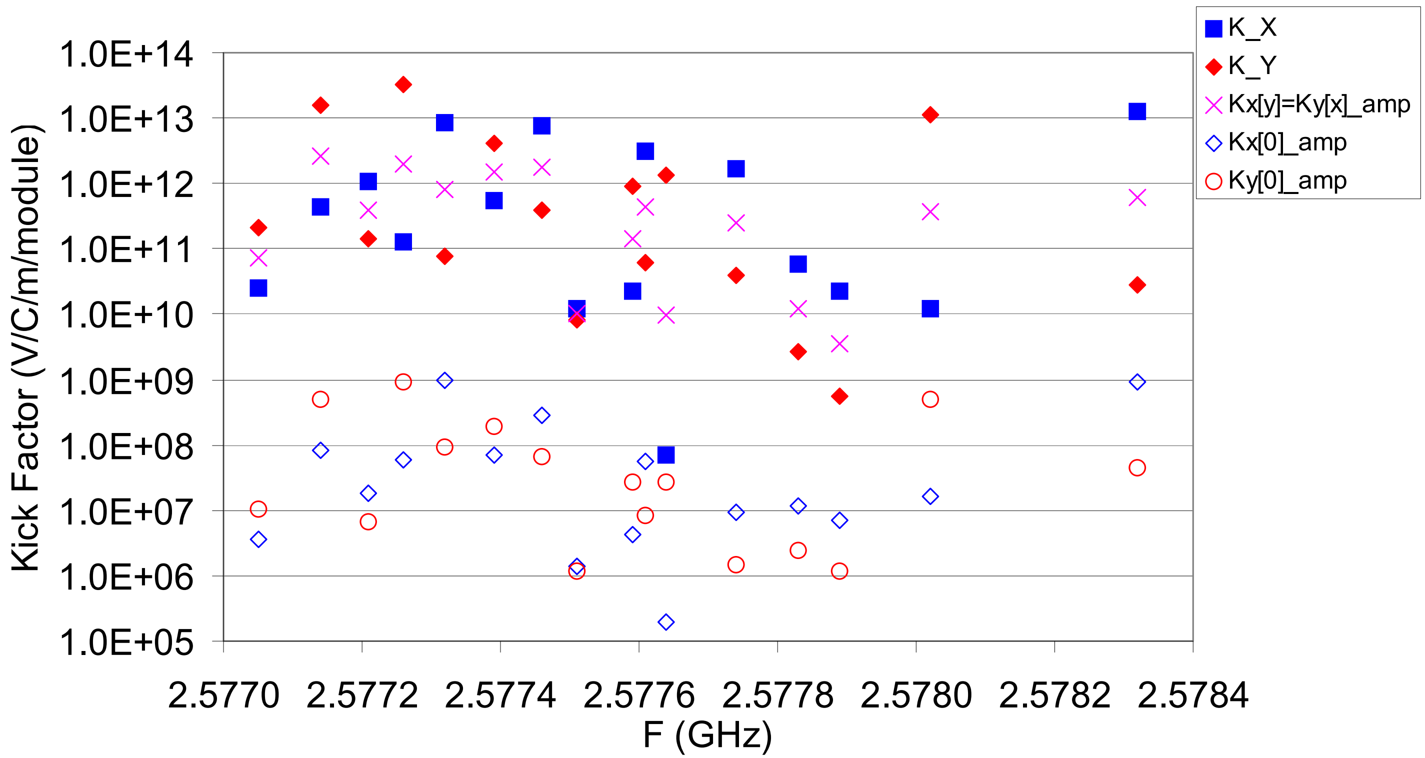
(R. Lee)



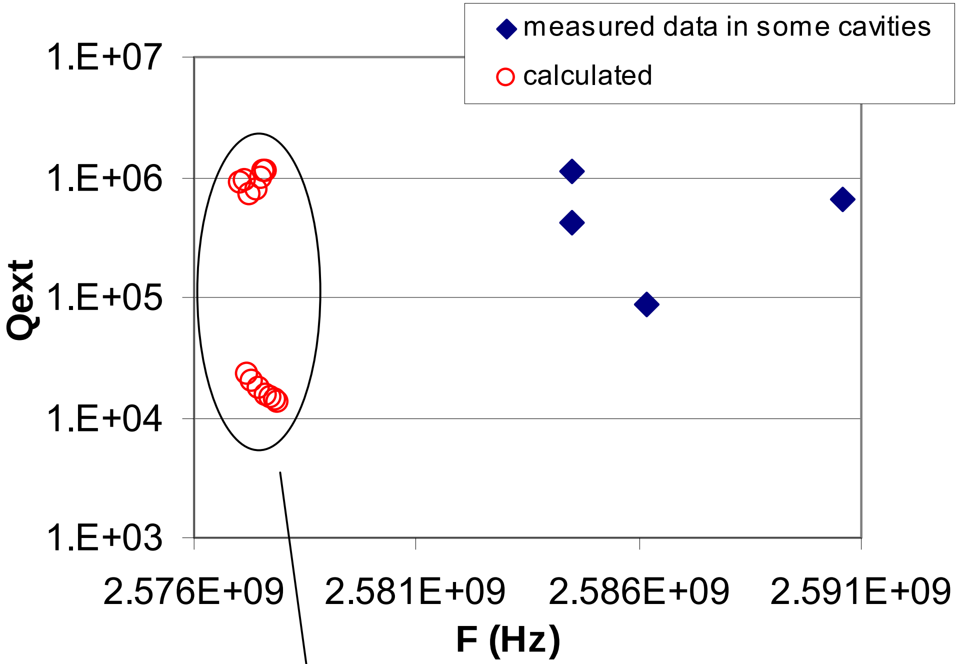
Calculated on NERSC Seaborg: 1500 CPUs, over one hour per mode

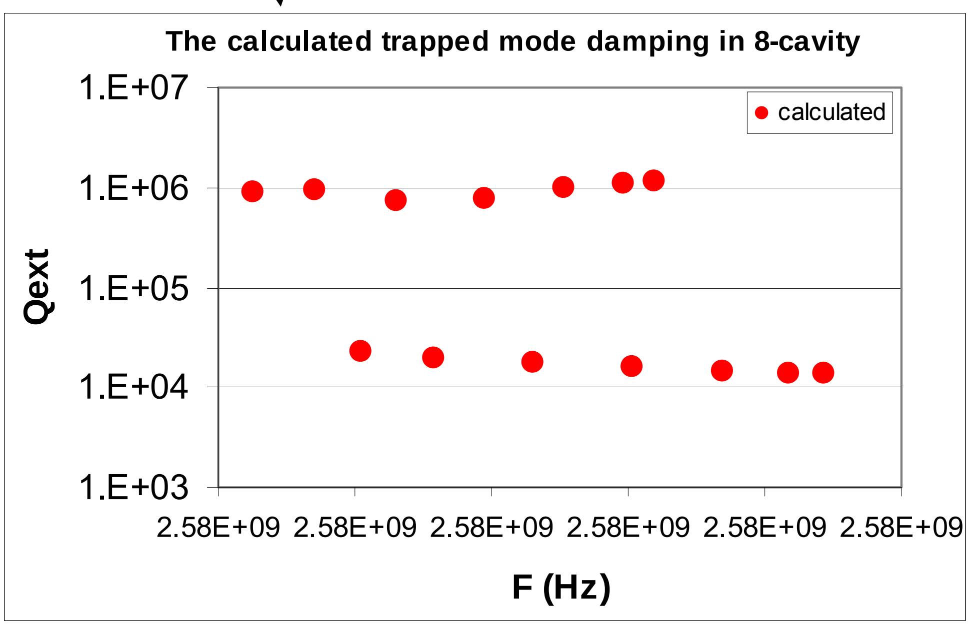
Kick Factor Of One Set Of 3rd Band Modes in the 8-Cavity TDR Module





- Modes above cutoff frequency are coupled through out 8 cavities
- Modes are generally x/y-tilted & twisted due to 3D end-group geometry
- Both tilted and twisted modes cause x-y coupling





One polarization mode is well damped.

INVESTIGATION OF A HIGH-Q DIPOLE MODE AT THE TESLA CAVITIES

N. Baboi*, M. Dohlus, DESY, Hamburg, Germany
C. Magne, A. Mosnier, O. Napoly, CEA, Saclay, France
H.-W. Glock, Uni Rostock, Germany

At TTF several experiments have been made in order to study the HOMs. By modulating the beam current [2], several high impedance modes have been found to have a very high Q [3]. Specially a mode around 2.585 GHz, the last of the 3rd dipole band, having an estimated impedance R/Q = 15 Ω/cm², was found to be badly damped in 2 cavities of the first module. Nevertheless, the other polarization of the same mode is better damped. It was found that this mode is badly damped in one of the cavities of the 2nd and 3rd modules as well. The results are summarized in Table. 1.

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	$1.1 \cdot 10^6$
#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	$6.5 \cdot 10^5$

Recent Advances in Solver and Meshing

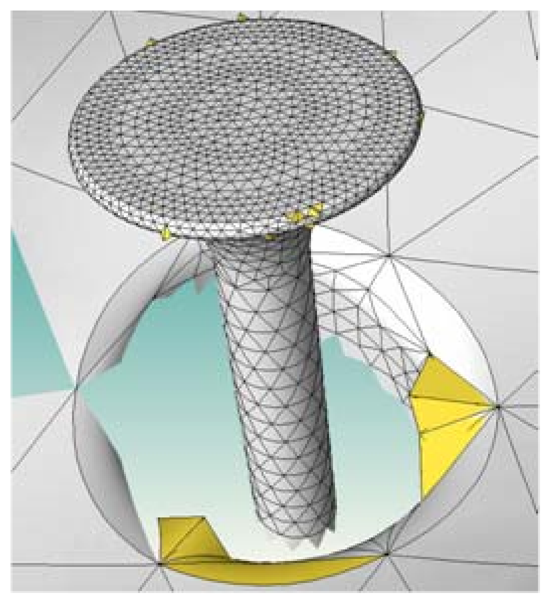
Linear Solver

Simulation capabilities limited by memory available even on DOE flagship supercomputers – develop methods for reducing memory usage

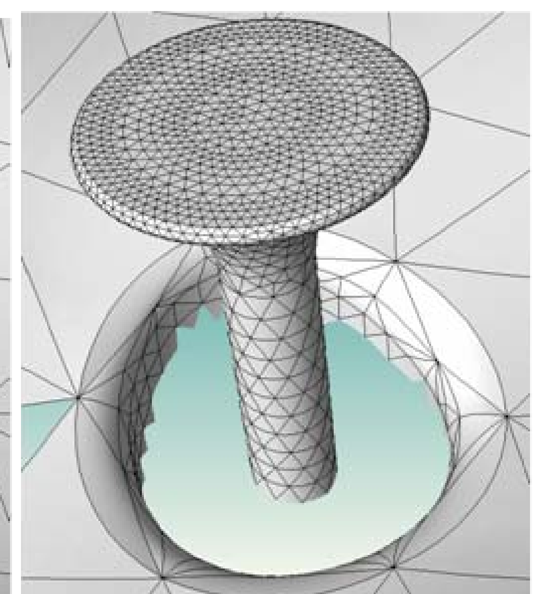
Method	Memory (GB)	Runtime (s)
MUMPS	155.3	293.3
MUMPS + single precision factorization	82.3	450.1

Meshing

- Invalid quadratic tets generated on curved surface
- Collaborated with RPI on a mesh correction tool
- Runtime of corrected model faster by 30% (T3P)



Invalid tets (yellow)



Corrected mesh

SLAC

SciDAC Scientific Discovery through Advanced Computing

SciDAC CS/AM Activities

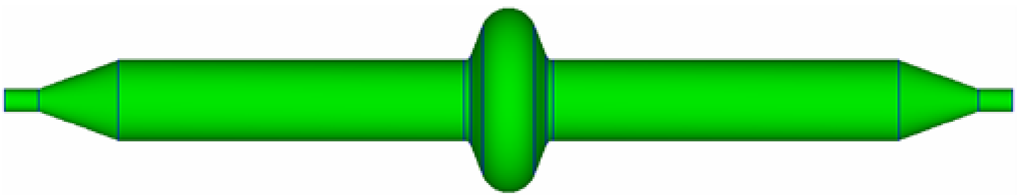
- Shape Determination & Optimization (TOPS/UT Austin, LBNL) – *Obtain cavity deformations from measured mode data through solving a weighted least square minimization problem*
- Parallel Complex Nonlinear Eigensolver/Linear Solver (TOPS/LBNL) – *Develop scalable algorithms for solving LARGE, complex, nonlinear eigenvalue problems to find mode damping in the rf unit complete with input/HOM couplers and external beampipes*
- Parallel Adaptive Mesh Refinement and Meshing (ITAPS/RPI, ANL) – *Optimize computing resources and increase solution accuracy through adaptive mesh refinement using local error indicator based on gradient of electromagnetic energy in curved domain*
- Parallel and Interactive Visualization (ISUV/UC Davis) – *Visualize complex electromagnetic fields and particles with large complex geometries and large aspect ratio*

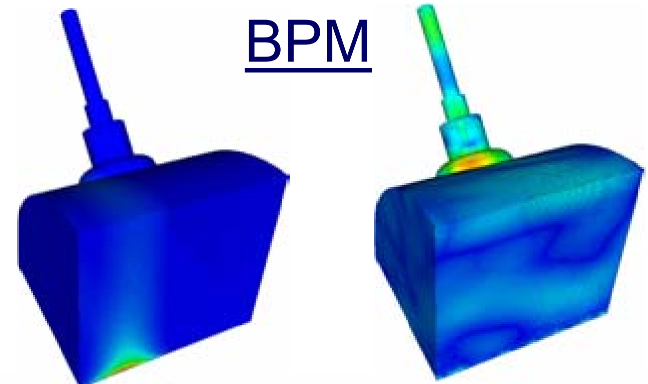
Summary

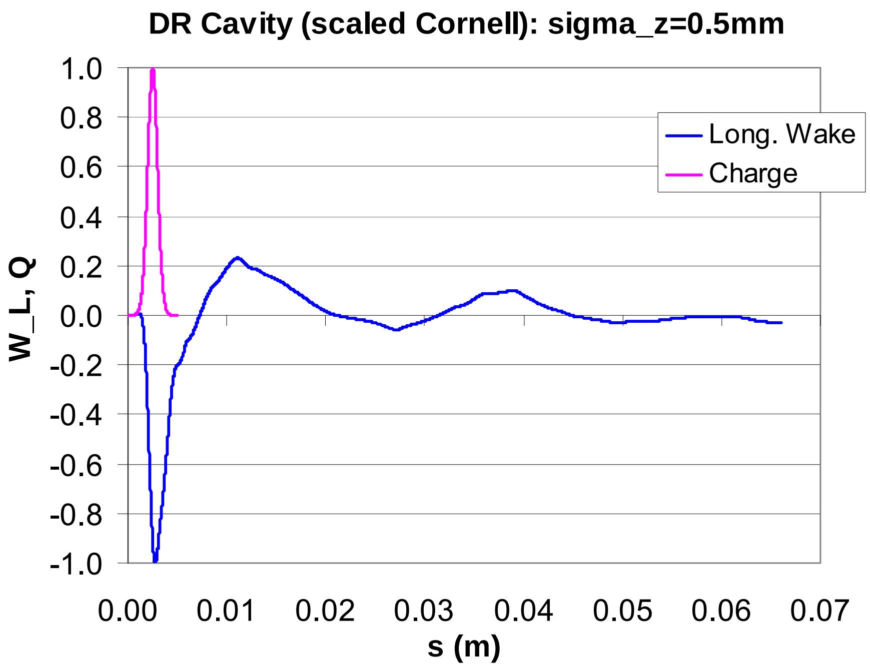
- A suite of parallel codes in electromagnetics and beam dynamics was developed for accelerator design, optimization and analysis
- Important contributions have been made using these codes to accelerator projects such as ILC, LHC, LCLS, SNS, etc…
- Through the SciDAC support and collaborations, advances in applied math and computer science are being made towards Petascale computing of large accelerator systems such as the ILC RF unit, etc

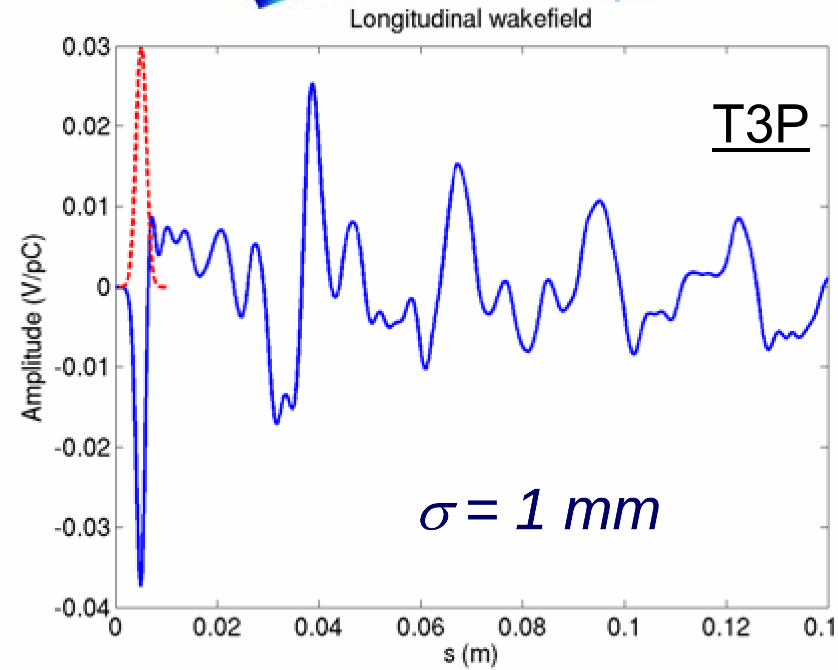
ILC Damping Ring Impedance Calculations

RF cavity









- *Components scaled from existing machines*
- *Determine pseudo Green's function wakefield for beam stability studies*