State of the Art in EM Field Computation

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SLAC

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SciDAC
Scientific Discovery through Advanced Computing

Outline

- ***US DOE SciDAC Program***
- *Parallel Finite Element EM Codes*
- *Applications to PEP-II, LCLS, ILC*
- *Petaflop Computing for a cryomodule*

What is SciDAC?

- ***Sci**entific **D**iscovery through **A**dvanced **C**omputing*
- *US DOE Office of Science (SC) Simulation Initiative*
- *Promote application of High Performance Computing to SC programs such as High Energy Physics (HEP)*
- *SciDAC-I (2001-2006), SciDAC-2 selections in progress*
- ***Multi-disciplinary approach** – computational scientists (CS & AM) work alongside application scientists*
- *HEP's Accelerator Simulation Project - 3 components:*

  ***Electromagnetics** (SLAC),*
  Beam Dynamics (LBNL),
  Advanced Accelerators (UCLA)

SciDAC Scientific Discovery through Advanced Computing

SciDAC's Accelerator Project

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)*

NERSC	**NLCF**
Seaborg IBM SP3	Phoenix Cray X1E
9 Tflops, 6 TB+	18 Tflops, 2 TB

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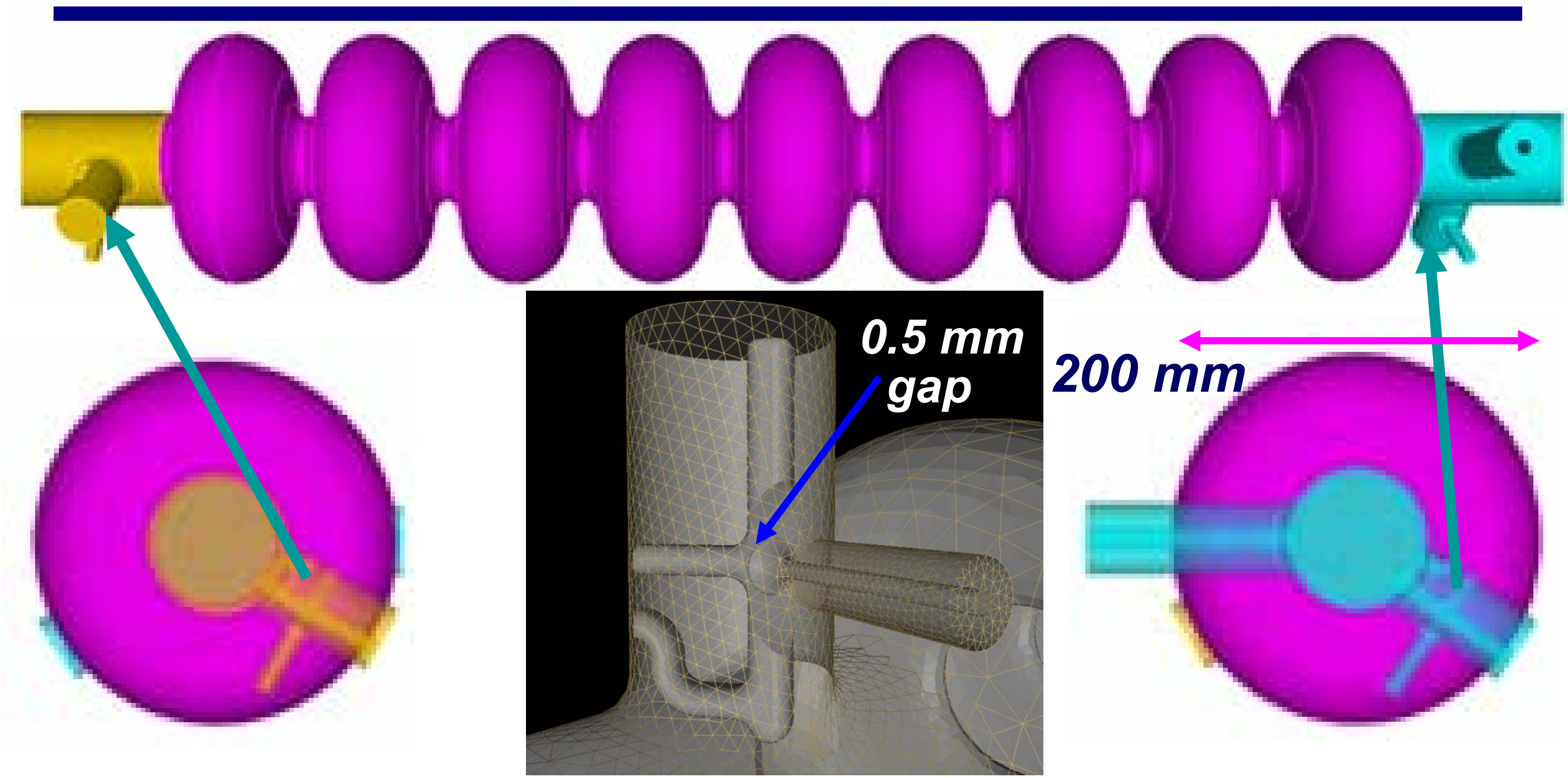
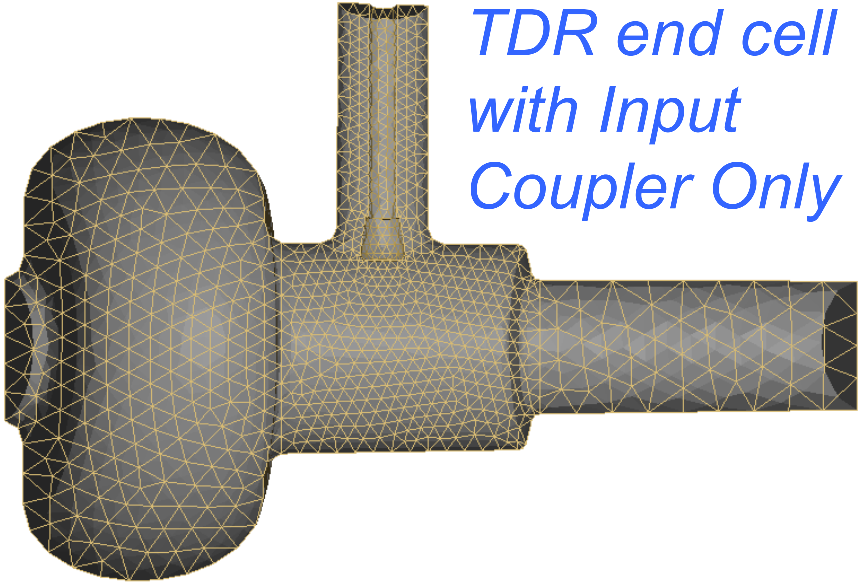
High Fidelity Modeling of TDR Cavity

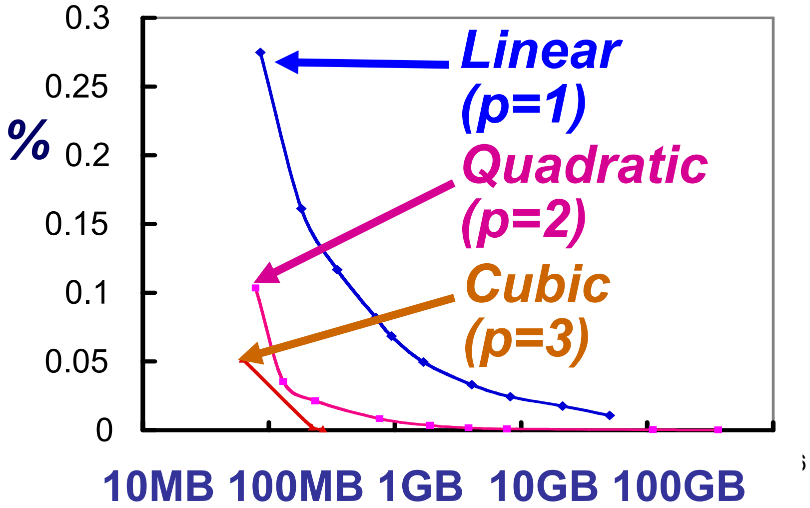


- ***Complexity*** – ***HOM coupler*** *(fine features)versus cell*
- ***Problem size*** – *multi-cavity structure, e.g. cryomodule*
- ***Accuracy*** – *10's kHz mode separation out of GHz*
- ***Speed*** – *Fast turn around time to impact designs*

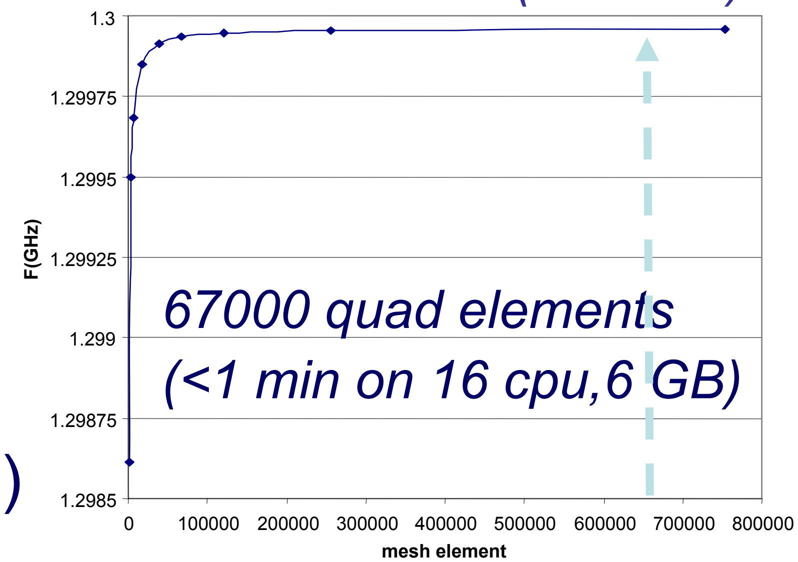
Higher-order FEM + Parallel Processing



TDR end cell with Input Coupler Only



Error ~ 20 kHz (1.3 GHz)



- Tetrahedral Conformal Mesh w/ quadratic surface
- Higher-order Finite Elements (p = 1-6)
- Parallel Processing (large memory &1/N speedup)

SLAC 3D Parallel FEM EM Codes

Tetrahedral Mesh with Finite-Element (up to 6th order basis)

T3P

Omega3P

S3P

Time Domain
With Beam
& Excitations

Frequency Domain
Mode Calculation

S- parameters
Computations

Track3P – Particle Tracking with Surface Physics

Dark Current
Multipacting

Under Dev.

Gun3P – Particle Tracking with Space Charge

DC Gun

Pic3P – Self-consistent Particle Simulation

RF Gun
Klystron

V3D – Visualization of Meshes, Particles & Fields

Programmed in C++ & MPI

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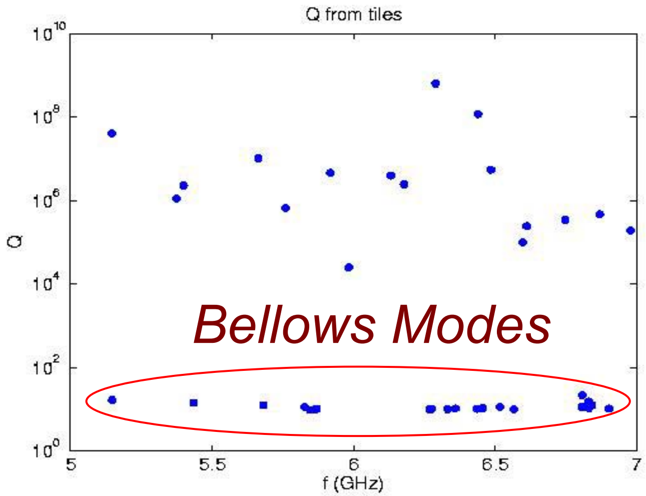
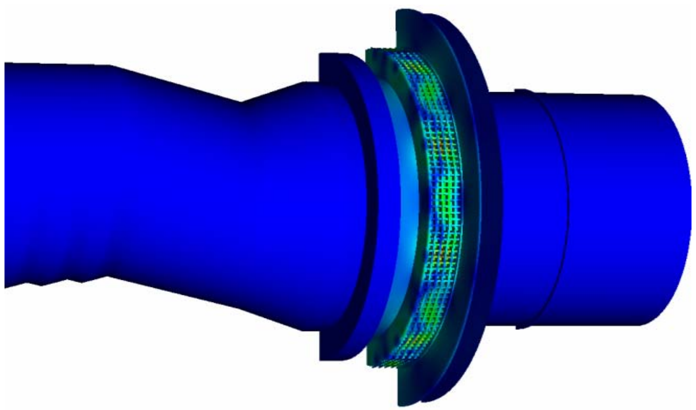
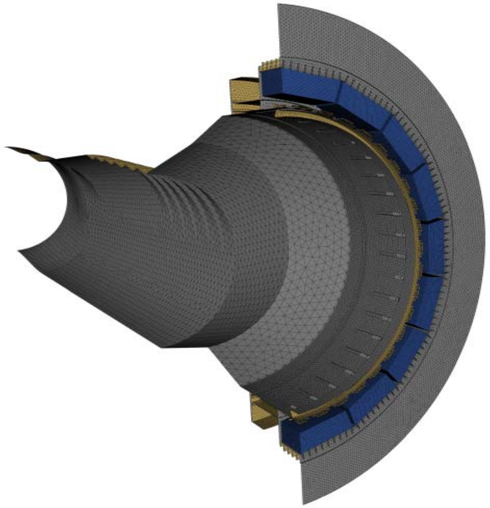
PEP-II Vertex Bellows Heating

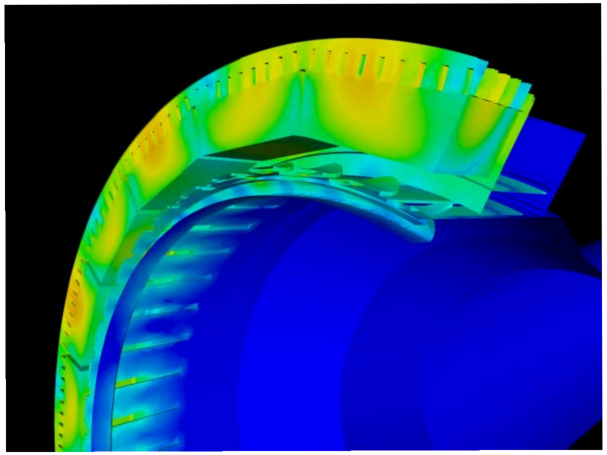
Omega3P *was used to evaluate the damping of localized modes by ceramic tiles mounted on the bellows convolution. Bellows modes were found to be damped to very low Qs*



Bellows mode   Ceramic tile absorber   Dielectric loss

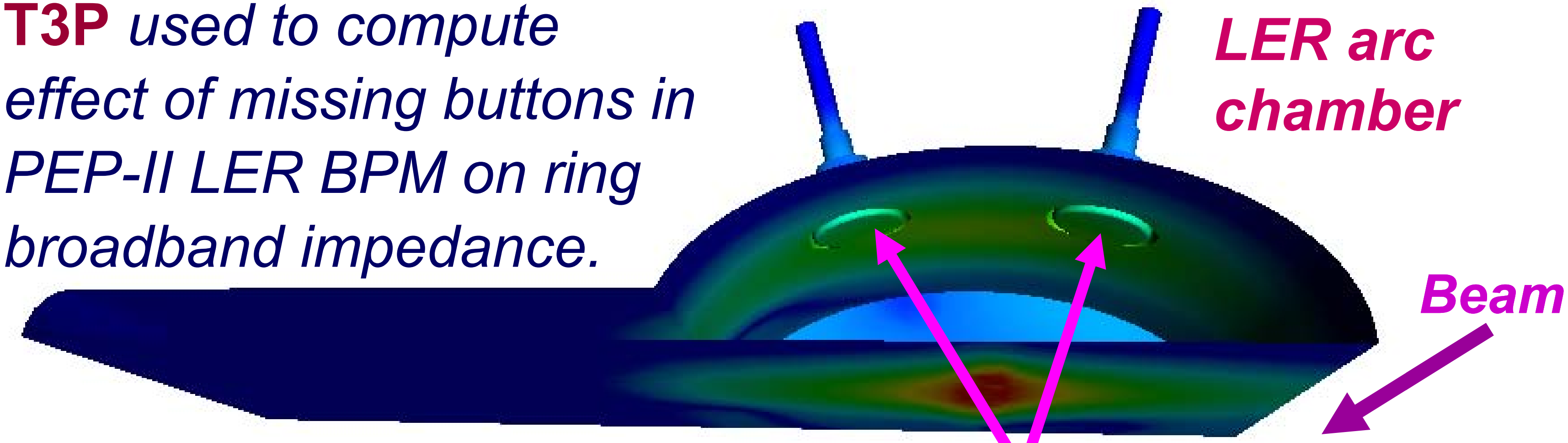


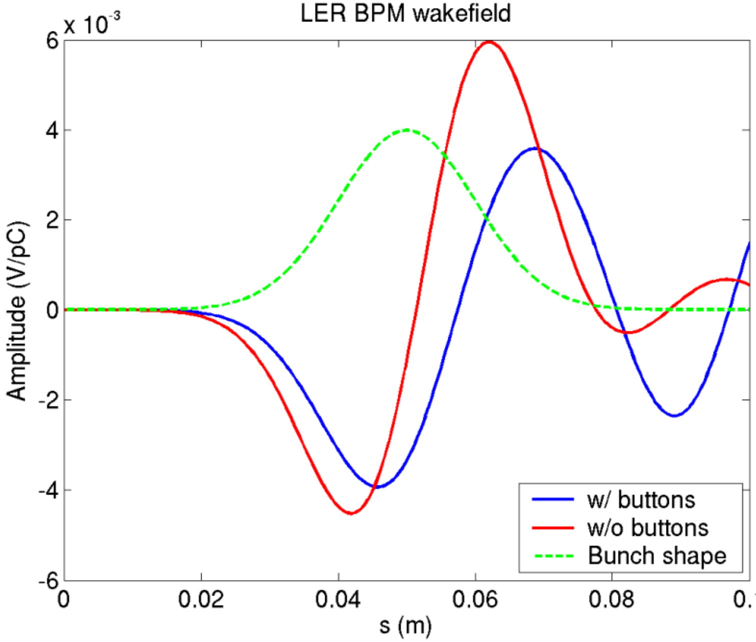


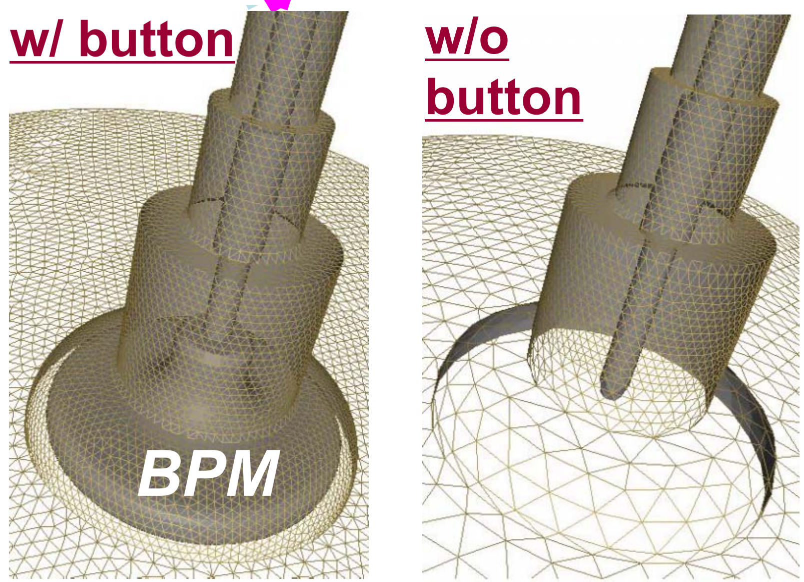


PEP-II LER BPM Broadband Impedance

T3P *used to compute effect of missing buttons in PEP-II LER BPM on ring broadband impedance.*

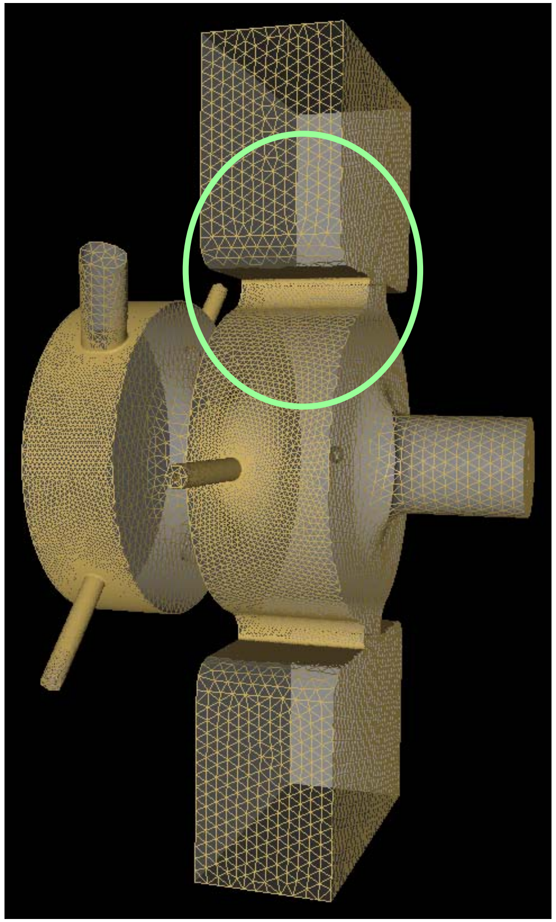




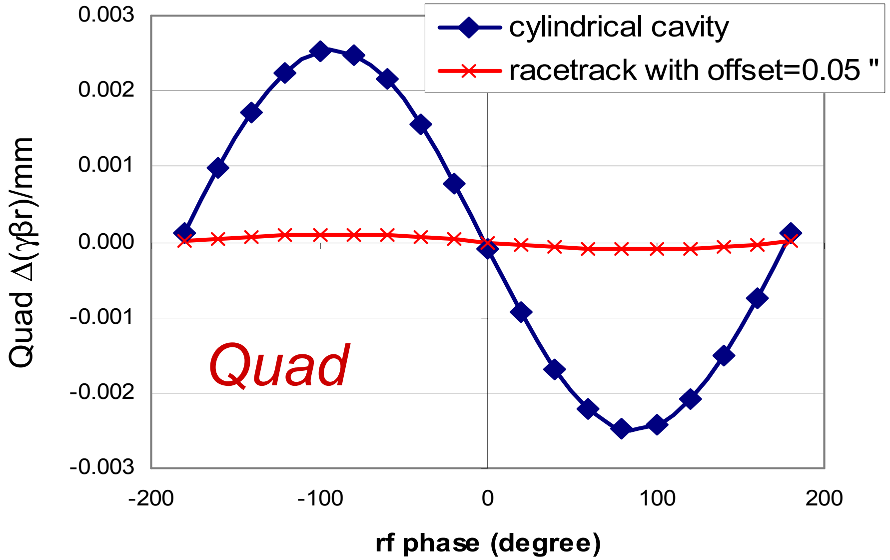


LCLS RF Gun Cavity

Omega3P/S3P *modeling provided the dimensions for the LCLS RF Gun cavity that meet two requirements:*



- reduce pulse heating by rounding of the z coupling iris
- minimize dipole & quadrupole fields via a racetrack dual-feed coupler design



1st Prototype: β = 1.97(2.1), Q_0 = 13200 (13500)

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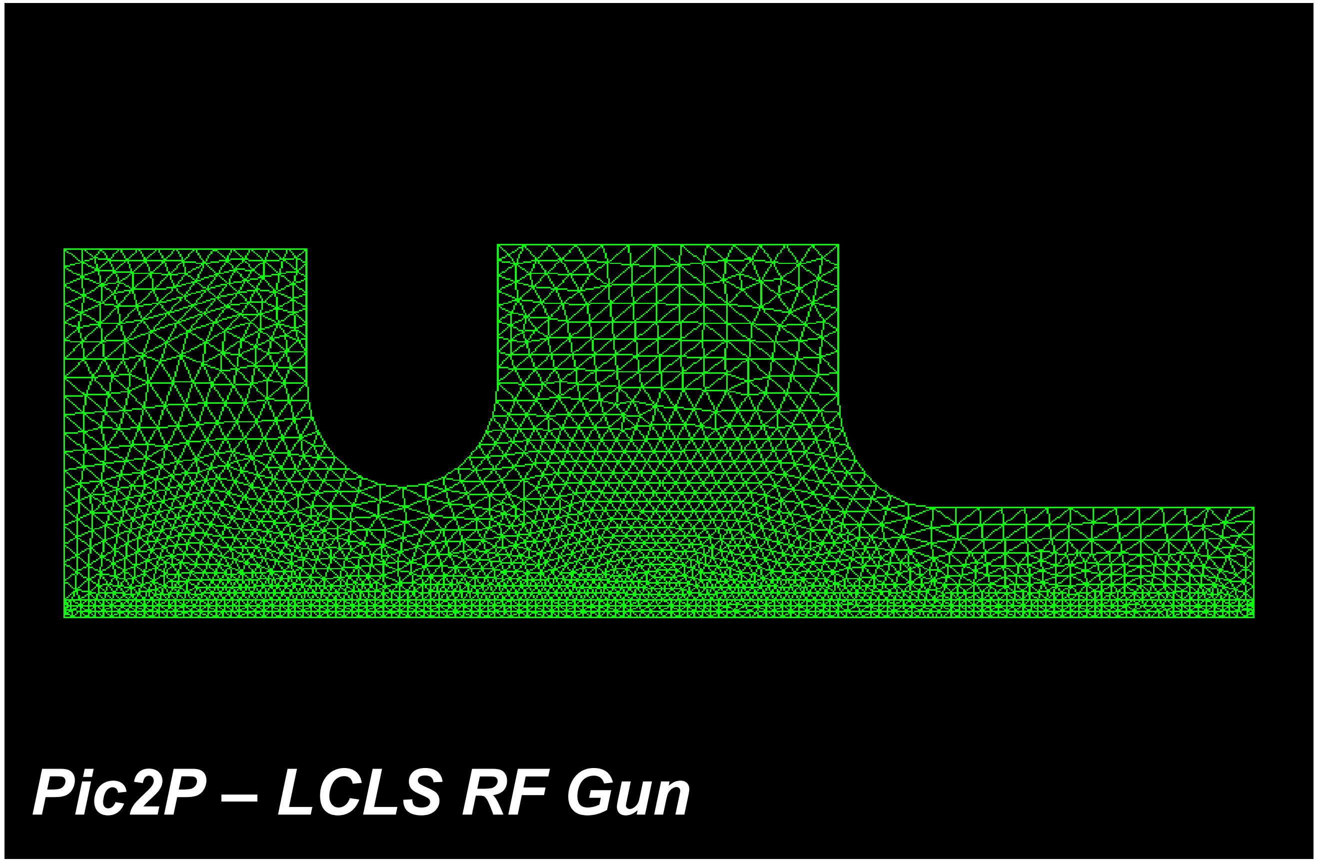
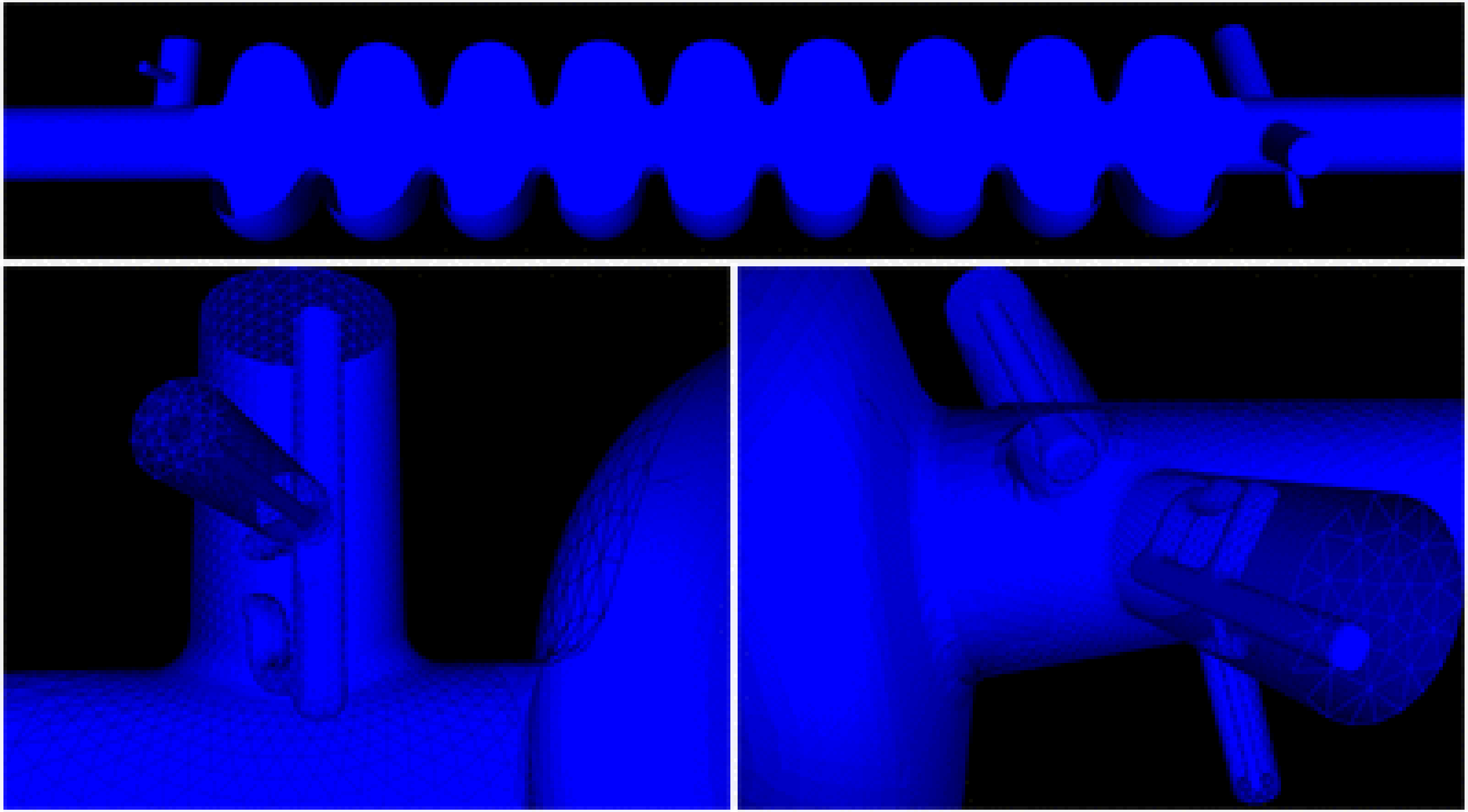
Particle Simulation on FEM Grid - Progress

- ***Parallel FEM*** *Particle-In-Cell (PIC) codes in 2 and 3D for RF guns and klystrons are under development*
- *Higher accuracy in fields and increased beam resolution*
- *Pic2P is presently being tested; Pic3P is next.*



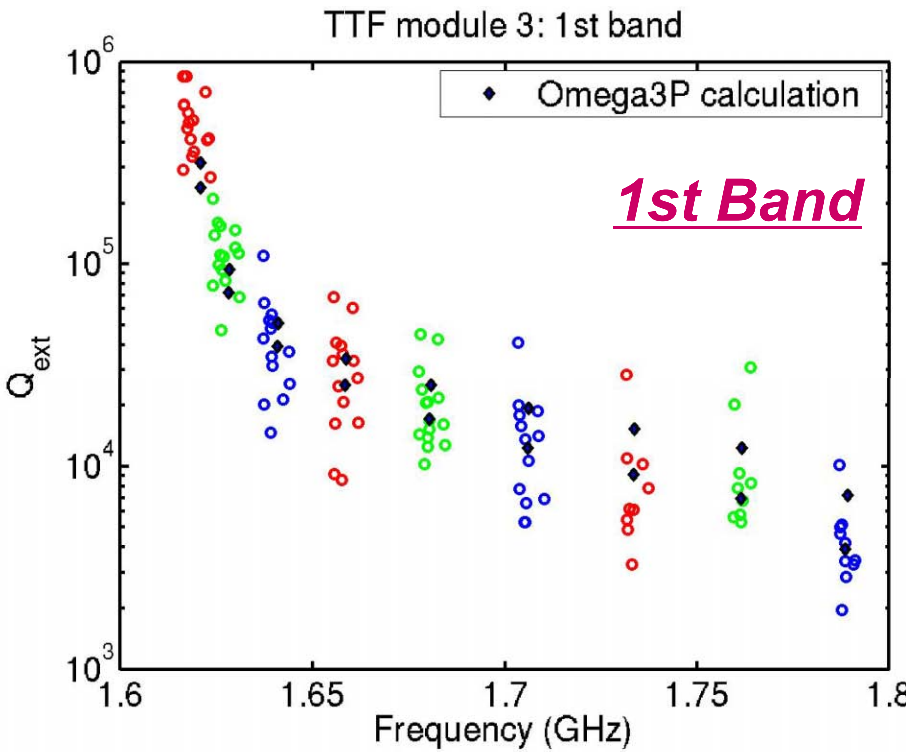
TDR Cavity – Wakefields (T3P)

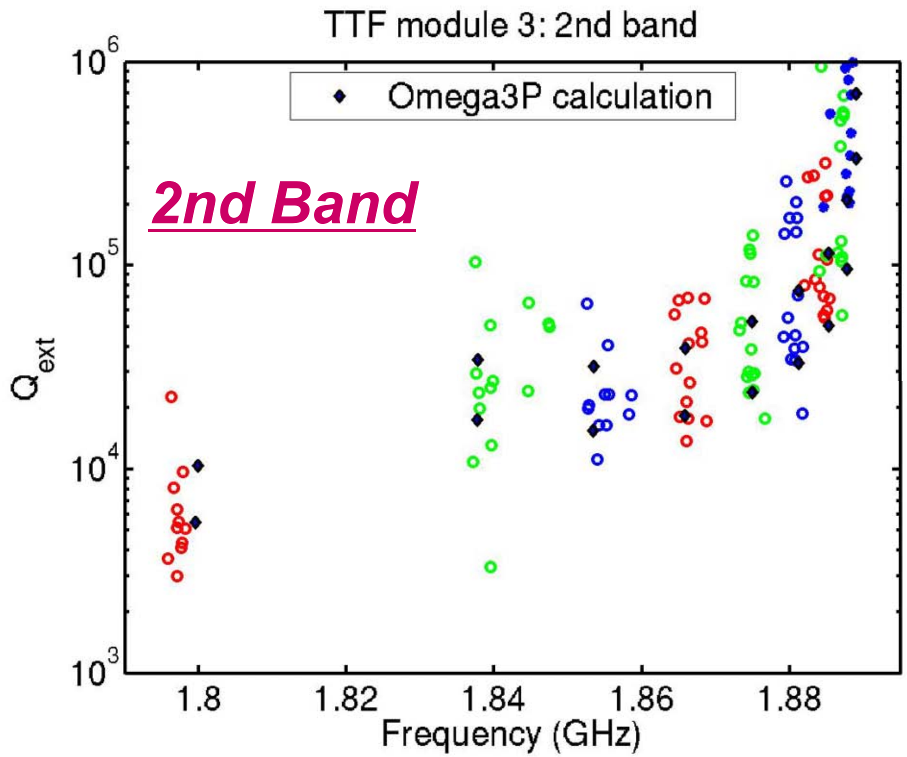


1.75 M quadratic elements, 10 M DOFs, 47 min per nsec on Seaborg 1024 CPU with 173 GB memory – CG and incomplete Cholesky preconditioner

TDR Cavity – HOM Damping (Omega3P)

*Comparing measurements (color) with **Omega3P** (black) complex eigenmode solutions ($Qe=f_{real}/2f_{imag}$) shows data scatter around ideal cavity results due to shape deformations*





0.53 M quadratic elements, 3.5 M DOFs, 512 CPU with 300 GB on Seaborg, Second Arnoldi with MUMPs, 1 hour per dipole band

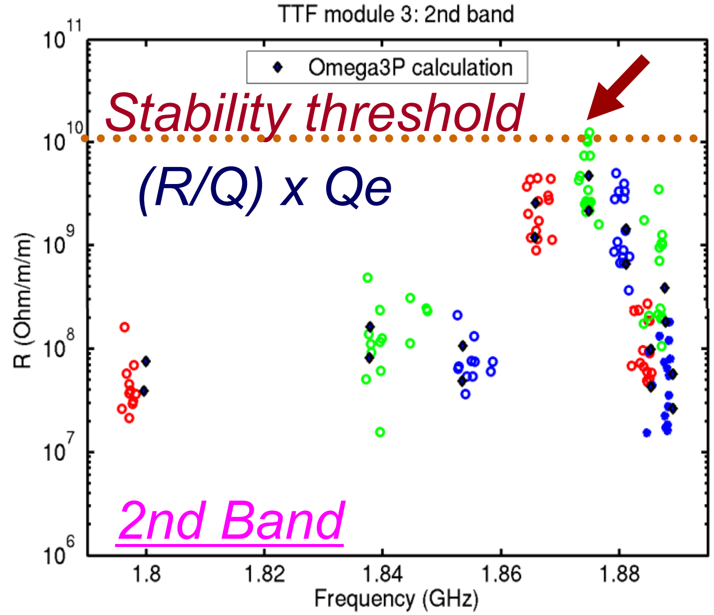
Shape Determination from Measurements

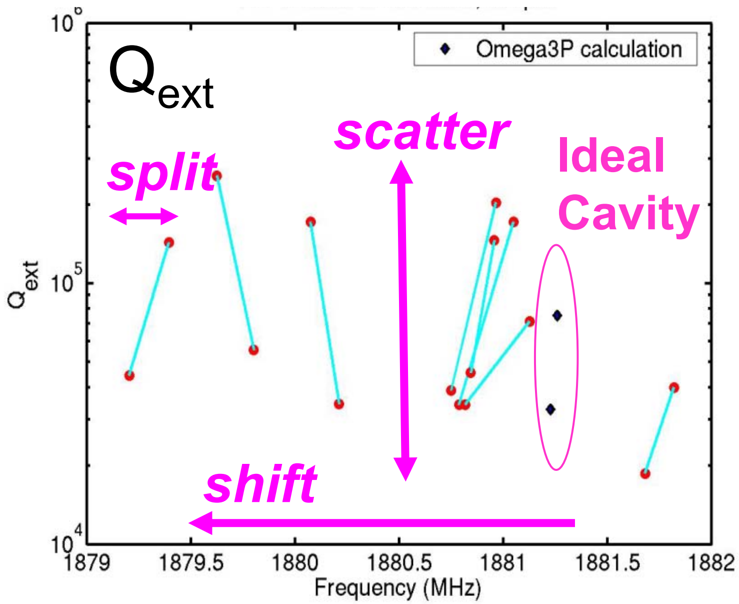
Effects of cavity deformations:

- *Mode splitting is 100s of kHz (10s of kHz in ideal cavity),*
- *Mode frequency is shifted by as much as few MHz,*
- *Qext scatter towards high side - may lead to dangerous modes.*

Shape determination:

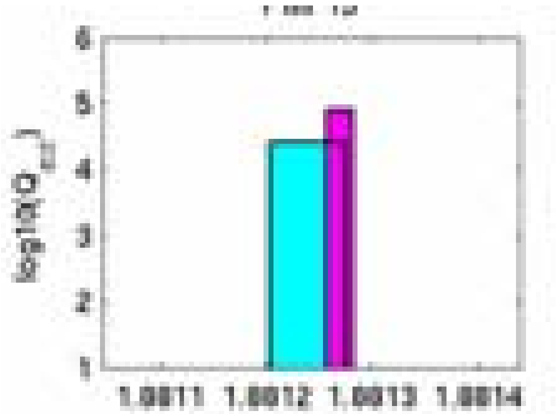
- *Solve an inverse problem to find cavity TRUE shape*
- *Use measurements from TESLA cavity data bank as input*
- *Goal to identify sensitivity of critical dimensions affecting Qe*





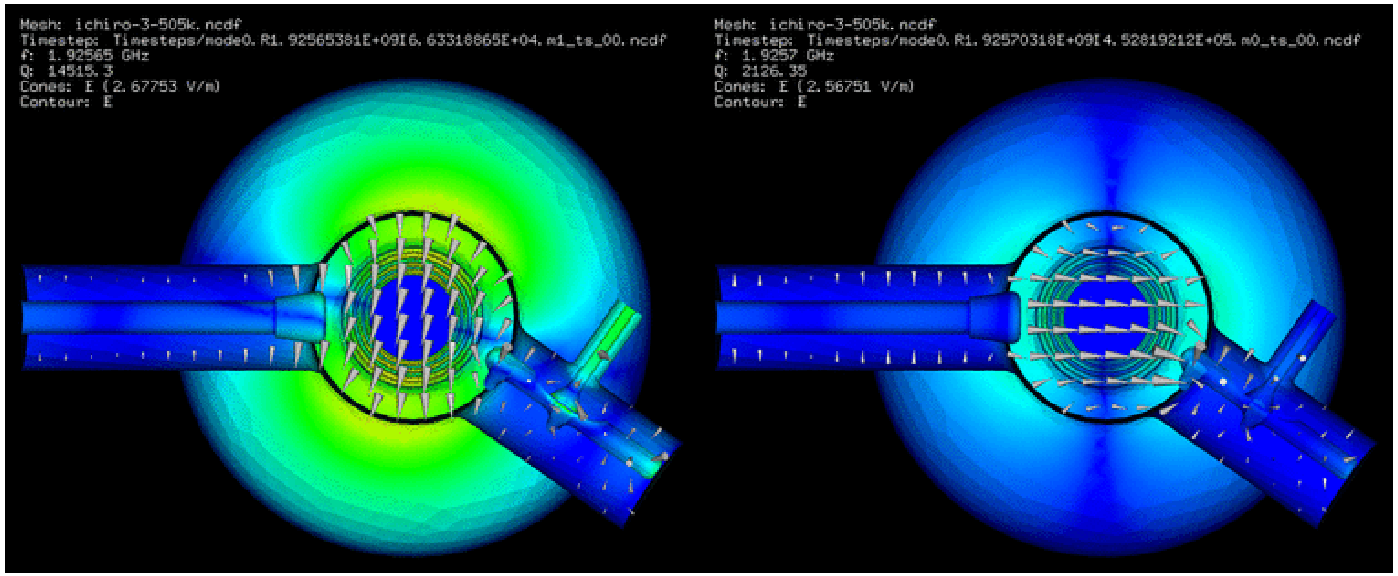
Mode Rotation in HOM pairs in ILC Cavity

The couplers split the dipole mode degeneracy in the ILC cavity. When the line widths of the mode pair overlaps due to damping, the modes become elliptically polarized and rotate in time.



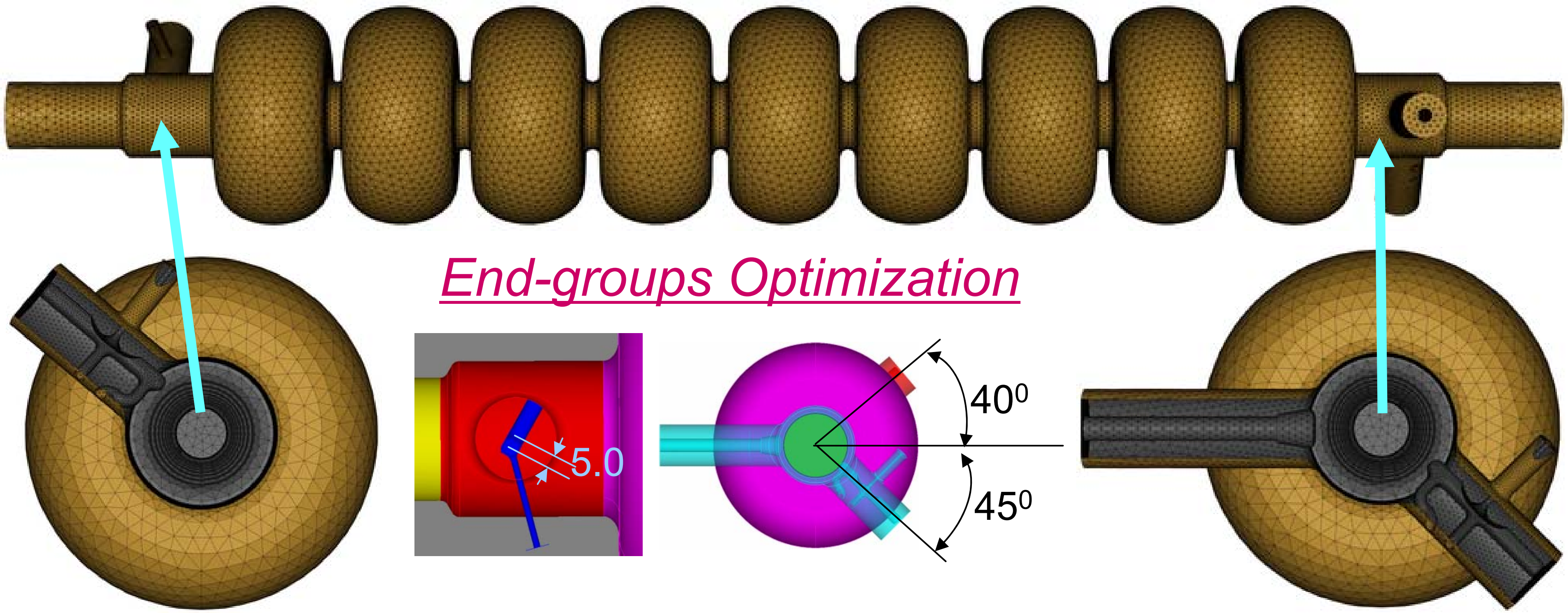
6th dipole mode pair in 2nd band

E field of rotating modes



Low-Loss Cavity - HOM Damping

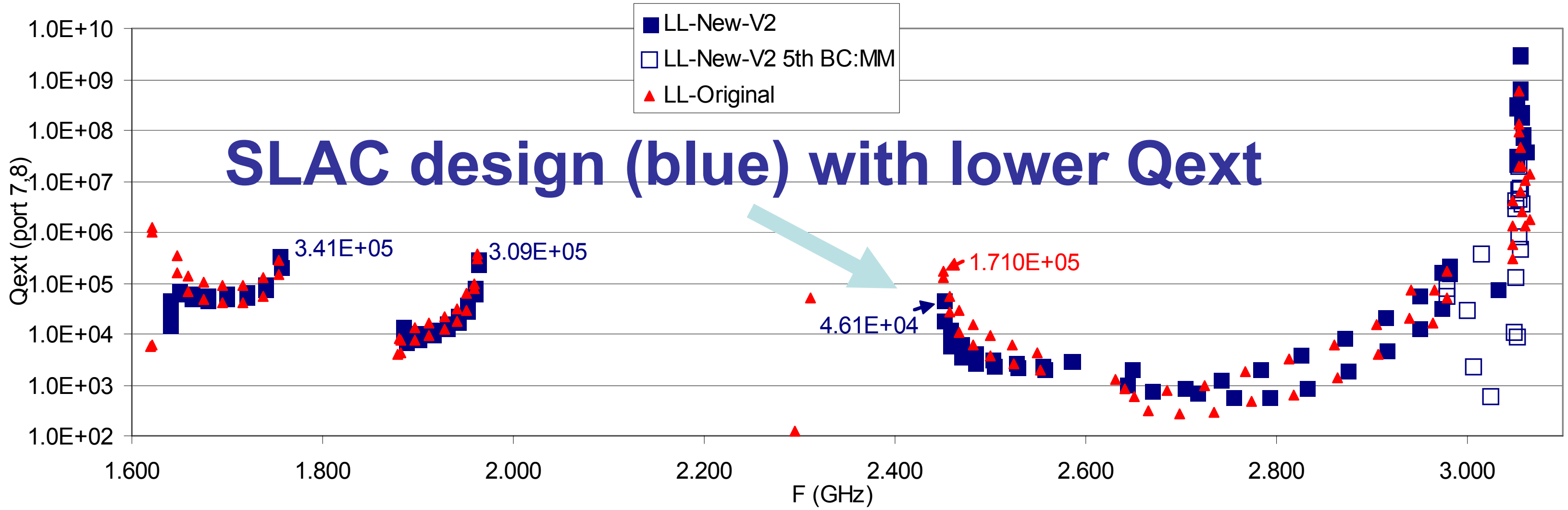
- *Low-Loss (LL) design has 20% cryogenic loss and higher shunt impedance than TDR cavity,*
- *TDR HOM coupler provides inadequate damping – dangerous mode in 3rd dipole band,*
- *Optimization of end-groups to improve design.*



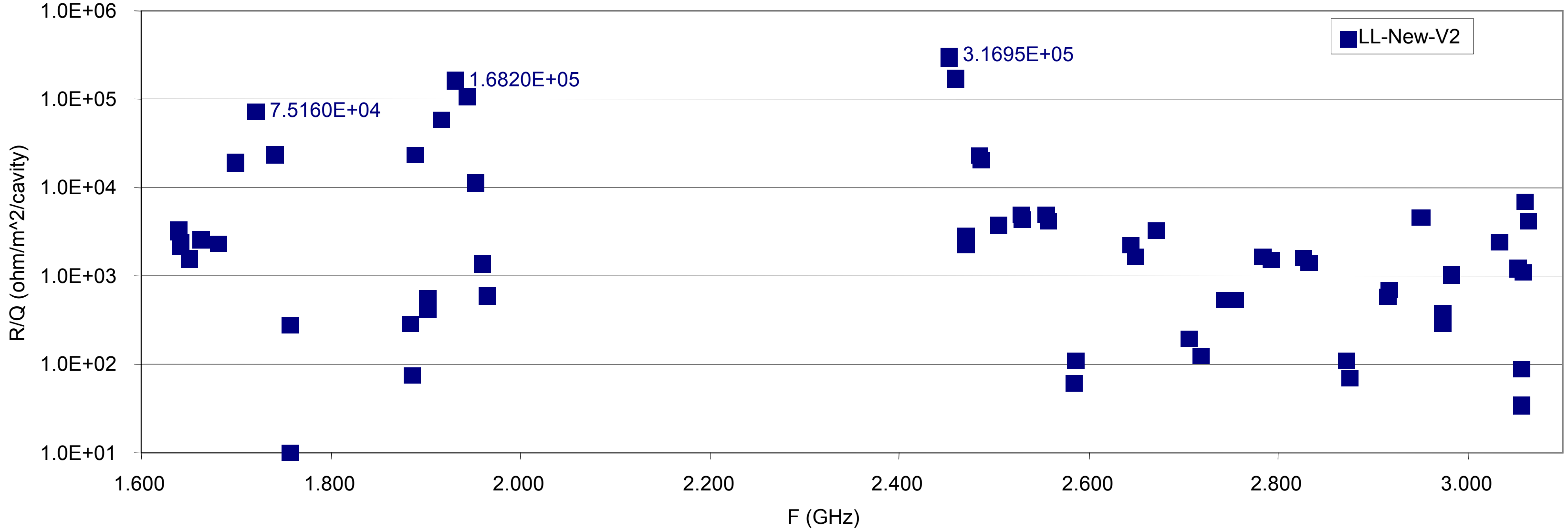
LL Cavity – End Groups Optimization

Similar Improvements carried out for the ICHIRO cavity

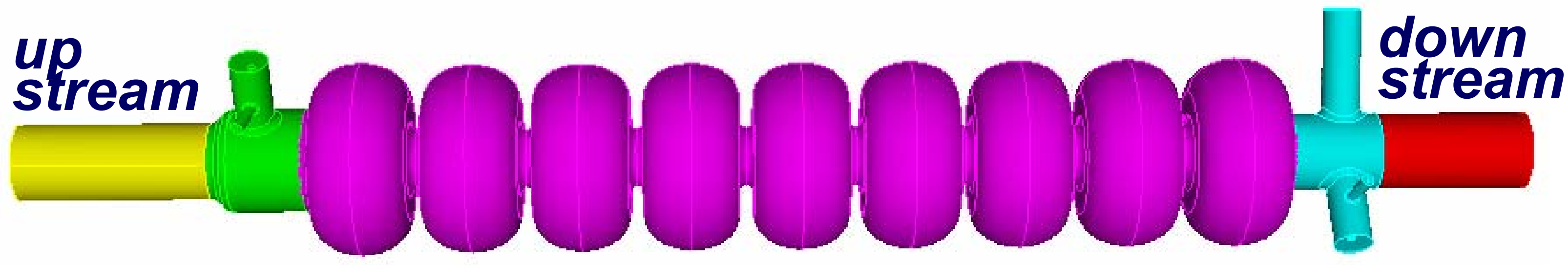
Qe

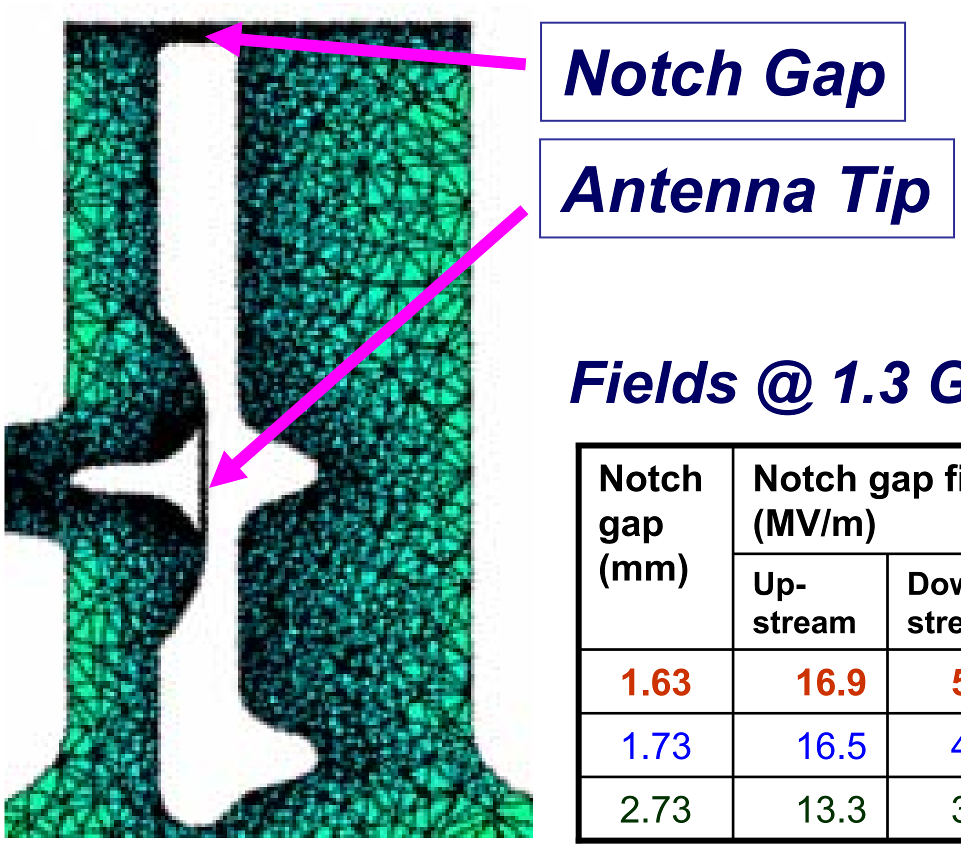


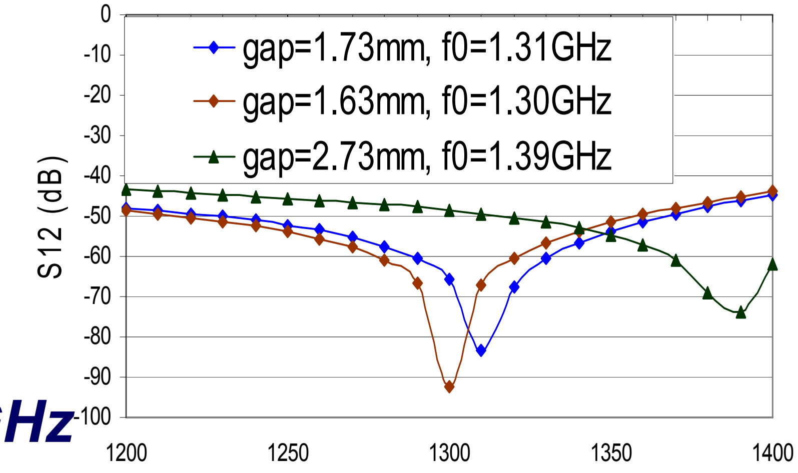
R/Q



ICHIRO HOM Coupler – Notch Filter





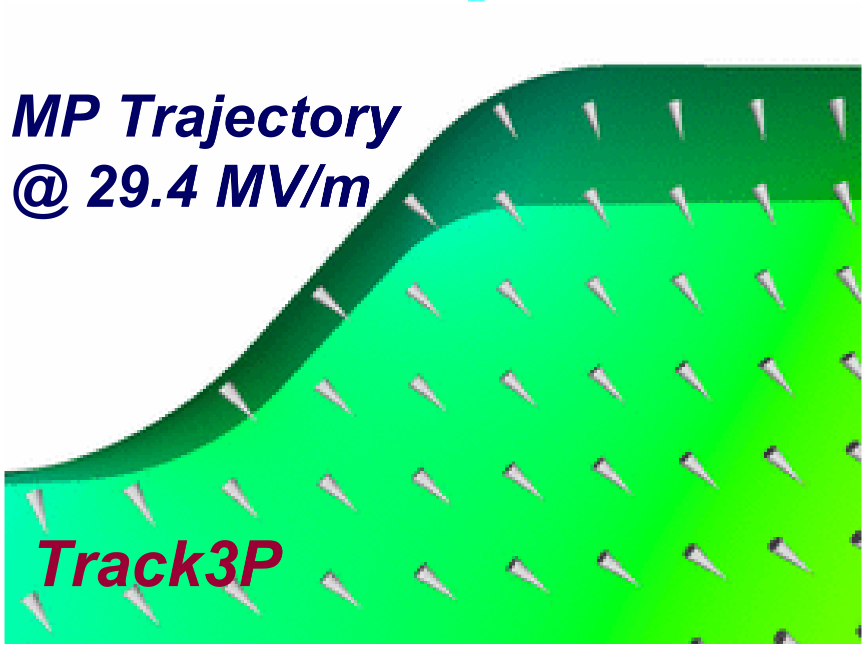


Fields @ 1.3 GHz

Notch gap (mm)	Notch gap field (MV/m)		Antenna tip Field (MV/m)		Qext of HOM port @1.3GHz	
	Up-stream	Down-stream	Up-stream	Down-stream	Up-stream	Down-stream
1.63	16.9	5.0	0.8	0.2	6.1e+9	1e+12
1.73	16.5	4.9	1.4	0.4	5.2e+8	9.e+9
2.73	13.3	3.9	6.1	3.0	1.4e+7	1.7e+8

ICHIRO Cavity – Multipacting Barriers

- ***ICHIRO** single cell reached ~ 50 MV/m @ KEK*
- *9-cell cavities can't process above 30 MV/m*

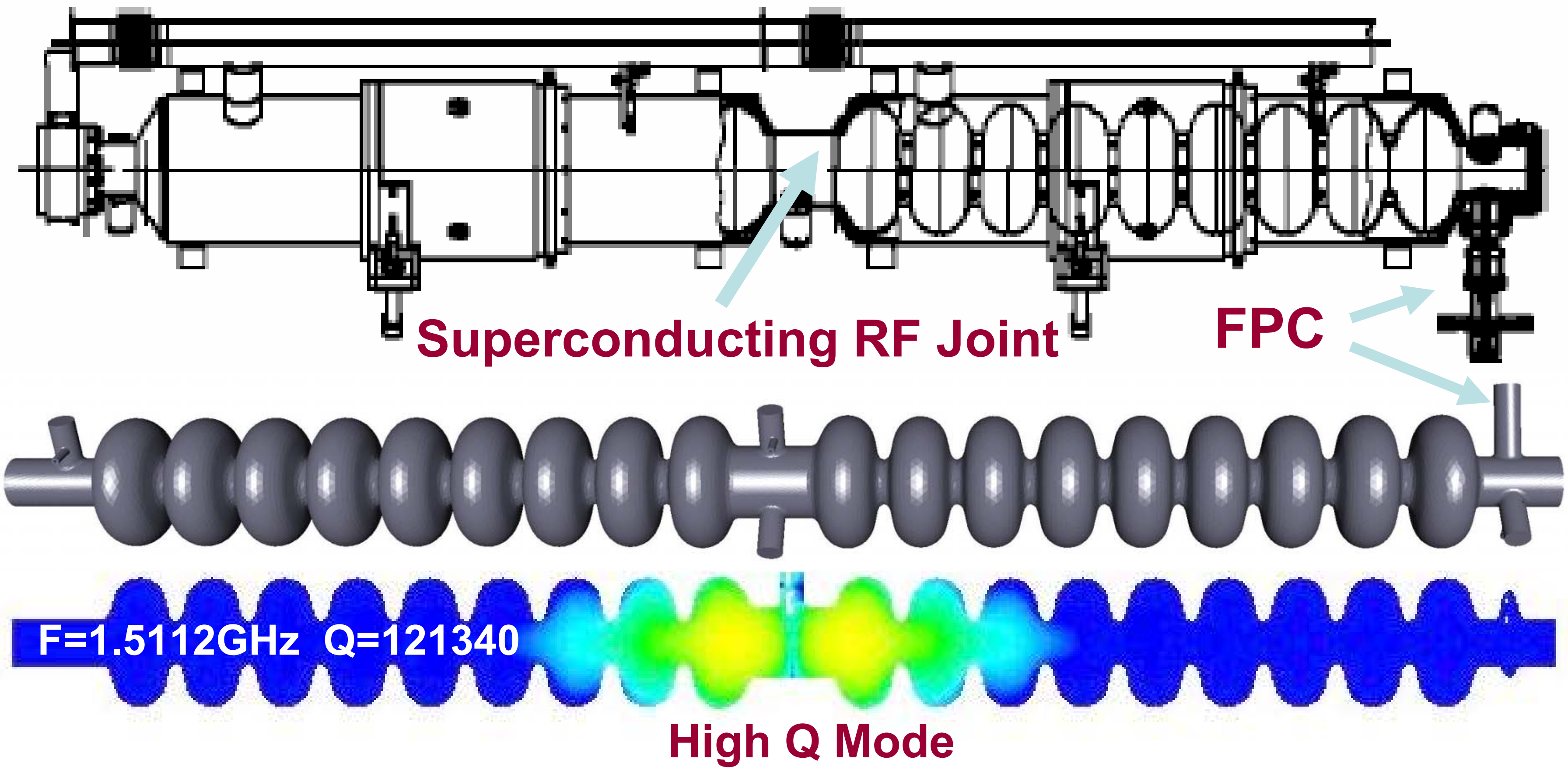


SLAC simulated MP levels [MV/m]	ICHIRO#0 X-ray barrier [MV/m]
	7.4, 9.0, 7-17
12.0	11-29.3, 12-18
13.9	13, 14, 14-18, 13-27, 13-27
16.8	(17, 18)
21.2	20.8
29.4	28.7, 29.0, 29.3, 29.4

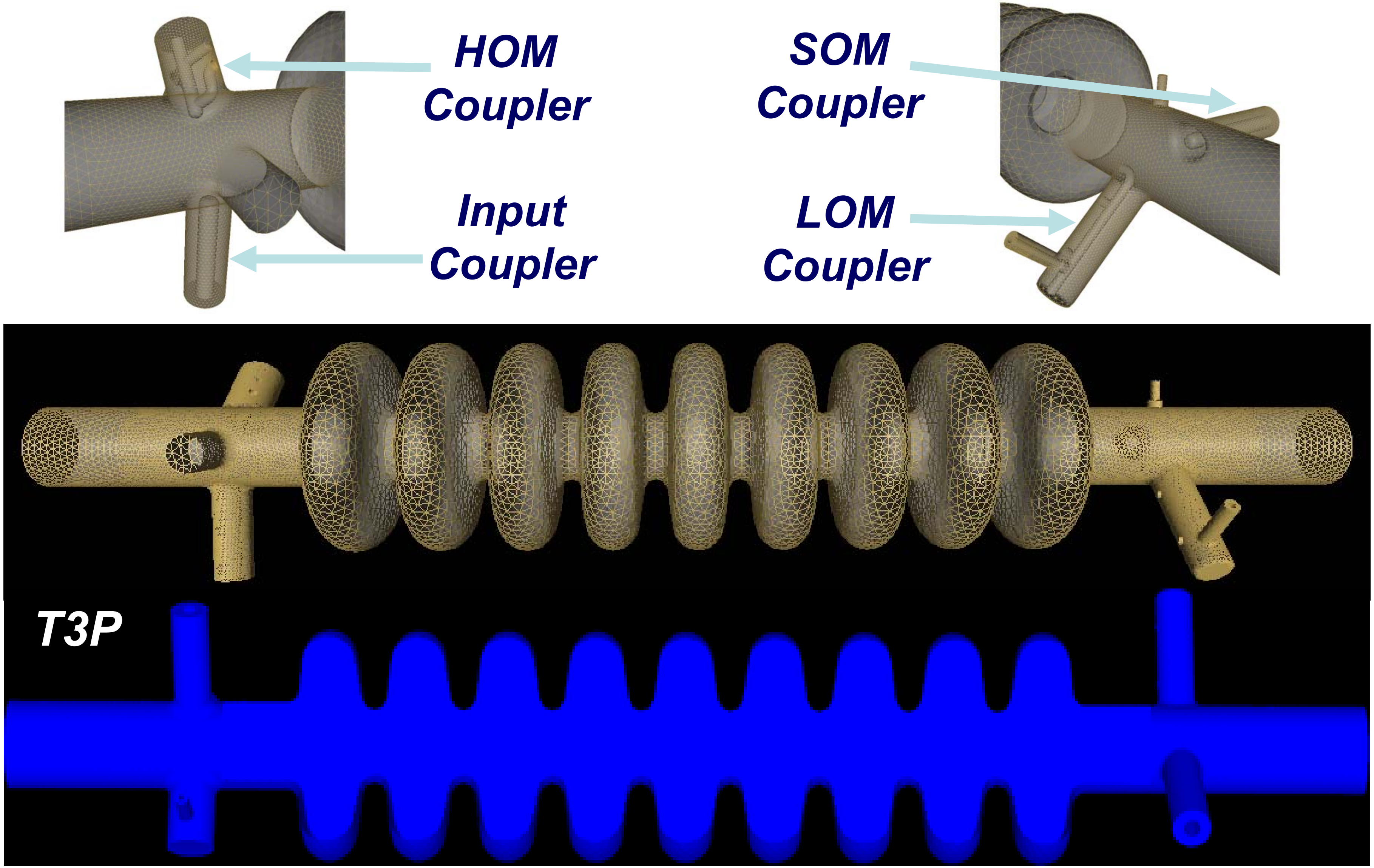
K. Saito (KEK)

Super-Structure – Trapped Modes

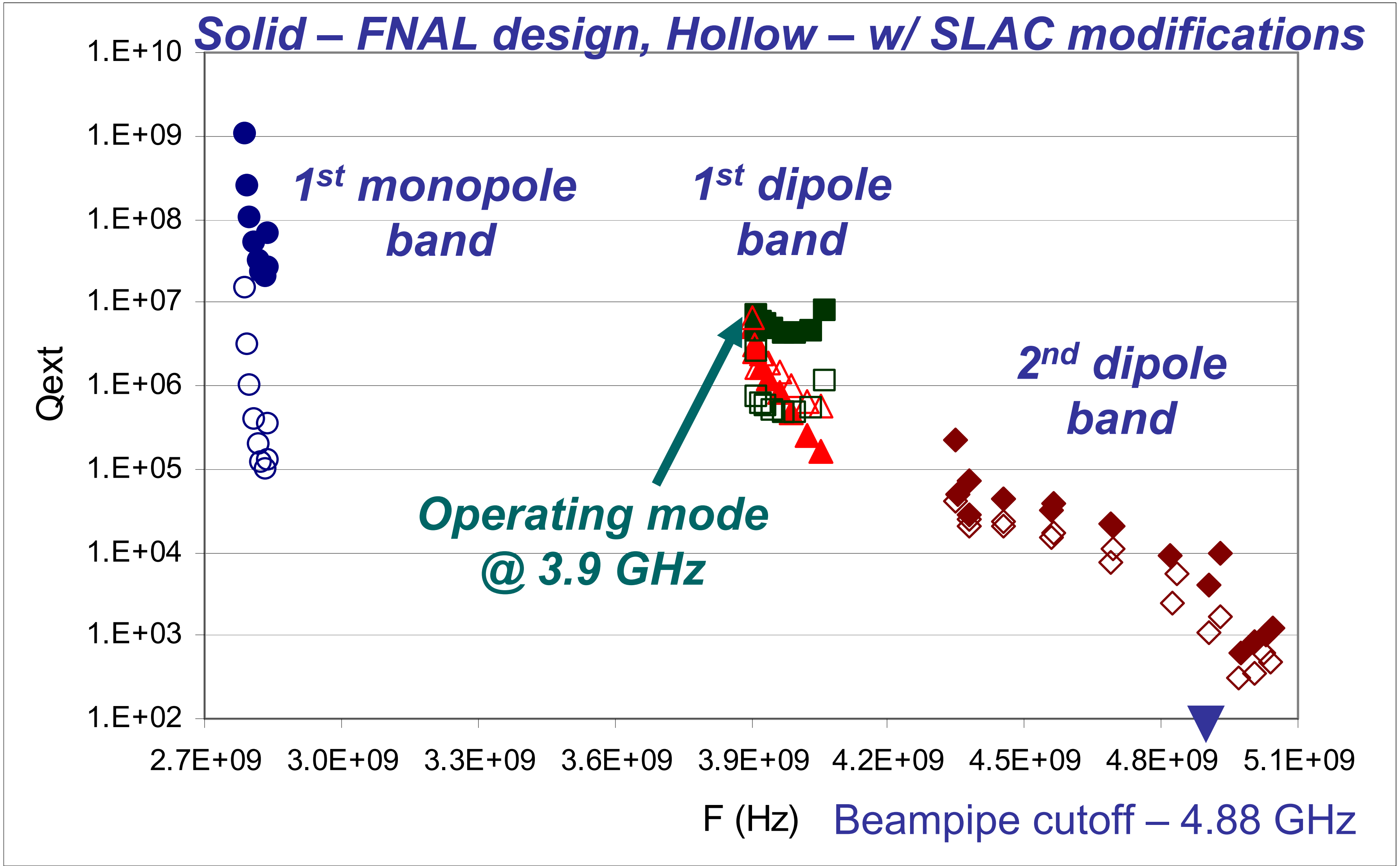
A <u>Super-Structure</u> combines two multi-cell cavities through a weakly coupling beam pipe into 1 unit to reduce # of input couplers and increase packing factor (w/ JLab)



FNAL 3.9 GHz Deflecting Cavity Design



Omega3P Analysis and 1st Improvements



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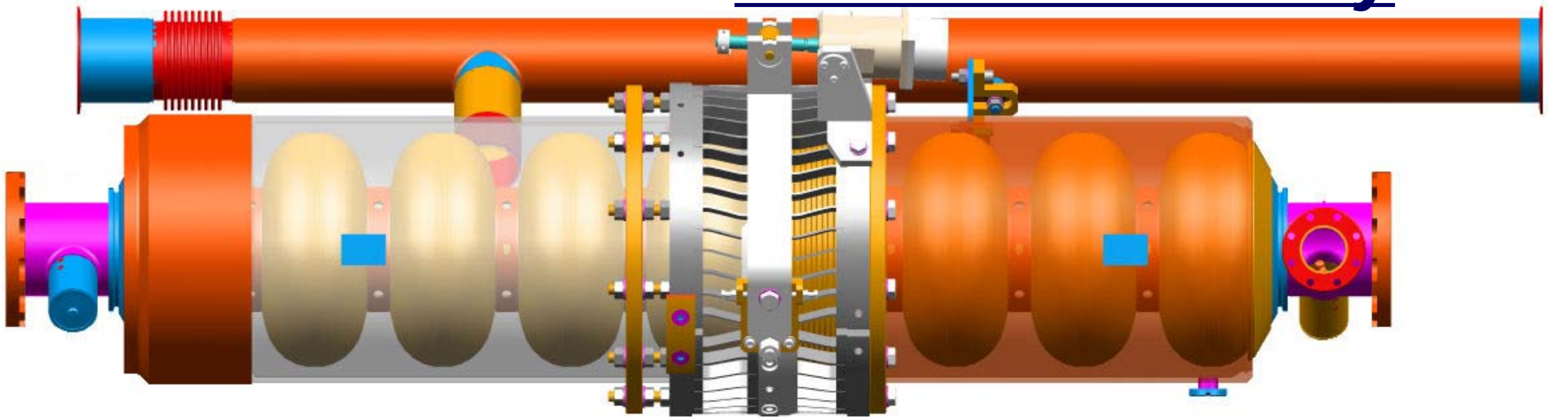
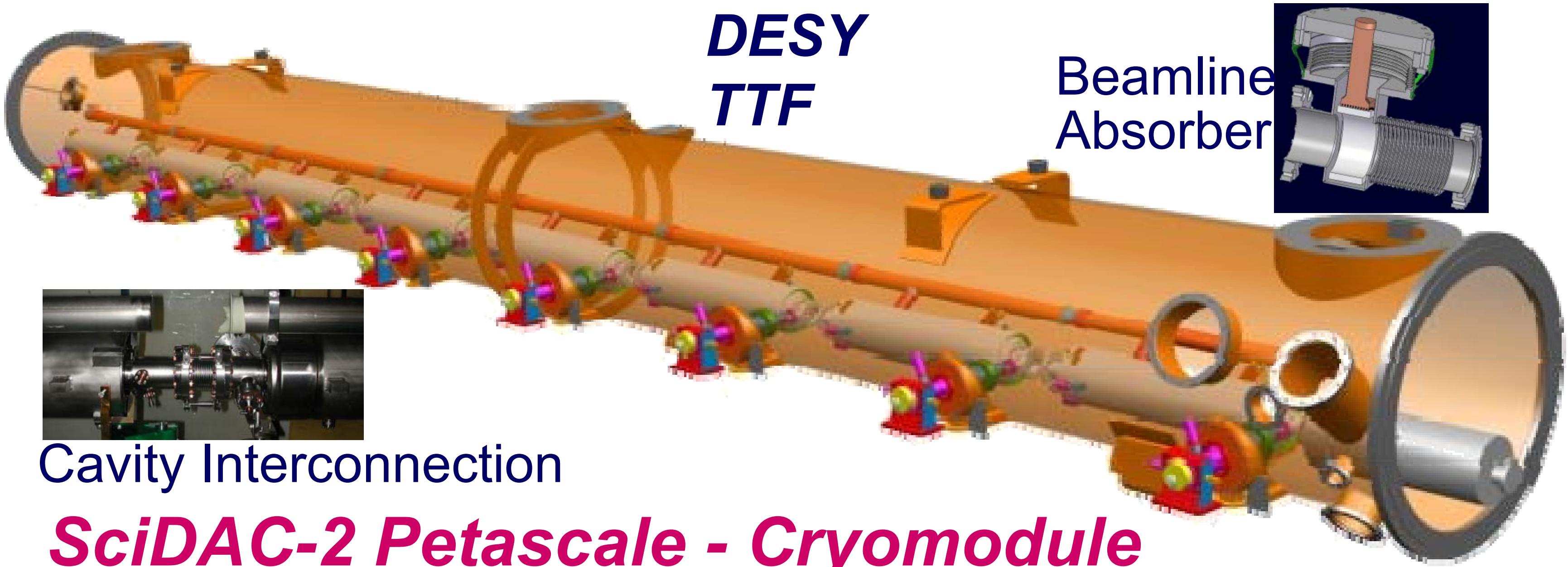
ILC – Cryomodule (8 Cavities)

SciDAC-1 Terascale - 9-cell SCRF Cavity



DESY TTF



Beamline Absorber

Cavity Interconnection

SciDAC-2 Petascale - Cryomodule

Cryomodule Computational Estimates

8-cavity cryomodule – 5 M quadratic elements, 30 M DOFs

For Omega3P (Mode Analysis):

To compute 1000 modes, given time complexity is about $N^{1.5}$ where N is number of DOFs, 2000 wall-clock hours required on a 1 teraflop computer with enough memory or ***2 hours on a 1 petaflop-peak machine per run***

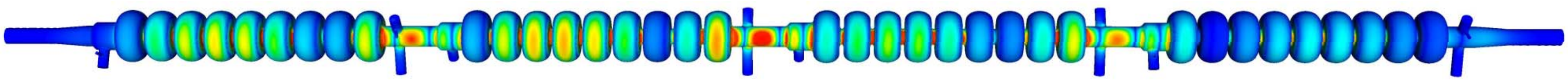
For T3P (Wakefields):

To simulate 1000ns, 3000 wall-clock hours needed on 1 teraflop computer, or
3 hours on a 1 petaflop-peak machine per run

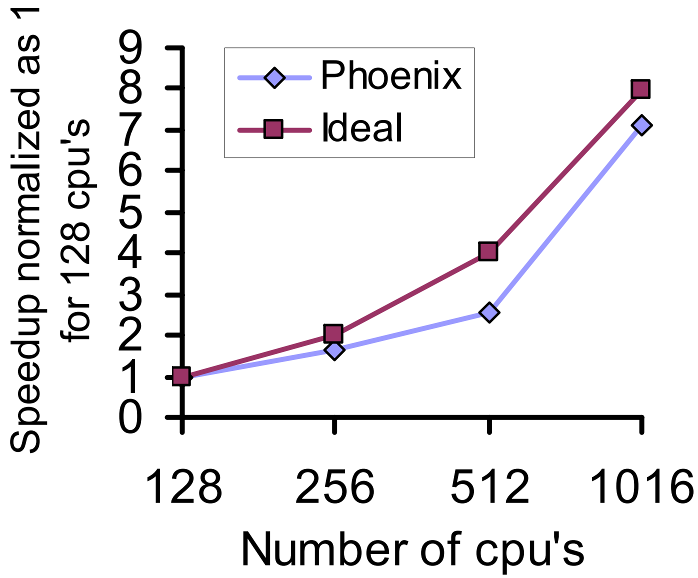
Towards Petascale Simulation

Omega3P - *A nonlinear eigensystem with > 15 million of DOFs was solved within 10 hours on 768 CPUs with 276 GB memory on NERSC's Seaborg as a 1st step towards modeling an entire cryomodule:*

4-cavity Structure



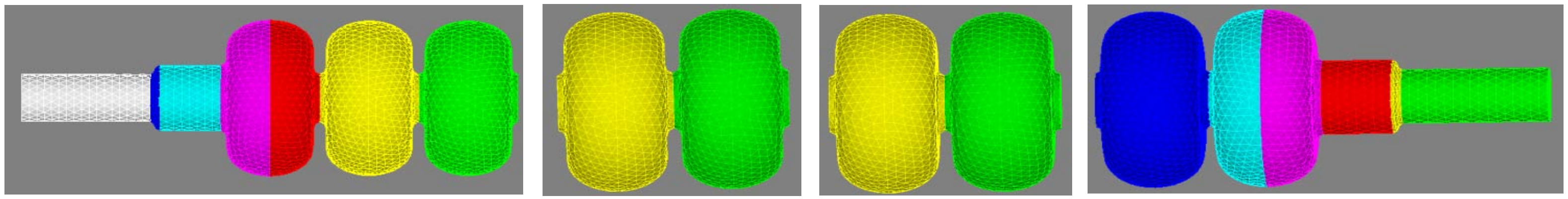
T3P – *Code has been improved to allow scalability to more than 1000 CPUs for a medium-size problem with close to linear speedup on NCCS's Phoenix*



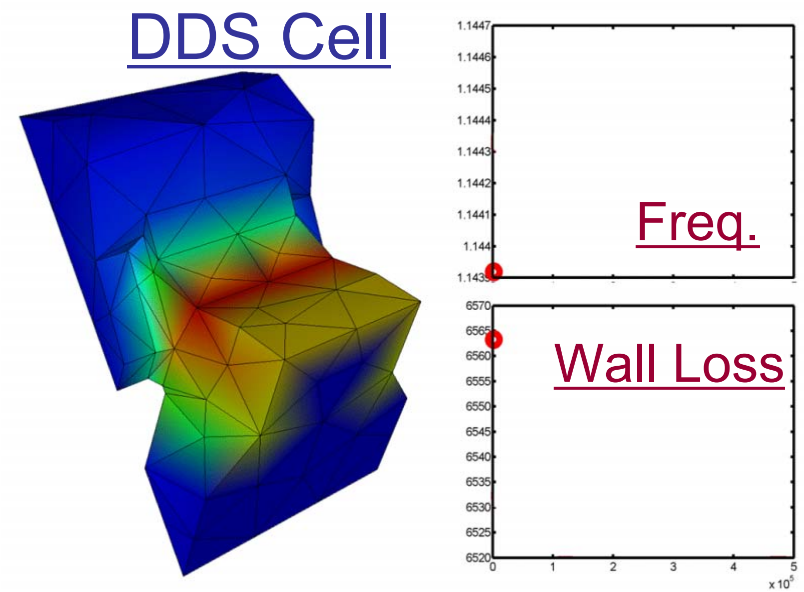
Parallel Meshing and Adaptive Refinement

Parallel meshing - *CAD-based partitioning is being used to generate LARGE meshes such as those required for modeling a chain of cavities within an ILC cryomodule*

Processor: 1 2 3 4



AMR - *Optimizes computing resources and increases solution accuracy through adaptive refinement using local error indicator based on gradient of electromagnetic energy density in curved domain*



ILC GDE, Cray XT3 & SciDAC-2