Towards Simulation of Electromagnetics and Beam Physics at the Petascale

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NCCS, ORNL

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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***

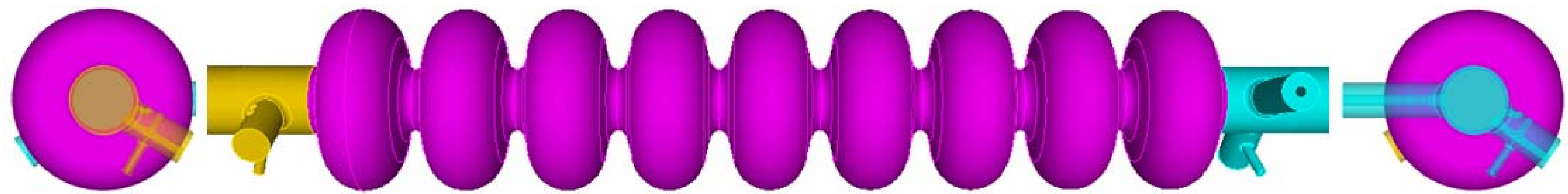
LCLS

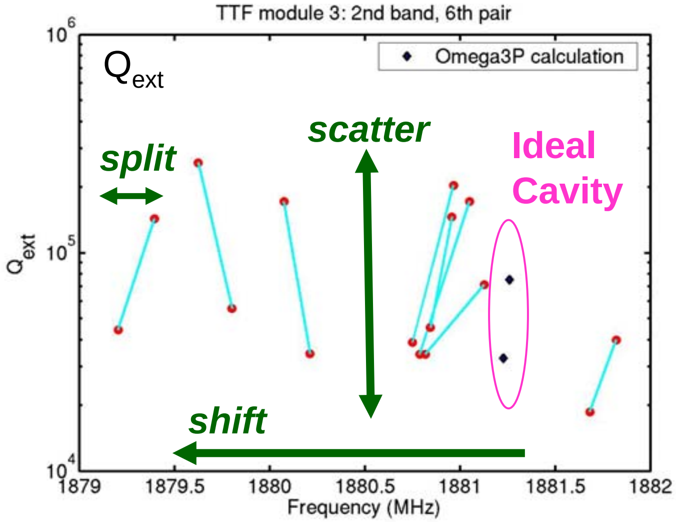
- ***RF gun – emittance calculations using PIC codes***

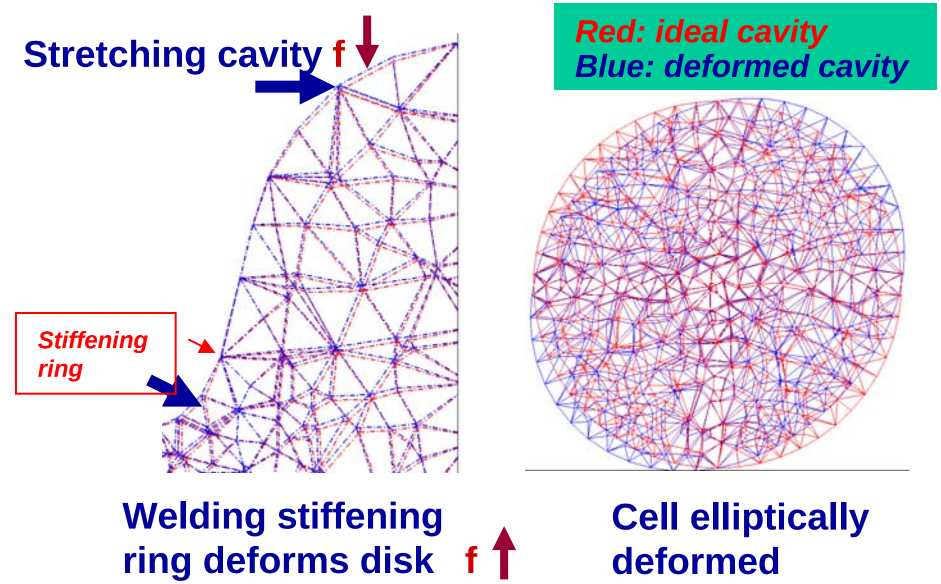
SNS

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

Imperfection Studies for ILC TDR Cavity







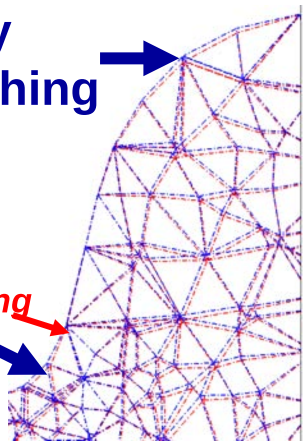
- Determine shape defromation from measured cavity data
- Evaluate wakefield effects on beam dynamics due to cavity imperfections

Effects of Cavity Imperfection

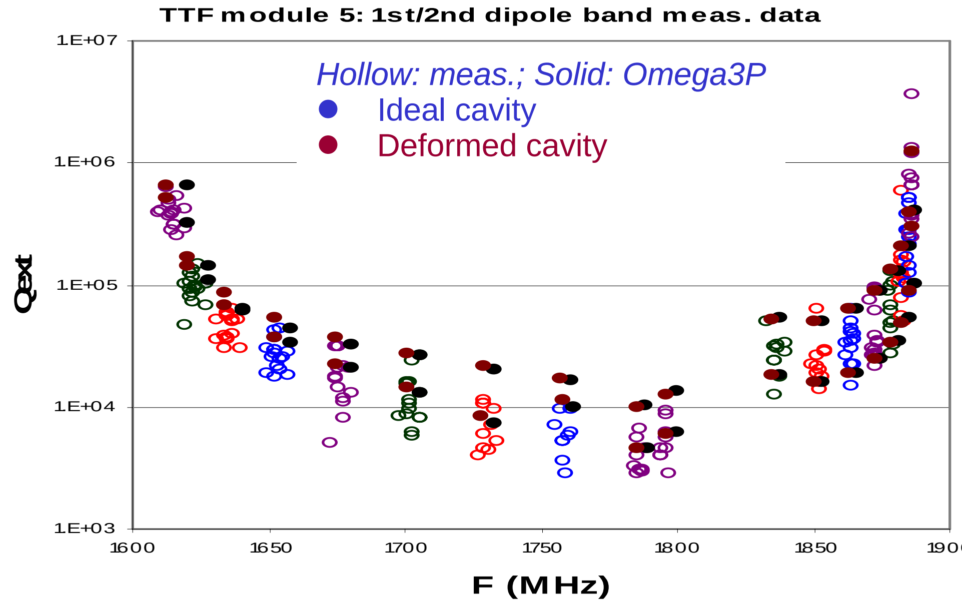
Cavity tuning due to fabrication errors

Cavity stretching

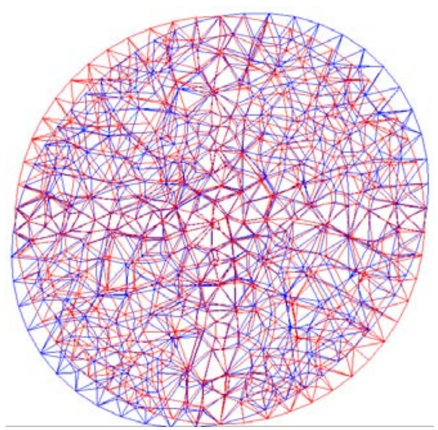
Stiffening ring



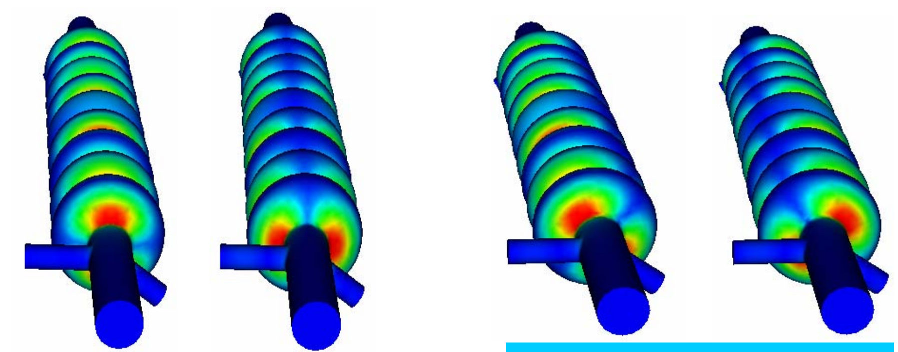
Frequency shift



Elliptical cell shape



Mode x-y coupling
& Qext scattering



ideal cavity

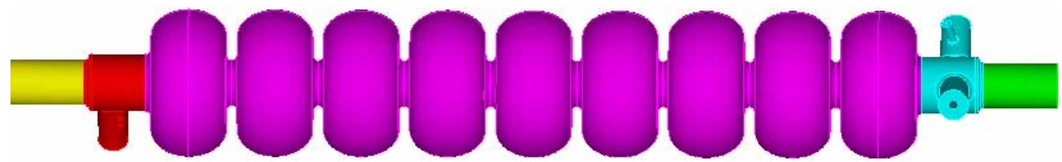
elliptically
deformed cavity

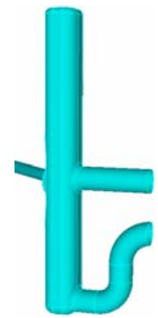
Poster: WEPMS048 - Modeling Imperfection Effects of TESLA Cavity on Dipole Modes -
L. Xiao et al.

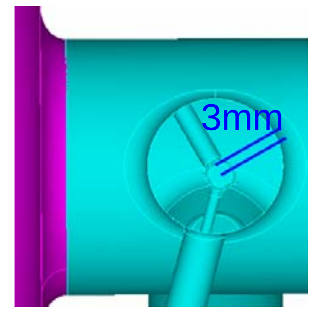
LL Cavity End-group Design

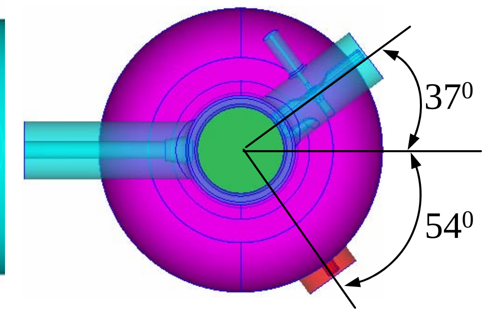
LL Shape
- >15% higher R/Q (1177 ohm/cavity)
- >12% lower Bpeak/Eacc ratio
- 20% lower cryogenic heating

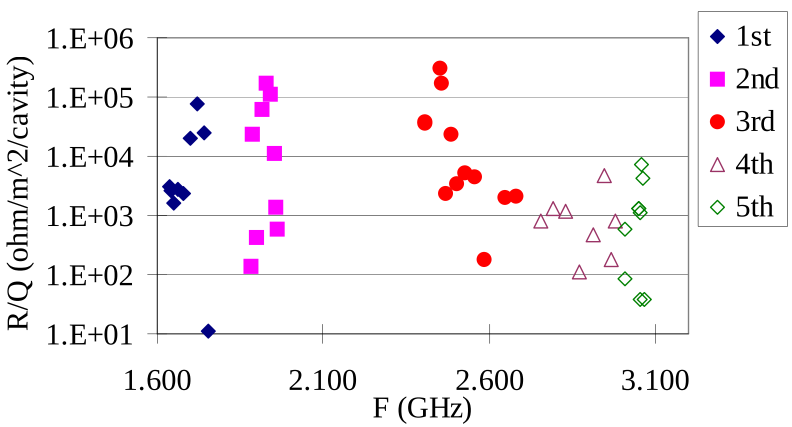
Effective damping achieved by optimizing:
- End-group geometry to increase fields in coupler region
- Loop shape and orientation to enhance coupling
- Azimuthal location for x-y mode polarization



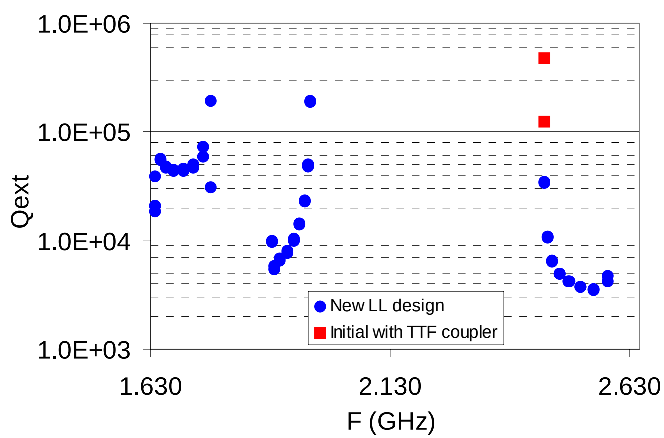




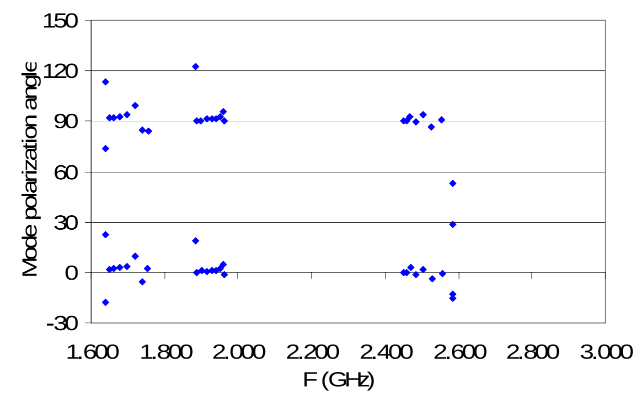




R/Q



Qext



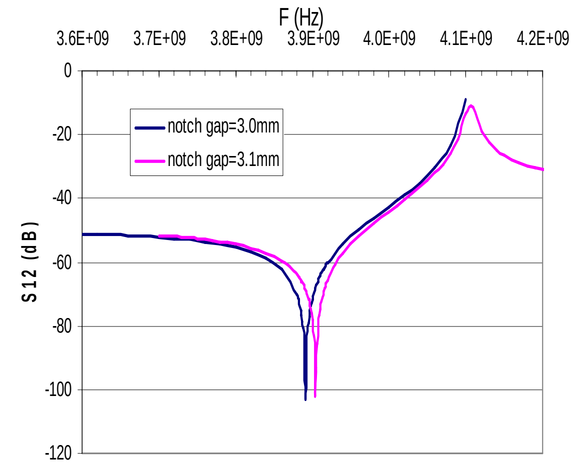
Polarization

Poster: WEPMS042 - Optimization of the Low-Loss SRF Cavity for the ILC - Z. Li et al.

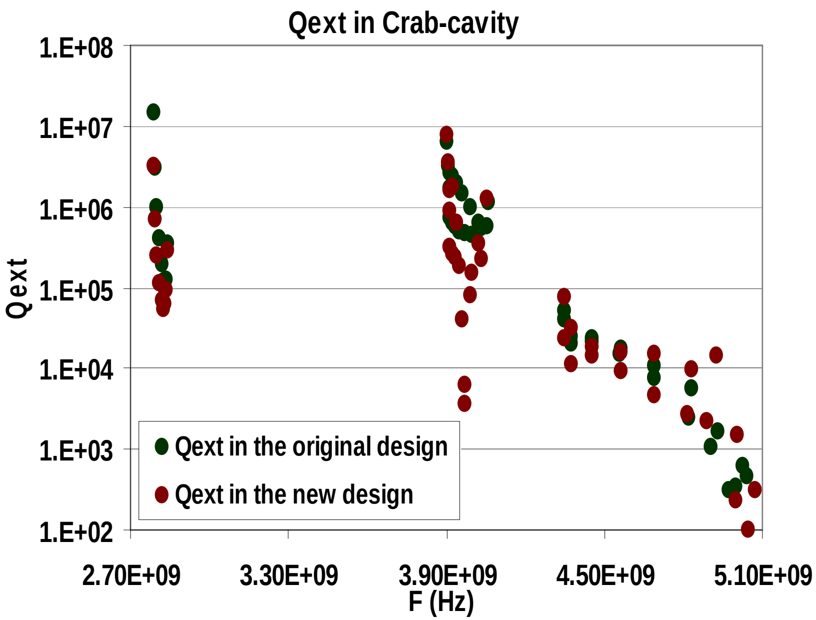
Crab Cavity Design for ILC BDS

Improved FNAL design

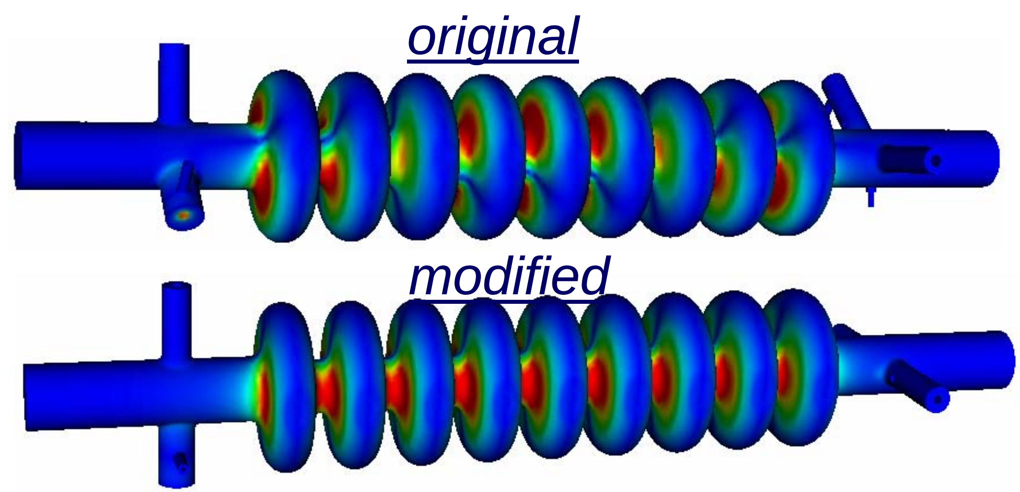
- *leads to better HOM, LOM and SOM damping*
- *reduces HOM notch gap sensitivity (to 0.1 MHz/μm from original 1.6 MHz/μm)*
- *eliminates LOM notch filter*
- *avoids x-y SOM coupling*



Notch gap sensitivity



Omega3P damping calculation

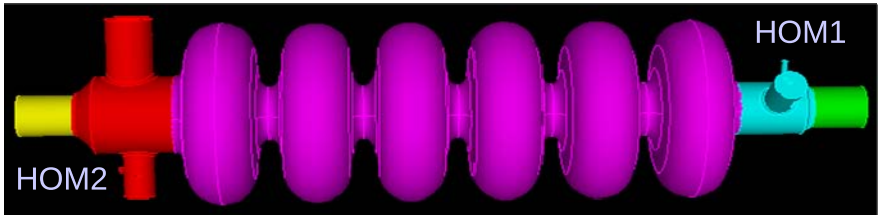


SOM x-y coupling

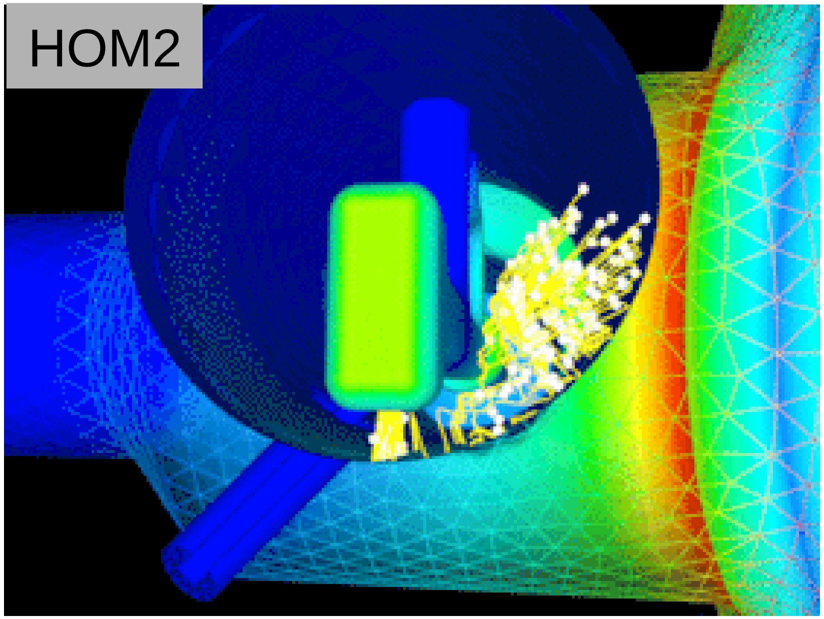
A copper model is being built in UK lab based on this design.

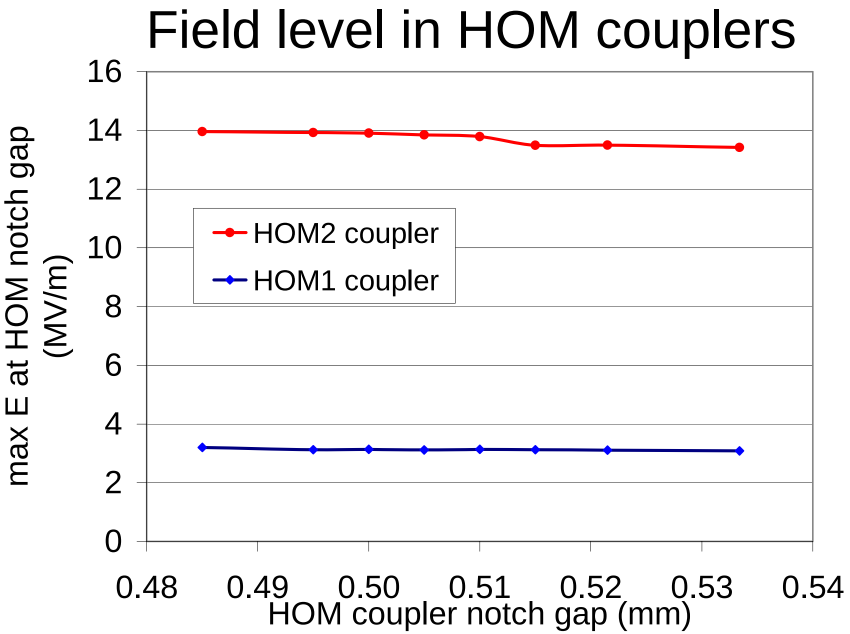
Poster: WEPMS050 - Crab Cavity Design for the ILC – L. Xiao et al.

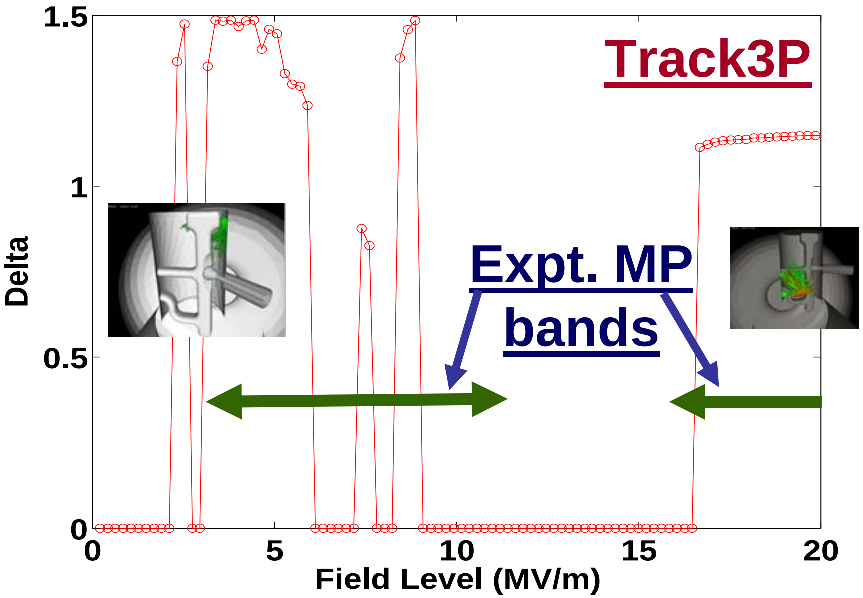
Multipacting in SNS HOM Coupler



- 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

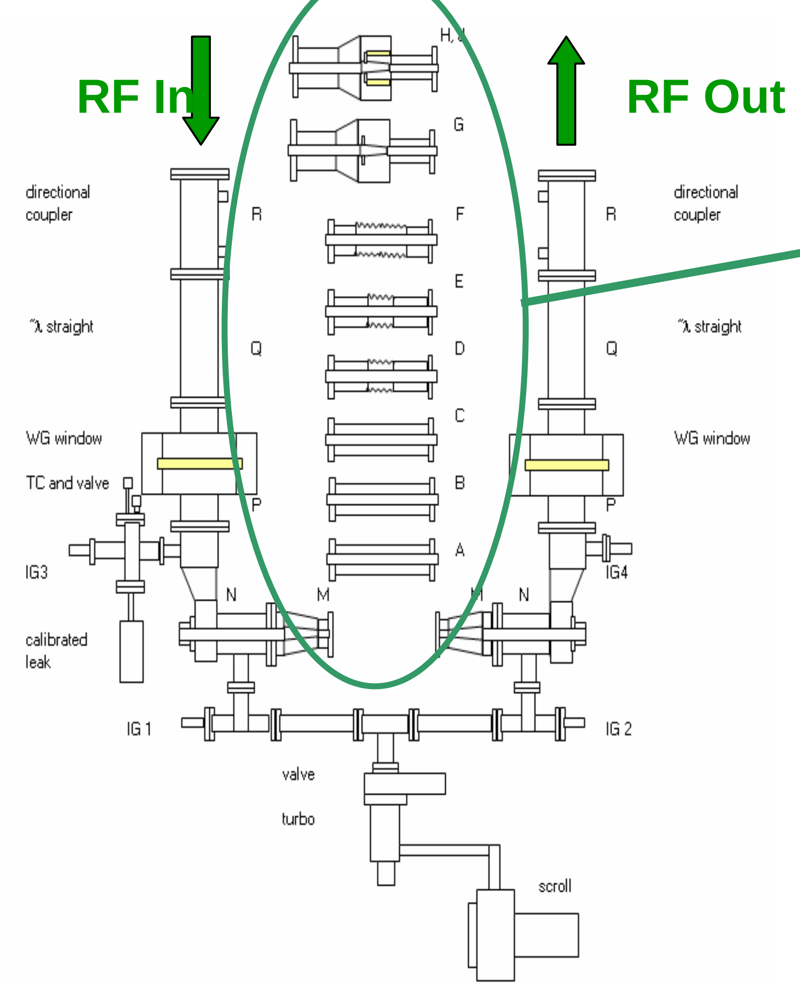


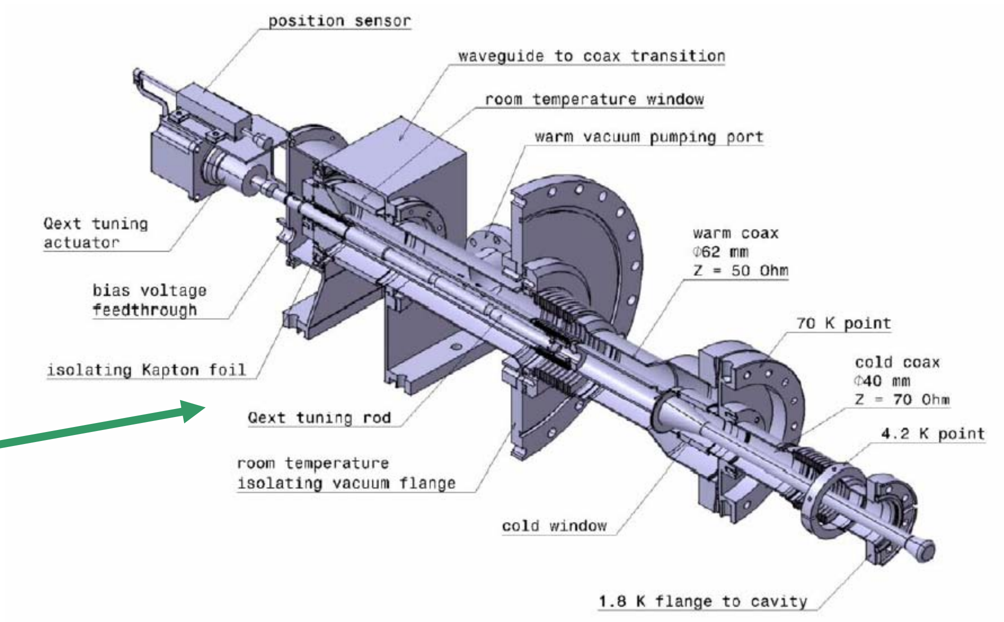


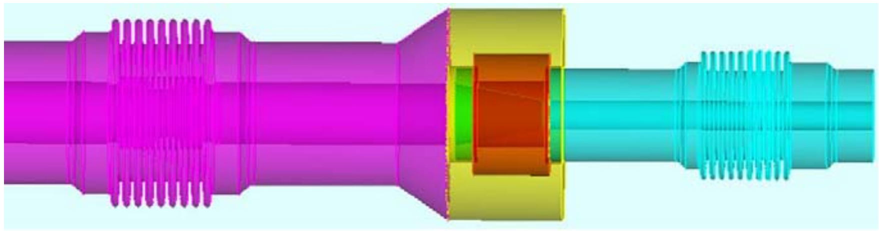


TTFIII Coupler – Multipacting Analysis

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



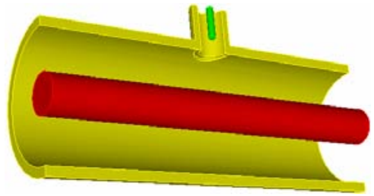




Track3P model

Mulitpacting in Coax of TTFIII Coupler

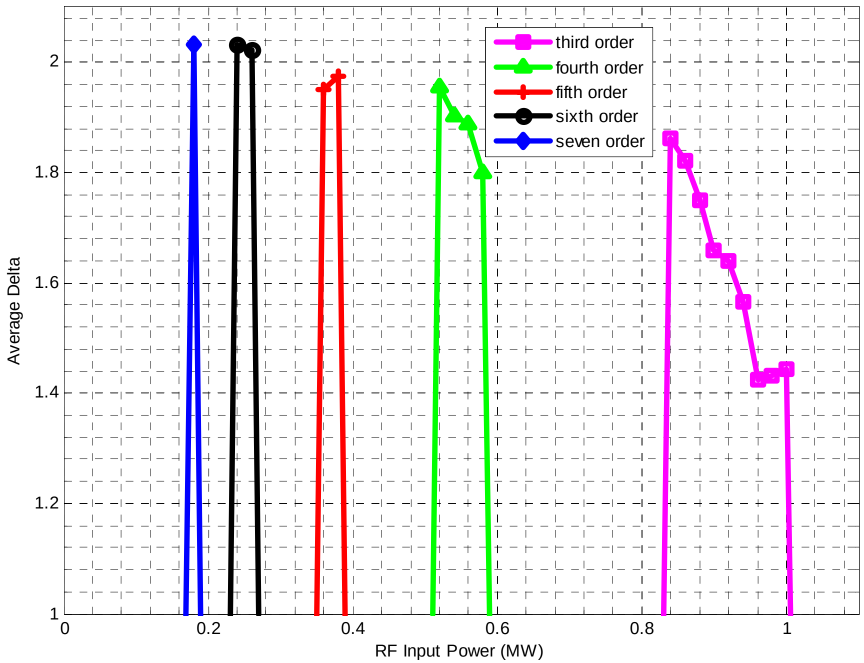
Cold coax

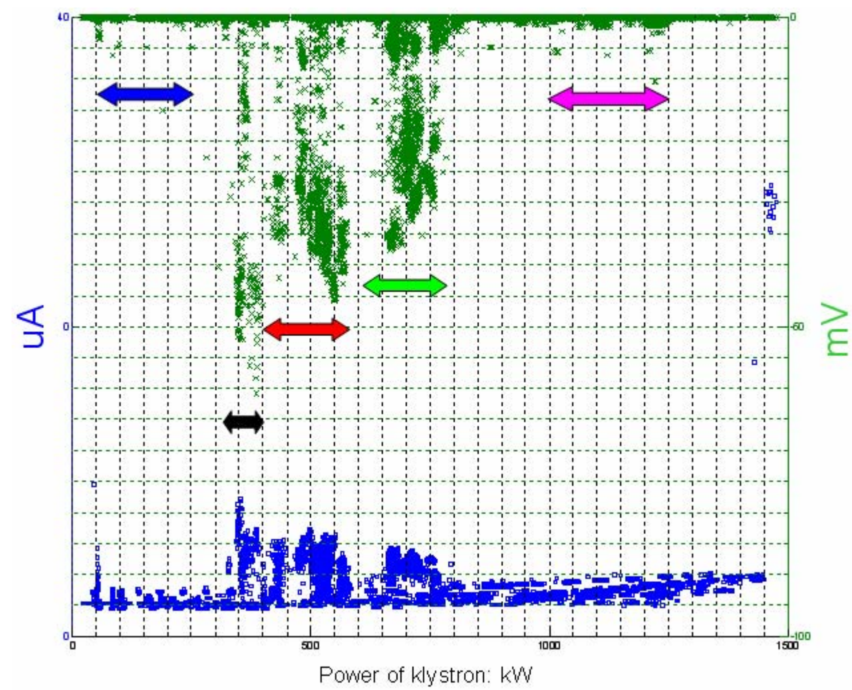


(F. Wang, C. Adolphsen, et. al)

After high power processing

Track3P simulation

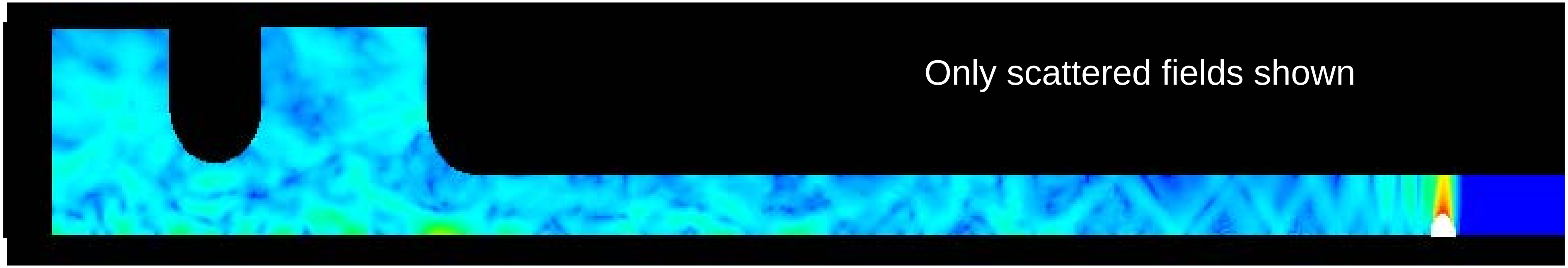




Simulated power (kW)	170~190	230~270	350~390	510~590	830~1000
Power in Coupler (kW)	43~170	280~340	340~490	530~660	850~1020
klystron power (kW)	50~200	330~400	400~580	620~780	1000~1200

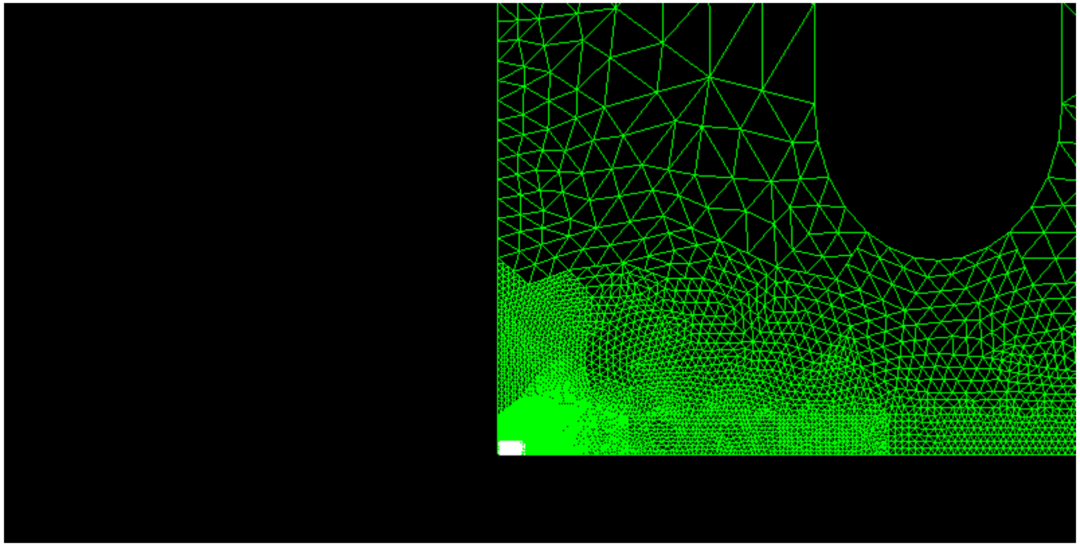
Posters: WEPMS041 - Multipacting Simulations of TTF-III Coupler Components – L. Ge et al.

Pic2P: Parallel FE 2.5D EM PIC Code

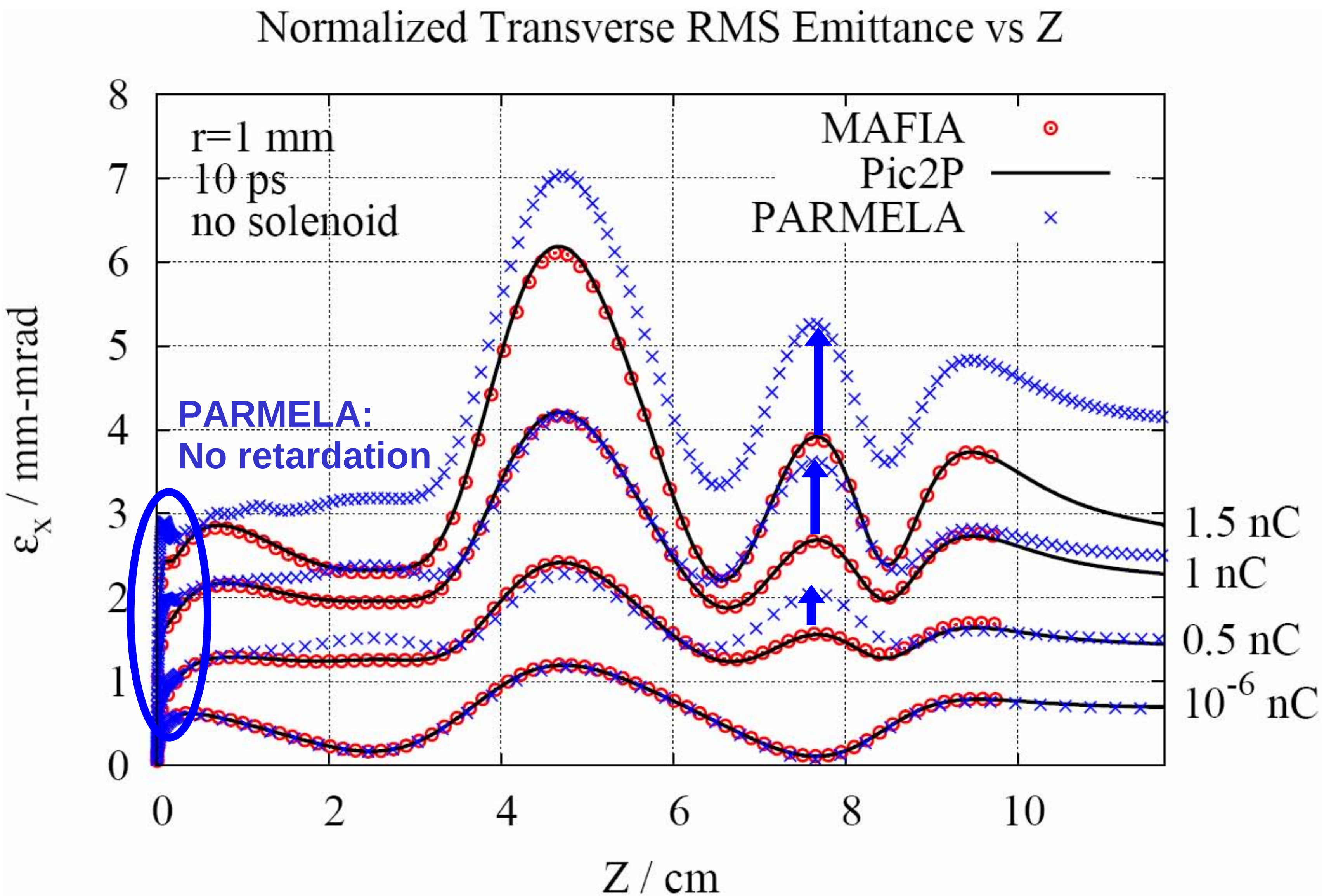


Pic2P: Parallel FE EM PIC code from first principles

- **Fully self-consistent**
- **Conformal mesh**
- **Adaptive *p*-refinement**
- **Up to 6th order basis**
- **Highest efficiency**
- **3D in development**

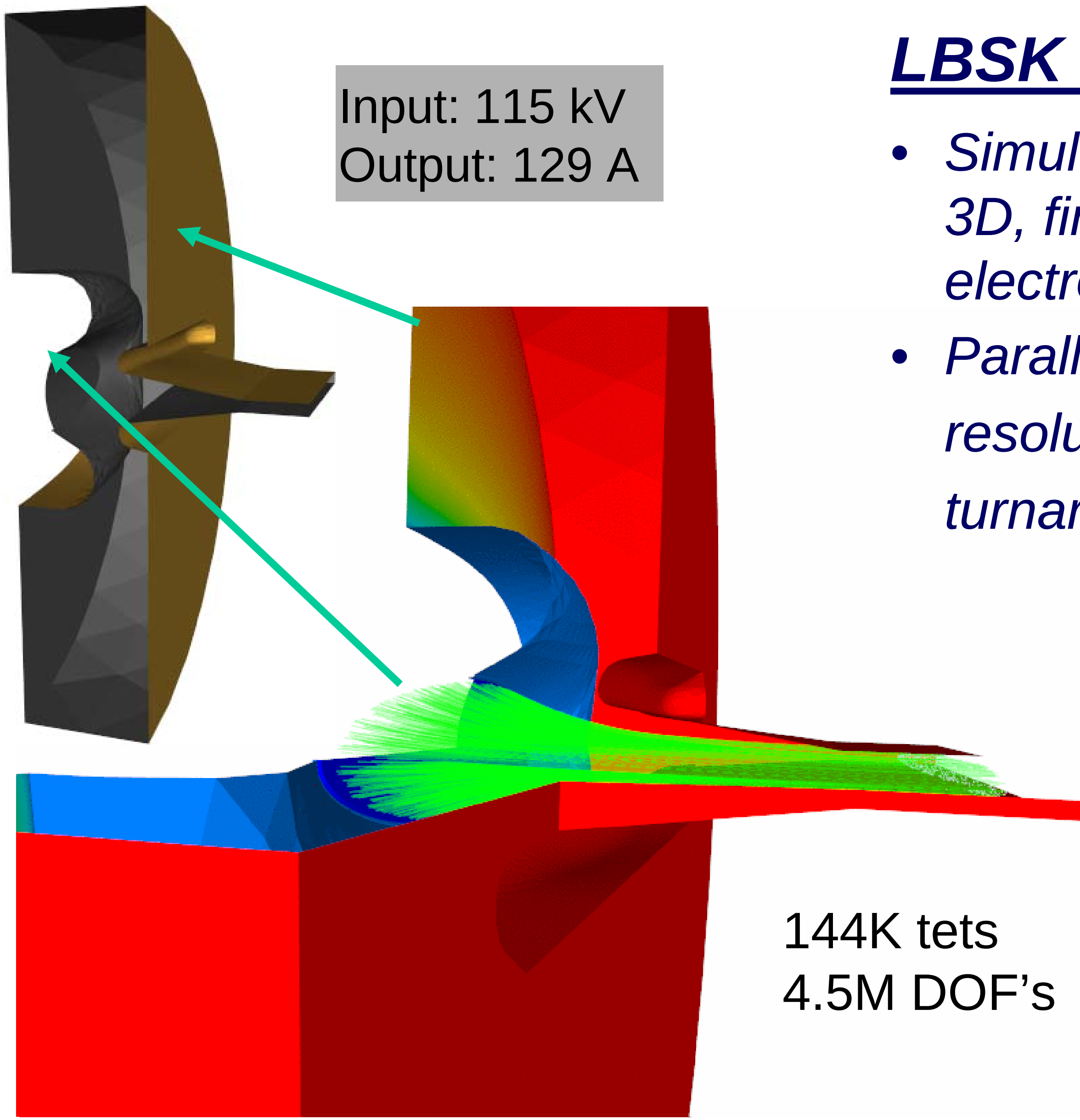


LCLS RF Gun Emittance



Talk: TUODC03 - Parallel Finite Element Particle-In-Cell Code for Simulations of Space-charge Dominated Beam-Cavity Interactions – Arno Candel et al.

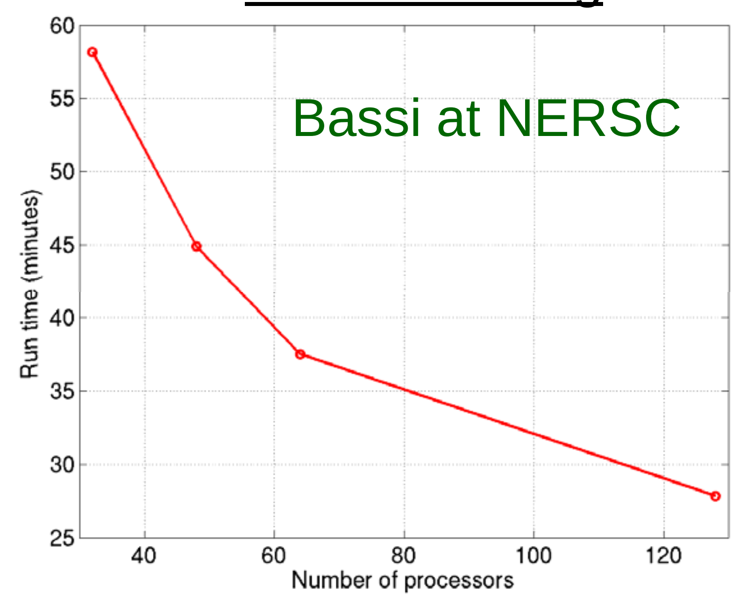
L-Band Sheet Beam Klystron



LBSK gun –

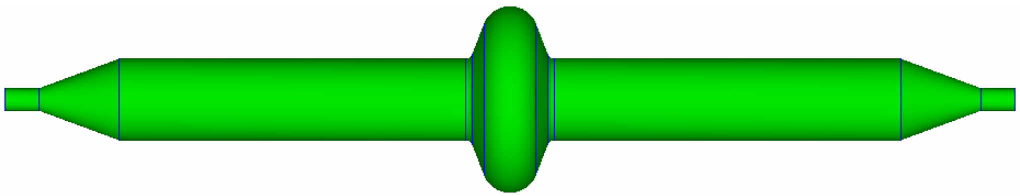
- *Simulated using GUN3P, a parallel, 3D, finite-element (up to 4th order) electron trajectory code*
- *Parallel computation allows high resolution simulation with fast turnaround time*

Parallel scaling

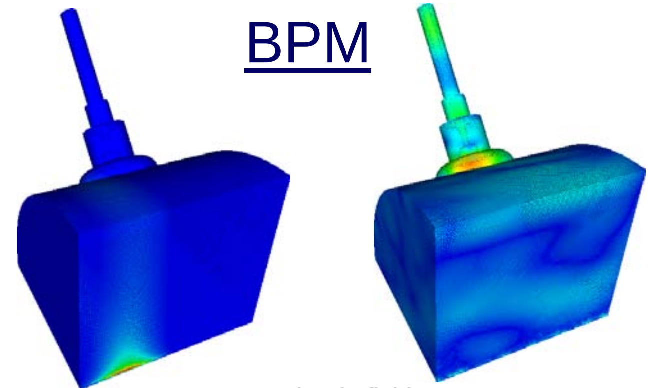


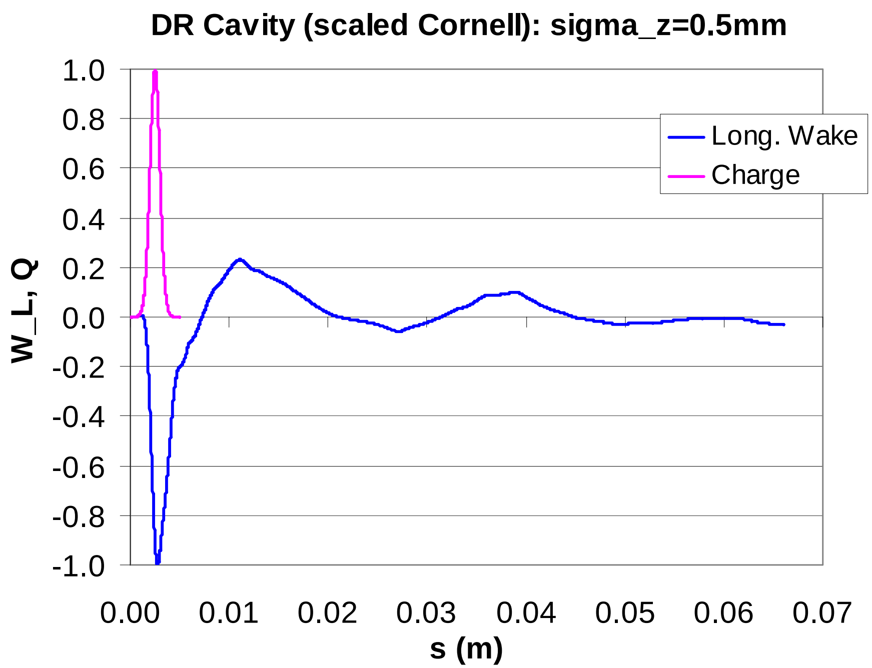
ILC Damping Ring Impedance Calculations

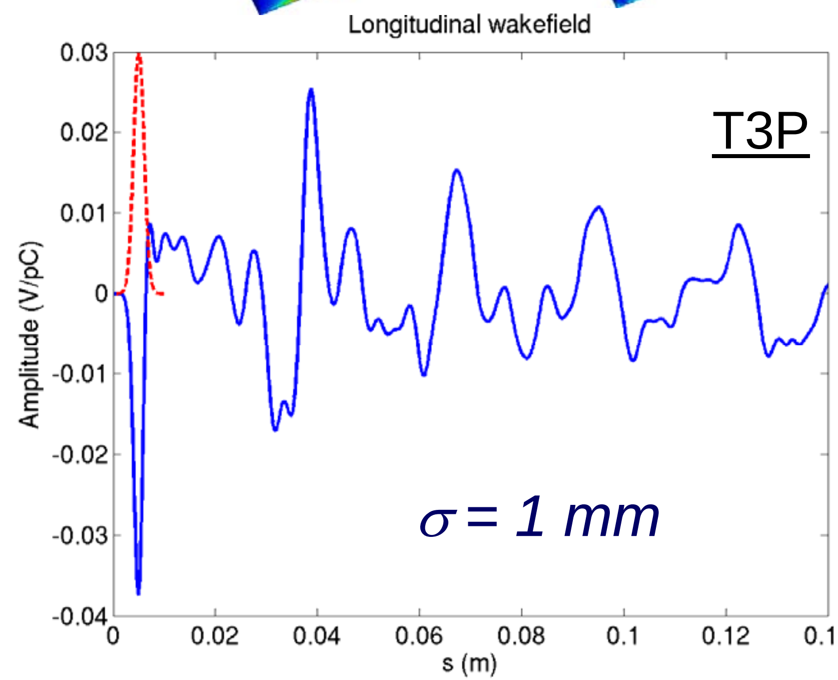
RF cavity



BPM







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

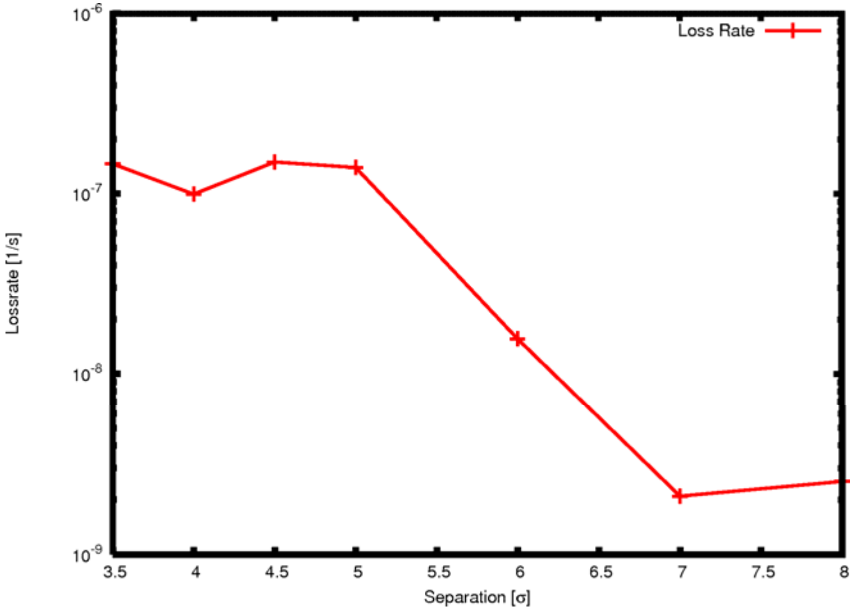
LHC beam-beam Effects

***Nimzovich** simulates strong-strong beam-beam interactions:*

- particle-in-cell for field computation
- full MAD-X compatible tracking
- several beam-beam models
- optimized for many parasitic crossings
- scales to thousands of processors
- currently benchmarking against wire-compensator experiments at RHIC

<u>High-resolution loss rate calculation for RHIC</u>

loss rate vs. beam separation



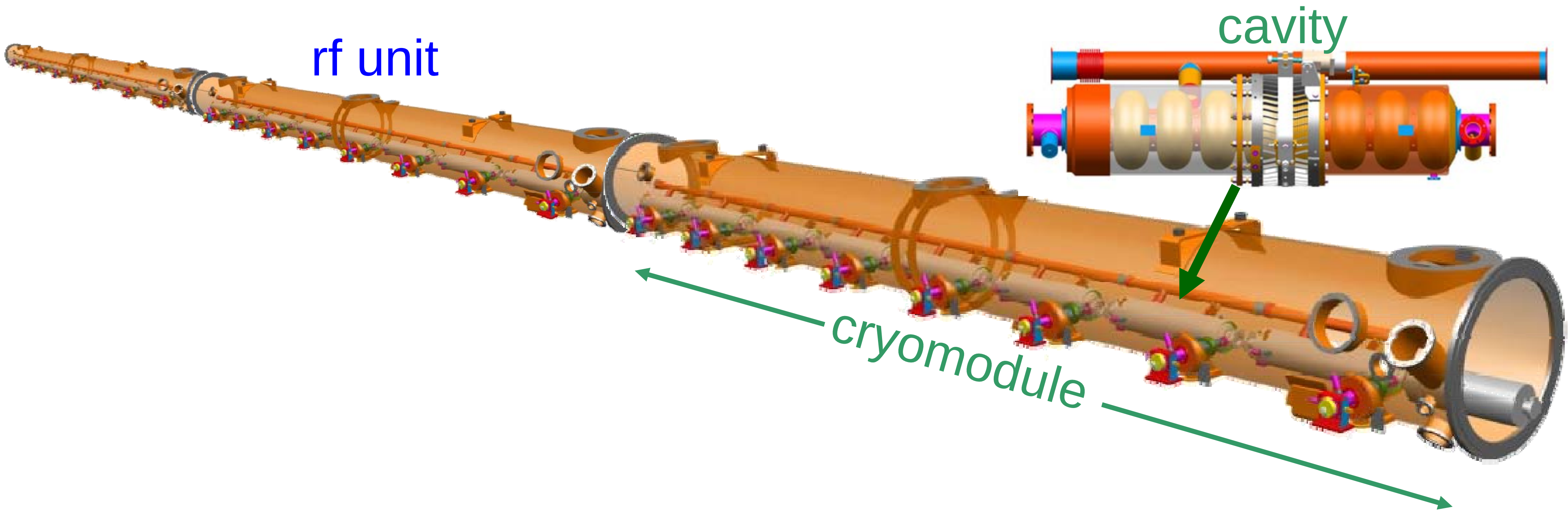
3 hours runtime using 64 processors

Poster: THPAS062 - Recent Progress in Beam-Beam Simulation Codes – A. Kabel et al.

SLAC

SciDAC Scientific Discovery through Advanced Computing

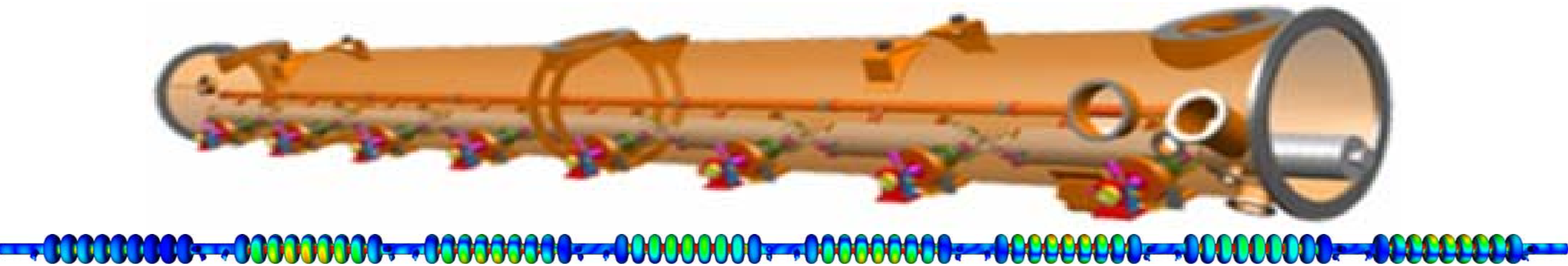
Modeling ILC Cryomodule & RF Unit



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 3rd 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*

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*

Recent Advances in Solver and Meshing

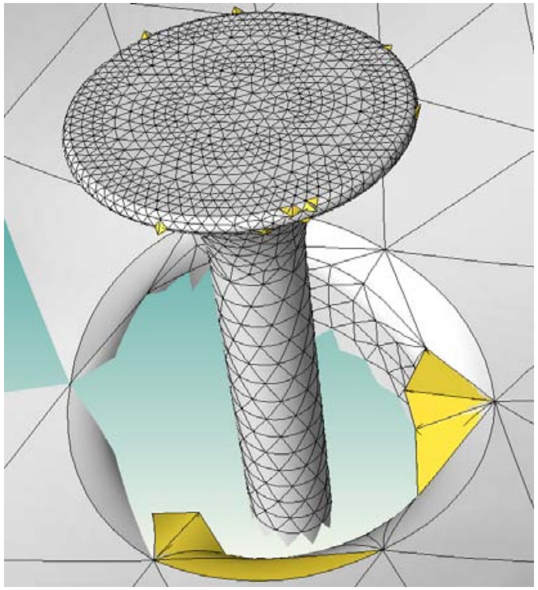
Linear Solver

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

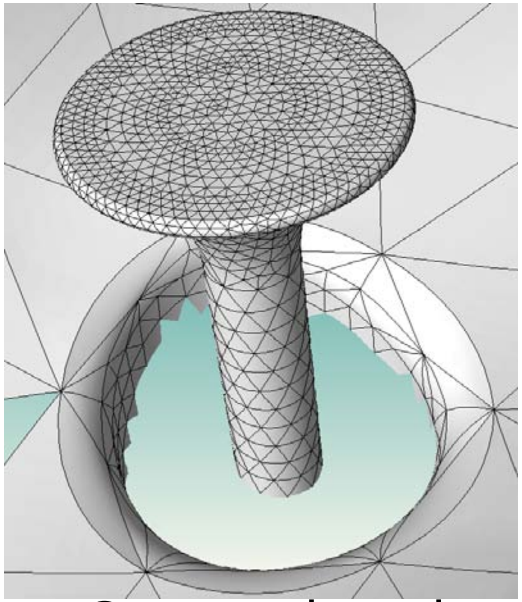
Method	Memory (GB)	Runtime (s)
MUMPS	155.3	293.3
MUMPS + single precision factorization	82.3	450.1

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

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

Related PAC07 Papers

TUODC03 - Parallel Finite Element Particle-In-Cell Code for Simulations of Space-charge Dominated Beam-Cavity Interactions – Arno Candel et al.

WEPMS041 - Multipacting Simulations of TTF-III Coupler Components – L. Ge et al.

WEPMS042 - Optimization of the Low-Loss SRF Cavity for the ILC - Z. Li et al.

WEPMS048 - Modeling Imperfection Effects of TESLA Cavity on Dipole Modes - L. Xiao et al.

WEPMS050 - Crab Cavity Design for the ILC – L. Xiao et al.

THPAS062 - Recent Progress in Beam-Beam Simulation Codes – A. Kabel et al