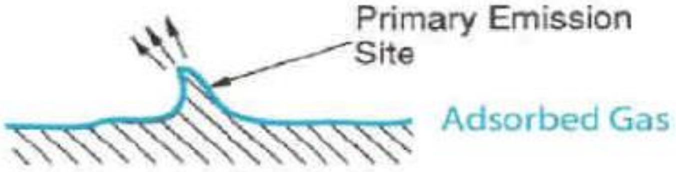
Fermilab

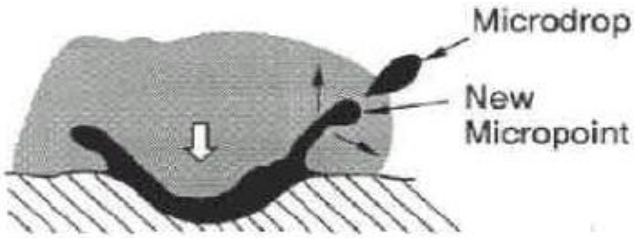
Managed by Fermi Research Alliance, LLC for the U.S. Department of Energy Office of Science

Advanced Simulation – Lecture 9

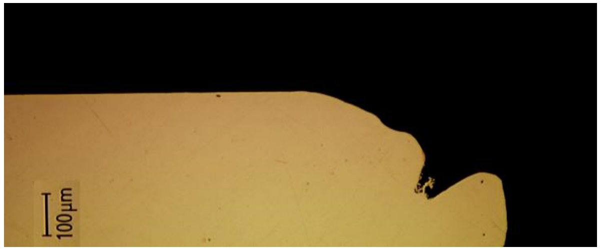
J.P. Holzbauer
Applied Electromagnetics - USPAS
2/3/2016

Conditioning limits

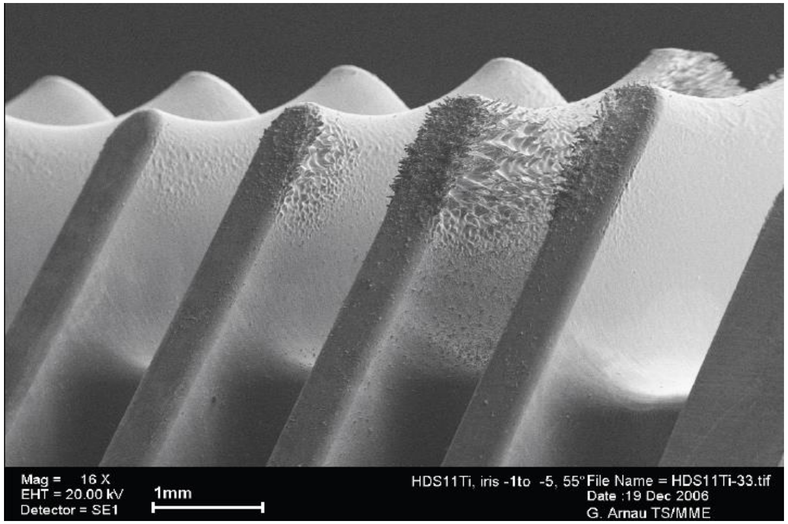




- More energy: electrons generate plasma and melt surface
- Molten surface splatters and generates new field emission points!
  $\Rightarrow$ limits the achievable field
- Excessive fields can also damage the structures
- Design structures with low E_{surf}/E_{acc}
- Study new materials (Mo, W)



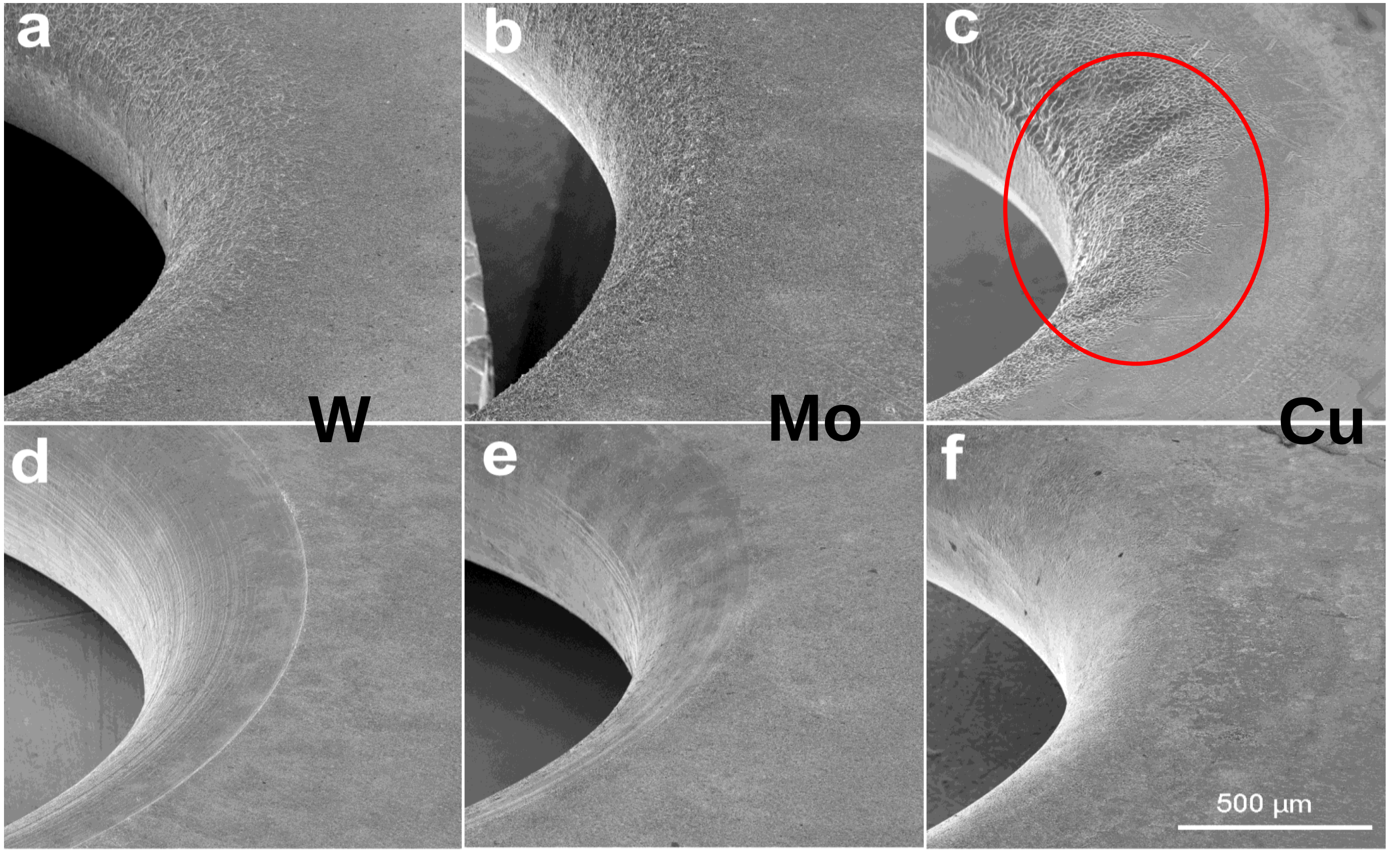
Damaged CLIC structure iris



Iris material tests in CTF2

First
iris

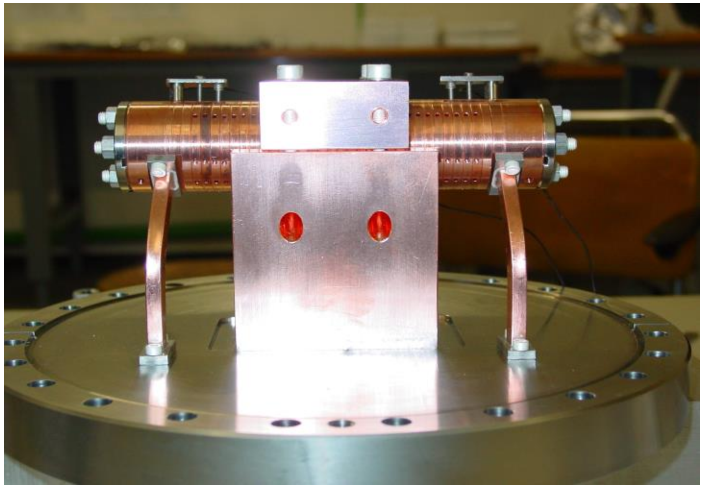
downstream
iris



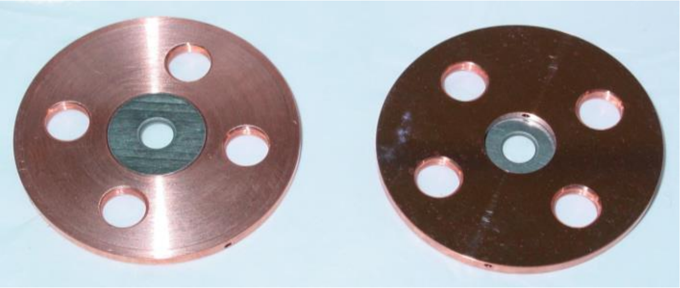
Damage on iris after runs of the 30-cell clamped structures tested in CTFII.
First (a, b and c) and generic irises (d, e and f) of W ,Mo and Cu structures respectively.

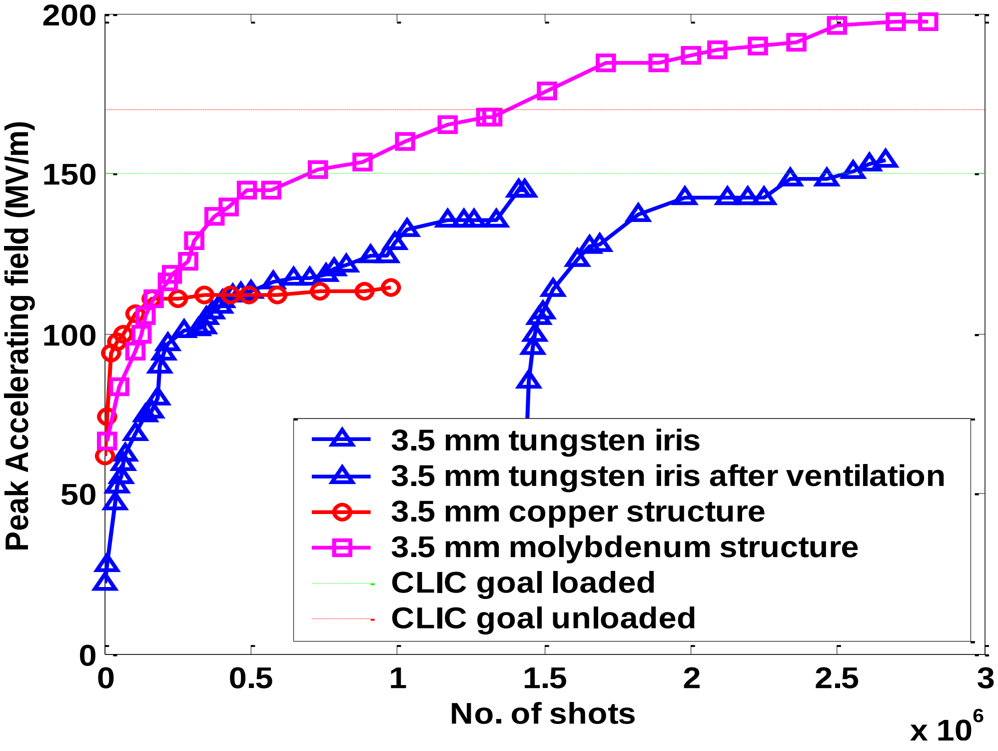
Achieved accelerating fields in CTF2

High gradient tests of new structures with molybdenum irises reached 190 MV/m peak accelerating gradient without any damage well above the nominal CLIC accelerating field of 150 MV/m but with RF pulse length of 16 ns only (nominal 200 ns)



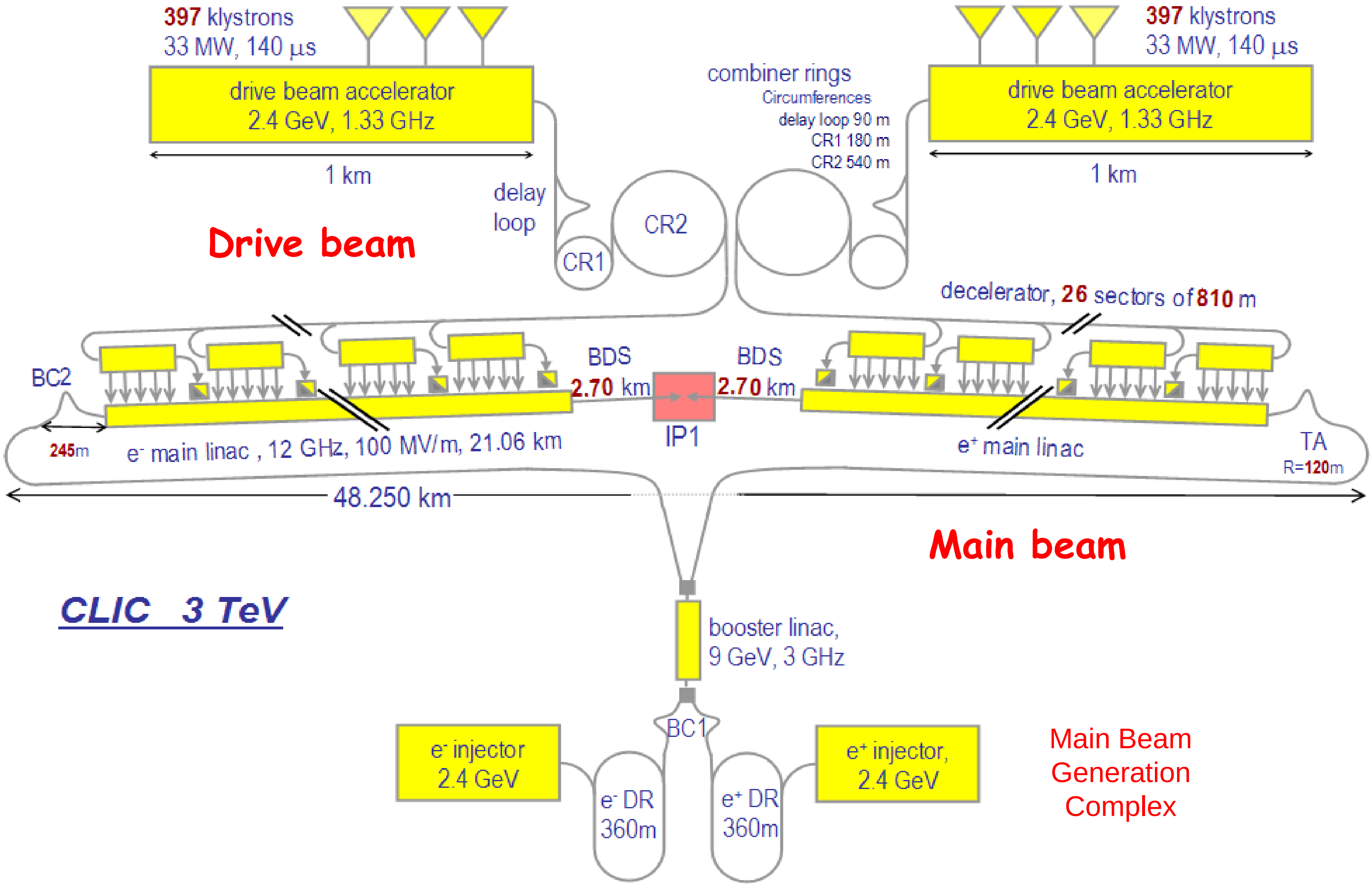
30 cell clamped tungsten-iris structure





A world record !!!

CLIC – overall layout

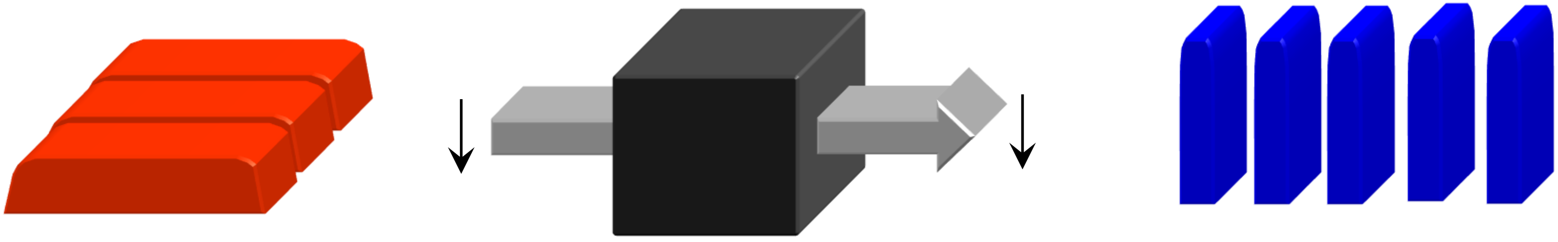


CLIC 3 TeV

Main Beam
Generation
Complex

CLIC scheme

- Very high gradients possible with NC accelerating structures at high RF frequencies (30 GHz → 12 GHz)
- Extract required high RF power from an intense e- “drive beam”
- Generate efficiently long beam pulse and compress it (in power + frequency)



‘few’ Klystrons
Low frequency
High efficiency

Power stored in
electron beam

Power extracted from beam
in resonant structures

Accelerating Structures
High Frequency – High field

Long RF Pulses
P_0 , ν_0 , τ_0

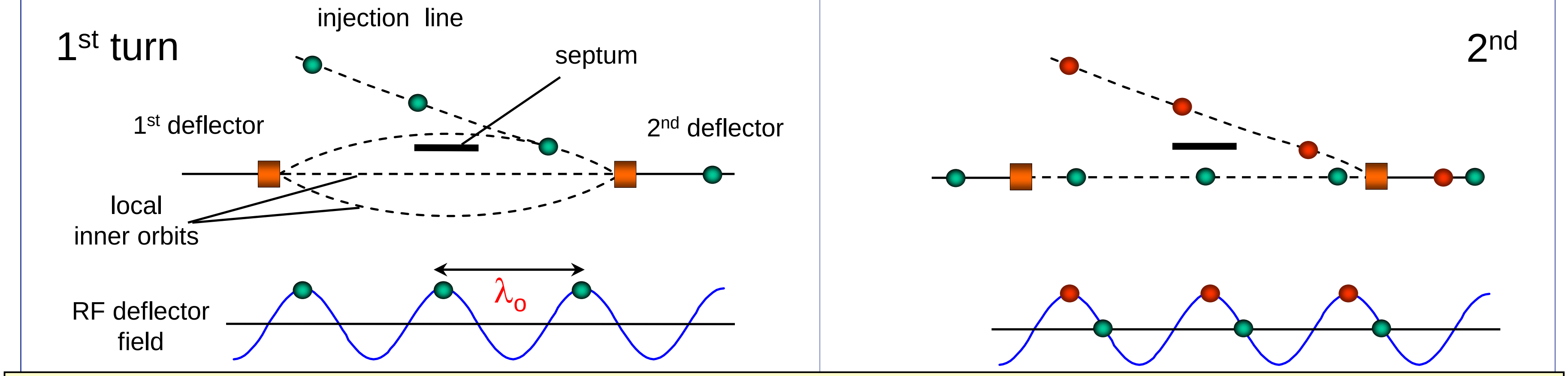
Electron beam manipulation
Power compression
Frequency multiplication

Short RF Pulses
$P_A = P_0 \times N_1$
$\tau_A = \tau_0 / N_2$
$\nu_A = \nu_0 \times N_3$

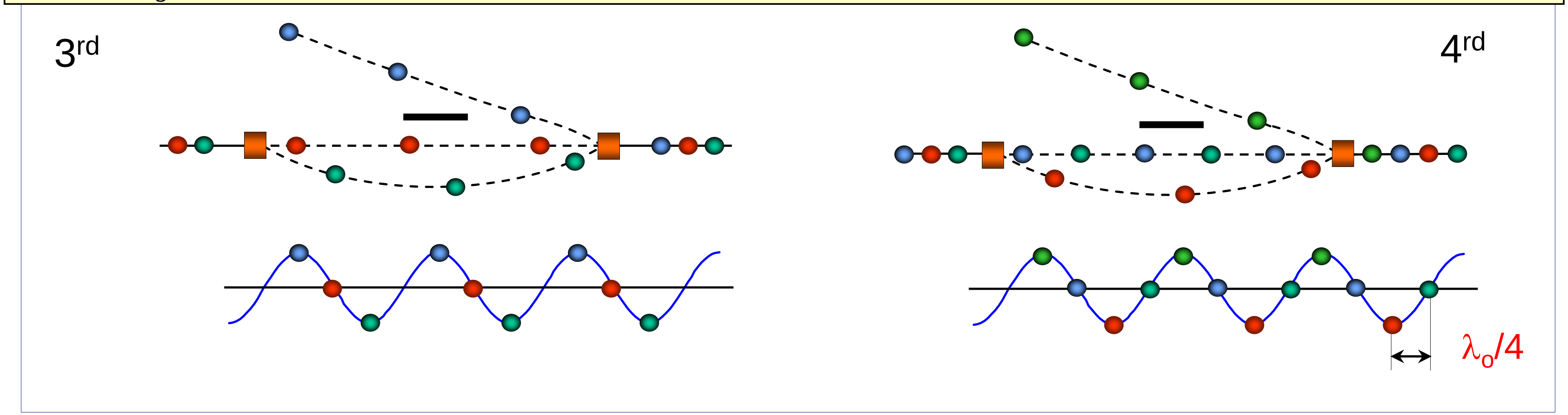
RF injection in combiner ring

- combination factors up to 5 reachable in a ring

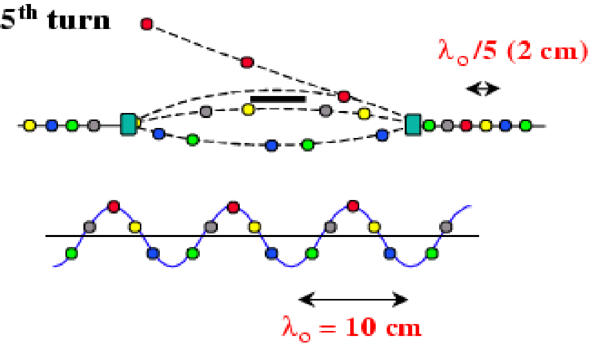
$$C_{ring} = (n + ¼)\,\lambda$$



C_{ring} has to correspond to the distance of pulses from the previous combination stage!

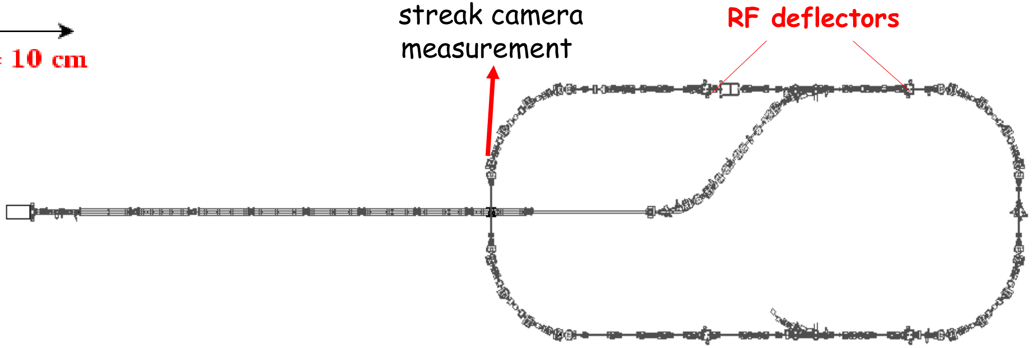


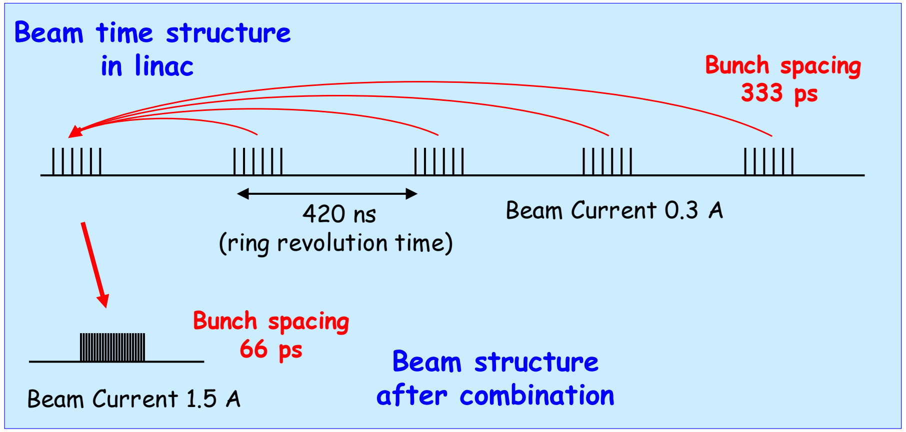
Demonstration of frequency multiplication



CTF3 - PRELIMINARY PHASE 2001/2002

Successful low-charge demonstration of electron pulse combination and bunch frequency multiplication by up to factor 5





Beam time structure in linac

Bunch spacing 333 ps

420 ns (ring revolution time)

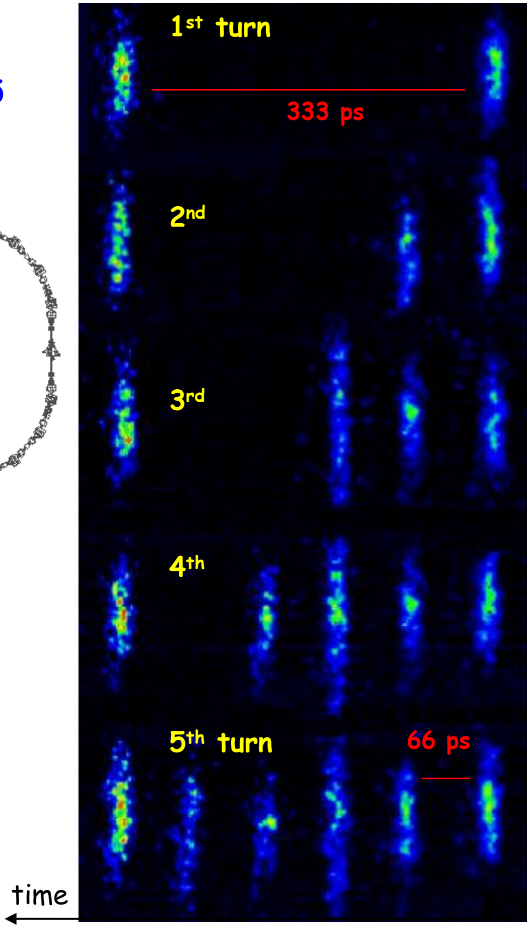
Beam Current 0.3 A

Bunch spacing 66 ps

Beam Current 1.5 A

Beam structure after combination

Streak camera image of beam time structure evolution



Software for EM Simulation

- CST-Microwave Studio
  - Standard for single computer simulation, some particle tracking, etc.
- ANALYST
  - Less common, but powerful scripting done by National Instruments
- ANSYS-APDL/HFSS
  - HFSS is now a module inside ANSYS-Workbench
  - Has the potential to do coupled simulation for Multiphysics
  - APDL is no longer supported, but very powerful Multiphysics solver (my preference, although I’m in the minority)
- COMSOL
  - Powerful Multiphysics solver, with high learning curve.

Distributed Computing

- All of these software choices are designed for single machine computing.
- You can spend tons of money on a single computer (64 GB RAM, 8-core with hyperthreading, etc.) and do significant amounts of R&D (think about the computing you've done with a standard computer).
- However, large simulations, complex geometries with symmetry, time domain/transient response, high precision simulation (perturbative) all are beyond single computer solvers.

ACE3P Group at SLAC

- At SLAC, they are building a code from the ground up to be used with distributed computing under the SciDAQ system.
- They have several computing clusters that they have tens of millions of core hours per year on.
- They've created modules to solve eigenmode, frequency domain, time domain, thermal, mechanical, particle in cell, and more.
- They run a workshop every hear called CW## (CW16 this year), which I recommend if you're interested.
- Thanks to Zenghai who provided me the following slides I'm showing today.

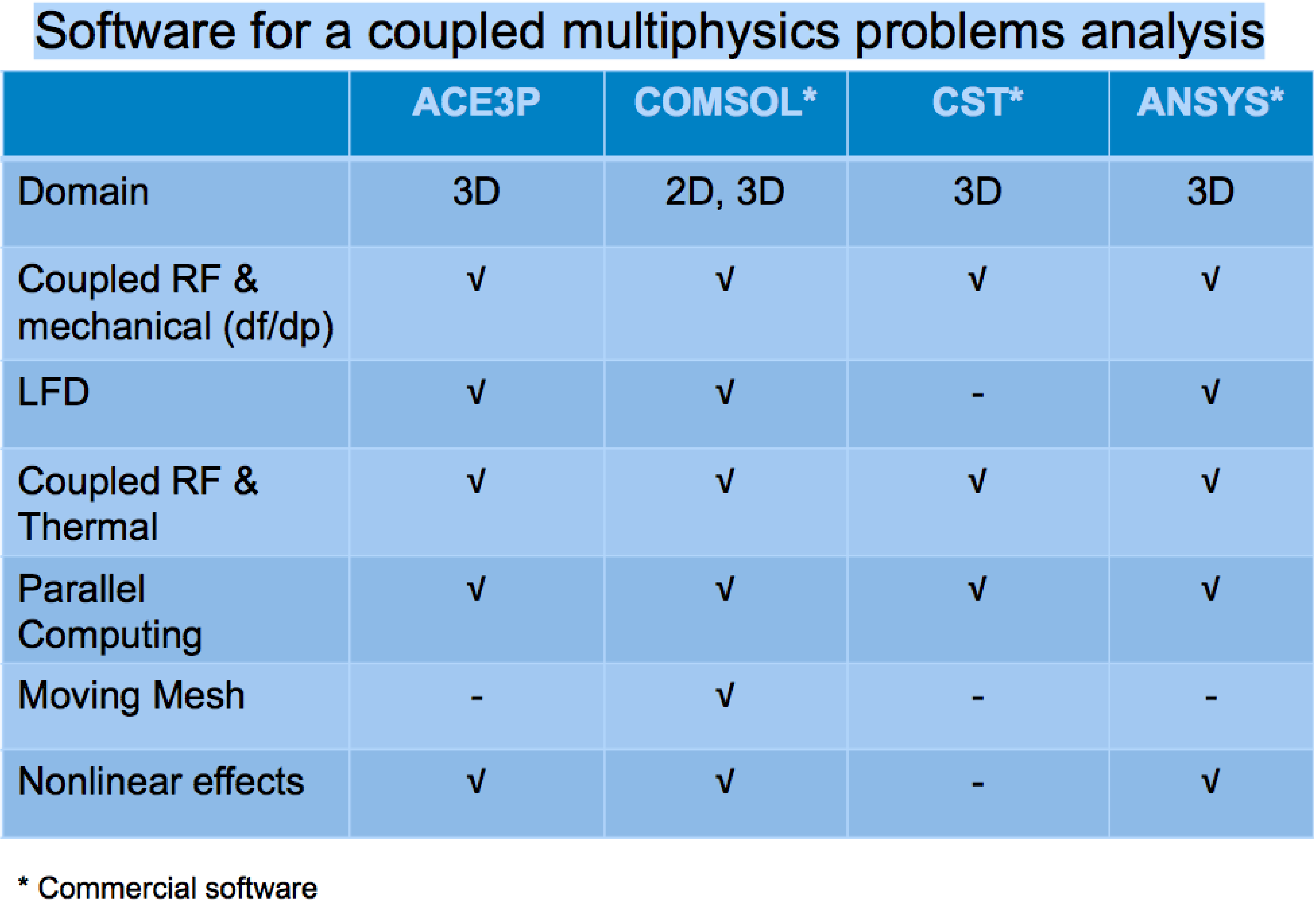
ACE3P

- CW14 is organized and hosted by Advanced Computations Department (ACD) to promote and disseminate ACE3P.

- ACD team members - Lixin Ge, Kwok Ko, Oleksiy Kononenko, Zenghai Li, Cho Ng, Liling Xiao

- ACD is supported by SLAC and DOE's High Performance Computing Initiatives
    - (1998–2001) HPC Accelerator Grand Challenge
    - (2001-2007) Scientific Discovery through Advanced Computation (SciDAC) - Accelerator Science and Technology (AST)
    - (2007-2012) SciDAC-2 - Community Petascale Project for Accelerator Science and Simulation (ComPASS)
    - (2012-2015) SciDAC-3 - ComPASS

1. 3D Electromagnetic Codes for Accelerator Modeling



Software for a coupled multiphysics problems analysis

	ACE3P	COMSOL*	CST*	ANSYS*
Domain	3D	2D, 3D	3D	3D
Coupled RF & mechanical (df/dp)	√	√	√	√
LFD	√	√	-	√
Coupled RF & Thermal	√	√	√	√
Parallel Computing	√	√	√	√
Moving Mesh	-	√	-	-
Nonlinear effects	√	√	-	√

* Commercial software

Courtesy: Andrei Lunin, ICAP 2012, August 19-24, 2012, Rostock-Warnemünde (Germany)

1. ACE3P Code Suite

- ACE3P is a comprehensive suite of parallel electromagnetic codes based on the conformal, high-order finite-element method and written in C++
- ACE3P consists of six application modules:

ACE3P (Advanced Computational Electromagnetics 3P)

Frequency Domain:	**Omega3P**	– Eigensolver (Damping)
	S3P	– S-Parameter
Time Domain:	**T3P**	– Wakefields & Transients
Particle Tracking:	**Track3P**	– Multipacting & Dark Current
EM Particle-in-cell:	**Pic3P**	– RF Guns & Sources (e.g. Klystron)
Multi-physics:	**TEM3P**	– EM, Thermal & Structural Effects

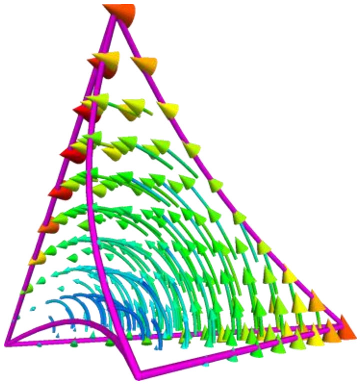
https://slacportal.slac.stanford.edu/sites/ard_public/bpd/acd/Pages/Default.aspx

- ACE3P uses Cubit for model and mesh generation
- ACE3P uses ParaView for visualization

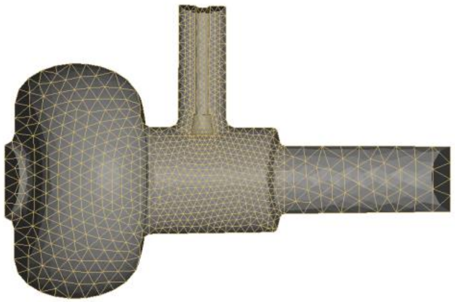
Development of ACE3P

ACE3P has been developed for the past 15 years under DOE SciDAC computing initiatives and SLAC program support. It has two unique features

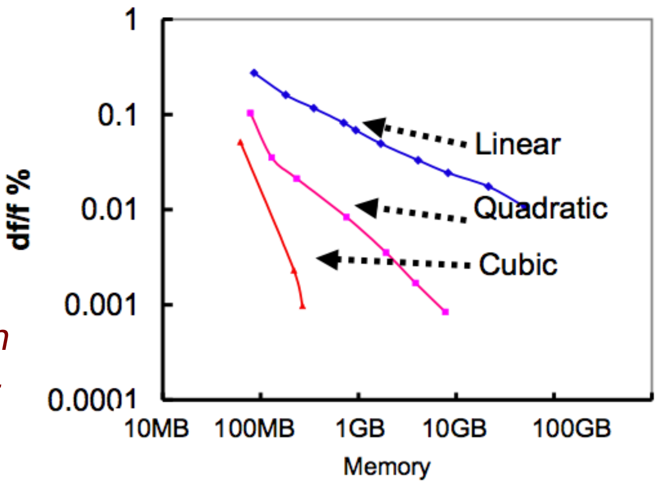
- Based on higher-order curved finite elements for ***high-fidelity modeling and improved solution accuracy***
- Implemented on massively parallel computers for ***increased memory (problem size) and speed***



Finite-element field representation



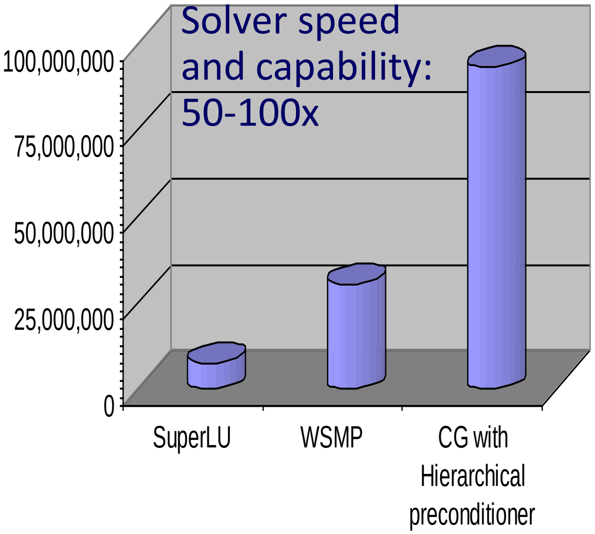
67k quad elements (<1 min on 16 CPU,6 GB) Error ~ 20 kHz (1.3 GHz)



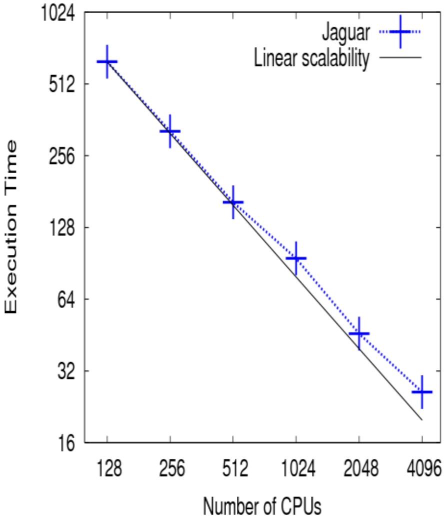
Parallel computation

2. SciDAC Collaborations in Computational Science

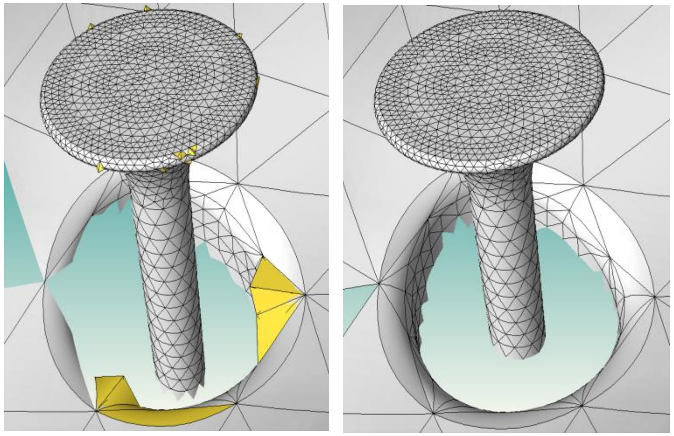
Eigensolver speed and scalability



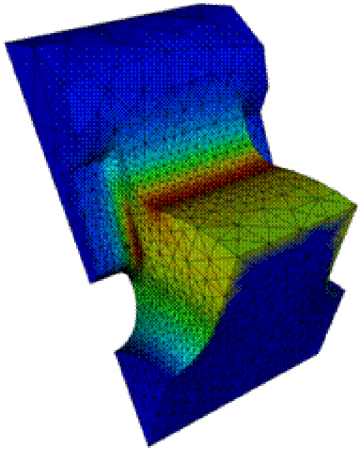
Solver speed and capability: 50-100x

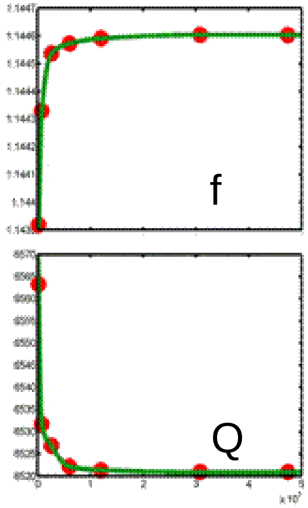


Mesh correction

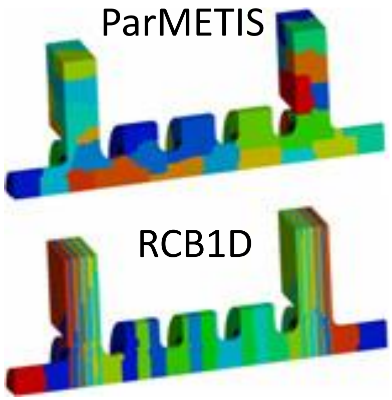


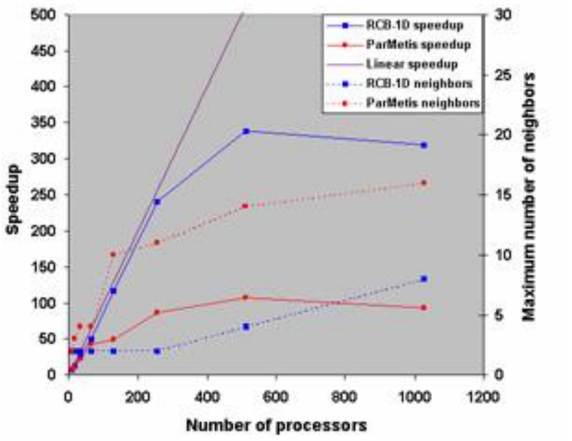
Adaptive mesh refinement





Partitioning scheme for load balancing



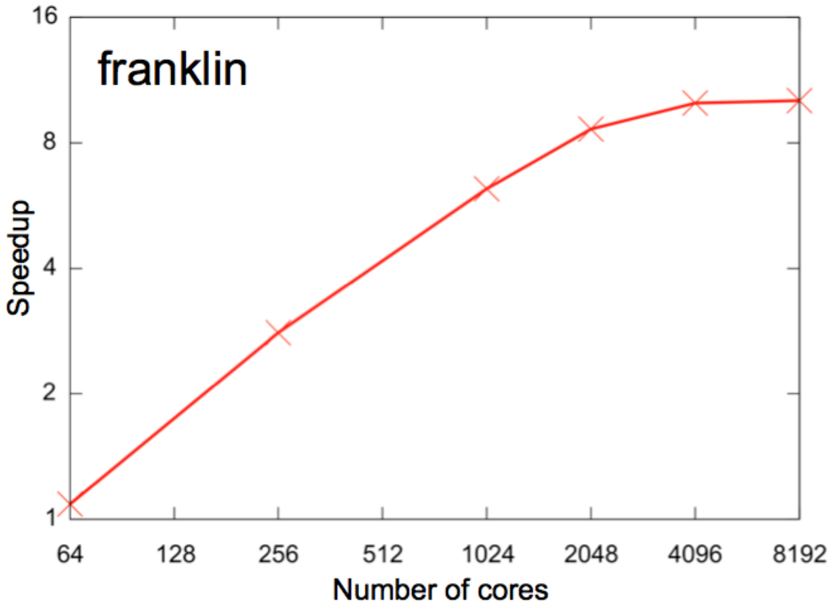


3. Massively Parallel Computing at NERSC

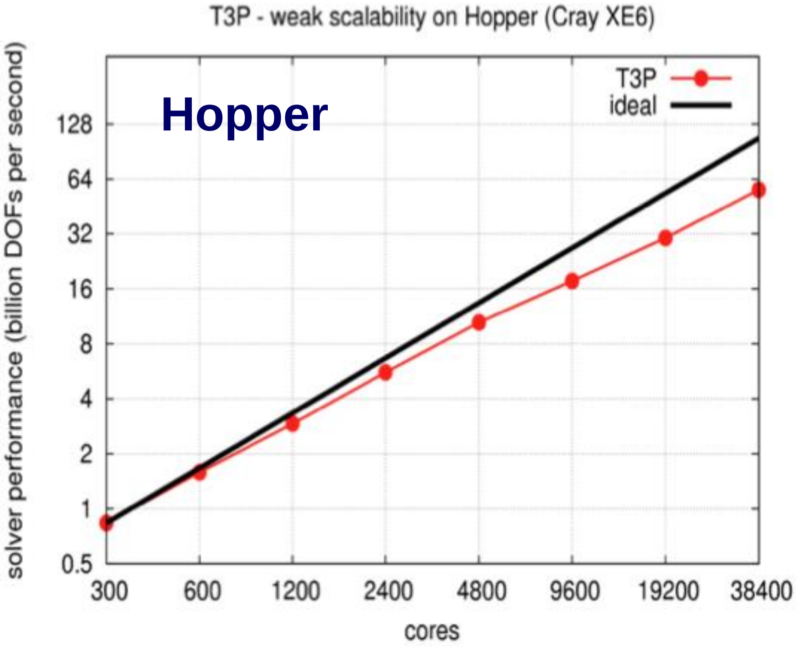
Hopper: Cray XE6
- 153,216 compute cores
- 212 terabytes of memory
- peak performance of 1.28 petaflops/sec

Edison: Cray XC30
- 124,800 compute cores
- 332 terabytes of memory
- peak performance of 2.39 petaflops/sec

Omega3P - Strong scaling of hybrid solver on Franklin

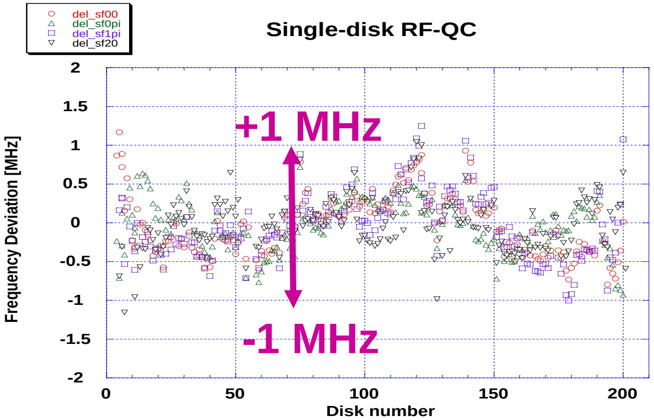


T3P – Weak scaling on Hopper

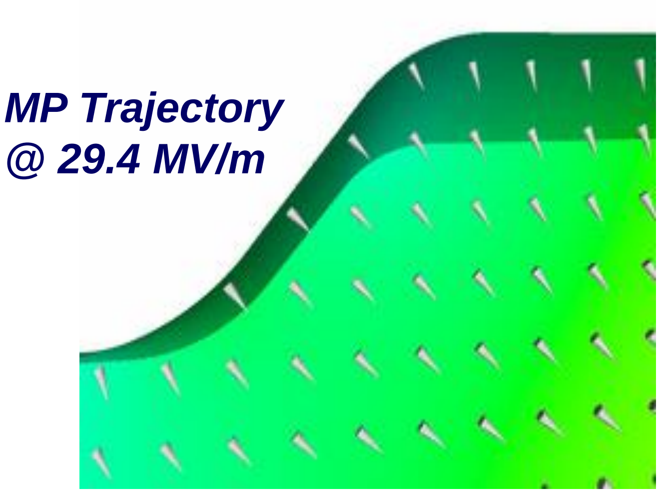


4. ACE3P – Accuracy and Complexity

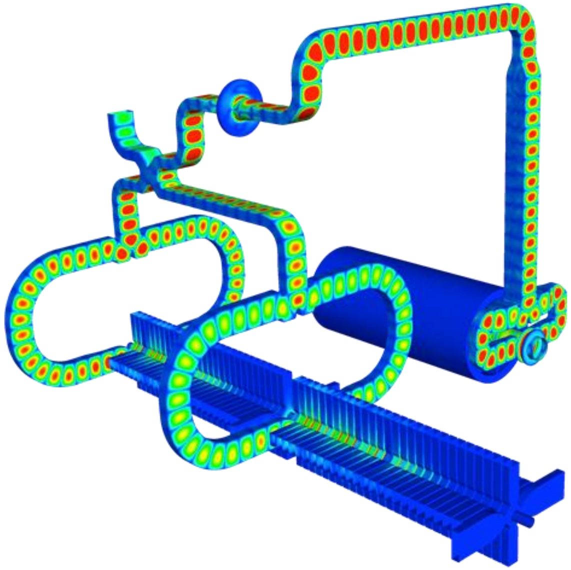
Omega3P – NLC structure cell design



Track3P – Prediction of multipacting barrier in Ichiro SRF cavity



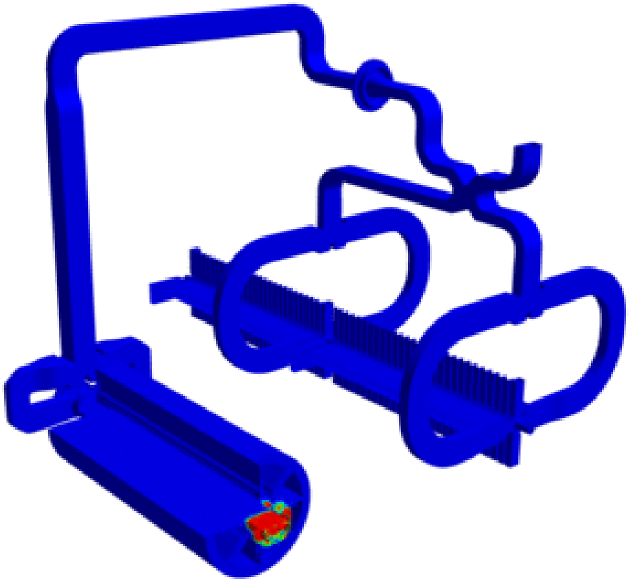
T3P - Wakefield coupling in CLIC two-beam module



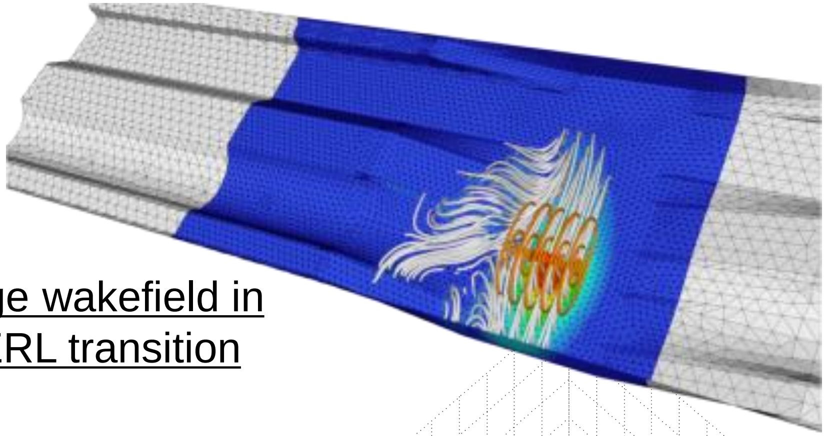
T3P Modeling Capabilities

Time domain

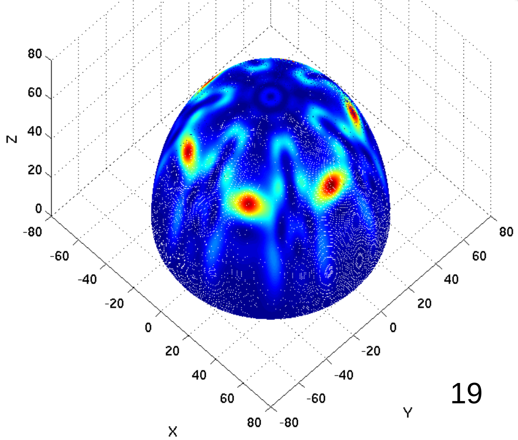
- Wakefield and HOM determination from beam excitation
- Moving window technique for short-range wakefield
- Absorbing boundary condition for far fields



Wakefield coupling in CLIC two-beam module



Short-range wakefield in Cornell ERL transition

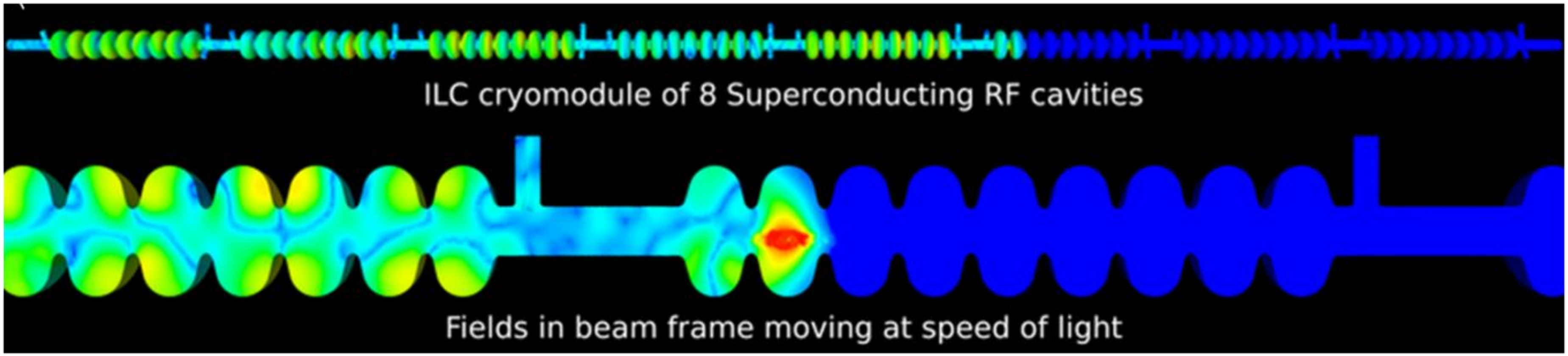


Far-field radiation from PBG fiber

4. ACE3P - Problem Size and Speed

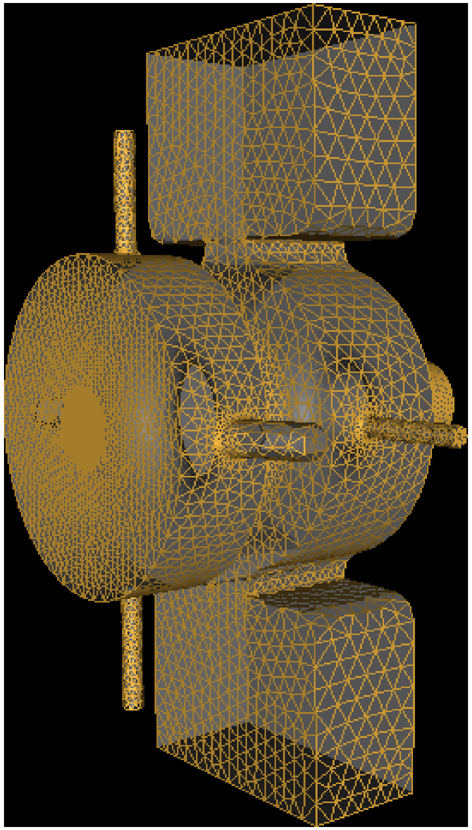
Simulating a cryomodule of 8 cavities for the ILC in frequency and time domain

Omega3P - 3 million-element mesh, ~20 million DOFs, 1024 CPUs (Seaborg), 300 GB memory, 1 hour per mode

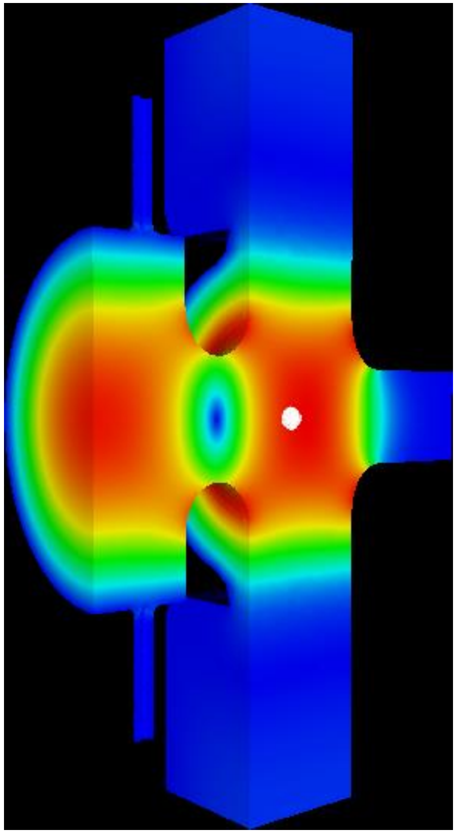


T3P - 80 million-element mesh, ~500 million DOFs, 4096 CPUs (Jaguar), 4 seconds per time step

Pic3P Example Case - LCLS RF Gun



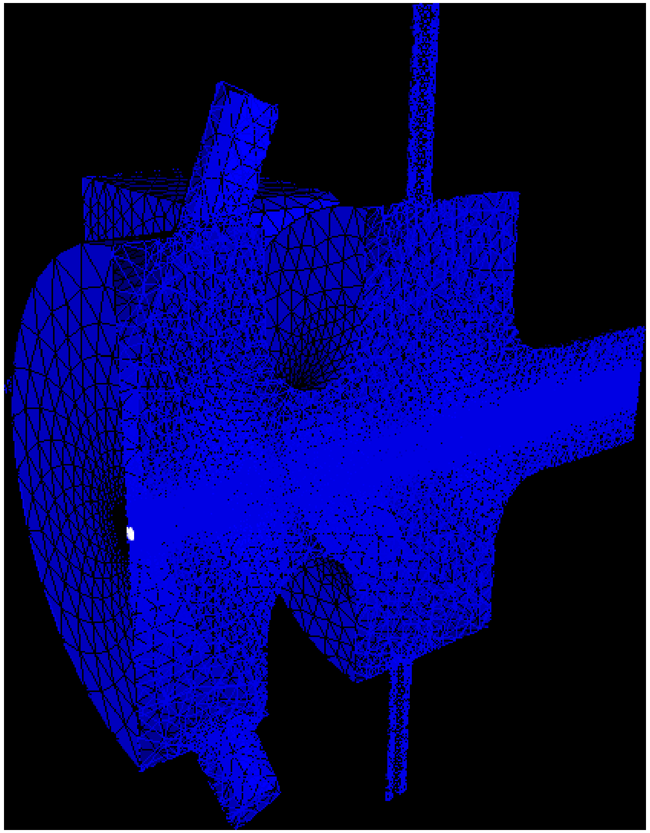
Unstructured mesh model of LCLS RF gun, generated with Cubit



Omega3P calculates RF drive fields, directly imported into Pic3P

π-mode 2.856 GHz

120 MV/m

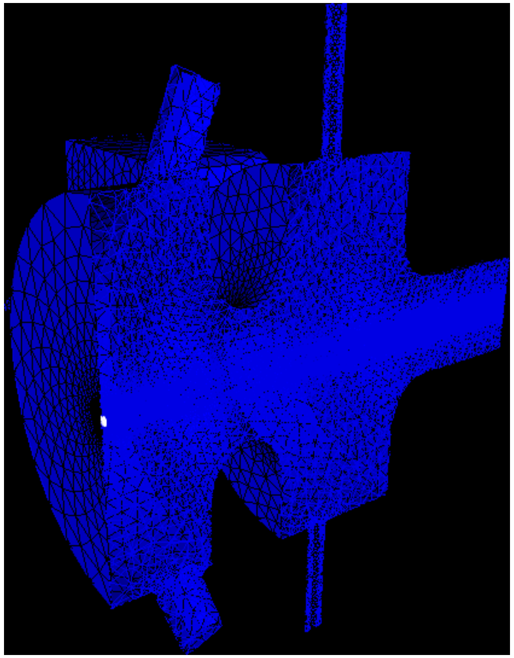


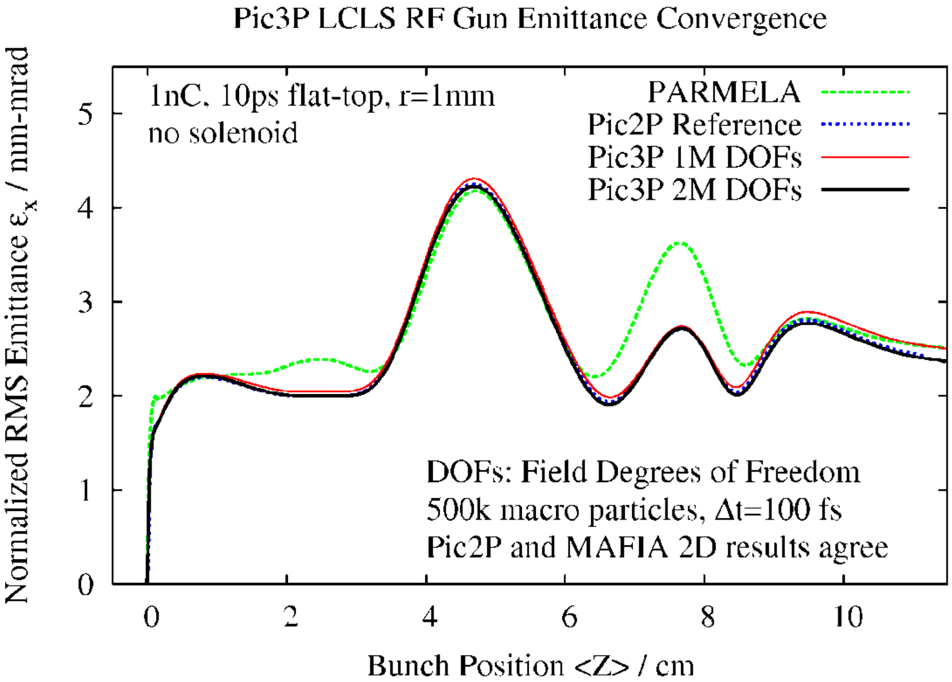
Temporal evolution of electron bunch and scattered self-fields as modeled with Pic3P

Pic3P Modeling Capabilities

Time domain

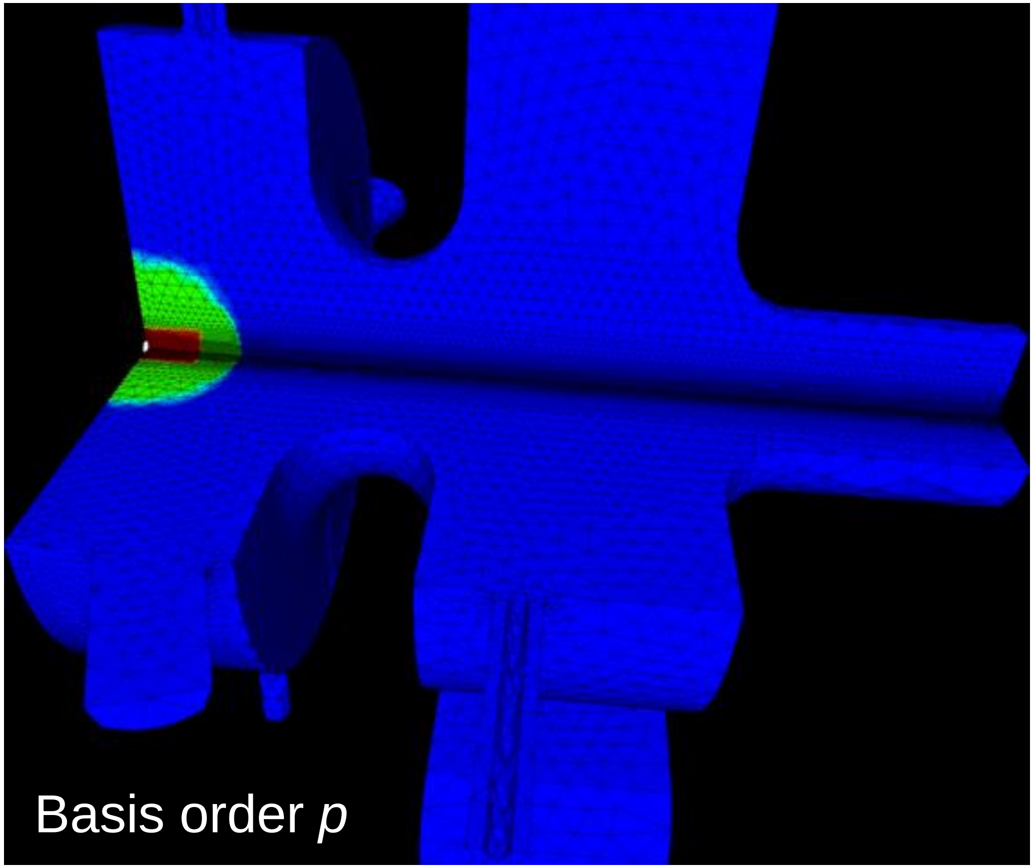
- Self consistent particle-in-cell modeling of beam-cavity interactions in space-charge dominated devices
- User-specified particle emission model





Emittance in LCLS RF gun

Causal Adaptive *p*-Refinement: Specify *p*



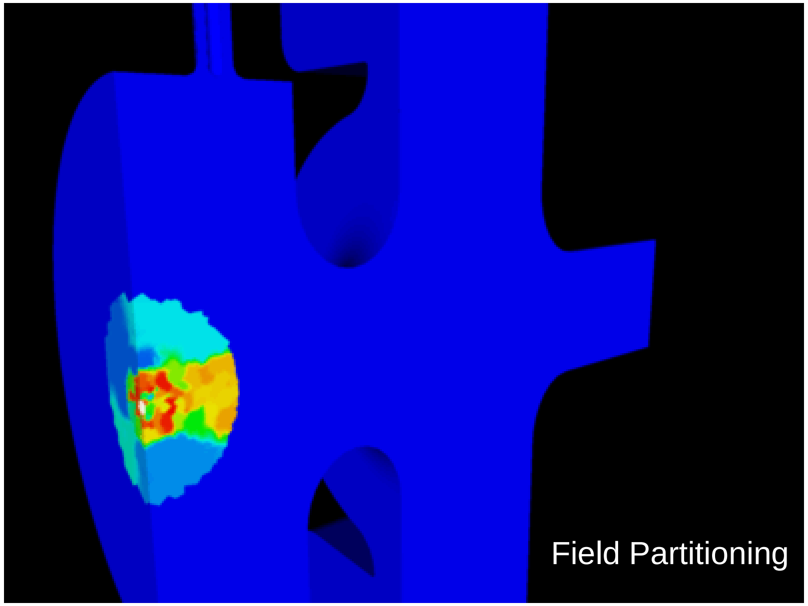
Blue: 0th order
Green: 1st order
Red: 2nd order

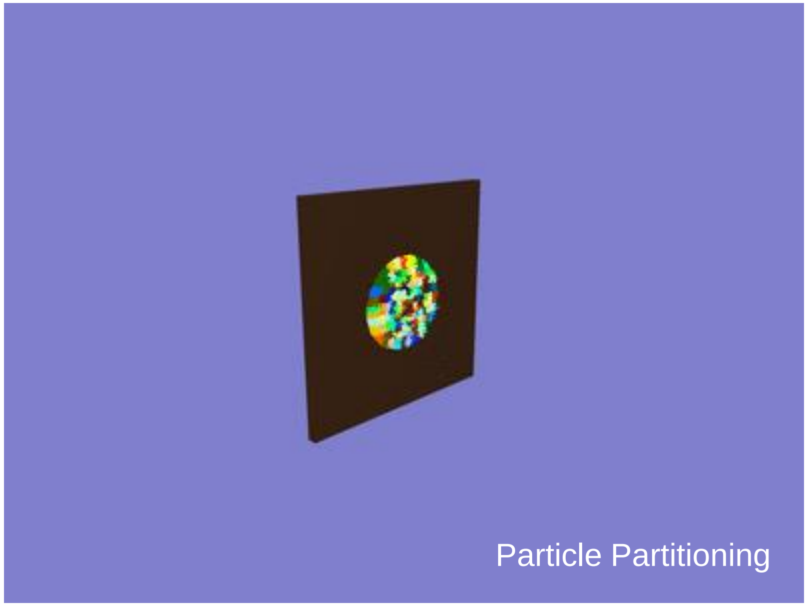
```
FiniteElement: {
  Order: 0
  Curved Surfaces: on
}

PRegion: {
  Type: PICCausality
  Order: 1
}

PRegion: {
  Type: PICDomain
  Order: 2
}
```

LCLS RF gun: Causal moving window reduces computational resource requirements *by orders of magnitude*

Ready for Supercomputers at NERSC

- Fields partitioned with graph-based methods (ParMETIS)
- Particles partitioned geometrically (Zoltan RCB 3D, SciDAC collaboration)
- Collective MPI on sub-communicators in disjoint regions, with optimized ordering to allow higher concurrency of communication


Field Partitioning


Particle Partitioning

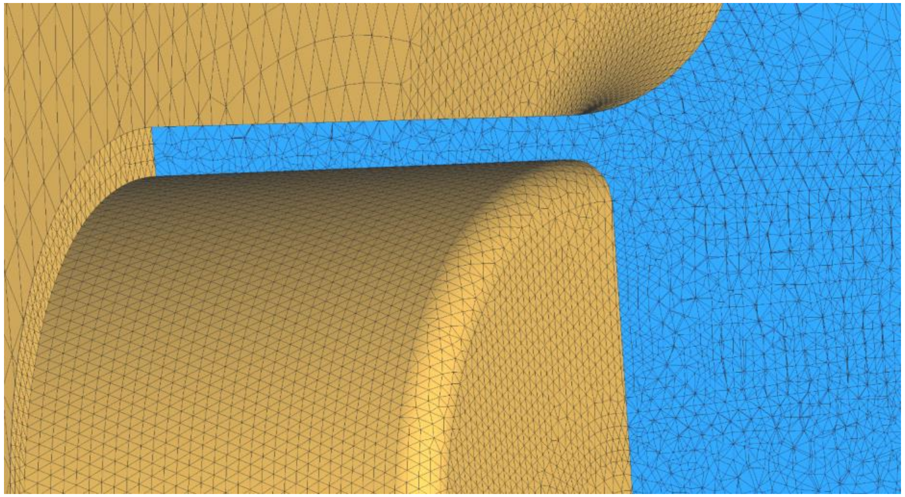
Example: LCLS RF gun, colors indicate distribution to different CPUs

Pic3P was tested on 24k CPUs: 750M DOFs, 5B particles

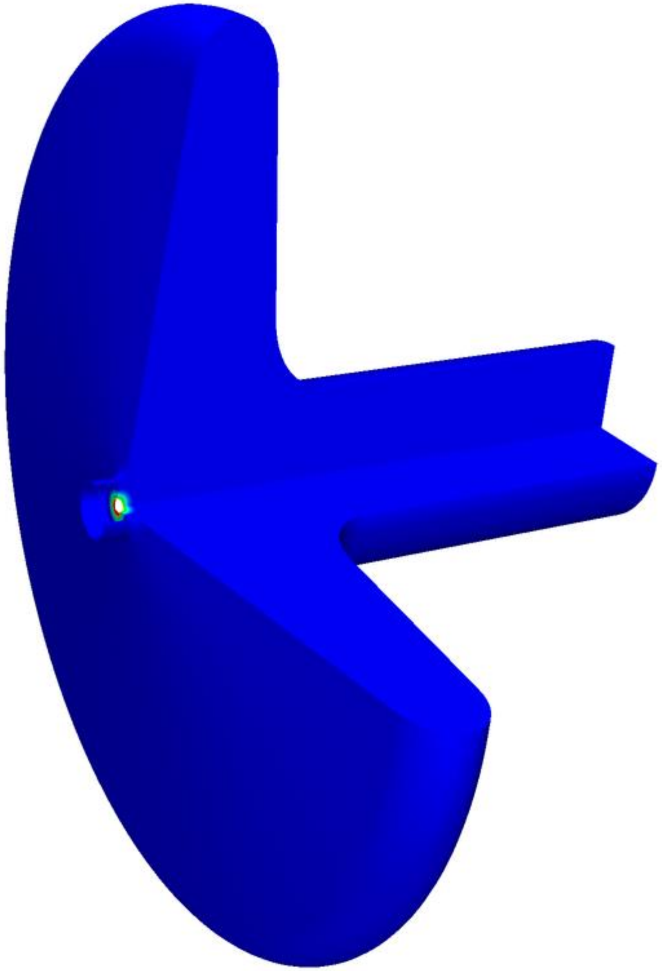
Larger problem: BNL Polarized SRF Gun

BNL Polarized SRF Gun (J. Kewisch)

½ cell, 350 MHz, 24.5 MV/m, 5 MeV, solenoid (18 Gauss), recessed GaAs cathode at T=70K inserted via choke joint, cathode spot size 6.5 mm, Q=3.2 nC, 0.4eV initial energy



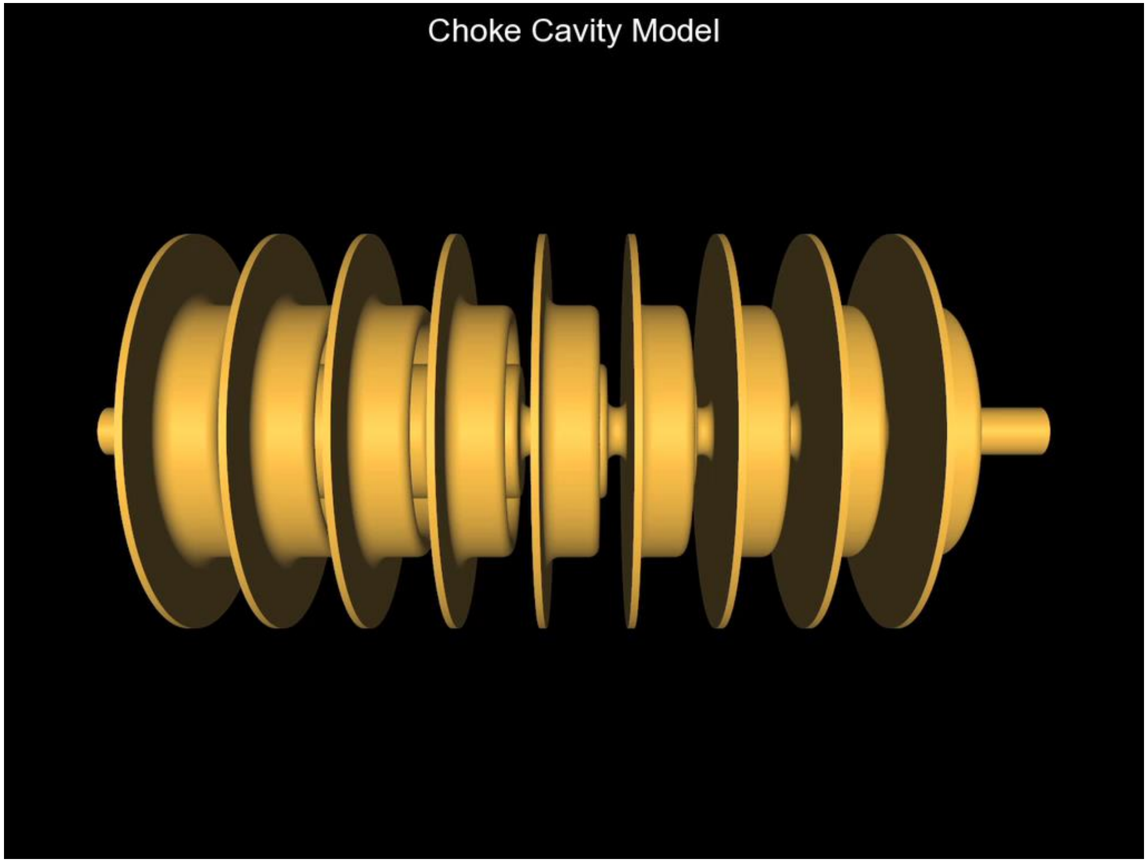
Cut-view of unstructured mesh near cathode



Self-fields during bunch transit

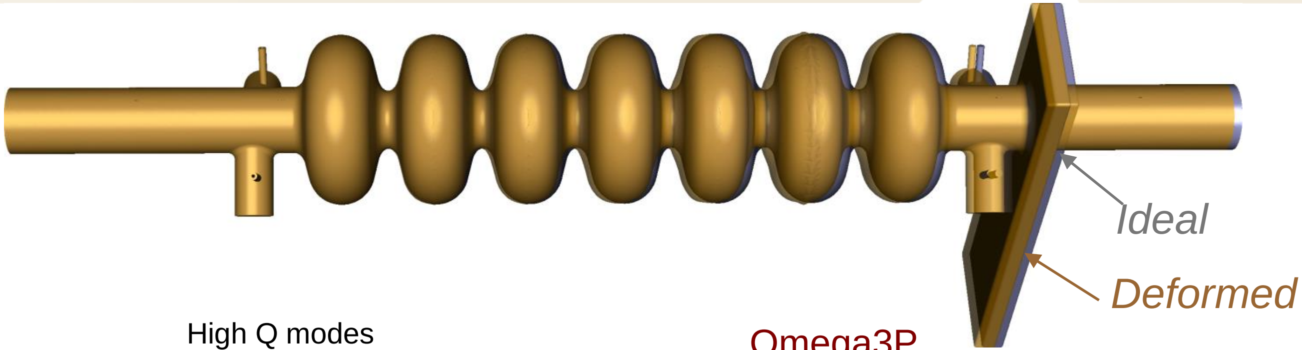
Optimization of Choke Mode Cavity

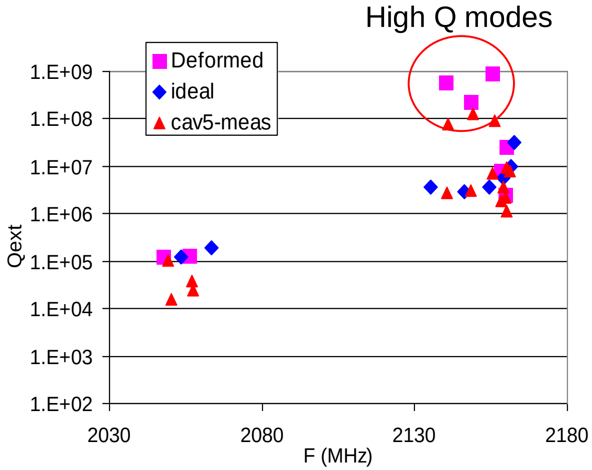
Optimize the performance of the choke mode cavity by improving the damping of the higher-order dipole modes.



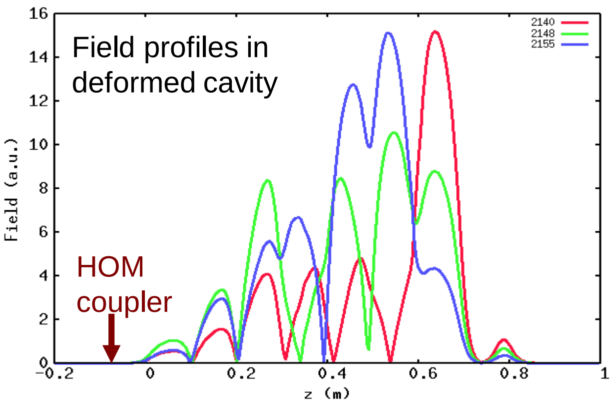
Shape Determination – Solving the CEBAF Beam Breakup Problem

A prototype cavity for CEBAF 12-GeV upgrade





Omega3P

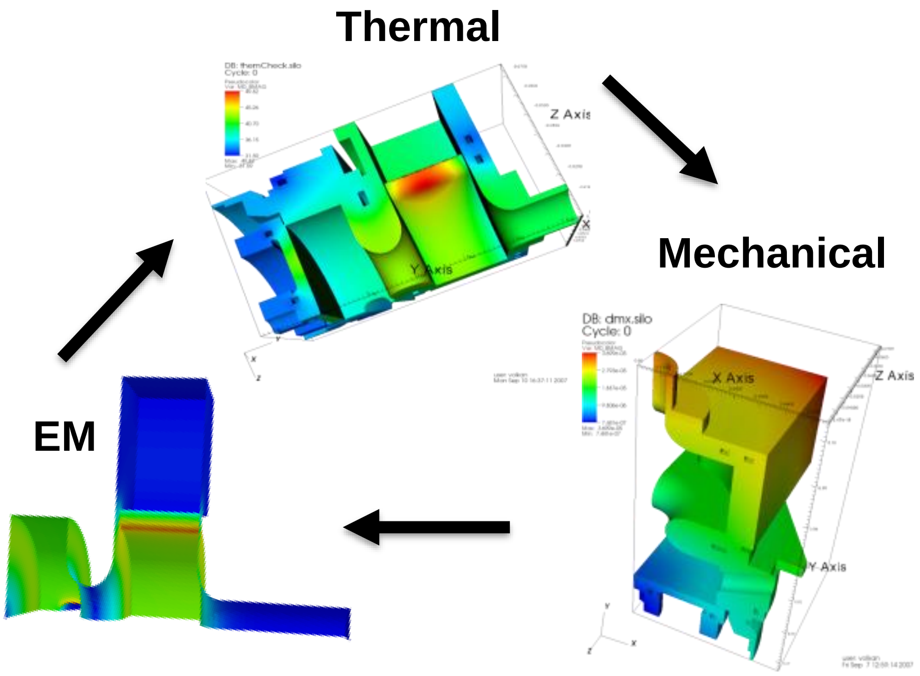


- Beam breakup (BBU) observed due to several high Q modes
- Used measured RF parameters such as f, Q_{ext}, and field profile as inputs to solve an inverse problem through an optimization algorithm.
- Identified shape imperfection that caused the high Q values, which was confirmed later from QC measurements.

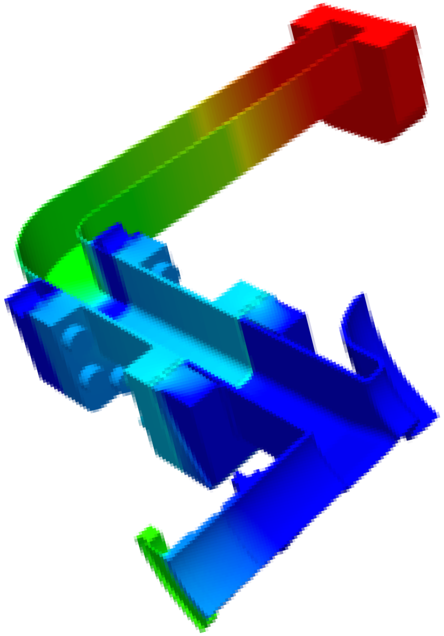
TEM3P Modeling Capabilities

Multi physics

- Integrated EM, thermal and mechanical effects
- Non-linear thermal conductivity for superconducting cavities
- Non-linear heat flux and convective boundary conditions
- Shell elements for surface coating

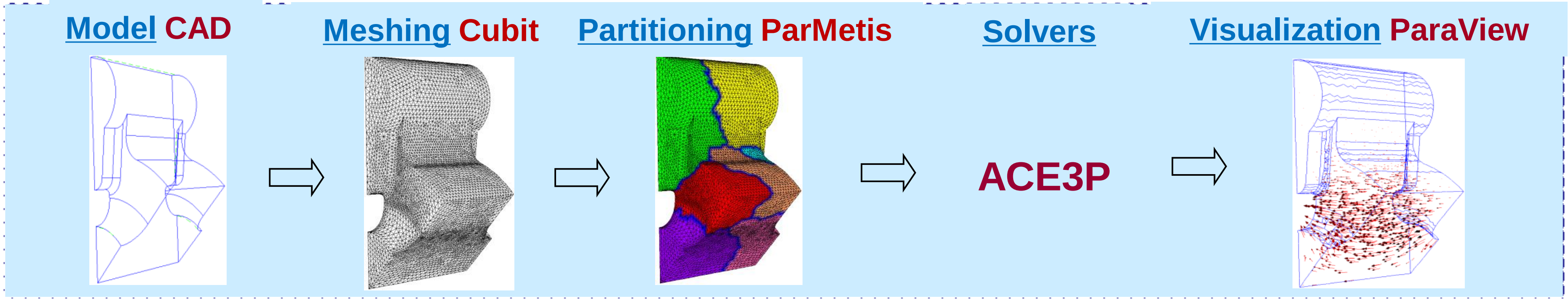


Integrated analysis of LCLS rf gun



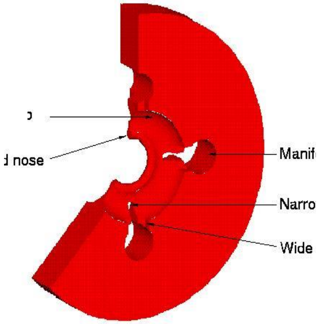
Temperature distribution in cold-warm transition of SRF cavity coupler at Jlab

4. ACE3P for Prototyping in RF Cavity Design



Component Scale

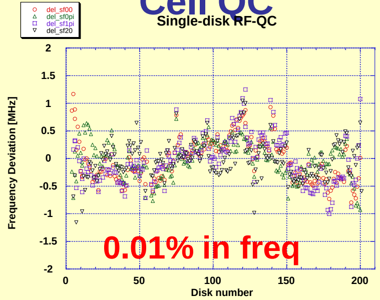
Determine dimensions of a cell



Constraint $f = f_0$;
Maximize (R/Q , Q)
Minimize (surface fields etc.)

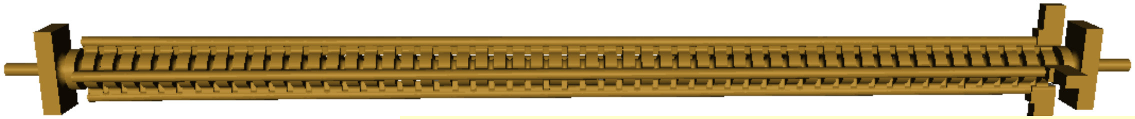
Fabrication

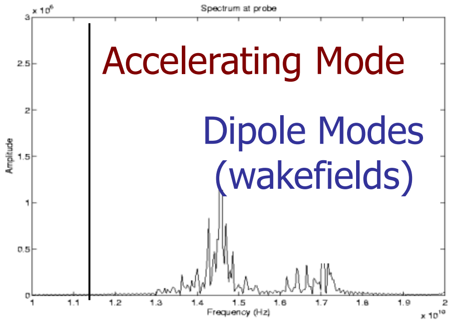
Cell QC



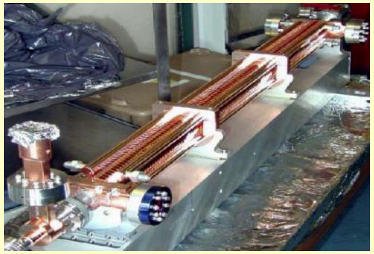
System Scale

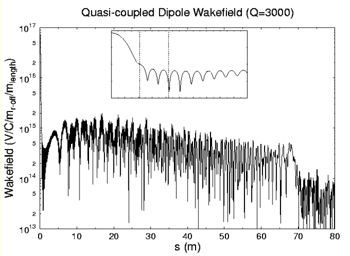
Minimize wakefields in the structure





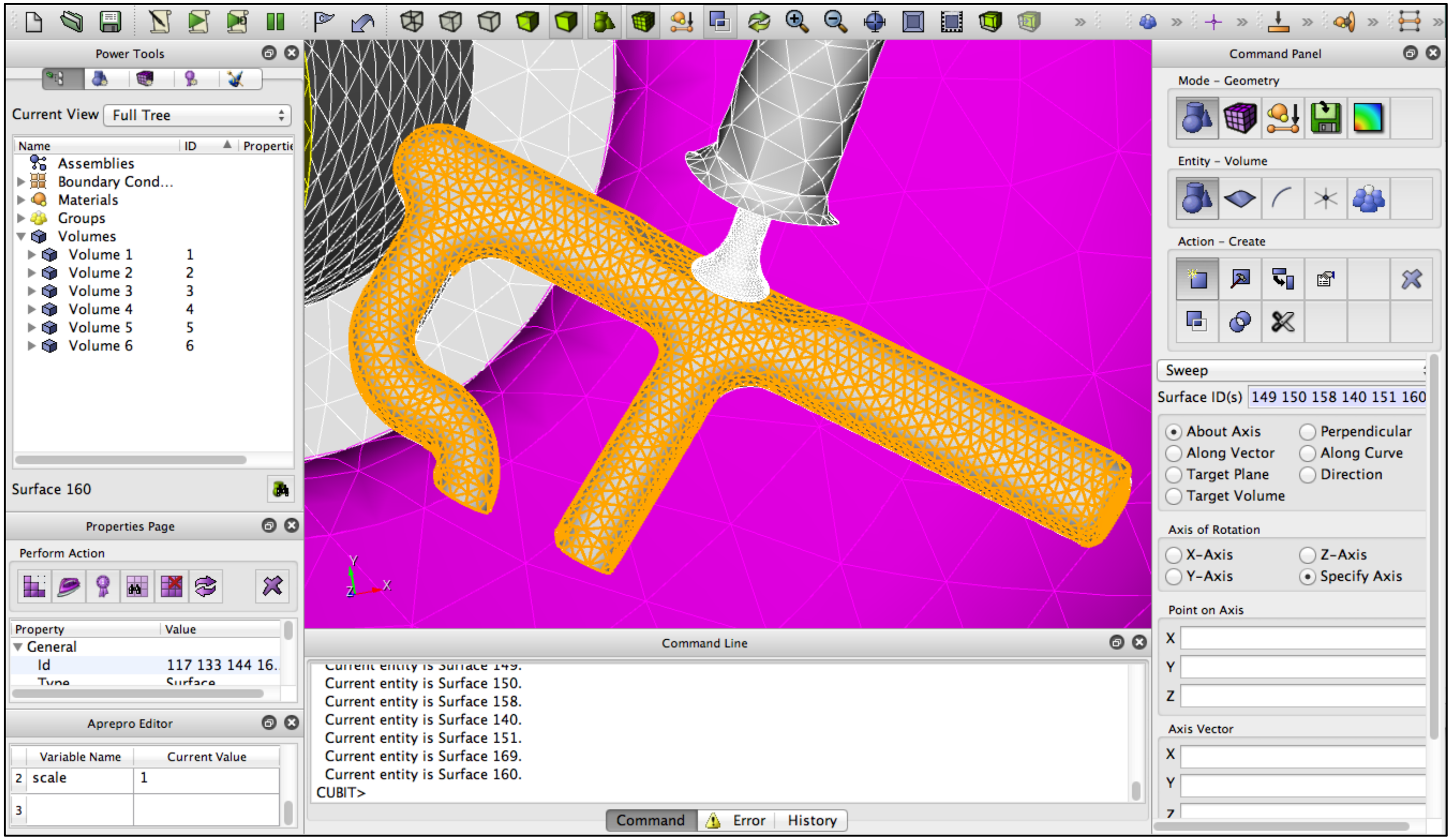
Wakefield Measurement





5. Simulation Workflow – Preprocessing

- Cubit builds CAD models and generates finite element meshes.
- ACE3P inputs curved finite-element meshes for high-fidelity representation of geometry.



Current View: Full Tree

Property	Value
General	
Id	117 133 144 16.
Type	Surface

	Variable Name	Current Value
2	scale	1
3		

Sweep

Surface ID(s): 149 150 158 140 151 160

● About Axis ○ Perpendicular
○ Along Vector ○ Along Curve
○ Target Plane ○ Direction
○ Target Volume

Axis of Rotation: ○ X-Axis ○ Z-Axis ○ Y-Axis ● Specify Axis

```
 Current entity is Surface 149.
 Current entity is Surface 150.
 Current entity is Surface 158.
 Current entity is Surface 140.
 Current entity is Surface 151.
 Current entity is Surface 169.
 Current entity is Surface 160.
CUBIT>
```

5. Simulation Workflow – Running ACE3P

- On NERSC computer facilities through submitting simple command files

Batch job script

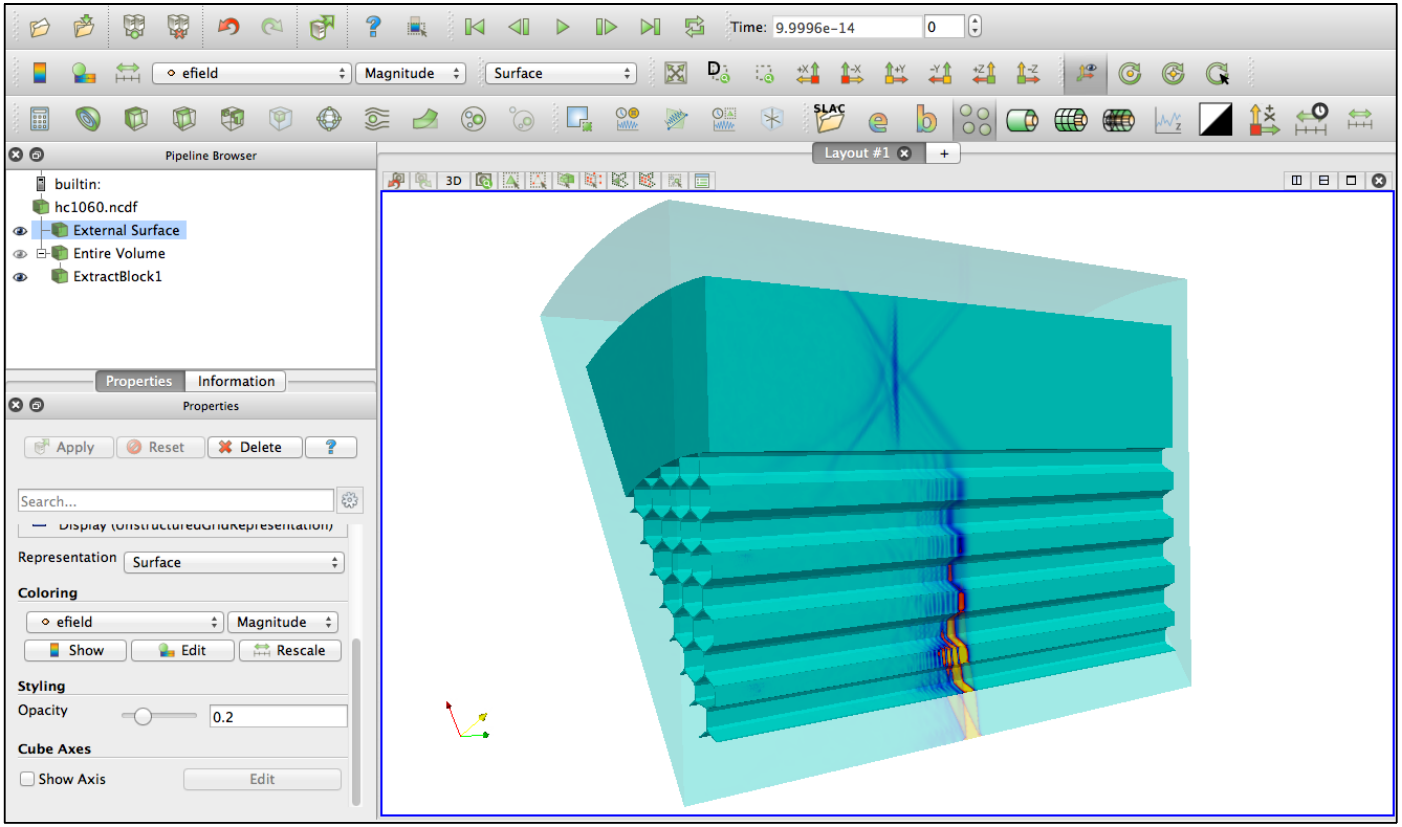
```
#!/bin/bash
#PBS -N pillbox
#PBS -q debug
#PBS -l mppwidth=120
#PBS -l mppnppn=24
#PBS -l walltime=00:10:00
#PBS -e fpb.$PBS_JOBID.err
#PBS -o fpb.$PBS_JOBID.out
#PBS -A m1779
#PBS -V

cd $PBS_O_WORKDIR

aprun –n 120 -N 24
/project/projectdirs/ace3p/hopper/omega3p
pillbox.omega3p
```

Omega3P input file

```
ModelInfo : {
   File: pillbox4.ncdf
   BoundaryCondition : {
      Magnetic: 1, 2
      Exterior: 6
   }
   SurfaceMaterial : {
      ReferenceNumber: 6
      Sigma: 5.8e7
   }
}
FiniteElement: {
   Order:          2
   CurvedSurfaces: on
}
EigenSolver : {
   NumEigenvalues: 2
   FrequencyShift:  1.0e9
}
```

5. Simulation Workflow – Postprocessing

- ParaView visualizes unstructured meshes, field and particle data.
- SLAC postprocessing tools for extracting rf parameters and field information



Time: 9.9996e-14 0

efield Magnitude Surface

Representation Surface

Coloring

efield Magnitude

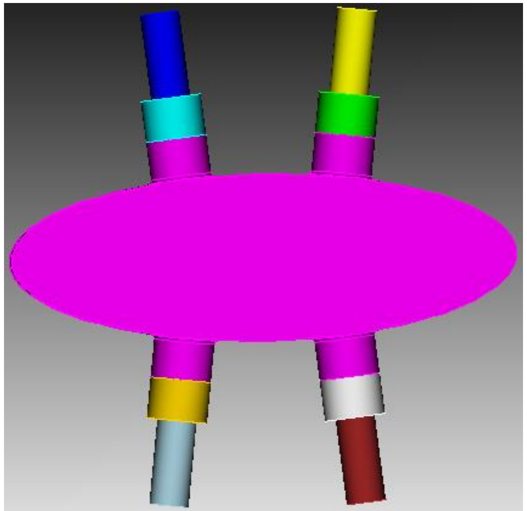
Styling

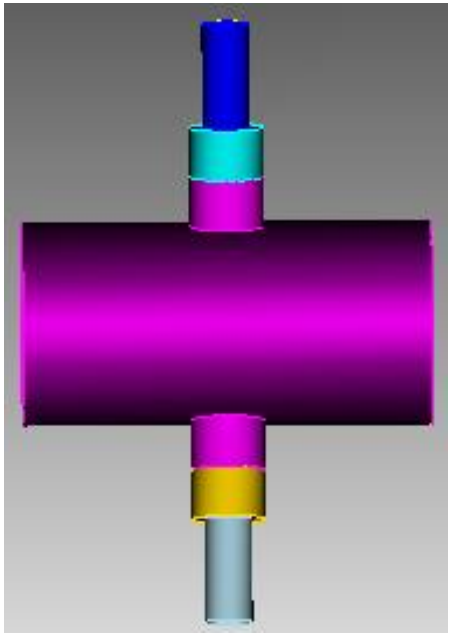
Opacity 0.2

Cube Axes

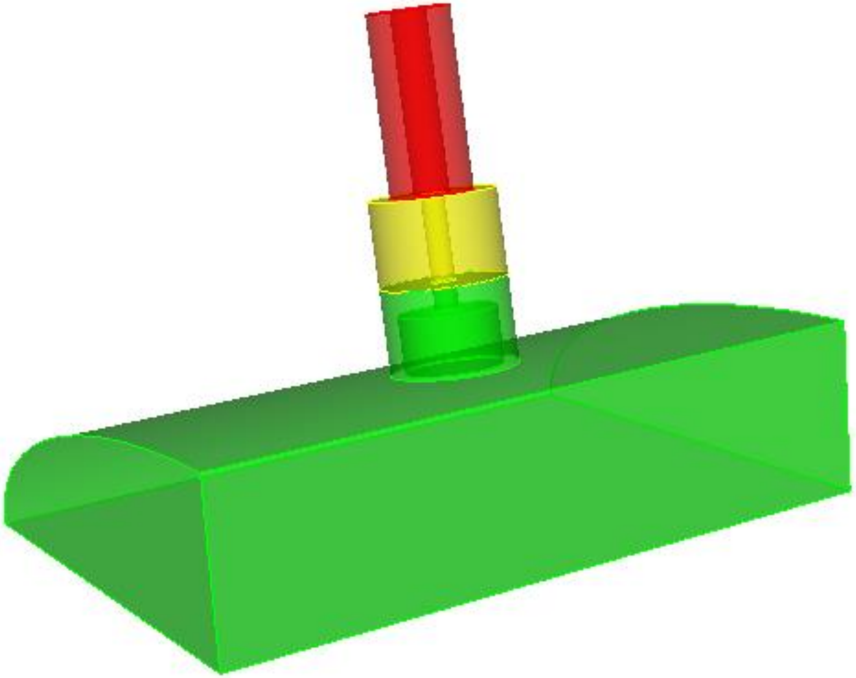
☐ Show Axis

BPM Model





Cubit: make-pepx-bpm.jou



Coax cable: Z=50ohm, εr=1

Ceramic window: Z=50ohm, εr=4.9

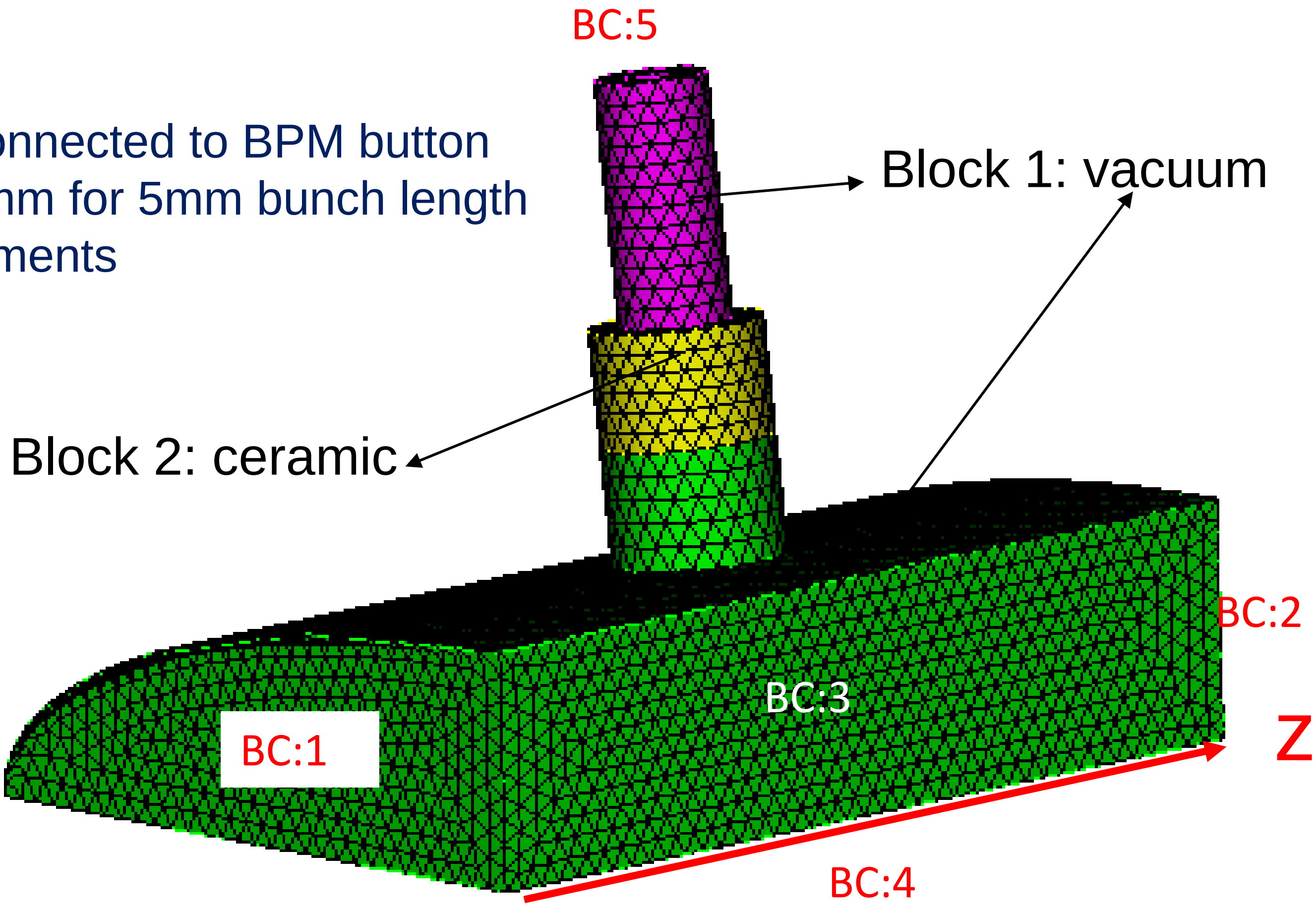
BPM button: diameter=7mm

BPM – Mesh

Cubit: mesh-pepx-bpm.jou

Mesh of ¼ model

- Elliptical chamber connected to BPM button
- Element size = 2.5 mm for 5mm bunch length
- Mesh size = 11k elements



BPM – T3P Run

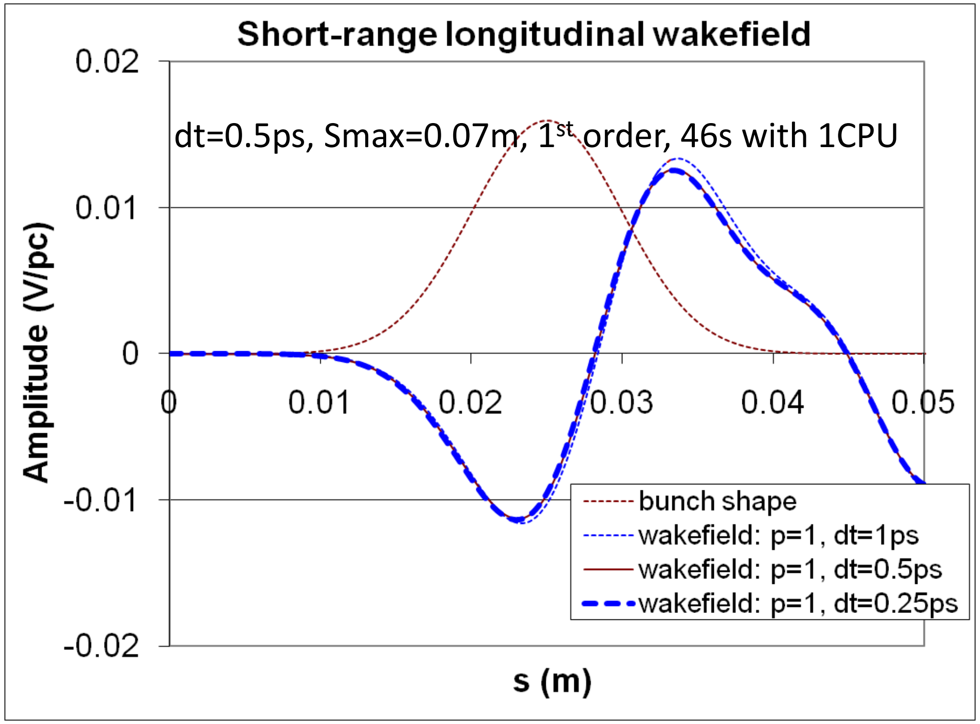
- Run T3P: **t3p bpm.input**
- Postprocess t3p output to obtain longitudinal wakefield

```
cd OUPTUT
acdtool postprocess wake_new wake.bnd wakefield.z.all.dat 0. 0.
```

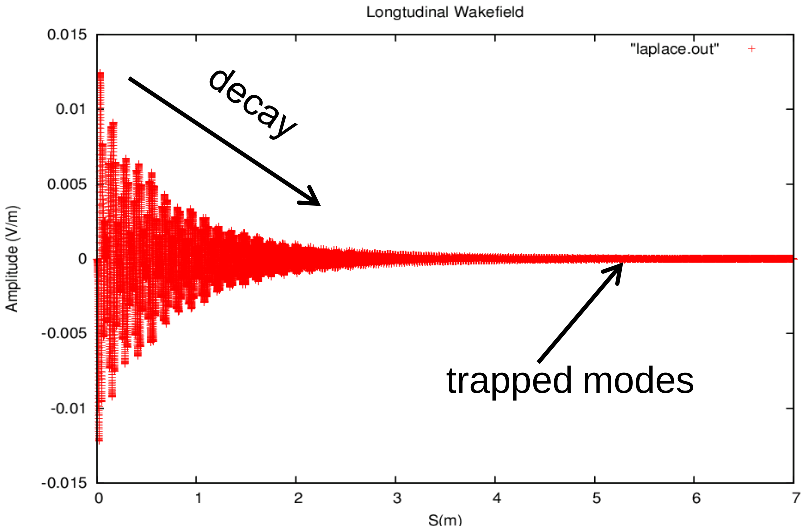
  – Wakefield data in output file ***wakes_new.out***,

- Plot the wakefield

Loss factor = 0.0037 V/pC

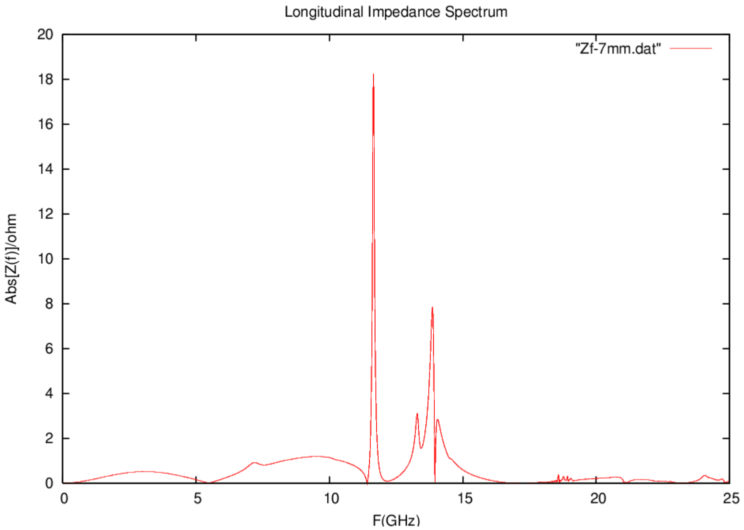


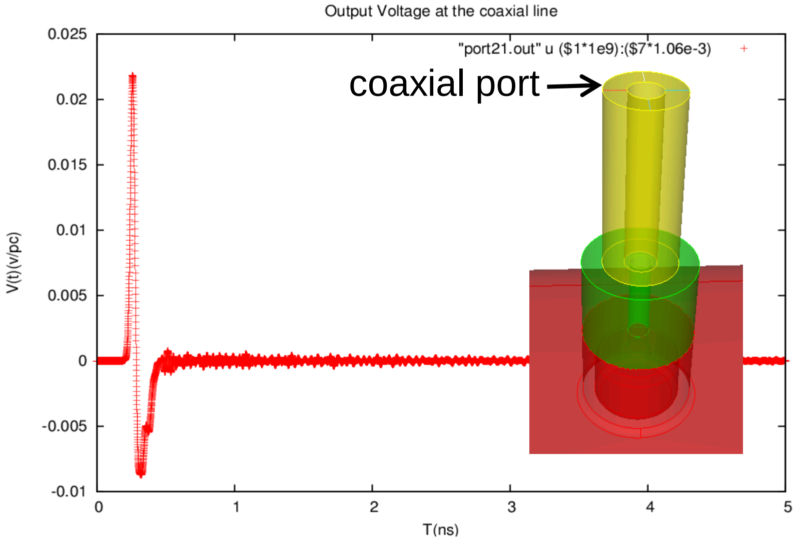
BPM Trapped Modes & Signal Sensitivity



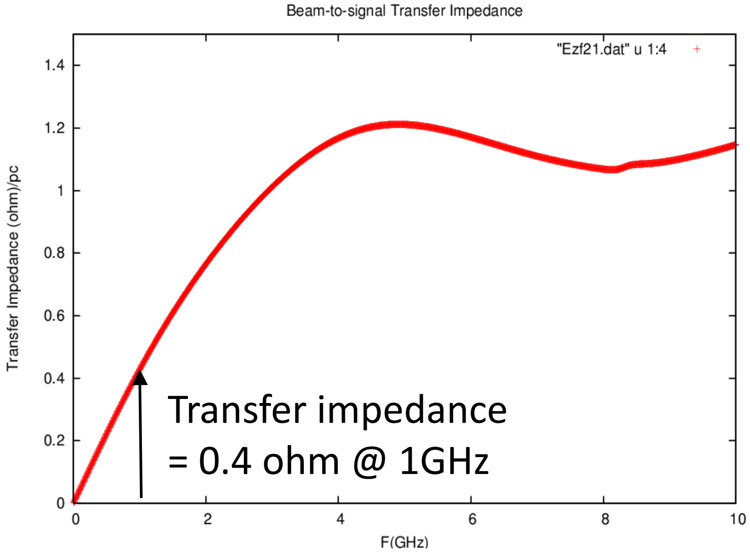
decay

trapped modes





coaxial port



Transfer impedance
= 0.4 ohm @ 1GHz

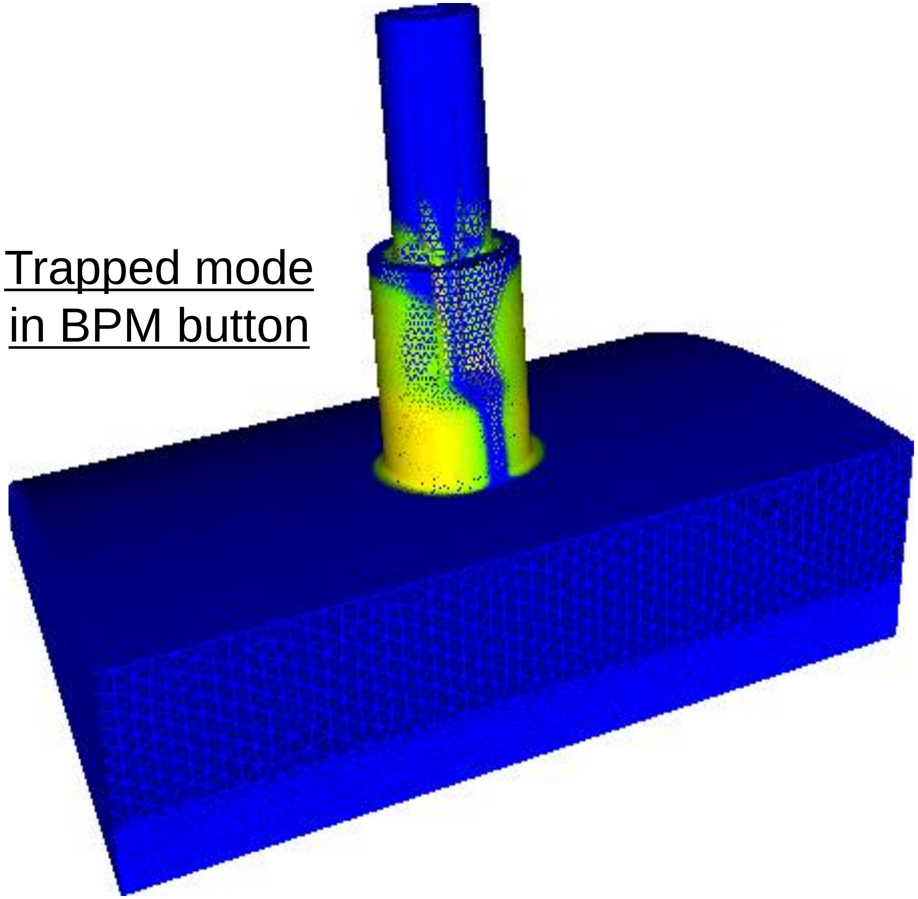
Identification of trapped modes and determination of signal sensitivity from time signals and their Fourier transforms.

BPM – Field Visualization

- Postprocess data for ParaView

  acdtool postprocess volmontomode bpm.input

  – Create *fs.out.mod in OUTPUT directory



Trapped mode in BPM button