Electromagnetic Systems Simulation (ESS)

Kwok Ko
(Representing the ESS team)

Advanced Computations Department
Stanford Linear Accelerator Center

SciDAC Project Review – 1/15-1/16, 2003
Berkeley, CA

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ADVANCED COMPUTATIONS

SciDAC ESS Focuses on:

- Parallel Electromagnetic Code Development
- Accelerator Modeling & Simulation
- Comp. Sci. & Appl. Math. Collaborations (E. Ng)
- Promoting Code Use (& Student Research)
- Summary/Future Plans

ESS Overview

Accelerator Modeling & Simulation | **Parallel Code Development** | **Appl. Math. & Comp. Sci.**

NLC
PEP-II
LCLS
Klystron
FNAL
PSI…

Comp. Math.
Accel. Mod.
Comp. Tech.

LBNL Stanford
SNL UCDavis
LLNL RPI

SBIR (STAR, Inc.) / USPAS / Grad & Undergrad Research

ADVANCED COMPUTATIONS

Contributors/Collaborators

(SciDAC/HENP – 715/1800 $K)

Accelerator Modeling

L. Ge, V. Ivanov, A. Kabel, K. Ko, Z. Li, C. Ng, L. Stingelin (PSI)

Computational Mathematics

Y. Liu, I. Malik, W. Mi, J. Scoville, K. Shah, Y. Sun (Stanford)

Computing Technologies

N. Folwell, A. Guetz, R. Lee, M. Wolf, G. Schussman (UCD), M. Weiner (Harvey Mudd)

SAPP- ***Stanford, LBNL, UCD***; **ISICs –** ***TSTT, TOPS***

(SciDAC/MICS ~ 400/655 $K)

LBNL (SCG)

E. Ng, P. Husbands, S. Li, A. Pinar

Stanford (SCCM)

G. Golub, O. Livne, Z. Su.

Sandia

P. Knupp, T. Tautges, L. Freitag, K. Devine

UCD (VGRG)

K. Ma, G. Schussman

LLNL (CASC)

D. Brown, K. Chand, B. Henshaw

RPI (SCOREC)

M. Shephard, Y. Luo

Parallel Electromagnetic Code Development

- **Need for accurate cavity design tools**
- **Unstructured grid + parallel processing**
- **Codes: Omega3P, Tau3P, Ptrack3D,** **S3P, Phi3P**

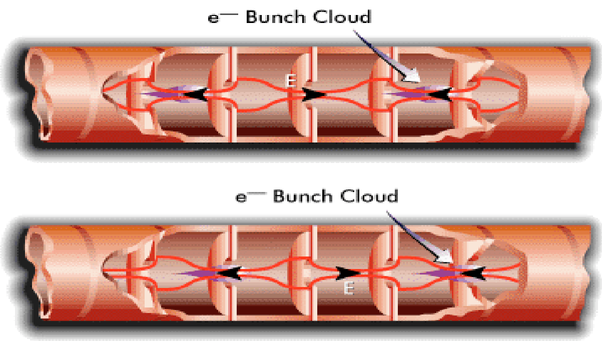
Challenges in EM Modeling of Accelerators

- **Accurate geometry is important due to tight tolerance**
  - needs unstructured grid to conform to curved surfaces
- **Large, complex electromagnetic structures**
  - large matrices after discretization (100's of millions of DOF), needs parallel computing
- **Small beam size ~** delta function excitation in time & space
  - ***Time domain*** **–** *needs to resolve beam size leading to huge number of grid points, long run time & numerical stability issues*
  - ***Frequency domain*** **–** *wide, dense spectrum to solve for thousands of modes to high accuracy*

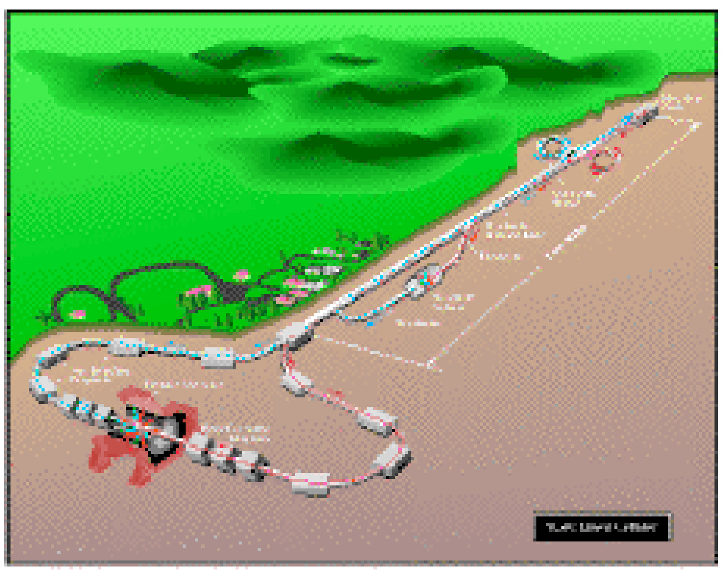
ADVANCED COMPUTATIONS

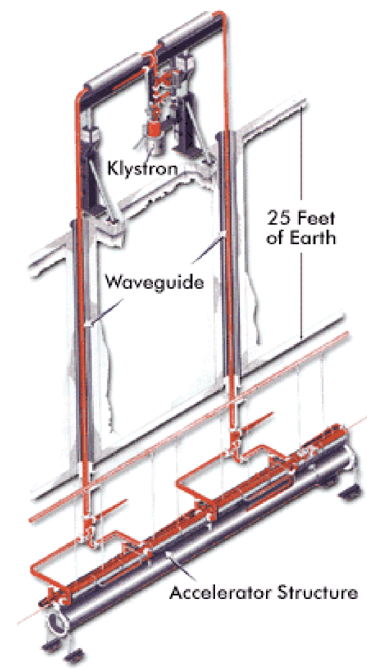
Stanford e+e- Linear Collider (SLC)

In the SLC, e+e- beams are accelerated by traveling waves in disk-loaded waveguide (DLWG) structures along the linac

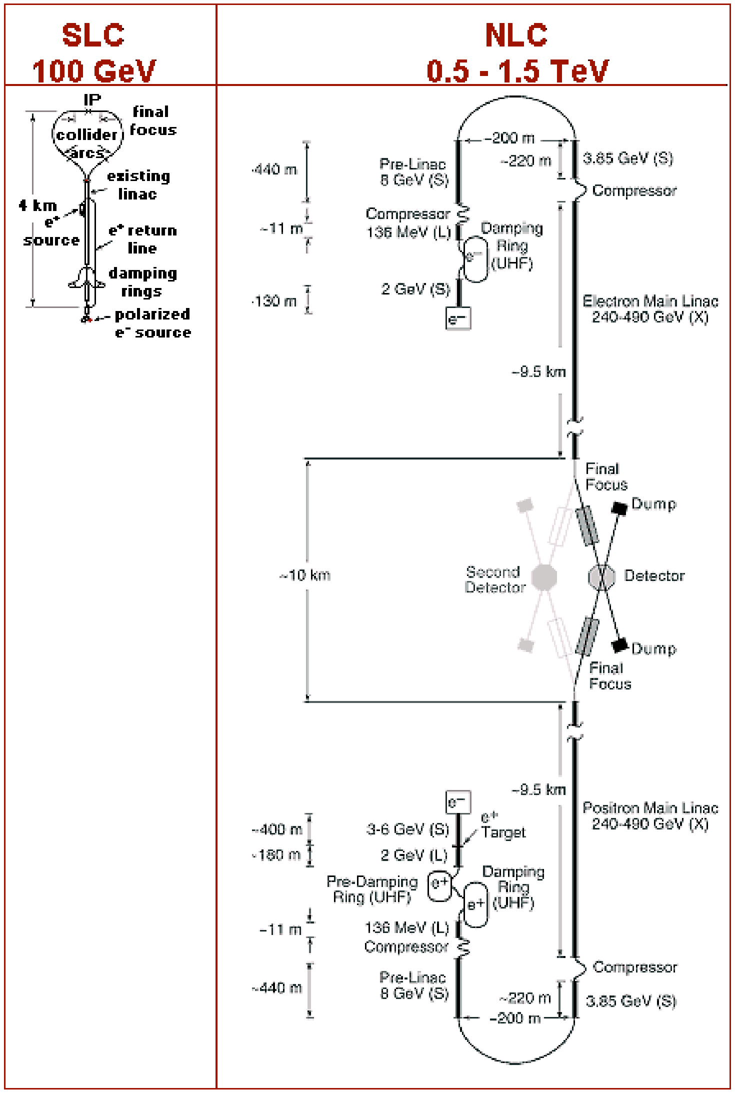


1/20,000,000,000 second later
(notice how far the bunches have moved)



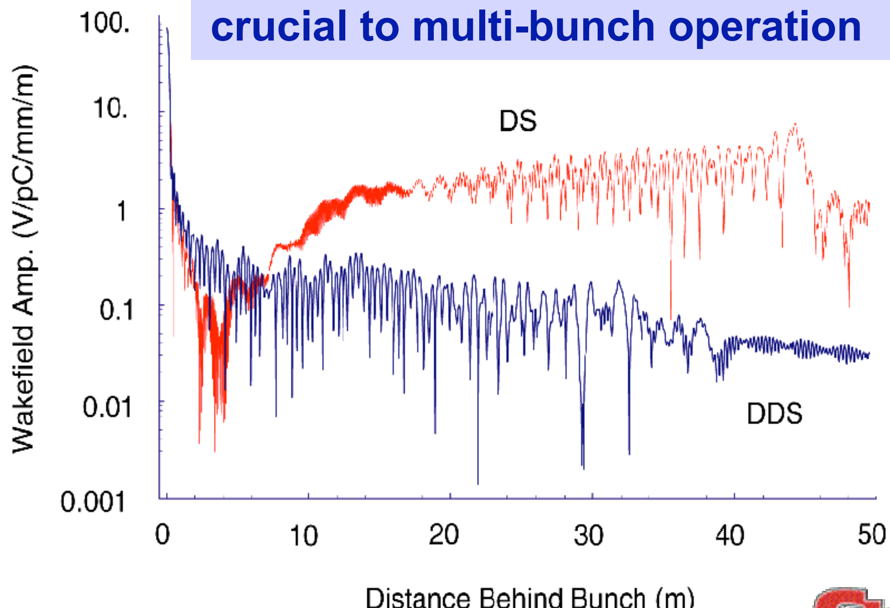


Next Linear Collider (NLC) – Wakefield Suppression



SLCNLCCenter of Mass100 GeV500 GeVBunches per pul:

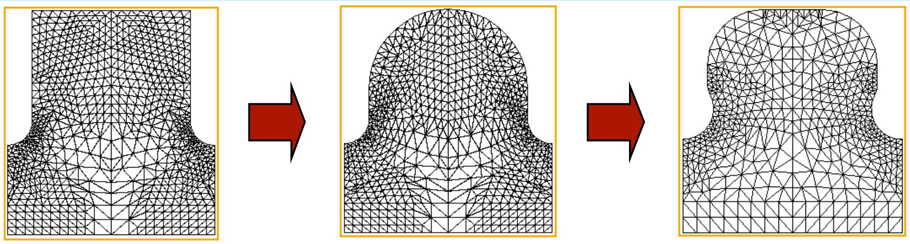
Control of Long Range Wakefield crucial to multi-bunch operation



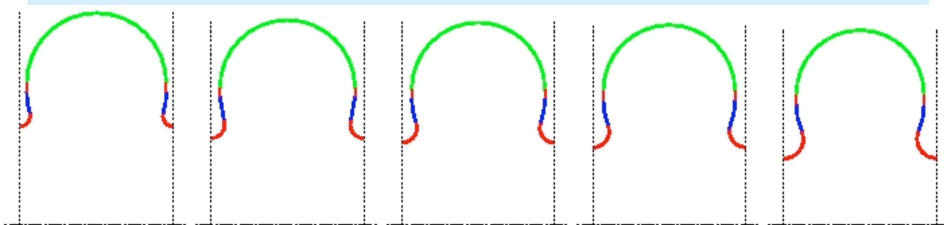
The NLC Accelerating Structure

206-Cell Round Damped Detuned Structure RDDS

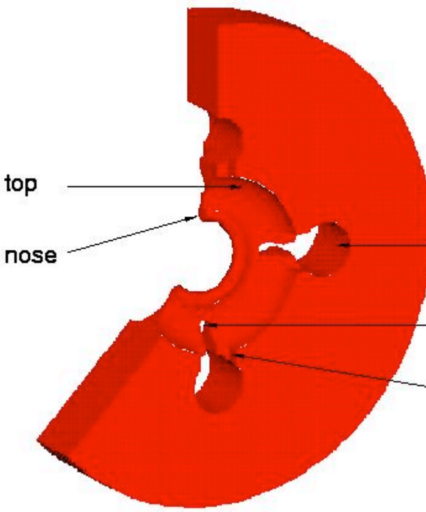
Cell optimized to increase shunt impedance (~14%) & minimize surface gradients



Cell to cell variation of order microns to suppress short range wakes by detuning



Manifold damping to suppress long range wakes



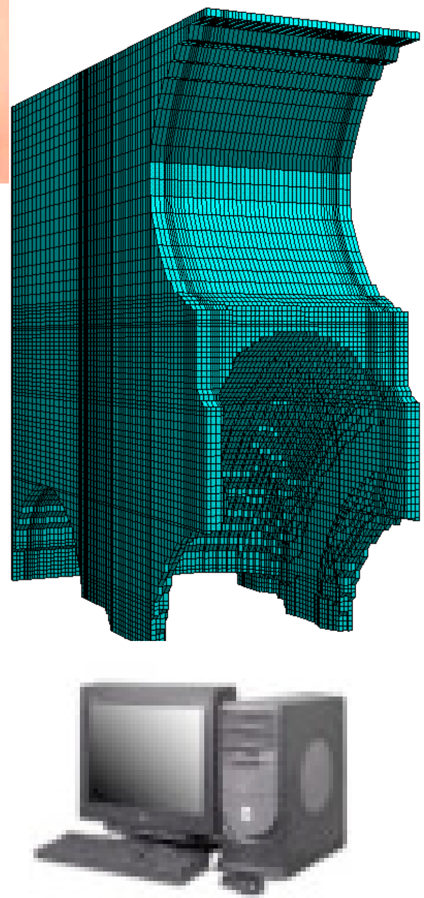
11 cavity dimensions

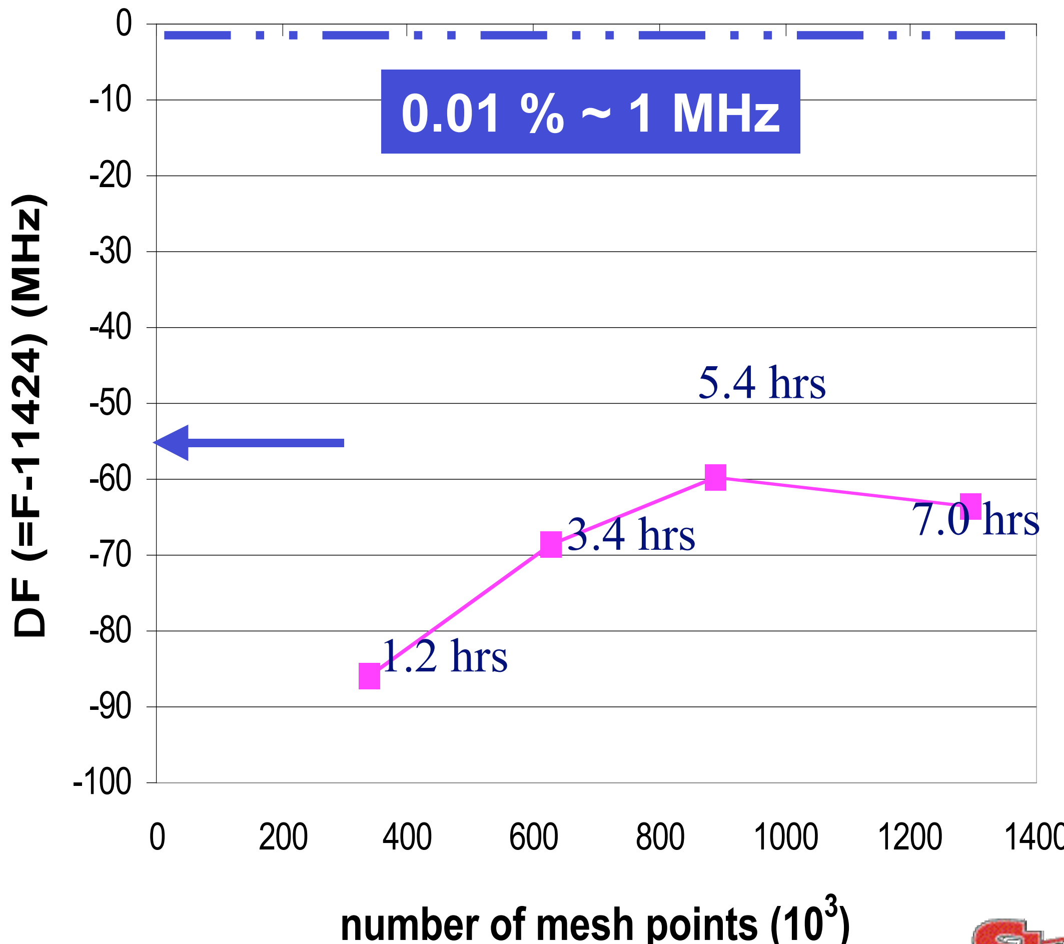
- **Needs accelerating frequency calculated to 0.01% accuracy to maintain structure efficiency**
- **Optimized design could save $100 million in machine cost**

ADVANCED COMPUTATIONS

Motivation for New EM Capability

Modeling RDDS Cell with standard community code MAFIA using Structured Grid on Desktops demonstrates the need for MORE ACCURATE EM codes





Parallel EM Code Development

Started with the NLC structure research, expanded under the DOE Grand Challenge, and is now fully supported by SciDAC with the emphasis on

>>> Modeling LARGE, COMPLEX structures to high accuracy using:

- **Unstructured Grids to conform to curved surfaces, and be able to increase resolution in regions of large field variation,**
- **Parallel Processing for big memory (mesh points) increase and speedup in simulation time.**

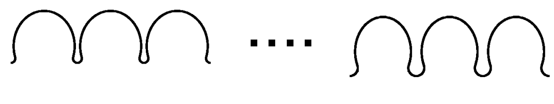
ADVANCED COMPUTATIONS

Eigensolver Development for Structure Design

- Round Detuned Cell

RF parameters *Omega2*

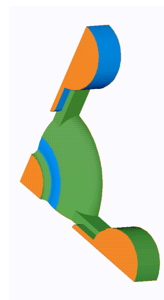
- Round Detuned Structure (RDS - 206 cells)



Transverse Wakefields *Omega2P*

----> DOE Grand Challenge

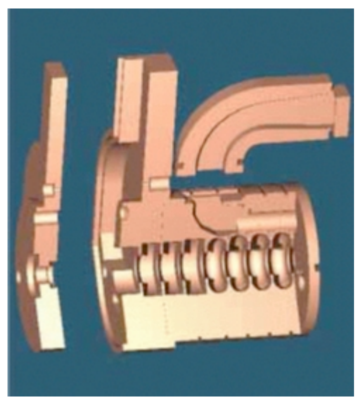
- Round Damped Detuned Cell



RF parameters *Omega3*

----> DOE SciDAC Project

- Round Damped Detuned Structure (RDDS - 206 cells)



Omega3P

Transverse Wakefields

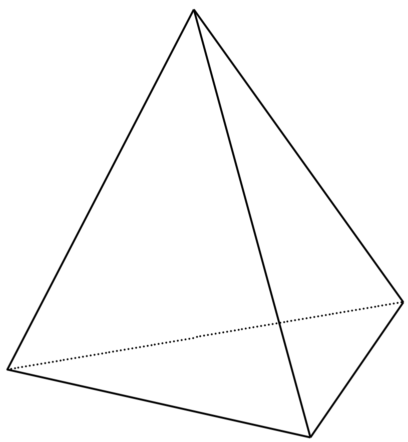
Omega3Pc

ACD ADVANCED COMPUTATIONS

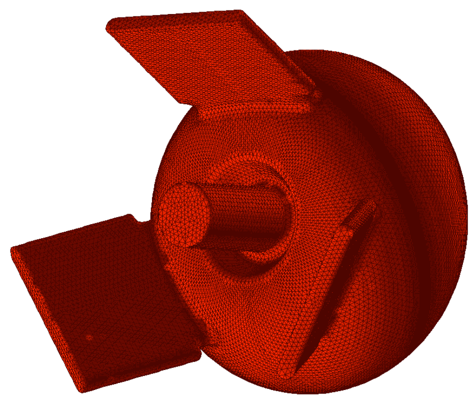
SLAC

Parallel Frequency-Domain Solver – Omega3P

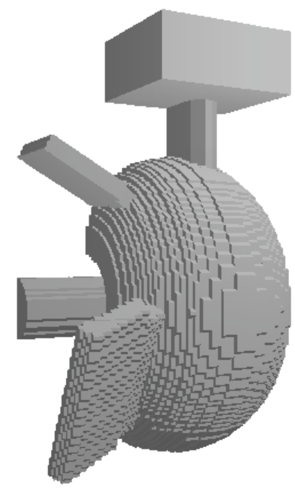
Calculates normal modes in lossless RF cavities using linear/quadratic finite elements on tetrahedral meshes.



Omega3P



MAFIA



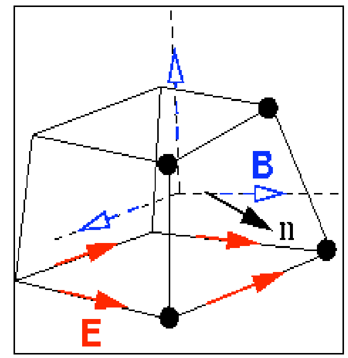
ADVANCED COMPUTATIONS

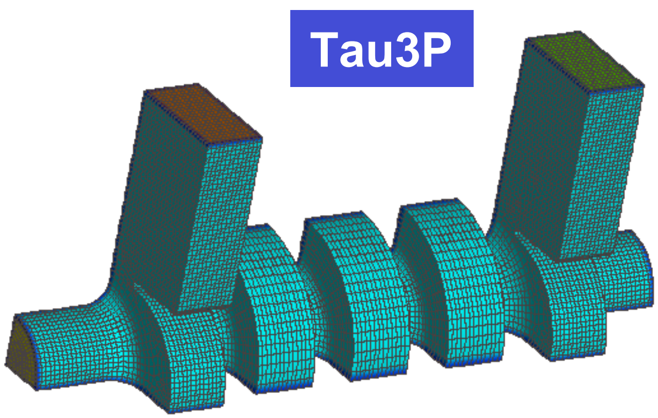
Parallel Time-Domain Solver – Tau3P

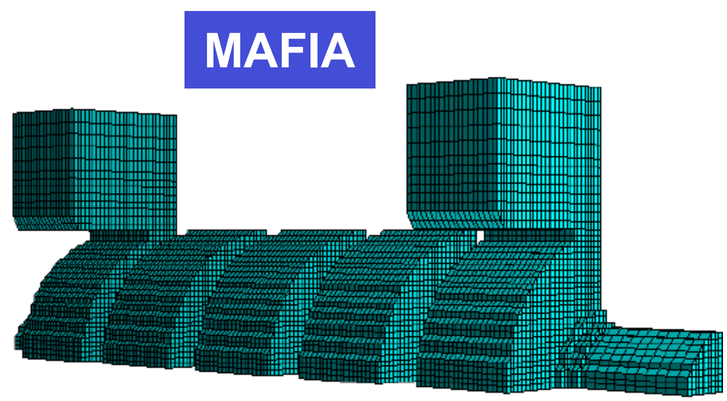
Follows evolution of E and H fields on dual meshes (hexahedral, tetrahedral and pentahedral elements) **using leap-frog scheme in time (DSI scheme)**

$$\oint E \bullet ds = -\iint \frac{\partial B}{\partial t} \bullet dA$$

$$\oint H \bullet ds^* = \iint \frac{\partial D}{\partial t} \bullet dA^* + \iint j \bullet dA^*$$



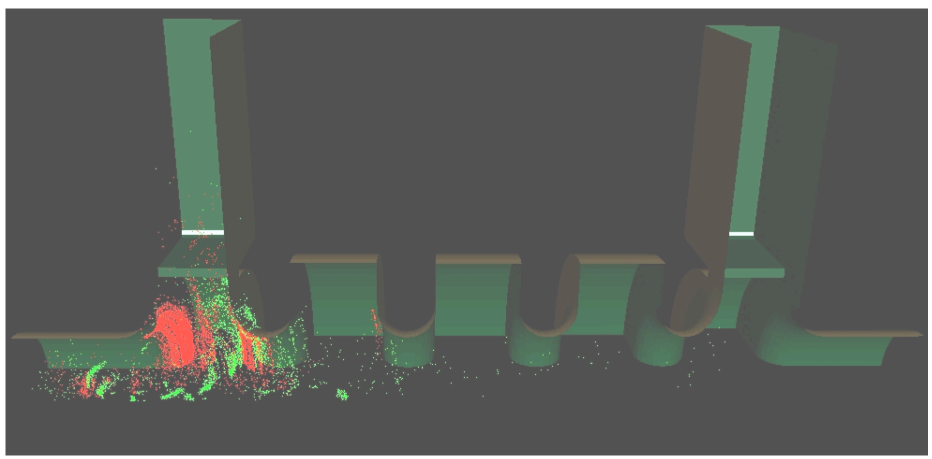




Particle Tracking Module – Ptrack3D

Calculate particle trajectories using E & B fields from Omega3P (for standing wave cavities**) or from Tau3P (**for traveling wave structures**) including surface physics (**injection, thermal emission, field emission**,** secondaries..**)**

$$\frac{d\vec{p}}{dt} = e\left(\vec{E} + \frac{1}{c}\left[\vec{v} \times \vec{B}\right]\right), \vec{p} = m\gamma\vec{v}, \gamma = \frac{1}{\sqrt{1 - v^2 / c^2}}$$



Ptrack3D – Surface Physics

- **Particle Injection**

$$I(t) = \frac{I_{\max}}{1 + \left(\left(\frac{v_0}{a} \right) t - \frac{\square_0}{\square} - iD_t \right)^2}$$

- **Thermal Emission (Child – Langmuir)**

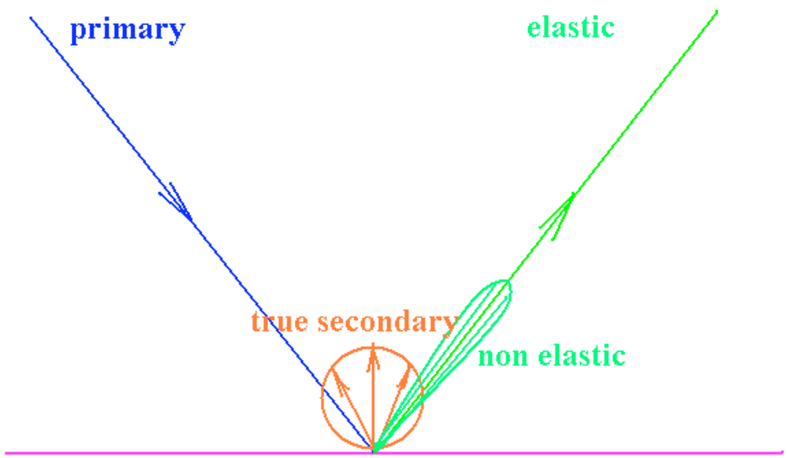
$$J(r,t) = \frac{4}{9} \varepsilon_0 \sqrt{\frac{2QE^2}{Md}}$$

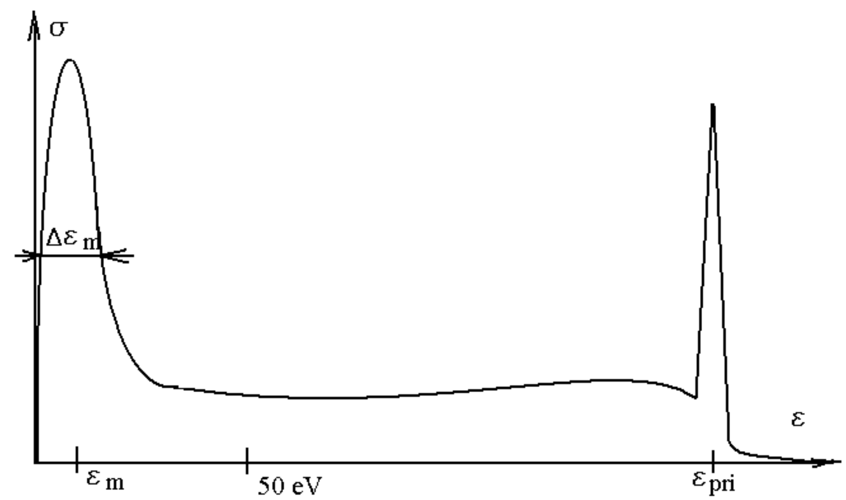
- **Field Emission (Fowler - Nordheim)**

$$J(r,t) = 1.54 \times 10^{\left(-6 + \frac{4.52}{\sqrt{\phi}} \right)} \frac{(\beta E)^2}{\phi} e^{\left(-\frac{6.53 \times 10^9 \phi^{1.5}}{\beta E} \right)}$$

Ptrack3D - Secondary Emission Model

- $\sigma = I_{secondary}/I_{primary} = \delta+\eta+r$;
- δ - true secondary emission (0-50 eV). $\varepsilon_m \approx$ 2-4.5 eV;
  $\Delta\varepsilon \approx$ 12-15 eV;
- η - non elastic reflection (50 eV-ε_{pri})
- r - elastic reflection; r = 0.05-0.5 for metals.

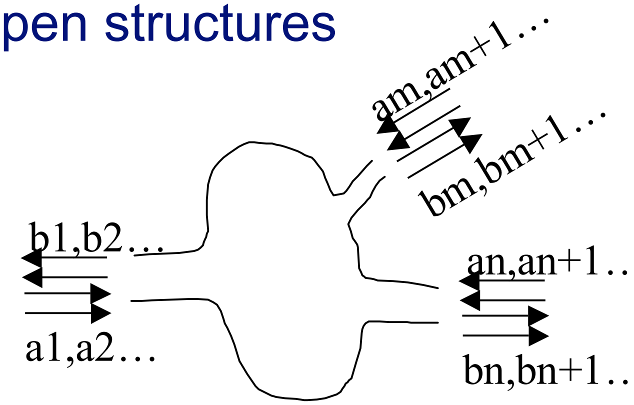




New Parallel Solvers

S3P – Frequency-domain solver based on **Omega3P** to calculate the Scattering Matrix S of open structures

$$\int_\Omega \frac{1}{\mu_r}(\nabla \times \vec{E})^* \cdot (\nabla \times \vec{h})dv - \frac{\omega^2}{c^2}\int_\Omega \vec{E}^* \cdot \vec{h}dv$$
$$= -i\omega\mu_0 \int_S (n \times \vec{H}_{excit})^* \cdot \vec{h}ds$$



Phi3P – Statics solver with field-based hybrid finite element (B on face, H on edge) for higher accuracy in fields & exact boundary condition description

Min 1/2 || $\underline{B}$ - _ $\underline{H}$ ||^2 s.t. div $\underline{B}$ = 0

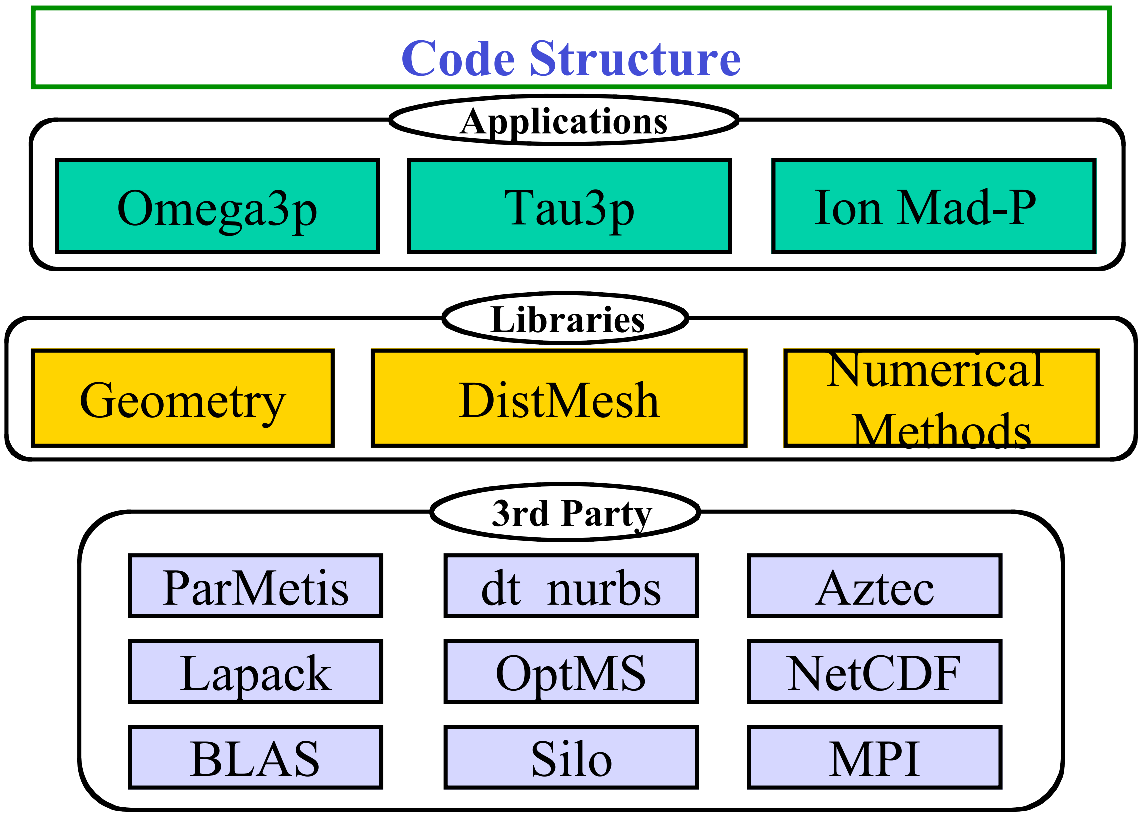
curl $\underline{H}$ = $\underline{J}$

$\underline{B} \bullet \underline{n} = f_B$

$\underline{H} \times \underline{n} = f_H$

Parallel Code Structure

- Written in C++ and use MPI for communication
- Share geometry data for mesh distribution & matrix assembly
- Reuse existing parallel libraries - ParMETIS, Aztec, …



Accelerator Modeling & Simulation

- **High resolution cavity design w/ Omega3P**
  (Accurate frequency & wall loss determination)
- **Numerical design & analysis w/ Tau3P**
- **System scale simulation w/ Omega3P & Tau3P**
- **Modeling dark current w/ Ptrack3D**

ACD ADVANCED COMPUTATIONS

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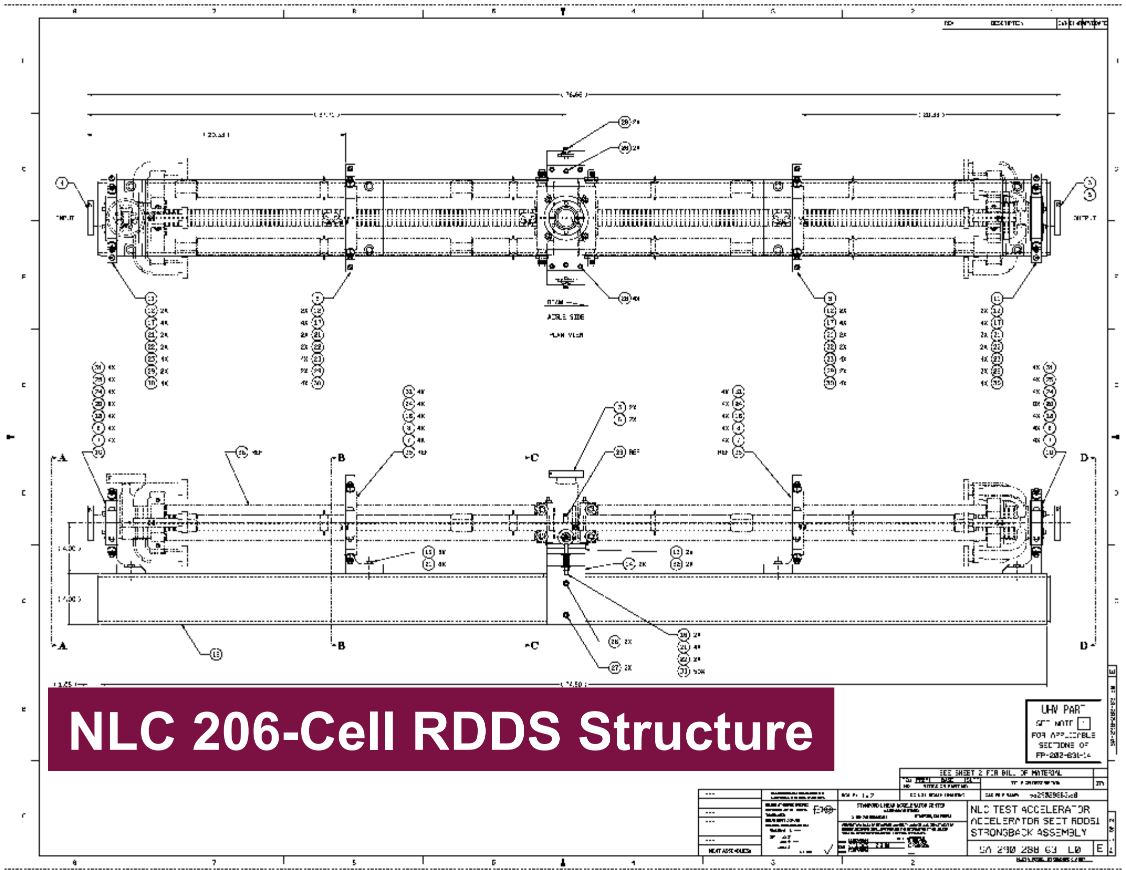
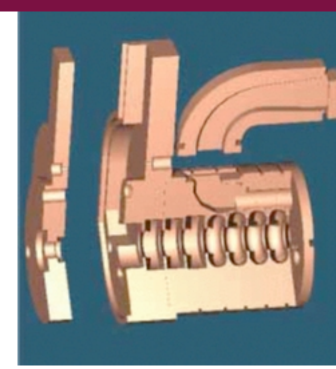
NLC Structure Design Requirements



NLC 206-Cell RDDS Structure

RDDS Cell

RDDS Section



- **RDDS Cell : Design to 0.01% accuracy in accelerating frequency,**
- **RDDS Section : Model damping/detuning of dipole wakefields.**

ACD ADVANCED COMPUTATIONS

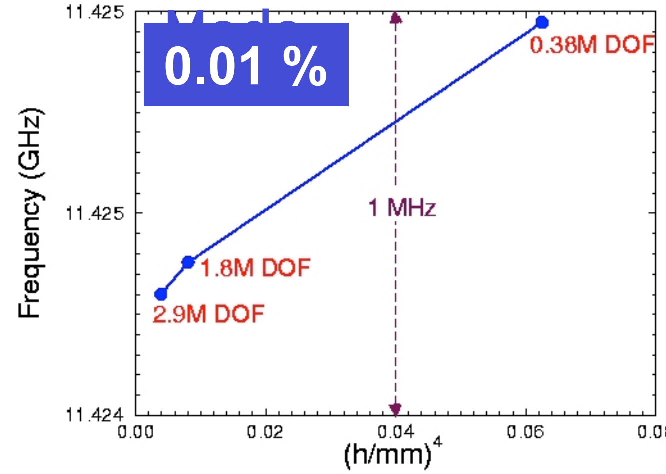
SLAC

Modeling RDDS Cell Design (Omega3P)

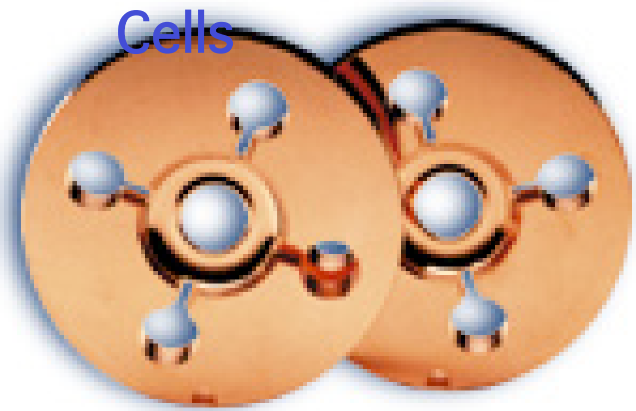
Omega3P Model

NERSC/T3E:
Elem=60K,
DOF=380K,
#proc=16,
T=19 min

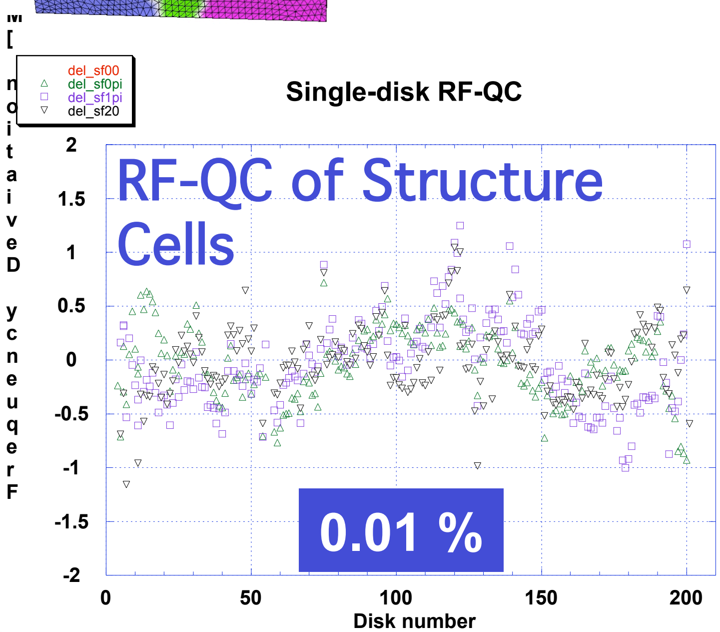
Accelerating Mode



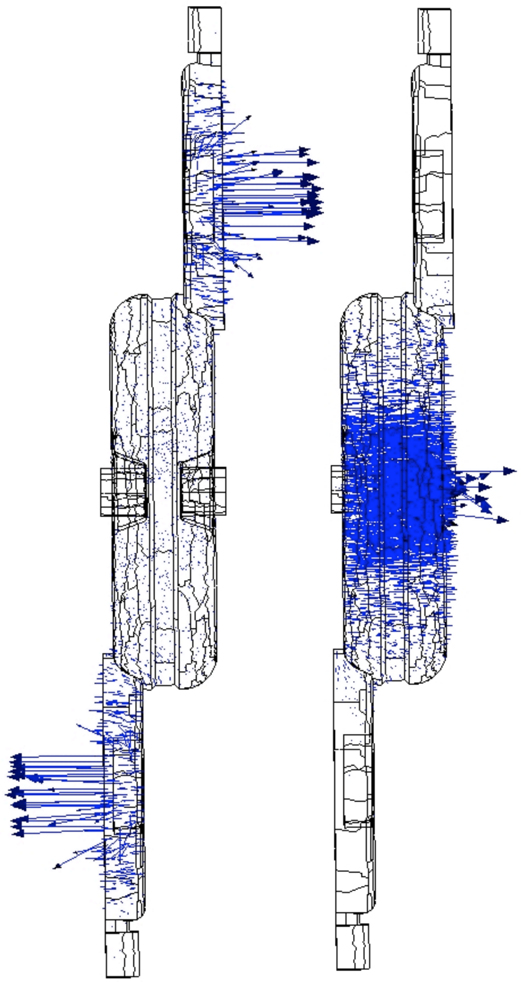
Fabricated Cells



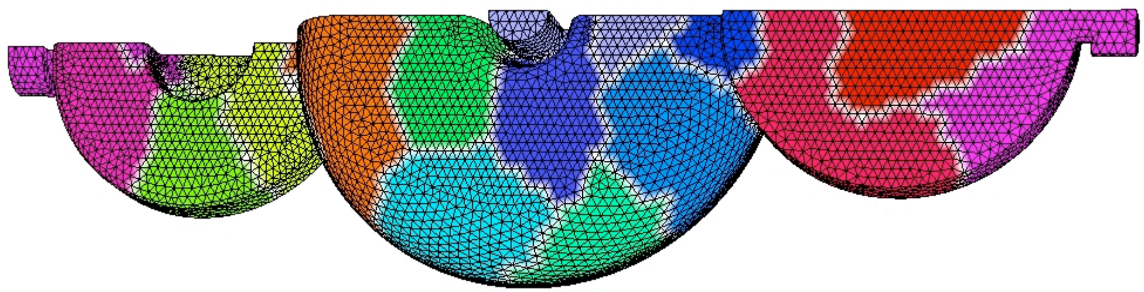
RF-QC of Structure Cells



APT Coupled Cavity Linac (Omega3P)



Omega3P Model



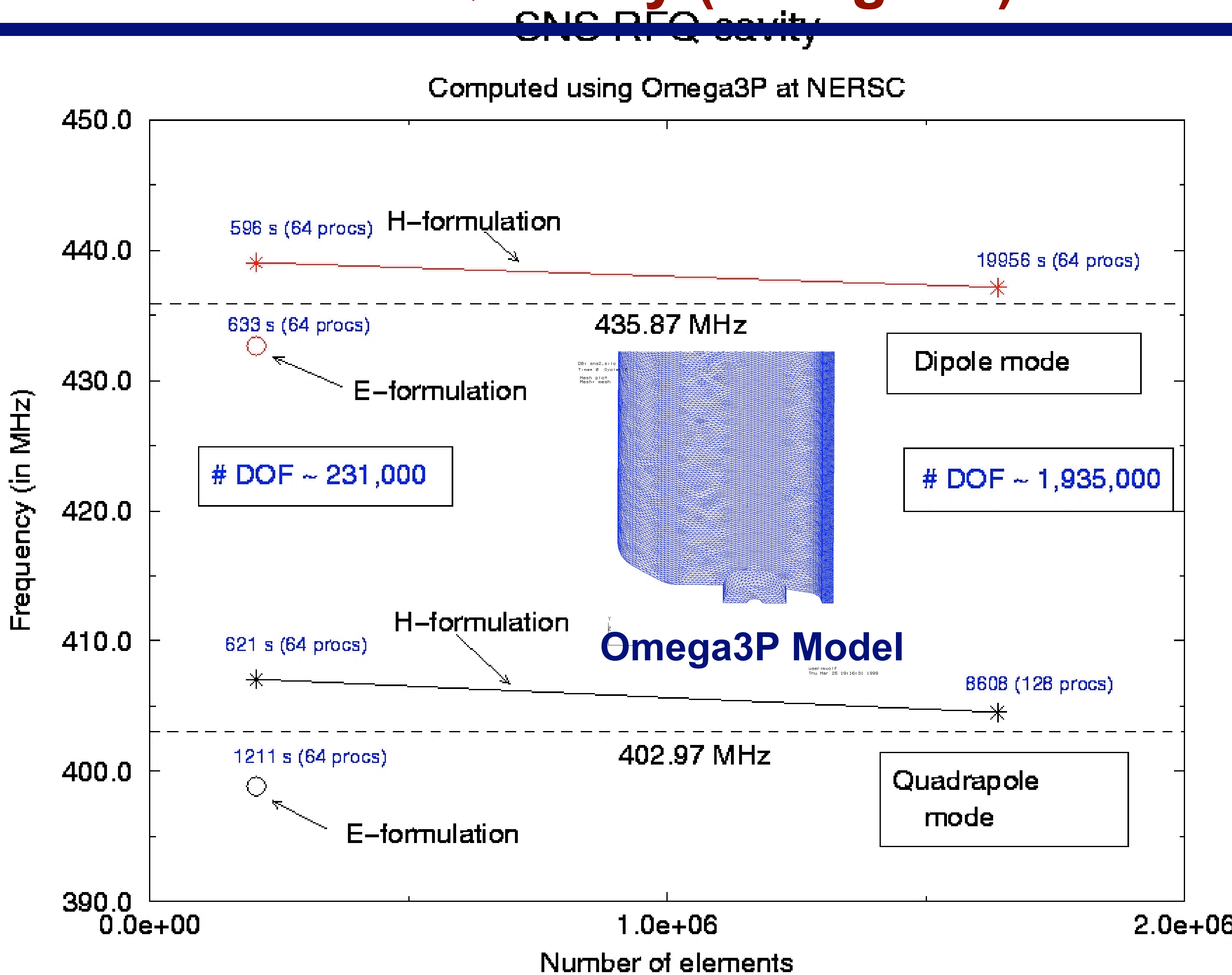
(MHz)	Frequency shift	Stop band
Measured	17.56	0.46
Ω3P	17.62	0.54

NERSC/SP2:
Elem=646K,
DOF=4M,
#proc=256,
T=1 hr

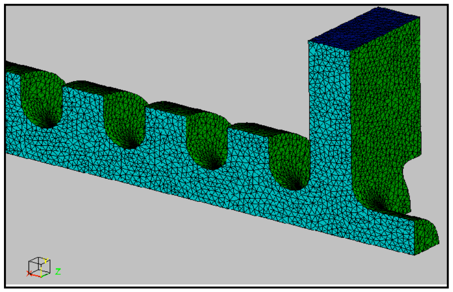
(MHz)	f_1^{uc}	f_1^c	f_2^c	k	k_1
Measured	1431.35	1413.79	1409.41	0.0376	-0.00556
Ω3P	1432.31	1413.73	1409.50	0.0382	-0.00523

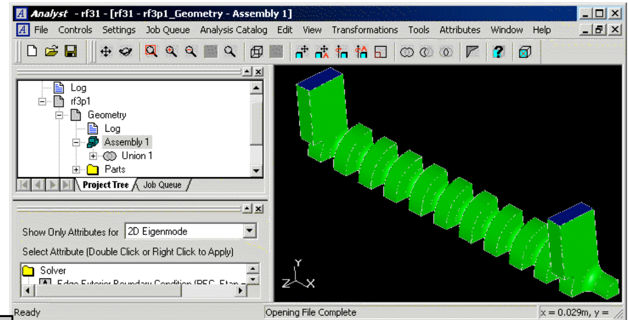
1432.35 (2D)

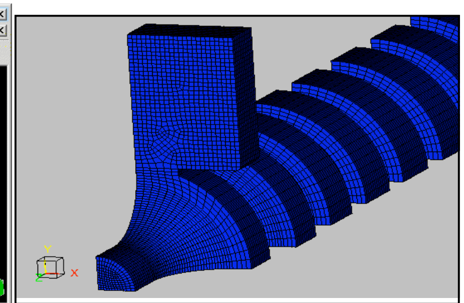
SNS RFQ Cavity (Omega3P)

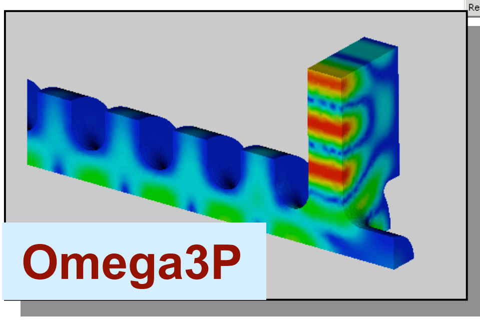


Promote Code use

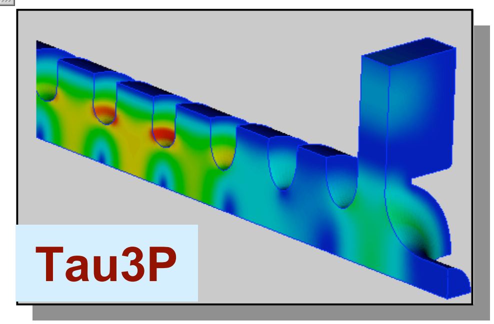








SBIR with STAR, Inc
Analyst provides an integrated GUI to Omega3P and Tau3P (FNAL,MSU,KEK,PSI)



US Particle Accelerator School (Stony Brook 2000, Yale 2002)

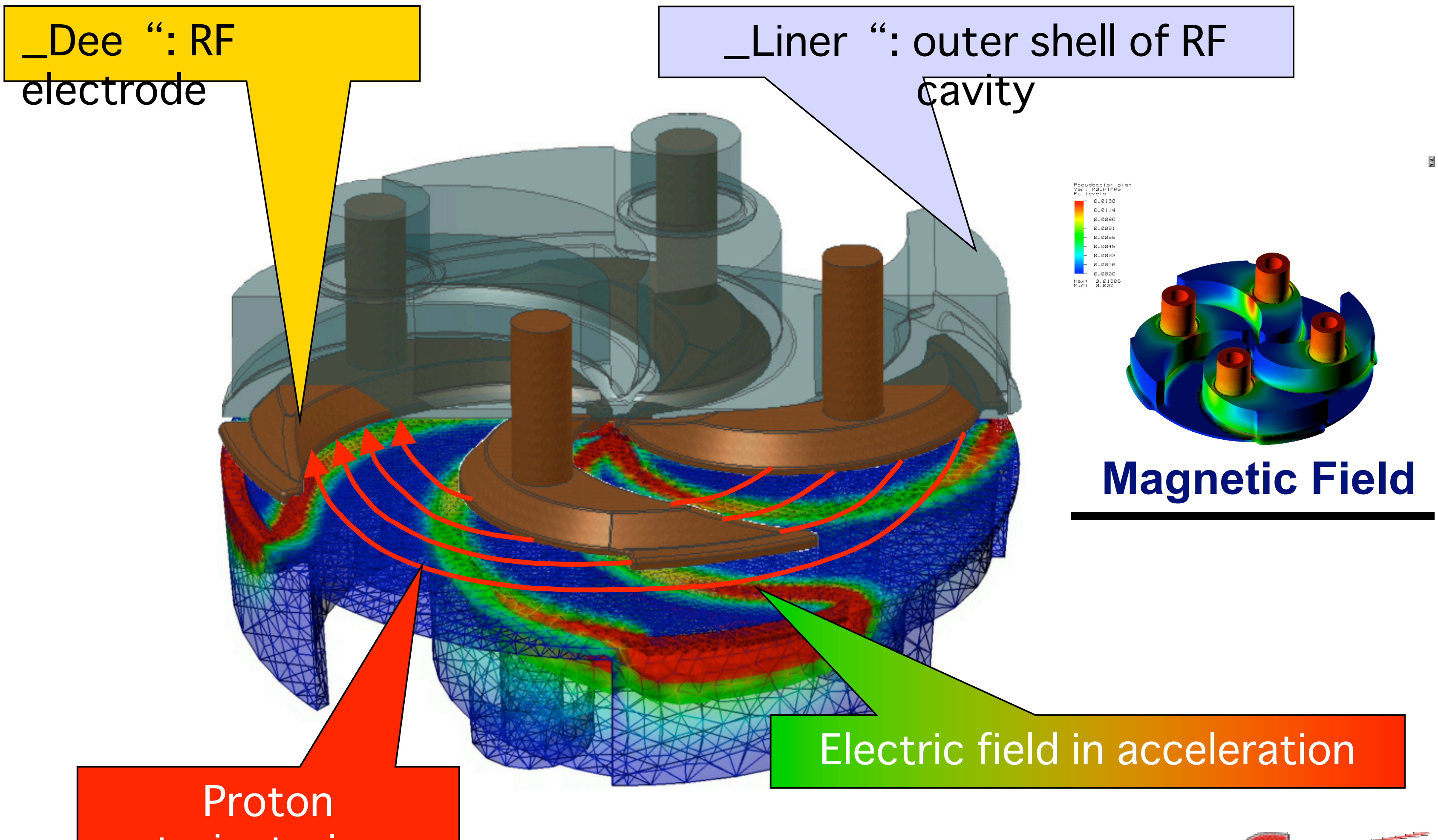
Computer Modeling:

(1) Electromagnetic Modeling in Accelerator Design & Analysis
(2) EM Codes _ Omega2P, Omega3P, RF3P, MAFIA, POISSON
(3) 2D Design _ SW Cavity & TW Structures
(4) 3D Design - External Q (SW) & Matching (TW)
(5) Vacuum Chamber, Beamline Components _ Performance & Failure Modes
(6) Computing Wakefields & Impedances
(7) Modeling Magnets & Eddy Currents

ADVANCED COMPUTATIONS

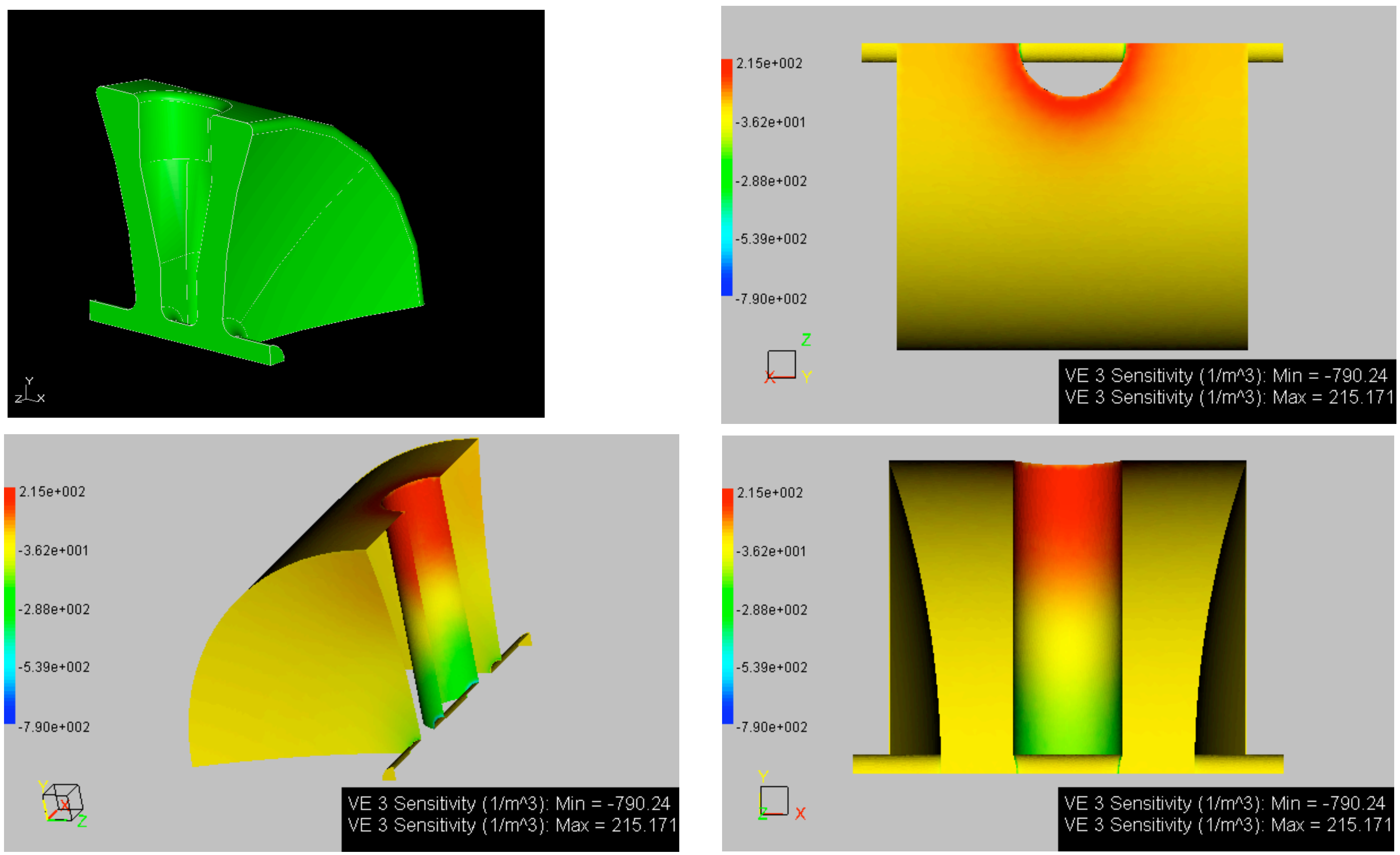
Cyclotron COMET (Omega3P)

First ever detailed analysis of an entire cyclotron structure
- L. Stingelin, PSI



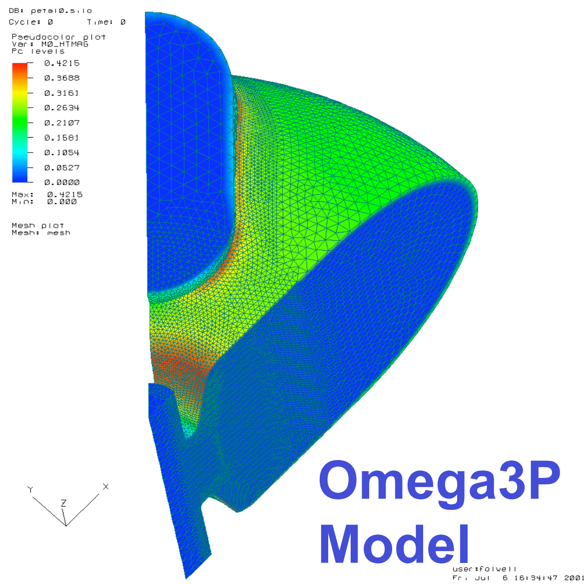
LANL Spoke Resonator (Omega3P)

Sensitivity analysis – J. DeFord (STAR, Inc.), F. Krawcyk (LANL)



Trispal CCL Cavity Design (Omega3P)

New Design with 4 Petal Coupling – P. Balleyguier (CEA)



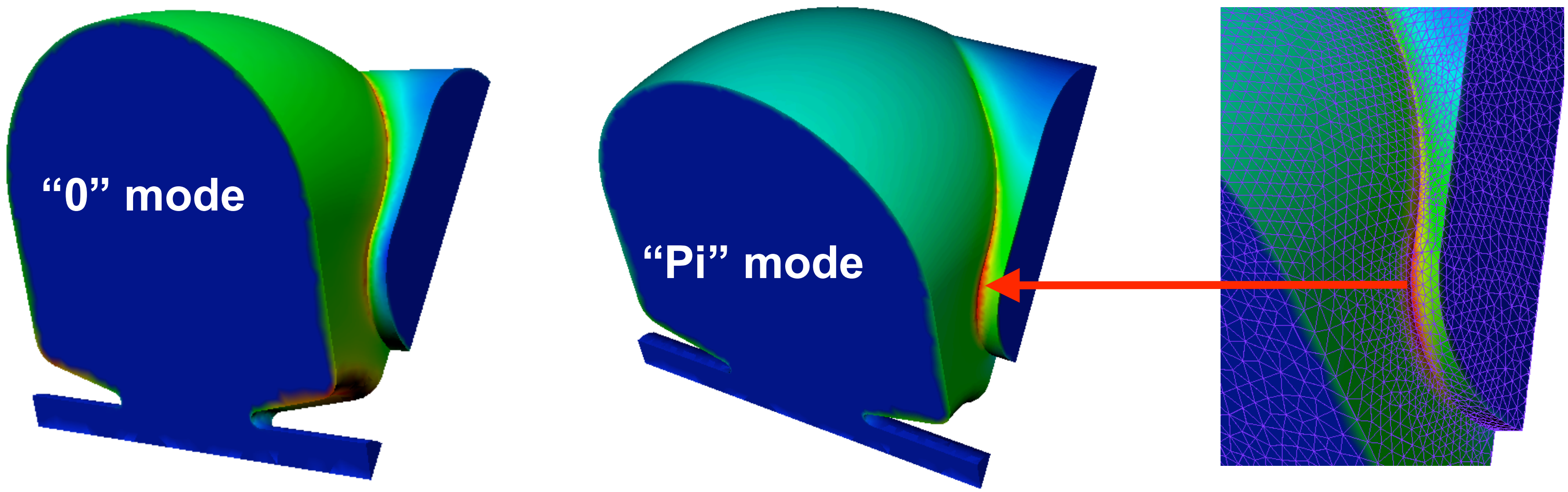
Frequency in MHz

Mode	Measured	Omega3P	Diff
Single	1080.841	1082.301	0.14%
Pi	1064.415	1066.106	0.16%
Zero	1072.412	1074.102	0.16%

Cavity openings perturb wall current leading to:

- **Increased wall loss that degrades shunt impedance**
- **Local RF heating that requires proper cooling**

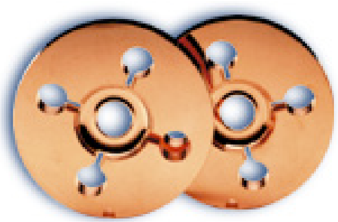
Accurate Wall Loss Determination (Omega3P)



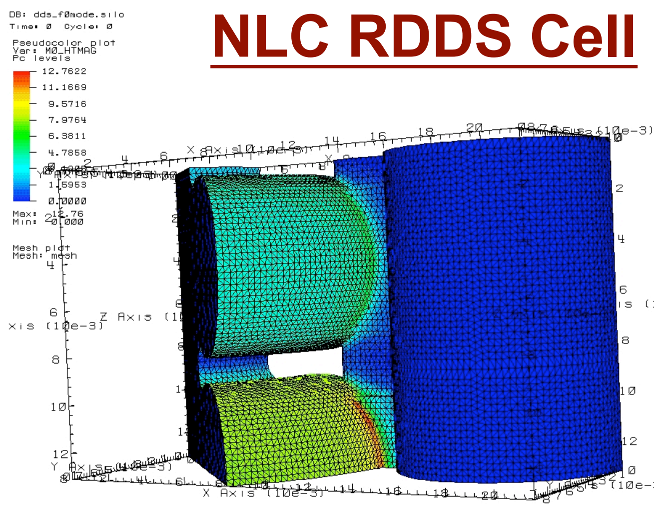
Mode	Meas.	dQ/Q	Omega3P	dQ/Q	MAFIA	dQ/Q
Single	12880		13509		12236	
Pi	11340	-22.5%	12111	-19.6%	11924	- 5.0%
Zero	12938	0.9%	13738	3.4%	12922	11.5%

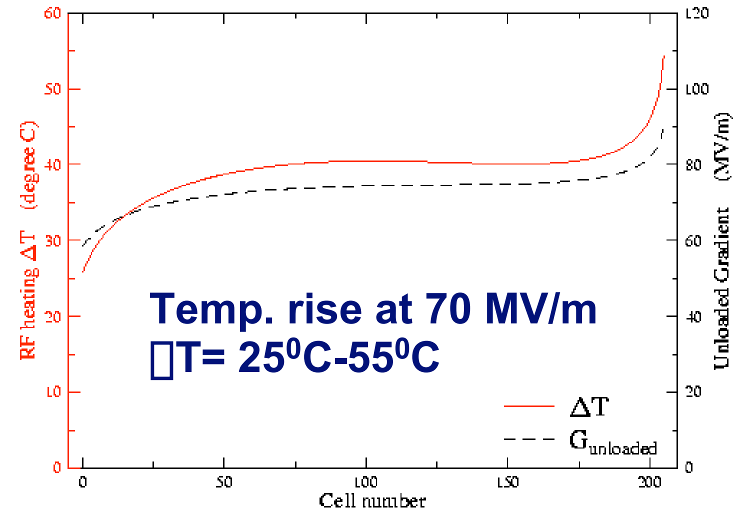
Omega3P enables new cavities to be designed with confidence

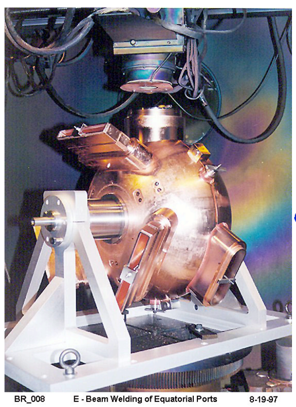
Local RF Heating (Omega3P)

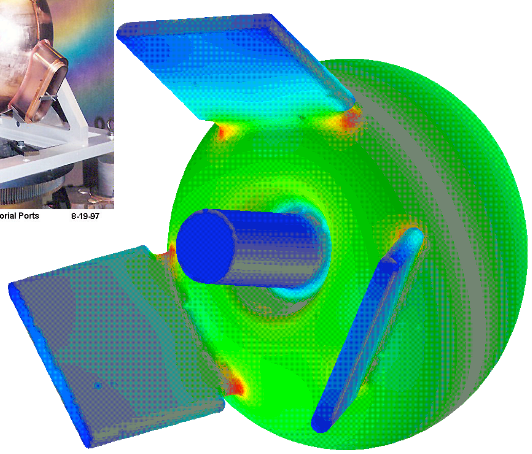


NLC RDDS Cell

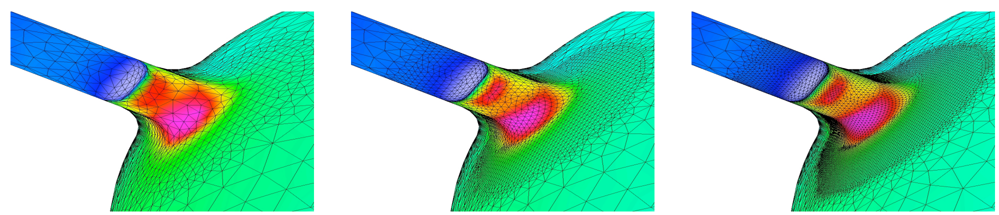








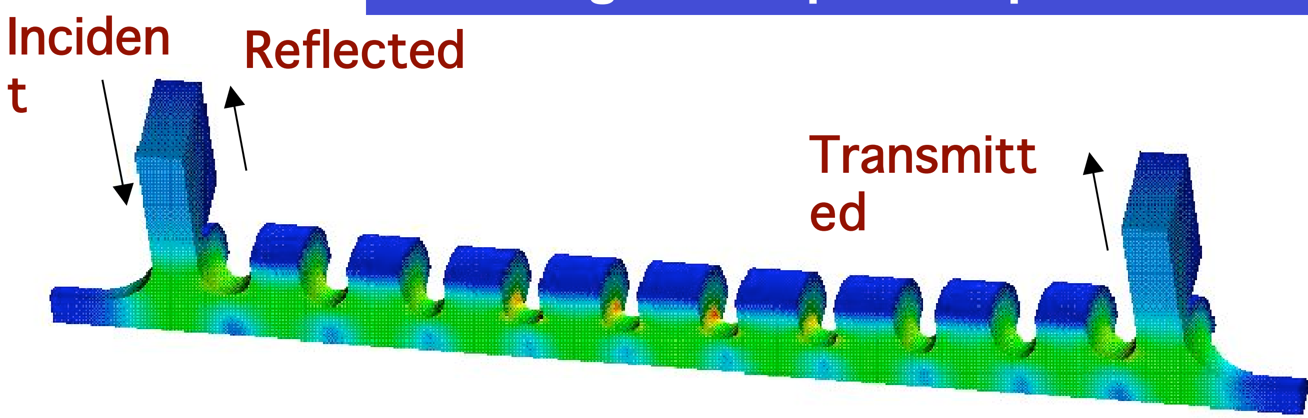
PEP-II RF Cavity

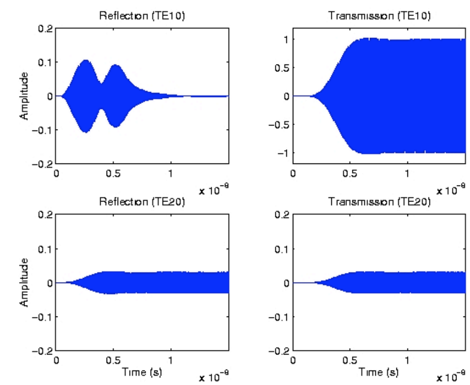


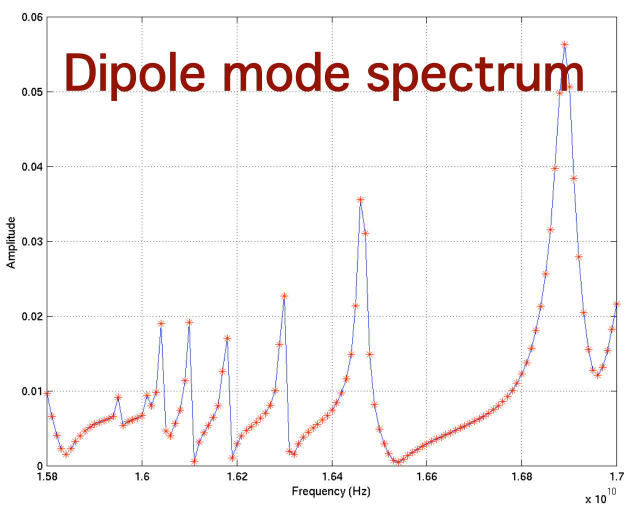
refined mesh size:	5 mm	2.5 mm	1.5mm
# elements :	23390	43555	106699
degrees of freedom:	142914	262162	642759
peak power density:	**1.2811 MW/m**	**1.3909 MW/m²**	**1.3959 MW/m²**

Time Domain Design & Analysis (Tau3P)

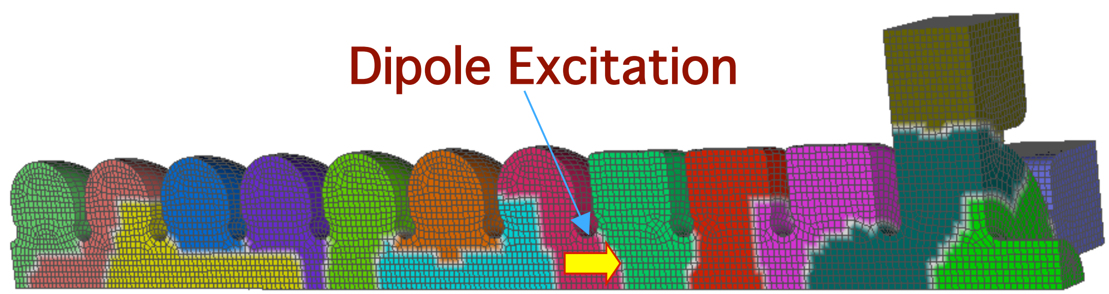
Matching NLC Input Coupler w/ Inline Taper







Output Coupler loading on HOM modes at the RDDS output end



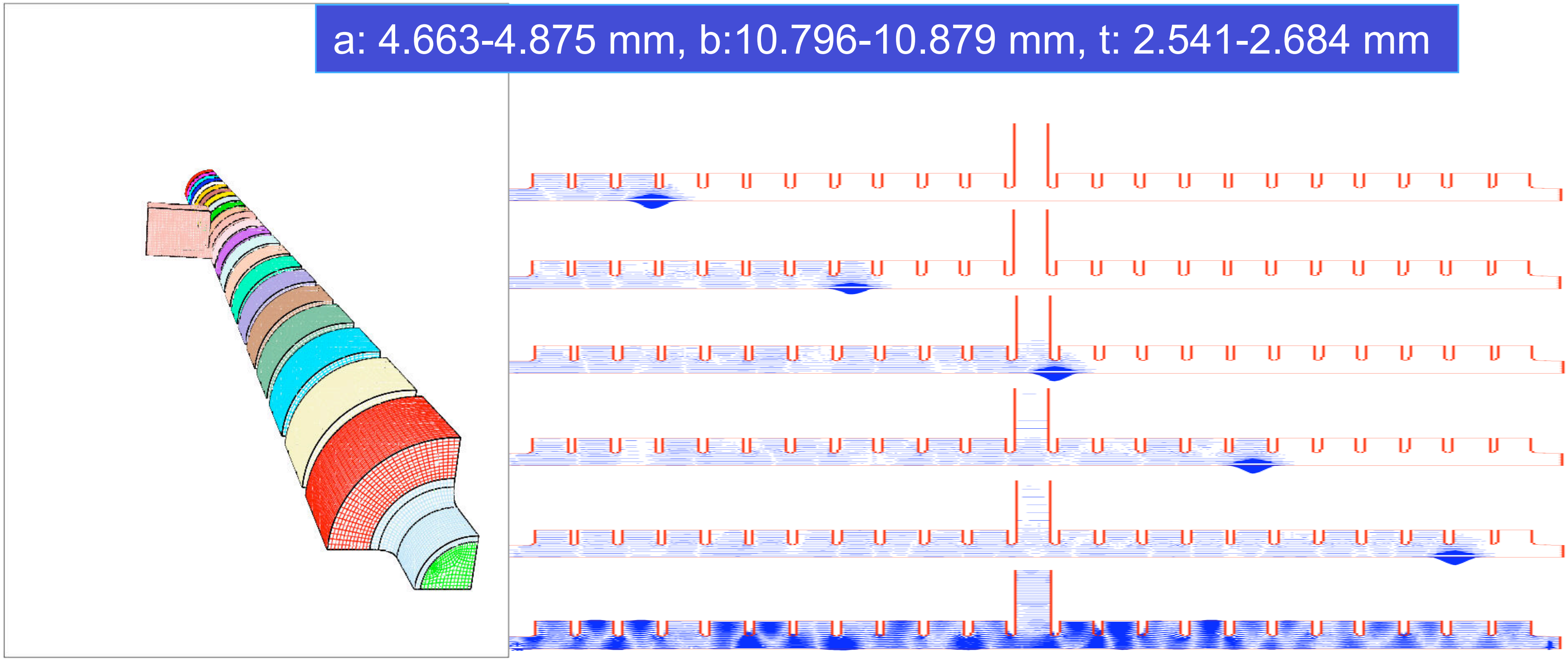
ACD ADVANCED COMPUTATIONS

SLAC

Wakefield Calculation (Tau3P)

- Response of a 23-cell X-Band Standing Wave Structure w/ Input Coupler & Tapered Cells to a transit beam in Tau3P.
- Direct wakefield simulation of exact structure to verify approximate results from circuit model.

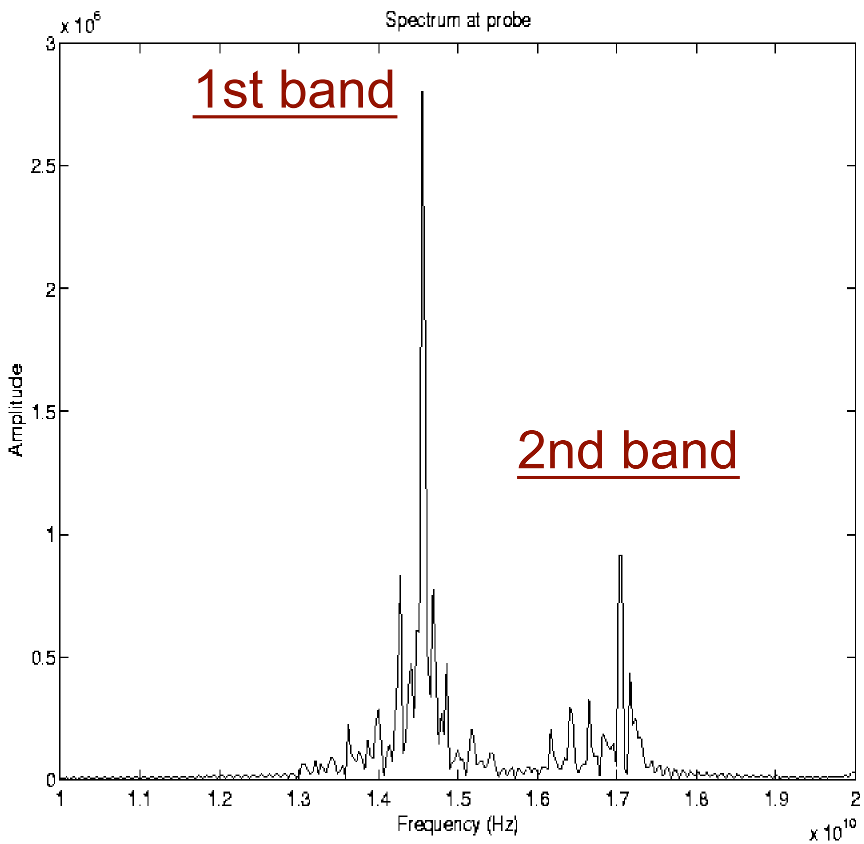
a: 4.663-4.875 mm, b:10.796-10.879 mm, t: 2.541-2.684 mm

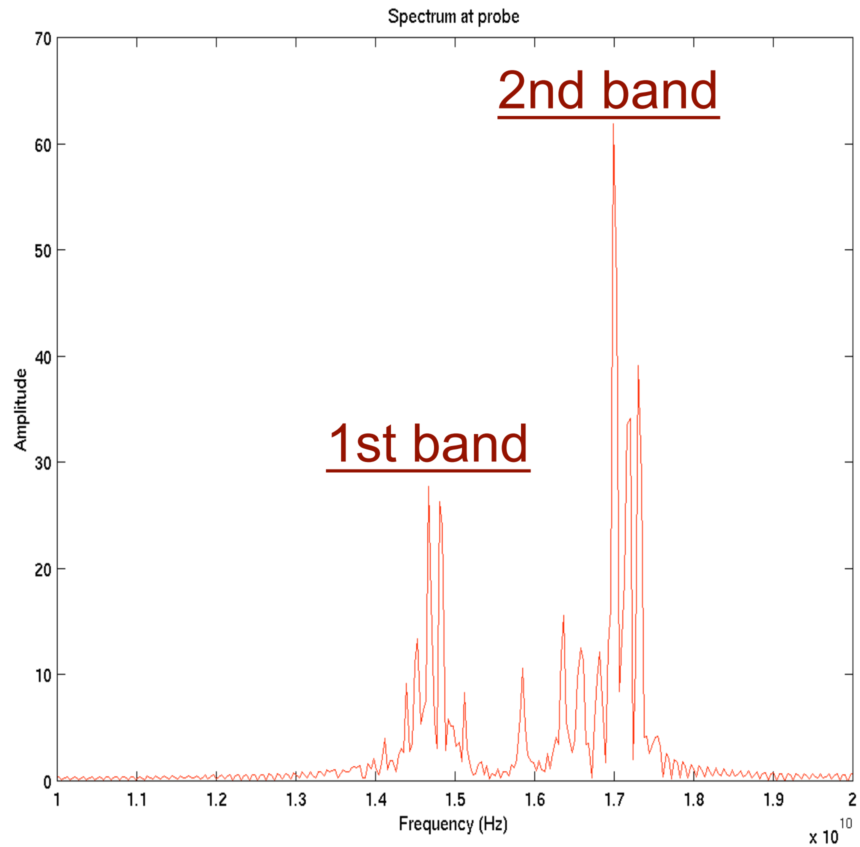


Beam Excited Dipole Mode Spectrum

Field inside Structure

Exit Field at Coupler Port

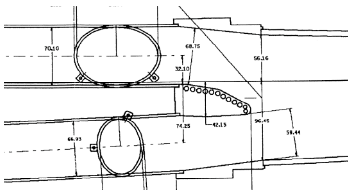




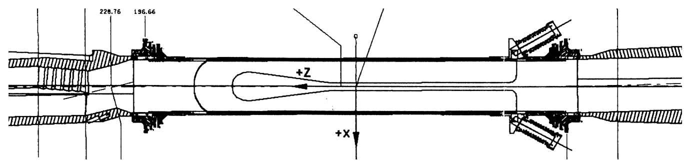
ADVANCED COMPUTATIONS

Heating in PEP-II Interaction Region

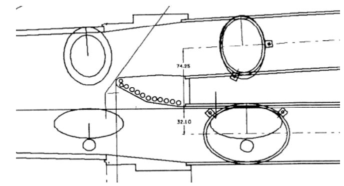
Left crotch | *Center beam pipe* | *Right crotch*



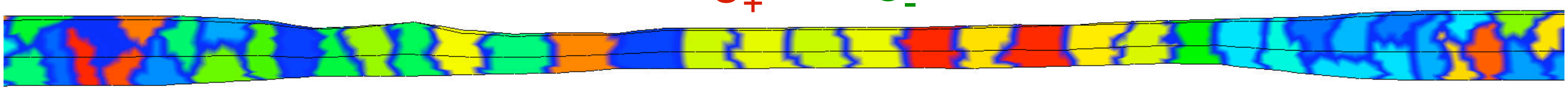
2.65 m

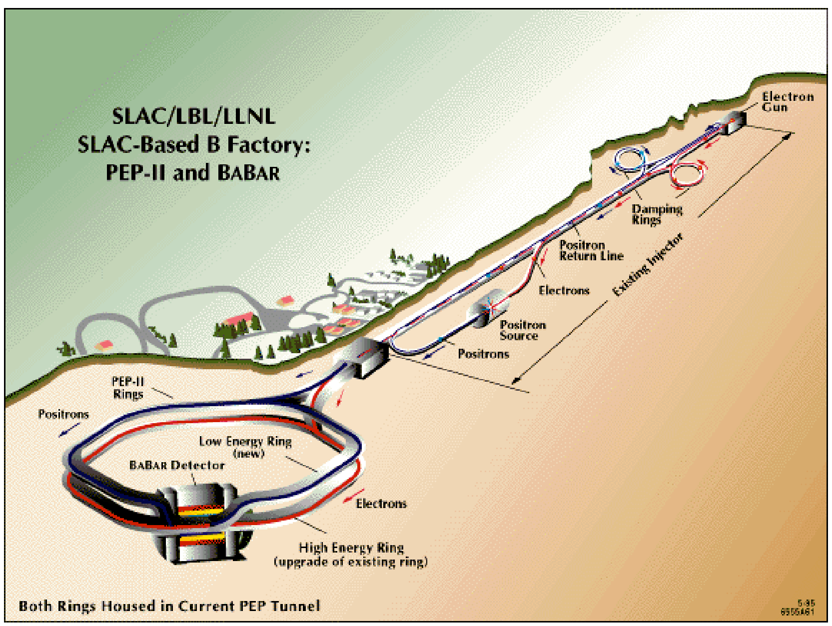


2.65 m



e_+ e_-

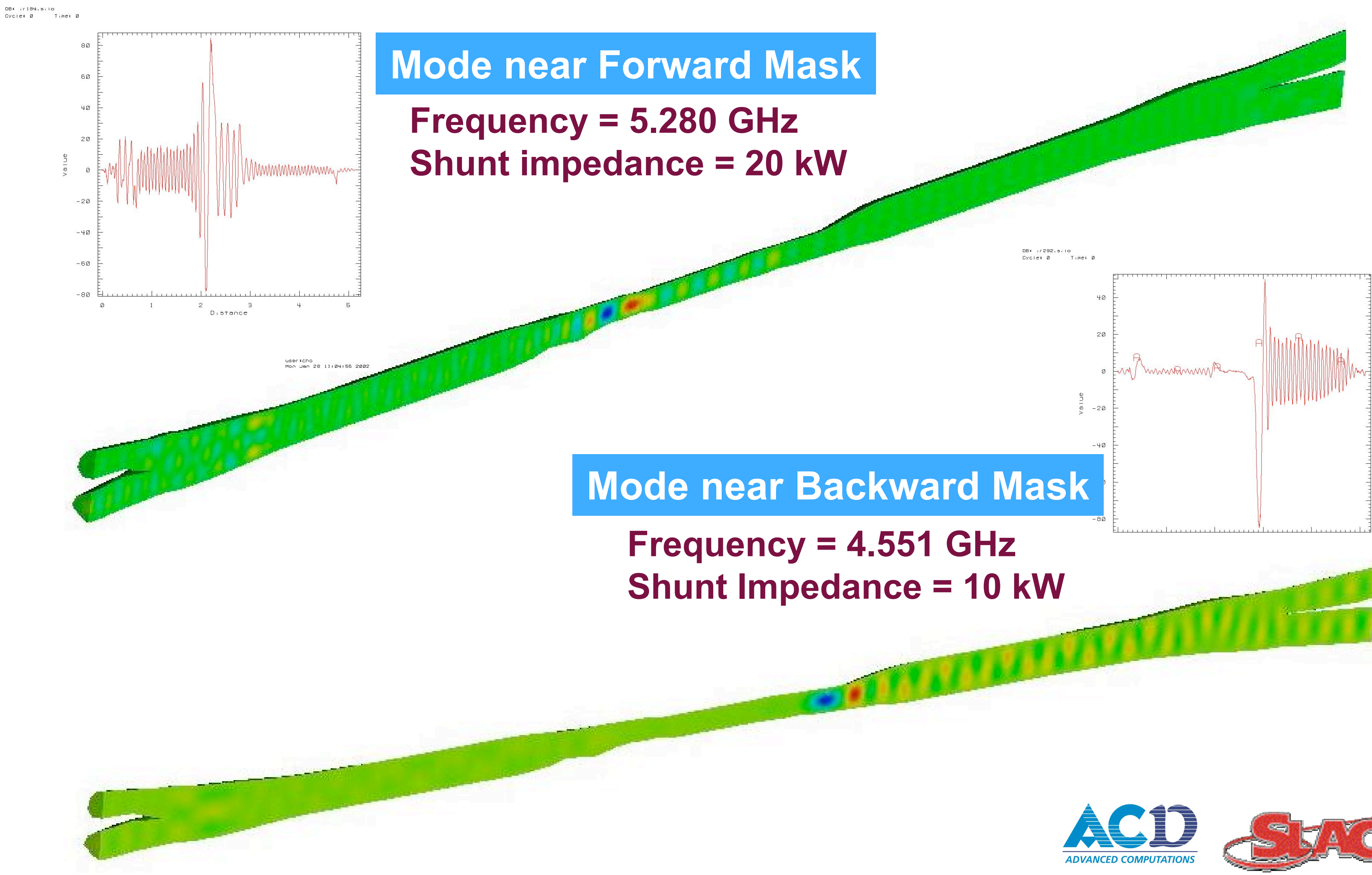




FULL-SCALE OMEGA3P MODEL FROM CROTCH TO CROTCH

Beam heating in the beamline complex near the IR limited the PEP-II from operating at high currents. Omega3P analysis helped in redesigning the IR for the upgrade.

Trapped Modes near the Masks (Omega3P)



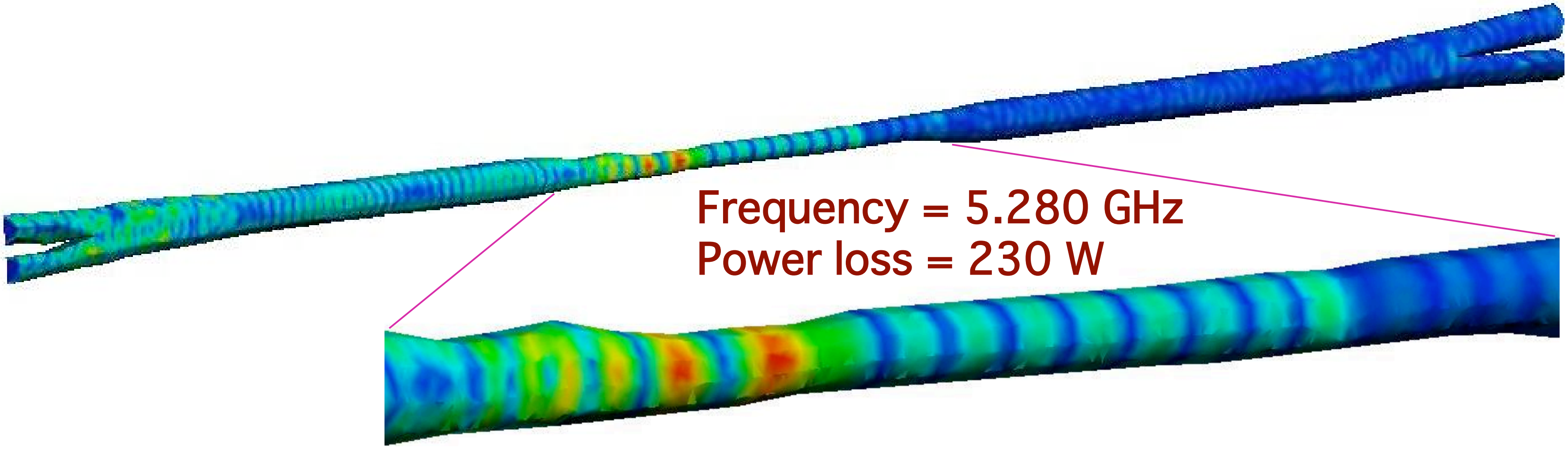
Mode near Forward Mask

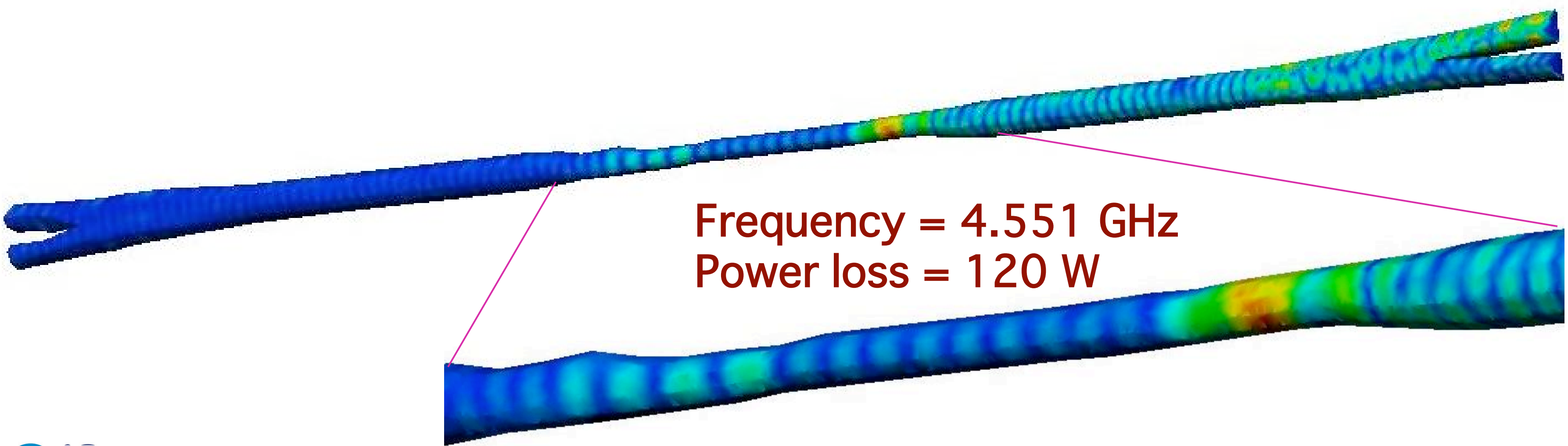
Frequency = 5.280 GHz
Shunt impedance = 20 kW

Mode near Backward Mask

Frequency = 4.551 GHz
Shunt Impedance = 10 kW

Trapped Mode Power Loss



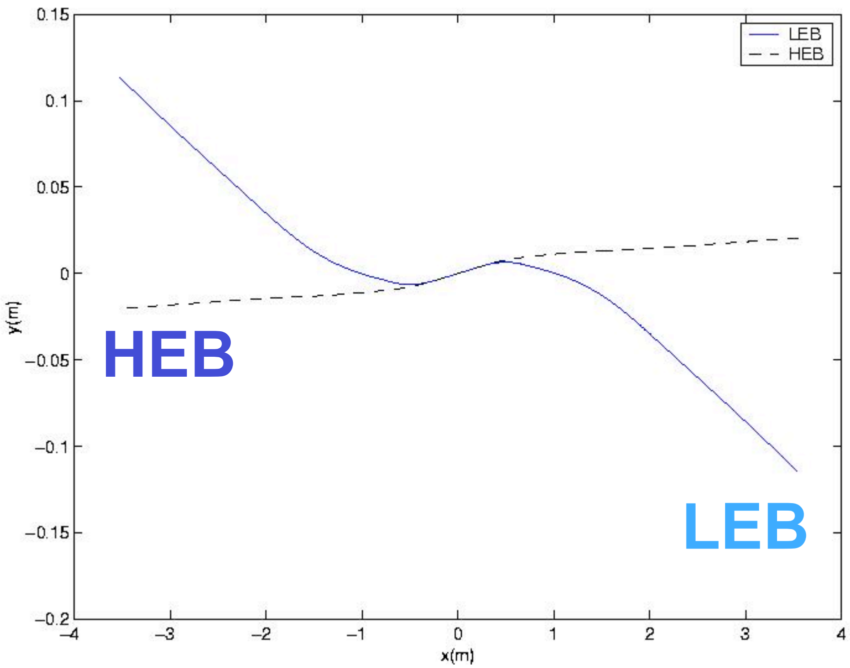


ADVANCED COMPUTATIONS

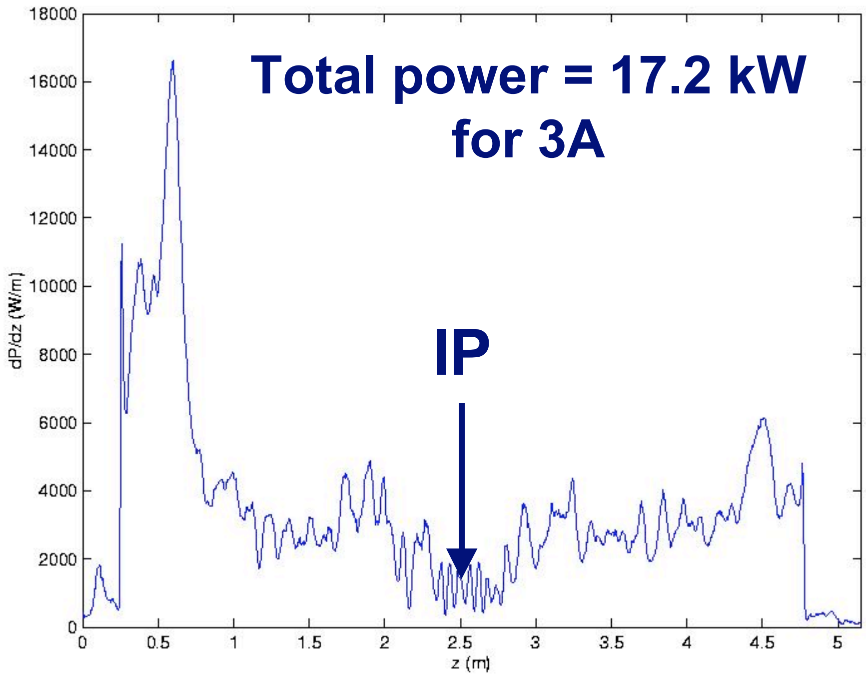
Power Distribution in PEP-II IR

- Sum power contributions from 330 localized modes in 2-6 GHz range (calculated along actual beam paths)
- Calculated power distribution agrees with measurement
- High loss mode identified near observed problem area

PEP-II Beam Paths



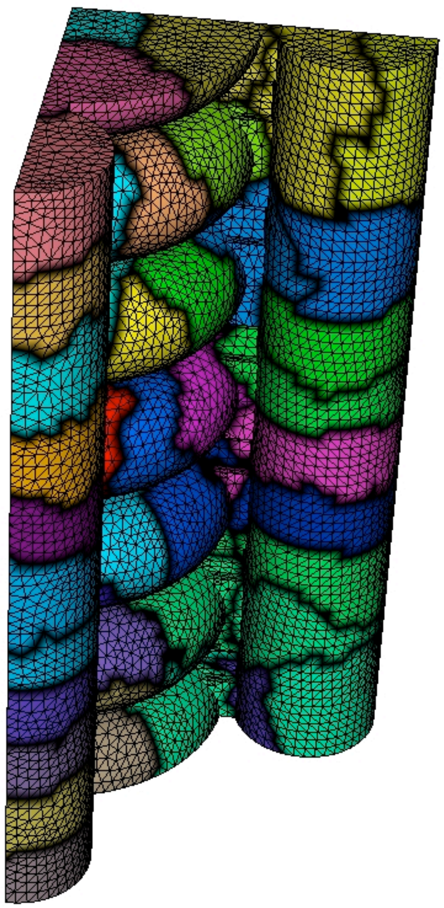
IR Power Distribution



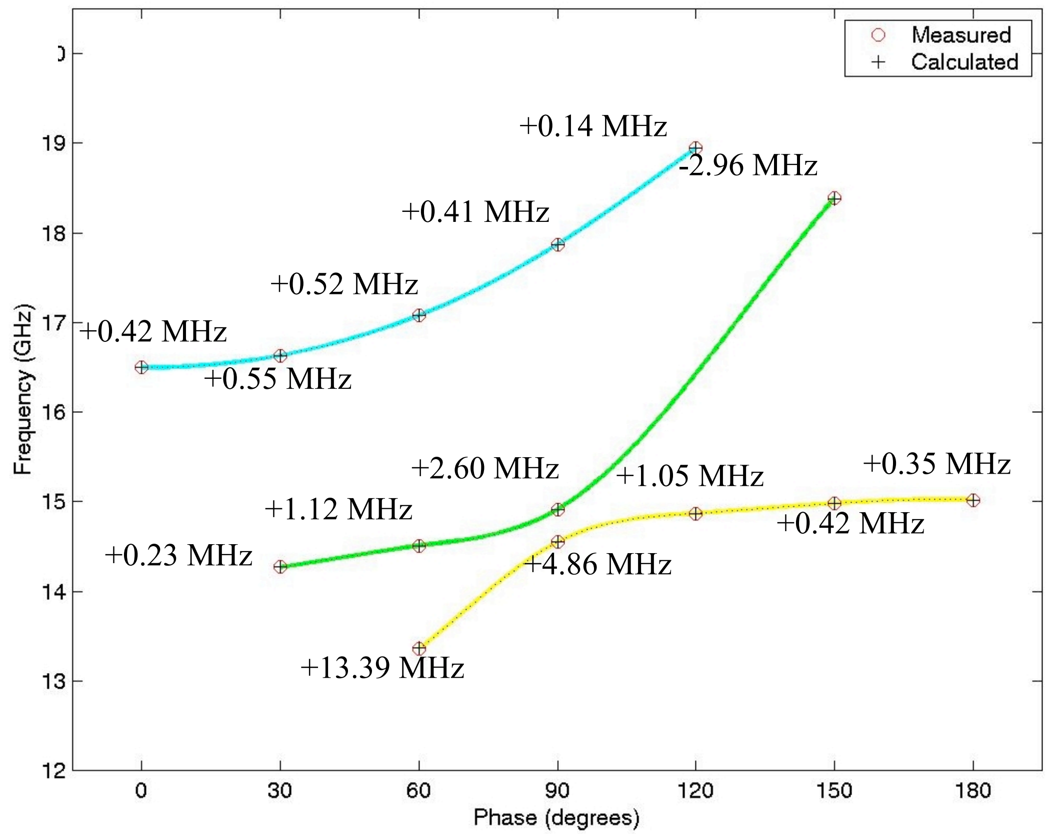
ADVANCED COMPUTATIONS

RDDS 6-cell Stack (Omega3P)

Omega3P model of a quadrant of the RDDS



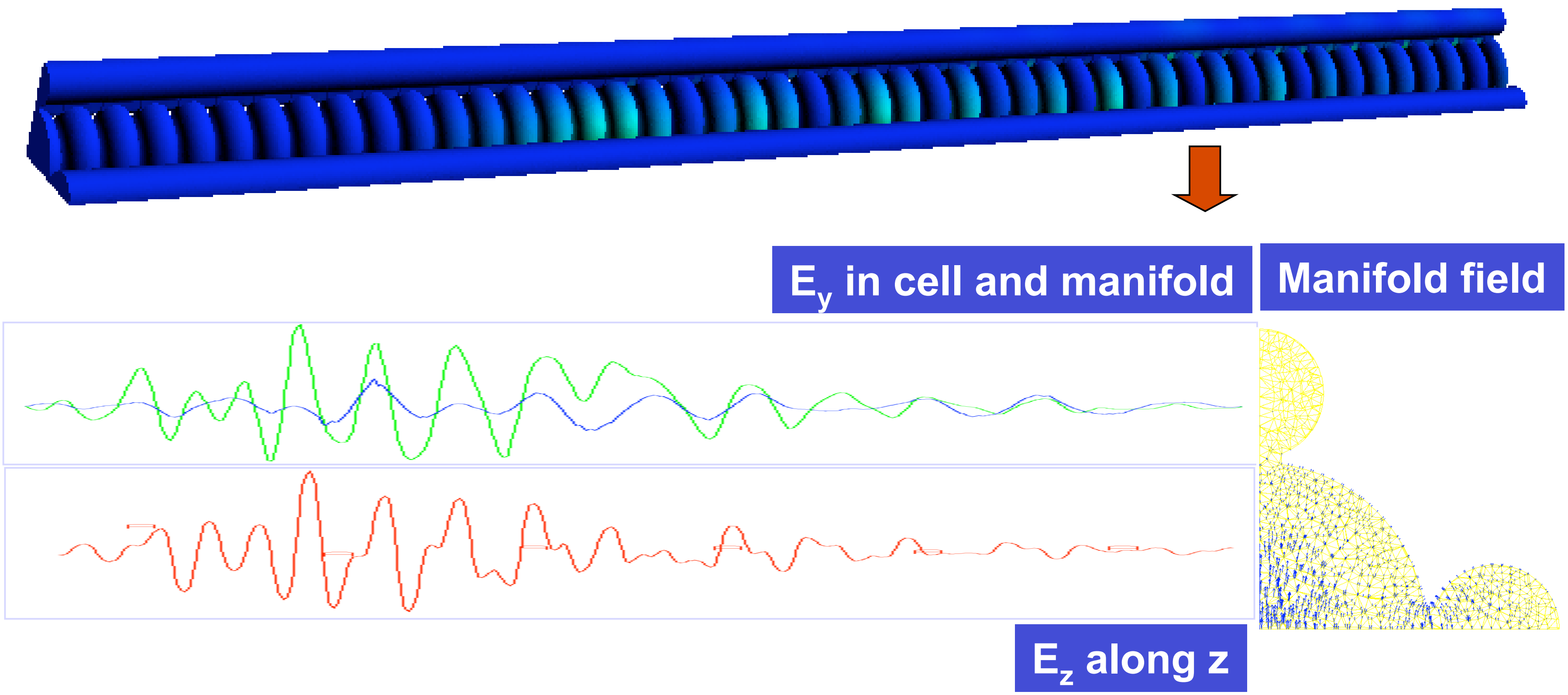
1st Two Dipole Bands & Manifold Modes



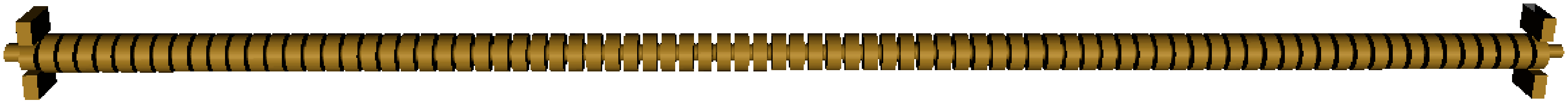
NERSC's IBM SP2: Elements = 275K, DOF = 1.7Million, Number of processors = 48, CPU Time = 1 hr

RDDS 47-cell Stack (Omega3P)

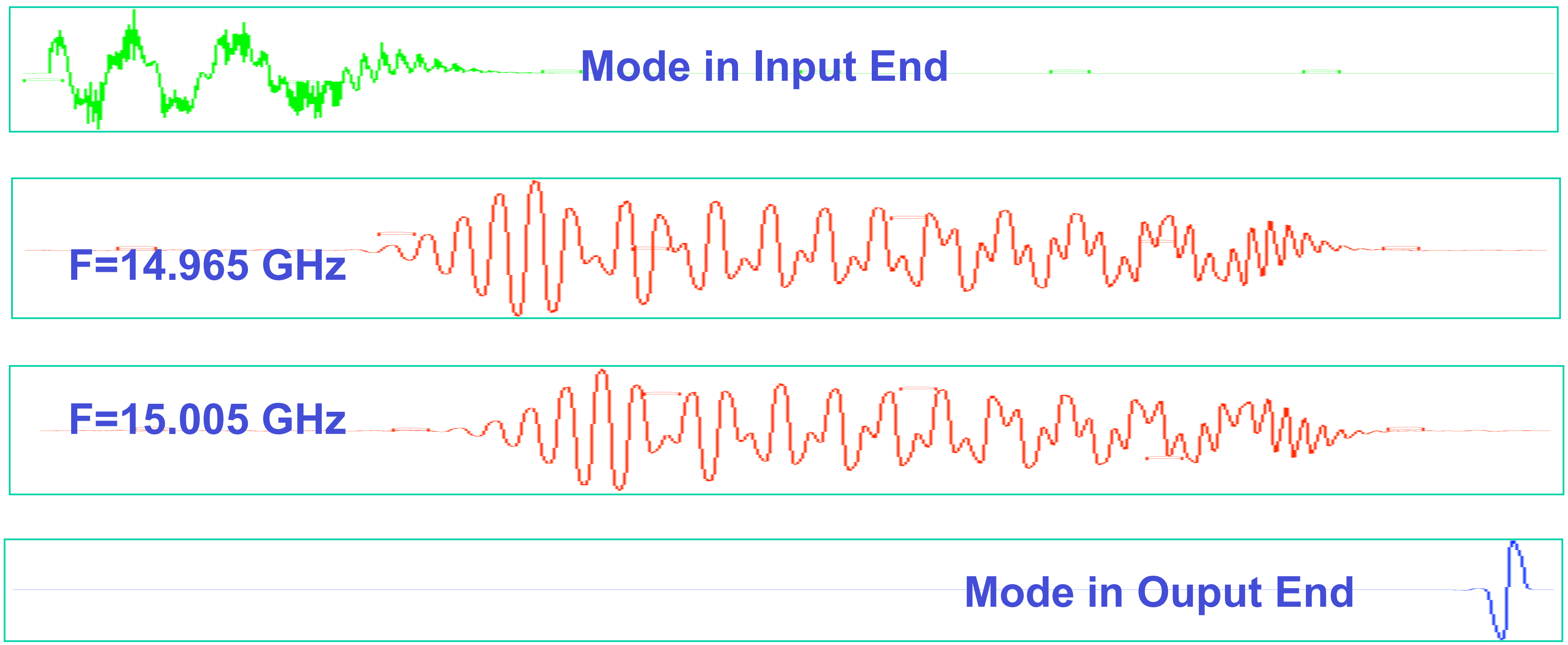
1st ever Field Calculation of a Localized Dipole Mode in the NLC RDDS section with actual structure dimensions and showing realistic fields in the cells and the manifold



H90VG5 83-cell Structure (Omega3P)

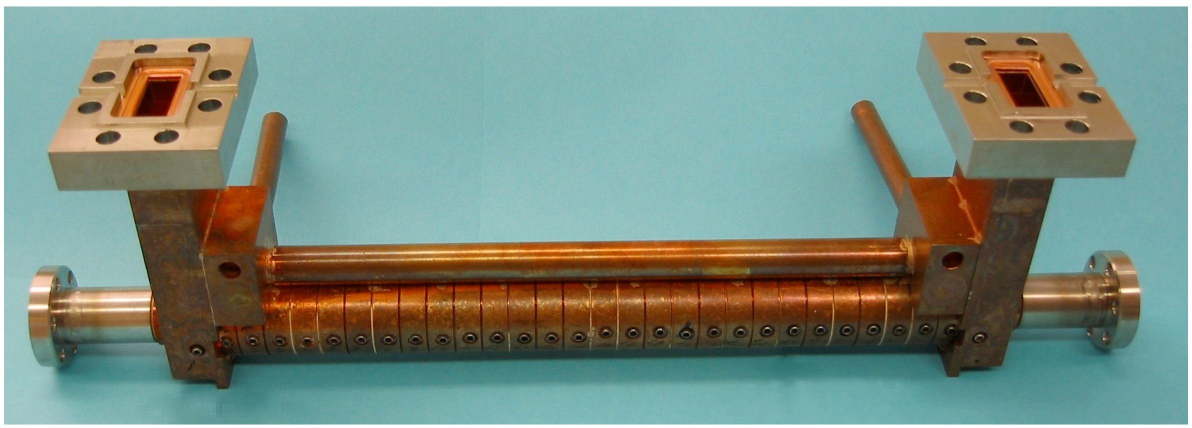


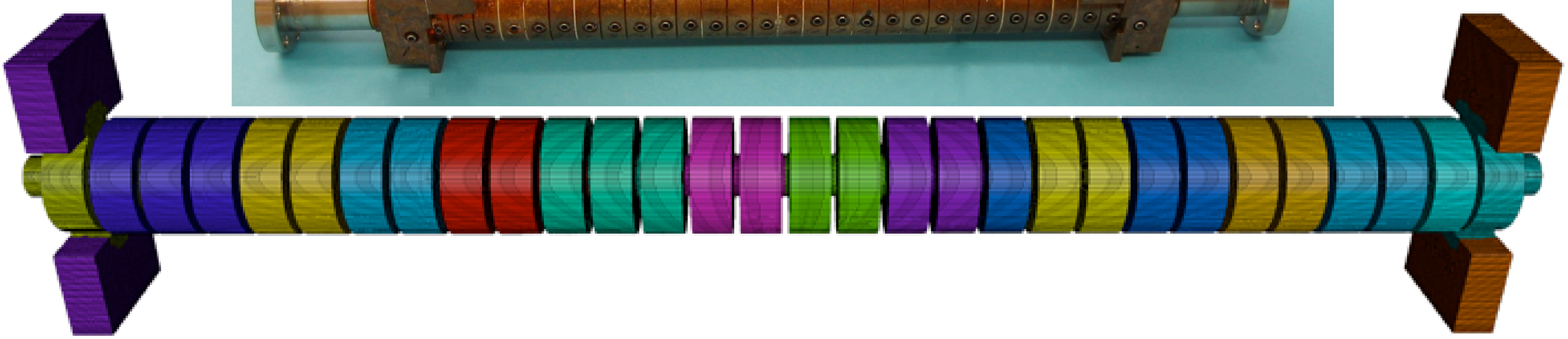
MODES IN 1st DIPOLE BAND



Full Scale modeling of 30-cell Structure

- **Distributed model on a mesh of half million hexahedral elements**
- **Study RF damage at high power X-Band operation using Tau3P & Ptrack3D**

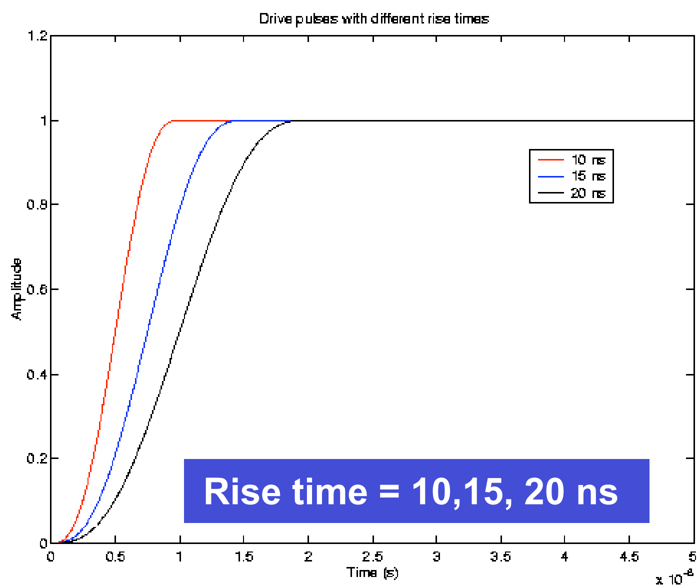




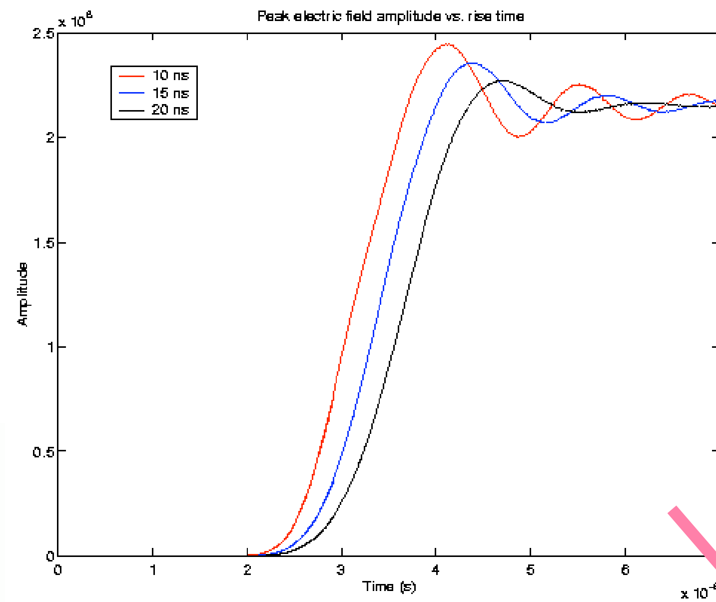
Determining Peak Fields (Tau3P)

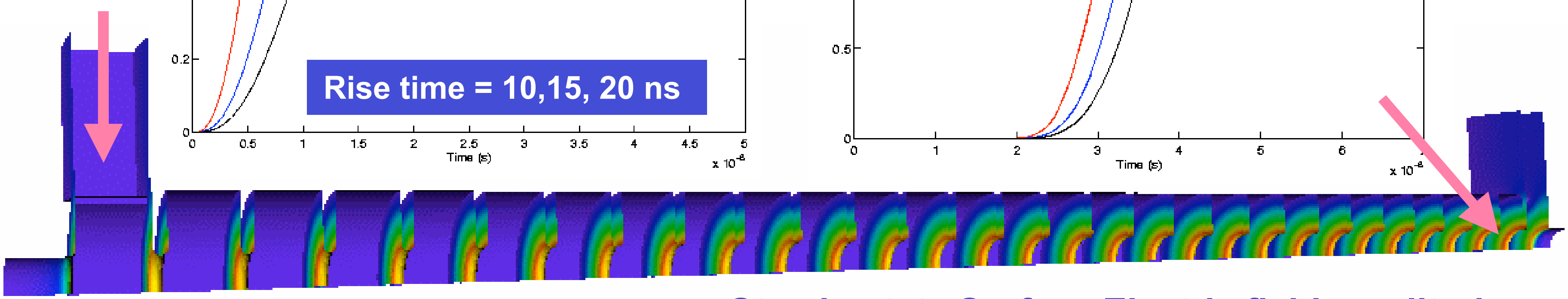
- When and where Peak Fields occur during the pulse?
- Transient fields 20% higher than steady-state value due to dispersive effects

Drive pulse



Electric field vs time

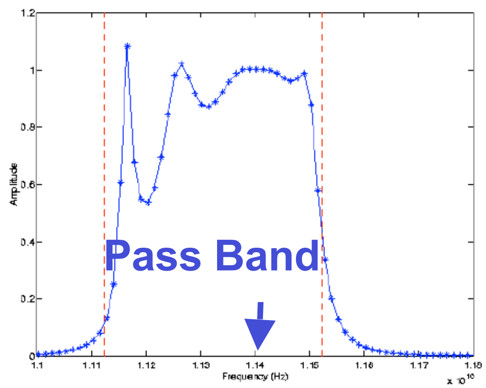




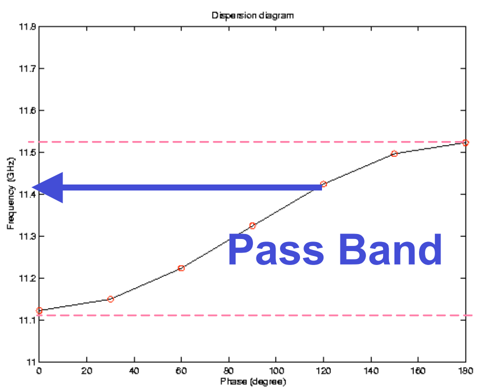
Steady-state Surface Electric field amplitude

Field Evolution in 30-cell Structure (Tau3P)

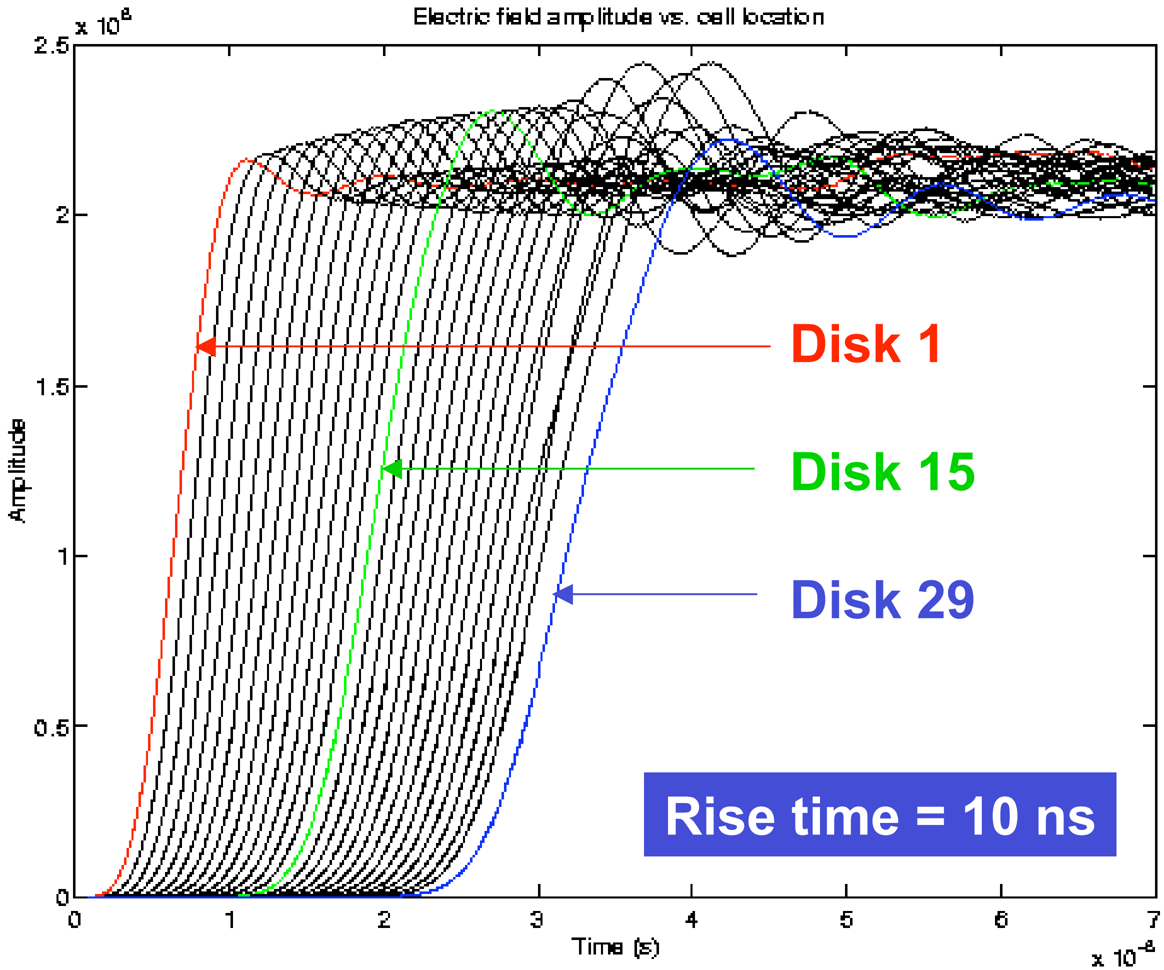
Input Spectrum



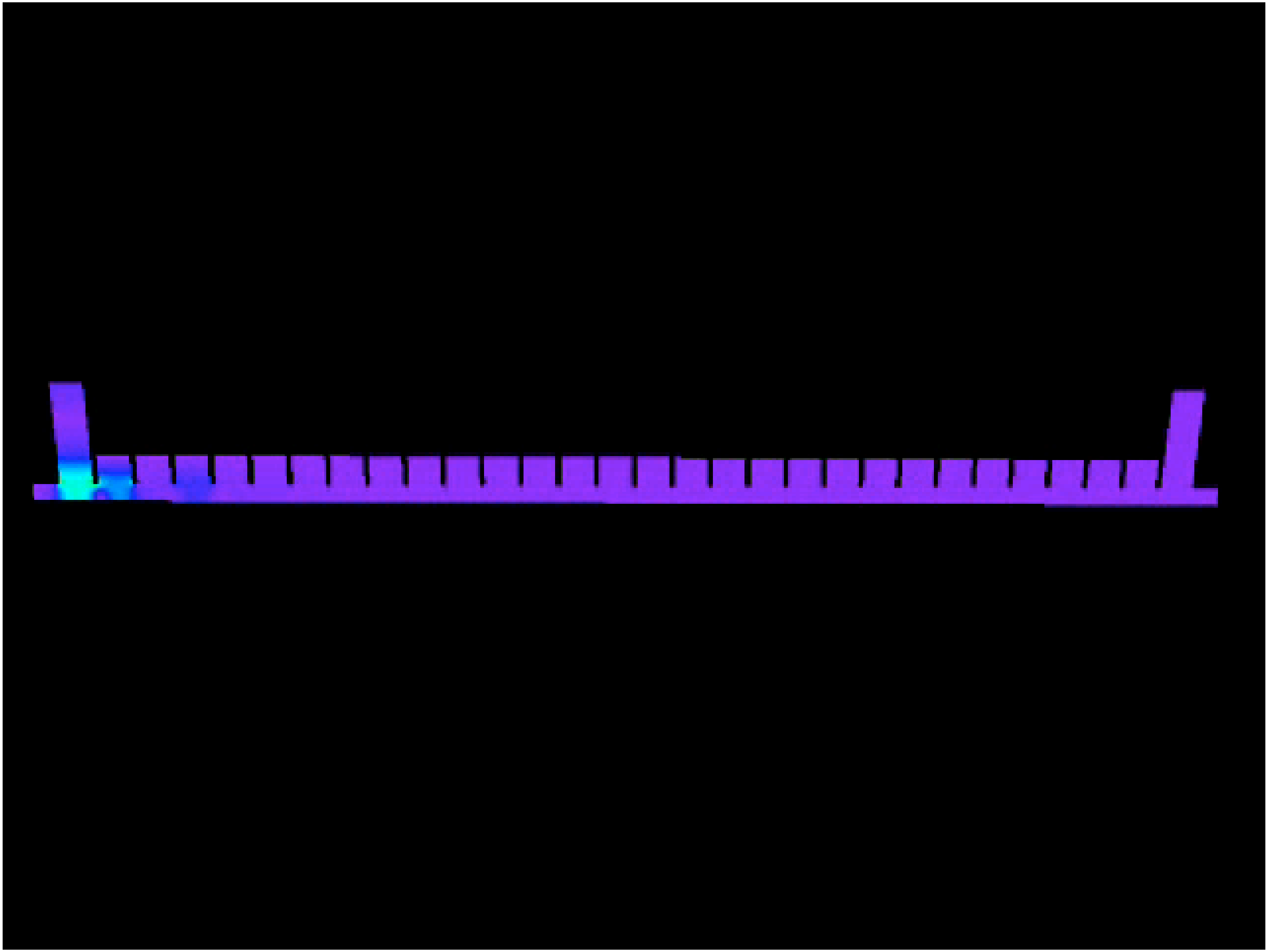
Dispersion Diagram

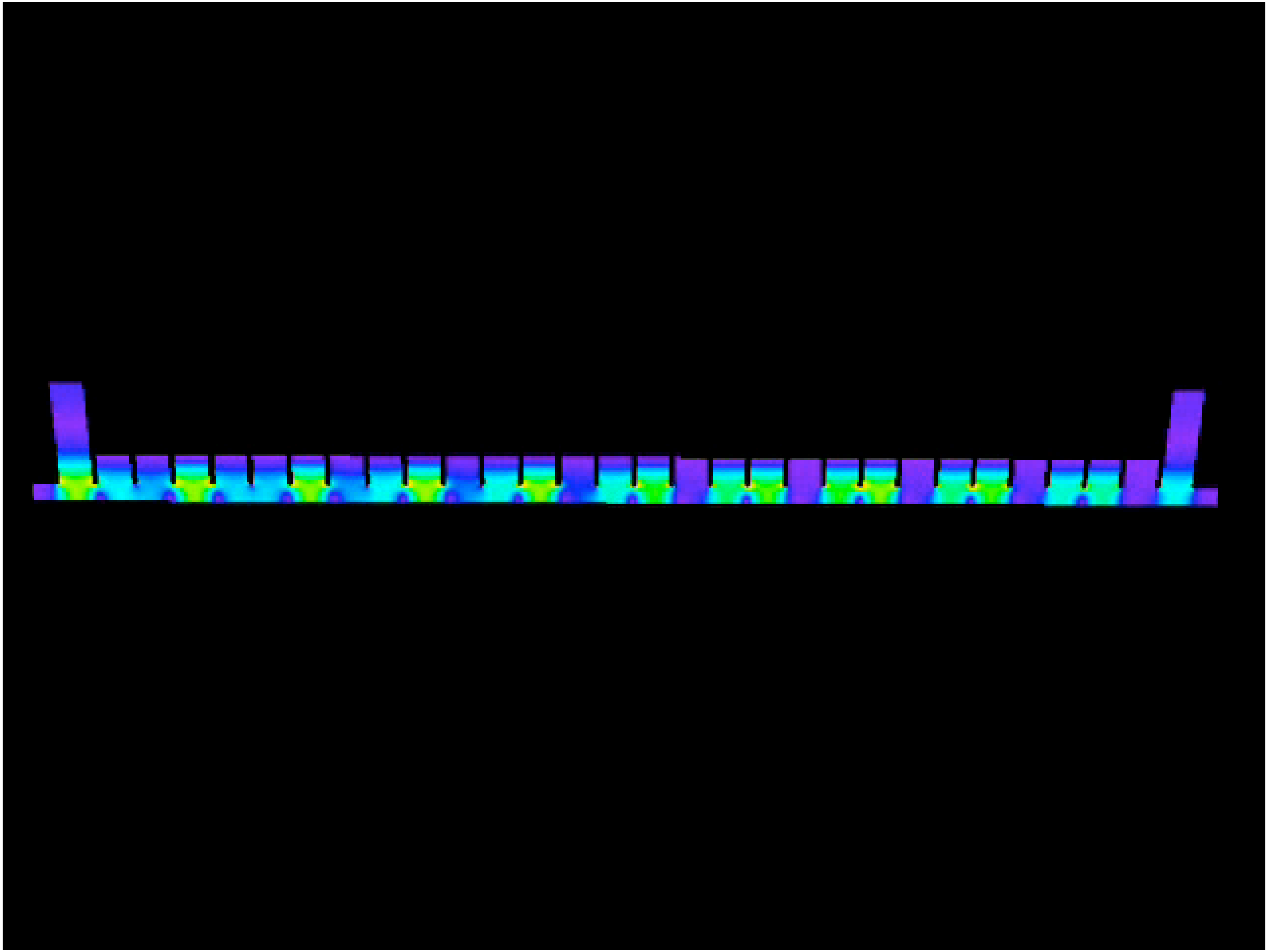


Electric field vs time

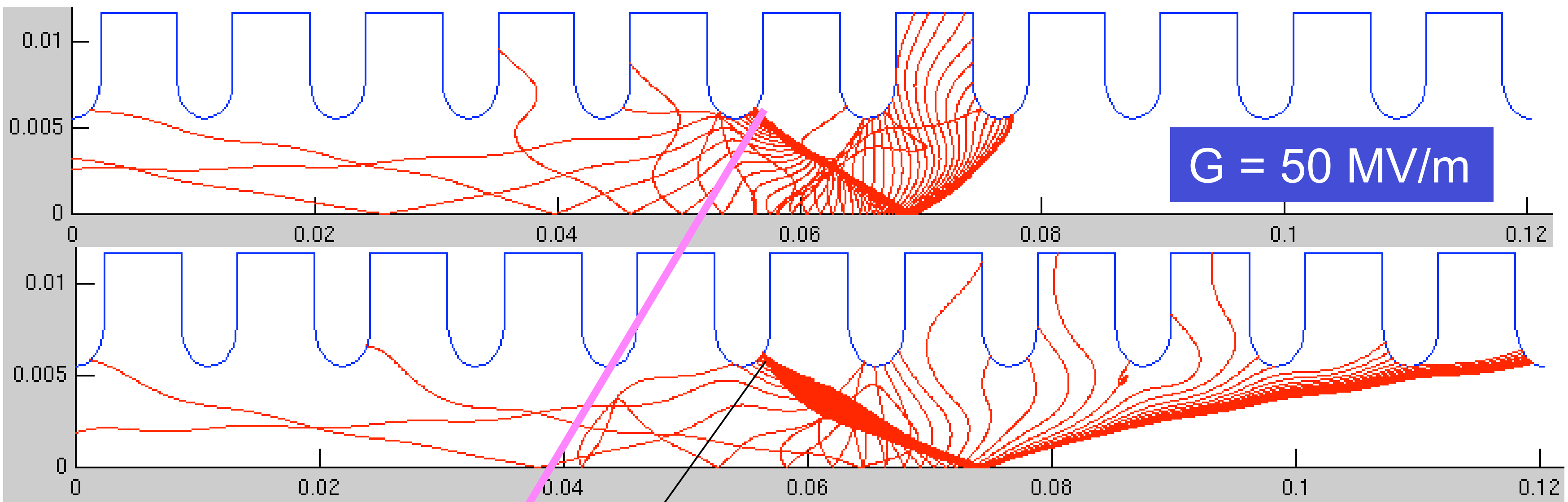


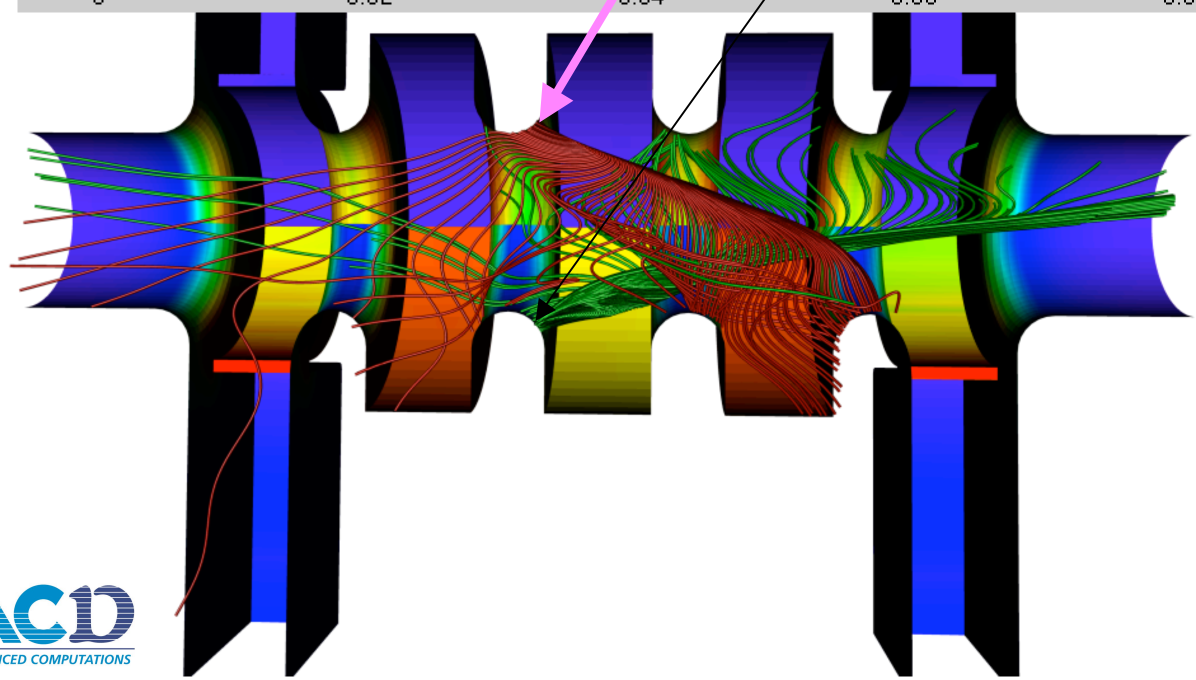
ADVANCED COMPUTATIONS



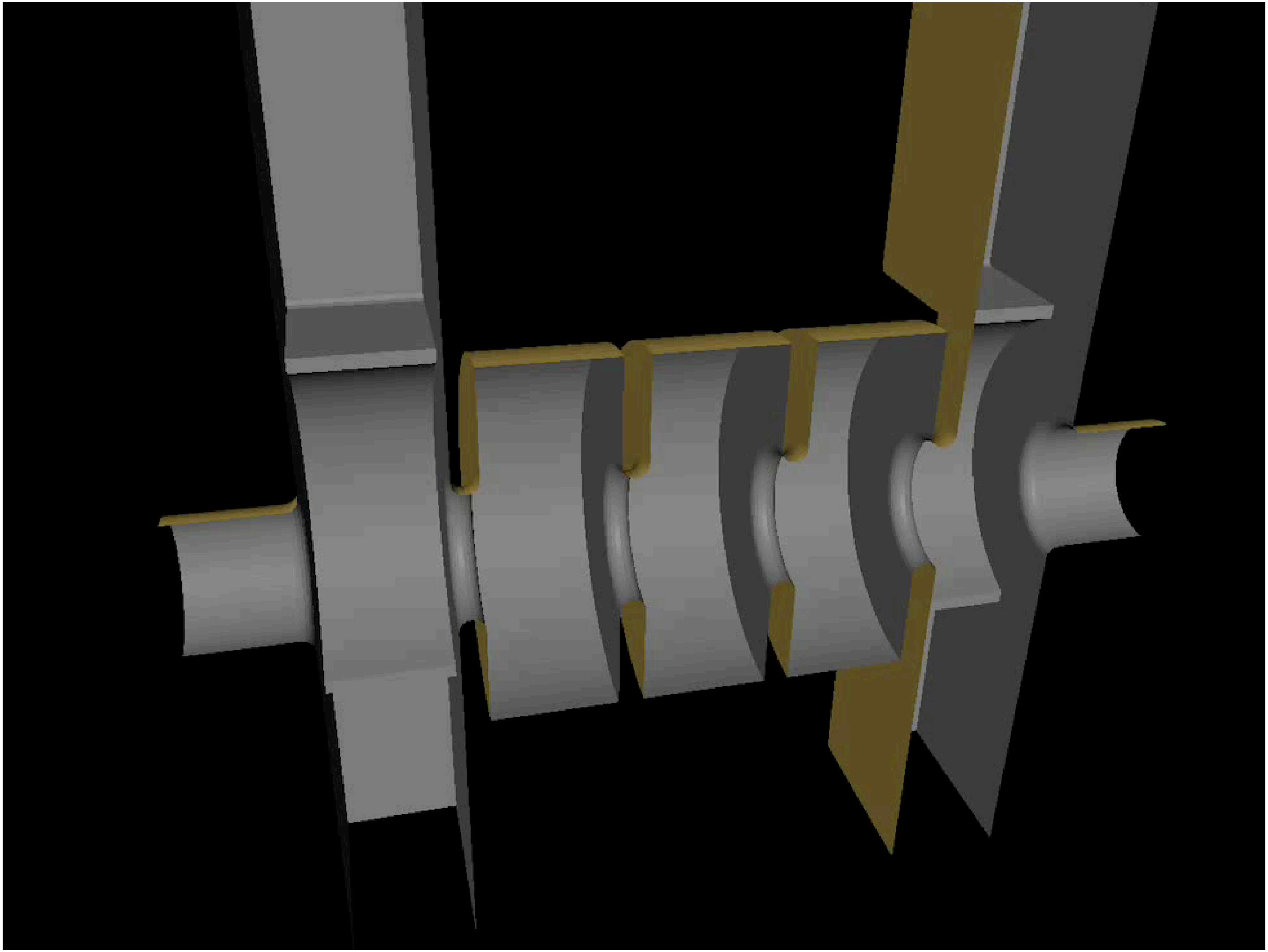


Particle Tracking in Structures (Ptrack3d)





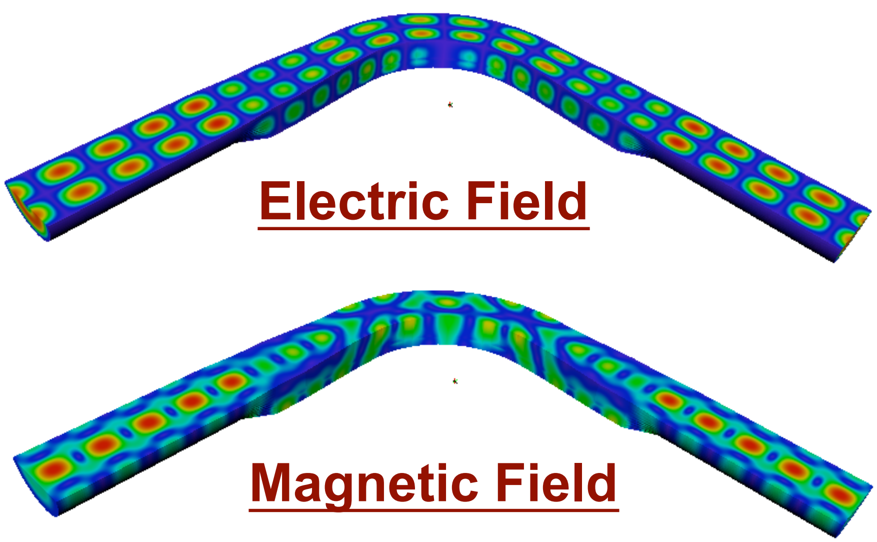
Benchmarking 3D trajectories against results from 2D model

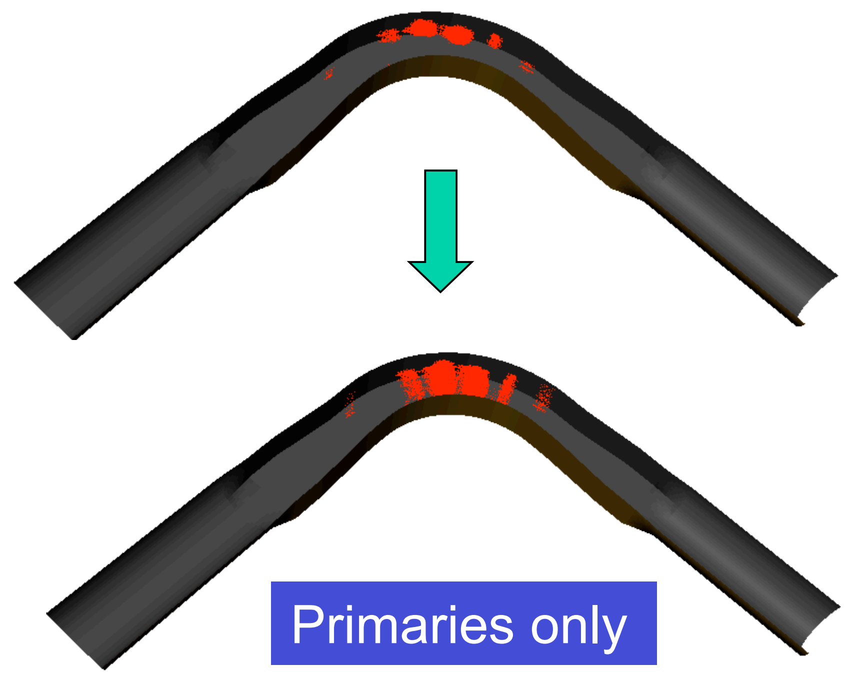


Benchmarking Ptrack3D

- **High power test on a 90 degree square bend provides measured data for benchmarking the secondary emission model in Ptrack3D on a simple geometry**

Using Fields from Tau3P



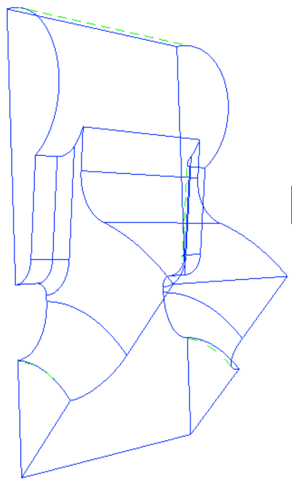


Comp. Sci. & Appl. Math. Collaboration

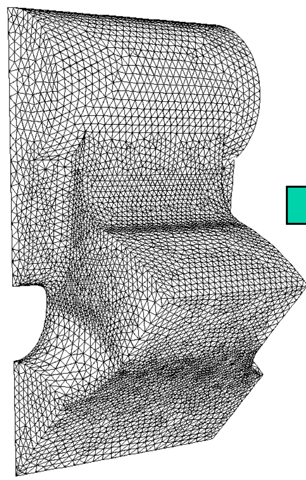
- Large Scale Electromagnetic Simulation
- SAPP Supported Ongoing Activities
- Ongoing/New Collaborations with the ISICs

CS/AM Issues with Parallel EM Simulation

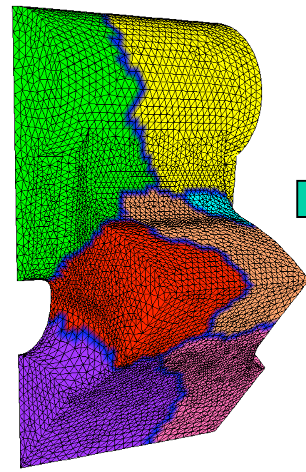
CAD Model



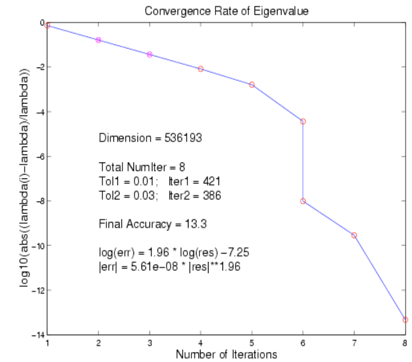
Meshing



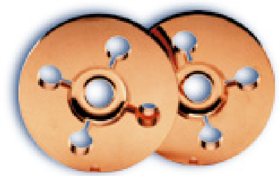
Partitioning



Solvers

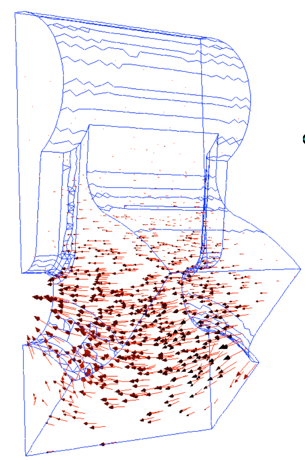


Verification

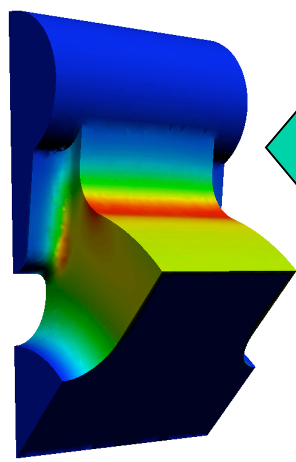


Cell	Numerical (MHz)	Meas. (MHz)	Diff. (MHz)
001	11420.57	11420.3	0.27
102	11420.35	11420.4	-0.05
203	11420.09	11419.7	0.39

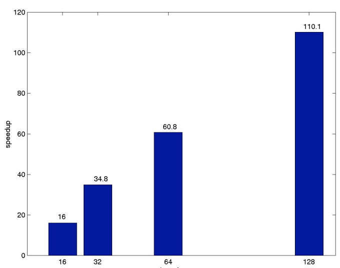
Visualization



Refinement



Parallel Performance



ADVANCED COMPUTATIONS

SLAC

CS/AM Activities – SAPP Supported

"Details covered in E. Ng's talk on CS/AM"

- **LBNL (E. Ng, P. Husbands, S. Li) –** Eigensolver, Linear Solvers
- **Stanford (G. Golub, O. Livne, Y. Sun, W. Mi) –** Eigensolver, Static Solver, Multigrid
- **SNL/SLAC (P. Knupp, N. Folwell) –** Mesh Quality Metrics
- **UCD (K. Ma, G. Schussman) –** Visualization, Multi-resolution Technique

CS/AM Activities – Collaboration w/ ISICs

"Details covered in E. Ng's talk on CS/AM"

- **TSTT (SNL: T. Tautges, L. Freitag; LLNL: K. Chand, B. Henshaw, D. Brown)** – CAD Model/Meshing
- **TSTT (RPI: M. Shephard, Y. Luo) –** Adaptive Refinement
- **TOPS (LBNL: A. Pinar, Sandia: K. Devine) –** Parallel Performance

ADVANCED COMPUTATIONS

Summary

- SciDAC coupled with institutional and programmatic leverage, supports a NEW scientific enterprise that benefits not only programs in HENP but those across the Office of Science,
- ESS developed a powerful NEW simulation capability that fundamentally changed the way business is done in Accelerator Design & Analysis and already has significant impact on both existing and planned facilities,
- SciDAC's multi-disciplinary team approach and its CS & AM resources foster collaborations that strengthen the computing and computational aspects of the ESS tools, thereby increasing the range and the speed of Scientific Discovery through Advanced Simulation.

ESS Goals for 2nd Half of Project & Beyond

Develop:

- Complex eigensolver
- Implicit time-domain FE solver
- PIC & advanced wakefield module

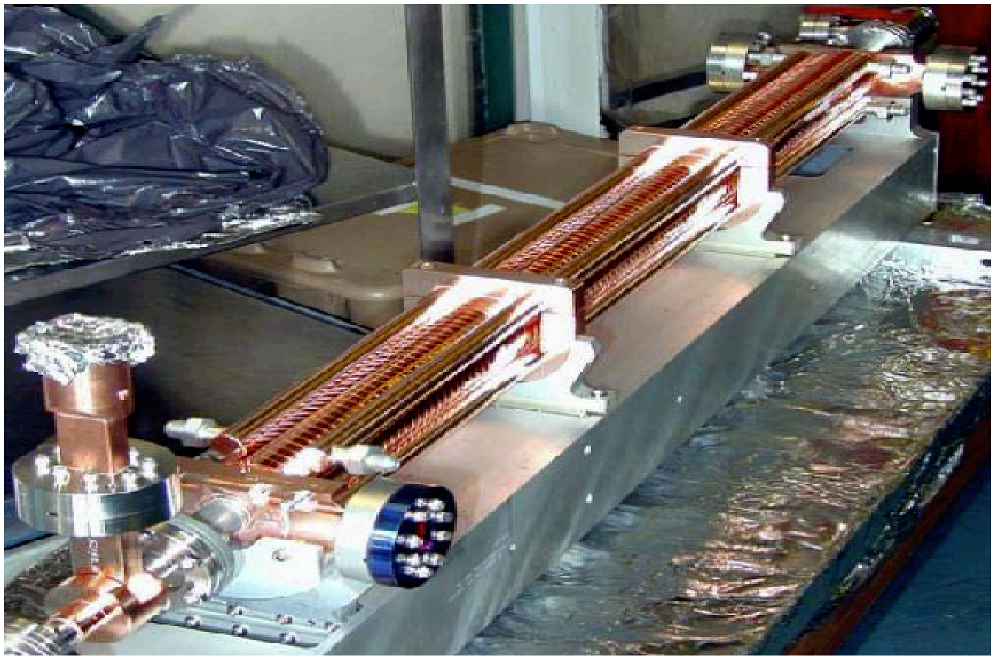
to:

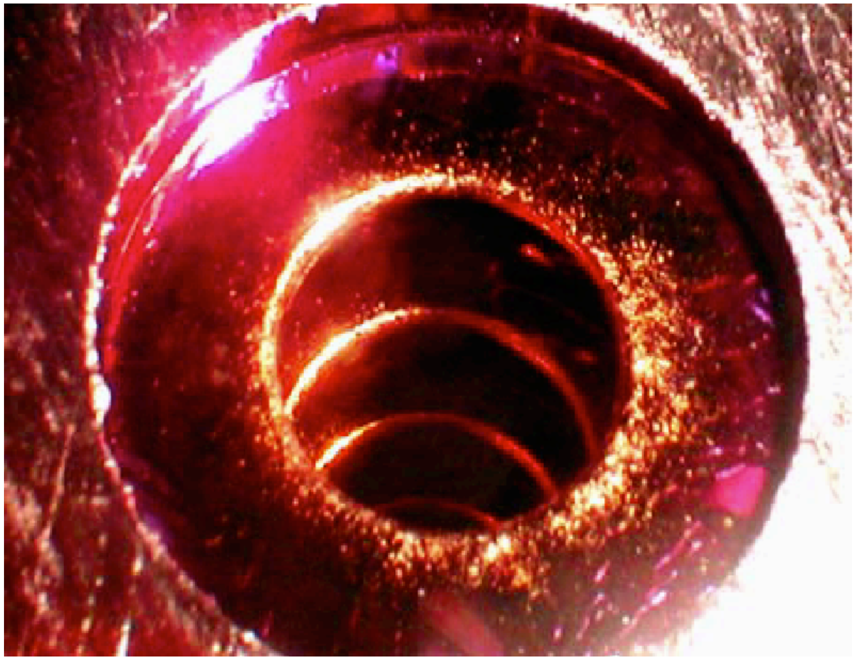
- Analyze wakefields in complete NLC structure
- Study RF breakdown & dark current
- Simulate an entire NLC klystron
- Model the RIA RFQ cavity

End-to-end NLC Structure Simulation

(J. Wang, C. Adolphsen – SLAC)

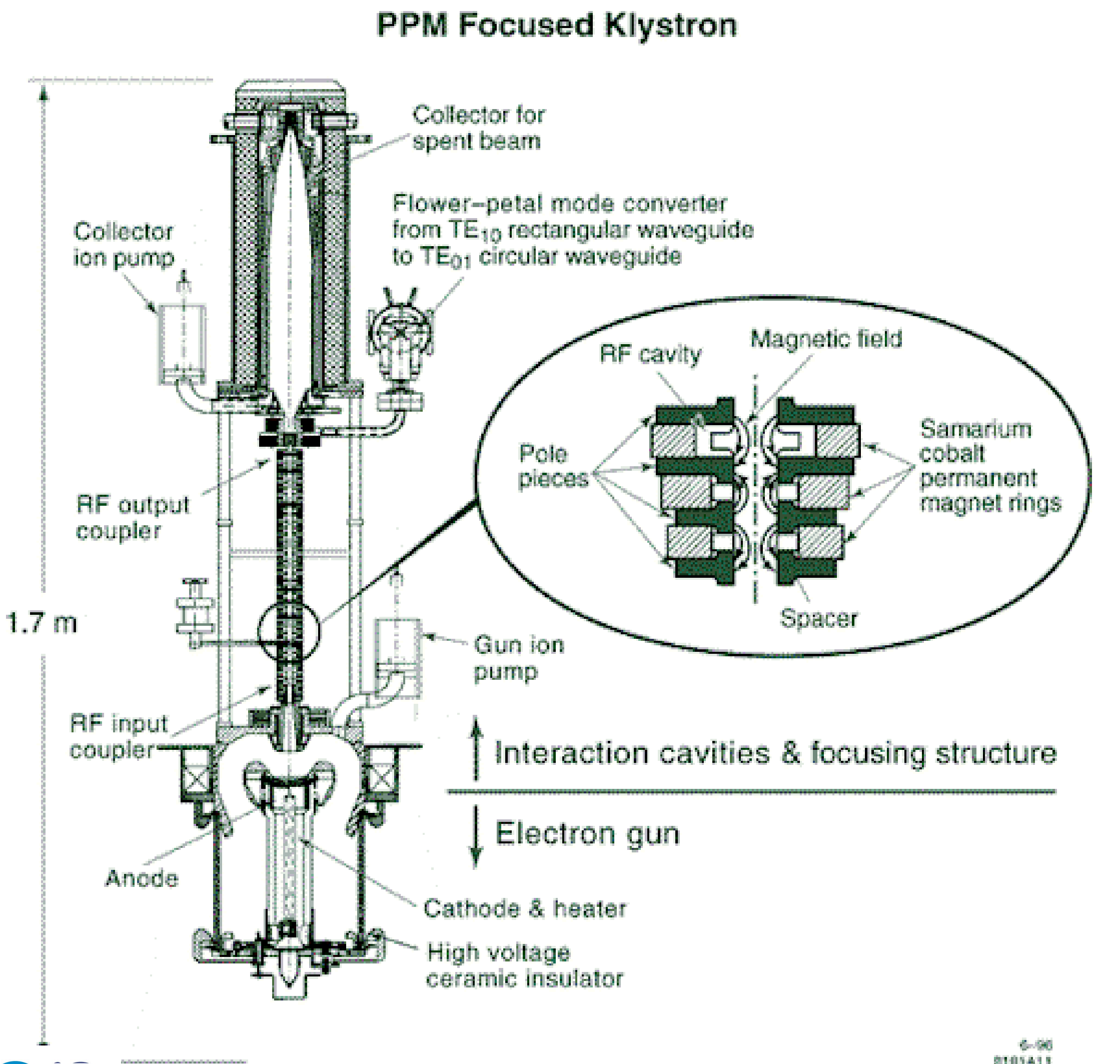
- NLC X-band structure showing damage in the structure cells after high power test
- Theoretical understanding of underlying processes lacking so realistic simulation is needed

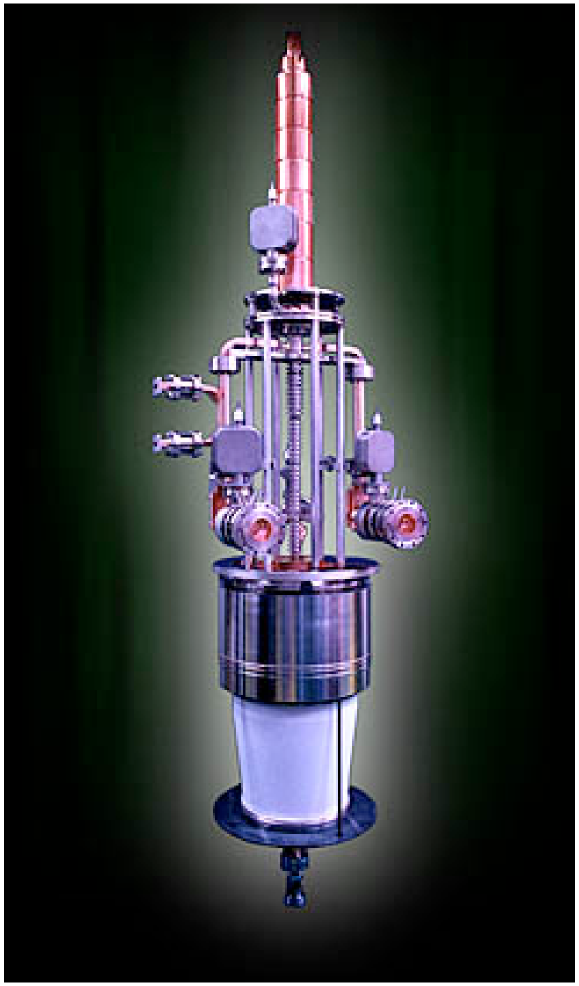




End-to-end NLC Klystron Simulation

Field and particle data estimated to be TB size





End-to-end RIA Hybrid RFQ Modeling

(J. Nolan, P. Ostroumov – ANL)