Application Specific Computing

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Advanced Computations Department

SLAC DOE Review – April 10, 2003

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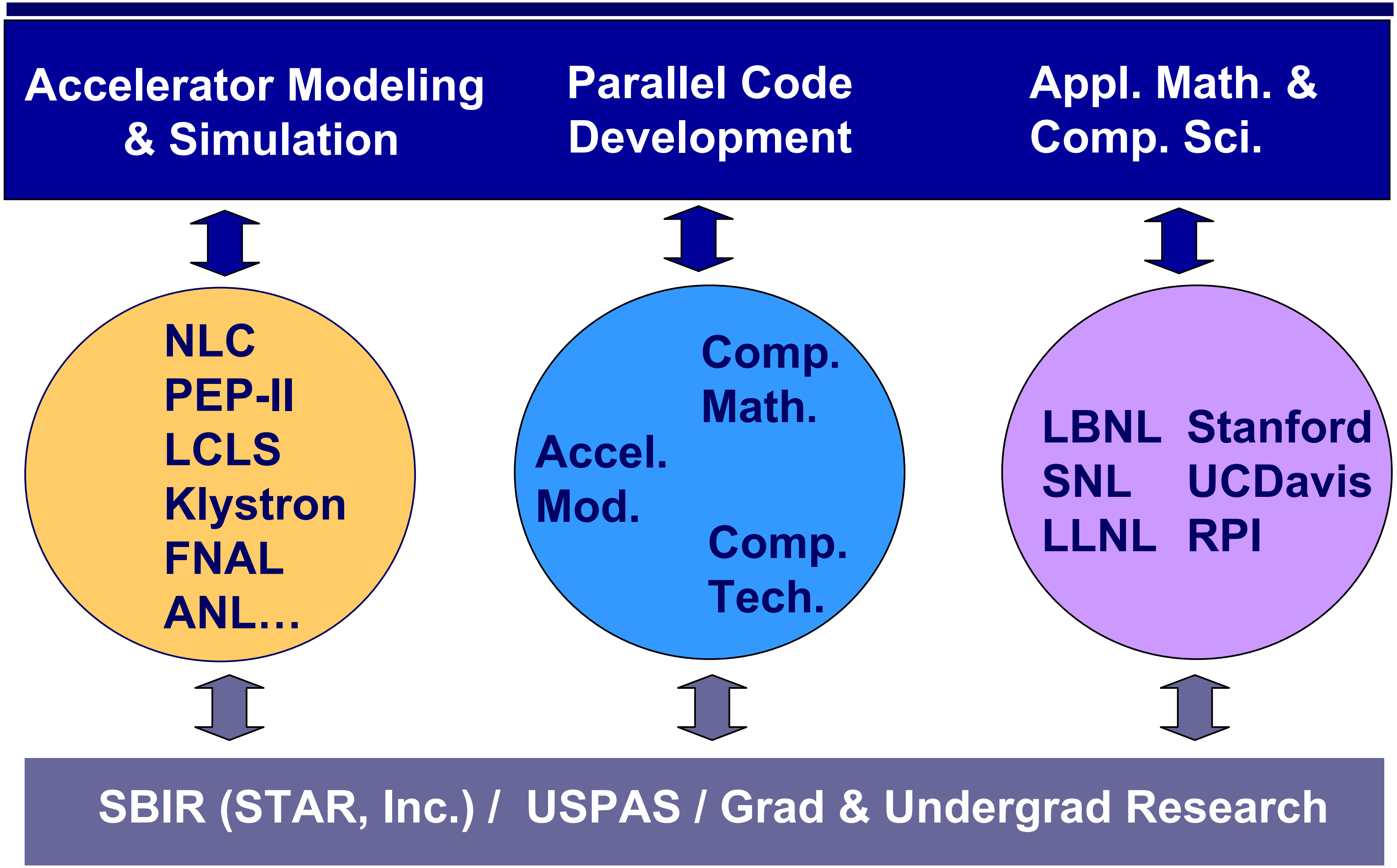
SciDAC Accelerator Simulation Project

SLAC leads the **Electromagnetic Systems Simulation** (**ESS**) component that

- Concentrates on developing **parallel tools** based on **unstructured grids** for the design, analysis, and optimization of complex electromagnetic components and systems in accelerators.
- Applies these tools to improve existing facilities (**PEP-II IR heating**, **Tevatron lifetime**), to design future accelerators (**NLC structure**), and to advance accelerator science (**Dark current**).
- Collaborates with **SAPP/ISIC** partners to target challenging electromagnetic problems that require **Large-scale simulations**, e.g. modeling small beams in long structures of complex geometry with high accuracy.

ACD Overview - SciDAC



Accelerator Modeling & Simulation

Parallel Code Development

Appl. Math. & Comp. Sci.

NLC
PEP-II
LCLS
Klystron
FNAL
ANL…

Comp. Math.

Accel. Mod.

Comp. Tech.

LBNL Stanford
SNL UCDavis
LLNL RPI

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

Contributors/Collaborators

(SciDAC - HENP/OASCR)

Accelerator Modeling

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Computational Mathematics

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

LBNL

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RPI

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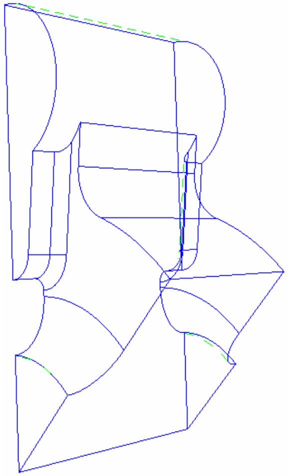
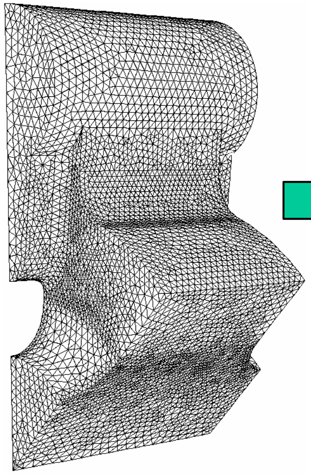
Parallel EM Simulation – CS/AM Issues

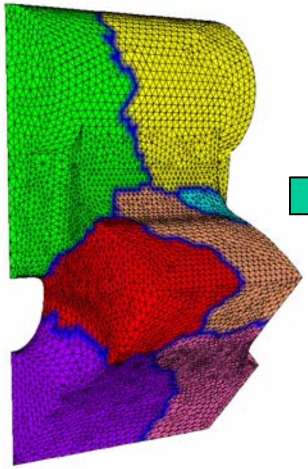
CAD Model



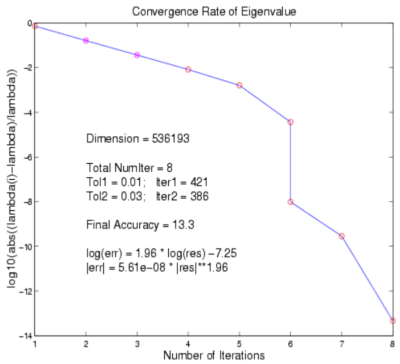
Meshing



Partitioning



Solvers



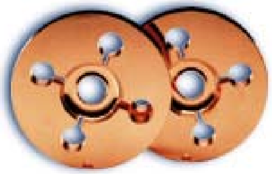
Dimension = 536193

Total NumIter = 8
Tol1 = 0.01;   Iter1 = 421
Tol2 = 0.03;   Iter2 = 386

Final Accuracy = 13.3

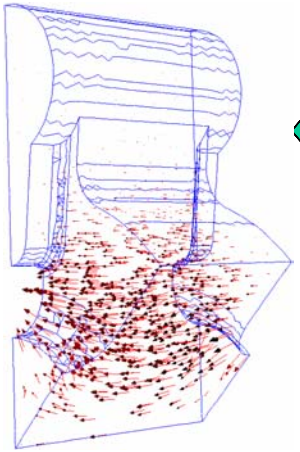
log(err) = 1.96 * log(res) −7.25
|err| = 5.61e−08 * |res|**1.96

Verification

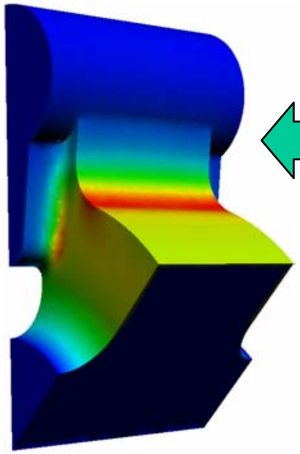


Cell	Numerical (MHz)	Meas. (MHz)	Diff. (MHz)
001	11420.57	11420.3	0.27
102	11420.35	11420.4	-0.05
203	11420.09	11419.7	0.39

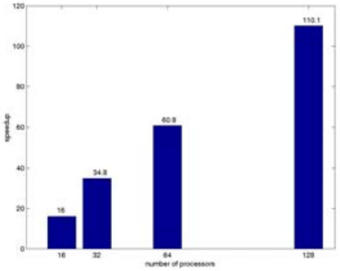
Visualization



Refinement



Parallel Performance



Code Development - Omega3P, Tau3P, Tfe3P

Omega3P (Parallel finite element eigensolver) –

(1) Improvements to ISIL solver for tackling tightly clustered eigenvalues that include Block algorithm, Deflation techniques, and Thick restart,
(2) AV formulation to accelerate convergence,
(3) ESIL solver (LBNL) as alternative and for verification.

(1) Periodic B.C.,
(2) More efficient filtering schemes,
(3) Complex eigensolver to treat lossy cavities.

Tau3P (Parallel time domain solver on modified Yee grid) –

(1) Wakefield version ported to NERSC's IBM SP2,
(2) Restart capability to enable long wakefield runs,
(3) Lossy dielectrics

Tfe3P (New parallel finite element time domain solver) –

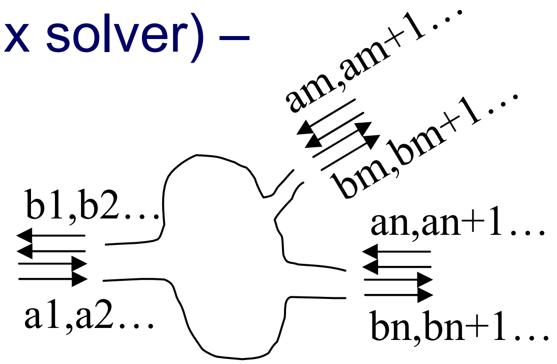
(1) Development of efficient linear solvers,
(2) Higher order elements and basis functions.

Code Development - S3P, Track3P

S3P (New parallel finite element scattering matrix solver) –

(1) Benchmarked against known solutions,
(2) Implementations on NERSC's IBM SP2.

(1) Higher order elements for improved accuracy,
(2) AWE technique to enable quick frequency sweep,
(3) Extension to include lossy material



Track3P (Particle tracking module) using **E & B** fields from

Omega3P (for standing wave cavities),
S3P (for open cavities), or
Tau3P (for traveling wave structures)

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

Surface physics - injection, thermal emission, field emission & secondaries.

Parallelization, Ionization, Collisions…..

Surface Physics - Track3P

- **Particle Injection**

$$I(t)=\frac{I_{\max}}{1+\left(\frac{v_0}{a}\left(t-\frac{\varphi_0}{\omega}-iD_t\right)\right)^2}$$

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

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

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

$$J(r,t)=1.54\times10^{\left(-6+\frac{4.52}{\sqrt{\varphi}}\right)}\frac{(\beta E)^2}{\varphi}e^{\left(\frac{-6.53\times10^9\varphi^{1.5}}{\beta E}\right)}$$

- **Secondary Emission**

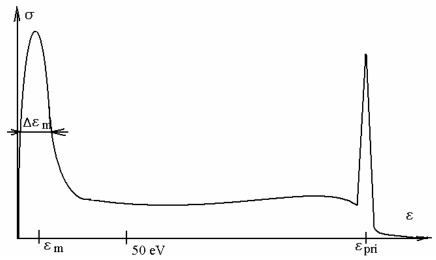
$\sigma = I_{secondary}/I_{primary} = \delta+\eta+r$;

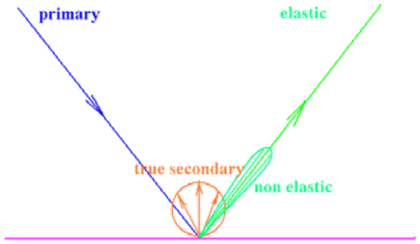
δ - true secondary emission (0-50 eV). $\varepsilon_m \sim$ 2-4.5 eV;

$\Delta\varepsilon \sim$ 12-15 eV;

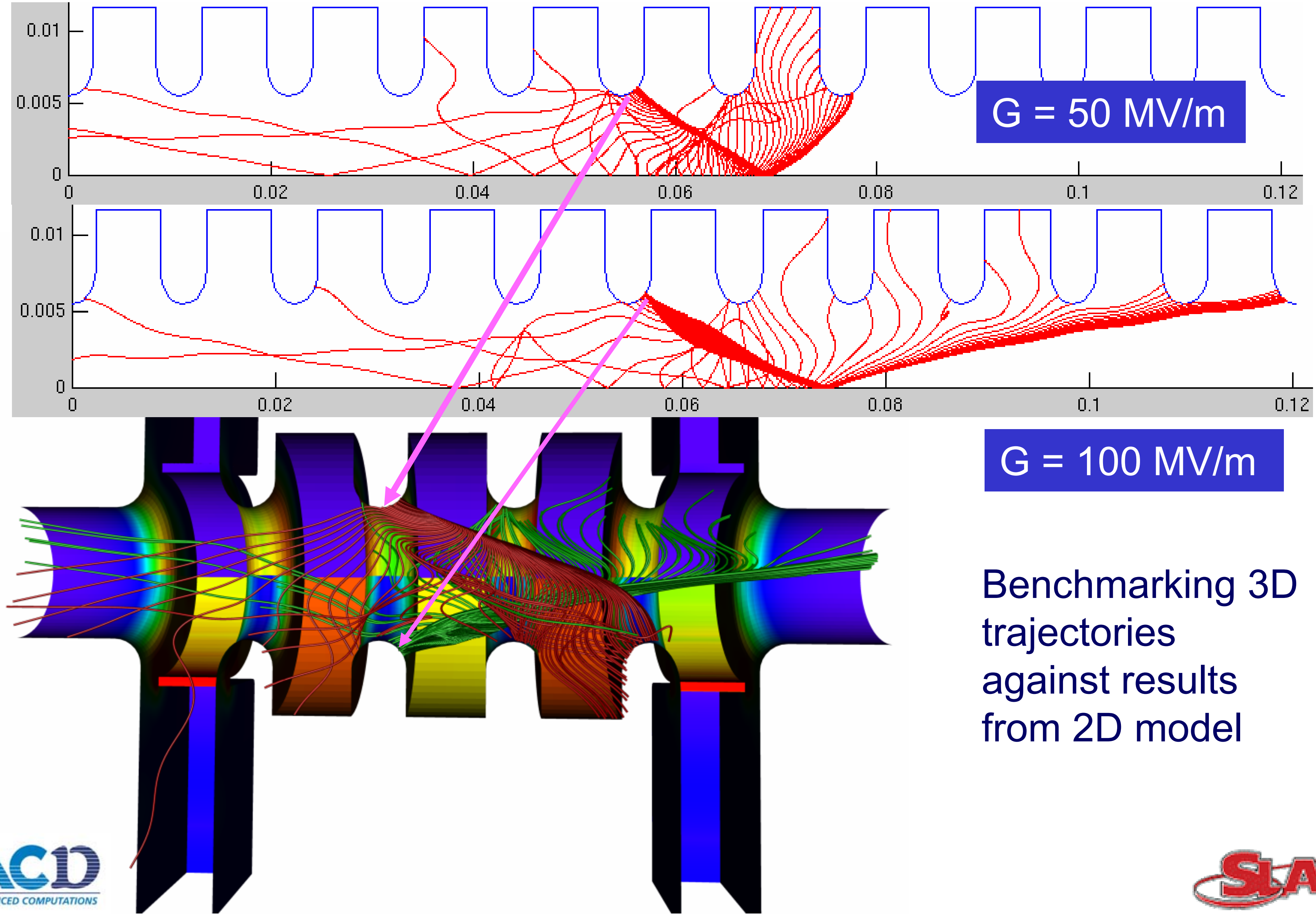
η - non elastic reflection (50 eV-ε_{pri})

r - elastic reflection; r = 0.05-0.5 for metals.





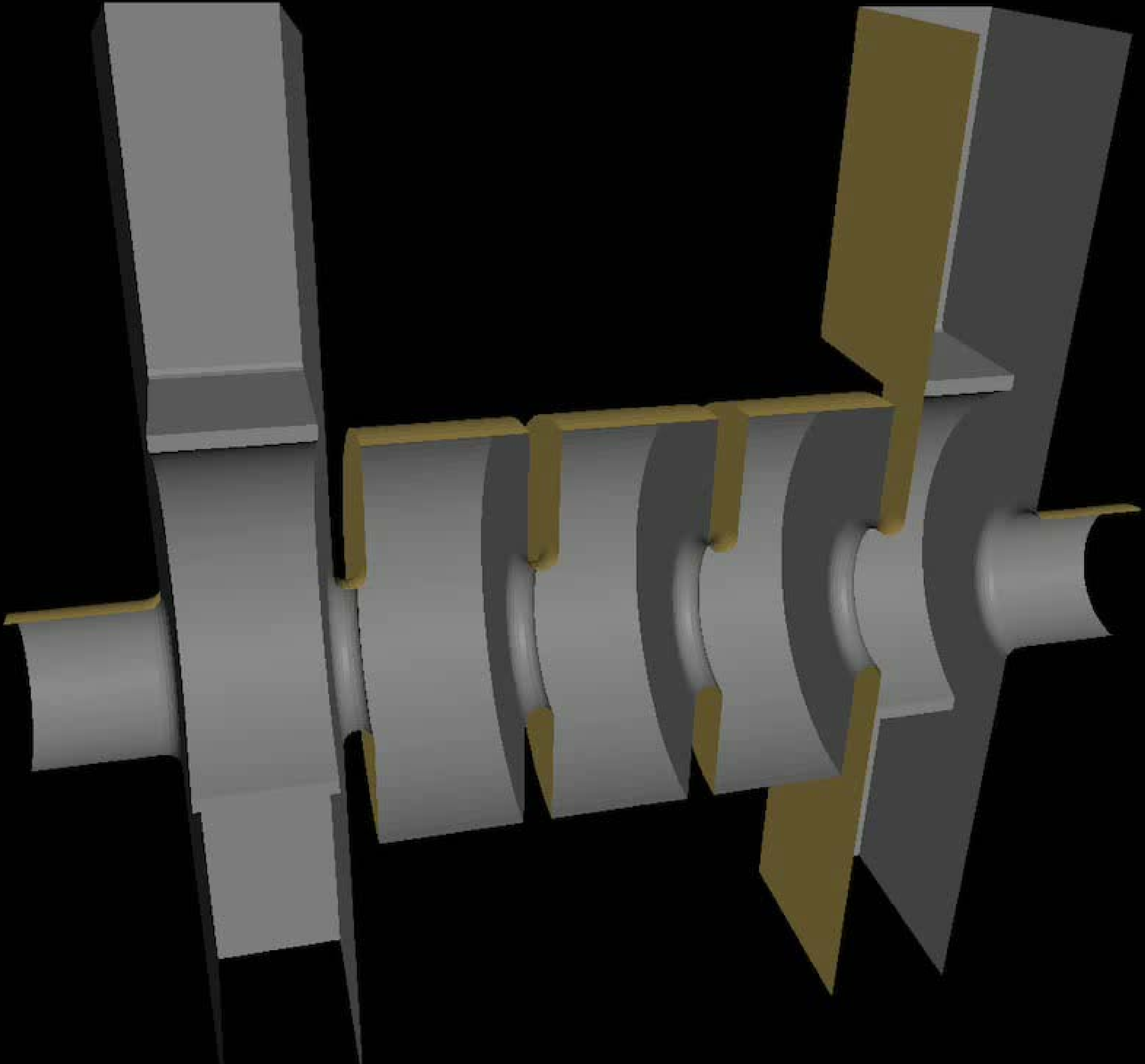
Particle Tracking – Track3P



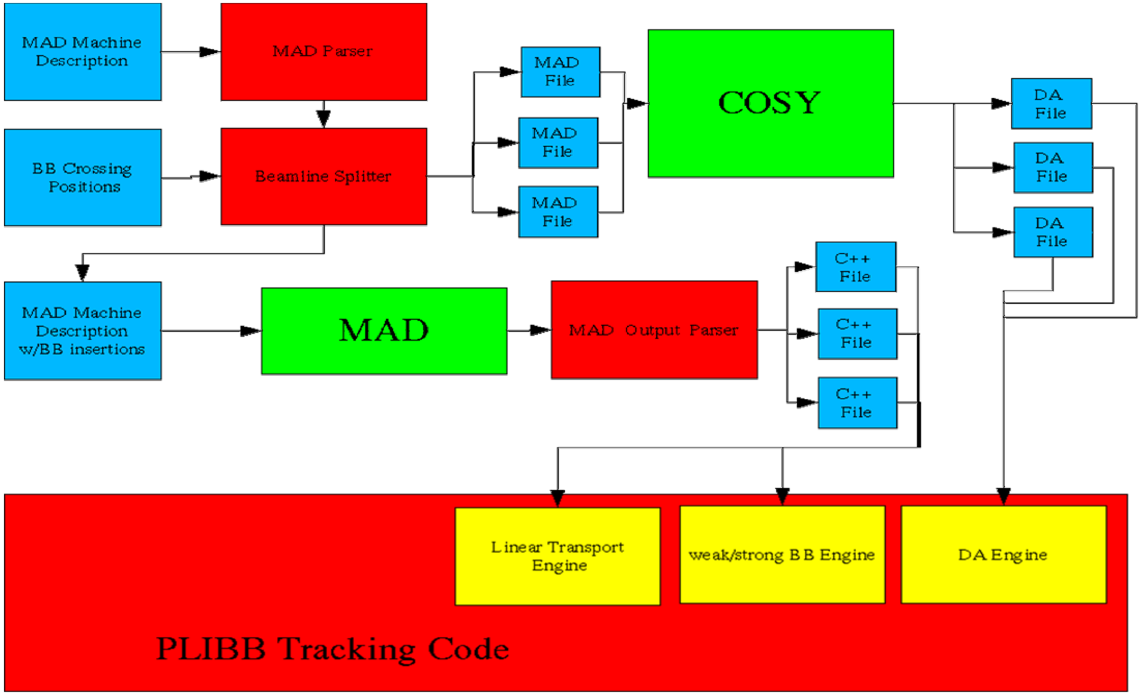
G = 50 MV/m

G = 100 MV/m

Benchmarking 3D trajectories against results from 2D model



Weak/Strong Beam-beam - PlibB



- Directly computes lifetimes in hadron machines, not dynamic apertures
- Does 10^{12} beam-beam interactions for typical Tevatron calculation (NERSC)
- Tracking and beam-beam kick engines designed for speed and fed by code generated data based on machine description
- Calculates lifetimes up to 10h for Tevatron with all 72 parasitic crossings

Code Development - PlibB

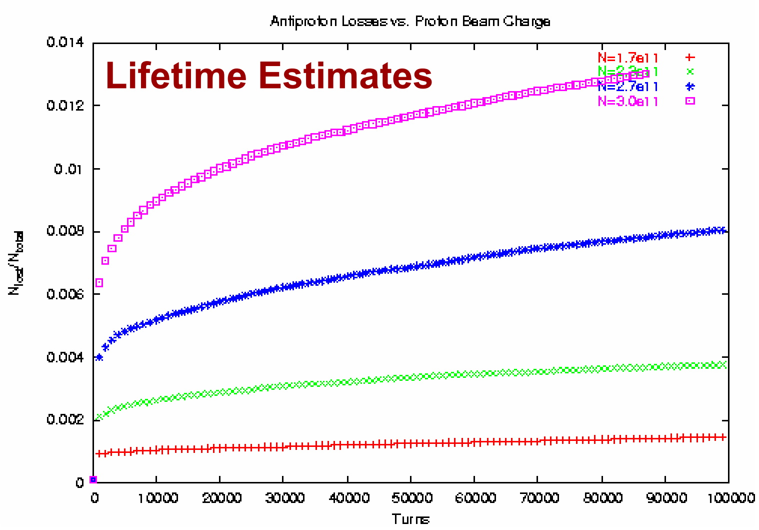
- Expanded to cover more physics:
  - Full 6-D coupling (linear case)
  - Chromaticity
  - Fast truncated power series tracking engine
  - Noise
- Accelerated BB-Engine
- Collaborated with FNAL to obtain DA map
- Running convergence studies for DA map

Future Plans:

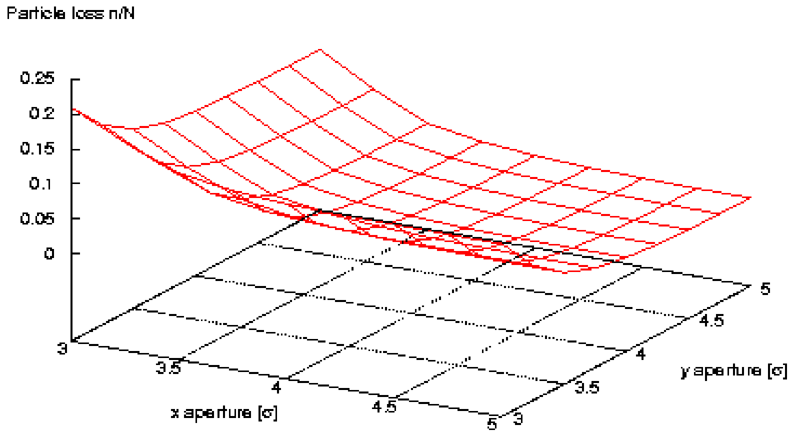
- Integrate w/ existing parallel strong/strong beam-beam-code PaBB
  - To simulate the Tevatron collision case
  - To simulate PEP-II w/inclusion of IP and parasitic crossings
- Combine PaBB with parallel PIC/Tracking modules
  - To simulate ECI and beam-beam effects in PEP-II and future accelerators

Tevatron Lifetime Estimates - PlibB

- Collaborating with FNAL on machine parameters (T. Sen, B. Erdalyi, M. Xiao)
- Currently running parameter scan studies for lifetime at Injection Stage (150GeV)
- Lifetime estimates track 400,000 particles for 100,000 turns on 256 processors on NERSC's IBM SP2
- Working with FNAL on tool suite to automatically create DA/MAD mappings

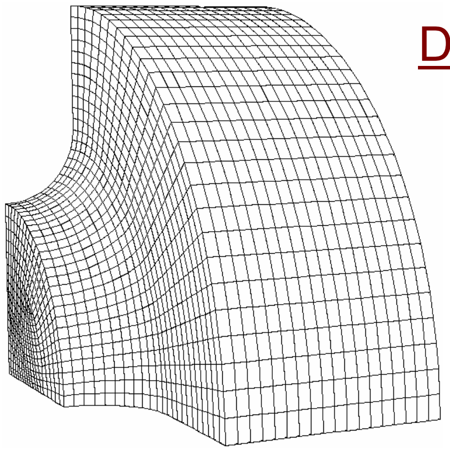


Lifetime Dependance on Physical Aperture



H60VG3 Structure - End-to-end Modeling

H60VG3 (55 cells including power couplers) is being considered as a baseline structure design for the NLC for which detuning and damping are planned to suppress dipole wakefields. **Entire** structure simulation has begun to calculate **long-range** wakefields in the detuned structure to be followed by modeling of the final damped, detuned design.



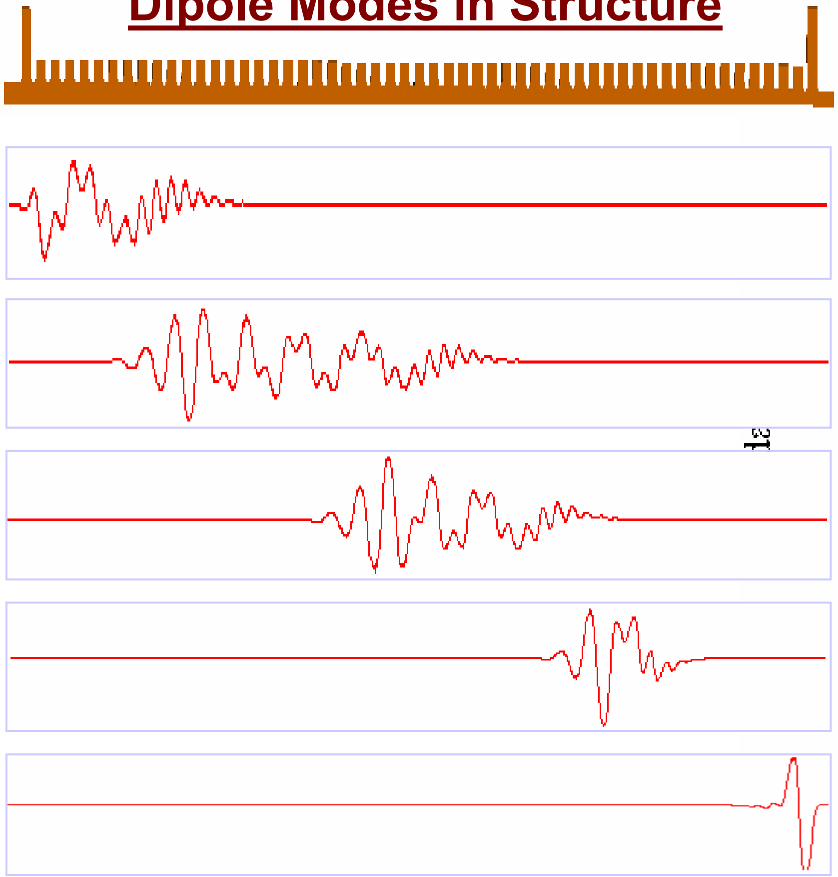
Detuned Cell

Damped, Detuned Cell

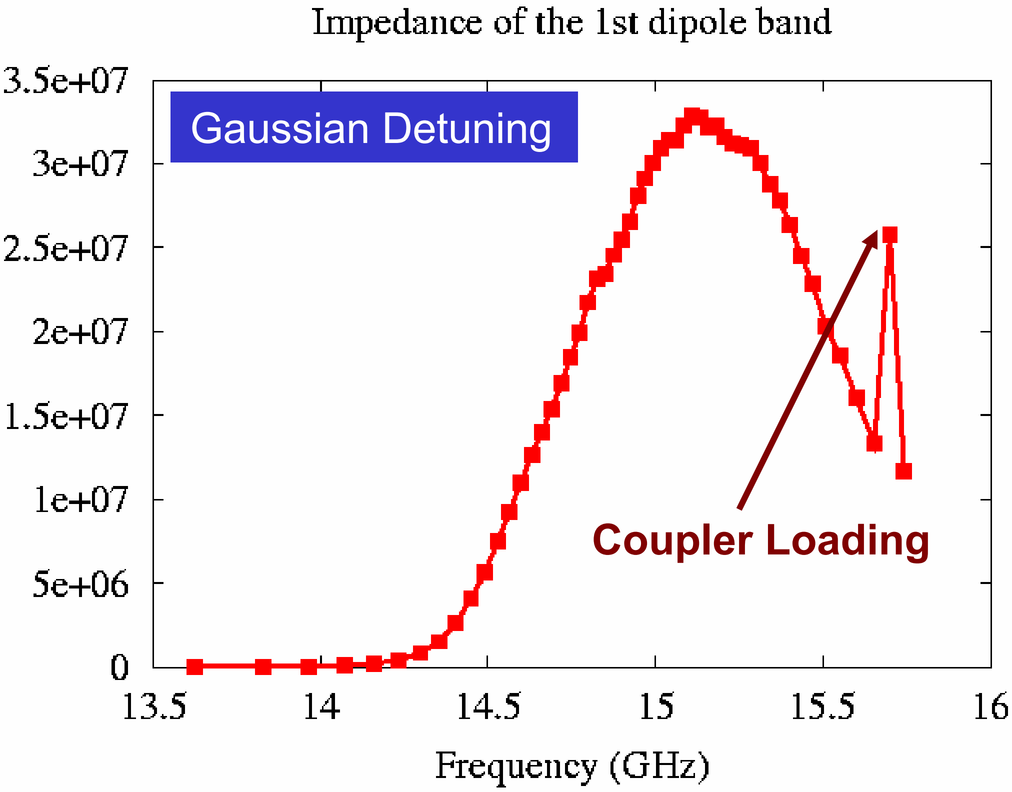
Eigenmodes in H60VG3 – Omega3P

Omega3P is used to find eigenmodes needed for calculating wakefields by mode summation – **1st Dipole Band**

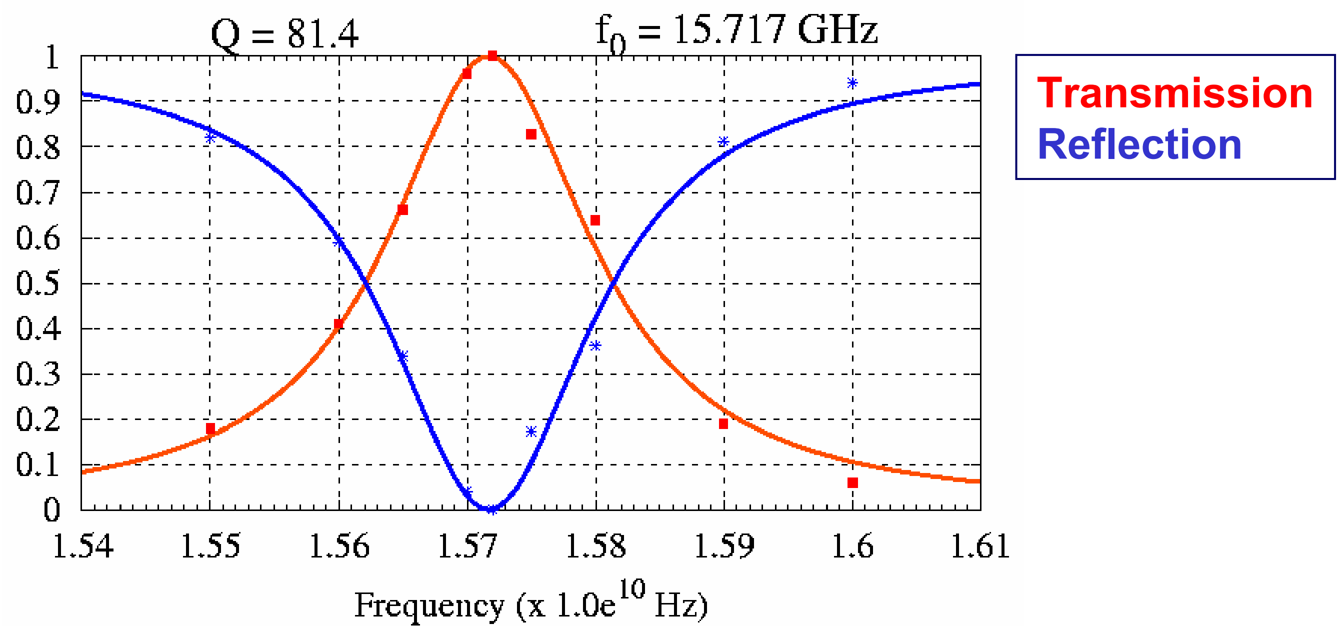
Dipole Modes in Structure

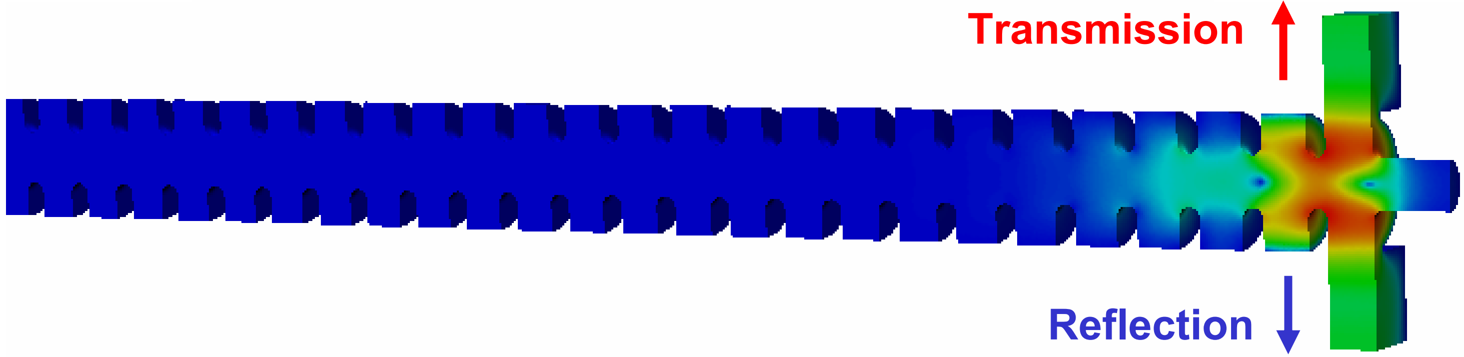


Impedance Spectrum



Coupler Loading on Dipole Mode – S3P

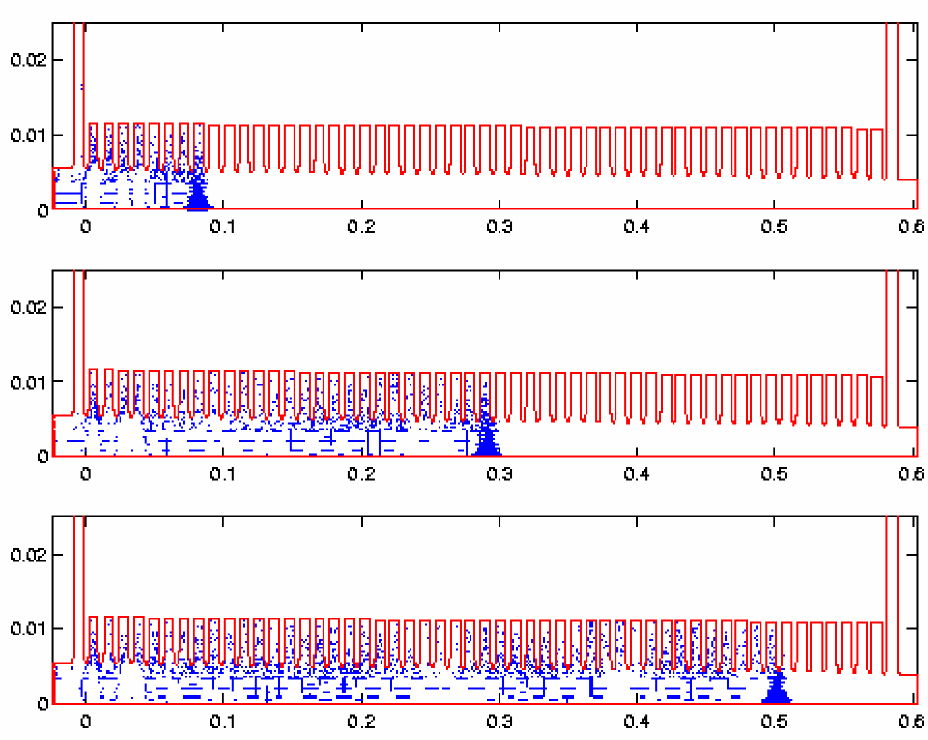




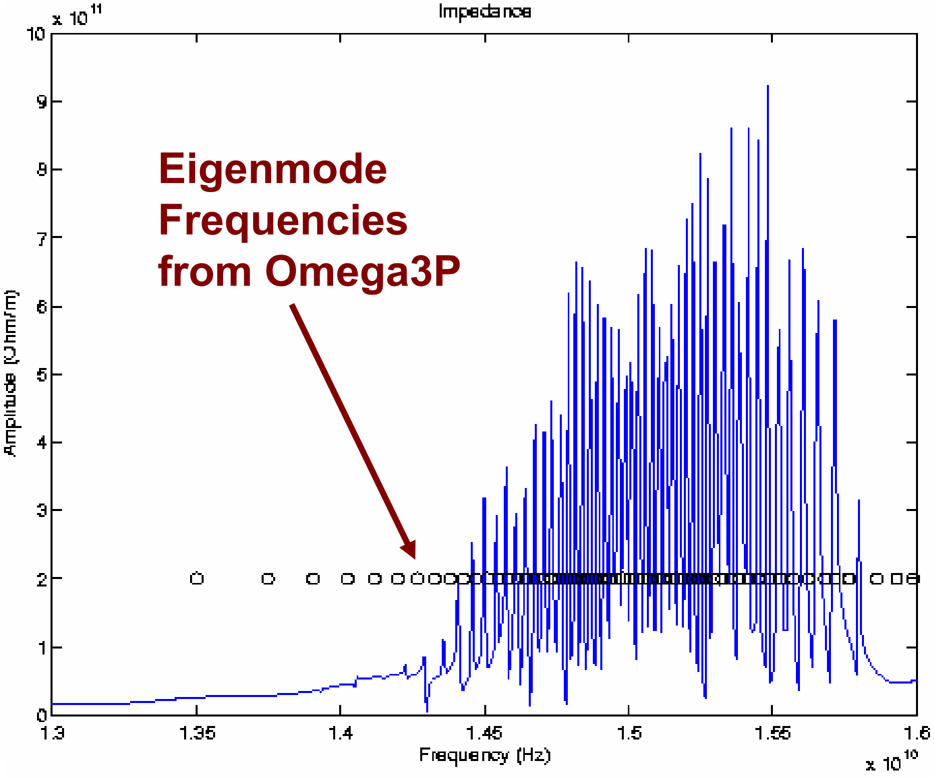
Beam Excitation of H60VG3 – Tau3P

Tau3P is used to excite wakefields directly by a transit beam and calculate the impedance spectrum covering all bands.

Beam Transit through Structure



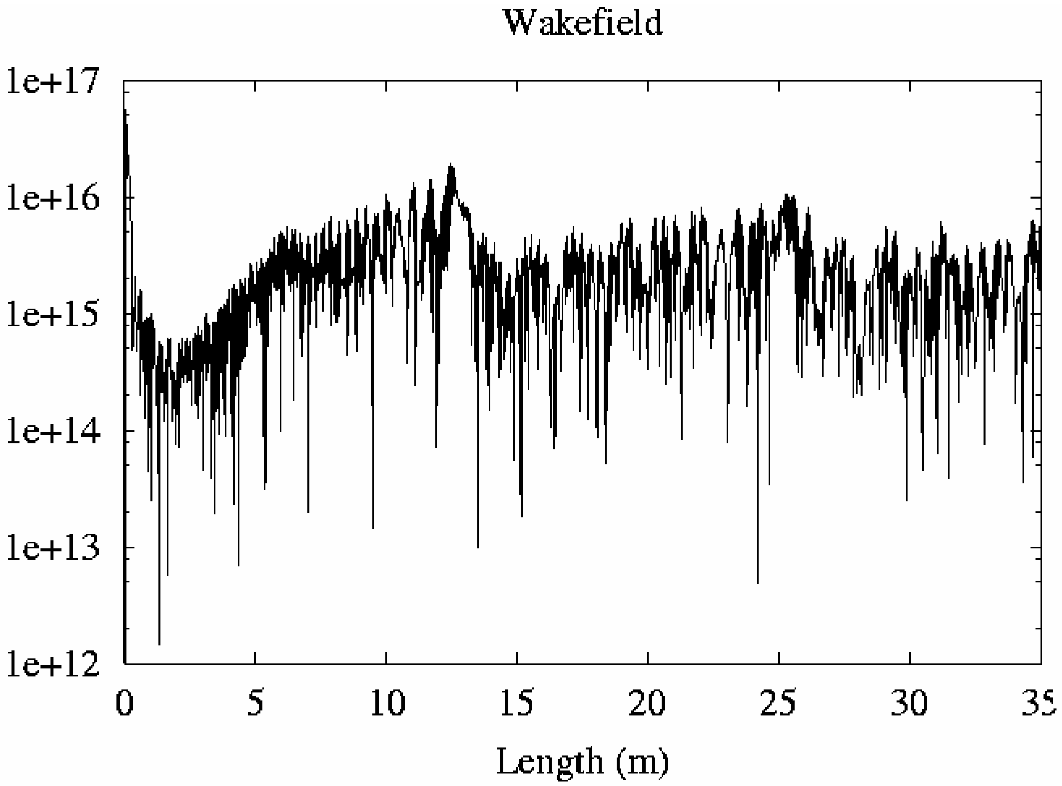
1st Band Impedance Spectrum



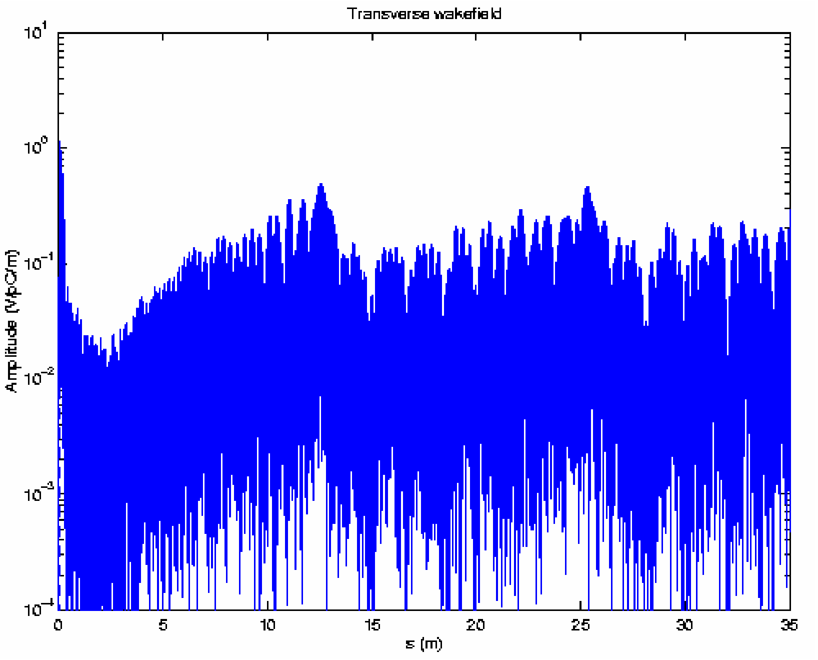
Eigenmode Frequencies from Omega3P

Dipole Wakefield in H60VG3

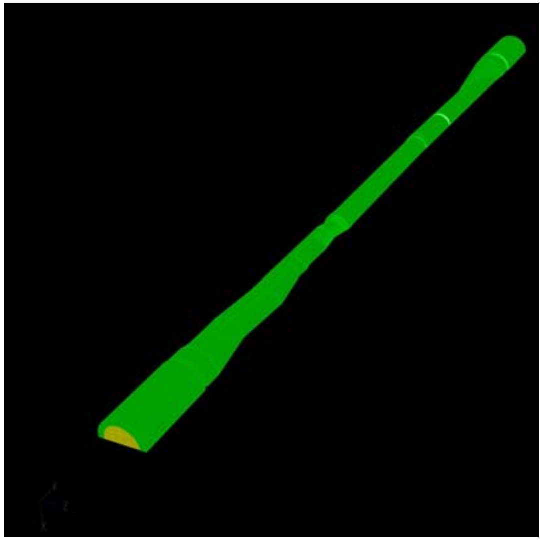
Omega3P – Sum of Modes from 1st Band



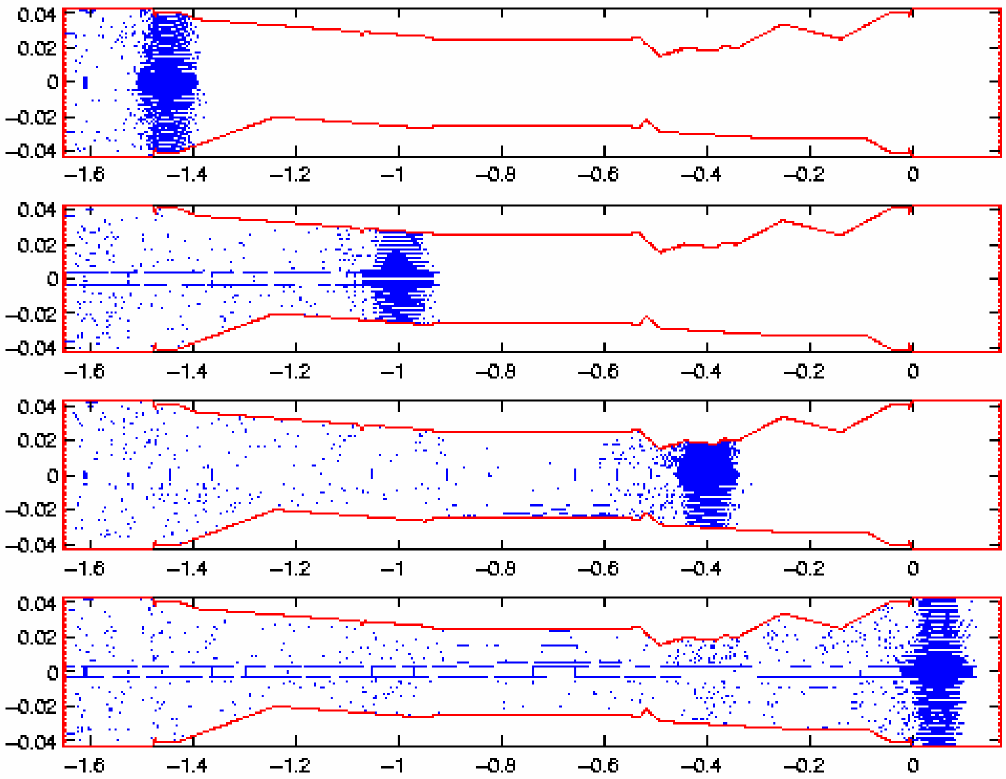
Tau3P – Direct Simulation



Trapped Modes in PEP-II IR – Tau3P

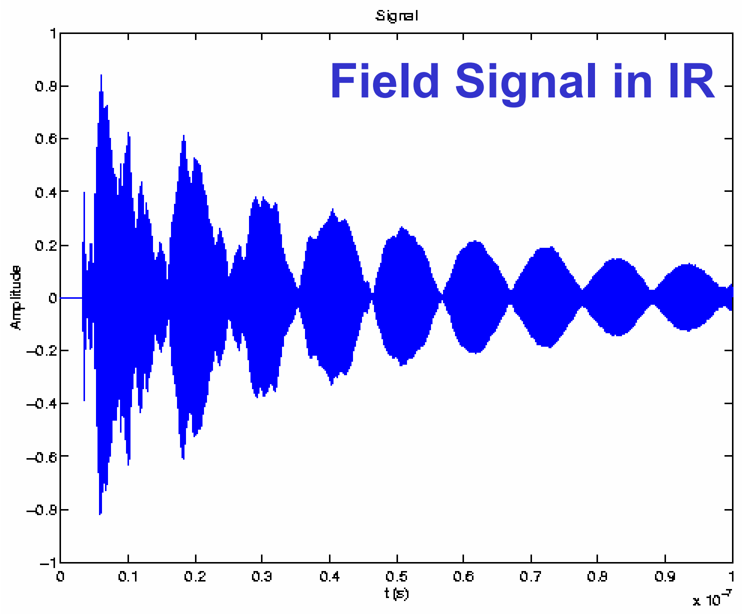


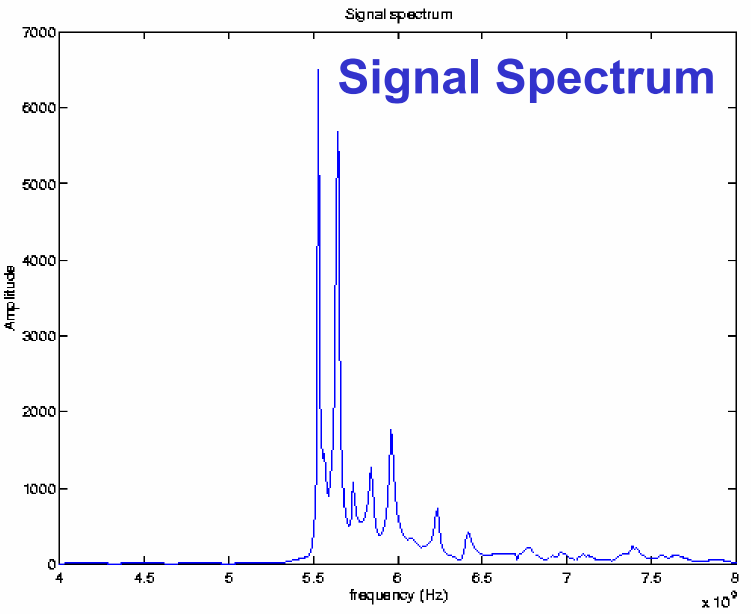
Find localized modes in IR complex for beam heating analysis by direct excitation (**Tau3P**) for comparison with eigenmodes found by **Omega3P**



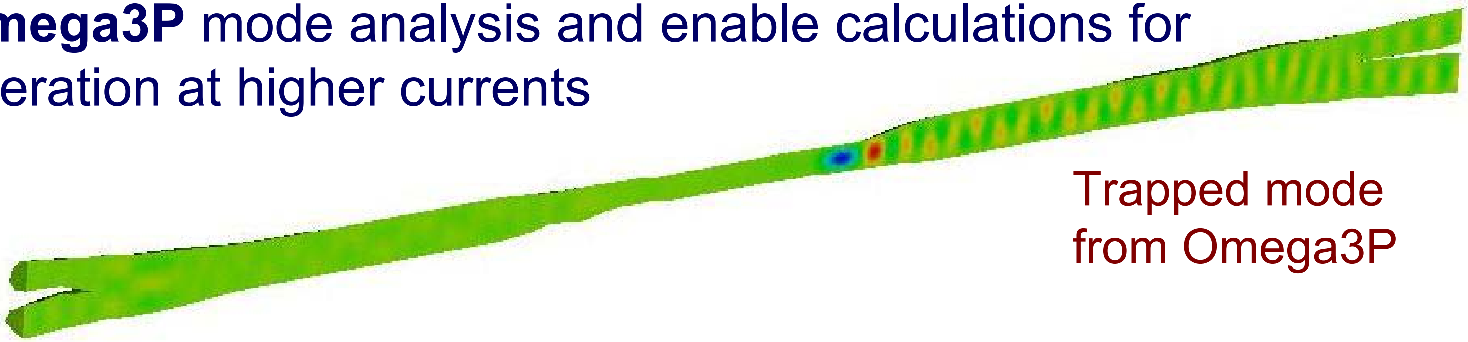
PEP-II IR Mode Spectrum – Tau3P

(S. Eckland, M. Sullivan – PEP-II)





Extension to Full IR model (crotch-to-crotch) will confirm **Omega3P** mode analysis and enable calculations for operation at higher currents

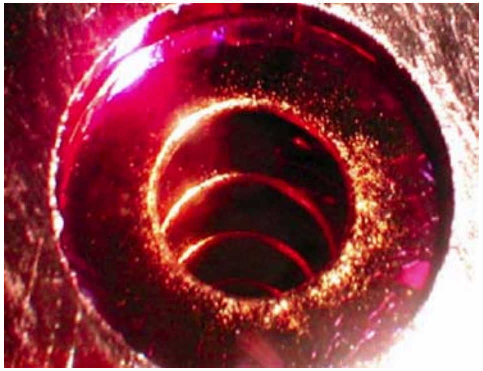


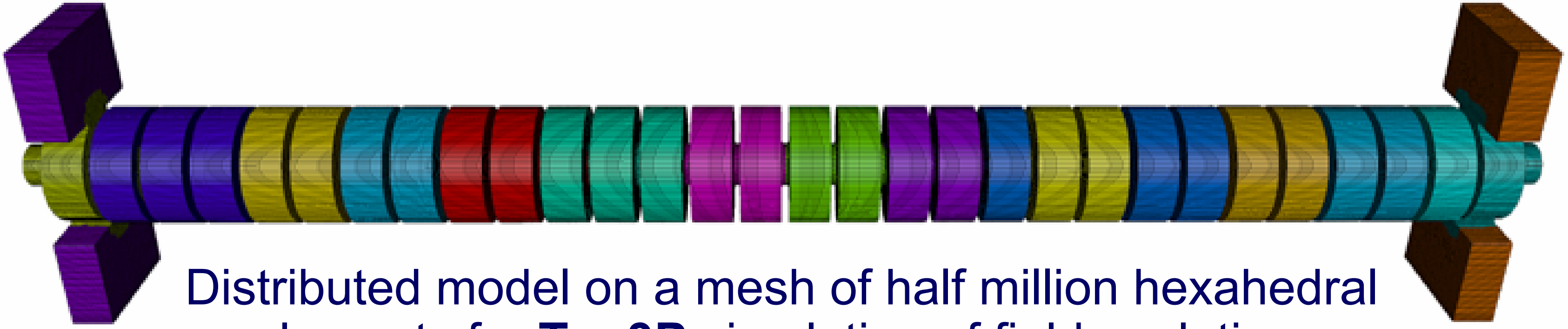
Trapped mode
from Omega3P

30-cell Structure – Tau3P

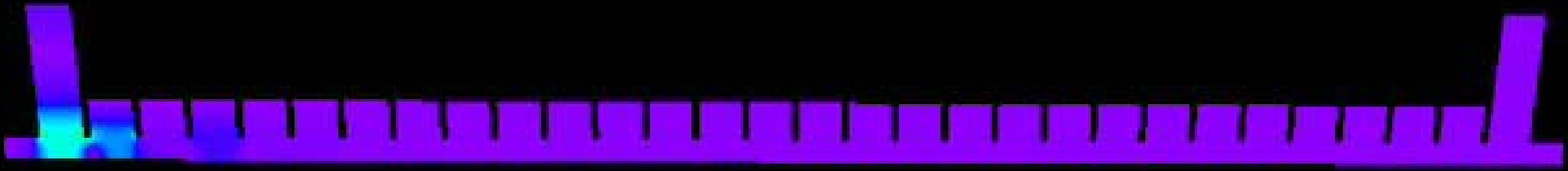
(J. Wang – ARDA)

- NLC X-band structure showing damage after high power test
- Realistic simulation needed to understand underlying processes



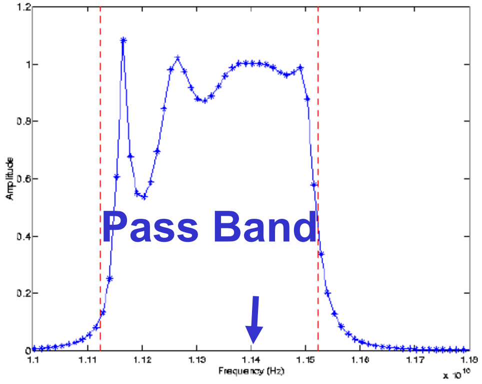


Distributed model on a mesh of half million hexahedral elements for **Tau3P** simulation of field evolution

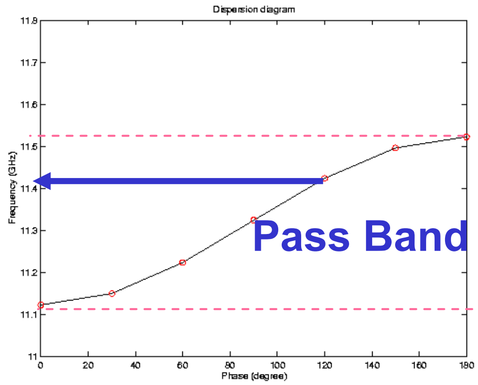


Transient Effect -Tau3P

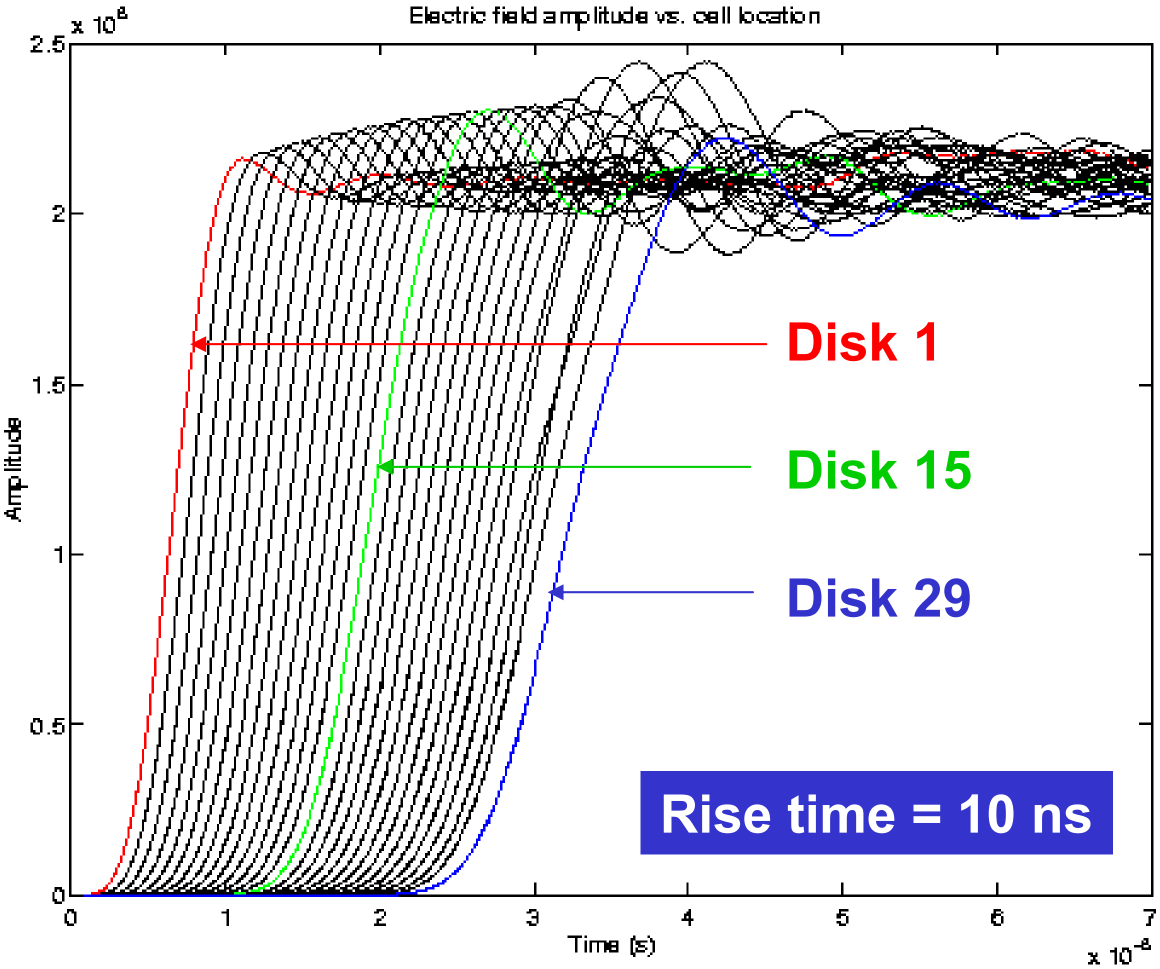
Power Spectrum



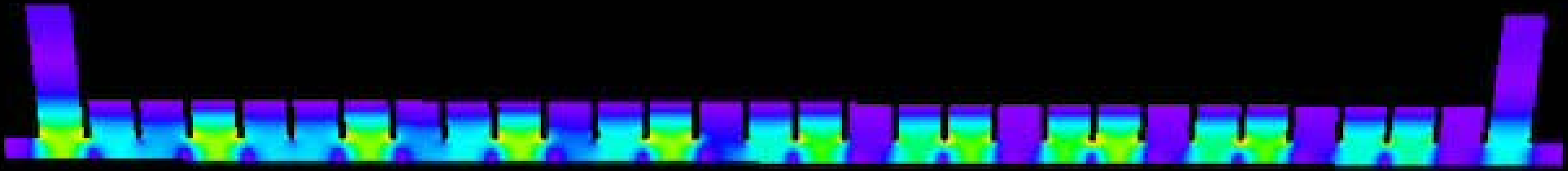
Dispersion Diagram



Electric field vs time



Rise time = 10 ns

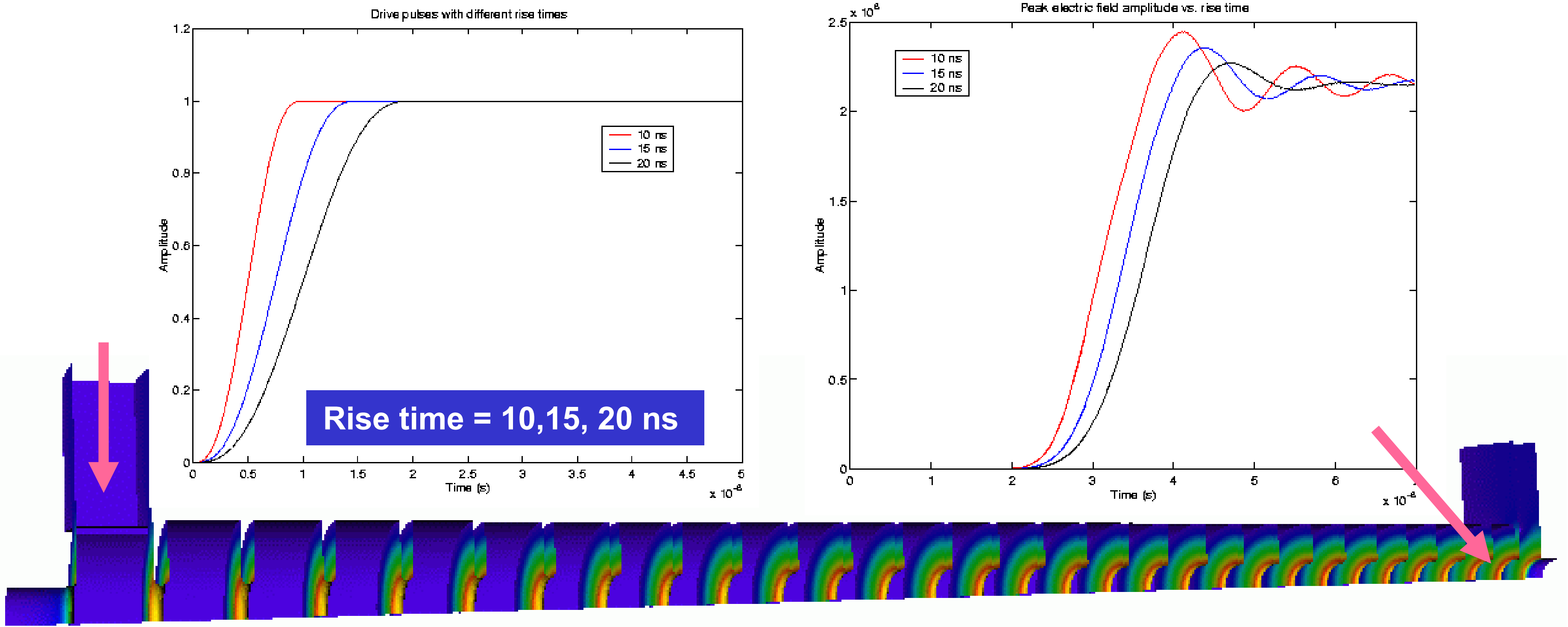


Peak Fields – Tau3P

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

Drive pulse

Electric field vs time



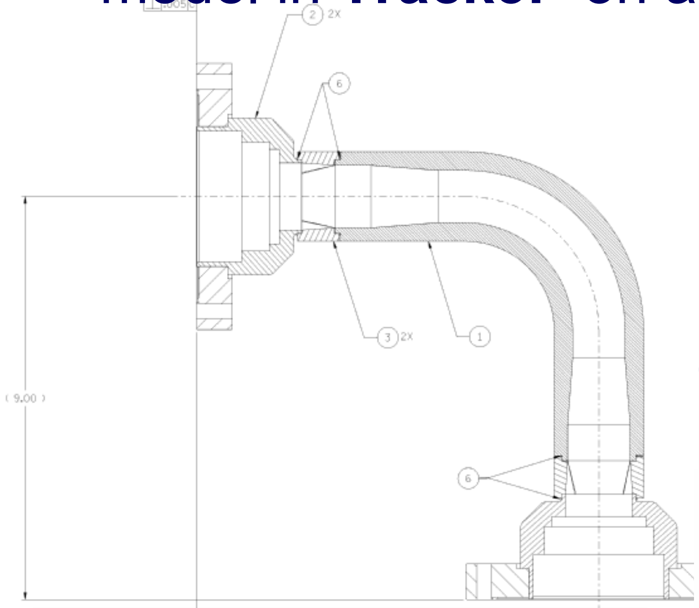
Rise time = 10,15, 20 ns

Steady-state Surface Electric field amplitude

Modeling High Power Test – Track3P

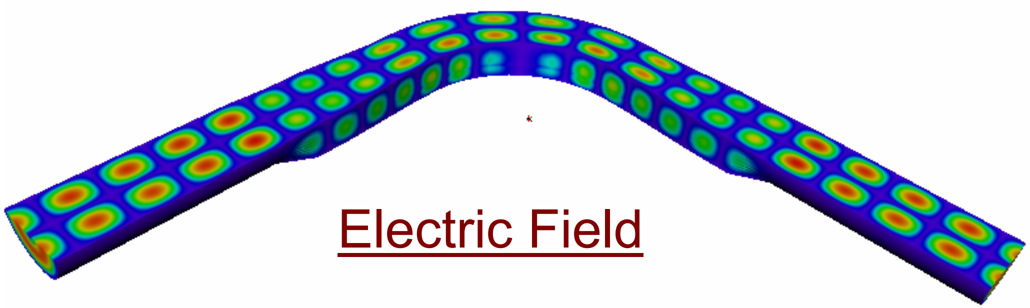
(C. Adolphson – NLC)

- High power test on a 90 degree square bend provides measured data for benchmarking the secondary emission model in **Track3P** on a simple geometry

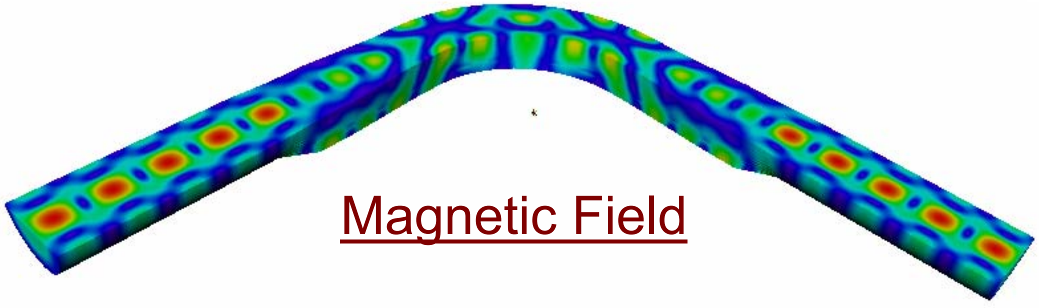


Square Bend Used at NLCTA to Transport SLED II Output Power to Structures

Using Fields from Tau3P



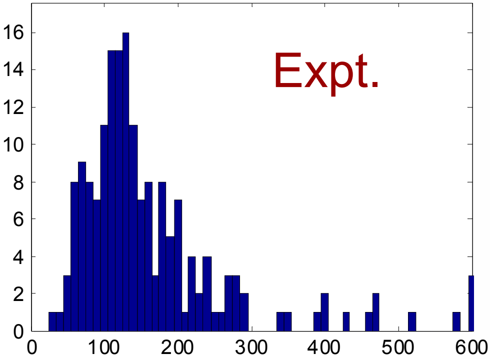
Electric Field

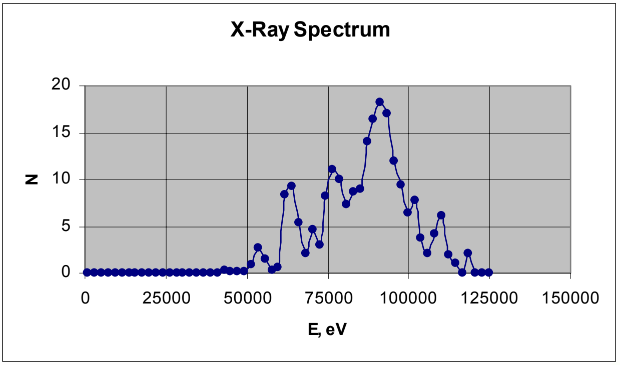


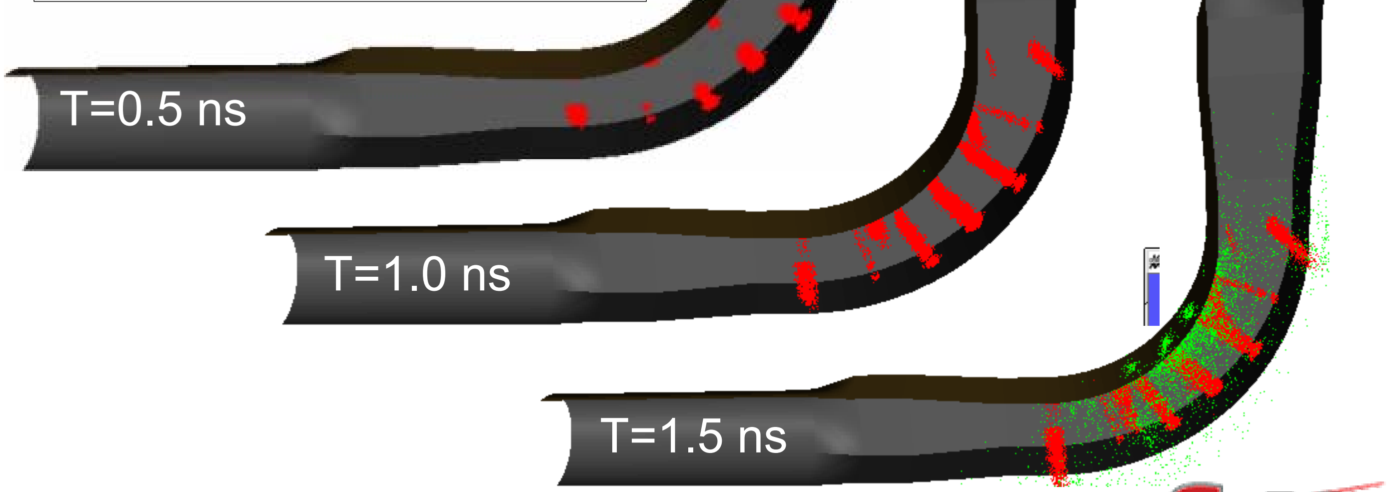
Magnetic Field

Benchmark Surface Physics – Track3P

X-Ray Energy Spectrum – Good agreement between Track3P and Measurement and simulation indicates high energy X-Ray is due to elastic scattered secondary electrons.





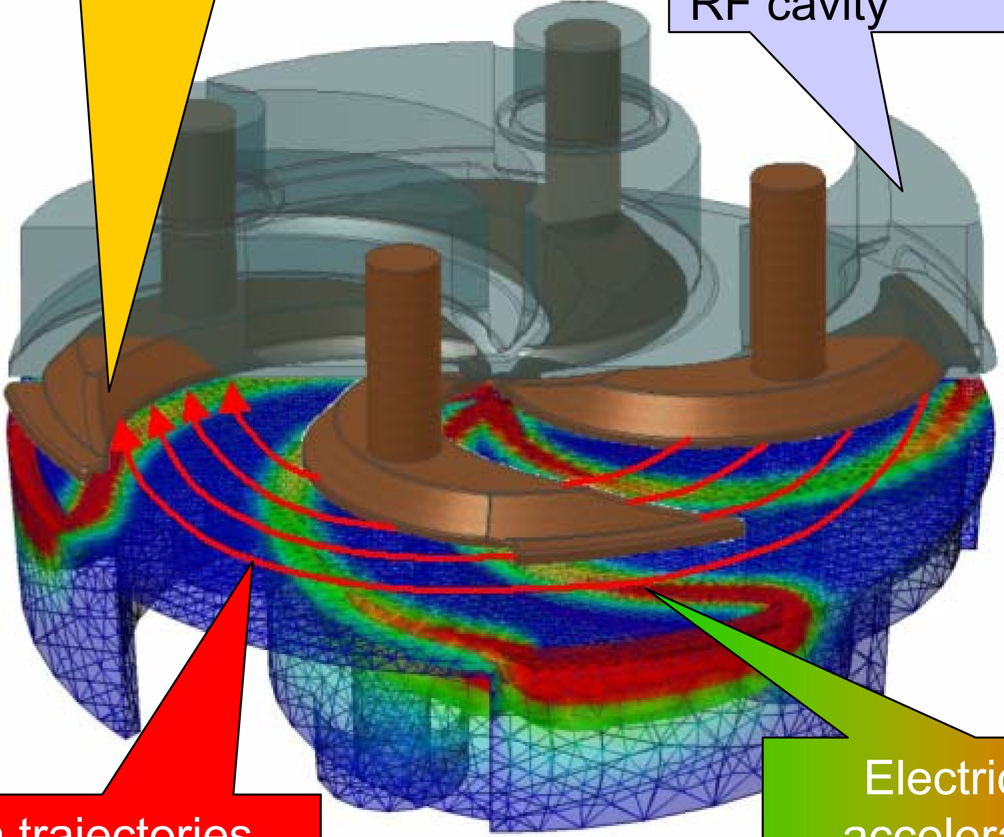


Cyclotron COMET - Omega3P

First ever detailed analysis of an entire cyclotron structure

- L. Stingelin, PSI

Fig 1. The cyclotron COMET

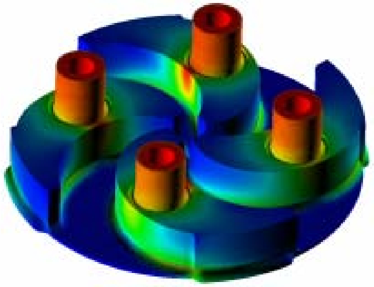


„Dee“: RF electrode

„Liner“: outer shell of RF cavity

Proton trajectories

Electric field in acceleration gap

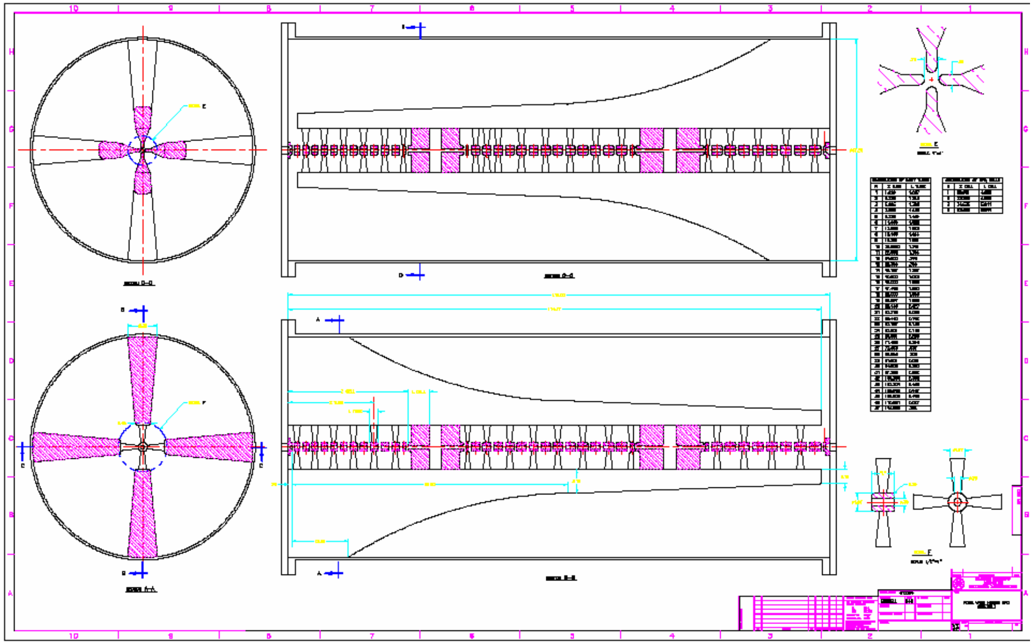


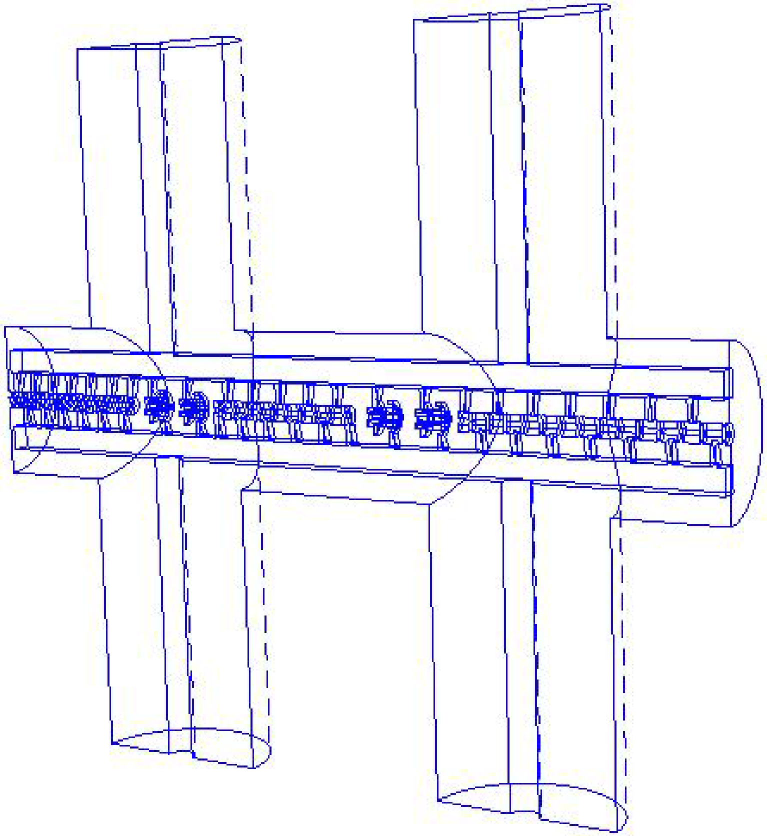
Magnetic Field

RIA Hybrid RFQ – Omega3P

(J. Nolan, P. Ostroumov – ANL)

Effort towards end-to-end modeling of the RFQ has started





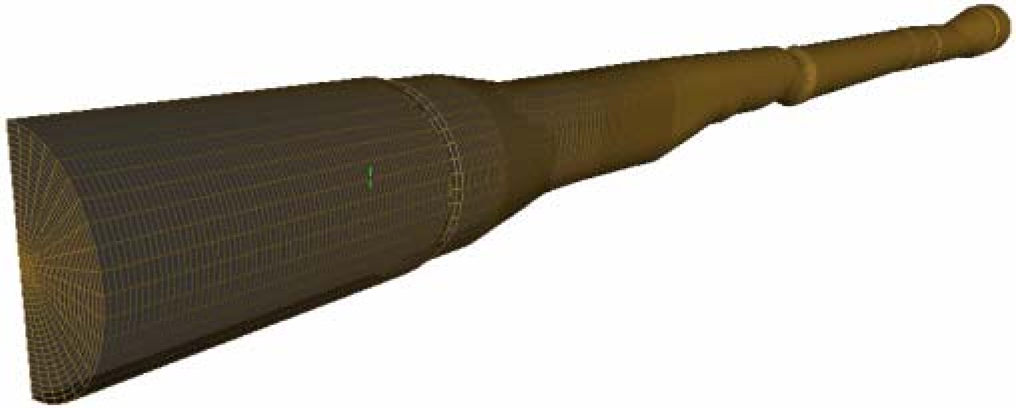
CS/AM Collaborations - SAPP, ISICs

- **CAD Model/Mesh Generation** – T. Tautges (SNL/TSTT)
- **Quality metrics to improve meshes** - P. Knupp (SNL/TSTT)
- **Improvements to the Eigensolver** – Y. Sun, G. Golub (Stanford);
  E. Ng, P. Husbands, X. Li,
  C. Yang (LBNL/TOPS)
- **Improvement studies for the DSI scheme** - B. Henshaw (LLNL/TSTT)
- **Visualization of multiple data sets** - G. Schussman, K. Ma (UCD/SAPP)
- **Parallel adaptive refinement** - Y. Luo, M. Shephard (RPI/TSTT)
- **Improving parallel performance** - A. Pinar (LBNL/TOPS), K. Devine (SNL)

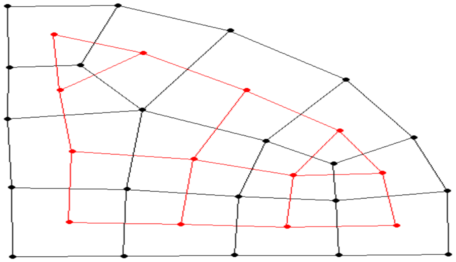
CAD/Mesh Issues - Tau3P

(T. Tautges – SNL/TSTT)

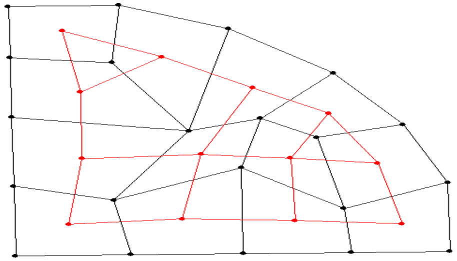
Fixing CAD model and Optimizing Tau3P Primary/Dual Mesh

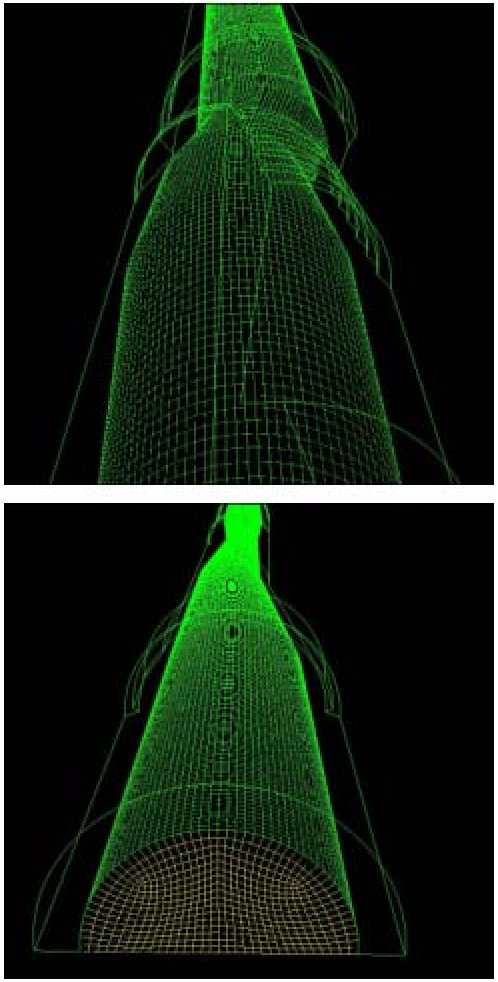


Worst deviation
= 41°



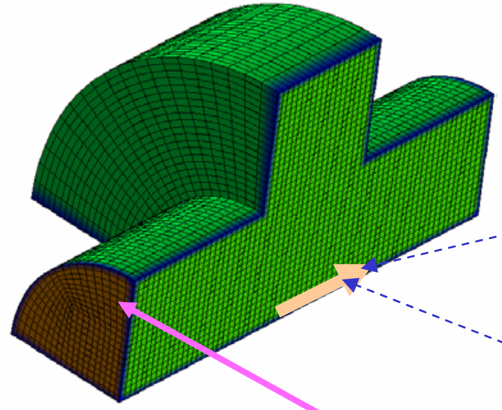
Worst deviation
< .001°

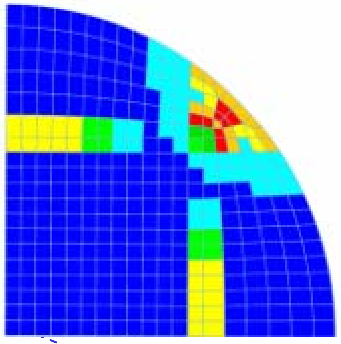


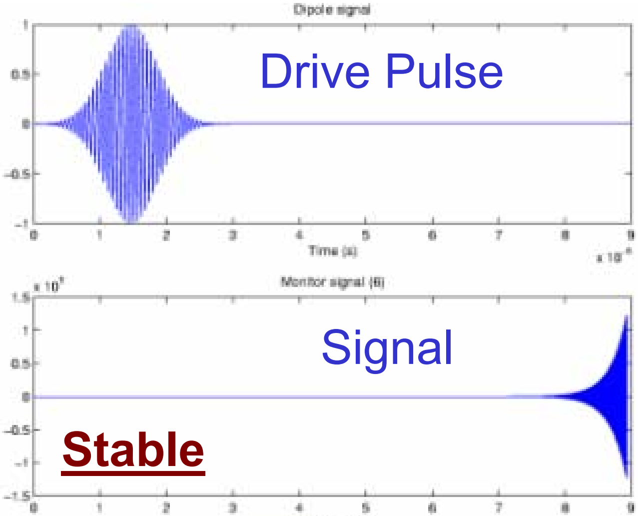


Mesh Effects on Stability – Tau3P

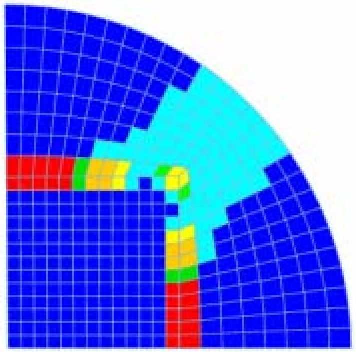
(P. Knupp – SNL/TSTT)

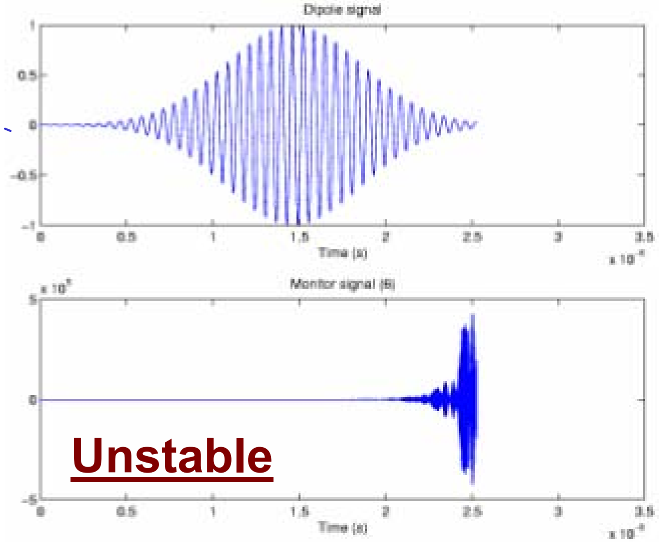






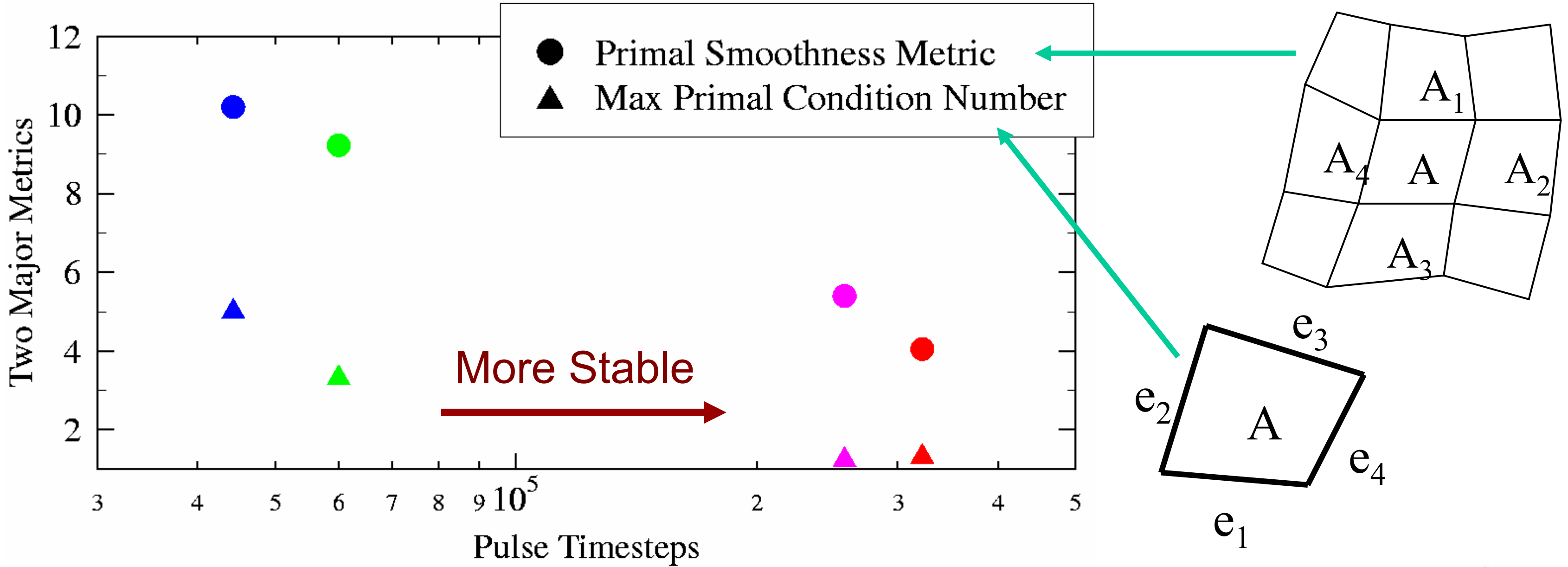
Stability is measured by the number of time steps before reaching a preset instability threshold (or error bound)

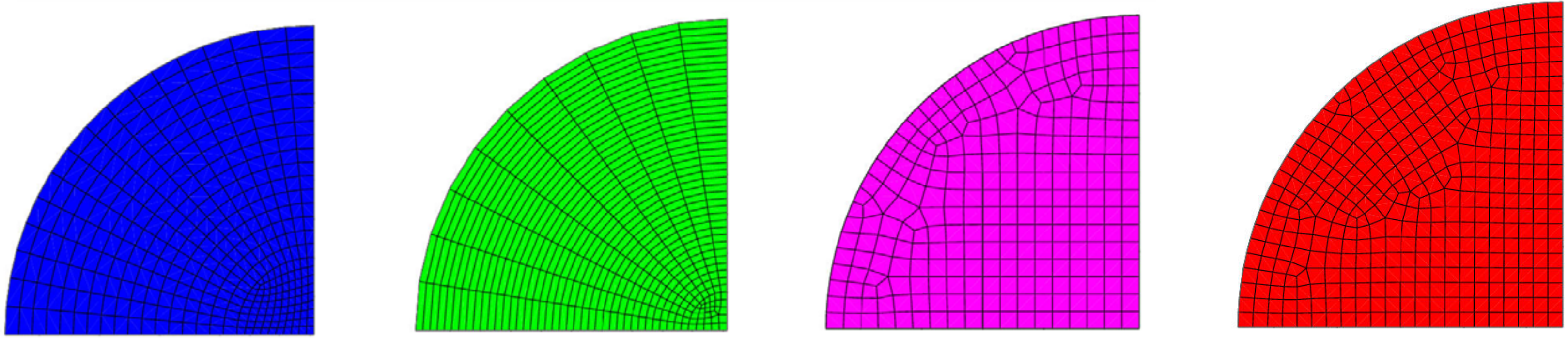




Mesh Quality Metrics – Tau3P

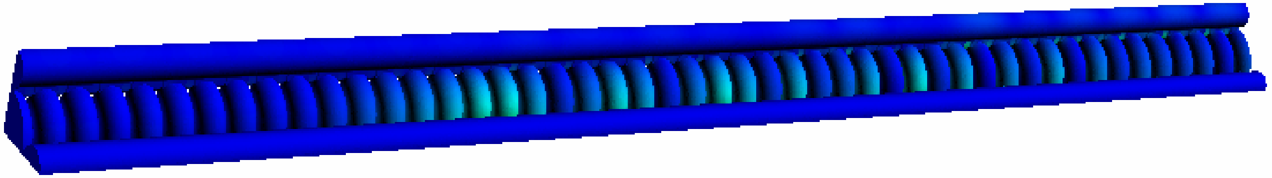
Selected quality metrics are being incorporated into **CUBIT** to aid in generating better meshes for **Tau3P**





ESIL Solver - Omega3P

(E. Ng, P. Husbands, X. Li, C. Yang – LBNL/SAPP, TOPS)



- Integrated an Exact Shift-Invert Lanczos (ESIL) eigensolver, developed by LBNL, into Omega3P
- Uses SuperLU for complete factorization of sparse matrices and combines with PARPACK to compute interior eigenvalues accurately
- Verifies Omega3P hybrid solver on a 47-cell structure calculation and can provide better efficiency at the expense of increased memory

	Omega3P	Omega3P with EISL	Omega3P with AV
Speed (larger is better)	1.0	2.57	3.41

Stable Algorithm Development – Tau3P

(B. Henshaw – LLNL/TSTT)

The **DSI** (Discrete Surface Integral) scheme in **Tau3P** exhibits instabilities for long time integration on non-orthogonal grids that result in non-self-adjoint operator. Explored 3 possible ways to develop a stable algorithm:

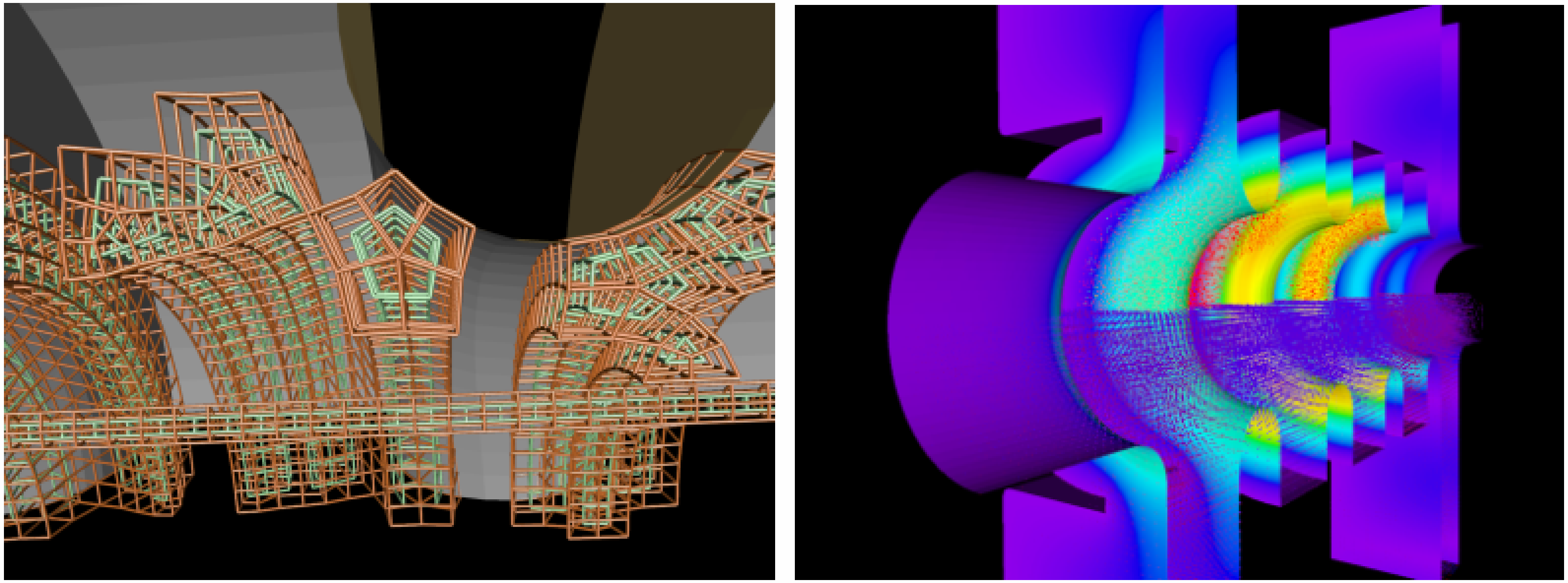
(1) **Spatial artificial dissipation** - Initial numerical experiments indicate that a sixth-order dissipation is very effective with very little damping of the energy over long times.

(2) **Dissipative time integration** - Studied the ABS3 (Adams-Bashforth Staggered-Grid Order-3) scheme but found it not suitable even though it improves the convergence properties.

(3) **A symmetric scheme** - developed 2nd-order and fourth-order accurate approximations that are self-adjoint but only for grids that are logically rectangular, not for general unstructured meshes. The fourth-order approximation could be used in the context of overlapping grids to give an accurate and very efficient solver.

Visualizing Mesh/Field/Particle – Track3P

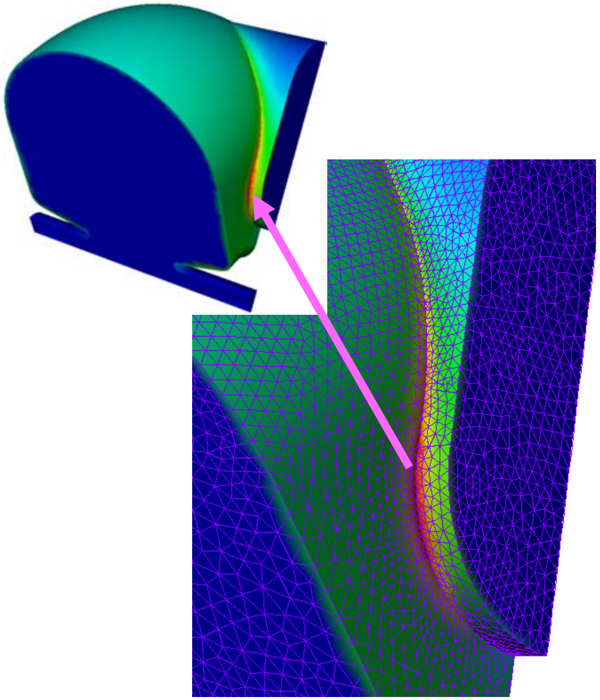
(G. Schussman, K. Ma – UCD/SAPP)



- Simultaneous rendering of field/particle data
- Extremely dense particle trajectories/field lines
- Complex data abstraction to overcome limited display resolution
- Interactive user interface needed to reveal structures

Optimization - Omega3P

(Y. Luo, M. Shephard – RPI/TSTT)



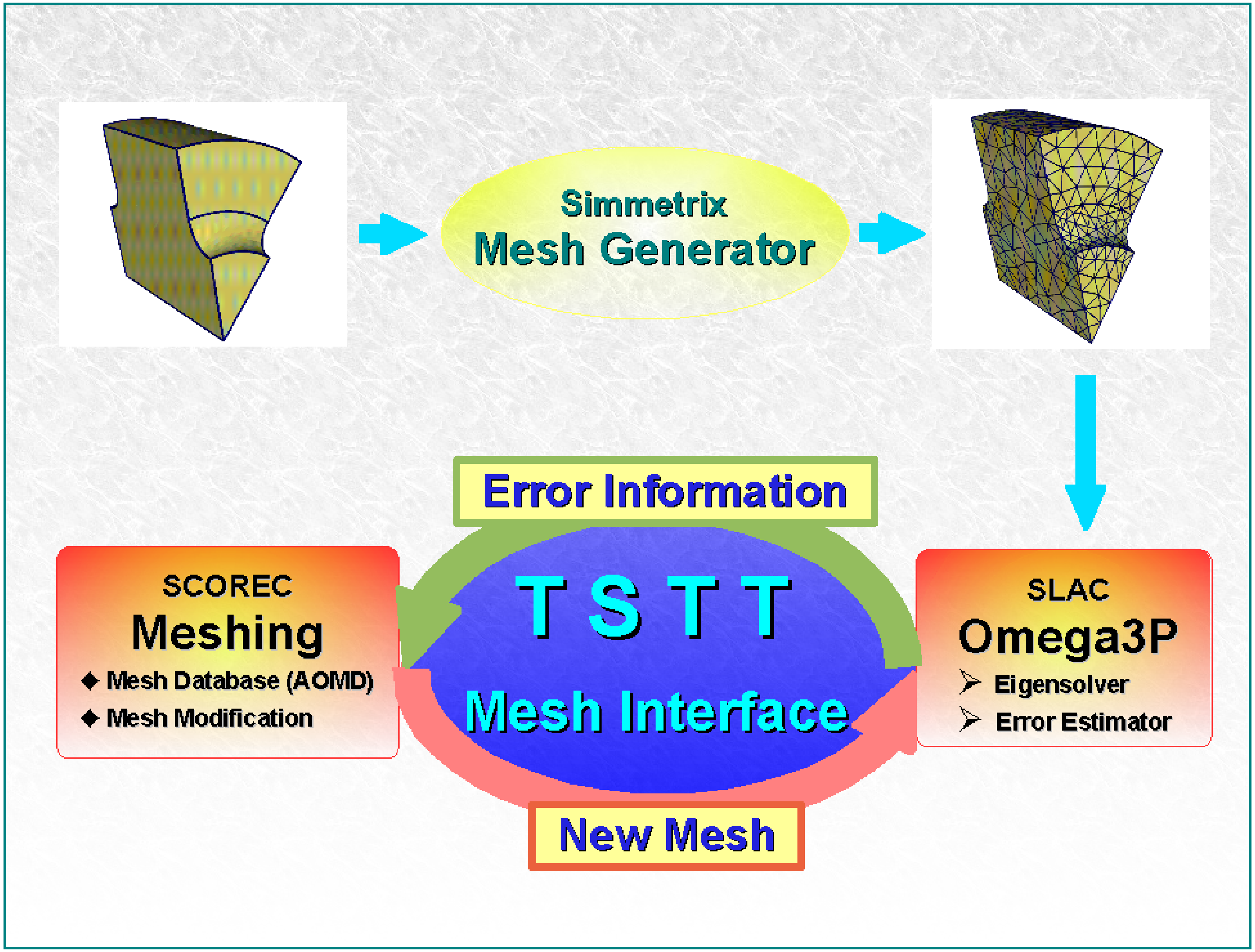
- Developing optimization strategy to obtain higher order accuracy in frequency & wall loss calculations in **most efficient** way
- Optimal use of solver and *h-p* adaptive refinement based on energy gradient error metric

$$r_e = \int_e |\nabla \cdot U|^2 dv \qquad U = \frac{\varepsilon}{2}|E|^2 + \frac{\mu}{2}|H|^2$$

- Integrate with RPI framework to deal with mesh partitioning and load balancing

h - mesh size	**p** – polynomial	**E** – solver converg.
1	1 (Linear)	1 (Lanzcos)
1/2	2 (Quadratic)	2 (Jacobi-Davidson)

Adaptive Refinement - Omega3P



Simmetrix
Mesh Generator

Error Information

T S T T
Mesh Interface

New Mesh

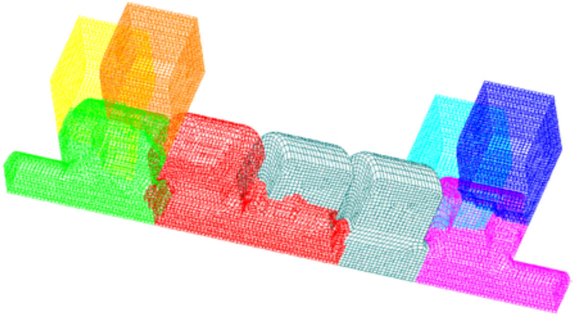
SCOREC
Meshing
- Mesh Database (AOMD)
- Mesh Modification

SLAC
Omega3P
- ➢ Eigensolver
- ➢ Error Estimator

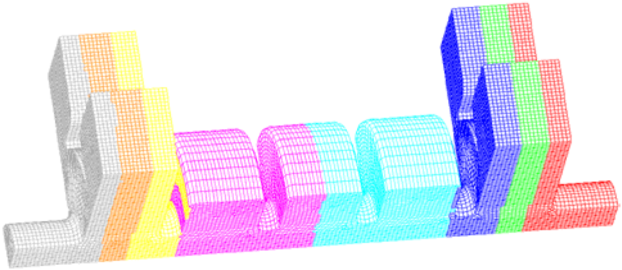
Domain Decomposition - Tau3P

(TOPS: K. Devine/SNL, A. Pinar - LBNL)

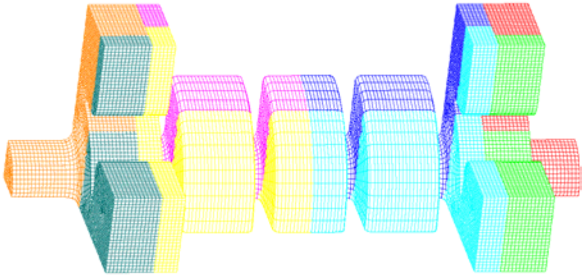
Sandia's **Zoltan** library is implemented to access better partitioning schemes for improved parallel performance over existing **ParMETIS** tool through reduced communication costs.



ParMETIS



RCB-1D



RCB-3D

8 processor partitioning comparison on Linux cluster

	Tau3P Runtime	Max. Adj. Procs.	Max. Bound. Objects
ParMETIS	140.6 sec	3	533
RCB-1D	126.4 sec	2	3128
RCB-3D	169.1 sec	5	1965

Summary

- Under SciDAC, ACD has developed a powerful suite of numerical tools for solving challenging electromagnetic problems facing existing and planned accelerators,
- These are parallel codes based on unstructured grids that target high accuracy design and system level studies,
- ACD's multi-disciplinary team approach mirrors the SciDAC concept and has been effective in accessing the computing and computational resources within the DOE,
- With SAPP/ISIC collaborators, ACD is building the high performance computing infrastructure needed to enable very LARGE (Ultra) scale simulations,
- New capability has been applied successfully to a range of applications and its potential to support DOE's mission is just beginning to be realized.