Numerical Methods

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CERN BE-RF

- What to compute
  - f_{res}, Q, R/Q, (V_{acc}, P, W) eigenmode solver + perturbation
  - but also $E_{max,surface}$, $H_{max,surface}$, $S_{max,surface}$
  - beam loading, loss factor, kick factor,
  - wakefields
- How?
  - if possible, analytic (Mathematica or Maple can help)
  - numerically
    - frequency domain – time domain
    - 2D – 3D
    - FEM - FD
- What else is important?
  - sensitivity analysis
  - knowledge/control of accuracy
  - consistency check

Time domain – frequency domain

- The Fourier transform allows to analyze in either *ω*- or *t*-domain (and to transform in the respective other) as long as the equations are **linear** (LTI: linear time-invariant).

FT:

$$g(t) \circ\!\!-\!\!\bullet\ G(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(t) e^{j\omega t} dt$$

IFT:

$$G(\omega) \bullet\!\!-\!\!\circ\ g(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} G(\omega) e^{-j\omega t} d\omega$$

- When one would prefer to use *ω*-domain:
  - With single frequency operation,
  - With large *Q*, the simulation in *t*-domain would take *Q* periods,
  - for beam impedance calculations.
- When one would prefer to use *t*-domain:
  - for transient responses (wide spectrum),
  - for wakefield calculations,
  - when simultaneously particles are tracked (or whenever things can become nonlinear) ...

Eigenmode solver + perturbation

Eigenmode solver finds solutions of the solutions ω^2 of

$$\nabla \times \left(\frac{1}{\mu} \nabla \times \vec{E} \right) - \omega^2 \varepsilon \, \vec{E} = 0$$

(e.g.), under the boundary conditions of a perfectly conducting closed cavity.

Perturbation ansatz for the losses:
Calculate H at the surface, from this the surface current density, and run this through the surface resistance

$$R_A = \sqrt{\frac{\omega\mu}{2\sigma}}$$

this allows to calculate the power lost in the wall.

Note that finding the complex eigenfrequency in presence of substantial losses, where the perturbation ansatz is not valid, is a much more difficult problem. The code HFSS can solve this problem.

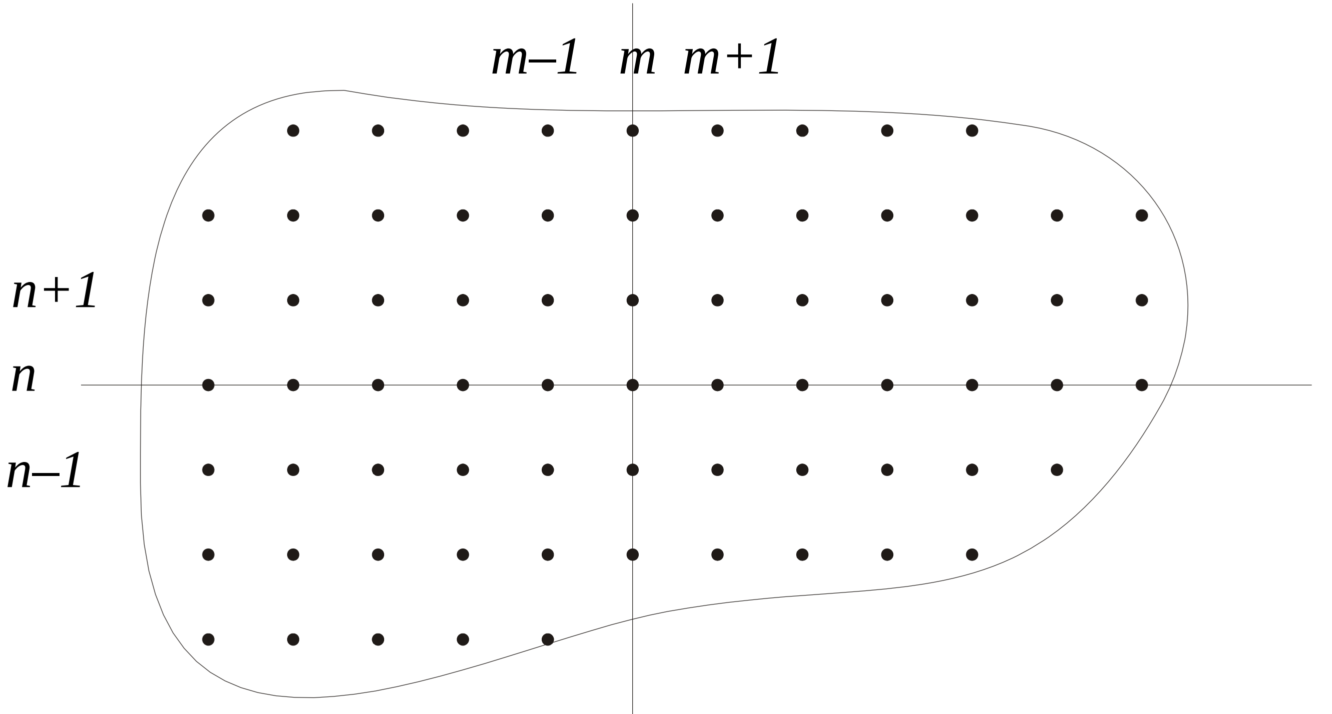
Parameters to calculate in *f*-domain

Acceleration voltage	$V_{acc} = \int E_z e^{\mathrm{j}\frac{\omega}{c}z} \mathrm{dz}$
Transit time factor	$TT = \frac{\left\|V_{acc}\right\|}{\left\|\int E_z \mathrm{dz}\right\|}$
Shunt impedance	$R = \frac{\left\|V_{acc}\right\|^2}{2\,P_{loss}}$
Q-factor	$Q = \frac{\omega_0 W}{P_{loss}}$
R-upon-*Q*	$\frac{R}{Q} = \frac{\left\|V_{acc}\right\|^2}{2\,\omega_0 W}$
Loss factor	$k_{loss} = \frac{\omega_0}{2}\frac{R}{Q} = \frac{\left\|V_{acc}\right\|^2}{4\,W}$

Finite Difference Method

Example: Laplace equation in 2D Cartesian: $\Delta\Phi \equiv \frac{\partial^2}{\partial x^2}\Phi + \frac{\partial^2}{\partial y^2}\Phi = 0$

First, discretize space (meshing) and write a difference equation for neighbouring points:

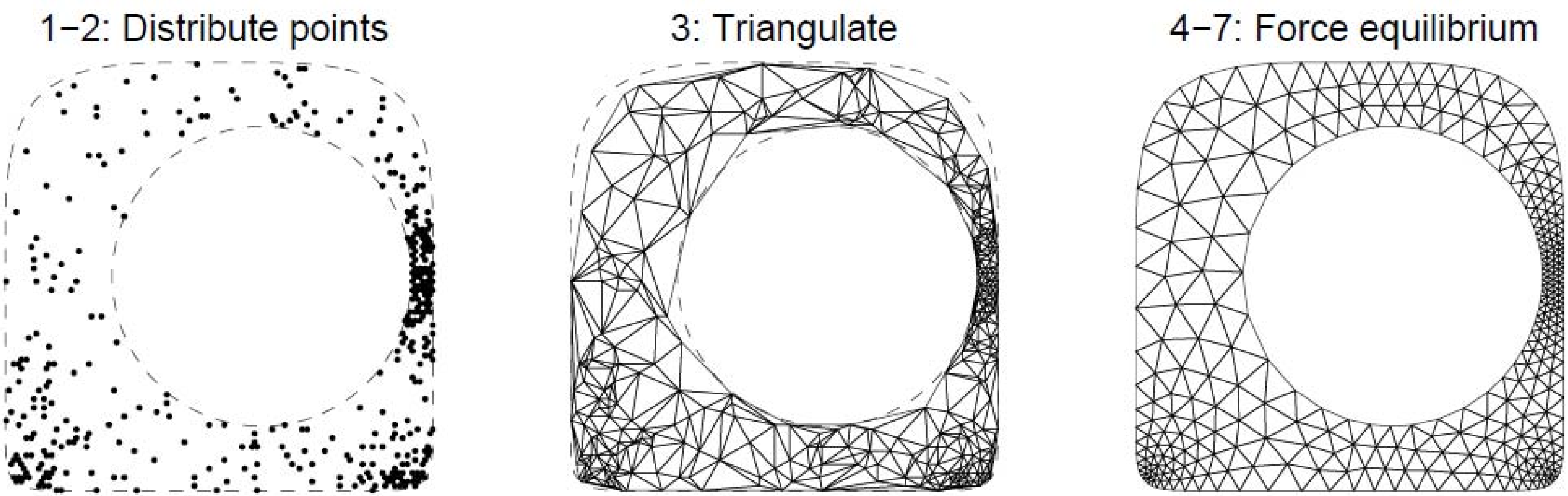


with the simplifying assumption $\Delta x = \Delta y$ this results in:

$$\Phi_{m+1,n} + \Phi_{m-1,n} + \Phi_{m,n+1} + \Phi_{m,n-1} - 4\Phi_{m,n} = 0$$

Mesh generation

In a more general case, mesh (grid) generation is an art of its own.



The mesh elements (here triangles, but more generally tetrahedra or hexahedra) should have a regular shape and approximate the geometry well.

Finite difference method (2)

These point equations can be written in matrix form (large sparse matrix):

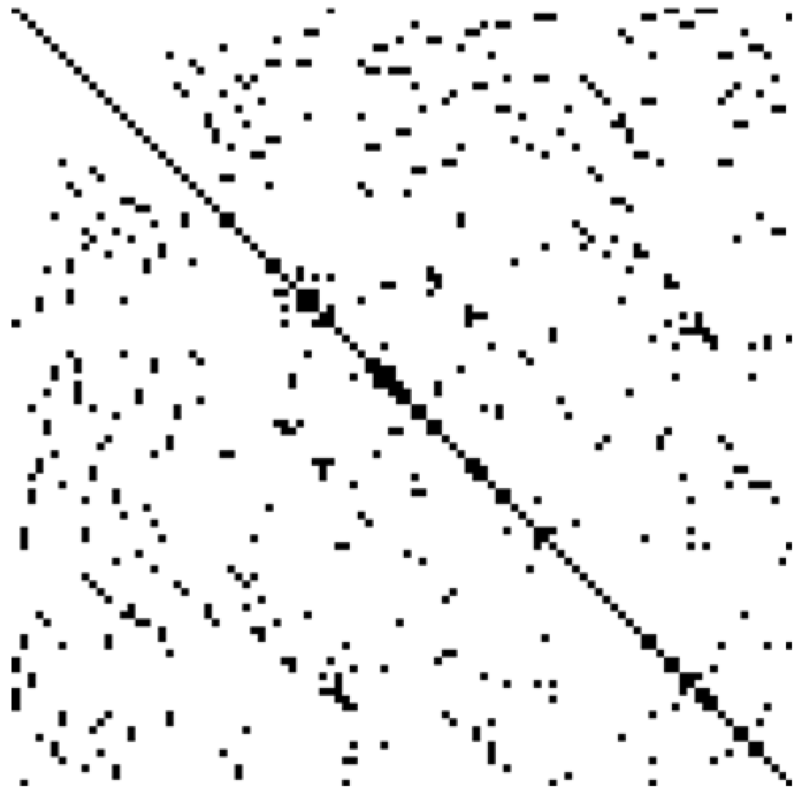
$$
\begin{pmatrix}
\ddots & \ddots & & & & \ddots & & & & & & \\
\ddots & \ddots & \ddots & & & & \ddots & & & & & \\
& \ddots & \ddots & \ddots & & & & \ddots & & & & \\
& & \ddots & \ddots & \ddots & & & & \ddots & & & \\
& & & \ddots & \ddots & \ddots & & & & \ddots & & \\
\ddots & & & & \ddots & \ddots & \ddots & & & & \ddots & \\
& 1 & & & & 1 & -4 & 1 & & & & 1 \\
& & \ddots & & & & \ddots & \ddots & \ddots & & & \\
& & & \ddots & & & & \ddots & \ddots & \ddots & & \\
& & & & \ddots & & & & \ddots & \ddots & \ddots & \\
& & & & & \ddots & & & & \ddots & \ddots & \ddots \\
& & & & & & \ddots & & & & \ddots & \ddots
\end{pmatrix}
\bullet
\begin{pmatrix}
\\
\Phi_{m,n-1} \\
\\
\\
\\
\Phi_{m-1,n} \\
\Phi_{m,n} \\
\Phi_{m+1,n} \\
\\
\\
\\
\Phi_{m,n+1}
\end{pmatrix}
=
\begin{pmatrix}
b \\ o \\ u \\ n \\ d \\ a \\ r \\ y \\ \\ \\ \\ \\
\end{pmatrix}
$$

Sparse matrices

There's a whole branch in computing science dealing with sparse matrices.

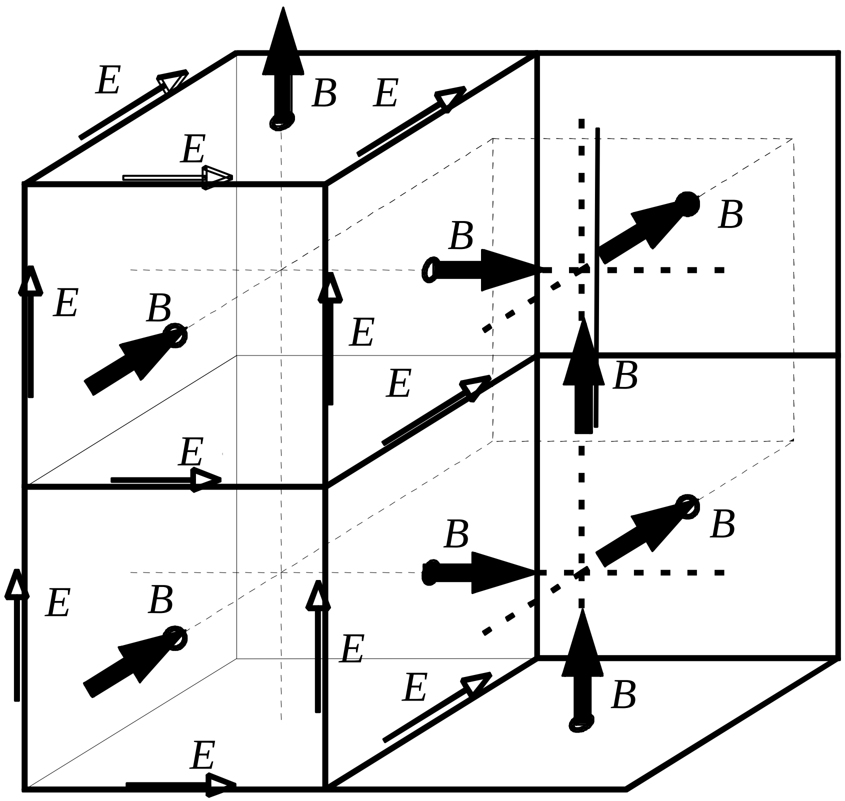
Methods to decompose or invert Sparse matrices:

QR factorization,
LU decomposition
Conjugate gradient method



Incidence plot of non-zero elements of a sparse matrix

FIT algorithm (CST MAFIA, CST Microwave Studio)



- Two interwoven grids
- Take *E, D, J* on grid,
- *B, H* on dual grid.
- In time domain, this is called "leap-frog"

Projection methods

Again you start with your partial differential equation: $D(\varphi) = 0$

for example: $\nabla \times \left(\frac{1}{\mu} \nabla \times \vec{E} \right) - \omega^2 \varepsilon \, \vec{E} = 0$

Assume that the solution has the form $\varphi = \sum_{n=1}^{N} a_n \varphi_n$,

where the φ_n are know basis functions (or trial functions).

Apply the differential operator on this assumed solution:

$$D\left(\sum_{n=1}^{N} a_n \varphi_n \right) = \sum_{n=1}^{N} a_n D(\varphi_n) = r$$

r is the residue.

Projection methods (2)

Now comes the "projection":

With the scalar product: $\langle \varphi, \psi \rangle = \iiint \varphi \, \psi^* \, \mathrm{d}V$

one can now "project" the residue r on the known weight (or test) functions ψ_m :

$$\langle \psi_m, r \rangle = \sum_{n=1}^{N} a_n \, \langle \psi_m, D(\varphi_n) \rangle = 0$$

This is a matrix equation for the coefficients a_n .

Different choices of basis functions/weight functions led to different methods:

if $\psi_m = \varphi_m$ → "Galerkin's method"

if $\langle \varphi, \psi \rangle = \delta_{m,n}$ → "spectral methods" (cf. Fourier series)

localized, simple φ_m → "Finite Element Method"

With localized basis/weight functions, the matrix becomes again sparse.

Specific simulation tools

• Superfish	2-D FDM, TM_{0n} eigenmodes http://laacg1.lanl.gov/laacg/services/services.phtml
• MAFIA (CST)	FIT, modular, versatile, superseded by CST Microwave studio and CST particle studio
• HFSS	FEM on TET's, f-domain, now owned by ANSYS http://www.ansoft.com/products/hf/hfss/
• GdfidL	Started of as "small MAFIA", improved, parallel http://www.gdfidl.de
• CST Microwave Studio, Particle Studio	FDTD, "perfect" boundary
• SuperLANS	"FEM version of Superfish"
• Concerto	(by Vectorfields), FDTD, suited? http://www.vectorfields.co.uk/
• ACE3P (Ω-3P, T-3P, Track-3P,...)	developed at SLAC, very powerful, parallel http://www.slac.stanford.edu/grp/acd/ace3p.html
• ANSYS Multiphysics	FEM, possibility to combine with thermal and stress analyses. http://www.ansys.com/products/multiphysics/default.asp

Simulation code errors

- Meshing: the simulated problem is not the real problem.
- Discretization of space
- Near boundaries: risk of systematic errors!
- The matrices to be inverted are very large: Conditioning!
- Rounding errors.

Comparing the codes – a simple benchmark

I took a simple spherical cavity, since the exact ***analytical solution*** is known.
Here how I calculate it with Mathematica:

Untitled-1 *

```
In[7]:= c0 = 299 792 458; MHz = 10^6; χ = x /. FindRoot[Evaluate[D[Sqrt[π x/2] BesselJ[3/2, x], x] == 0], {x, 2.7}];

In[8]:= ω = χ c0/a; f = ω/(2 π);

In[3]:= ψ[ρ_, θ_] := Sqrt[π k ρ/2] BesselJ[3/2, k ρ] Cos[θ]

In[4]:= Hφ[ρ_, θ_] := -1/ρ ∂θ ψ[ρ, θ]; Simplify[Hφ[ρ, θ]];

In[9]:= P = Sqrt[ω μ/(2 σ)] (-Cos[ka] + Sin[ka]/ka)^2 /. ka → χ; W = μ a/ka ∫_0^ka (Sin[kρ]/kρ - Cos[kρ])^2 dkρ /. ka → χ;
        Q = ω W/P;

In[6]:= {f/MHz, Q} /. {μ → 4 π 10^-7, σ → 5.8 10^7, a → .5}

Out[6]= {261.823, 89 899.1}
```

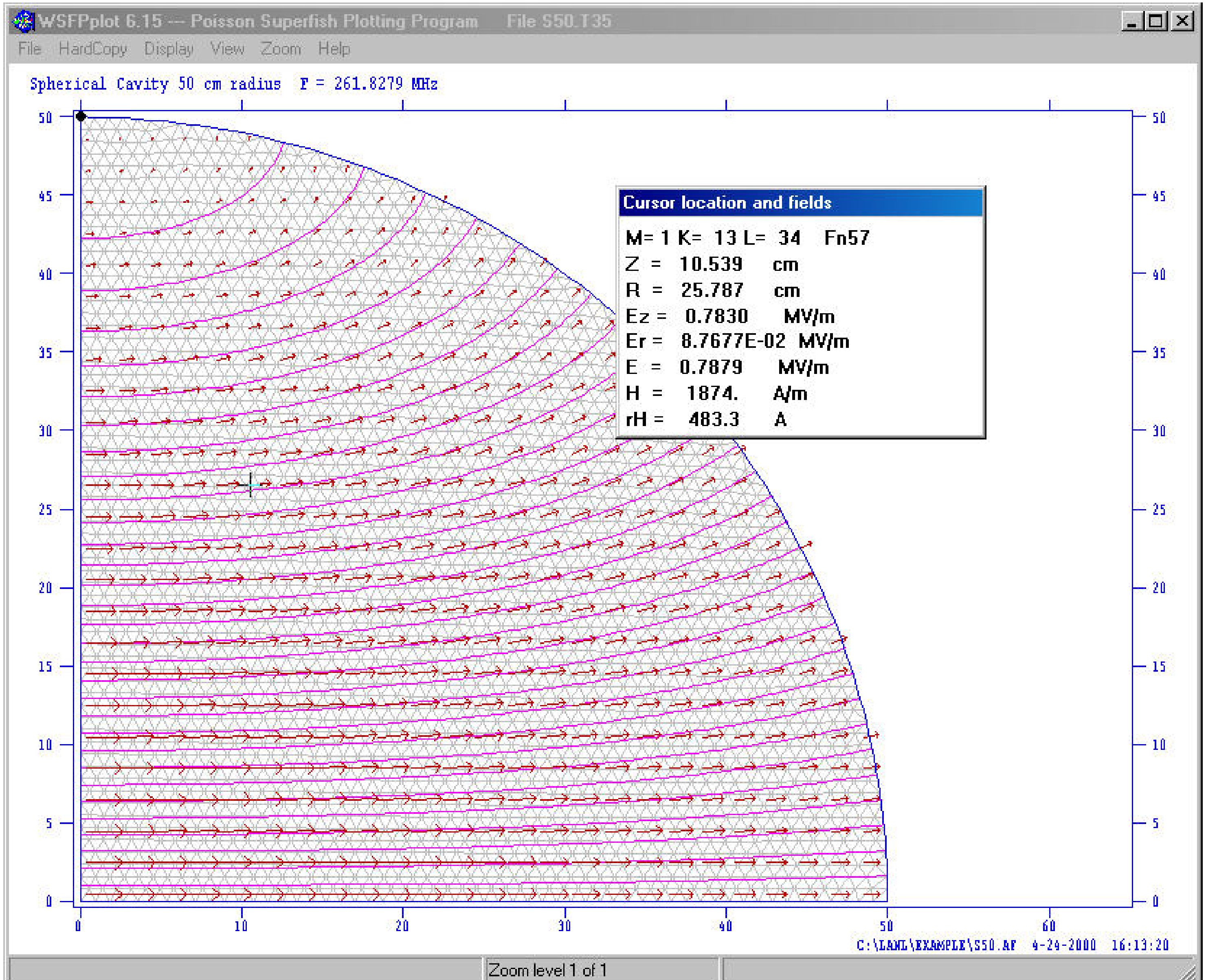
150%

Cu conductivity: 58 MS/m

radius 50 cm

f: 261.823 MHz, *Q*: 89,899.1

Sphere benchmark: Superfish



Superfish output:

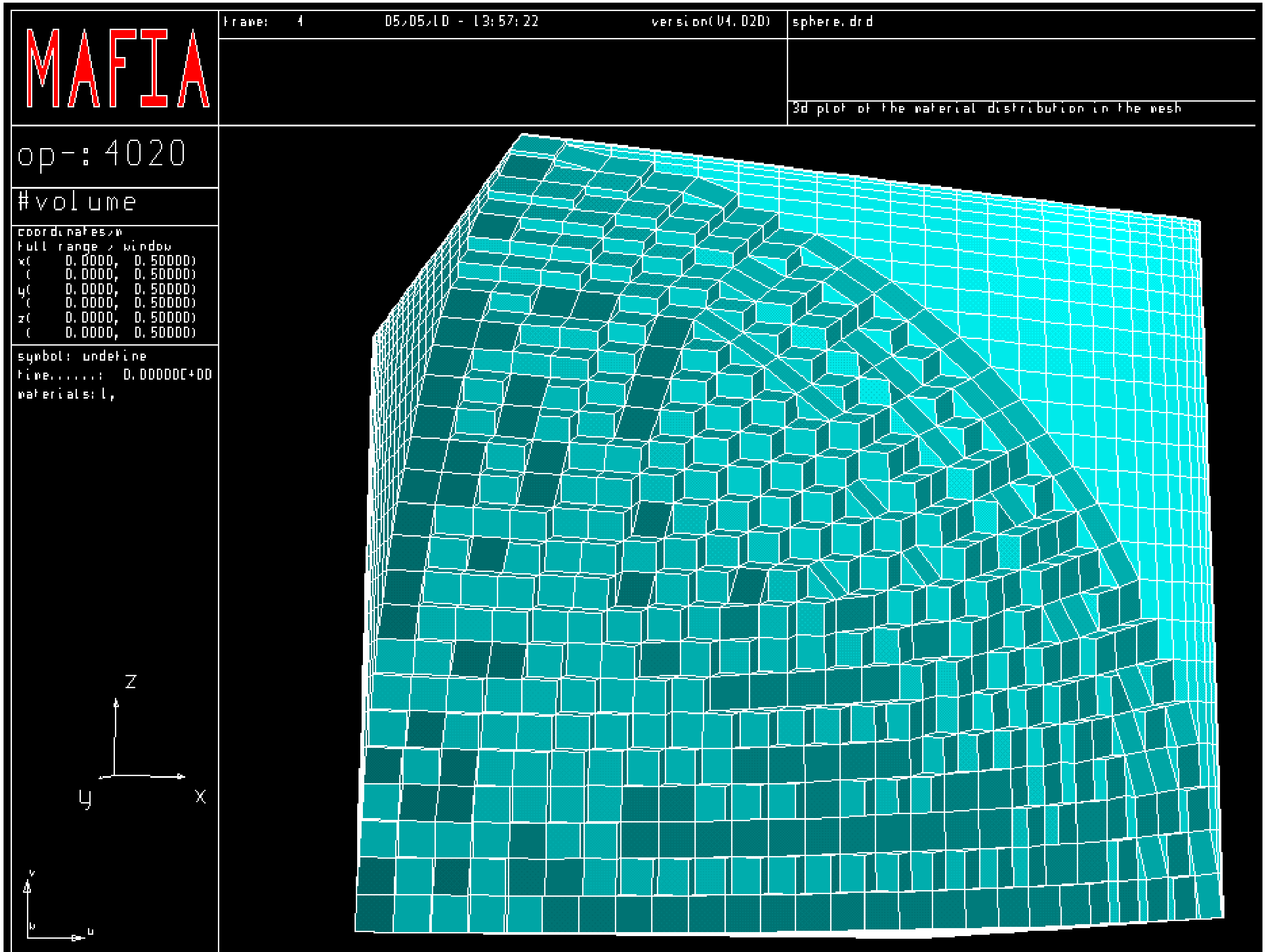
```
Superfish output summary for problem description:
Spherical Cavity
Uses NT=5 option to draw arc of specified radius
[Originally appeared in 1987 Reference Manual C.12.1]
Problem file: C:\LANL\EXAMPLES\RADIOFREQUENCY\SPHERICALCAVITY\SPHERE.AF  6-06-2010
15:12:02
-------------------------------------------------------------------------------
All calculated values below refer to the mesh geometry only.
Field normalization (NORM = 0):     EZERO =      1.00000 MV/m
Frequency                                 =    261.82697 MHz
Particle rest mass energy                 =   938.272029 MeV
Beta =  0.8733608          Kinetic energy =      988.072 MeV
Normalization factor for E0 =  1.000 MV/m =     7389.860
Transit-time factor                       =    0.1572027
Stored energy                             =    0.4646490 Joules
Using standard room-temperature copper.
Surface resistance                        =      4.22151 milliOhm
Normal-conductor resistivity              =      1.72410 microOhm-cm
Operating temperature                     =      20.0000 C
Power dissipation                         =    8504.5782 W
Q    =   89880.7          Shunt impedance =       58.792 MOhm/m
Rs*Q =   379.433 Ohm                Z*T*T =        1.453 MOhm/m
r/Q  =     8.082 Ohm  Wake loss parameter =      0.00332 V/pC
Average magnetic field on the outer wall  =      1957.35 A/m, 808.673 mW/cm^2
Maximum H (at Z,R = 0.779989,49.9939)     =      1961.31 A/m, 811.952 mW/cm^2
Maximum E (at Z,R = 50,0.0)               =     0.542516 MV/m, 0.033147 Kilp.
Ratio of peak fields Bmax/Emax            =       4.5430 mT/(MV/m)
Peak-to-average ratio Emax/E0             =       0.5425
```

MAFIA

- Used to be most widely used in accelerator community
- FD method with FIT algorithm
- Eigenmode and time domain.
- Cartesian mesh, problematic near round boundaries and non-orthogonal geometries.
- For special cases also rz and rφz-coordinates.
- Modular: O, M, S, H3, E, W3, T2, T3, TL3, TS2, TS3, P

  (the modules needed for RF design are underlined)
- To our knowledge, the only program today which can include particle dynamics (selfconsistent PIC)
- Evaluated from well known URMEL, TBCI.
- GUI & Macros (first use GUI, then start from logged macro)
- Runs on unix and derivates
- I do not recommend the use for future developments!

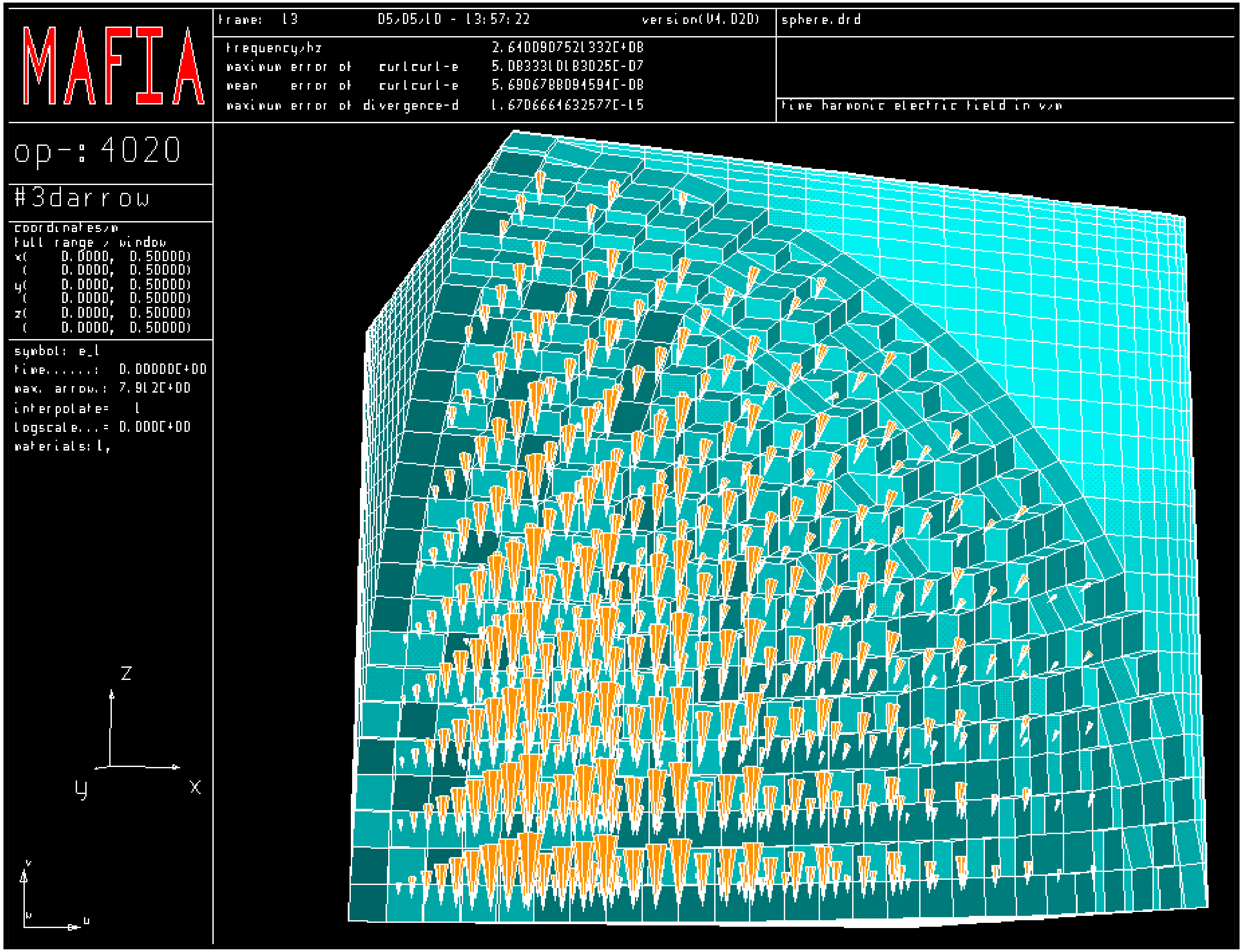
Spherical resonator in MAFIA



How MAFIA meshes the spherical resonator

curved boundaries are problematic!

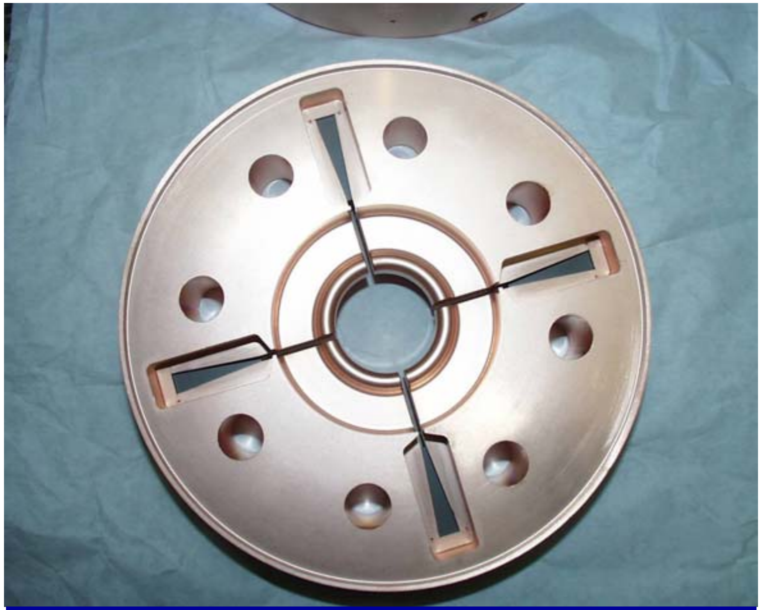
Spherical resonator in MAFIA (2)



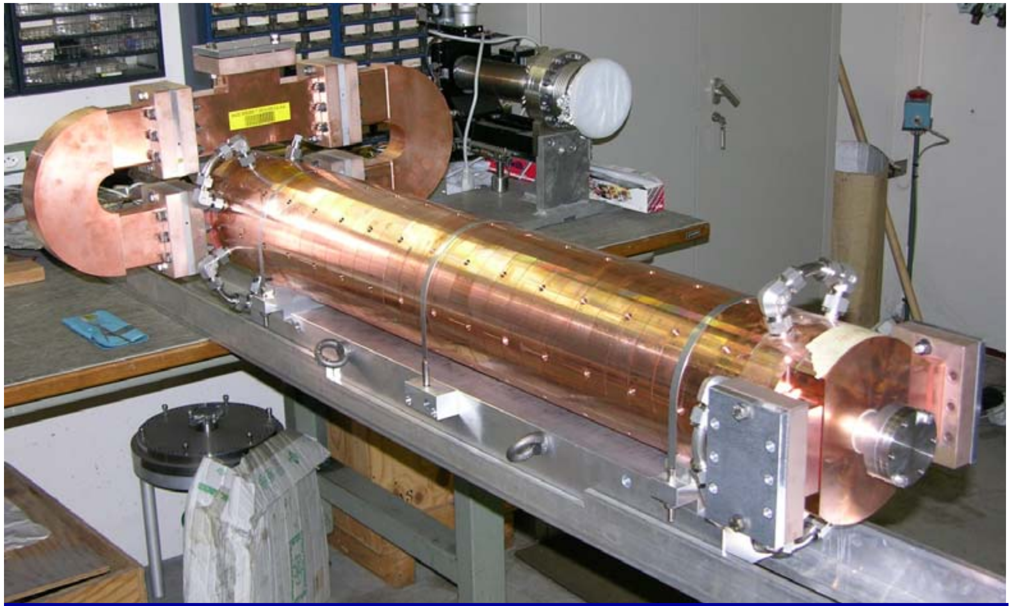
Time harmonic electric field, first mode of the above example.

MAFIA: transverse wakefield calculation (1/4)

The example: the CTF3, 3 GHz drive beam accelerating structures which need strong damping of the transverse wakefield.

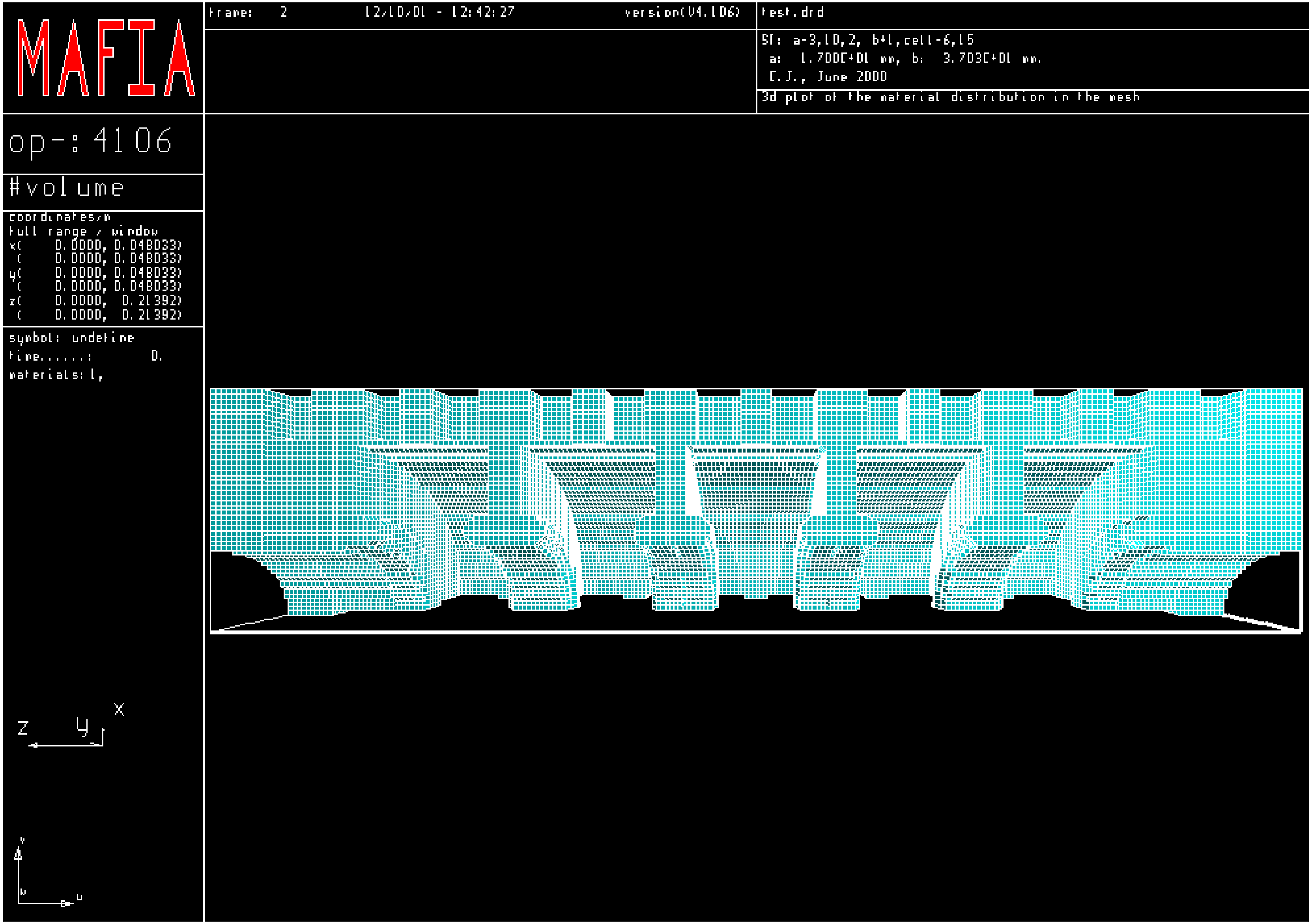


SICA: Slotted Iris – Constant Aperture. Photograph of one cell



18 of these are used in CTF3 to accelerate the Drive Beam.

MAFIA: transverse wakefield calculation (2/4)

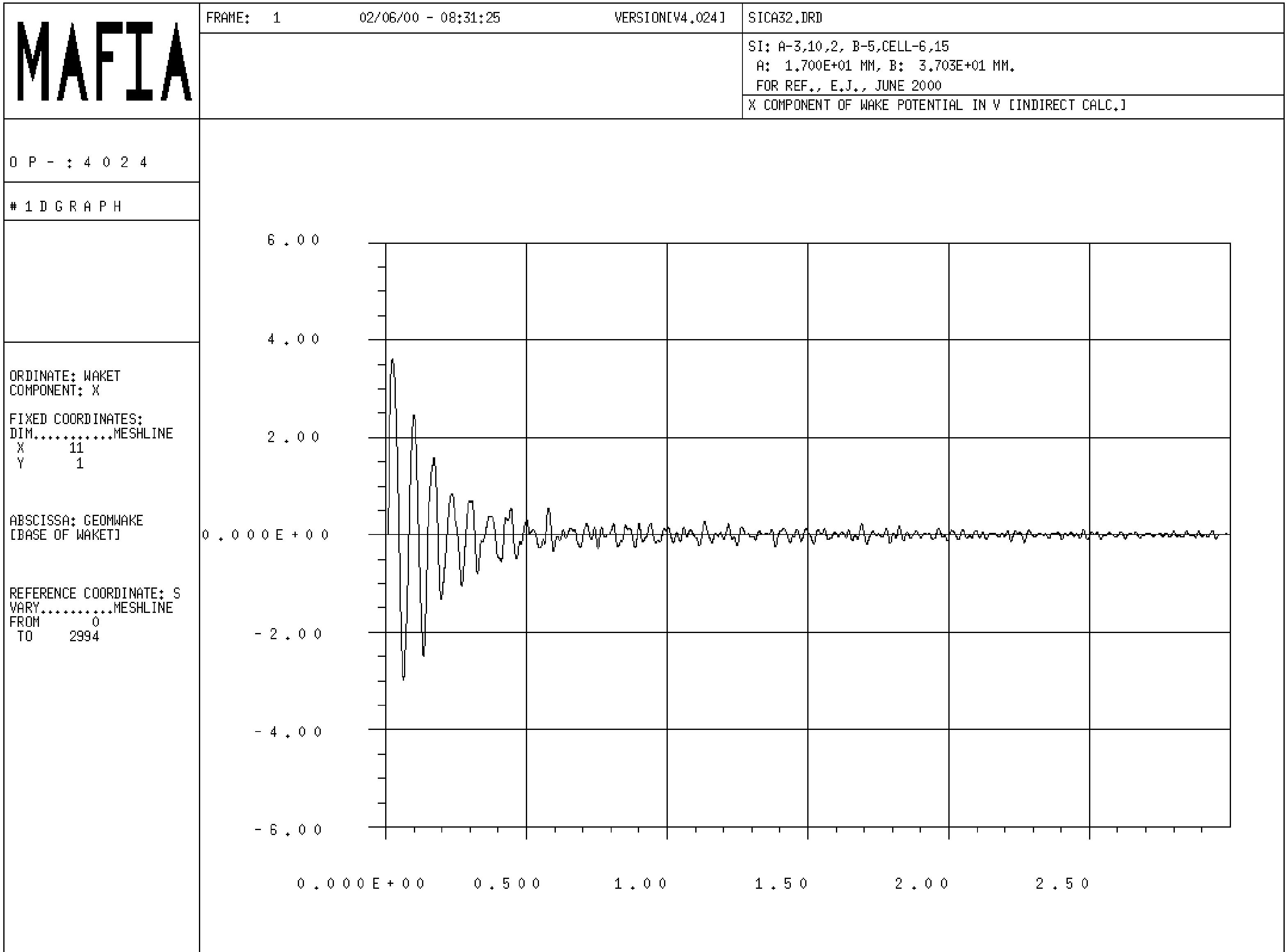


MAFIA: transverse wakefield calculation (3/4)

```
#ot3
def sigma 2.5e-3
def xoff 10e-3
def shi 3.
#cont delcalc
#mate mat 0 ty nor mat 1 ty el
#bound xb ele wav
       yb mag wav
       zb wav wav
#time tstep "@real02*.7" tend "(totl+5*sigma)/@c0"
def fg="(fband/2.0)/sqrt(log(1000))"
def tpuls="sqrt(log(1000))*2/@pi/fg"
#waveg mode 1 power 0 signal user p1 fcent p2 fg
       p3 "tpuls/2" p4 "@pi/2" func pulse freq fcent
       low "fcent-fband/2.0" upp "fcent+fband/2.0"
       reflec 1e-4
for icav=1,ncav1
  def pname "portname(2*icav-1)"
  makesymb chs pname 1
  cha chs port pname mode 1 where xmax power 0 ex
  def pname "portname(2*icav)"
  makesymb chs pname 1
  cha chs port pname mode 1 where ymax power 0 ex
endfor
#beam beamd z xpo xoff ypo 0. beta=1.0
  bun gaussian charge 1e-12 sigma sigma isig 5
#time nend "@integer03+@integer05" mt 4
#mon type wake symb waket comp x wind signal
xpo xoff ypo 0 islo 0 isst 1 shi shi ex
#time nend @integer00
#cont delcalc usebuf y window beam dumps no
ex
```

Excerpt of MAFIA Macro language – T3 module, calculation of transverse wake

MAFIA: transverse wakefield calculation (4/4)



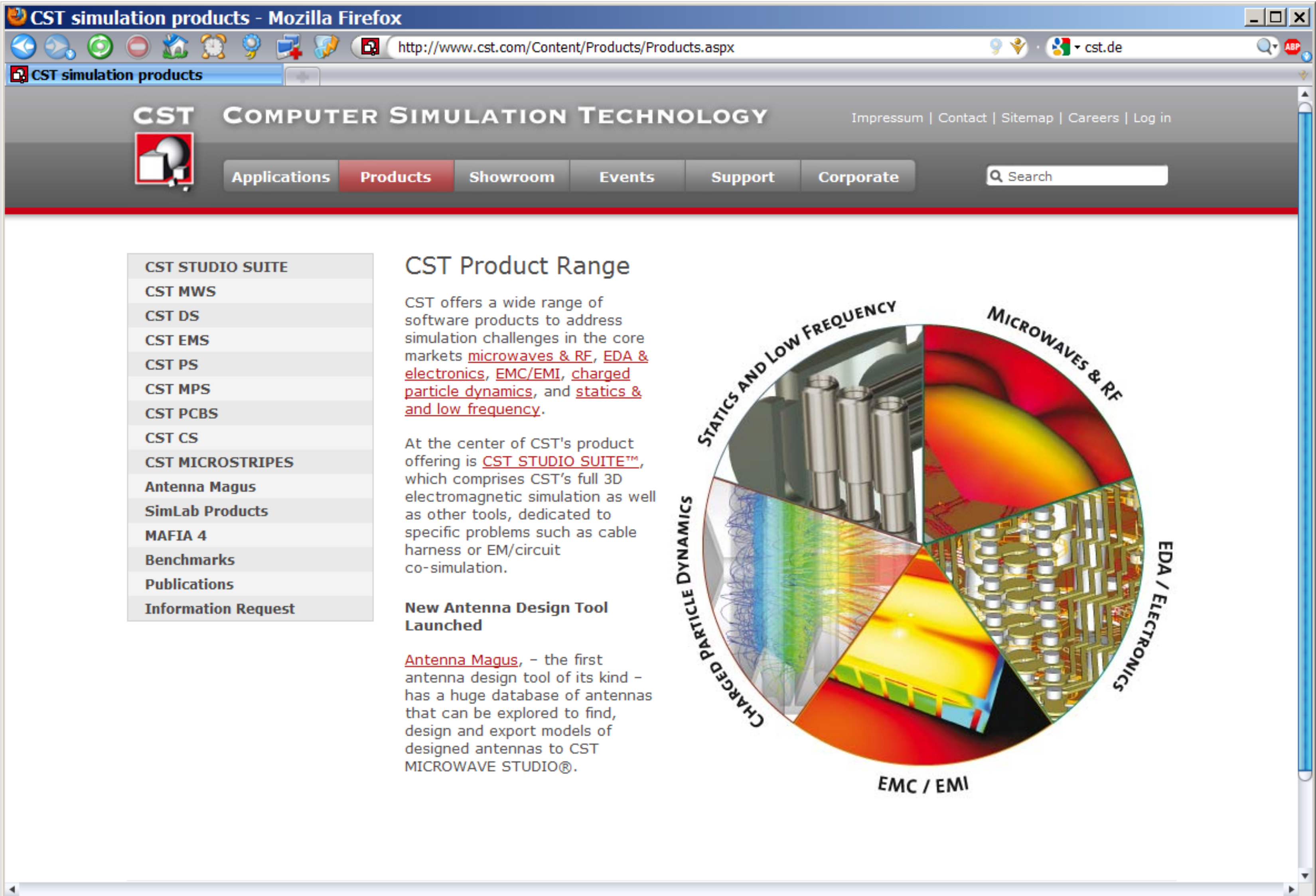
GdfidL

- Started off as a “small MAFIA”, but has much improved features.
- FDTD method with FIT algorithm
- Eigenmode and time domain
- Cartesian mesh, but allows diagonal fillings.
- Macro language similar to MAFIA
- Allows absorbing boundaries (PML) and periodic boundaries
- http://www.gdfidl.de
- Runs on Unix and Linux
- Strong point: a parallel version exists, which allows to solve very large problems.
- It is heavily used at CERN for CLIC structure design and for calculation of spurious impedances.

CST Studio Suite

- Consists of Microwave Studio and Particle Studio
- "Successor" of MAFIA
- FDTD with FIT algorithm, cartesian mesh, but with much improved PBA (perfect boundary approximation)
- Eigenmode and time domain (transient solver).
- Allows radiation bundary for antenna problems
- Uses Visual basic as Macro language
- http://www.cst.com
- Actual version: CST Studio Suite 2010
- runs on Windows

CST


CST simulation products - Mozilla Firefox
http://www.cst.com/Content/Products/Products.aspx
cst.de
CST simulation products
CST
COMPUTER SIMULATION TECHNOLOGY
Impressum | Contact | Sitemap | Careers | Log in
Applications
Products
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Events
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CST STUDIO SUITE
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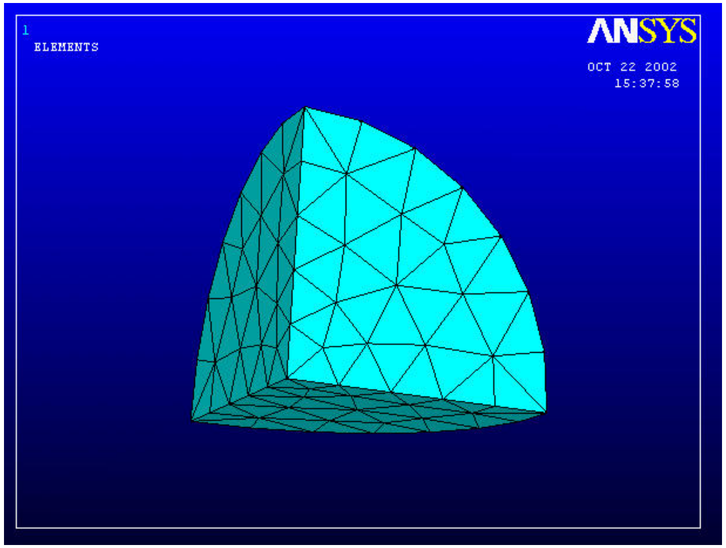
CST Product Range
CST offers a wide range of software products to address simulation challenges in the core markets microwaves & RF, EDA & electronics, EMC/EMI, charged particle dynamics, and statics & and low frequency.
At the center of CST's product offering is CST STUDIO SUITE™, which comprises CST's full 3D electromagnetic simulation as well as other tools, dedicated to specific problems such as cable harness or EM/circuit co-simulation.
New Antenna Design Tool Launched
Antenna Magus, – the first antenna design tool of its kind – has a huge database of antennas that can be explored to find, design and export models of designed antennas to CST MICROWAVE STUDIO®.
STATICS AND LOW FREQUENCY
MICROWAVES & RF
EDA / ELECTRONICS
EMC / EMI
CHARGED PARTICLE DYNAMICS

ANSYS Multiphysics – Electromagnetics

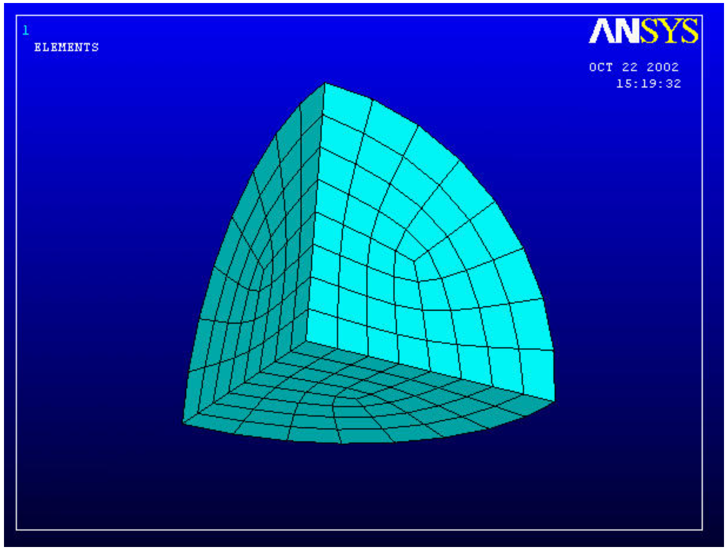
- 3-D, tetrahedra or hexahedra, excellent mesher
- FEM, 1st and 2nd order interpolation
- Eigenmodes lossless + perturbation
- *f*-domain driven solutions, ports not well integrated.
- Macro language exists
- Strong point: Allows to integrate structural, fluid, thermal and electromagnetic simulations.
- No periodic boundary conditions.
- No direct control of obtained precision.
- http://www.ansys.com/products/multiphysics/default.asp
- Actual version 12
- runs on Windows and Unix.

Sphere benchmark: ANSYS

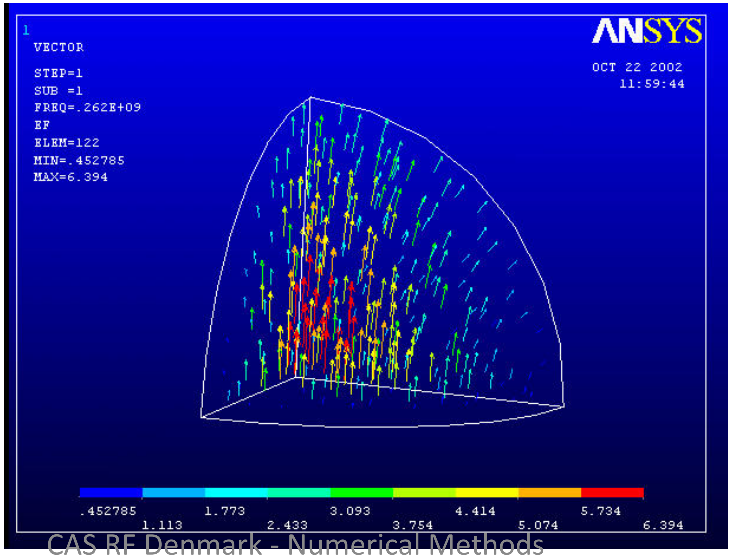
tetrahedra



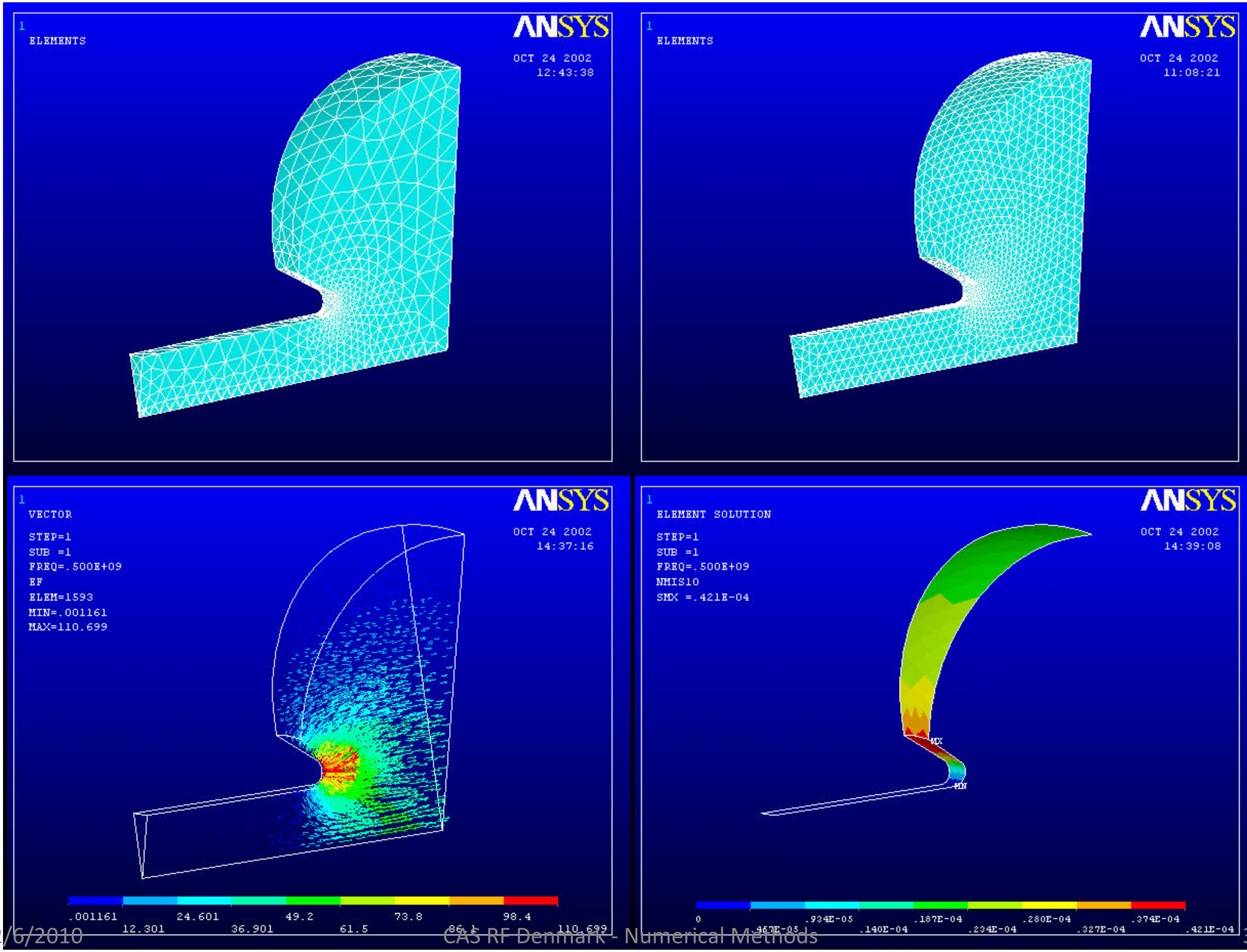
hexahedra



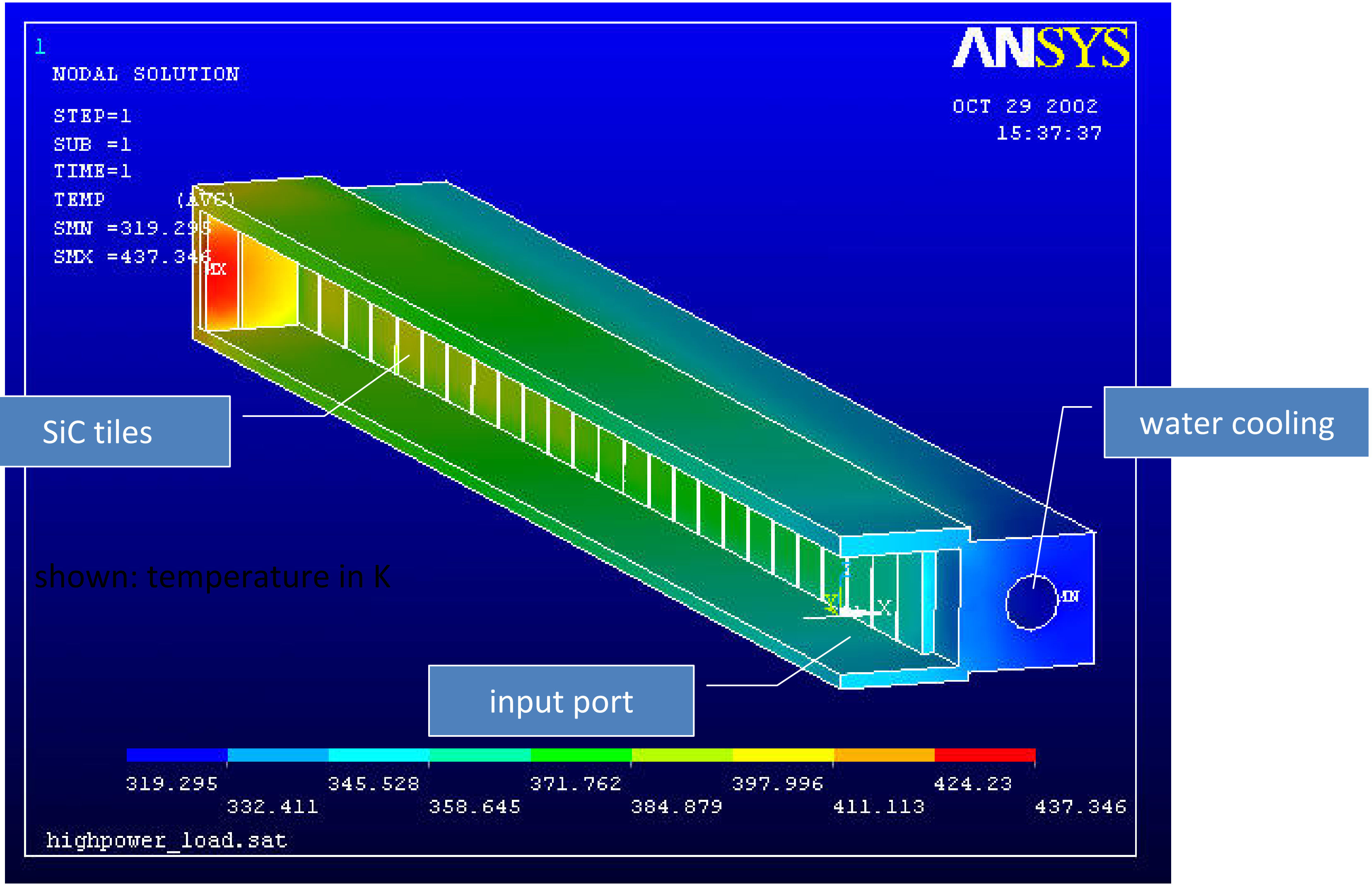
E-field vector display



ANSYS example: KEK photon factory cavity



Example suiting ANSYS: High power load



shown: temperature in K

ANSYS calculations by M. Eklund

HFSS


RF Design - Mozilla Firefox
http://www.ansoft.com/rf_design.cfm
cst.de
CST simulation products
RF Design
PRODUCTS INDUSTRIES SUPPORT ANSYS
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Our RF design software helps engineers design, simulate, and validate the behavior of complex high-performance RF, microwave, and millimeter-wave devices in next generation wireless communication and defense systems. Designers of high-frequency components, circuits, and systems must adopt a new generation of design strategies and tools to meet demanding specifications for performance and reliability while optimizing size, weight, power and cost.
Ansoft technology delivers transistor-level detail for complex, highly nonlinear circuits and 3D full-wave accuracy for components to enable modern RF/mW design. By leveraging advanced electromagnetic-field simulators dynamically linked to powerful harmonic-balance and transient circuit simulation, Ansoft software breaks the cycle of repeated design iterations and lengthy physical prototyping. With Ansoft, engineering teams consistently achieve best-in-class design in a broad range of applications including antennas, phased arrays, passive RF/mW components, integrated multi-chip modules, advanced packaging, and RF PCBs.
View the Design Flow
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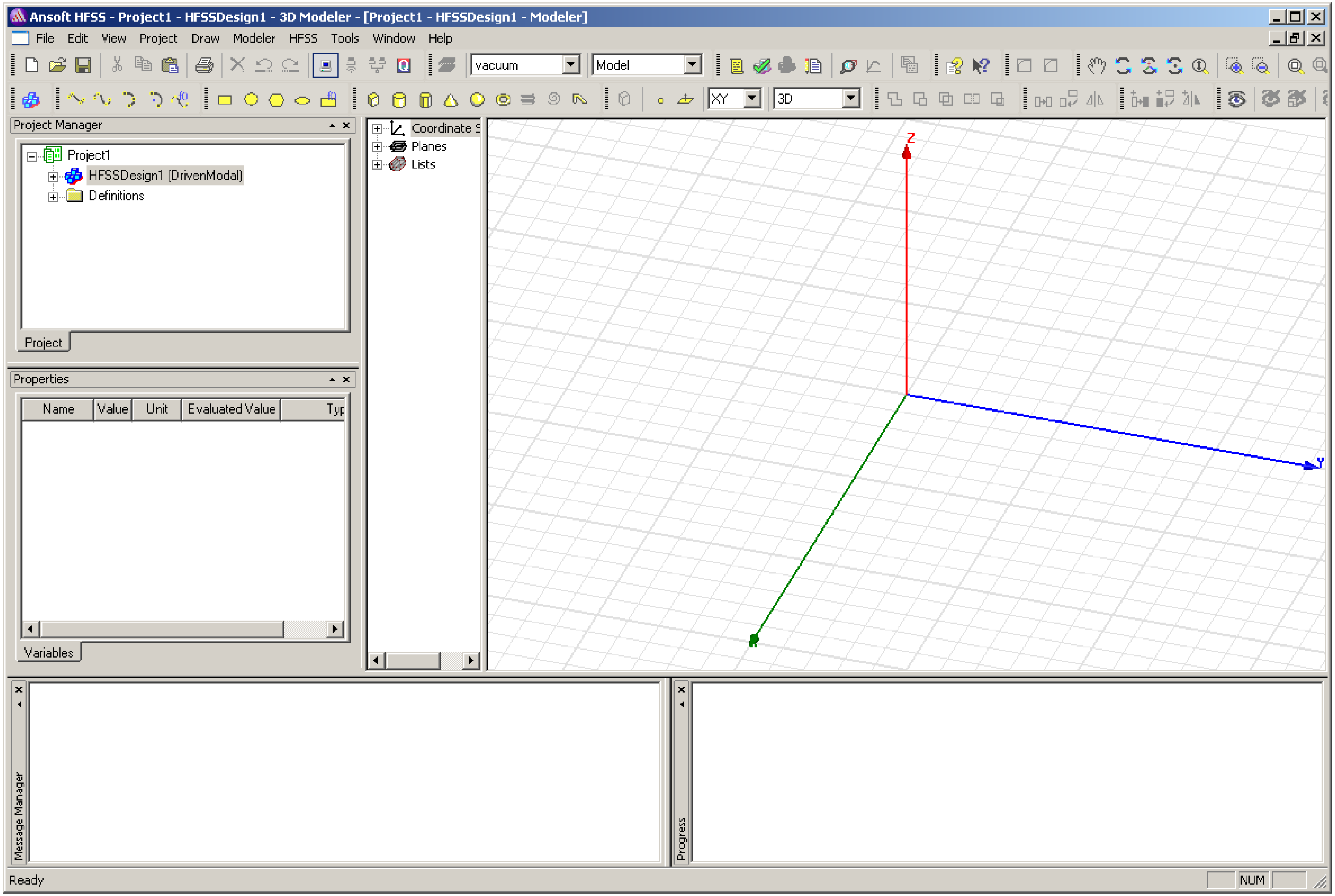
Designer RF
RF and Microwave Product Suite
Nexxim®
Transient and Harmonic-balance circuit simulation
ELECTROMAGNETICS
HFSS™
3D full-wave solver
Full-Wave SPICE™
High-frequency SPICE Models
Q3D Extractor®
3D quasi-static solver
AUTOMATION
Optimetrics™
Parametric optimization
Distributed Solve
Distributed parametric computation
AnsoftLinks™
WHITE PAPERS
Multiphysics Simulation of Satellite Dish
RFID Radio Circuit Design in CMOS
60 GHz Transceiver IC Design Using High-Mobility .15-micron GaAs Process - Taiyo Yuden
RFIC Design White Paper - 0.13um RF CMOS Solution
RECENT MATERIAL
AMI Design Kit for IBM HSS15 Core Technology
HFSS 12.0 Tips and Techniques for HFSS project setup and solve
Introducing HFSS Version 12
Maxwell and HFSS Coupling to ANSYS 12.0
RF Power Amplifier Design Using Coupled Circuit, EM, and Thermal
POPULAR MATERIAL
Microwave Simulation, Macro Benefits
AMI Design Kit for IBM HSS15 Core

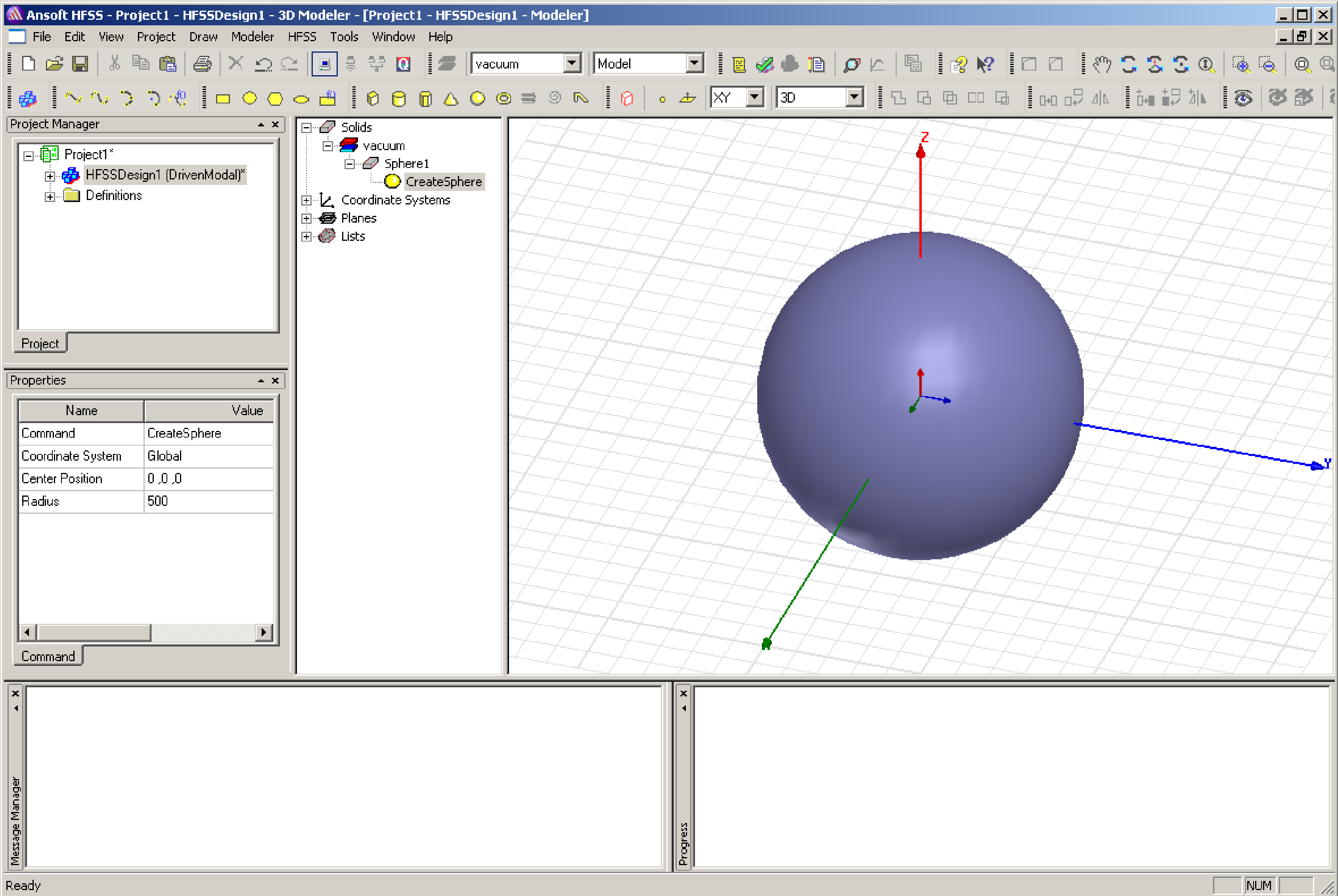
HFSS

- 3-D, tetrahedra, mesher with “lambda refinement”
- FEM, 1st and 2nd order interpolation, curved surfaces
- Eigenmodes lossless + lossy (complex solver)
- *f*-domain driven solutions.
- Good GUI
- Macro language is Visual Basic
- Allows periodic boundary conditions
- Allows also radiation boundary and PML
- Good control of obtained precision (adaptive refinement).
- http://www.ansoft.com/products/hf/hfss/index.cfm
- Actual version 12
- Runs on Windows and Linux
- Since 2009, Ansoft belongs to ANSYS

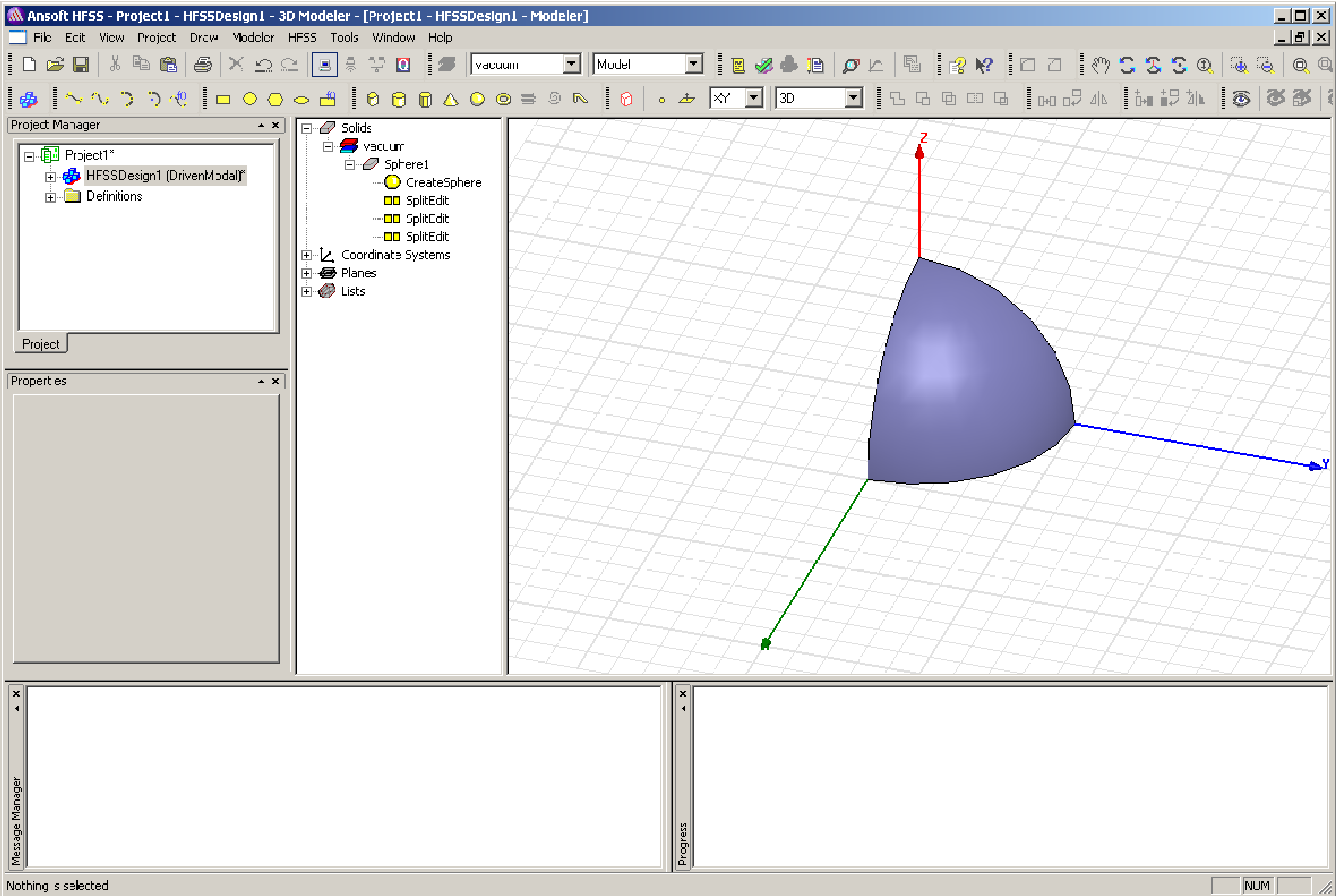
HFSS Sphere (1/9)



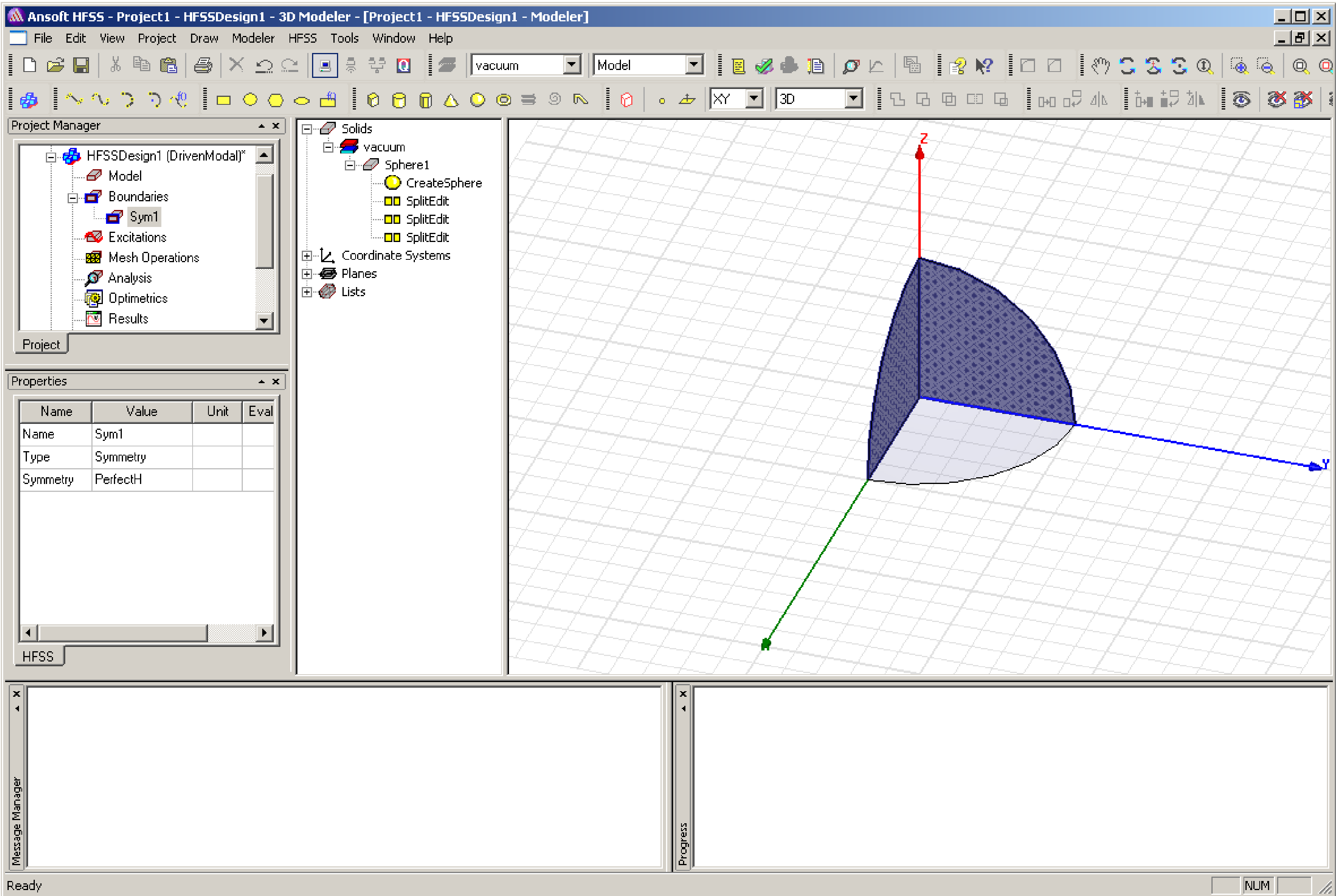
HFSS Sphere (2/9)



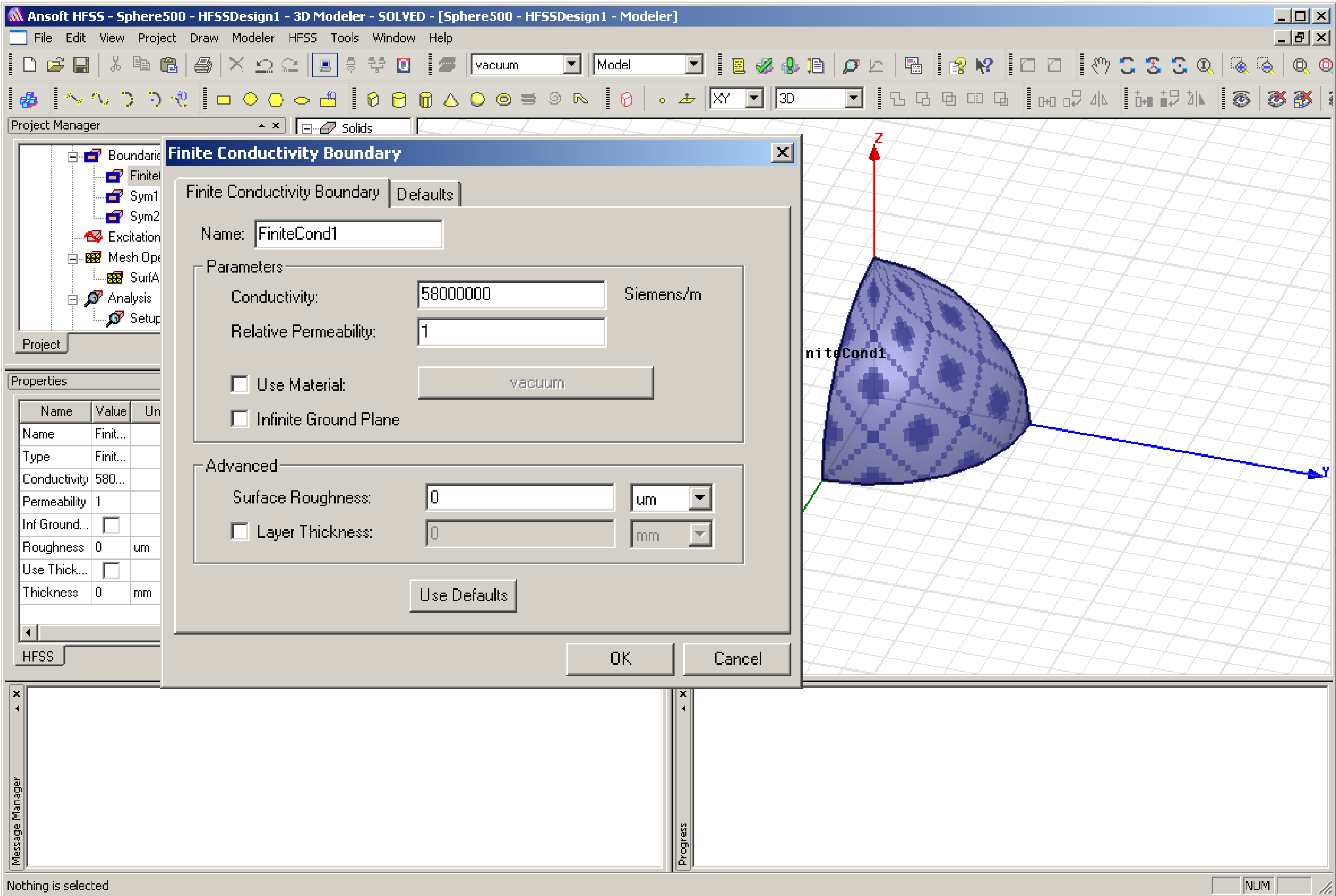
HFSS Sphere (3/9)



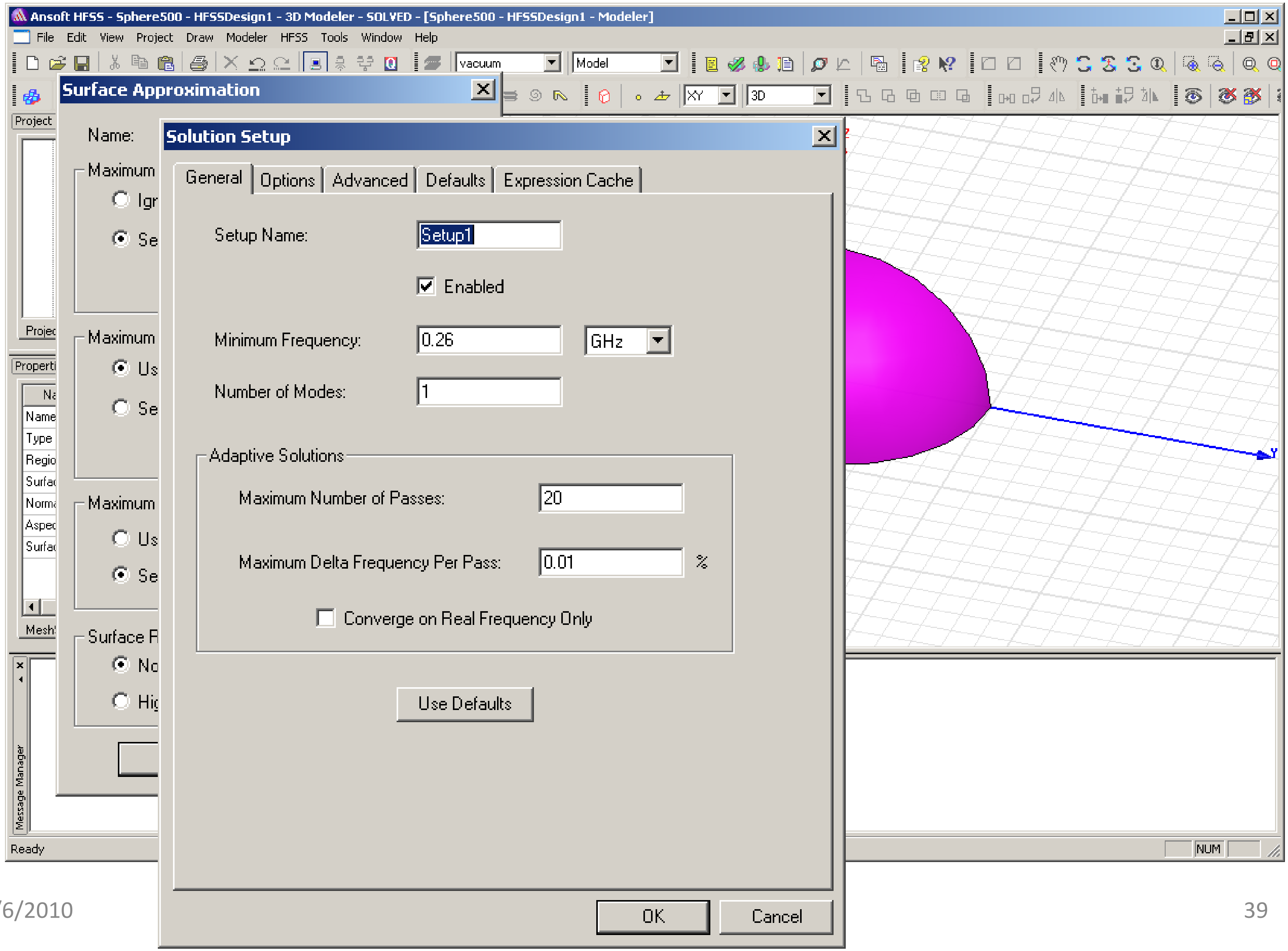
HFSS Sphere (4/9)



HFSS Sphere (5/9)

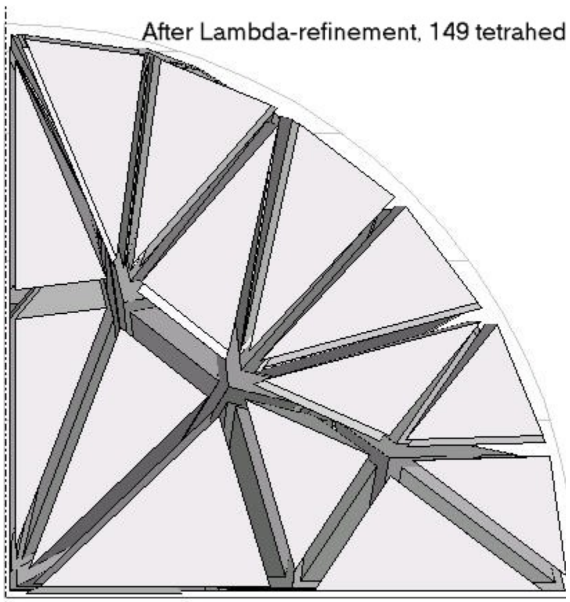


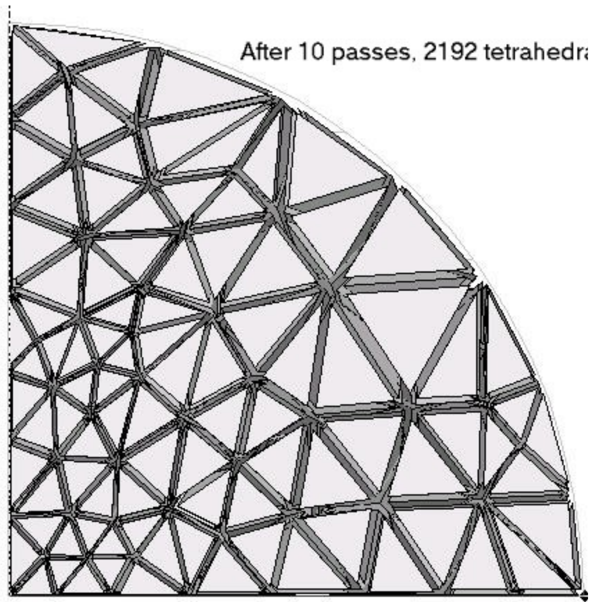
HFSS Sphere (6/9)

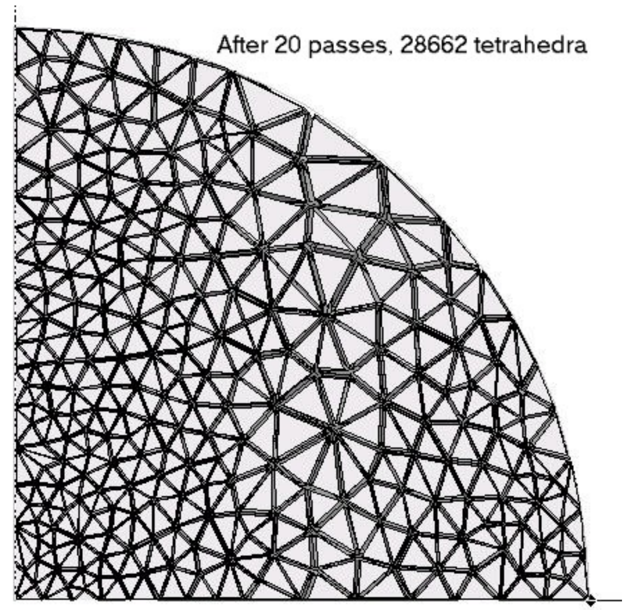


HFSS Sphere (7/9)

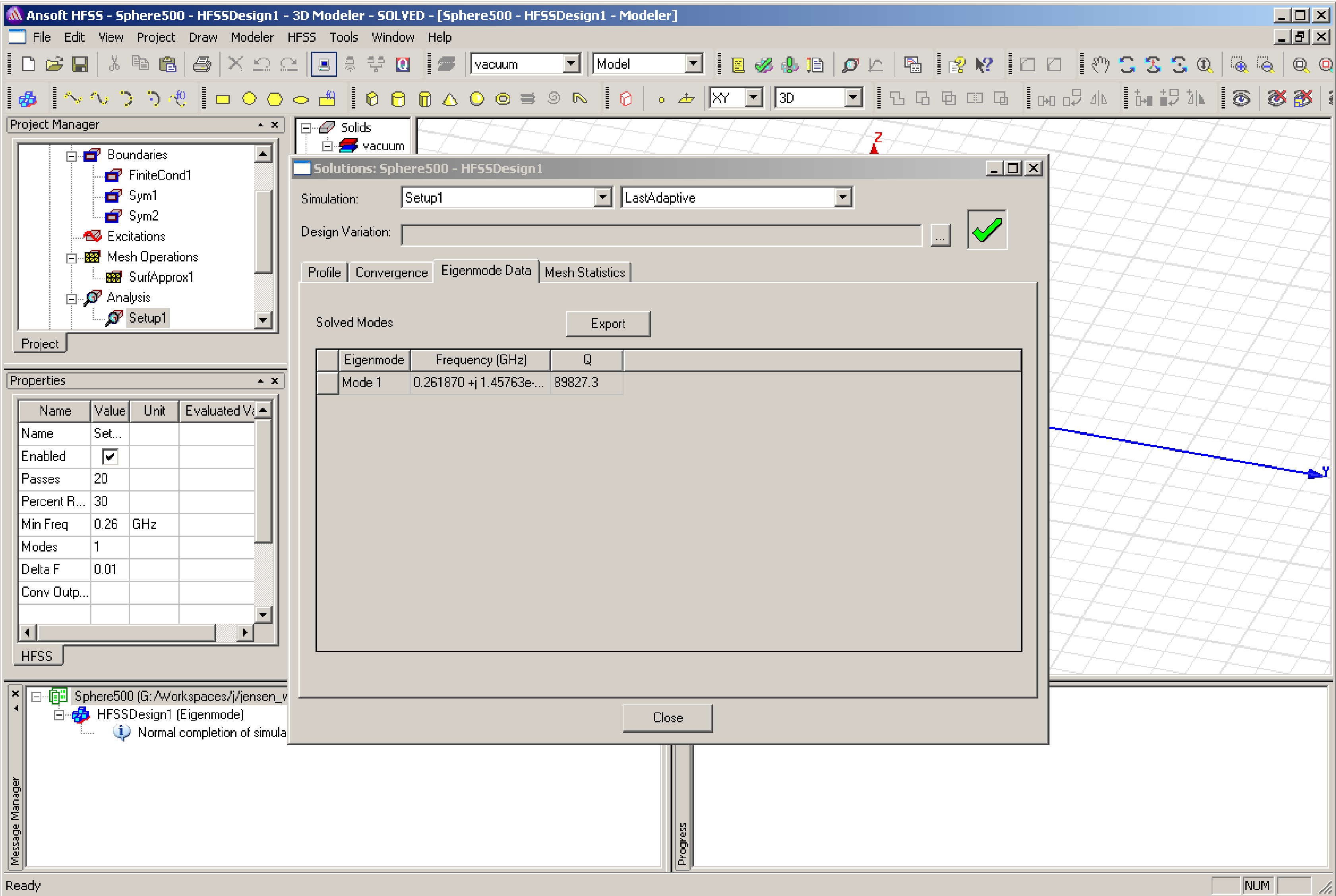
Mesh refinement



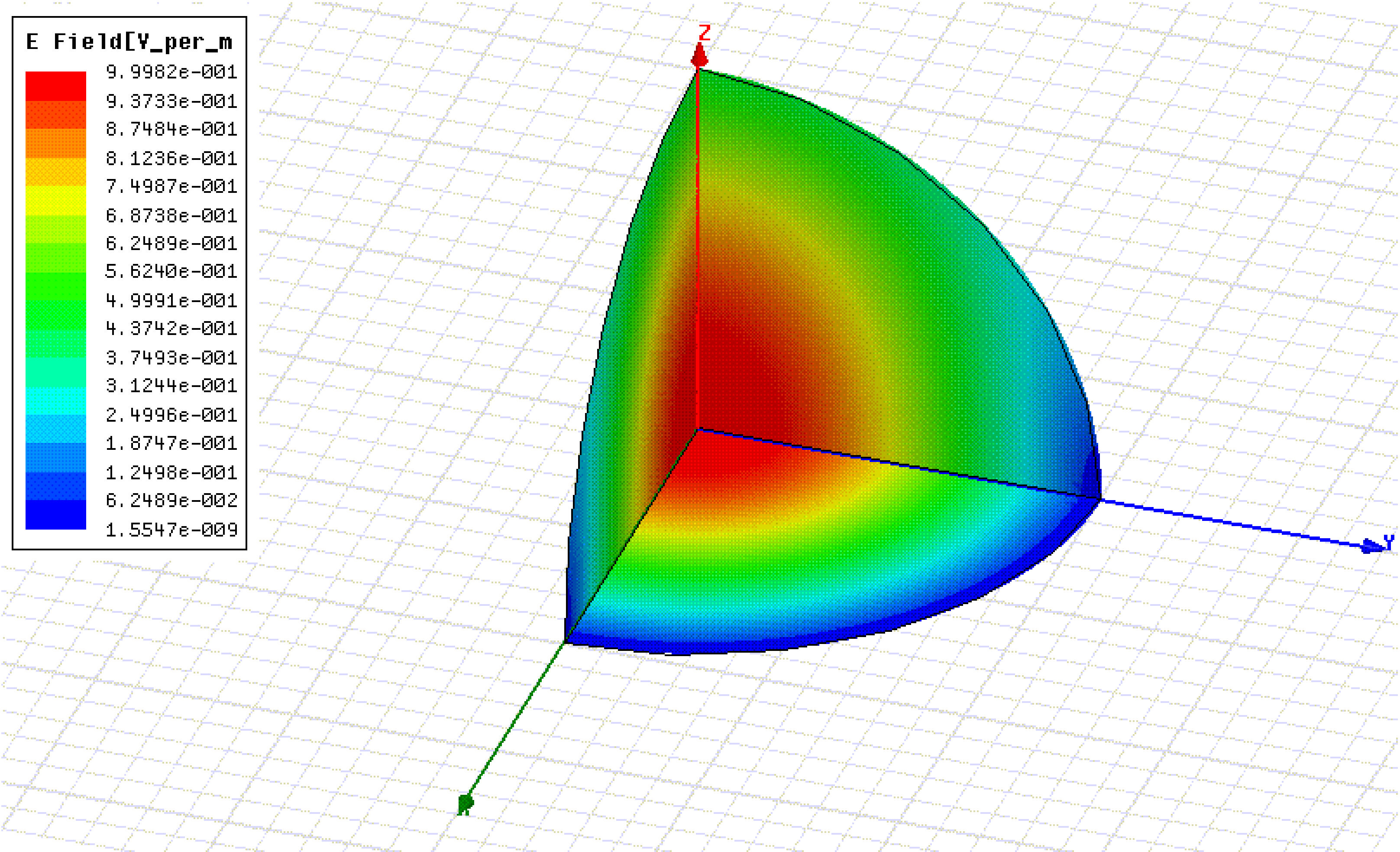




HFSS Sphere (8/9)



HFSS Sphere (9/9)

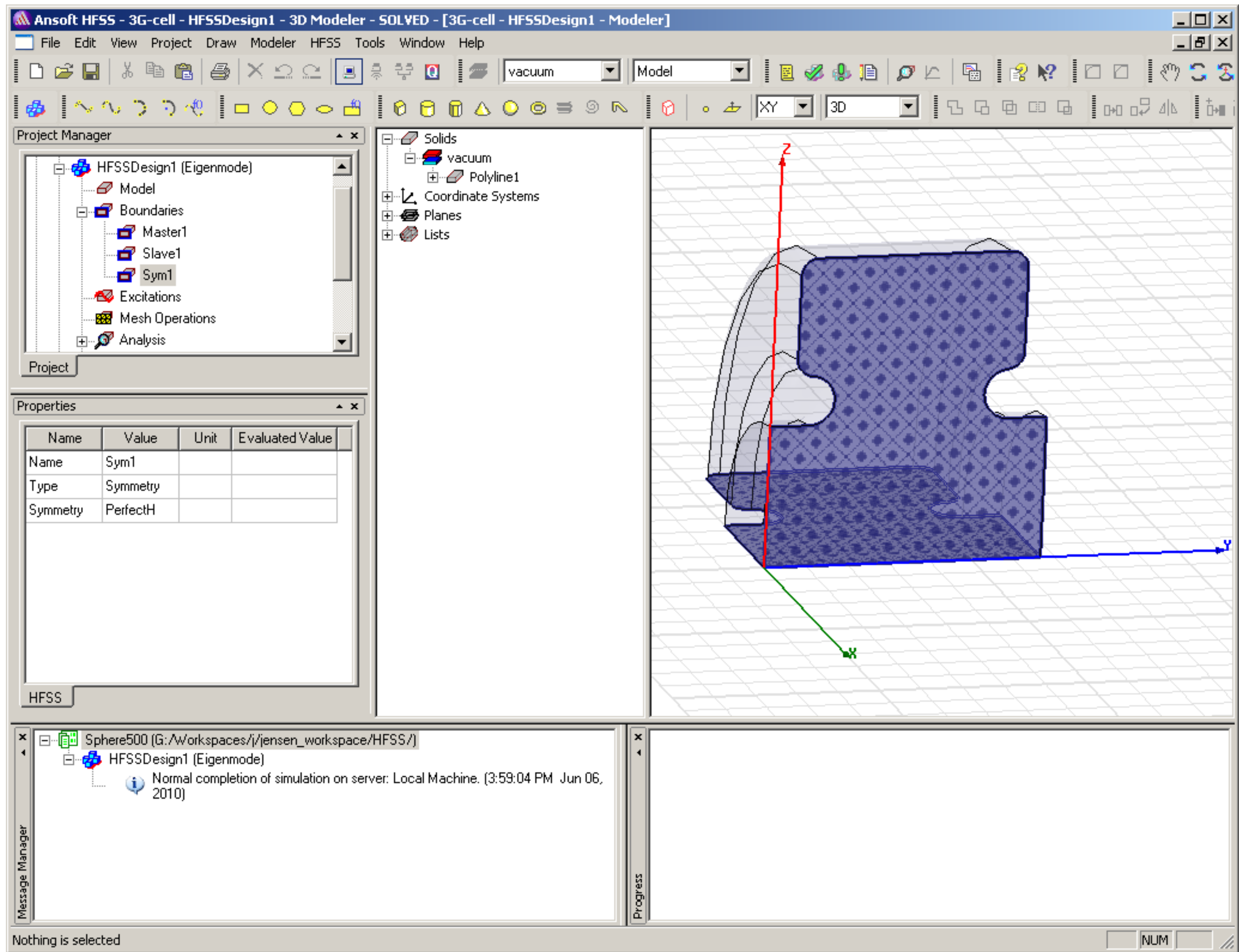


HFSS example: periodic structure (1/5)

In HFSS, select Solution Type “Eigenmode”

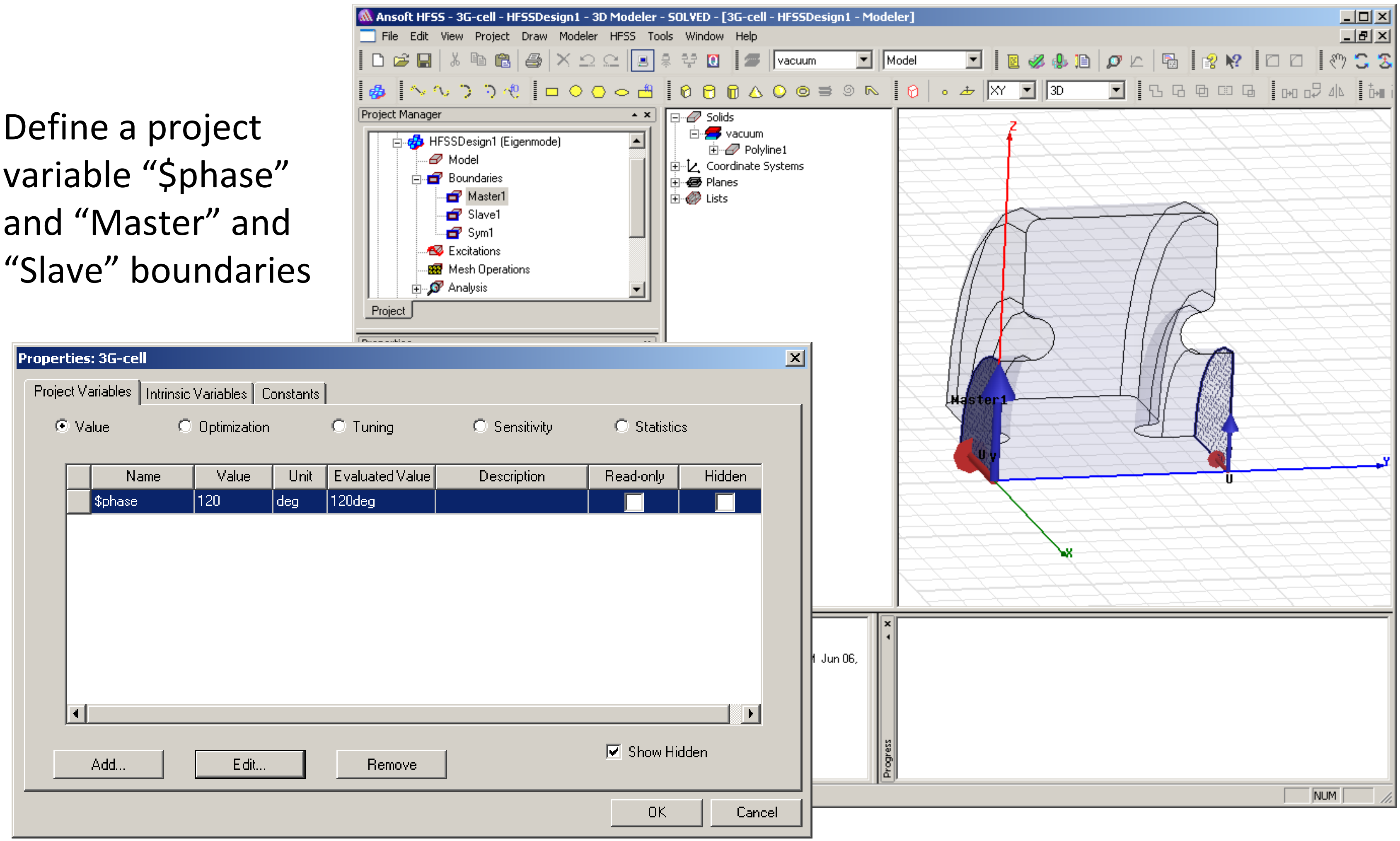
Input the geometry of the cell of the periodic structure.

Use symmetries!



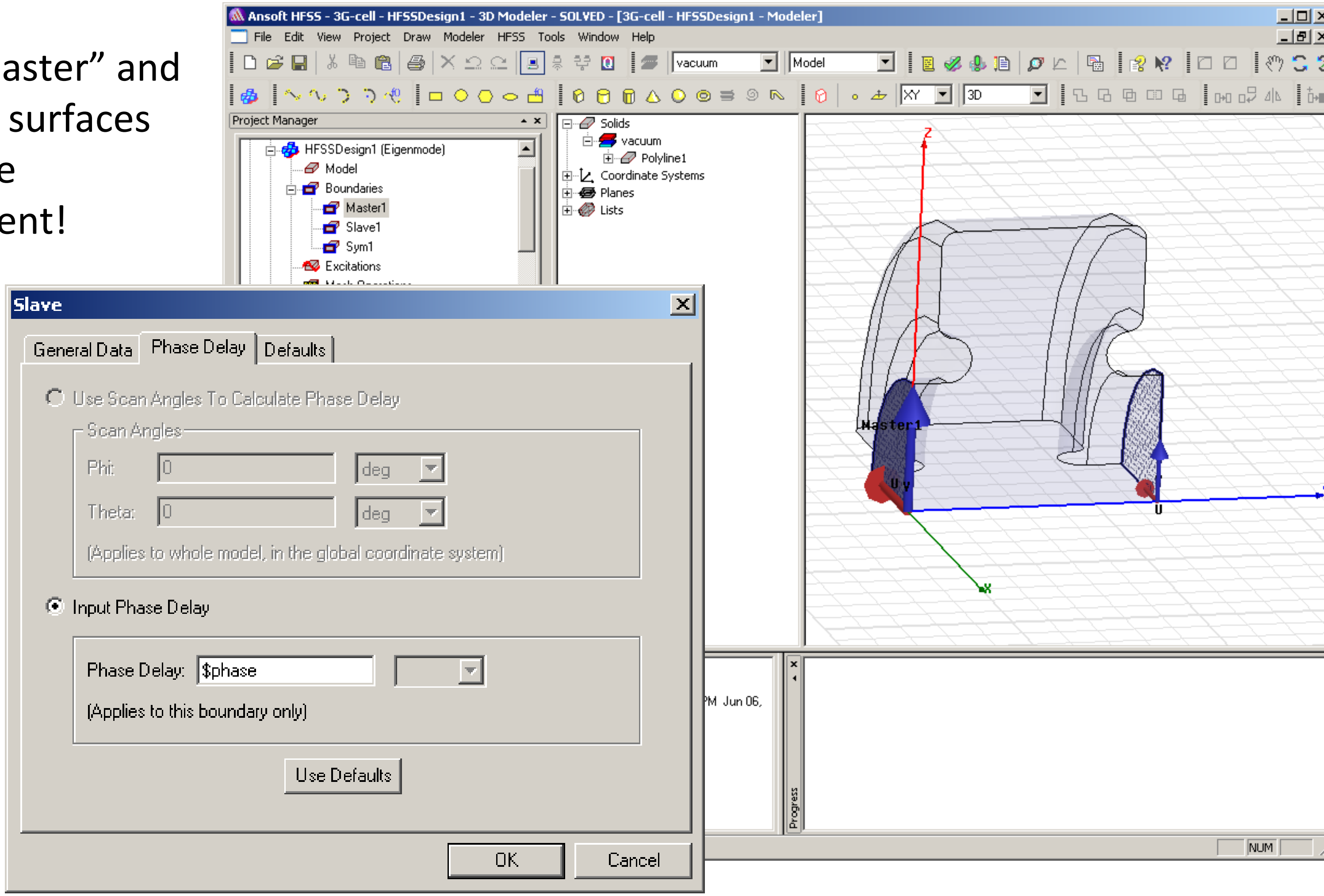
HFSS example: periodic structure (2/5)

Define a project variable “$phase” and “Master” and “Slave” boundaries



HFSS example: periodic structure (3/5)

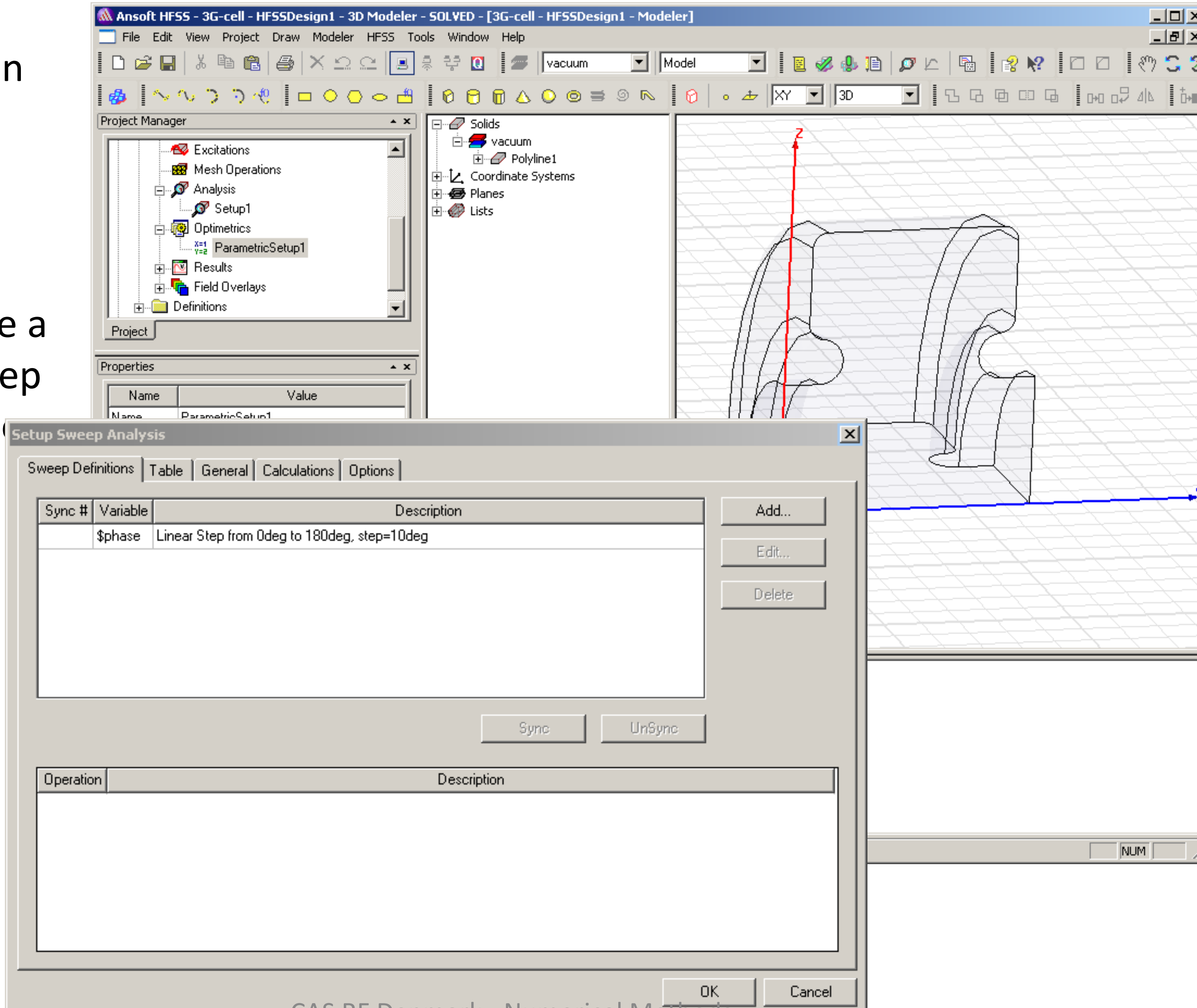
The "master" and "slave" surfaces must be congruent!



HFSS example: periodic structure (4/5)

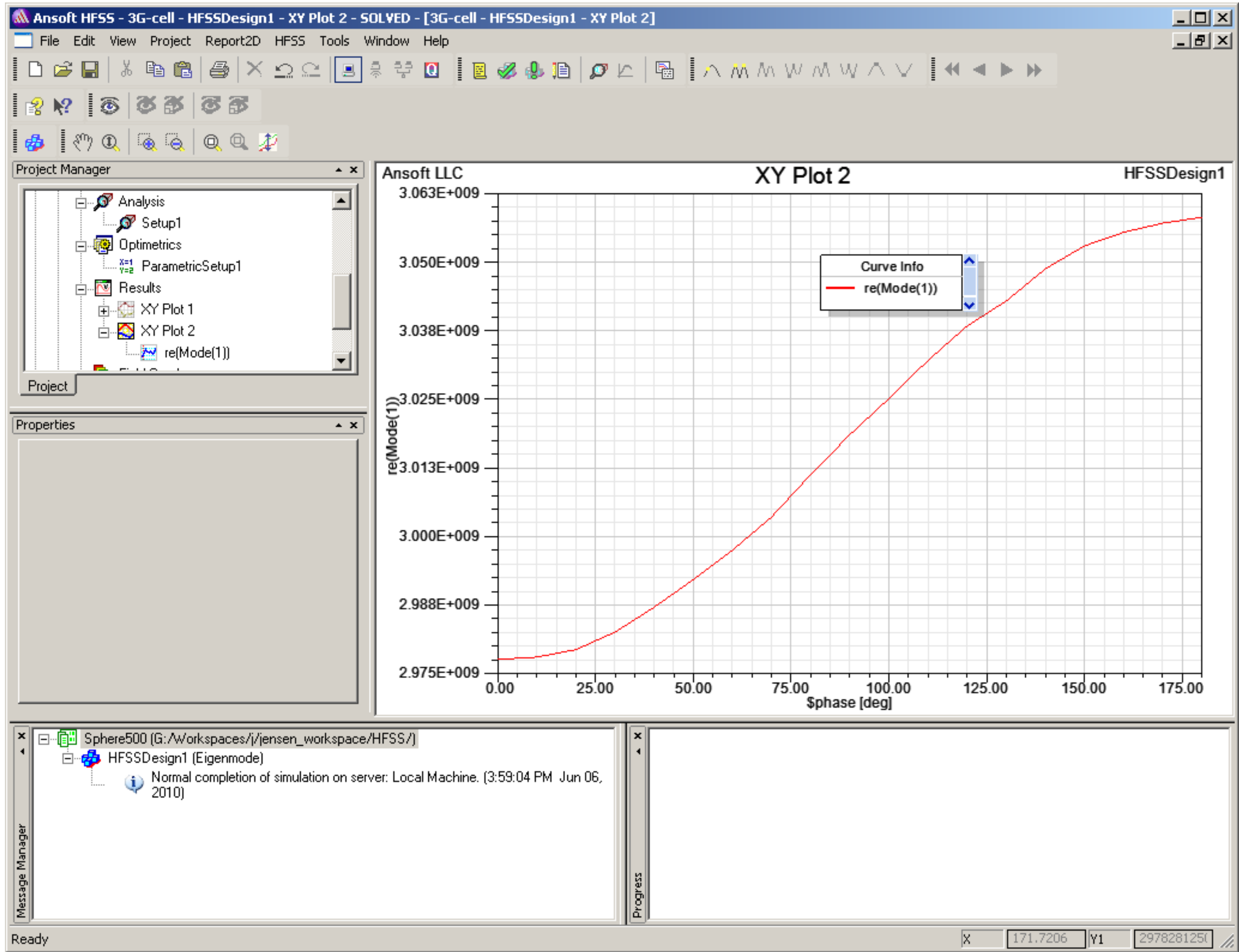
Define a solution setup.

Under “Optimetrics Analysis”, define a parametric sweep with the variabl “$phase”



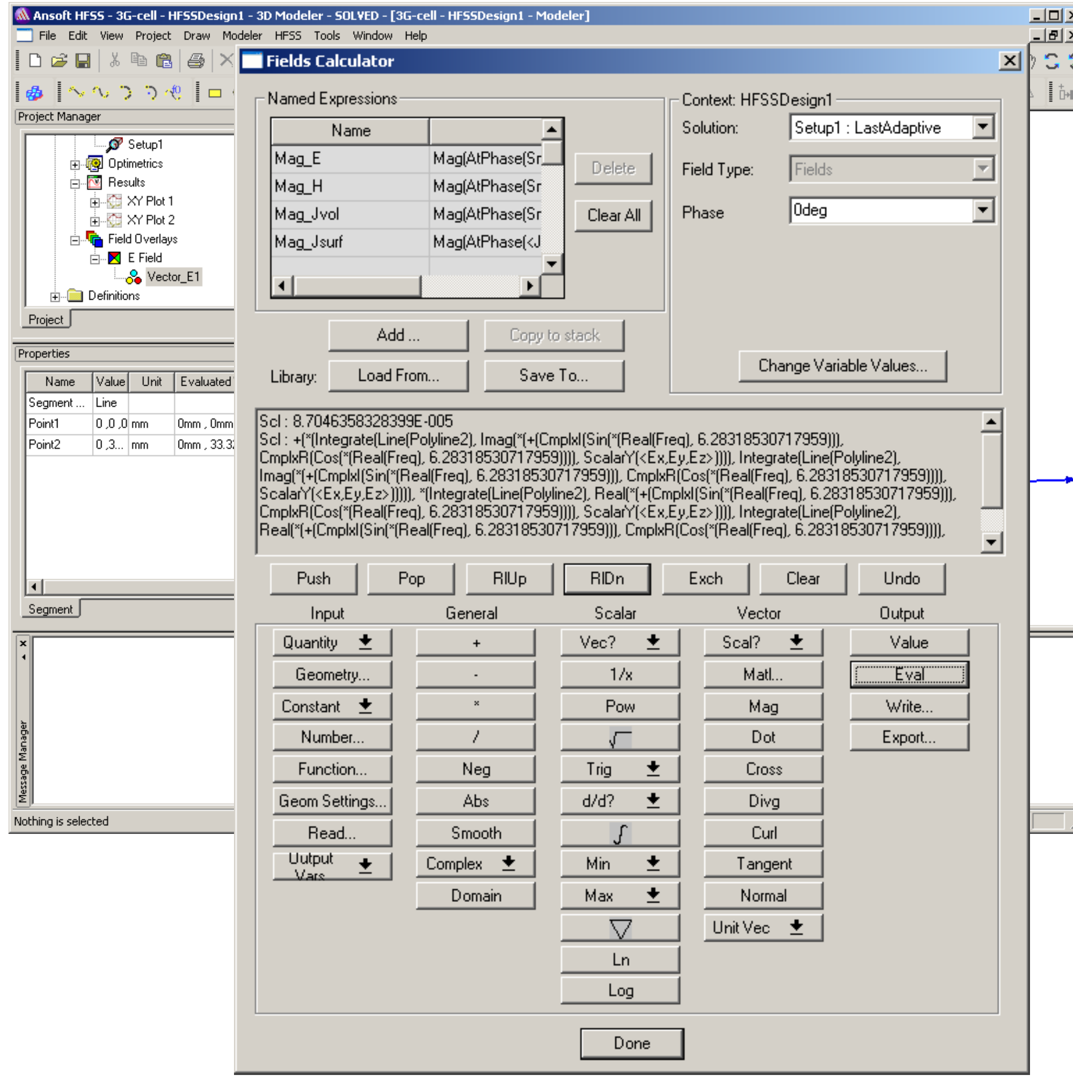
HFSS example: periodic structure (5/5)

The solution is directly the dispersion diagram!



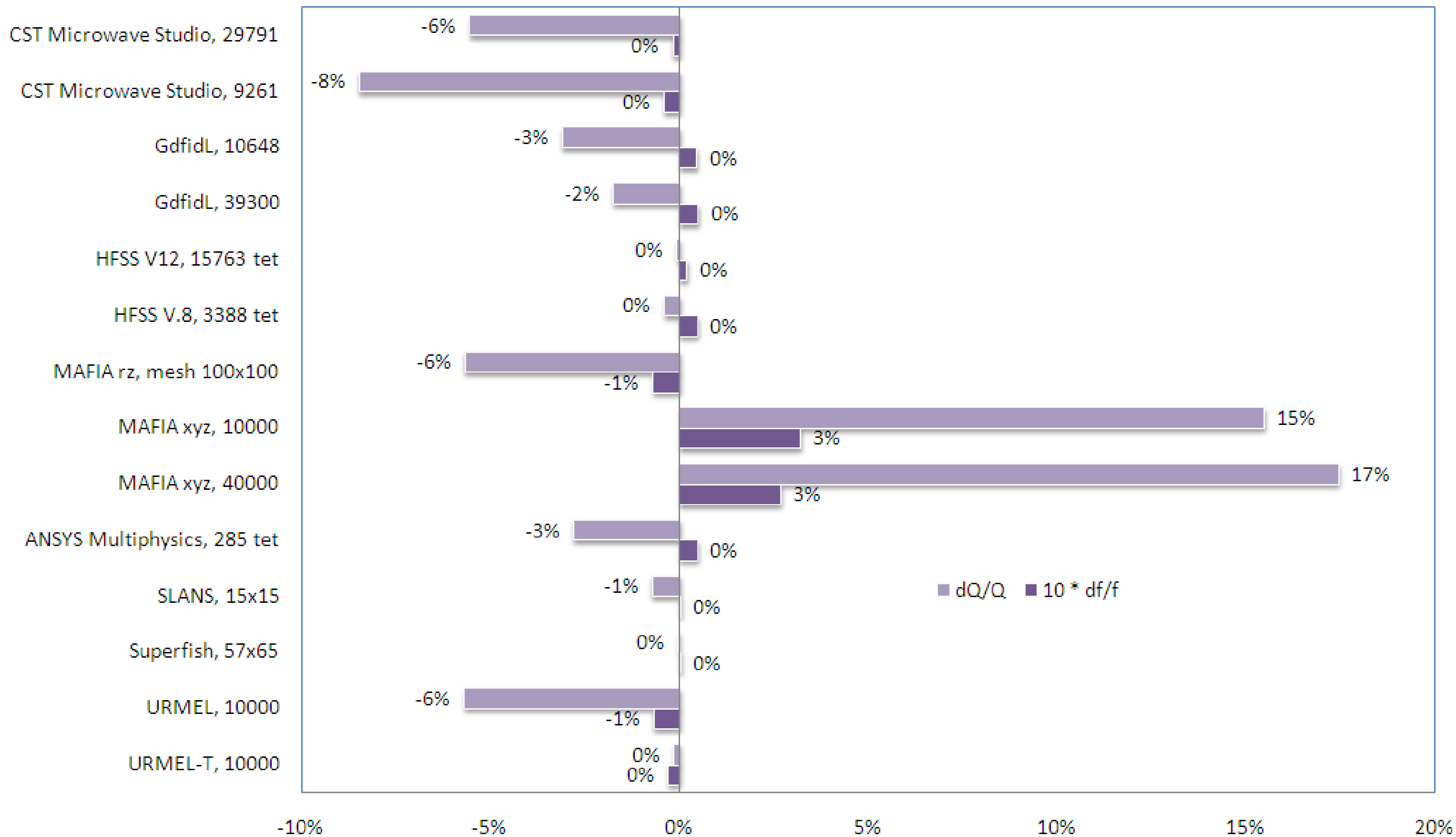
How to calculate cavity parameters with HFSS

Example: How to calculate the acceleration voltage:
Make a “Polyline” describing the beam axis (Polyline2)
Select: HFSS – Fields – Calculator
Output Vars: Freq, Complex Real
Number Scalar 2
Constant Pi
twice “*”
Function Y, *,Constant C, /
Push, Trig Sin, Complex CmplxI
Exch, Trig Cos, Complex CmplxR
+
Quantity E, VectorScal? y, *
Push Real Exch Imag
Geometry, Line, Polyline2
Integrate, Push,*,RlDn
Geometry Line Polyline2
Integrate, Push,*,
+ , Sqrt, Eval



It’s a little clumsy, but works well.

Outcome of the benchmark



Note: some of the calculations were made years ago, so the accuracy data might not be up to date.

... to give you an idea of what one can do today with good hardware:

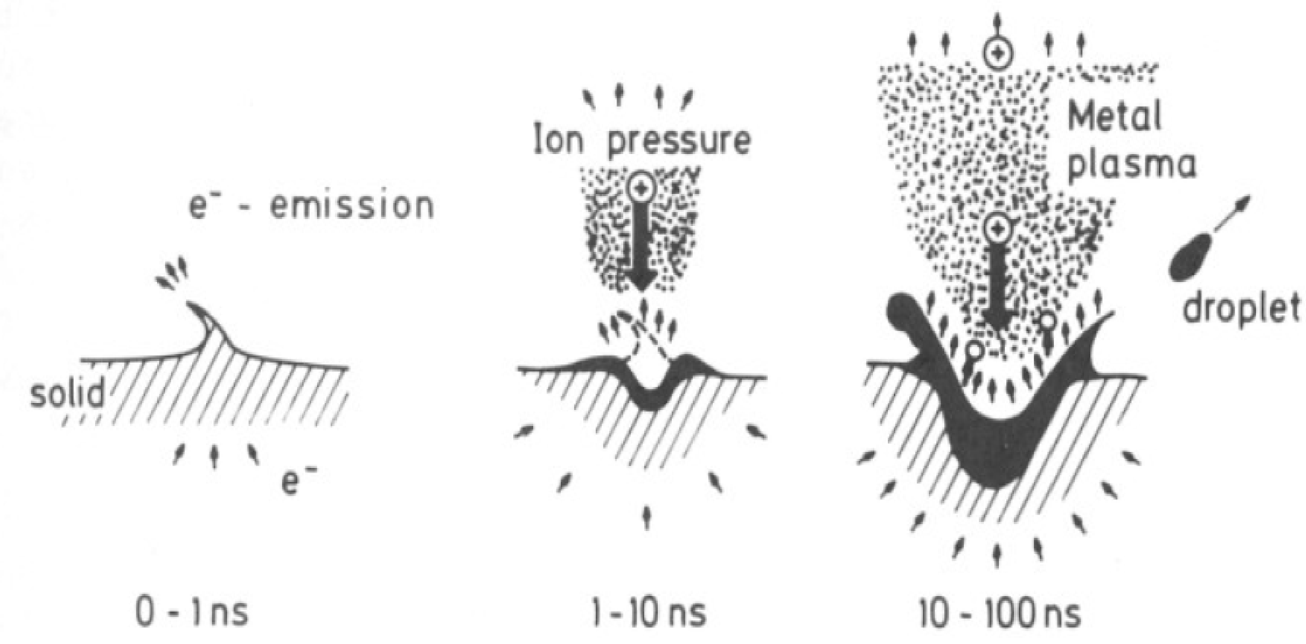
NOW FOR THE SERIOUS STUFF ...

Breakdown simulations

As mentioned in "Cavity Basics", it is not well understood what happens when electrical discharge (breakdown) occurs.

Numerical methods can help the **understanding** breakdown physics phenomena.

Physics involved include electromagnetics (RF and DC fields), plasma physics, surface physics and molecular dynamics.



1. Onset
2. Build-up of plasma
3. Surface damage, new spots

Multiscale model

… developed by Helsinki University

Stage 0: Onset of tip growth; Dislocation mechanism
Method: MD, Molecular Statics… ~ sec/min

Stage 1: Charge distribution @ surface
Method: DFT with external electric field ~few fs

Stage 2: Atomic motion & evaporation
Method: Hybrid ED&MD model ~few ns

- Classical MD+Electron Dynamics: Joule heating, screening effect
- Solution of Laplace equation

Stage 3: Evolution of surface morphology due to the given charge distribution
Method: Kinetic Monte Carlo ~ sec/hours

Onset of plasma

=> Electron & ion & cluster emission ions

Plasma build-up

Stage 4: Plasma evolution, burning of arc
Method: Particle-in-Cell (PIC) ~10s ns

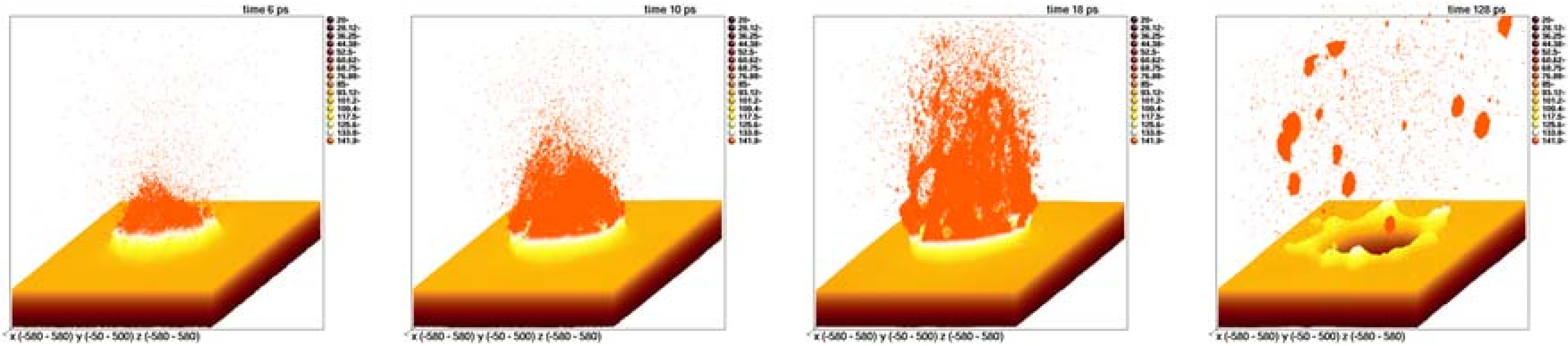
=> Energy & flux of bombarding ions

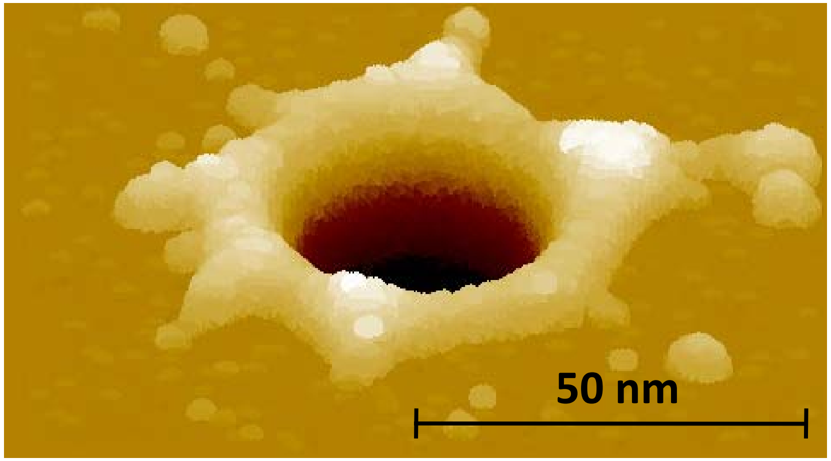
Surface damage

Stage 5: Surface damage due to the intense ion bombardment from plasma
Method: Arc MD ~100s ns

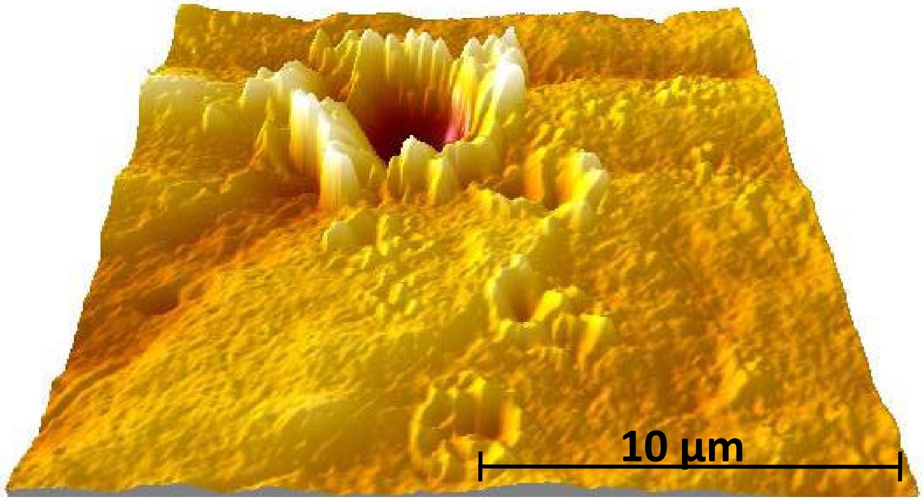
Encouraging results

Erosion and sputtering simulations with MD (molecular dynamics):





Simulation results



Experimental results (SEM)

Advanced Computations

What follows is taken – with his kind permission – from a presentation that **Dr. Arno Candel** from SLAC gave at CERN on May 4th 2010 during the "4th Annual X-band Structure Collaboration Meeting". It will allow you to see what is possible today with EM simulation!

Arno's group includes the accelerator physicists

Arno Candel, Andreas Kabel, Kwok Ko, Zenghai Li, Cho Ng, Liling Xiao

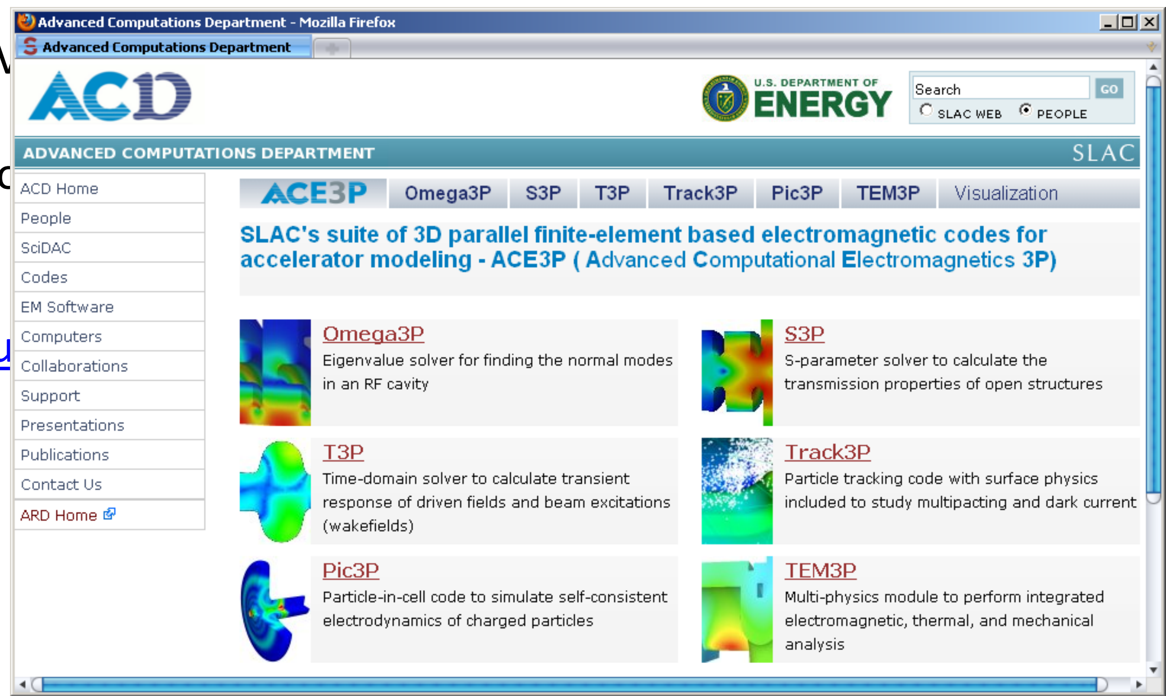
And the computer scientists

Lixin Ge, Rich Lee, V

Full credits to the following gr

See here

http://www.slac.stanford.edu



Parallel Finite Element EM Code Suite ACE3P

- Support from SLAC and DOE's HPC Initiatives – Grand Challenge (1998-2001), SciDAC1 (2001-06), SciDAC2 (2007-11)

- Developed a suite of conformal, higher-order, C++/MPI-based parallel finite-element based electromagnetic codes

ACE3P (Advanced Computational Electromagnetics 3P)

Frequency Domain:	**Omega3P**	**– Eigensolver (damping)**
	S3P	**– S-Parameter**
Time Domain:	**T3P**	**– Wakefields and Transients**
Particle Tracking:	**Track3P**	**– Multipacting and Dark Current**
EM Particle-in-cell:	**Pic3P**	**– RF gun (self-consistent)**

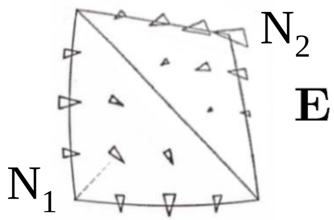
Visualization: **ParaView** **– Meshes, Fields and Particles**

Goal is the Virtual Prototyping of accelerator structures

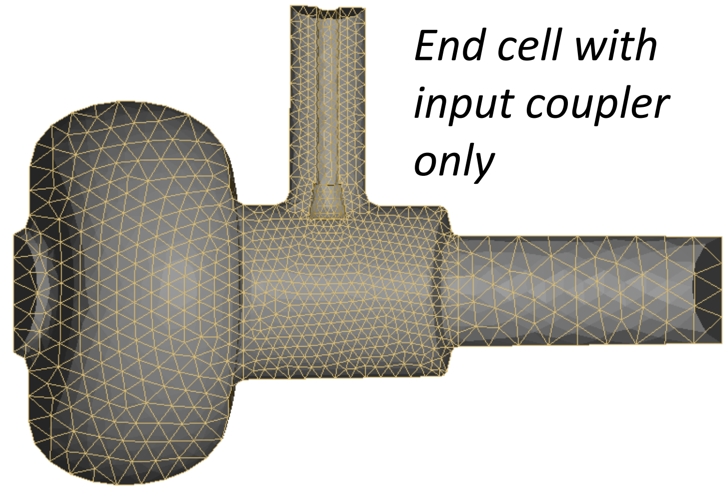
SciDAC Scientific Discovery through Advanced Computing

Parallel Higher-order Finite-Element Method

Discretization with finite elements -

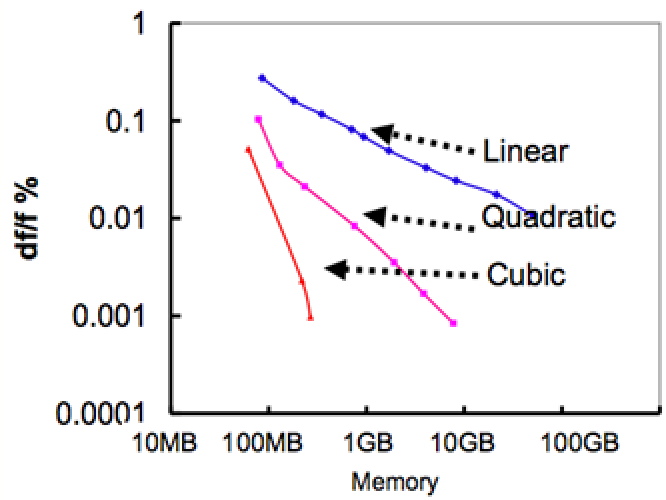


$$\mathbf{E}\left(\mathbf{x}, t\right) = \sum_i e_i\left(t\right) \cdot \mathbf{N_i}\left(\mathbf{x}\right)$$

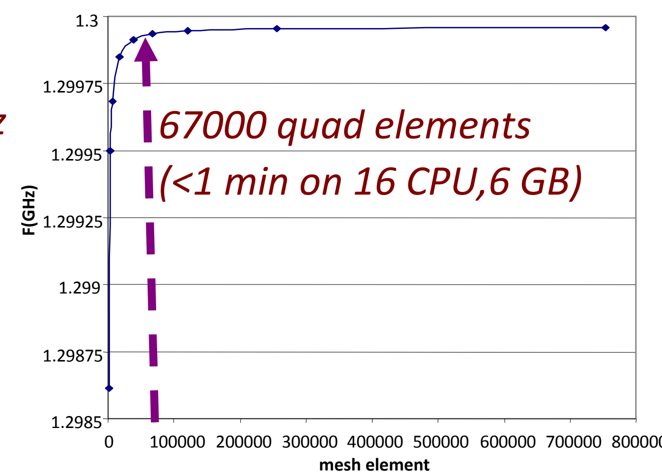


End cell with input coupler only

- **Tetrahedral conformal mesh with quadratic surface**
- **Higher-order elements (p = 1-6)**
- **Parallel processing (memory & speedup)**



Error ~ 20 kHz (1.3 GHz)

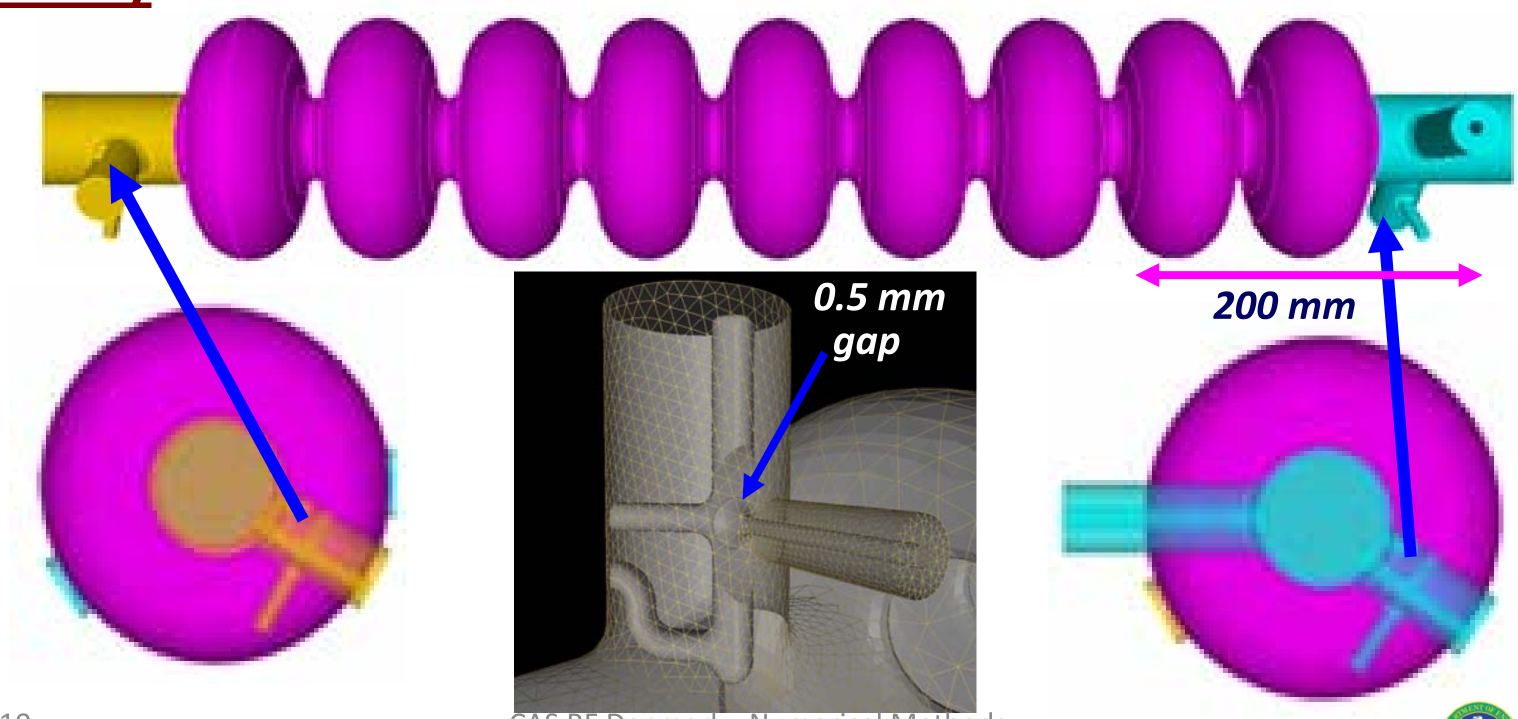


Virtual Prototyping of Accelerator Structures

Modeling challenges include:

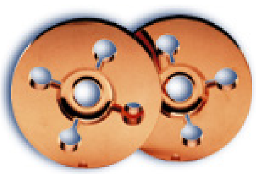
- **Complexity** – HOM coupler (fine features) versus cavity
- **Problem size** – multi-cavity structure, e.g. cryomodule
- **Accuracy** – 10s of kHz mode separation out of GHz
- **Speed** – Fast turn around time to impact design

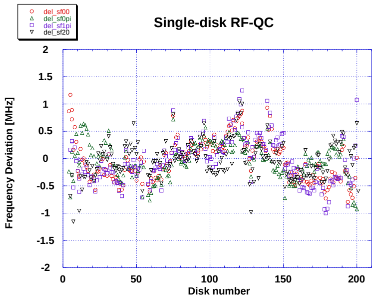
ILC Cavity



Accelerator Modeling Achievements in **SciDAC-1**

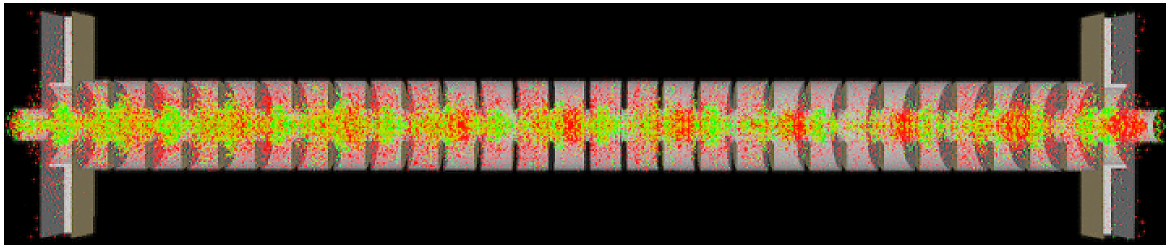
Omega3P





NLC cell design to machining accuracy

Track3P

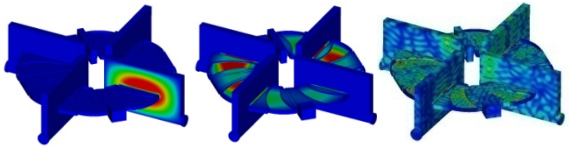


Dark current in 30-cell accelerator structure

T3P

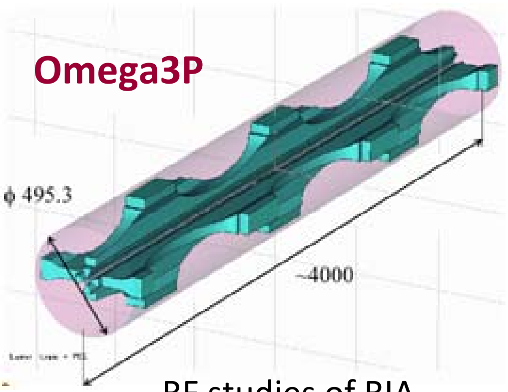
Beam heating analysis of PEP-II interaction region

Omega3P

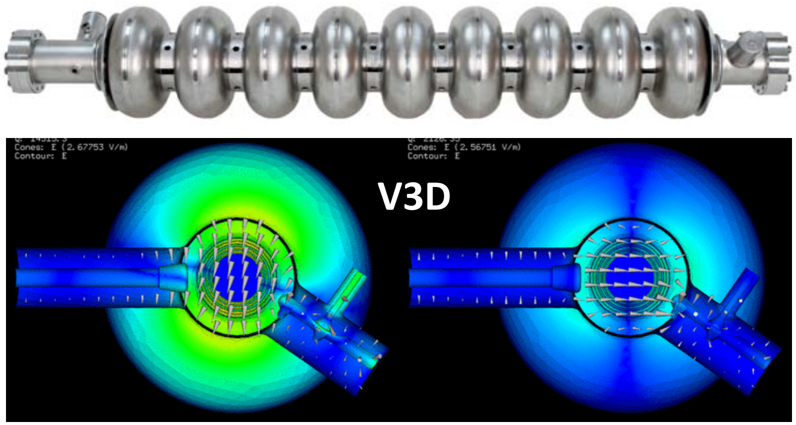


Simulation of entire cyclotron

Omega3P

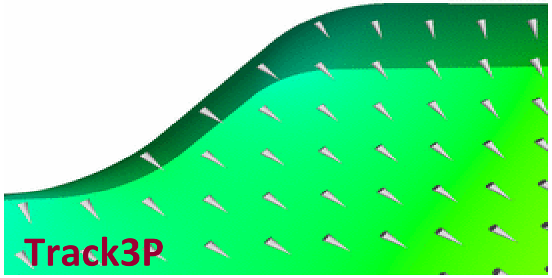


RF studies of RIA RFQ



Discovery of mode rotation in superconducting cavity

MP Trajectory @ 29.4 MV/m

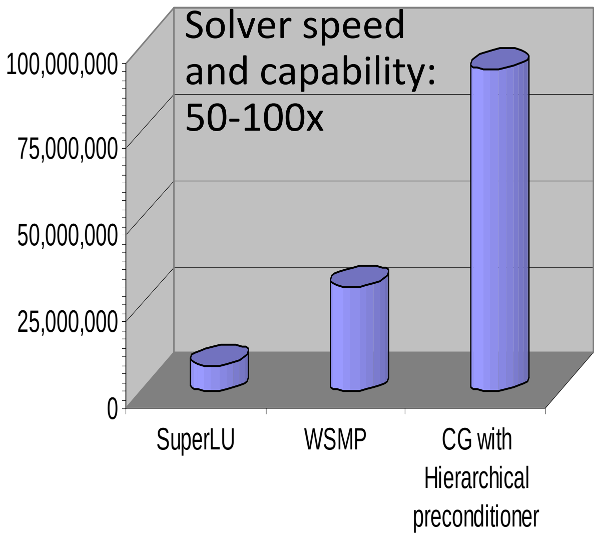


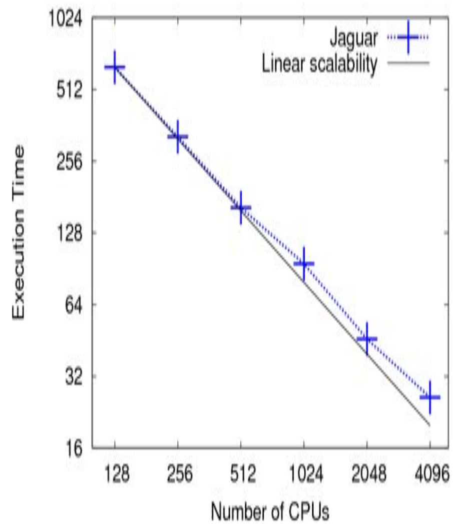
Prediction of multipacting barriers in Ichiro SRF cavity

SciDAC Scientific Discovery through Advanced Computing

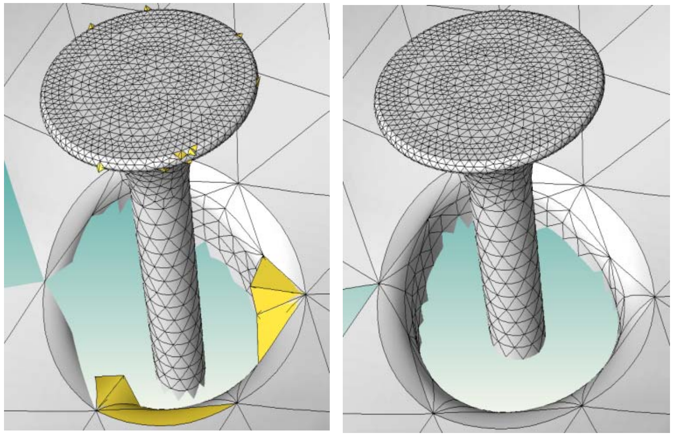
SciDAC Advances in Computational Science

Eigensolver speed and scalability

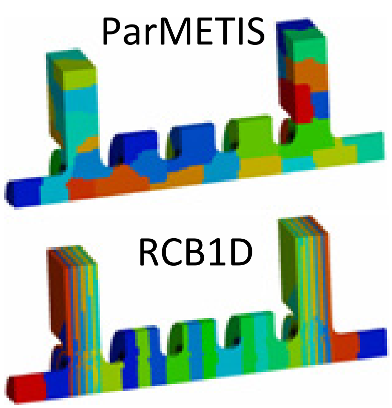


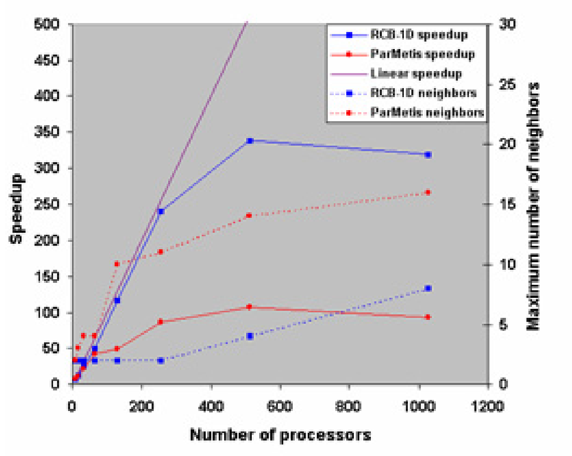


Mesh correction

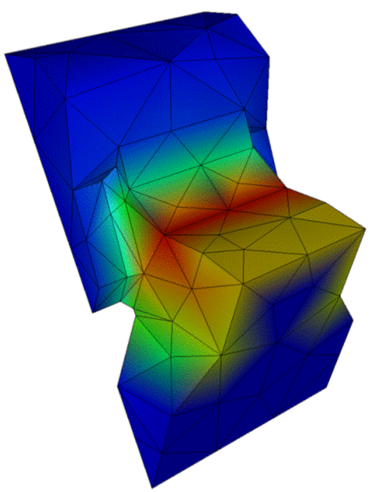


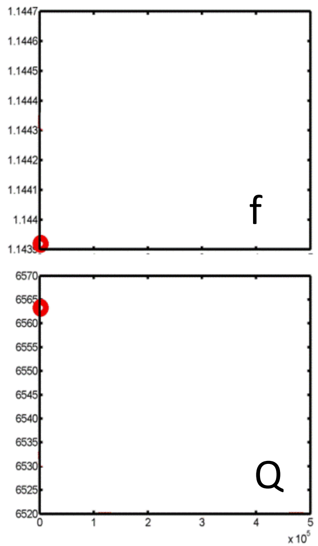
Partitioning scheme for load balancing





Adaptive mesh refinement





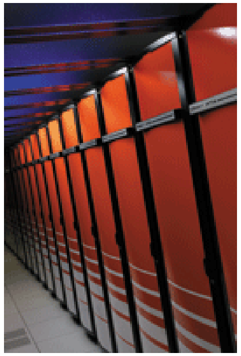
High-performance Computing for Accelerators

DOE Computing Resources:

Computers -

NERSC at LBNL - Franklin Cray XT4, 38,642 compute cores, 77 TBytes memory, 355 TFlops

NCCS at ORNL - Jaguar Cray XT5, 224,256 compute cores, 300 TBytes memory, 2331 TFlops 600 TBytes disk space



Allocations –

NERSC - *Advanced Modeling for Particle Accelerators* - **1M CPU hours**, renewable
- *SciDAC ComPASS Project* – **1.6M CPU hours,** renewable (shared)
- *Frontiers in Accelerator Design: Advanced Modeling for Next-Generation BES Accelerators* - **300K CPU hours**, renewable (shared) each year

NCCS - *Petascale Computing for Terascale Particle Accelerator: International Linear Collider Design and Modeling* - **12M CPU hours** in FY10

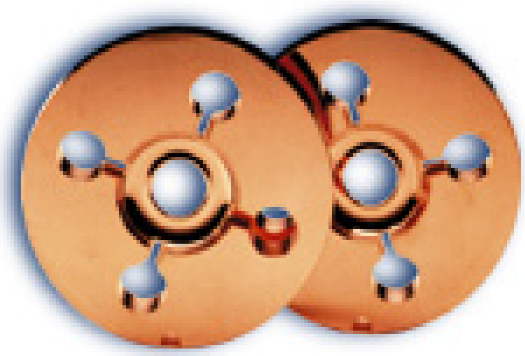
SciDAC Scientific Discovery through Advanced Computing

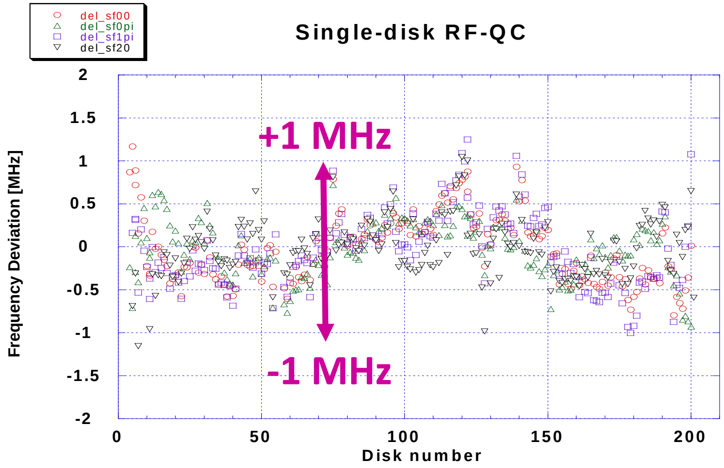
Omega3P Capabilities

- Omega3P finds eigenmodes in lossless, lossy, periodic and externally damped cavities

Code validated in 3D NLC Cell design in 2001

- *Microwave QC verified cavity frequency accuracy to 0.01% relative error (1MHz out of 11 GHz)*

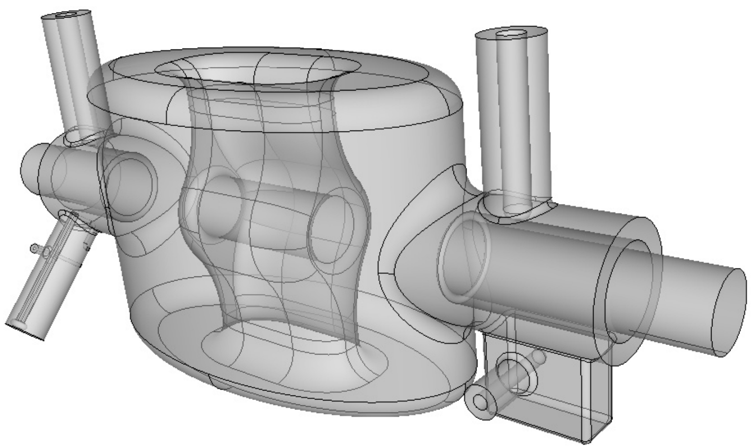


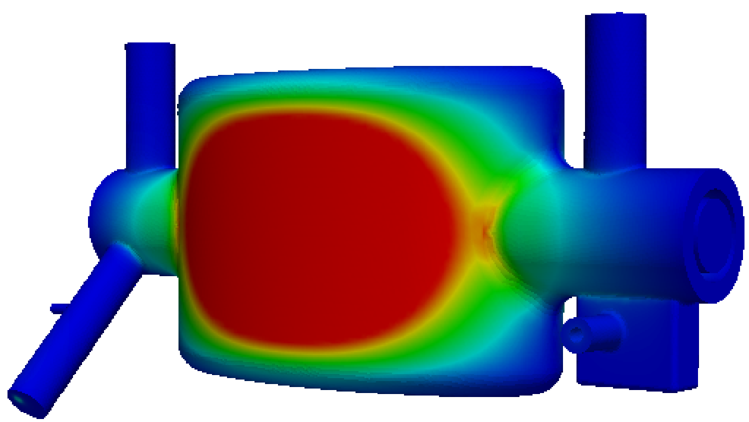


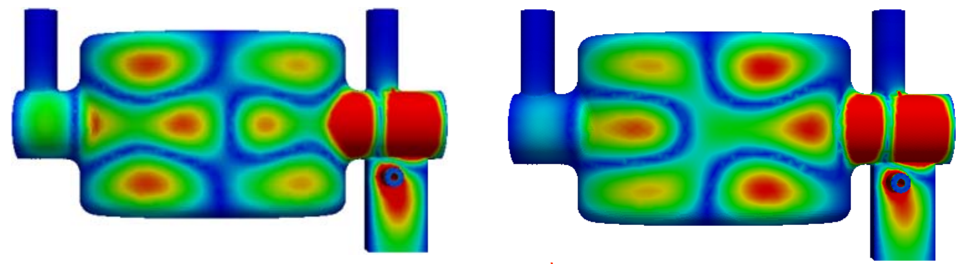
- Omega3P can be used to
  - optimize RF parameters,
  - reduce peak surface fields,
  - calculate HOM damping,
  - find trapped modes & their heating effects,
  - design dielectric & ferrite dampers, etc....

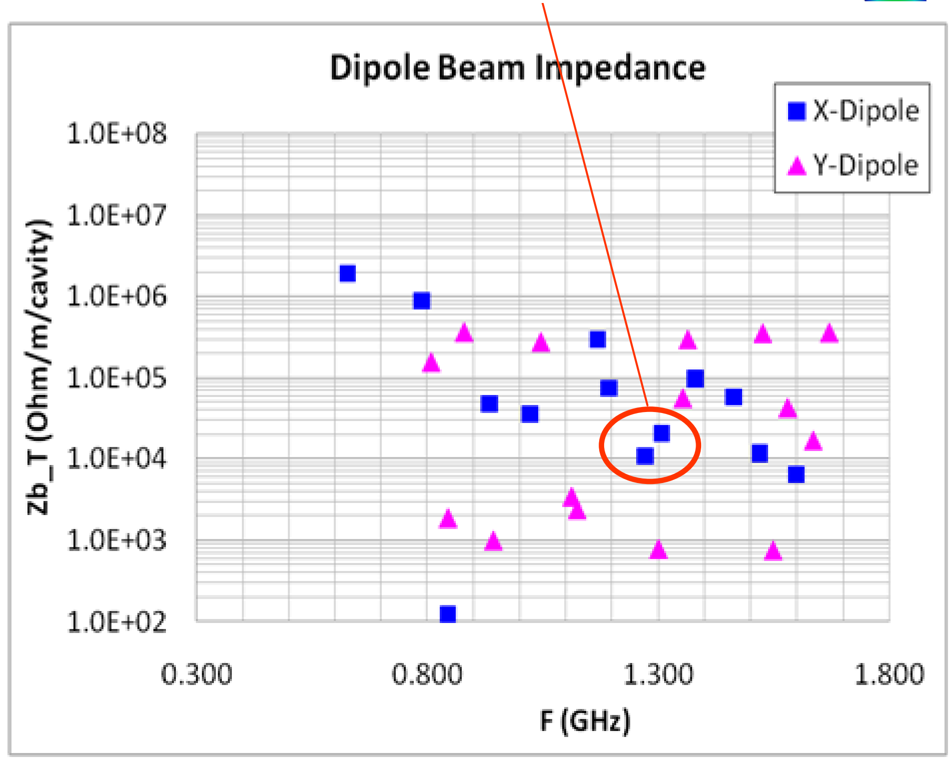
SciDAC Scientific Discovery through Advanced Computing

Omega3P – HOMs in LARP Deflecting Cavity





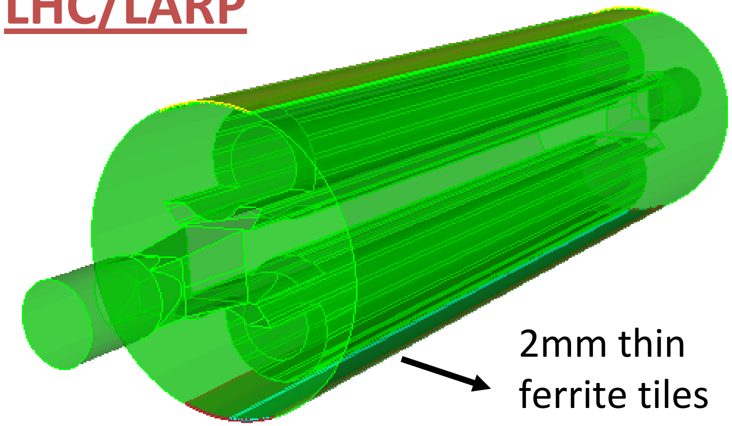


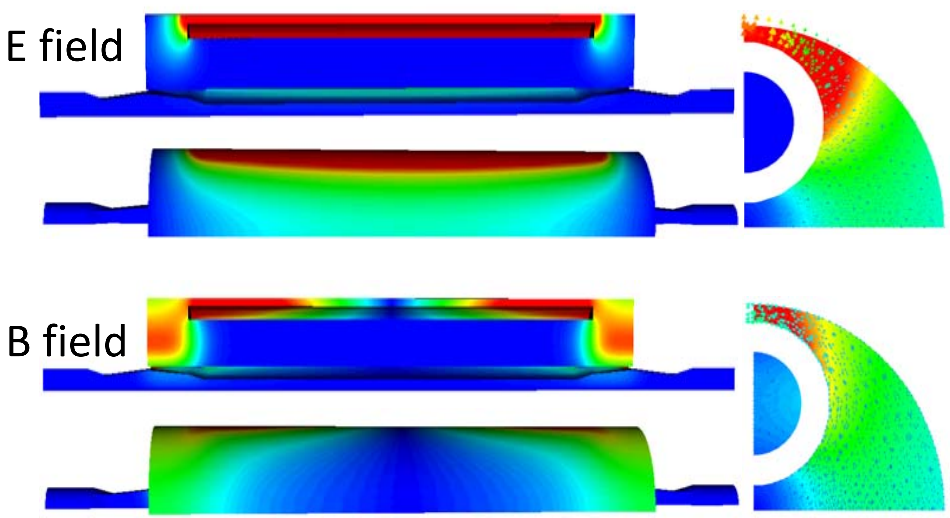


Omega3P – Trapped Modes in LARP Collimator

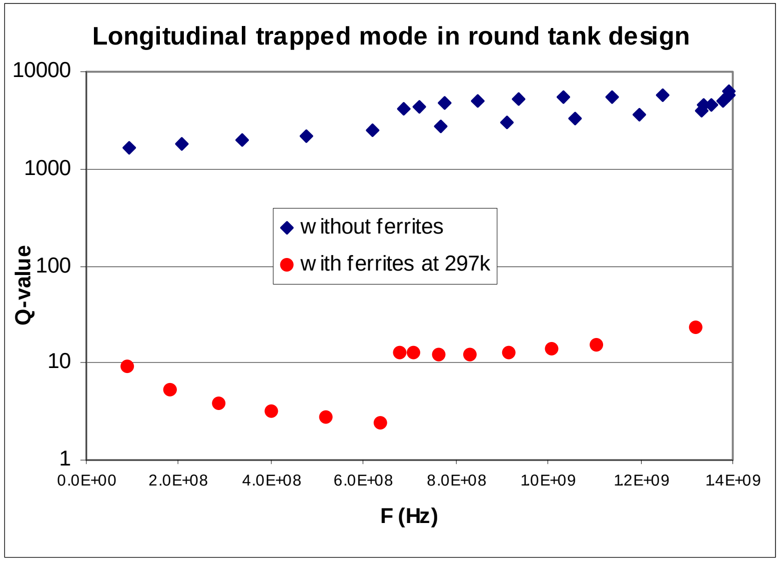
- Trapped modes found in circular design may cause excessive heating
- Adding ferrite tiles on circular vacuum chamber wall strongly damp trapped modes
- Further analysis needed on ferrite's thermal and mechanical effects

LHC/LARP





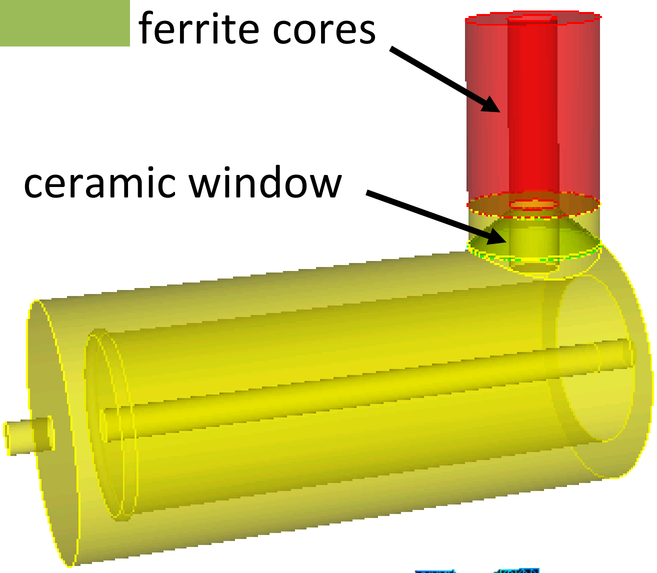
Q of resonant modes w/ and w/o ferrite



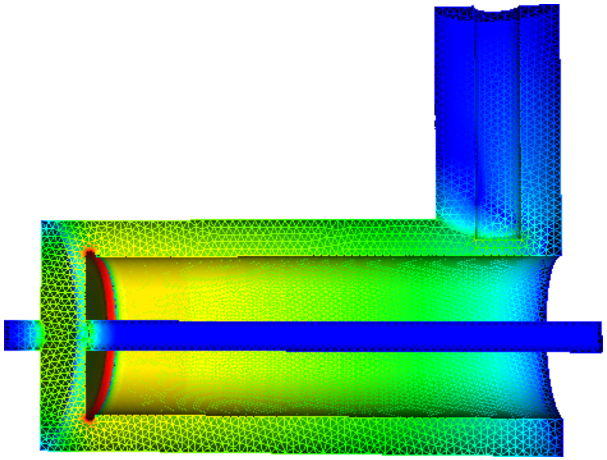
Omega3P – Project-X Main Injector Cavity

Lossy dielectric and ferrite calculation

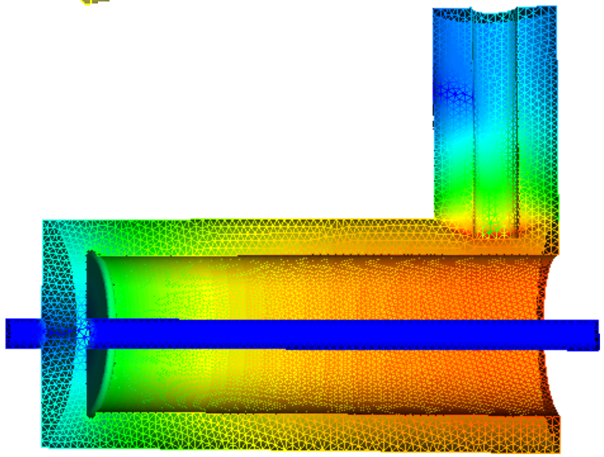
- Determine cavity RF parameters and peak surface fields
- Evaluate HOM effects
- Identify possible multipacting zones
- Investigate effectiveness of **ferrite core** in fundamental mode tuning



E-field

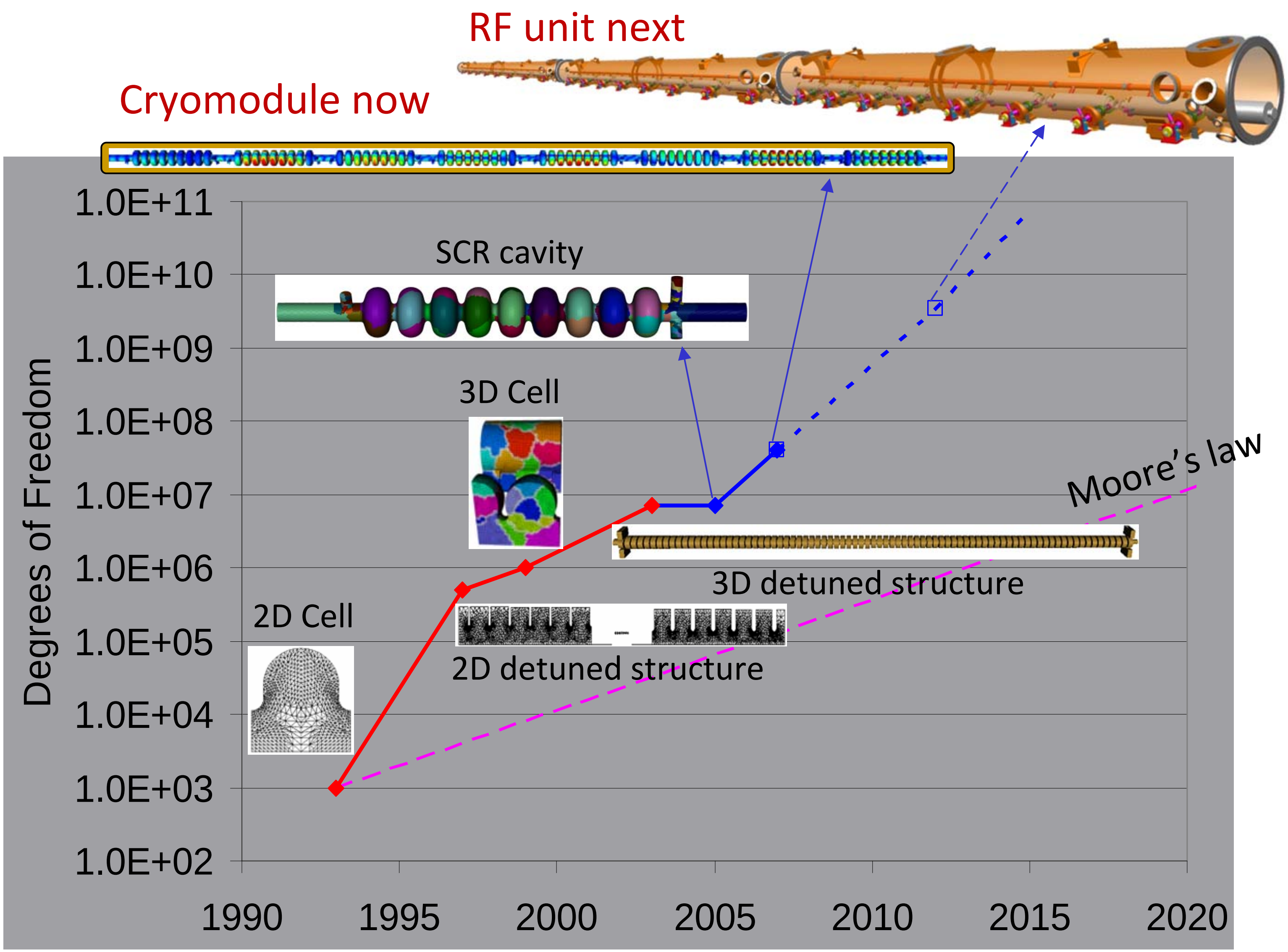


B-field



In collaboration with FNAL

Omega3P – Towards System Scale Modeling



Track3P Capabilities

- Multipacting can cause
  - Low achievable field gradient
  - Heating of cavity wall and damage of RF components
  - Significant power loss
  - Thermal breakdown in SC structures
  - Distortion or loss of RF signal

- Track3P studies multipacting in cavities & couplers by identifying MP barriers, MP sites and the type of MP trajectories.

- MP effects can be mitigated by modifying the geometry, changing surface conditions to reduce SEY and applying DC biasing.

Track3P – Multipacting in ICHIRO Cavity

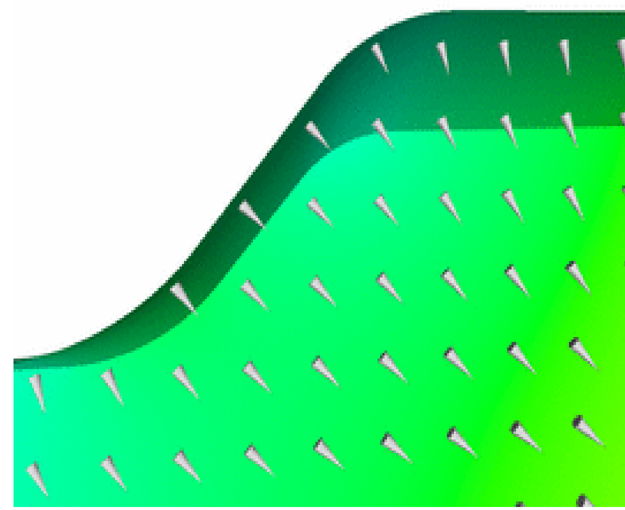
ICHIRO cavity experienced

- Low achievable field gradient
- Long RF processing time

- **Hard barrier at 29.4 MV/m field gradient with MP in the beampipe step**
- **First predicted by Track3P simulation**

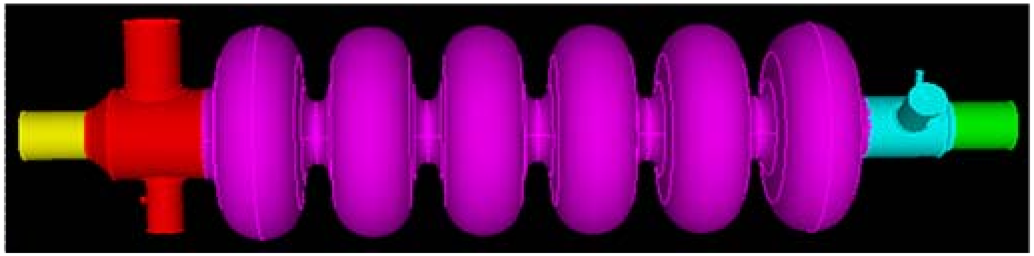
ICHIRO #0	Track3P MP simulation	
X-ray Barriers (MV/m)	Gradient (MV/m)	Impact Energy (eV)
11-29.3 12-18	12	300-400 (6^{th} order)
13, 14, 14-18, 13-27	14	200-500 (5^{th} order)
(17, 18)	17	300-500 (3^{rd} order)
20.8	21.2	300-900 (3^{rd} order)
28.7, 29.0, 29.3, 29.4	29.4	600-1000 (3^{rd} order)

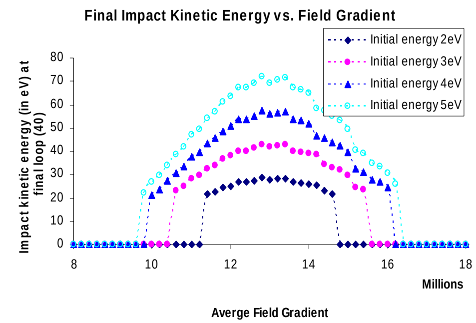
MP Trajectory @ 29.4 MV/m



K. Saito, KEK

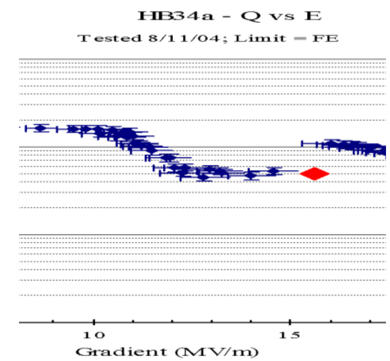
Track3P – Multipacting in SNS Cavity/HOM Coupler





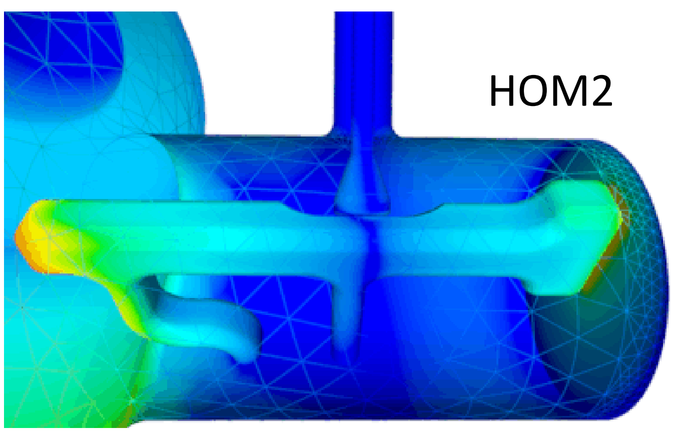
SNS Cavity

- Both Experiment and Simulation show same MP band: 11 MV/m ~ 15MV/m

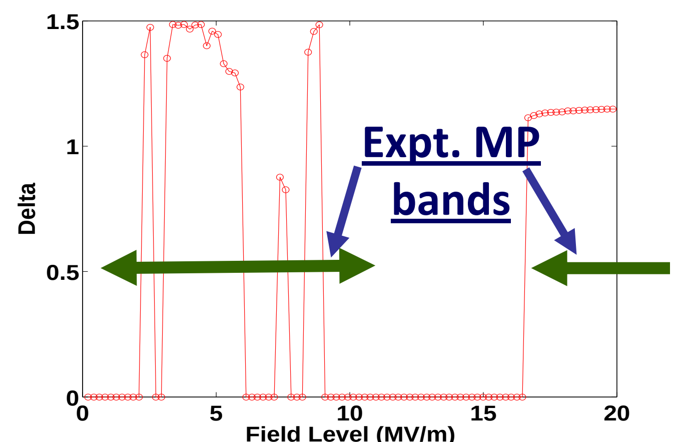


SNS Coupler

- SNS SCRF cavity experienced rf heating at HOM coupler
- 3D simulations showed MP barriers close to measurements



HOM2

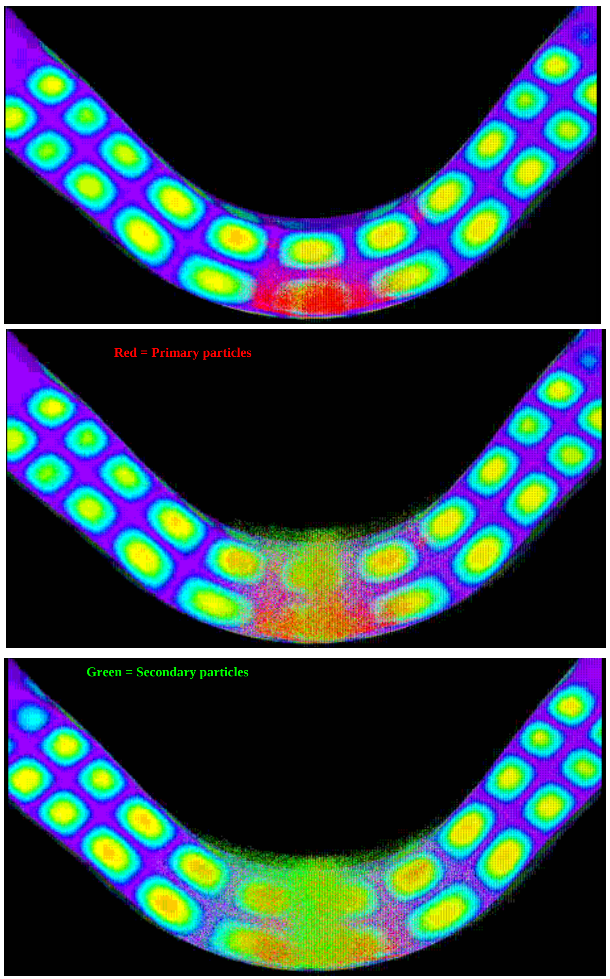


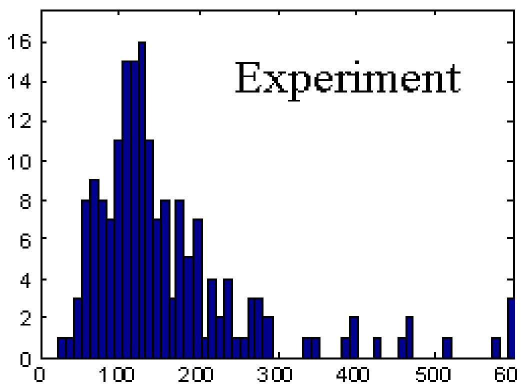
Track3P – Dark Current in Waveguide Bend

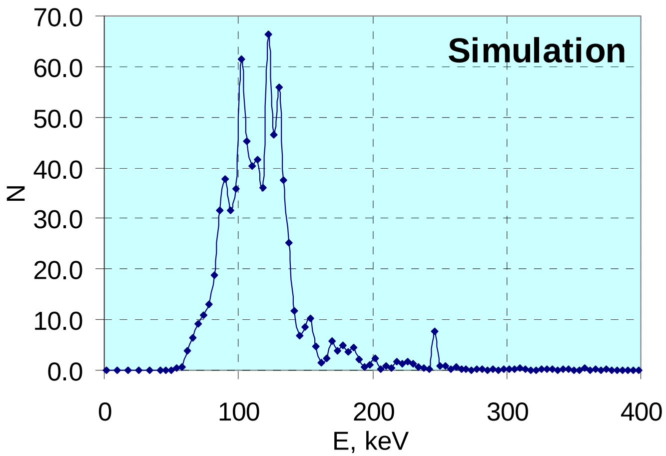
High power tests on a NLC waveguide bend provided measured data on the X-ray spectrum with which simulation results from **Track3P** can be compared.

This allows the surface physics module in **Track3P** consisting of primary and secondary emission models to be benchmarked.

Evolution to steady -state

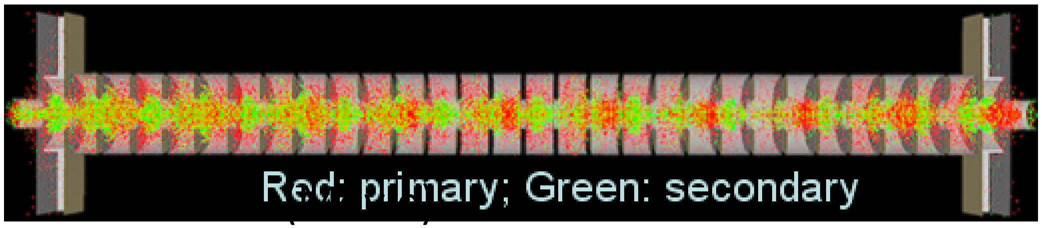


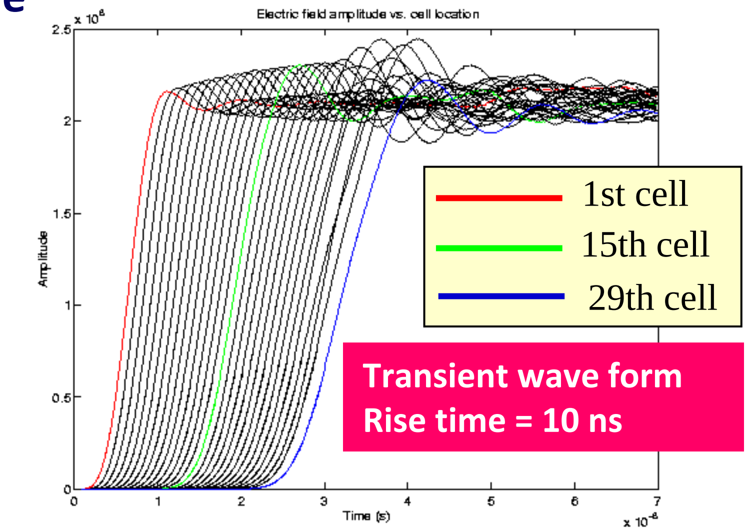


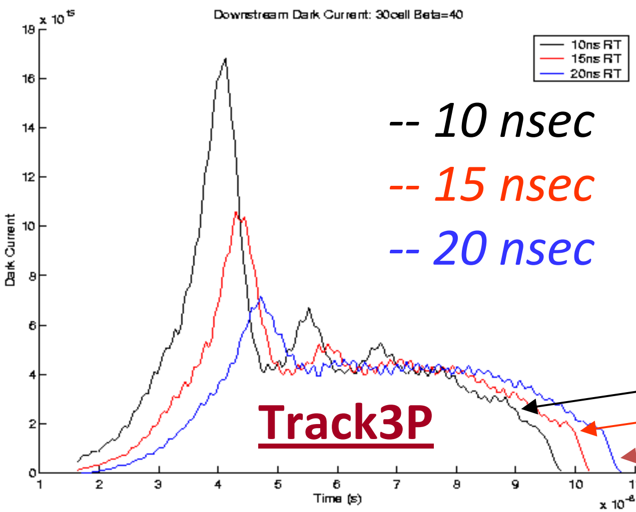


Track3P – Dark Current in X-Band Structure

Dark current pulses were simulated for the **1st time** in a 30-cell X-band structure with **Track3P** and compared with data. Simulation shows increase in dark current during pulse risetime due to field enhancement from dispersive effects.







Dark current @ 3 pulse risetimes

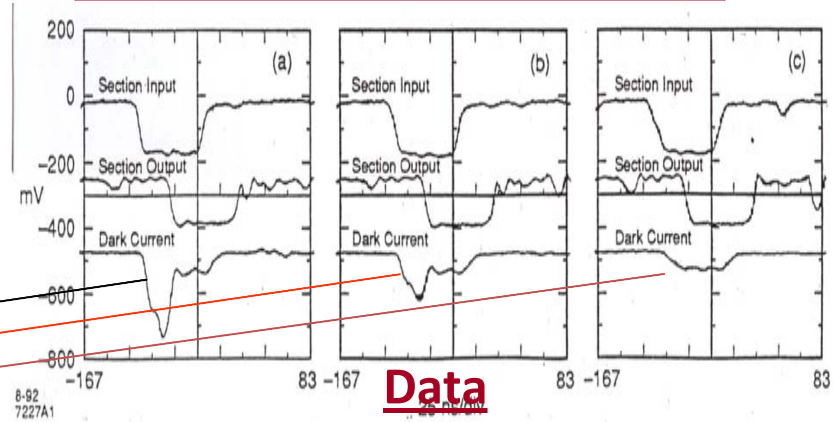


Fig. 7. Pulse shapes of section input, output and dark current for three different rise times of the RF pulse for 30-cavity TW section tests.

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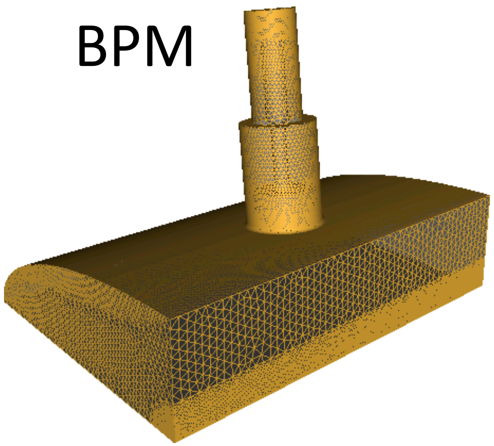
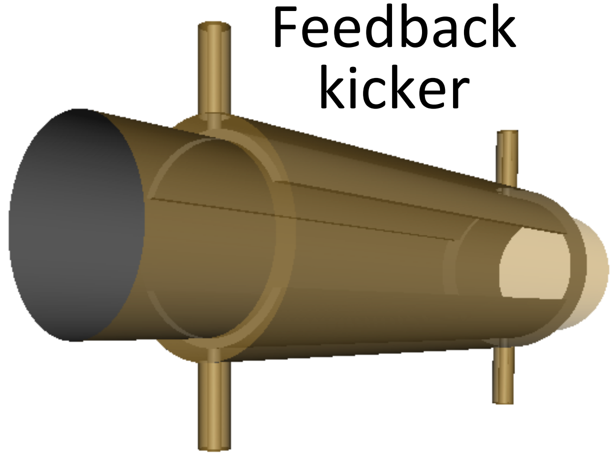
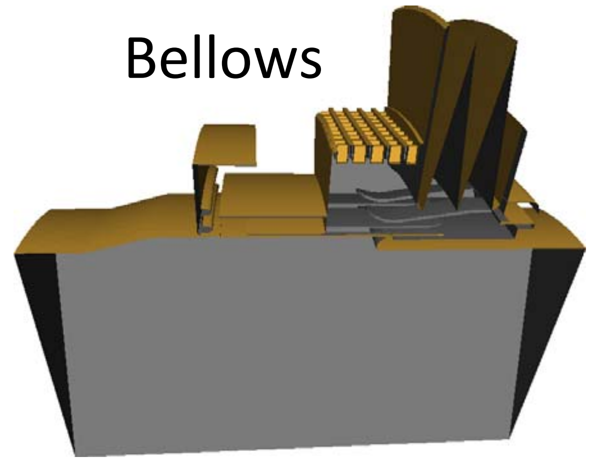
T3P Capabilities

- T3P uses a driving bunch to evaluate the broadband impedance, trapped modes and signal sensitivity of a beamline component.





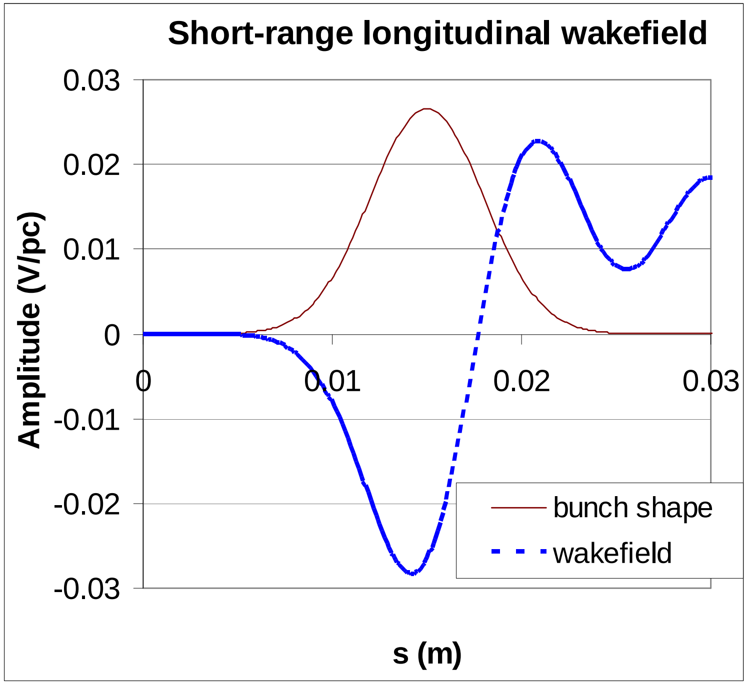


- T3P computes the wakefields of Short bunches with a moving window in 3D Long tapered structures.

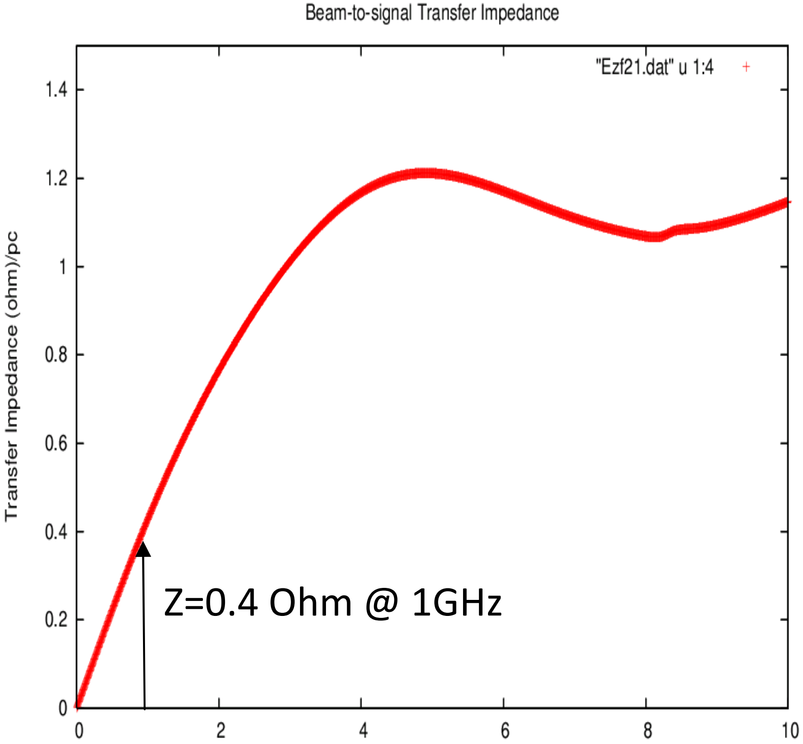
- T3P simulates the beam transit in Large 3D complex structures consisting of lossy dielectrics and terminated in open waveguides (broadband waveguide boundary conditions).

T3P - PEP-X BPM Transfer Impedance

- Evaluate contribution to broadband impedance budget
- Identify trapped modes that can contribute to beam heating and coupled bunch instability
- Determine signal sensitivity



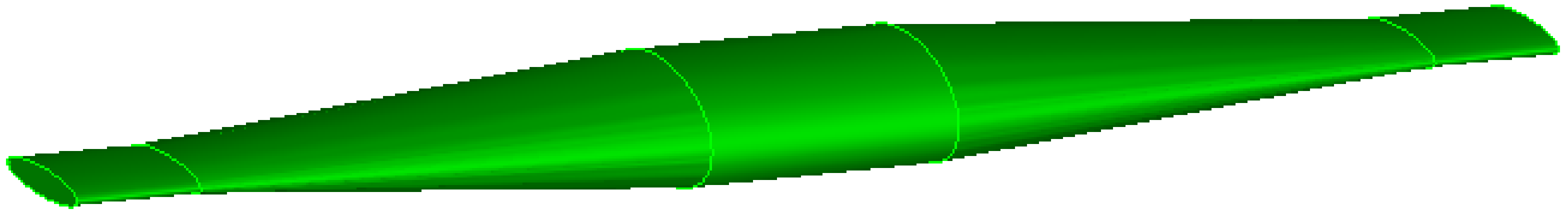
Wakefield



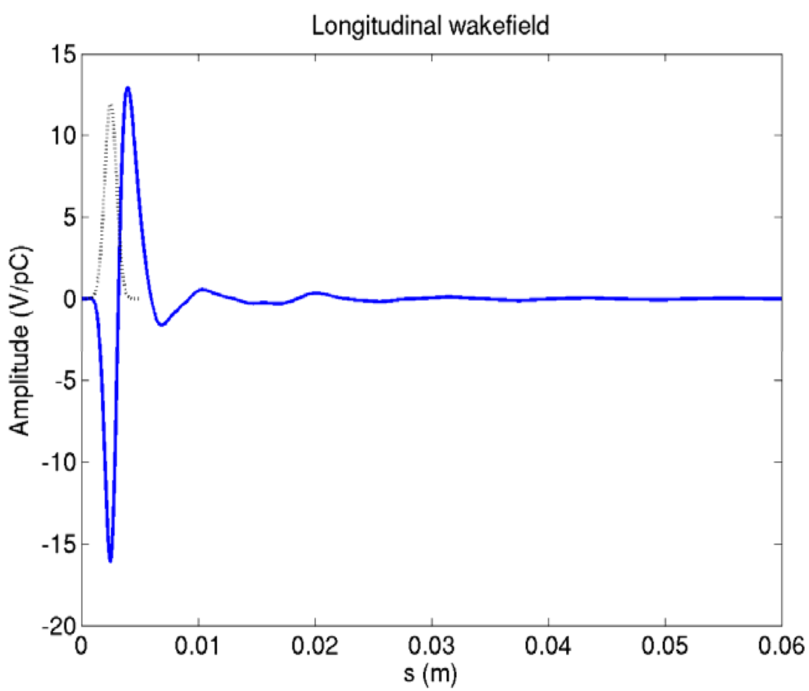
Transfer impedance

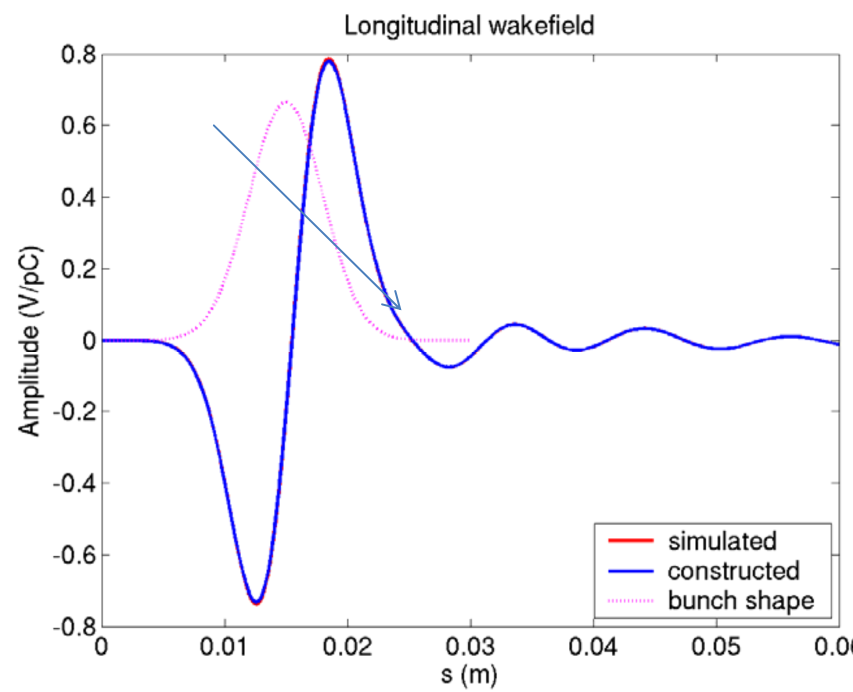
T3P - PEP-X Undulator Vacuum Chamber

Wakefields of Ultra-short bunch beam in Long 3D taper



<u>0.5mm bunch</u> → 3mm bunch





<u>Reconstruction of wakefield for long bunch verifies that for short bunch.</u>

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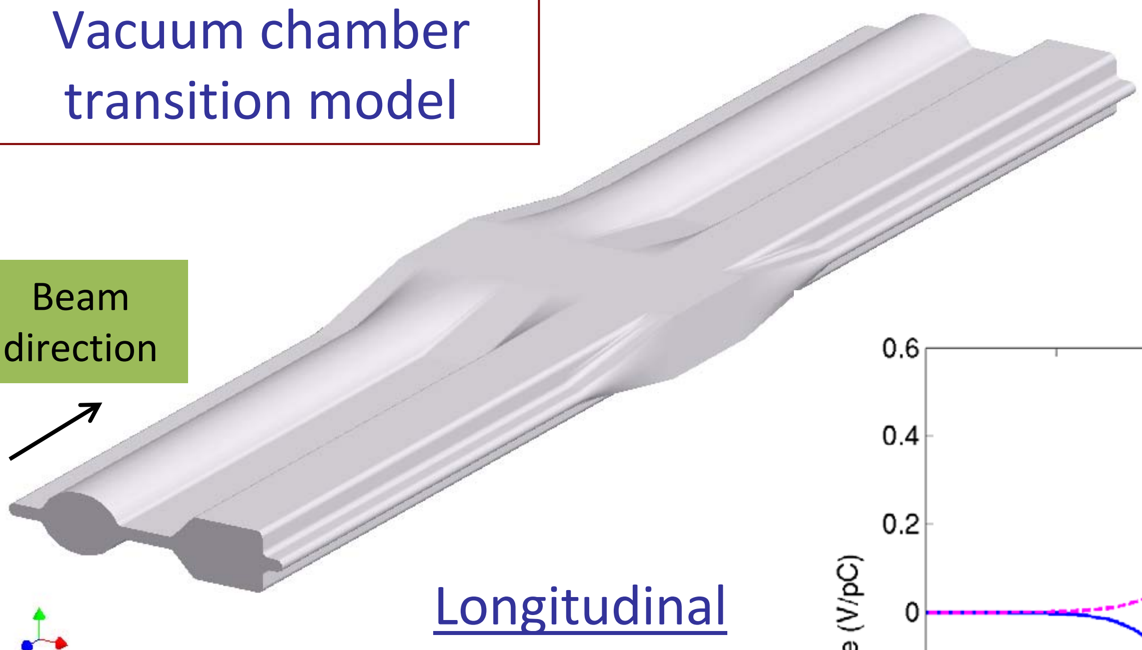
T3P - ERL Vacuum Chamber Transition

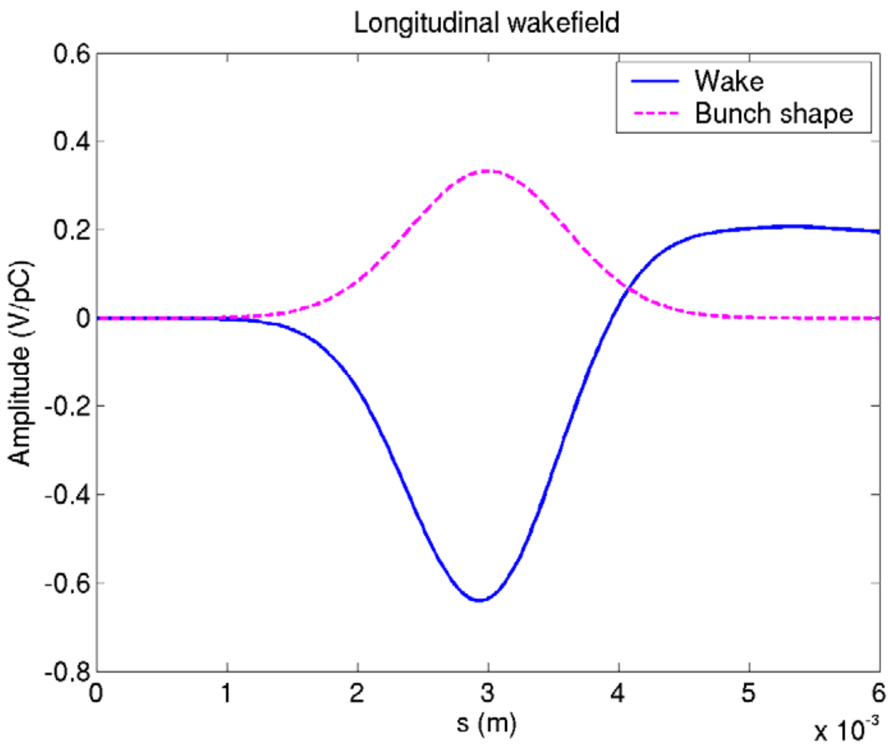
Vacuum chamber transition model

Beam direction



Longitudinal wakefield

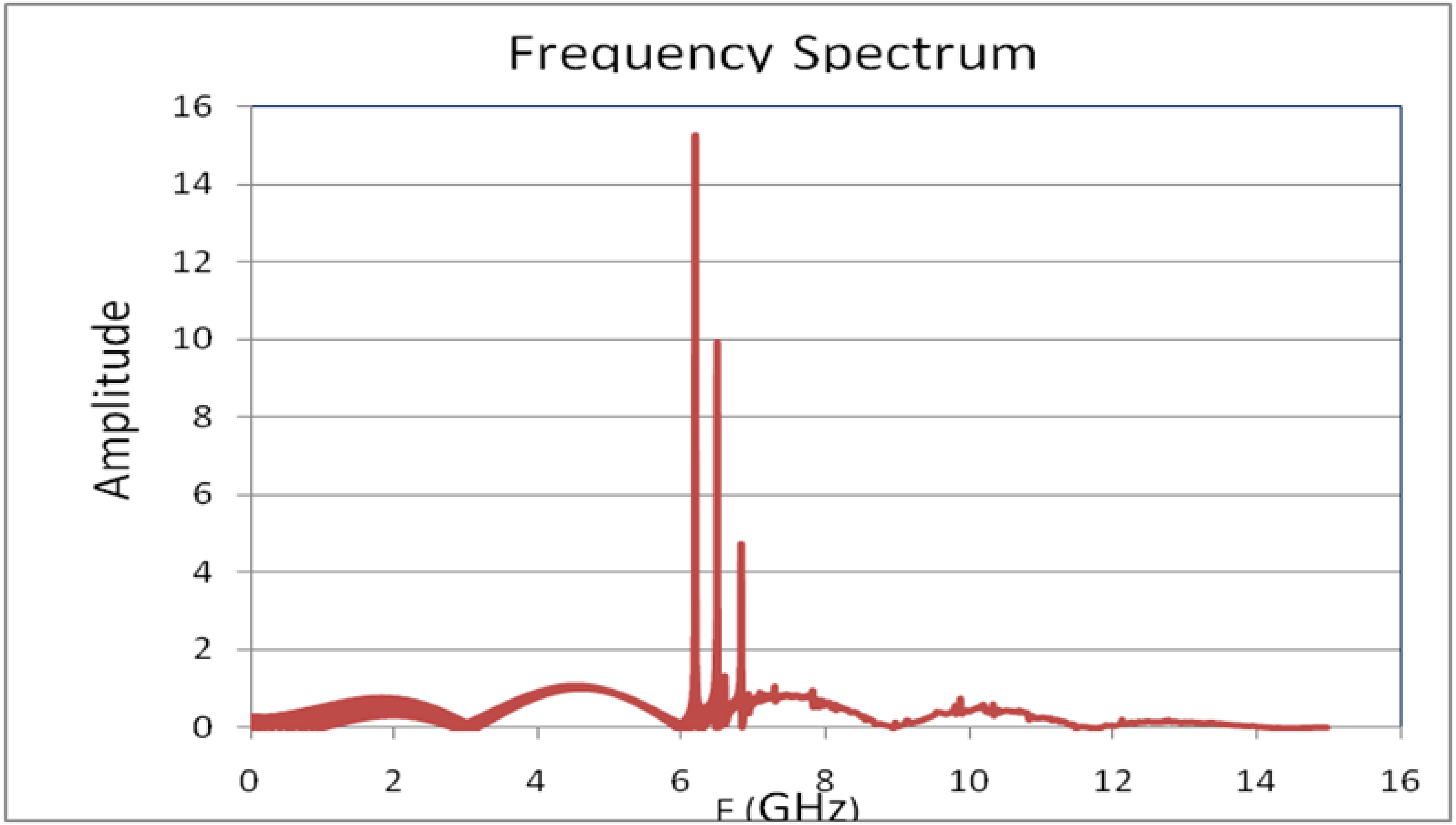
Loss factor = 0.413 V/pC for 0.6 mm bunch length



In collaboration with Cornell

T3P – ERL Trapped Modes from Beam Transit

Three longitudinal trapped modes between 6 ~ 7GHz found from beam excitation in the vacuum chamber with a **10 mm bunch**.



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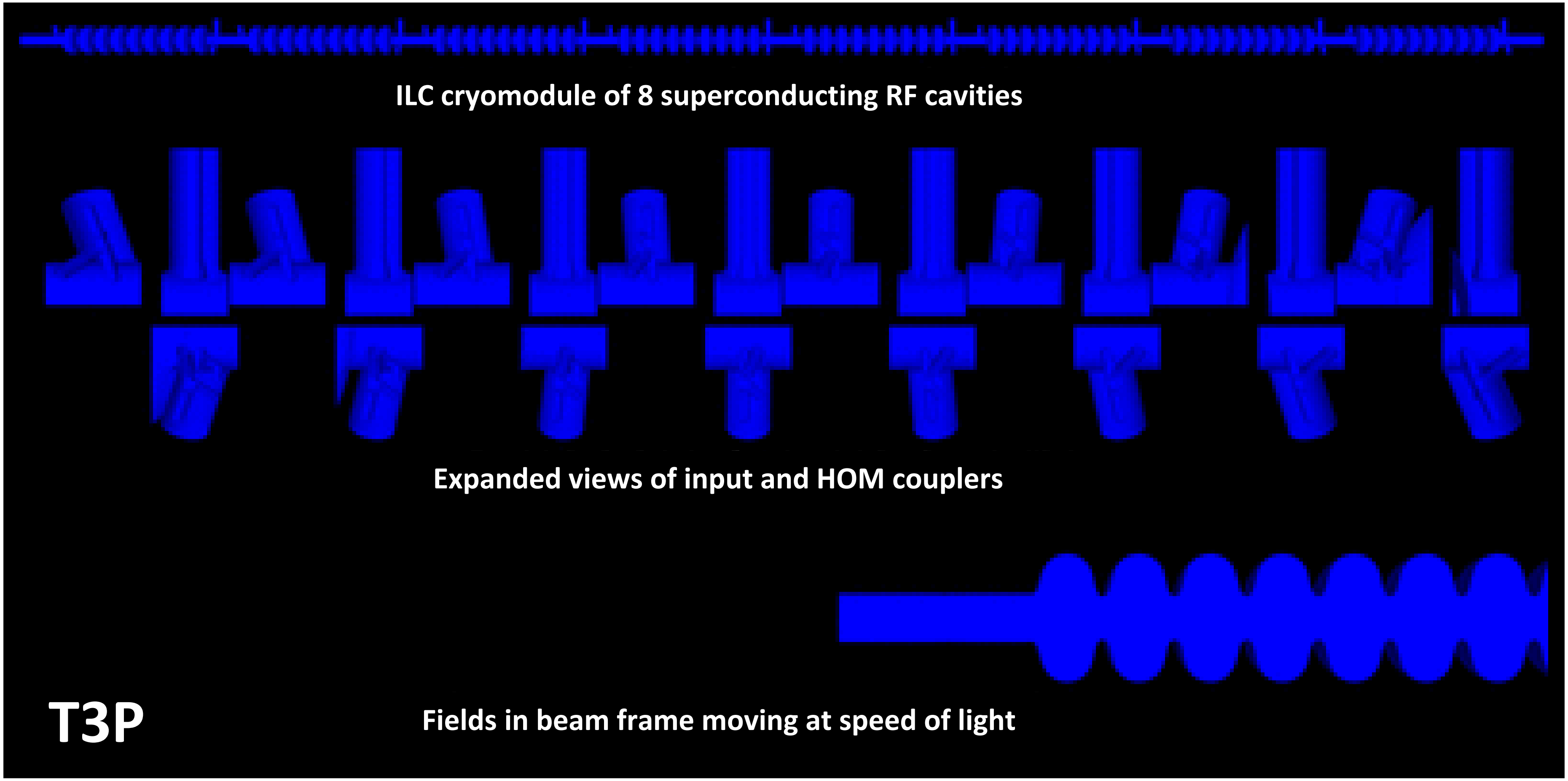
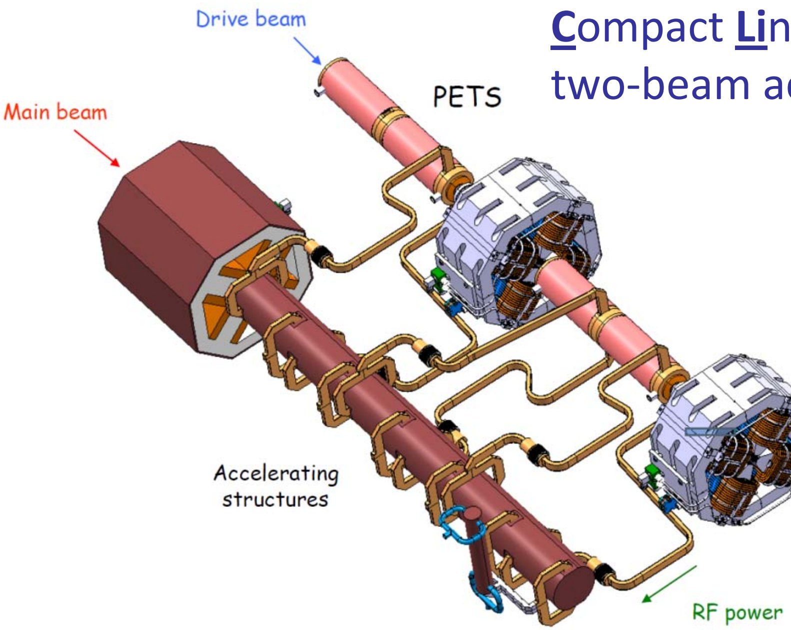
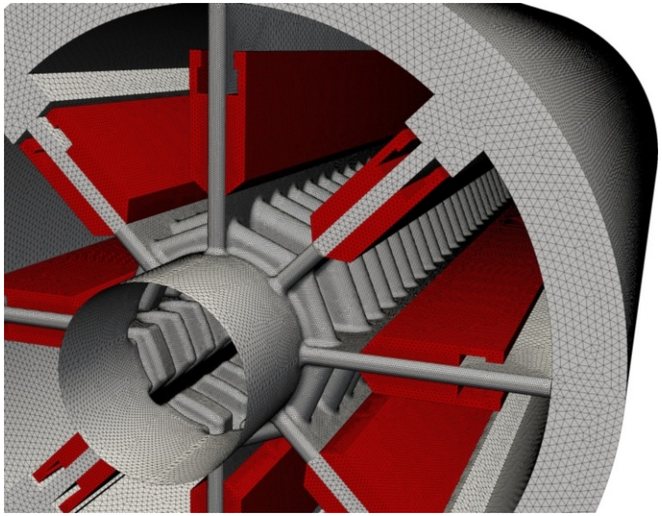
T3P – ILC Beam Transit in Cryomodule



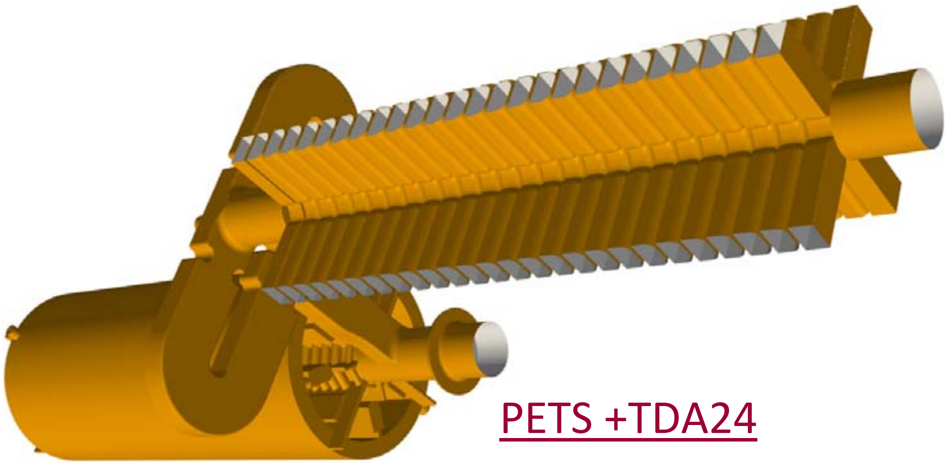
T3P – CLIC Two-Beam Accelerator

Compact Linear Collider
two-beam accelerator unit

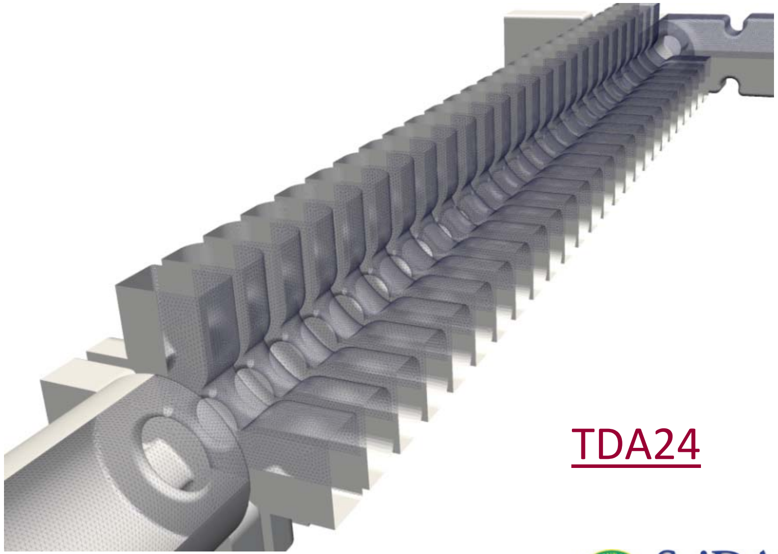




PETS



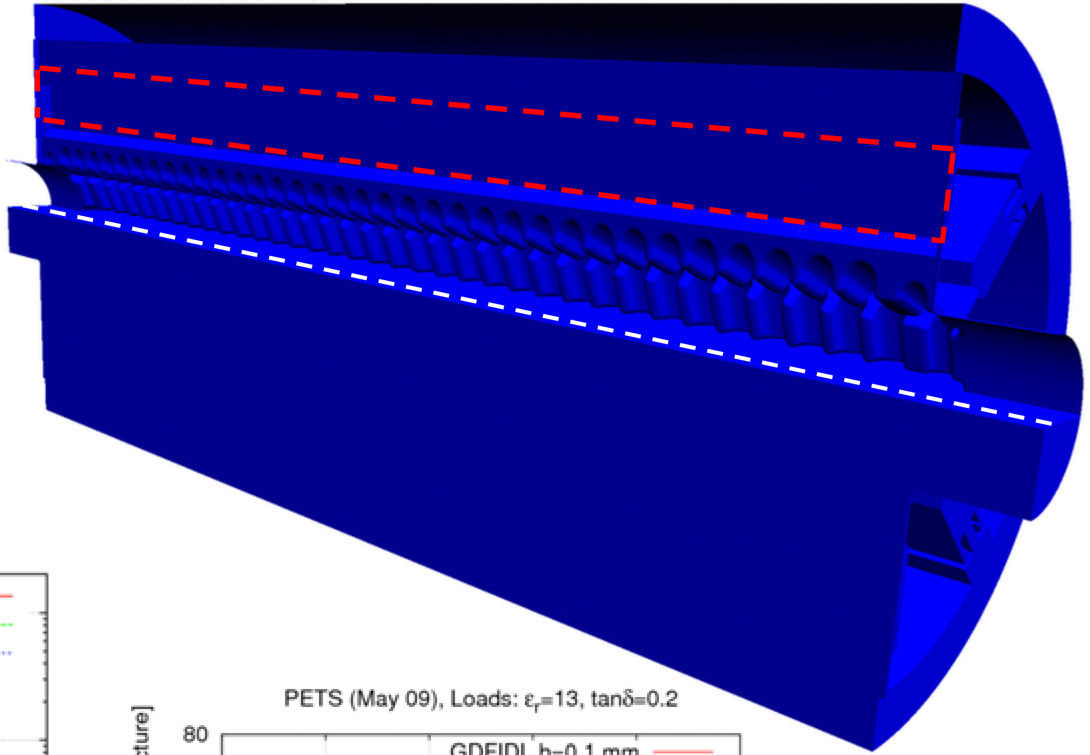
PETS +TDA24

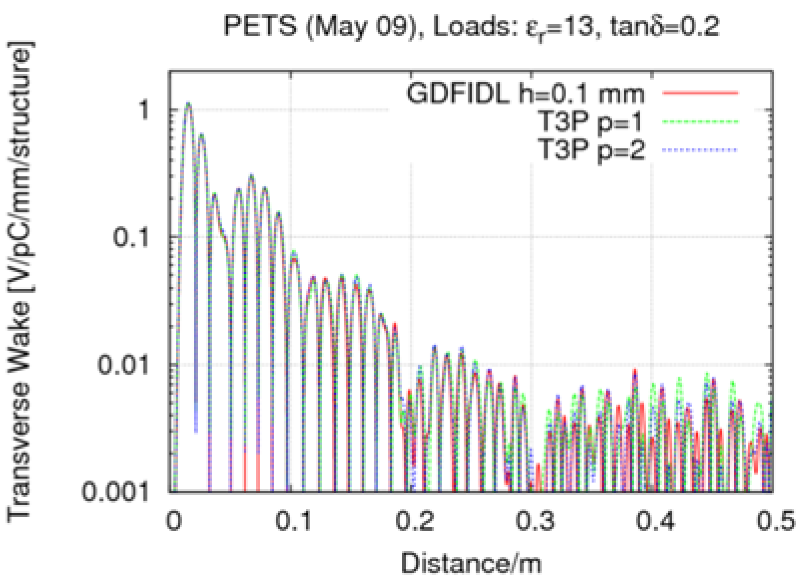


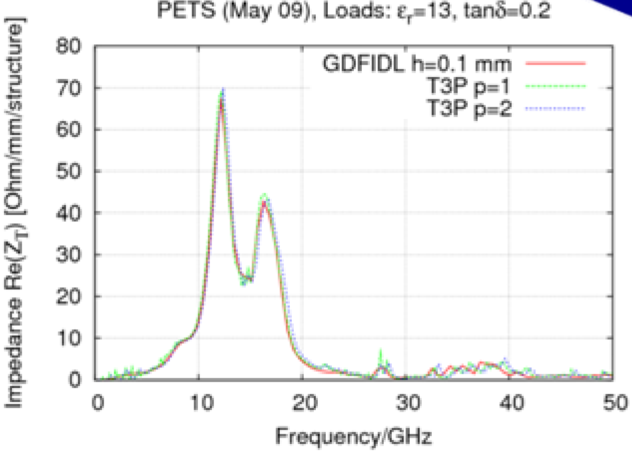
TDA24

T3P – CLIC PETS Bunch Transit

Dissipation of transverse wakefields in dielectric loads: eps=13, tan(d)=0.2







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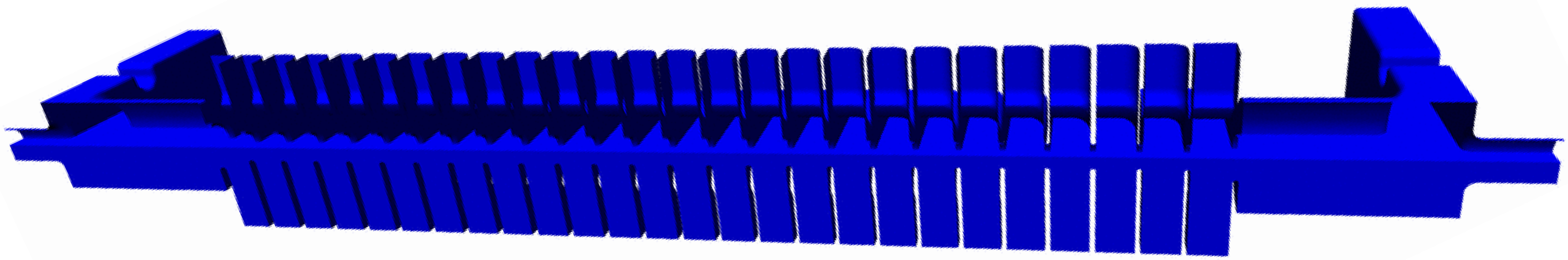
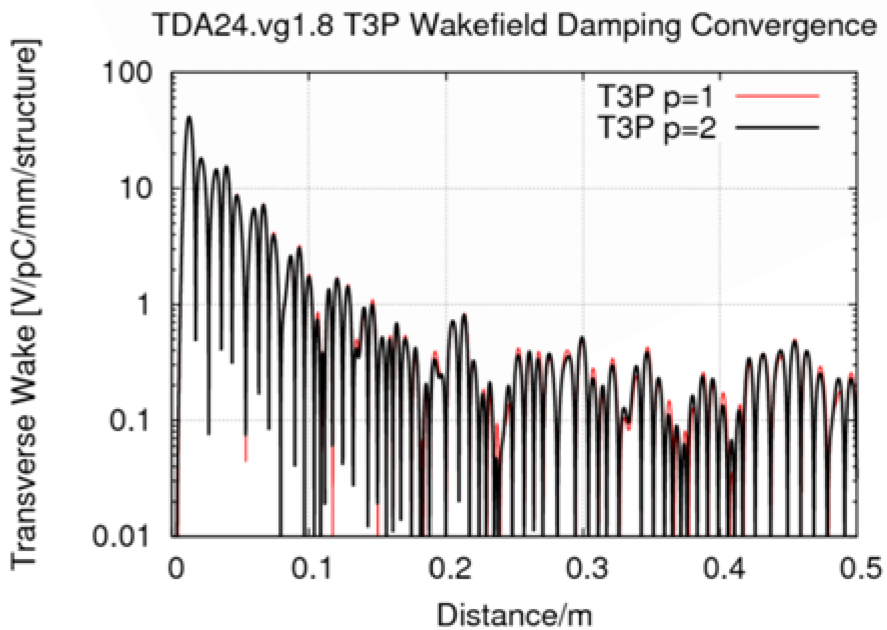
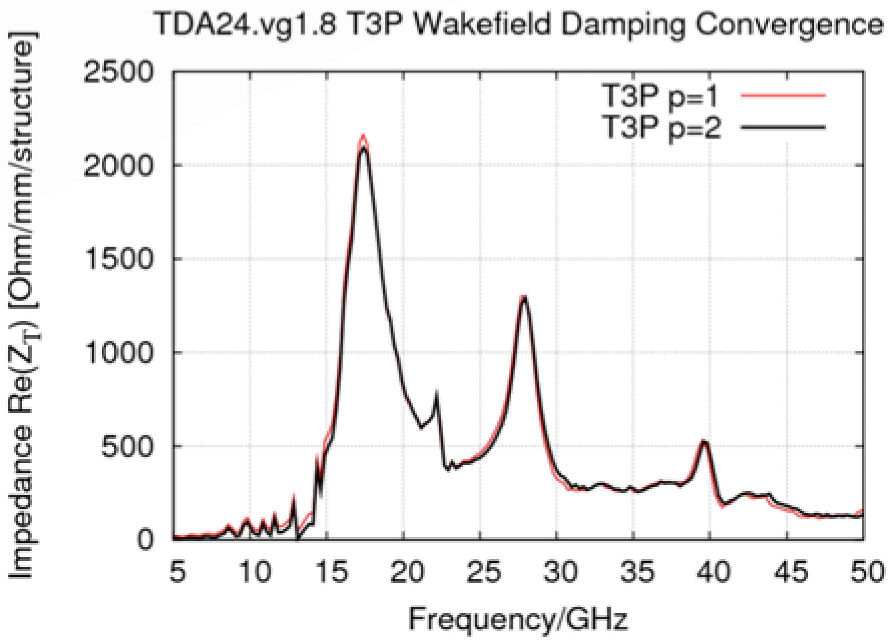
T3P – CLIC TDA24 Bunch Transit







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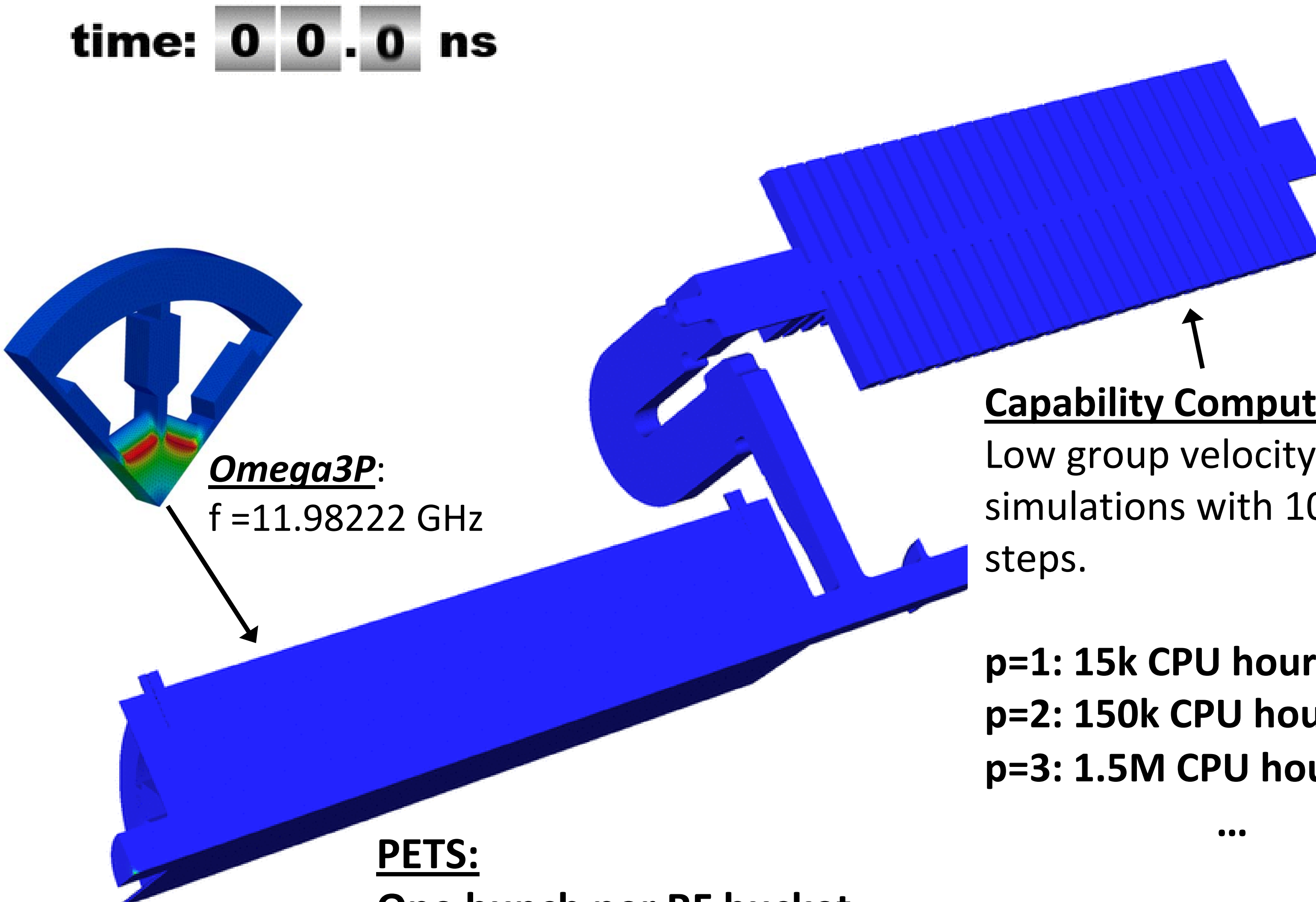
T3P – RF Power Transfer in Coupled Structure



Omega3P:
f =11.98222 GHz

PETS:
One bunch per RF bucket

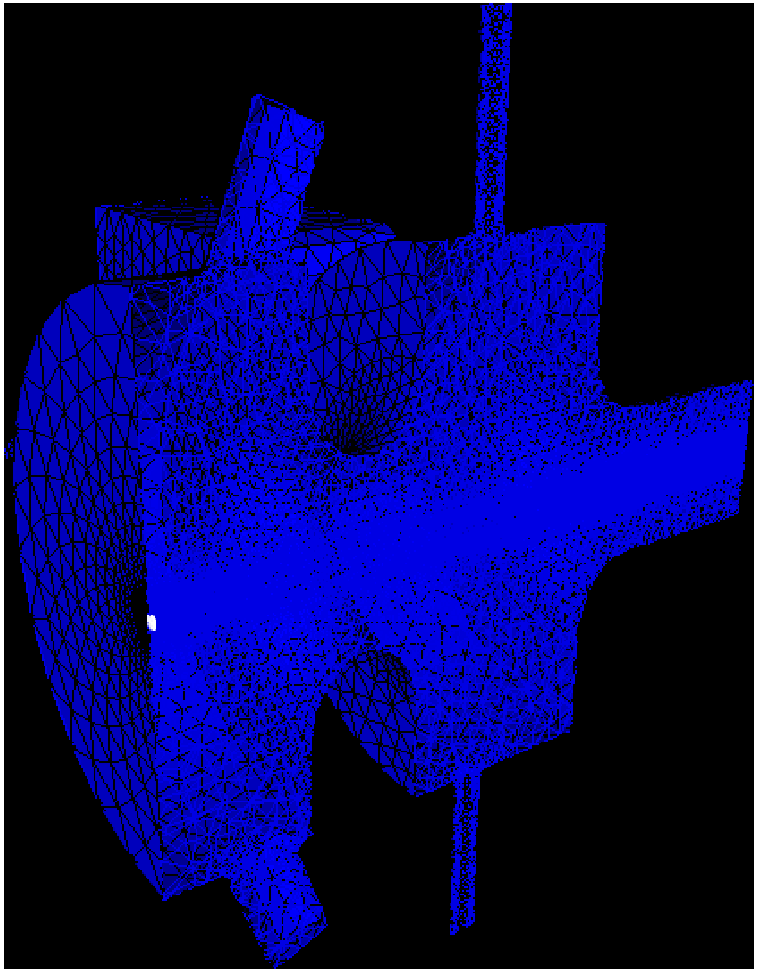
<u>Capability Computing:</u>
Low group velocity requires simulations with 100k time steps.

p=1: 15k CPU hours
p=2: 150k CPU hours
p=3: 1.5M CPU hours
…

Pic3P Capabilities

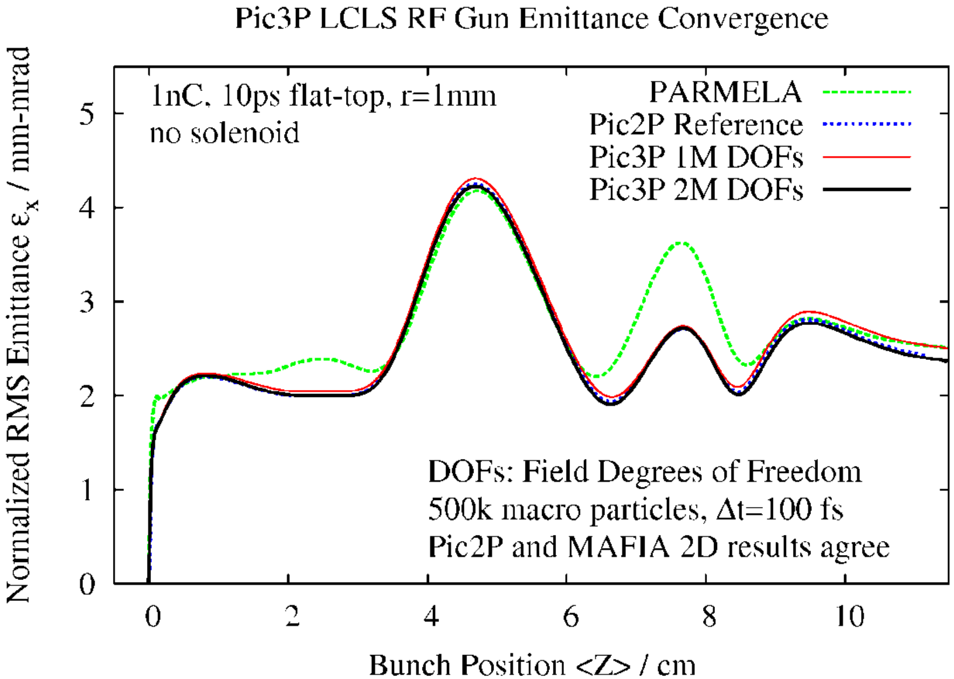
- **Pic3P** simulates beam-cavity interactions in space-charge dominated regimes
- **Pic3P** self-consistently models space-charge effects using the electromagnetic Particle-In-Cell method
- **Pic3P** delivers unprecedented simulation accuracy thanks to higher-order particle-field coupling on unstructured grids and parallel operation on supercomputers
- **Pic3P** was applied to calculate beam emittance in the LCLS RF gun and in the BNL polarized SRF gun and fast solution convergence was observed

Pic3P – LCLS RF Gun



Temporal evolution of electron bunch and scattered self-fields

Racetrack cavity design: Almost 2D drive mode. Cylindrical bunch allows benchmarking of 3D code Pic3P against 2D codes Pic2P and MAFIA



Unprecedented Accuracy thanks to Higher-Order Particle-Field Coupling and Conformal Boundaries

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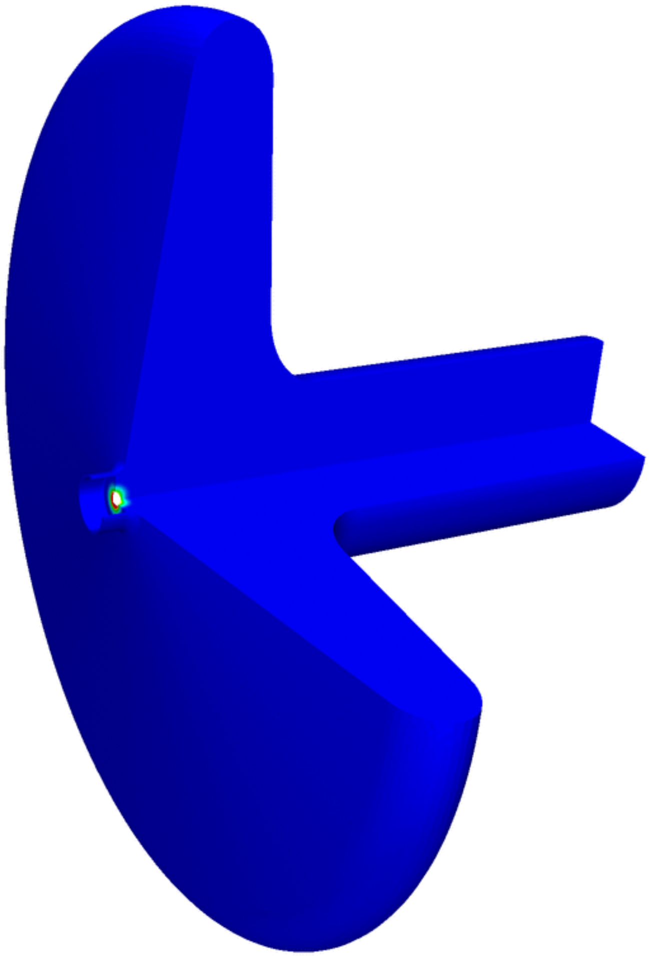
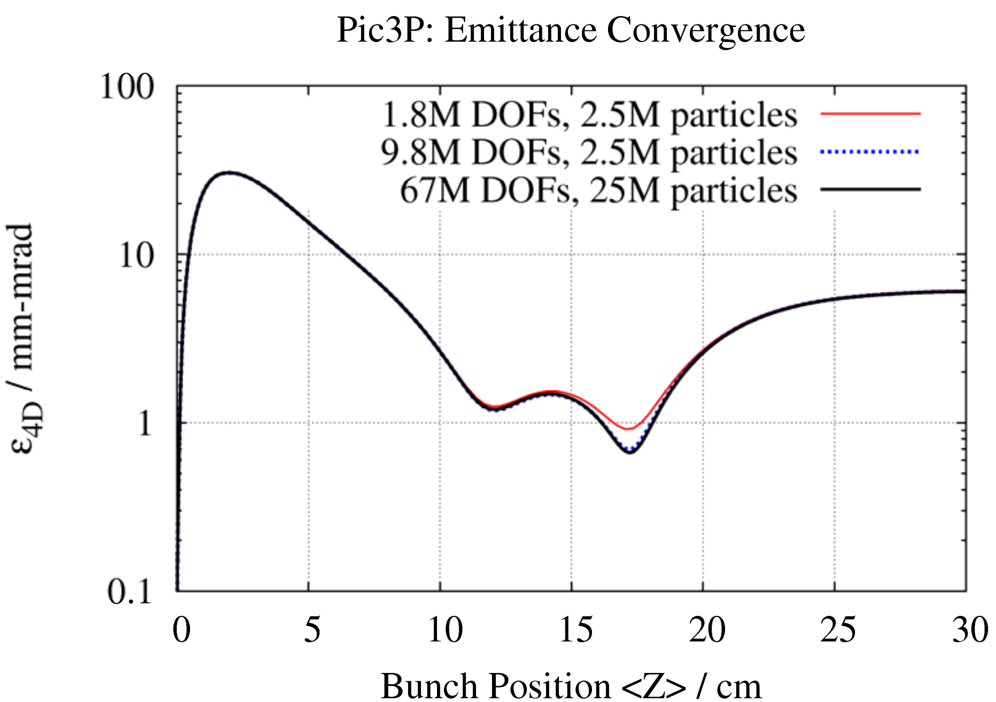
Pic3P – BNL Polarized SRF Gun

Bunch transit through SRF gun (only space-charge fields shown)



BNL Polarized SRF Gun:

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



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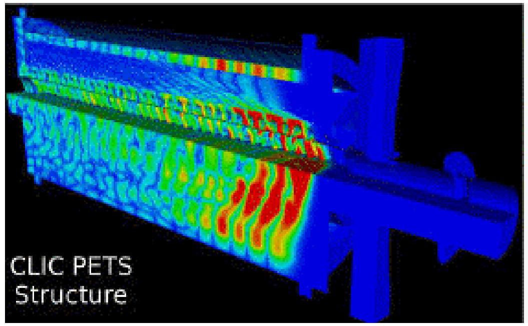
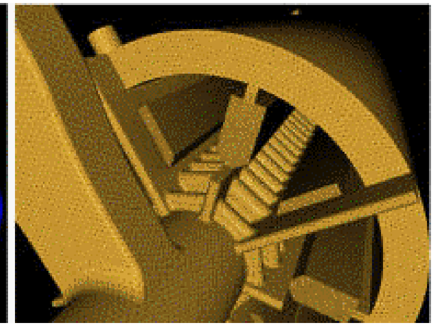
ACE3P User Community – CW10 Code Workshop

CW10 ACCELERATOR CODE WORKSHOP | SLAC NATIONAL ACCELERATOR LABORATORY

- Home
- Agenda
- Attendees
- Software
- Worshop Materials
- SLAC Computer Accounts





Accelerator Code Workshop (CW10) at SLAC for the ACE3P (Advanced Computational Electromagnetics 3P) Code Suite organized by the Advanced Computations Group (ACG)

Date — September 20-22, 2010
Time — TBD
Place — SLAC National Accelerator Laboratory
Menlo Park, California

Contact — ACG-CW10@slac.stanford.edu
650-926-2864
650-926-4603 (FAX)

SLAC ACCESS

All visitors must have a valid photo ID to enter the Laboratory. The SLAC Main Gate is open 24 hours a day, 7 days a week.

MAPS AND DIRECTIONS

» More Information

SLAC GUEST HOUSE

» More Information

SLAC National Accelerator Laboratory, Menlo Park, CA
Operated by Stanford University for the U.S. Dept. of Energy

Office of Science

(http://www-conf.slac.stanford.edu/CW10/default.asp)

SciDAC Scientific Discovery through Advanced Computing

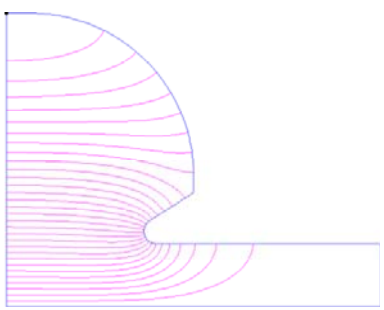
... after this excursion, now back to basics:

PREPARING FOR THE EXERCISE

Would *you* like to design a cavity?

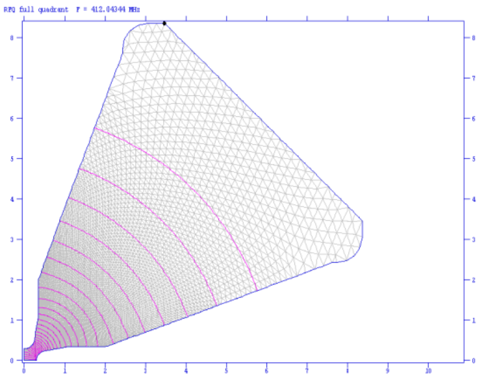
- Superfish is 2-D. The 2 coordinates can be R-Z in cylindrical or X-Y in cartesian.
- Losses must be small (perturbation method).
- Please come up with ***your own ideas*** of what you would like to do!
- Examples for your inspiration:

Nose cone cavity:

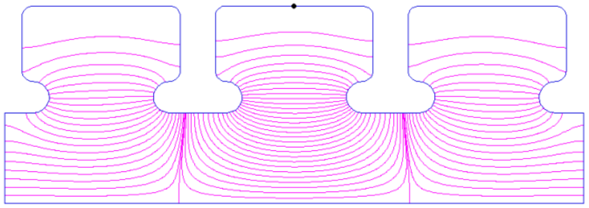


Ferrite cavity:

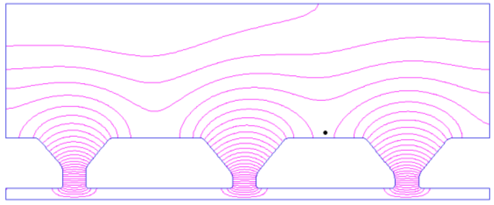
RFQ:



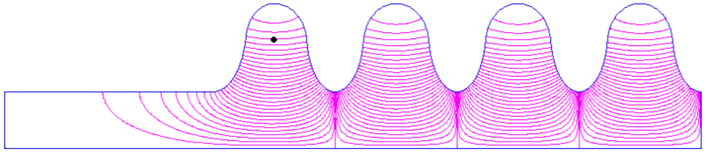
2pi/3 TW structure:



DTL:



Elliptical cavities:



Poisson/Superfish

The history of these codes starts in the sixties at LBL with Jim Spoerl who wrote the codes “MESH” and “FIELD”. They already solved Poisson’s equation in a triangular mesh.
Ron Holsinger, Klaus Halbach and others from LBL improved the codes significantly; the codes were now called “LATTICE”, “TEKPLOT” and “POISSON”.
From 1975, when Holsinger came to Los Alamos, development continued there and Superfish came to life (French *poisson* = English *fish*). It could do eigenfrequencies!
Since 1986, the Los Alamos Accelerator Code Group (LAACG) has received funding from the U.S. Department of Energy to maintain and document a standard version of these codes.
In 1999, Lloyd Young, Harunori Takeda, and James Billen took over the support of accelerator design codes, which were heavily used in the design of the SNS.
The codes were ported to DOS/Windows from the early nineties, the latest version 7 is from 2003. To my knowledge, other versions are presently not supported.

The Los Alamos Accelerator Code group maintain these codes still today with competence and free of charge.
http://laacg1.lanl.gov/laacg/services/services.phtml