THE DOE GRAND CHALLENGE IN COMPUTATIONAL ACCELERATOR PHYSICS: ELECTROMAGNETICS COMPONENT*

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THE DOE GRAND CHALLENGE IN COMPUTATIONAL ACCELERATOR PHYSICS

Collaborating Institutions:

Beam Dynamics - LANL (R. Ryne), UCLA (V. Decyk), ACL (J. Reynders)

Electromagnetics - SLAC (K. Ko), Stanford (G. Golub), NERSC (E. Ng)

Goals:

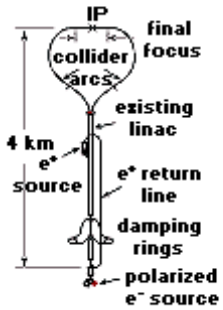
- ***Develop*** a new generation of accelerator modeling tools targeted to high performance computing platforms

- ***Apply*** tools to present and future accelerator applications of national importance

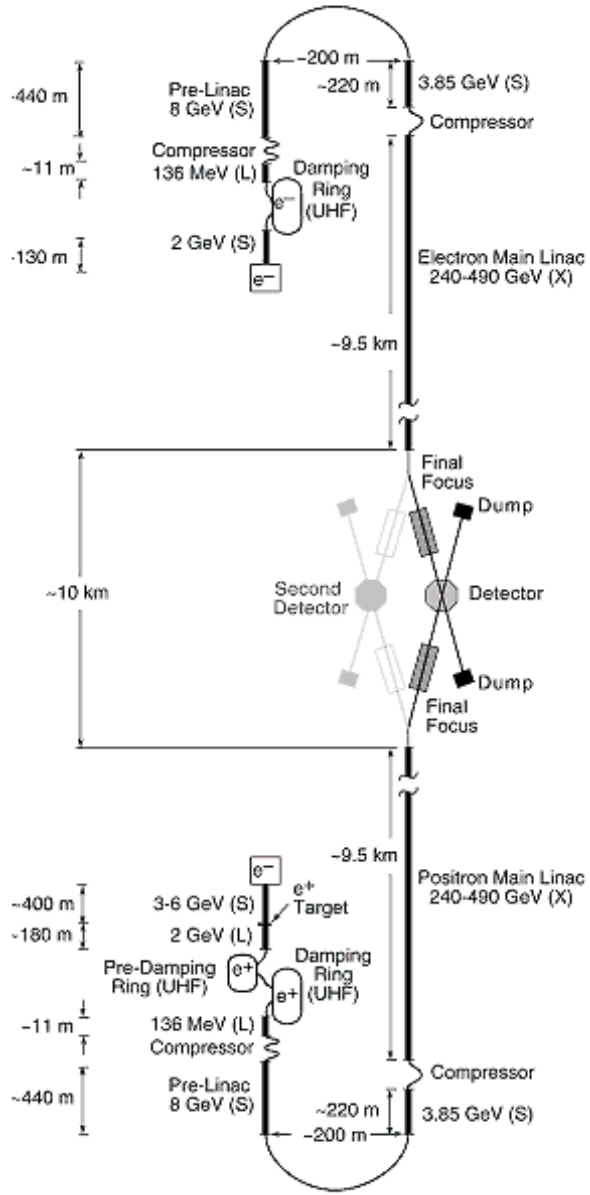
Outline

- **Next Linear Collider Structure Design**
- **DOE Grand Challenge Achievements**
- **Large Scale Simulation Components**
- **Summary**

SLC
100 GeV

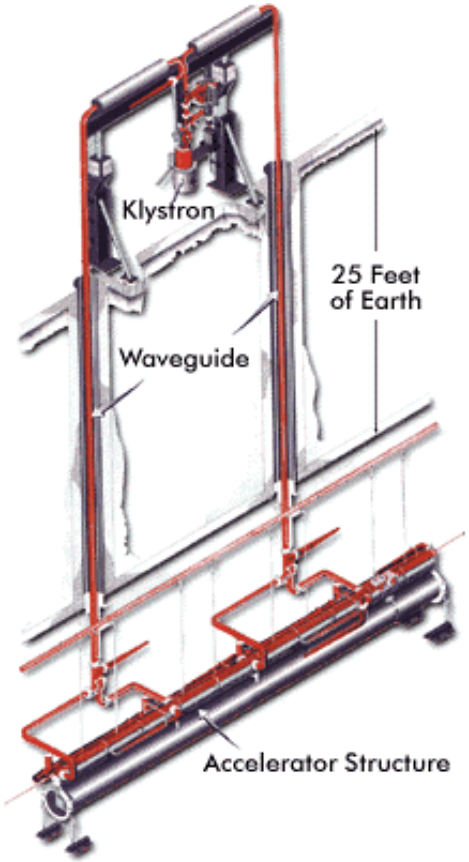


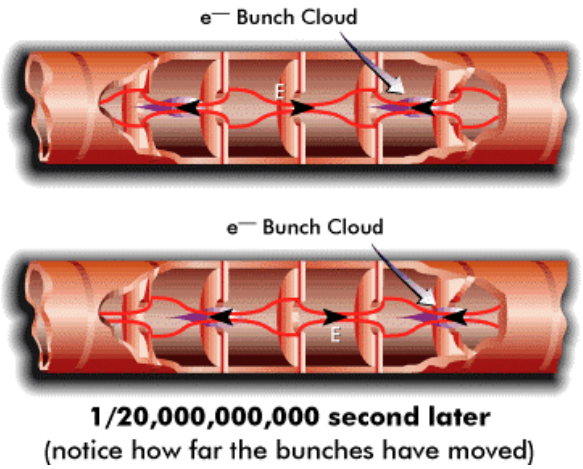
NLC
0.5 - 1.5 TeV

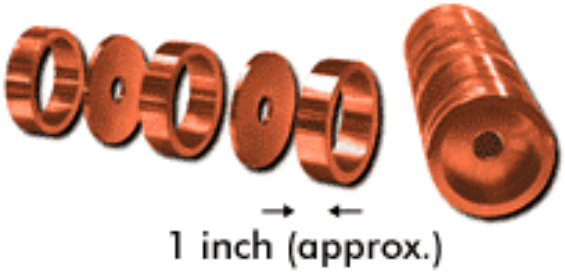


SLC Linac Structure

Accelerating Structure - Cylindrically symmetric Disk-Loaded WaveGuide (DLWG)







Main Linac Comparison

	SLC	NLC
Center of Mass	100 GeV	500 GeV
Bunches per pulse	1	95
Operating Frequency	(S) 2.856 GHz	(X) 11.424 GHz
Number of Cavities	80,000	2 million
Post-Tuning	yes	No

NLC Linac Structure - Design Requirements

Electrical:

- Maximize shunt impedance of Accelerating Mode to increase structure efficiency
- Minimize wakefields due to Higher-Order-Modes to preserve low emittance of multi-bunch trains

Mechanical:

- Improvement in vacuum conductance
- Precision machining to micron tolerances
- Manufacturability for mass production

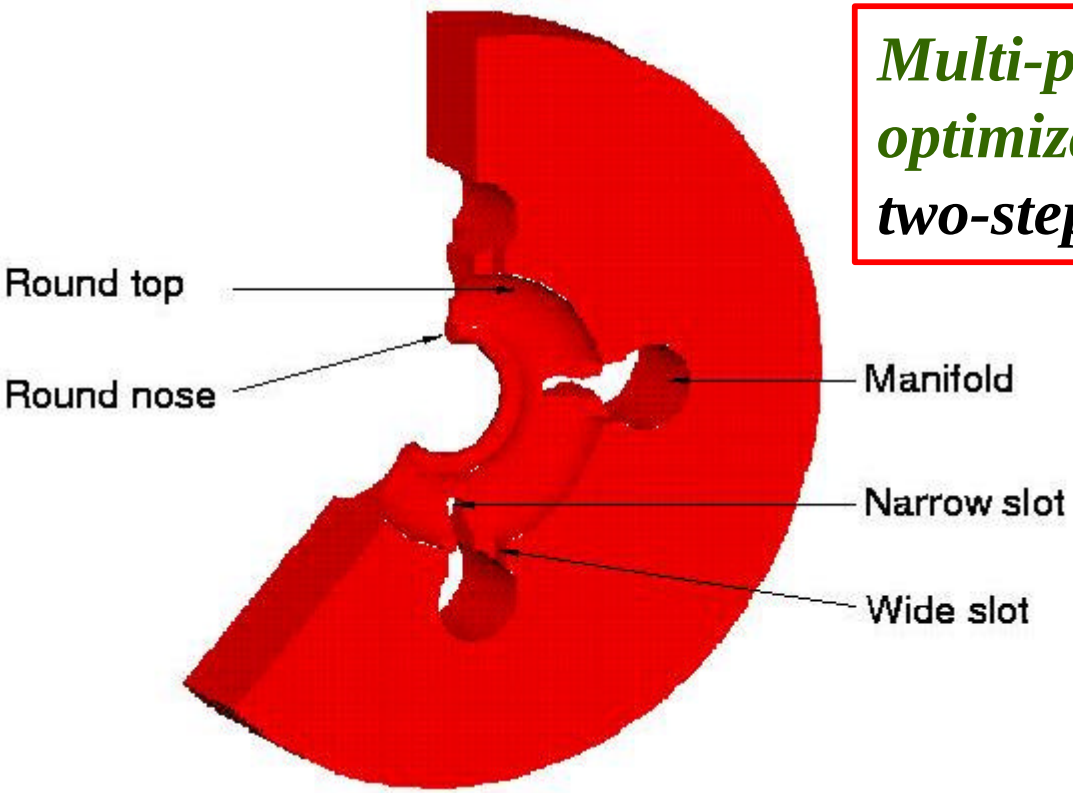
Goal is to Optimize Performance, Lower Cost & Reduce Risk

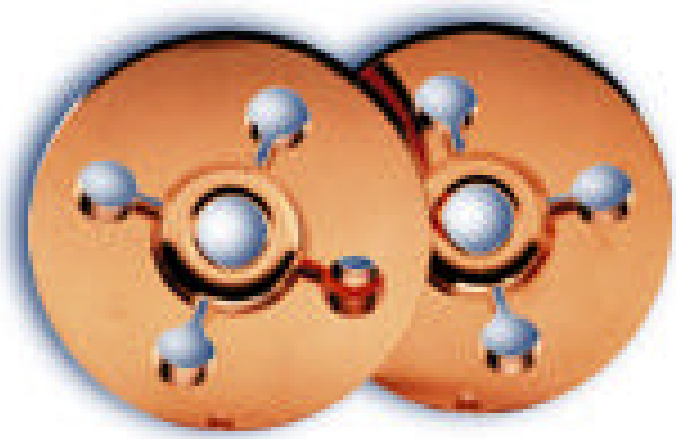
NLC Accelerating Structure

Round **D**amped **D**etuned **S**tructure: **(RDDS)**

- Fully *three-dimensional*
- *Eleven* cell dimenions

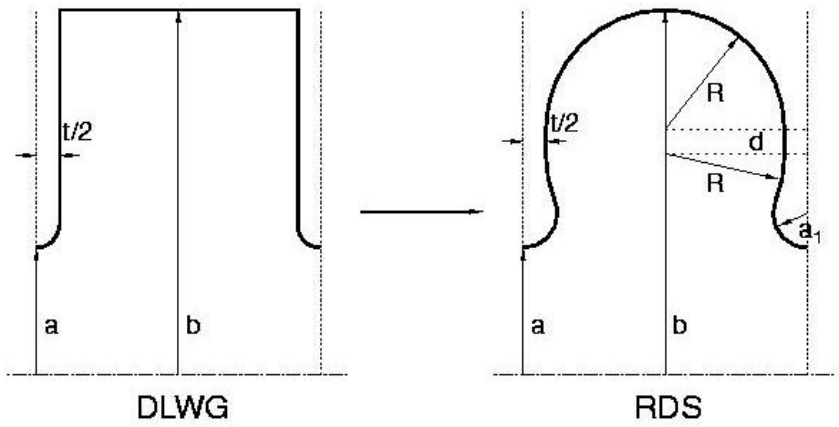
***Multi-parameter, multi-constraint optimization problem* solved by a two-step design procedure!**



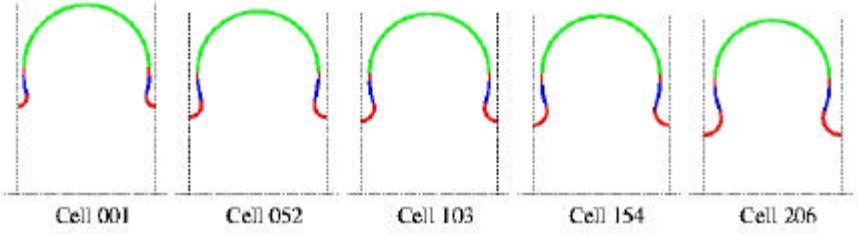


Cell Shape Optimization - 2D

- Round cavity contour to increase shunt impedance of Accelerating Mode by 15% (negligibly more expensive with computer controlled machining)

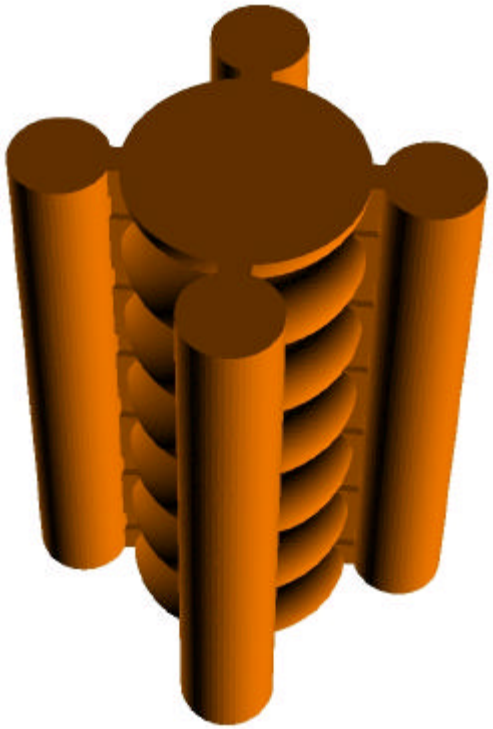


- Cell-to-cell variation in dimensions (order of microns) to detune Higher Order Modes and reduce wakefields by factor of >100



*Developed 2D finite element codes **Omega2** and **Omega2P** to design **RDS cell** and study wakefields in **206-cell section***

Round Damped Detuned Structure - 3D



- Add Damping Manifold to suppress long-range wakefields but retain RDS performance
- Require 0.01% frequency accuracy to maintain structure efficiency
- Existing 3D codes on desktop computers cannot deliver the required accuracy & resolution

Parallel *field solver that can model* ***Large, Complex*** *electromagnetic structures to* ***high accuracy*** *is needed!*

Linear Collider Structure Simulation

- **Round Detuned Cell**

RF parameters Omega2

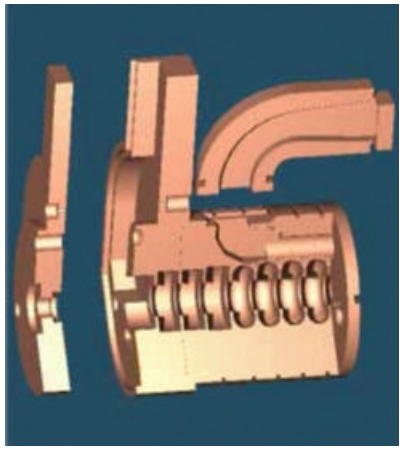
- **Round Detuned Structure (RDS - 206 cells)**

Transverse Wakefields Omega2P

- **Round Damped Detuned Cell**

RF parameters Omega3P

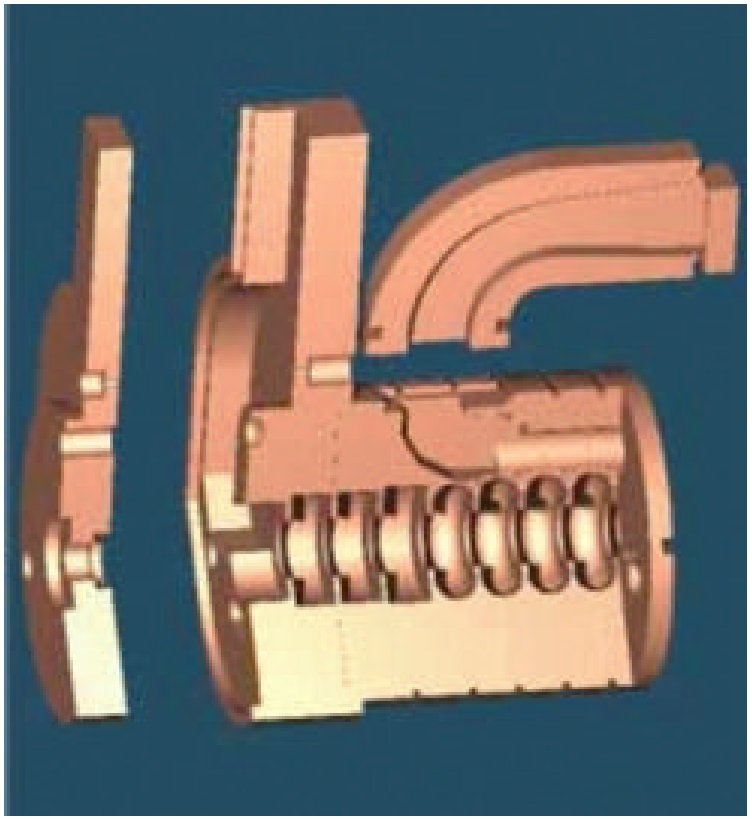
- **Round Damped Detuned Structure (RDDS - 206 cells)**



Transverse Wakefields Omega3Pc

Large-Scale Electromagnetic Simulations

RDDS for the NLC



- **Cell Design** requires frequency error of 1 part in 10,000 - mesh size close to fabrication tolerance
- **Wakefield Analysis** needs 206-cell section to verify RDDS scheme in preserving emittance

10^6 to 10^9 degrees of freedom

"High-Resolution" design, "System-Scale" analysis *only possible on* ***very large scale*** *computers*

DOE Grand Challenge - Parallel Codes

Under the **DOE Grand Challenge**, two application codes were developed:

- ***Omega3P* - *3D Parallel Finite Element Eigensolver*** *to find normal modes of RF cavities*
- ***Tau3P* - *3D Parallel Time Domain Solver*** *to calculate the transmission properties of electromagnetic structures*

Common features:

- Object-Oriented Design - C++ implementation
- Message Passing Interface (MPI) for communication
- Unstructured Grid for conformal meshes

Omega3P: Frequency-Domain on Finite Element Grid

Omega3P consists of 2 main modules:

DIstMesh - C++ Library for distributed 3D unstructured mesh operations via MPI that supports a comprehensive set of finite element shapes (Tetrahedra, Prisms, Pyramids, and Hexahedra) using the NURBS geometry representation, and their partitioning onto processors.

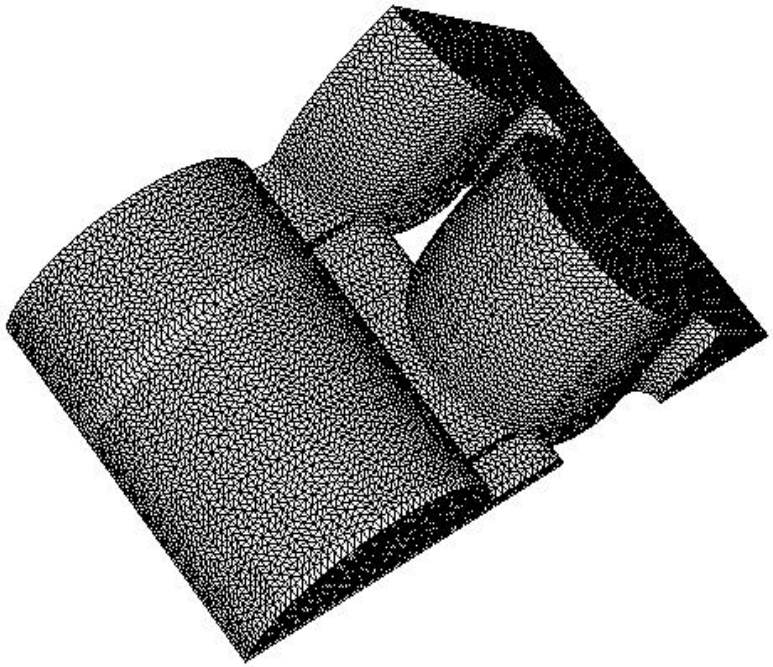
Eigensolve - Designed to solve the Generalized Eigenvalue problem (K x = ë M x) in parallel for very large sparse matrices with a new filtering algorithm that combines:

- Spectrum transformation and band pass polynomial filtering
- Inexact Krylov subspace projection
- Modified Jacobi-Davidson local refinement

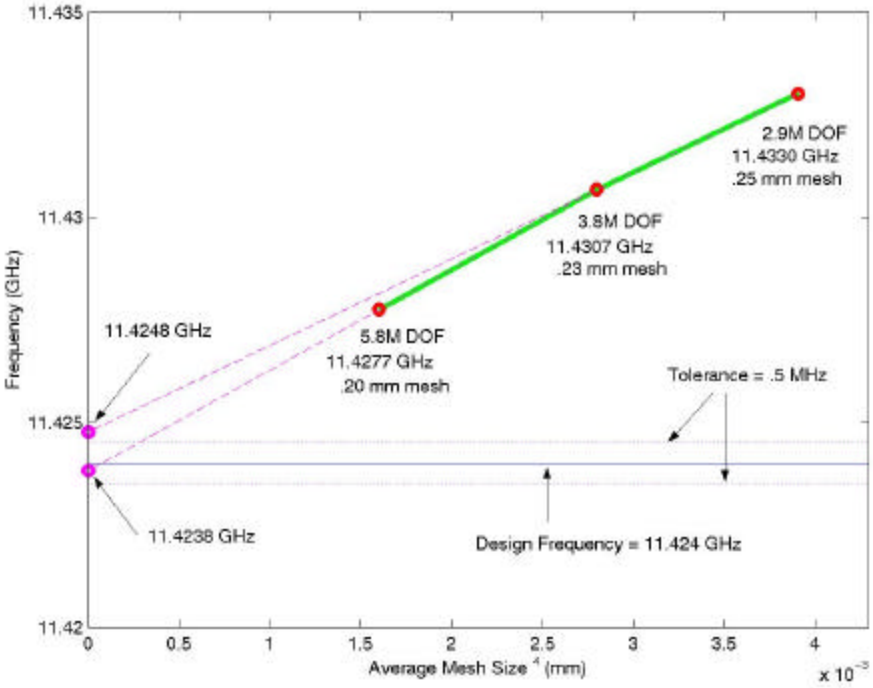
to provide superior accuracy and convergence over other solvers

Omega3P Modeling of RDDS Cell

RDDS Mesh



Accelerating Mode

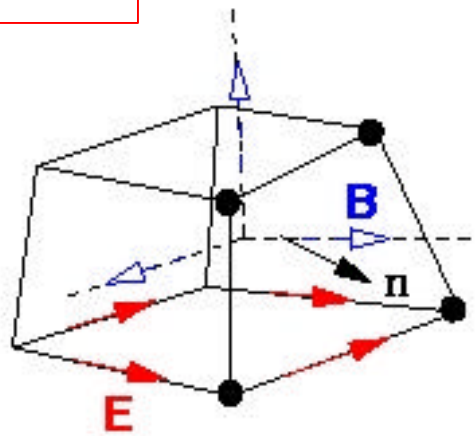


Frequency accuracy to 1 part in 10,000 is achieved

Tau3P: Time-Domain on Unstructured Grid

Discrete Surface Integral Method

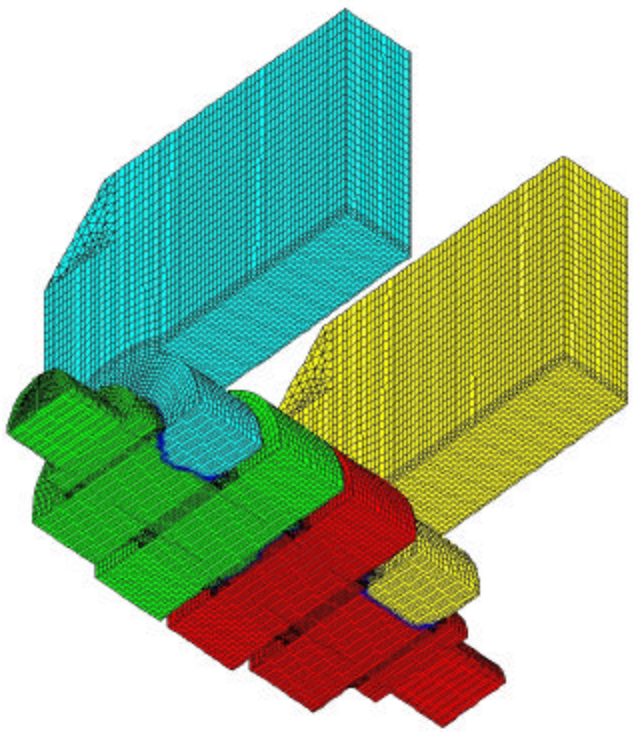
- Non-orthogonal dual grid (**E** on primary, **B** on dual)
- Fields on grid averaged over neighboring cells



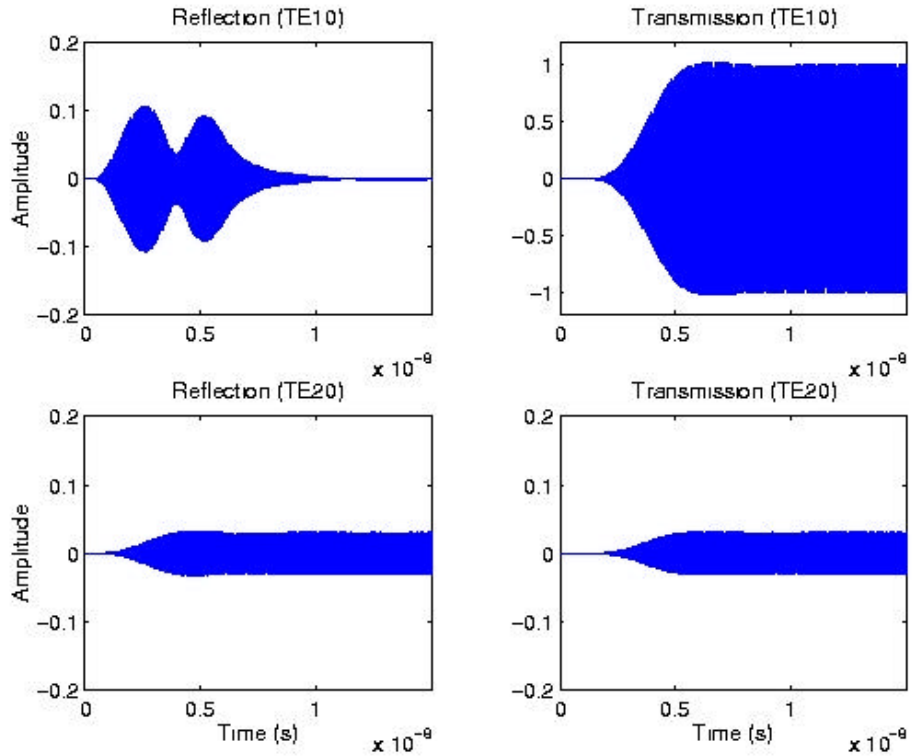
- *DistMesh Library for unstructured mesh distribution*
- *Leapfrog time advancement scheme with filtering*
- *broadband matched impedance B.C. at waveguide ports to model pulse propopation*

Tau3P Modeling of RDDS Input Coupler

Input Coupler Mesh



Match at 11.424 GHz



Excellent agreement between measurement & simulation

Grand Challenge Achievements

- Developed Parallel Application codes that utilize NERSC HPC resources to solve a challenging design problem for the NLC (important milestone in project)

- Improved accelerating structure design (RDDS) leads to savings in NLC machine cost ~$100 million (higher gradient results in shorter linac length ~ 6%)

- New capability enables Simulations orders of magnitude greater than previously possible (***Omega3P*** on T3E can model millions of DOF's in minutes - much shorter design cycle)

- Applied to other projects : PEP-II, ALS, APT & SNS

Large Scale Simulations - Components

Large Scale Electromagnetic Simulation consists of many computing technologies each of which has to be optimized for it to be an effective modeling tool for accelerator design:

- Parametric Geometry - CAD models to facilitate optimization
- Mesh Generation - impacts matrix conditioning/time-stepping
- Domain Decomposition - partitioning tools for load balancing
- Parallel Solvers - scalable algorithms with fast convergence
- Adaptive Refinement - improve accuracy/optimize resources
- Visualization - efficient post-processing of large data sets
- Performance/Error Analysis - computer science/applied math

Multi-Disciplinary Approach

Success of Large Scale Simulation depends on integrating the combined efforts of a multi-disciplinary team that includes application scientists, applied mathematicians, computer scientists, software engineers, geometry builders, visualization experts etc.

SLAC's Numerical Modeling Group consists of:

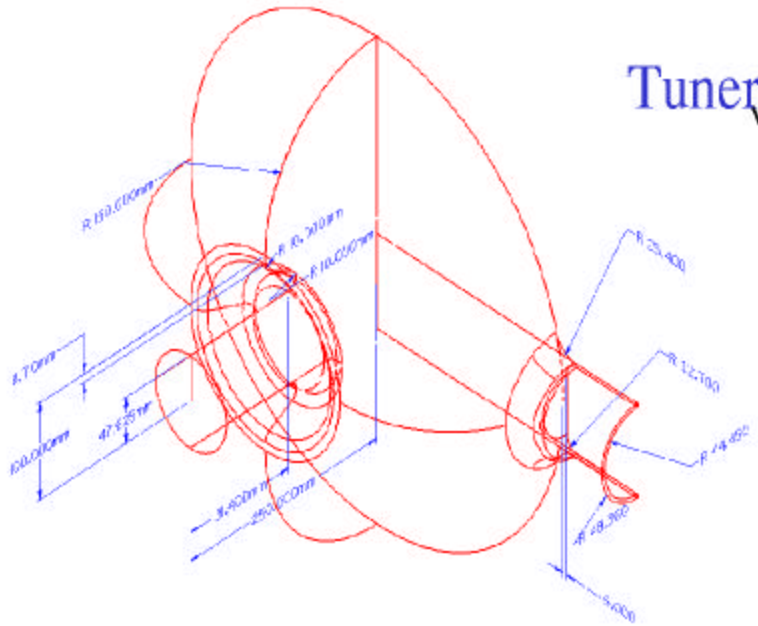
Accelerator Physicists - Kwok Ko, Cho Ng, Zenghai Li

Computer Scientists/Software Engineers - Brian McCandless, Nate Folwell, Michael Wolf

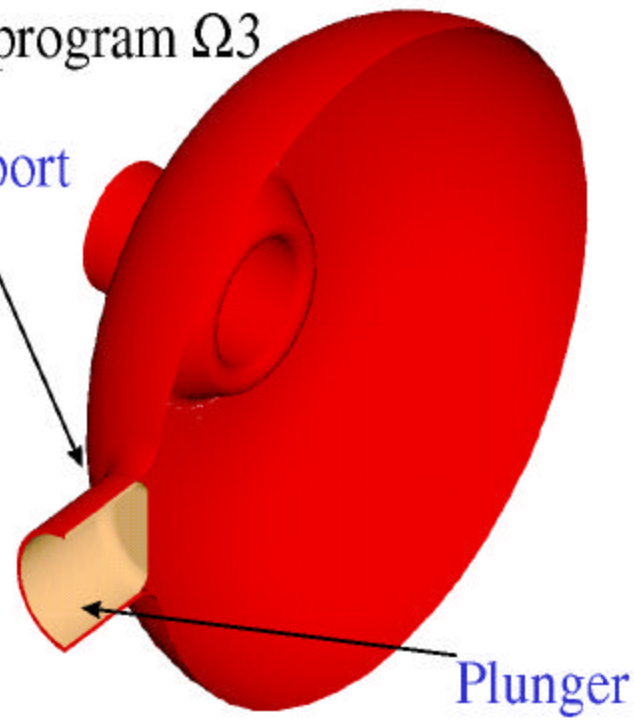
Applied Mathematicians - Yong Sun, Wanjun Mi, Misha Saparov (Graduate students from Prof. Gene Golub's SCCM Program)

Parameterized solid model

– Analyze cavity with tuner using program Ω3



Engineering drawing



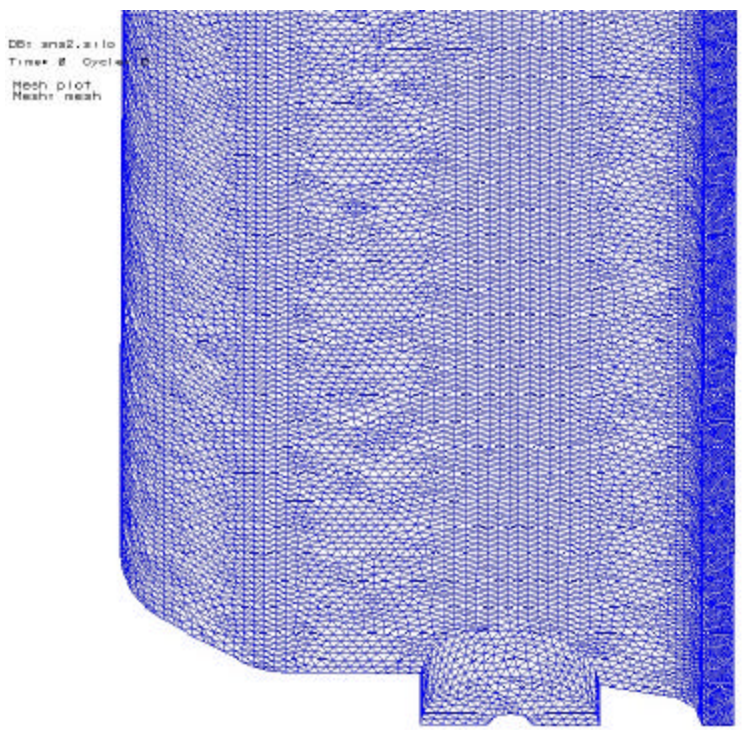
Parametric Solid model

- Interface to a variational solid modeler EMS/Intergraph
- Can resolve necessary features (e.g., small distance between the tuner port and the plunger)
- Easy to change plunger position

Mesh Generation

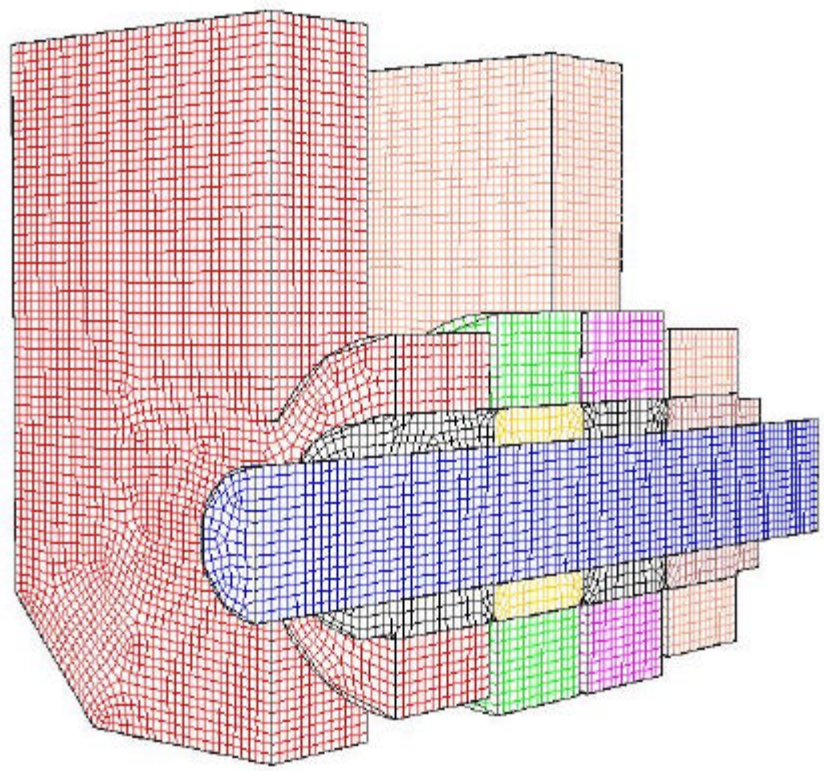
Parallel Mesh Generation is needed for large geometries

Tetrahedral mesh for ***Omega3P*** from ***SIMAIL*** (Simulog)



RFQ Cavity for SNS

Hexahedral mesh for ***Tau3P*** from ***CUBIT*** (Sandia)

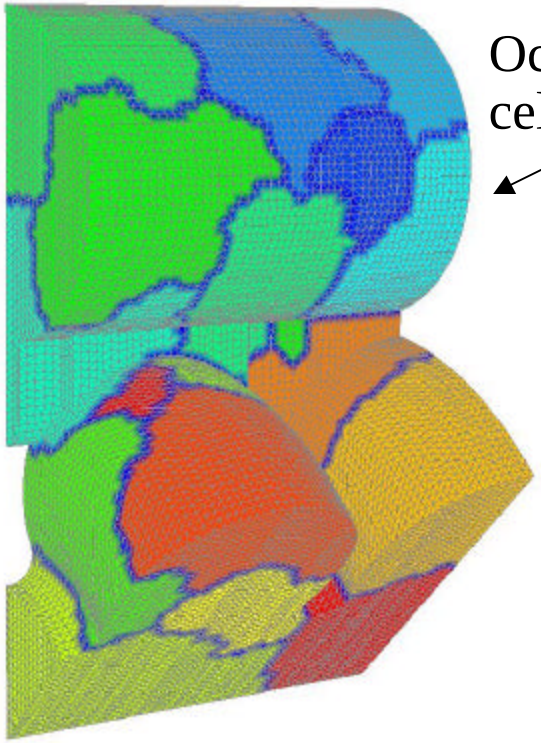


Input Coupler for NLC

Domain Decomposition

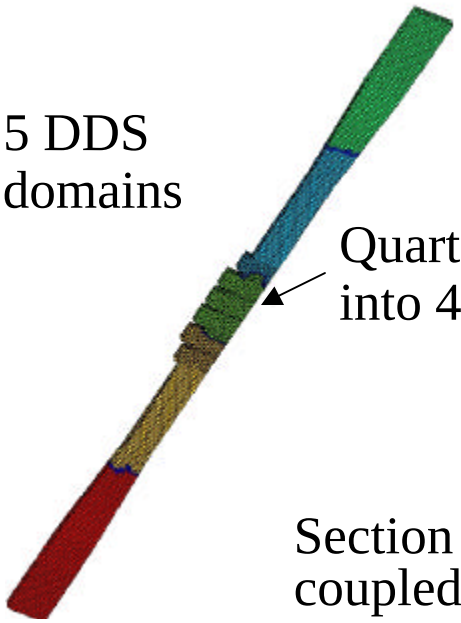
Load Partitioning uses ParMETIS from ACTS Toolkit

Omega3P



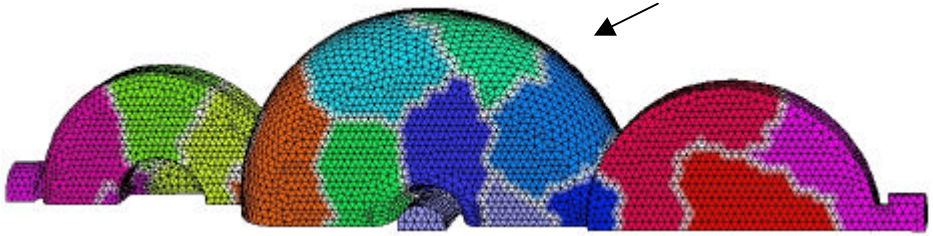
Octant of 1.5 DDS cell into 16 domains

Tau3P



Quarter of RF choke into 4 domains

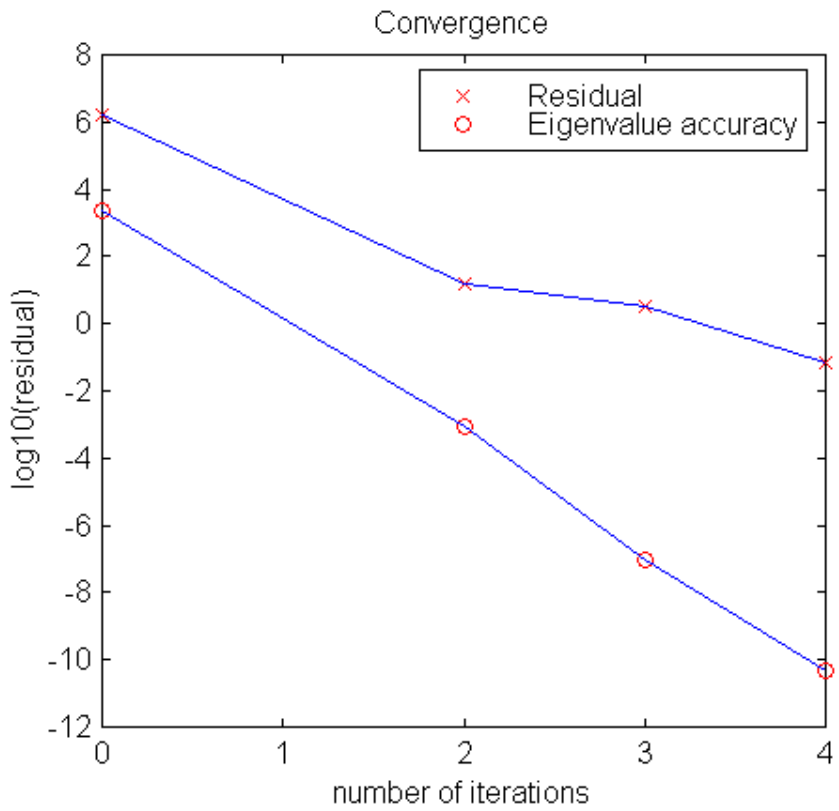
Section of APT side-coupled cavity



Parallel Solver

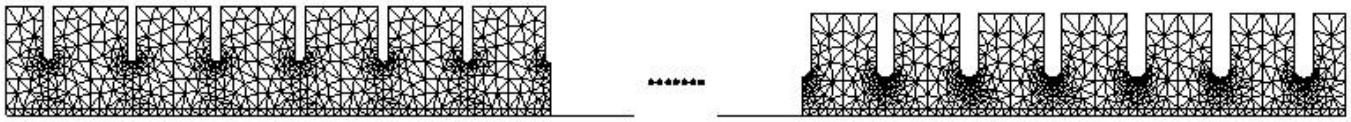
Parallel Linear Algebra uses Aztec from ACTS Toolkit

Omega3P convergence on DDS example with 1 Million DOF's

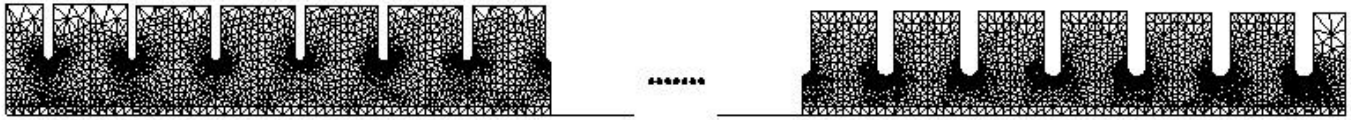


Simulation Results for NLC Detuned Structure

- initial mesh:



- adaptive refinement:

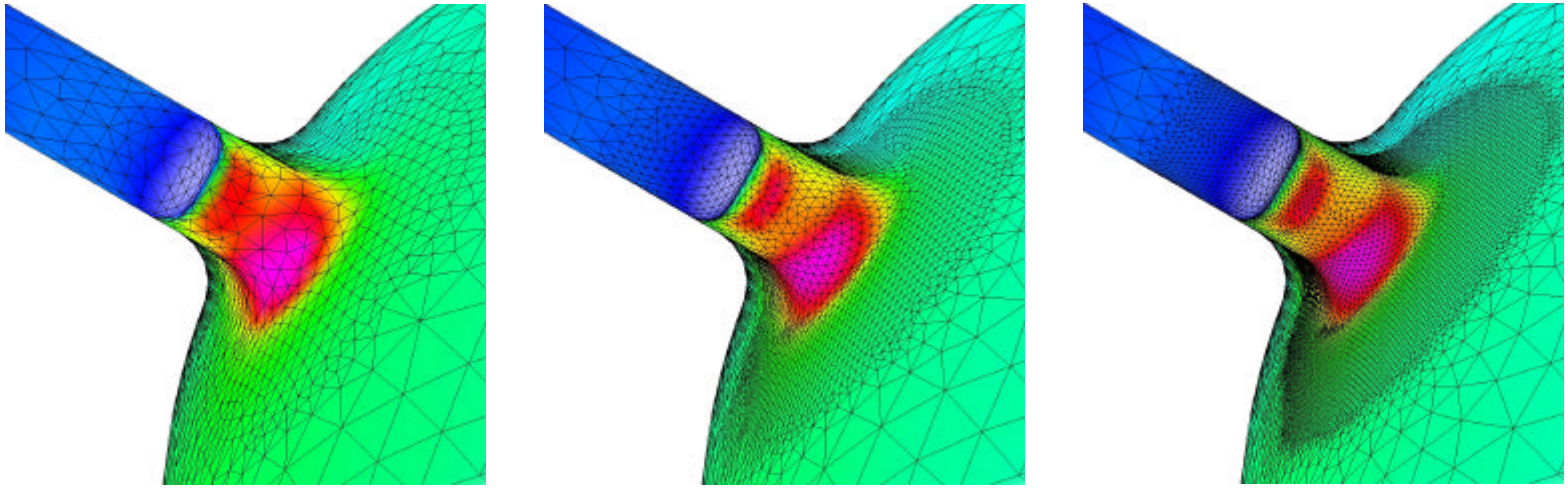


Mesh level	DOF	Solution time	Memory
0	227,769	25 minutes	4.0 GB
1	651,194	98 minutes	6.2 GB

3D Mesh Refinement

Parallel Adaptive Mesh Refinement is desired to optimize resources

Wall Loss in PEP-II Waveguide-Damped RF cavity

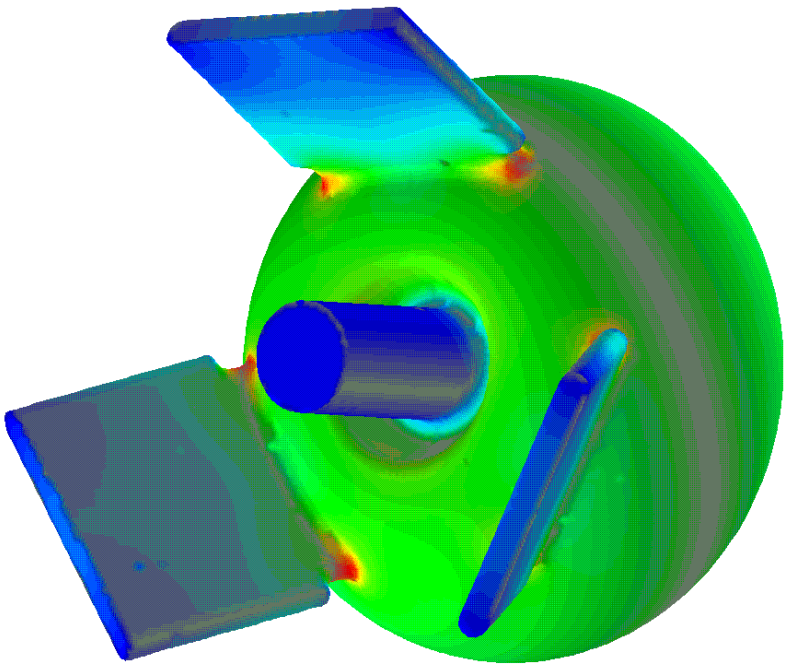


refined mesh size:	5 mm	2.5 mm	1.5mm
# elements :	23390	43555	106699
degrees of freedom:	142914	262162	642759
peak power density:	1.2811 MW/m^2	1.3909 MW/m^2	1.3959 MW/m^2

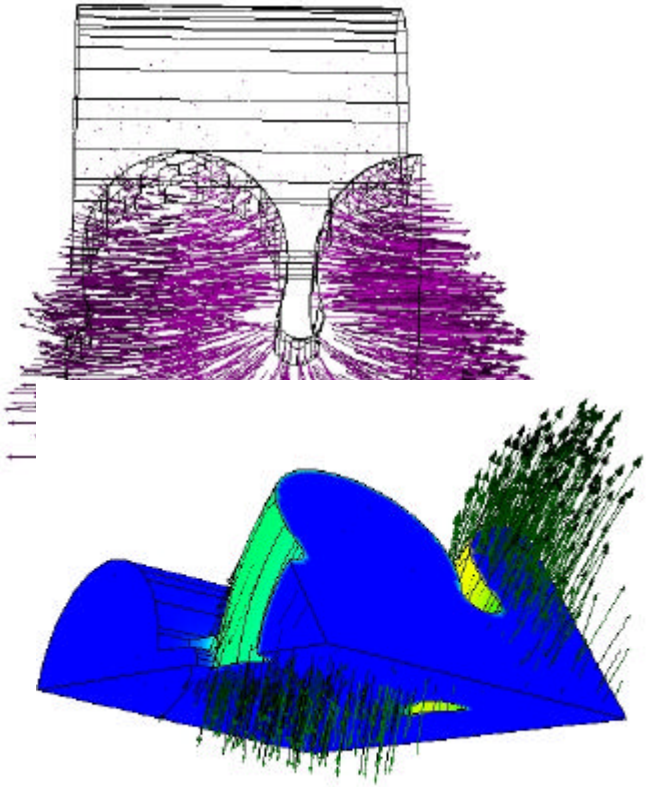
Visualization

Interactive Visualization using CUMULVS under development

MODULEF (INRIA)



MESHTV (LLNL)

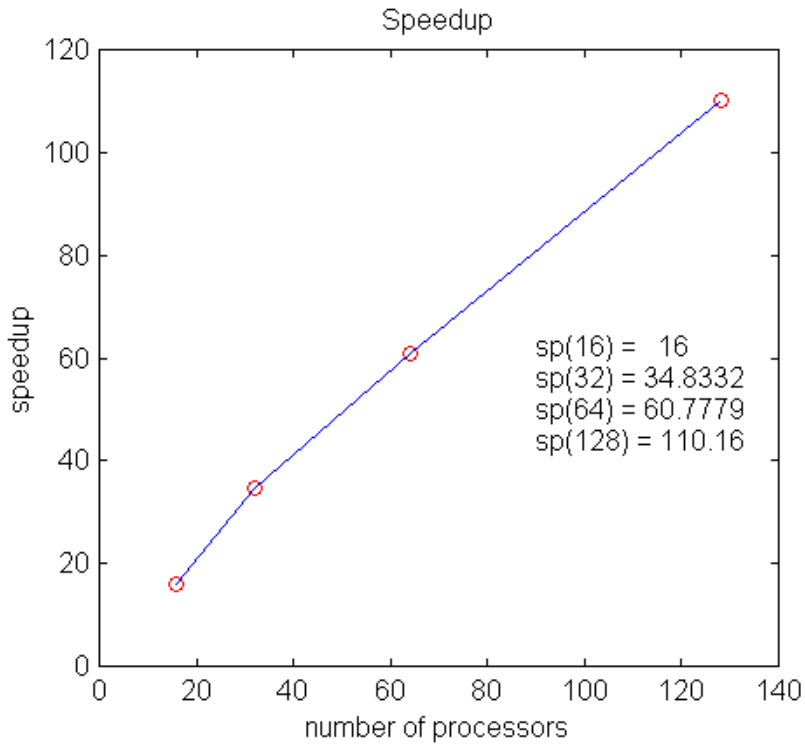


Parallel Performance

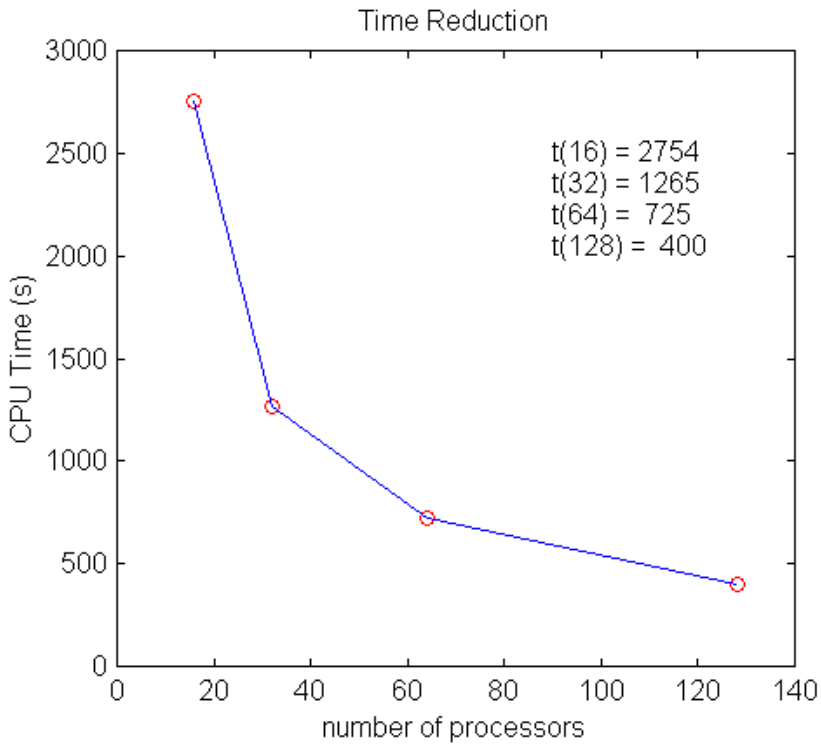
Sparse Matrix-Vector Multiplication Kernel to improve speedup

Omega3P performance on RDDS example with 1 Million DOF's

Speedup



CPU Time



64-node PC Linux Cluster

SLAC (ARDA, SCS, BaBar) & NERSC Collaboration

- Omega3P running on cluster using MPI
- Performance is within 25% of T3E up to 16 processors
- Effective resource for NLC structure design to narrow parameter space
- Economical alternative to supercomputers for medium-scale problems

Summary

- **DOE Accelerator Grand Challenge supported by NERSC resources has enabled Simulations with dramatic impact on the NLC project**

- **Demonstrates that Simulations can be a powerful tool for accelerator design, in addition to Theory & Experiment**

- **Multi-disciplinary approach is required to solve *LARGE*, *COMPLEX* problems**