SAND2015-9433PE

Exceptional service in the national interest

Sandia National Laboratories

Computational Electromagnetics at Sandia National Laboratories - Current Code Capability

Dr. J. D. Kotulski

Sandia National Laboratories – Organization 1352

Oct. 30, 2015

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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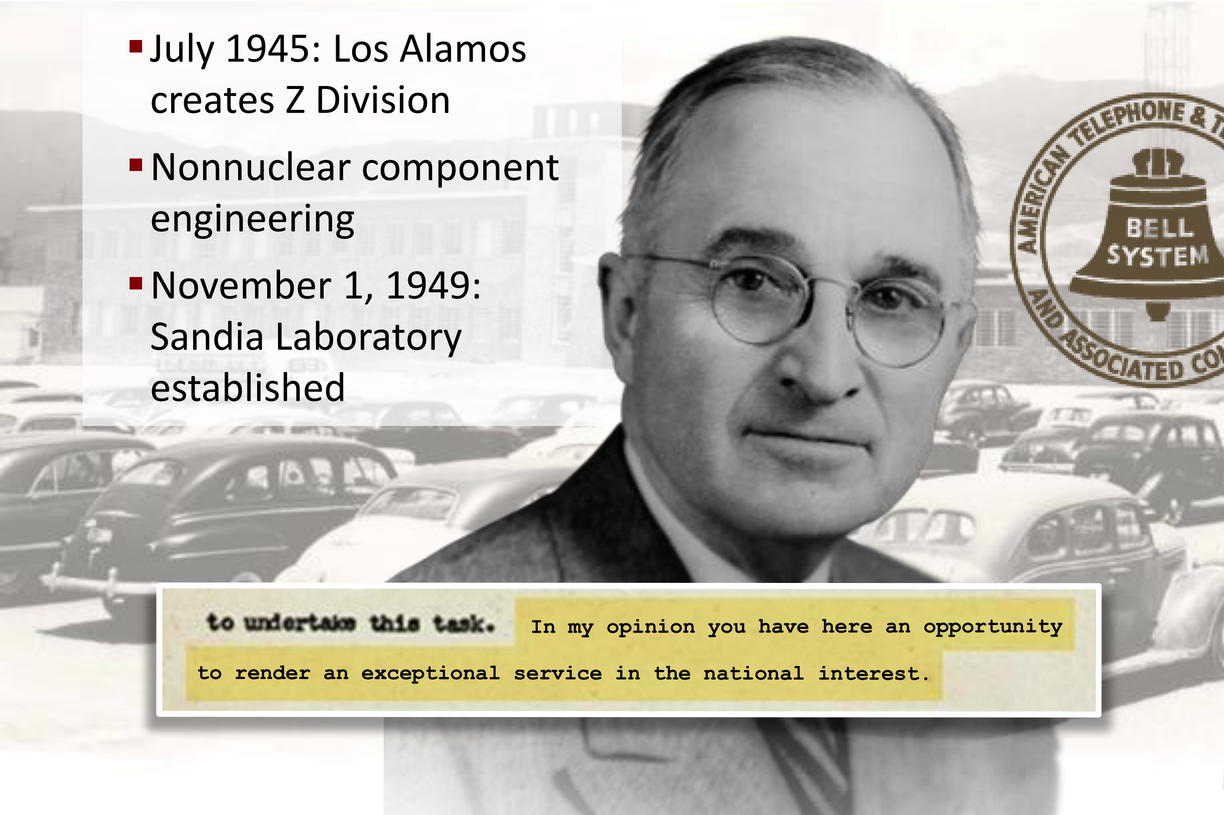
Outline

- Overview of Sandia National Labs
  - Electromagnetic Theory Organization
- Electromagnetic Environments
- Solution Process
- Computational Electromagnetics
  - Focus on Method of Moments – EIGER
    - Thin-slot Algorithm
    - Matrix Compression
- Conclusions / Future Work

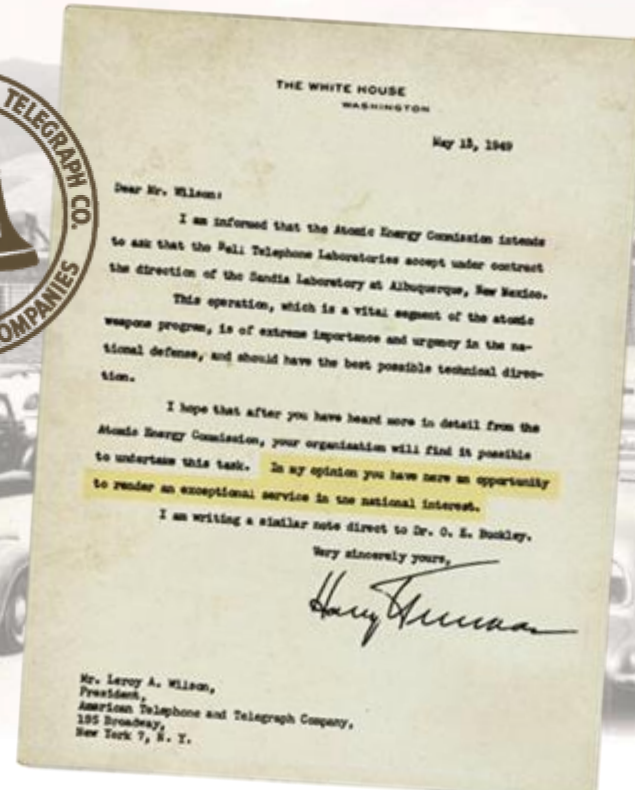
Sandia's History

Exceptional service in the national interest

- July 1945: Los Alamos creates Z Division
- Nonnuclear component engineering
- November 1, 1949: Sandia Laboratory established



to undertake this task. In my opinion you have here an opportunity to render an exceptional service in the national interest.



THE WHITE HOUSE
WASHINGTON

May 13, 1949

Dear Mr. Wilson:

I am informed that the Atomic Energy Commission intends to ask that the Bell Telephone Laboratories accept under contract the direction of the Sandia Laboratory at Albuquerque, New Mexico.

This operation, which is a vital segment of the atomic weapons program, is of extreme importance and urgency in the national defense, and should have the best possible technical direction.

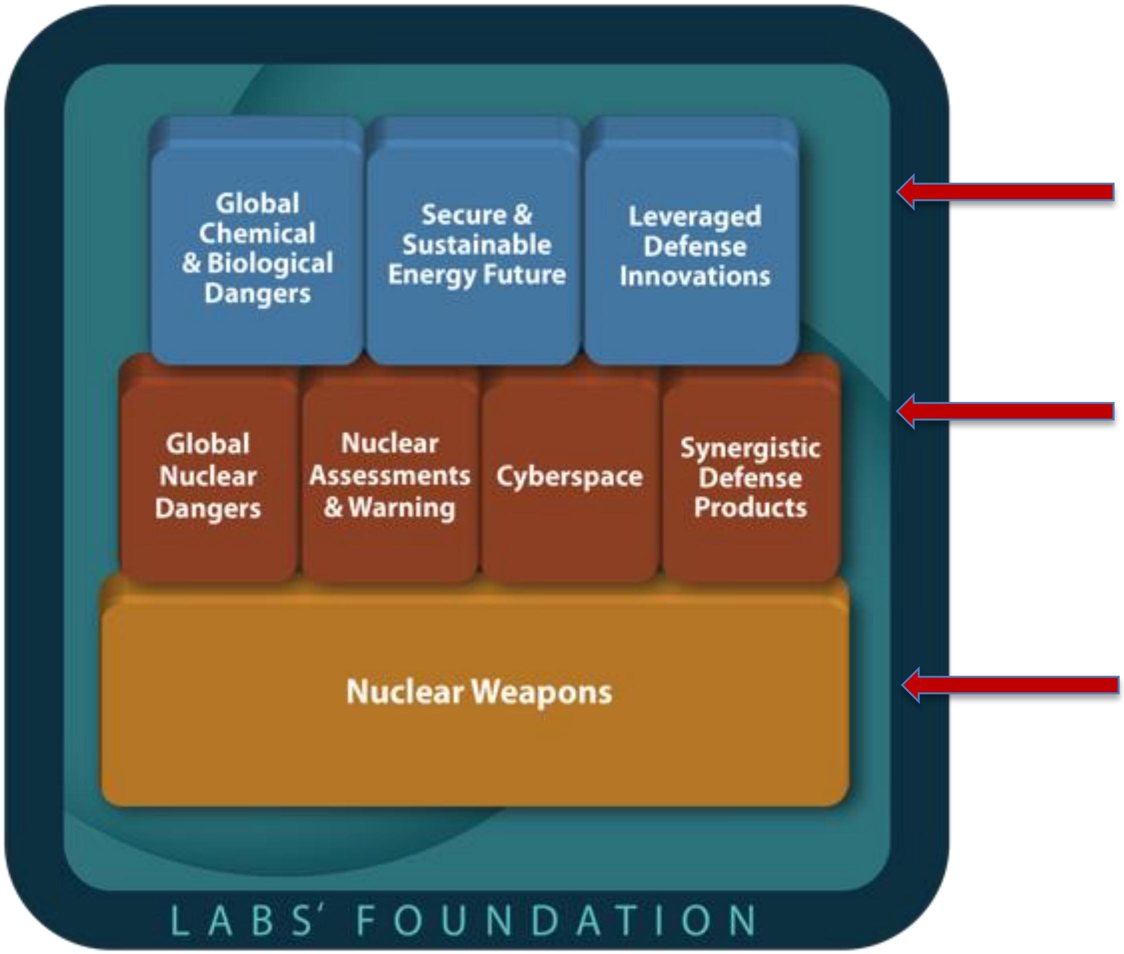
I hope that after you have heard more in detail from the Atomic Energy Commission, your organization will find it possible to undertake this task. In my opinion you have here an opportunity to render an exceptional service in the national interest.

I am writing a similar note direct to Dr. O. E. Buckley.

Very sincerely yours,

Mr. Leroy A. Wilson,
President,
American Telephone and Telegraph Company,
195 Broadway,
New York 7, N. Y.

National Security Mission Areas



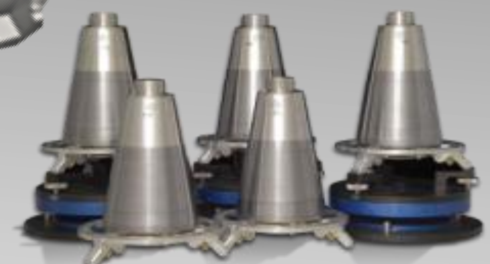
- Top row: Critical to our national security, these three mission areas leverage, enhance, and advance our capabilities.
- Middle row: Strongly interdependent with NW, these four mission areas are essential to sustaining Sandia's ability to fulfill its NW core mission.
- Bottom row: Our core mission, nuclear weapons (NW), is enabled by a strong scientific and engineering foundation.

Sandia's Current Nuclear Weapons Activities

Warhead Systems Engineering and Integration

Gas Transfer systems

Design Agency for Nonnuclear Components

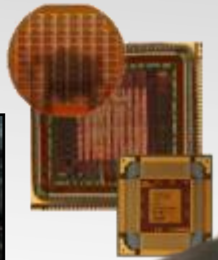


Arming, fuzing, and firing systems

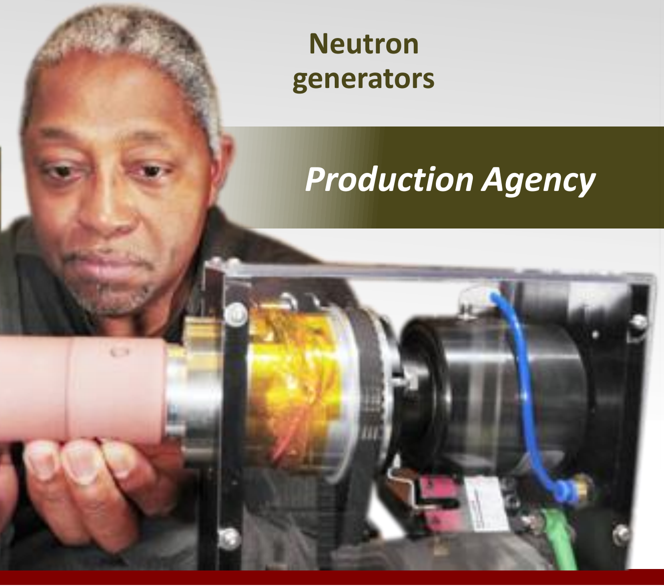
Safety systems

An extensive suite of multi-disciplinary capabilities are required for Design, Qualification, Production, Surveillance, Experimentation / Computation

MESA Microelectronics



Neutron generators



Production Agency

Major Environmental Test Facilities and Diagnostics

Z Machine

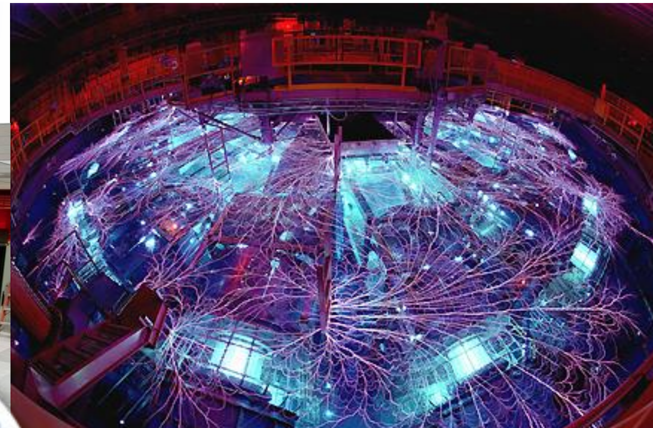
Light Initiated High Explosive

Annular core research reactor

Our Research Framework

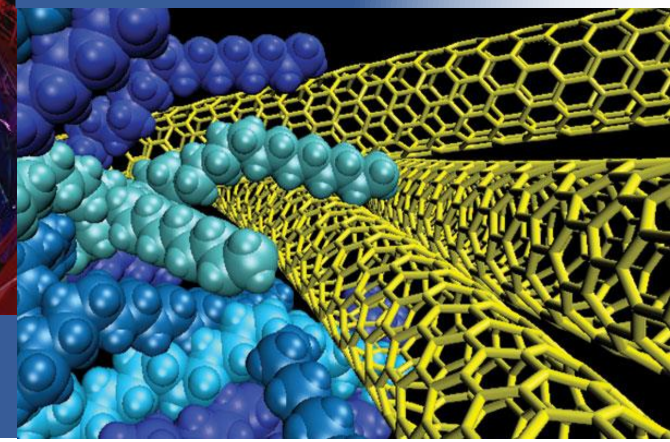
Strong research foundations play a differentiating role in our mission delivery

Computing & Information Sciences

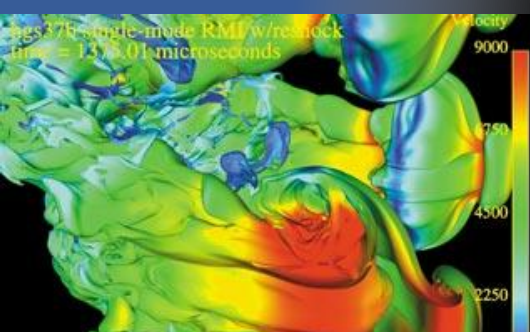


Radiation Effects & High Energy Density Science

Materials Sciences

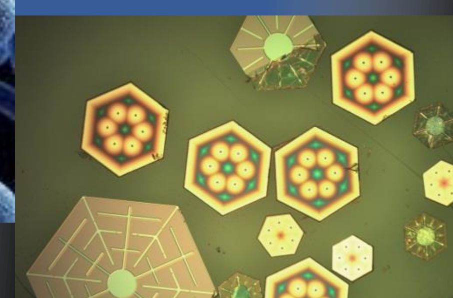


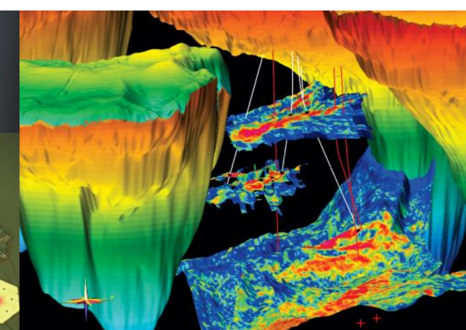
Engineering Sciences



Bioscience

Nanodevices & Microsystems



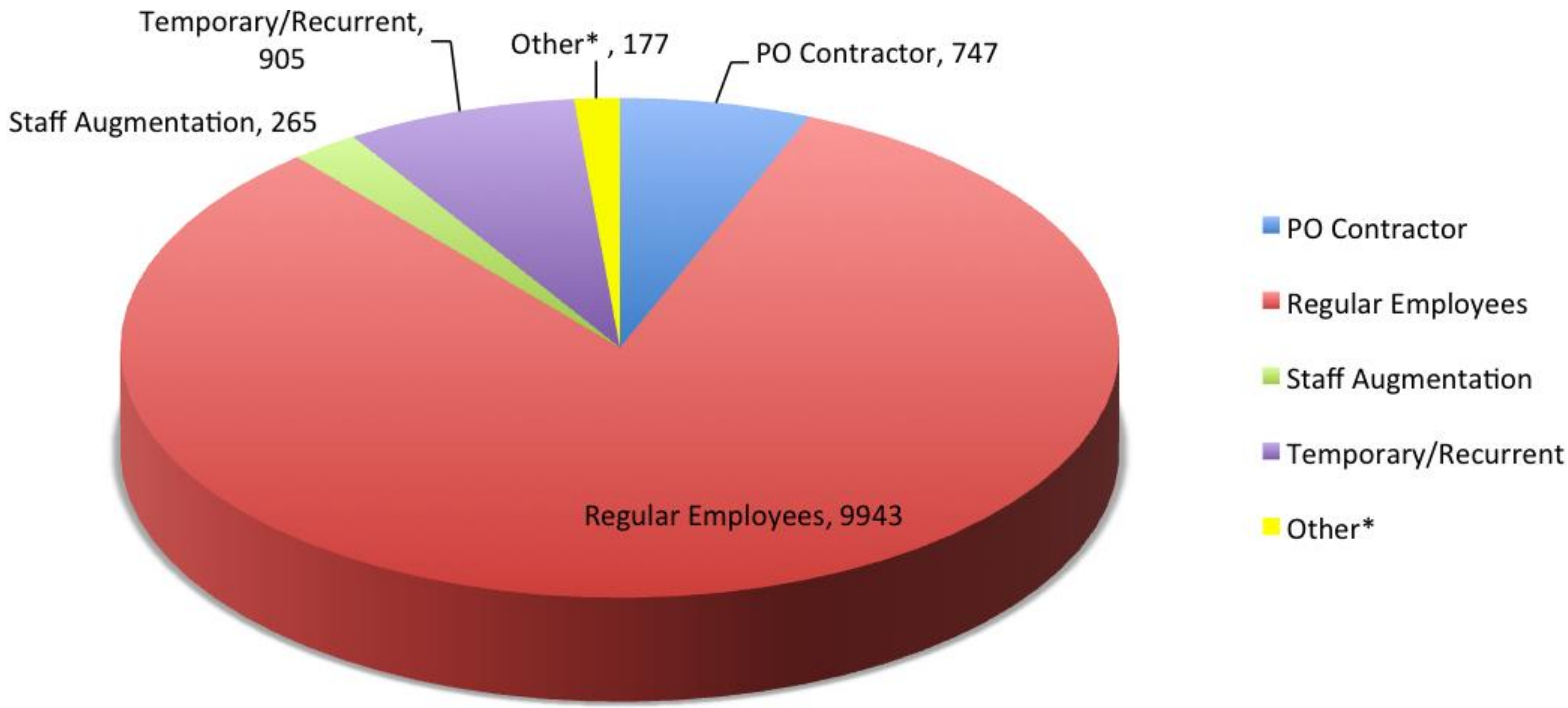


Geoscience

Our Workforce

- Total Sandia workforce: 12,037
- Regular employees: 9,943
- Advanced degrees: 5,703

Data as of August 25, 2014



Organization 1352 - Big Picture

- **What?**
  - **Provide high-fidelity, robust, computational tools based on Maxwell's Equations.**
- **Why?**
  - **To aid in weapons qualification in conjunction with experiments.**
  - **Weapon component and subsystem modeling.**
  - **In addition can be used to address problems for DoD customers.**
- **How?**
  - **Time-domain finite element formulation.**
    - **EMPHASIS**
  - **Frequency domain boundary element formulation.**
    - **EIGER**

Electromagnetic Environments

- Electromagnetic Interference
  - Radars, etc.
- Lightning
  - Nearby, direct strike
- System Generated EMP (SGEMP)
  - High-energy particles produce currents and fields.

Solution Process

- Geometry to appropriate mesh for analysis.
  - CUBIT – SANDIA Mesh Software
- Boundary conditions and excitations applied
  - Computational Electromagnetic Codes in Organization 1352
    - EMPHASIS/EIGER
    - EMPHASIS/NEVADA
    - Solver Technology
      - TRILINOS – SANDIA Solver Technology
- Computational
  - CIELO - LANL
  - SEQUOIA – LLNL
  - SANDIA Computational Resources

Radiation Suite of Tools

- **RAMSES (Radiation Analysis, Modeling and Simulation for Electrical Systems) framework includes Emphasis, Xyce, Charon and Sceptre**

- **EIGER**
  - **Frequency domain, boundary element**

- **EMPHASIS**
  - **Transient, volumetric finite-element, particle-in-cell**

- **QUICKSILVER**
  - **Transient, volumetric finite-difference, particle-in-cell (Legacy)**

EMPHASIS

- Time-domain
- Volumetric (space between parts) mesh
  - Unstructured finite-element
  - Structured finite-difference (stair-stepped)
  - Hybrid combination
- Requires truncation of simulation domain
- Formulation results in sparse matrix
  - Limited by ability to generate large mesh

EMPHASIS Features

- Finite-Element Time-Domain (FETD) solver
  - Full-field (no approximations)
  - Arbitrary geometry subject to meshing limitations
- Two formulations for field solve
  - Unconditionally stable, 2nd order Helmholtz
  - Conditionally stable, 1st order Curl-Curl (generalization of structured Finite-Difference Time-Domain (FDTD))
- Vector finite elements-Edge & Face based
  - Advantageous field-continuity and boundary properties
  - Divergence-free, avoiding spurious solutions
- Sub-element algorithms for slots and wires

Emphasis – Solution FETD

- Newmark-Beta approximation for time derivatives.

- Implicit solution
  - Matrix solve each time step
    - Symmetric positive definite
      - Conjugate gradient can be used
  - Unconditionally stable
    - Theoretically independent of Δt

Common Emphasis - EIGER Features

- General purpose based on Maxwell's equations (3D).
- Full-wave formulations.
- Include separate electrostatic components.
- Massively parallel capable.
- Slot, thin wire, and lumped element models.
  - Sub-cell models
- Wide variety of sources and boundary conditions.

EIGER

- Frequency-domain method of moments solution
  - Steady state solution
  - F90 code – Object Oriented Design
- Boundary element formulation
  - Mesh surfaces of parts – interface between regions
- Exact radiation boundary condition
  - Due to Green's function
- Formulation results in dense (fully populated) matrix
  - Simulations can be limited by available memory
  - Entries are double precision complex

EIGER – Basic Formulation

$$\bar{E}^{scatt} = -\left[j\omega\bar{A} + \nabla\phi \right]$$

$$\bar{A}(r) = \mu\int \bar{J}(r')g(R)ds'$$

Surface Current

$$\phi(r) = \frac{1}{\varepsilon}\int \sigma(r')g(R)ds'$$

Surface Charge

Relationship between current and charge

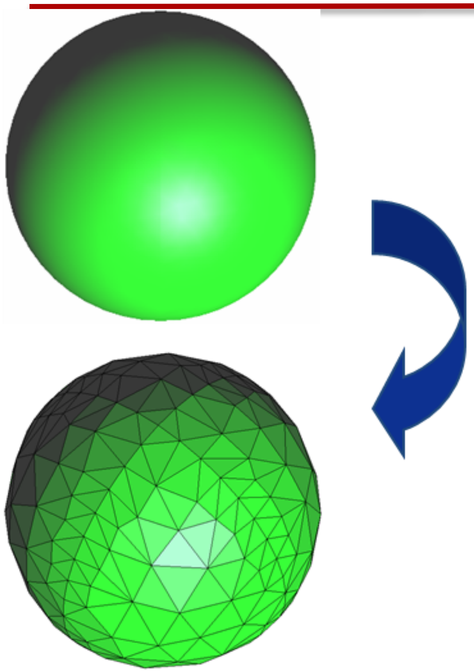
$$j\omega\sigma = -\nabla\cdot\bar{J}$$

Free space Green's Function

$g(R)$

Note : example is for the electric field integral equation

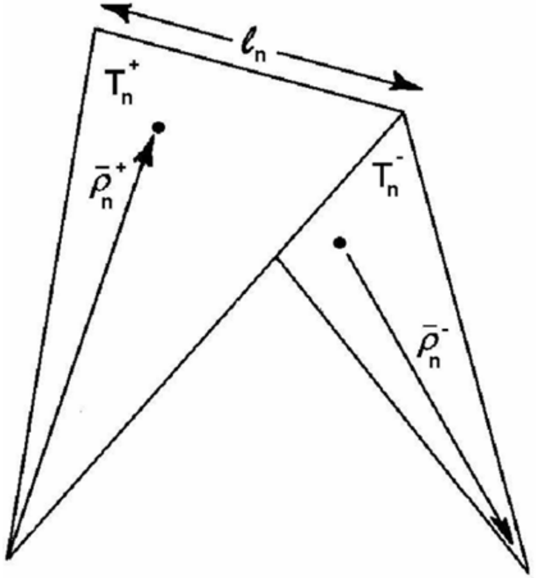
EIGER – Numerical Implementation



$$\bar{J}(\boldsymbol{r}) = \sum_{j=1}^{N} I_j \bar{f}_j(\boldsymbol{r})$$

Discretize object

$$\boldsymbol{f}_n(\boldsymbol{r}) = \begin{cases} \frac{l_n}{2A_n^+}\rho_n^+ & \boldsymbol{r} \in T_n^+ \\ \frac{l_n}{2A_n^-}\rho_n^- & \boldsymbol{r} \in T_n^- \\ 0 & \text{otherwise} \end{cases}$$



Div-conforming Rao-Wilton-Glisson (RWG) basis functions

EIGER – Numerical Implementation

- **The integral equation is (on the surface):**

$$T(\bar{J}) = \bar{E}_{scatt}\Big|_{\tan} = \bar{E}_{incident}\Big|_{\tan}$$

- **The currents are expanded in terms of the Rao-Wilton-Glisson expansion functions (~ 10 per wavelength) :**

$$\bar{J}(r) = \sum_{n} I_n \bar{f}_n(r)$$

- **Test the integral equation with the basis functions:**

$$\langle \bar{f}_m, \mathrm{T}(\bar{J}) \rangle \Rightarrow \int_{surface} \bar{f}_m \cdot T(\bar{J}) ds$$

EIGER – Numerical Implementation

- **The integral equation through discretization has become a matrix equation:**

$$\bar{\bar{Z}}\,\bar{I} = \bar{V}$$

- **Implications:**
  - **The matrix Z is fully populated – a dense matrix.**
  - **This method is memory limited.**

EIGER

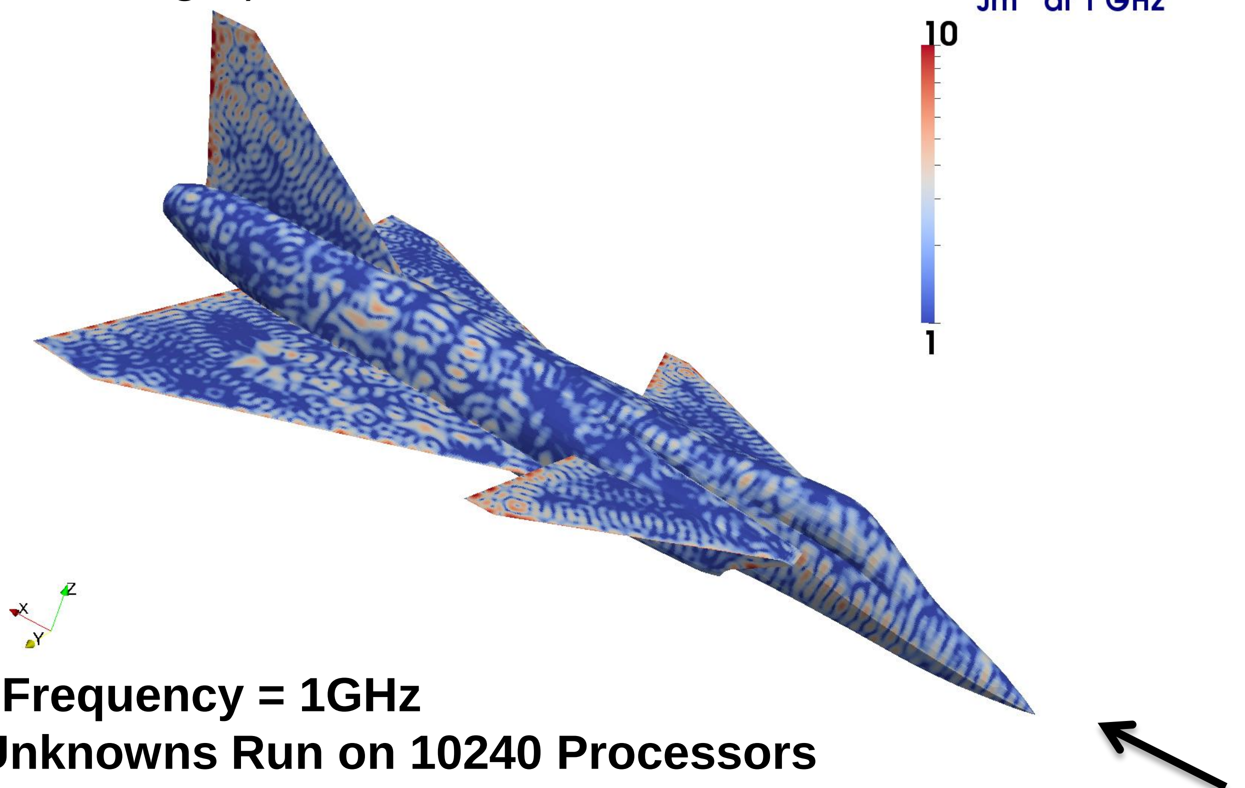
- The boundary element code EIGER:
  - Validated with:
    - Measurements (slot in a box)
    - Analytical solutions (sphere)
  - Used for weapon qualification
  - Additional customers

- The method is memory limited.
  - Limits size of the problem (with respect to frequency)

- Path Forward -> Compression techniques:
  - Relaxes the memory limit issue.
    - Increases the size of the problem (with respect to frequency) that now can be solved.

Results – External Problem
(Direct Solve on CIELO)

External Problem
VFY 218 (50.6 ft. length)



Frequency = 1GHz
930,000 Unknowns Run on 10240 Processors
Memory Requirement 13.8 TBytes

Direction of Incident Field

Direct Solve Information

Geometry	Max Frequency (GHz)	Unknowns	Solve Time (per frequency)	Number of Processors	Flop Rate (Gflops per Processor)
#1	5.	389756	13529	1600	7.3
#1	12.	1855082	65875	40000	6.5
#2	16.5	2474989	83575	80000	6
#3	2.	226647	7271	640	6.7
#3	12.5	858826	33375	7600	6.7
#3	12.5	858826	30364	8000	6.9

EIGER Thin-Slot Formulation

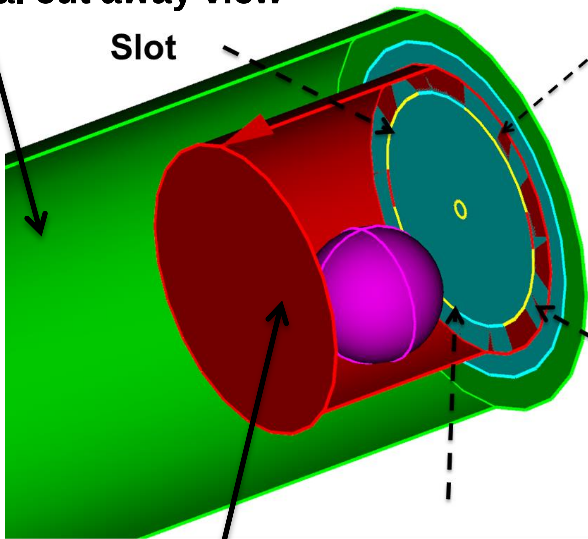
- **This modeling feature enables the incorporation of potential penetration points on a structure that couple fields into a cavity without gridding the slot explicitly.**

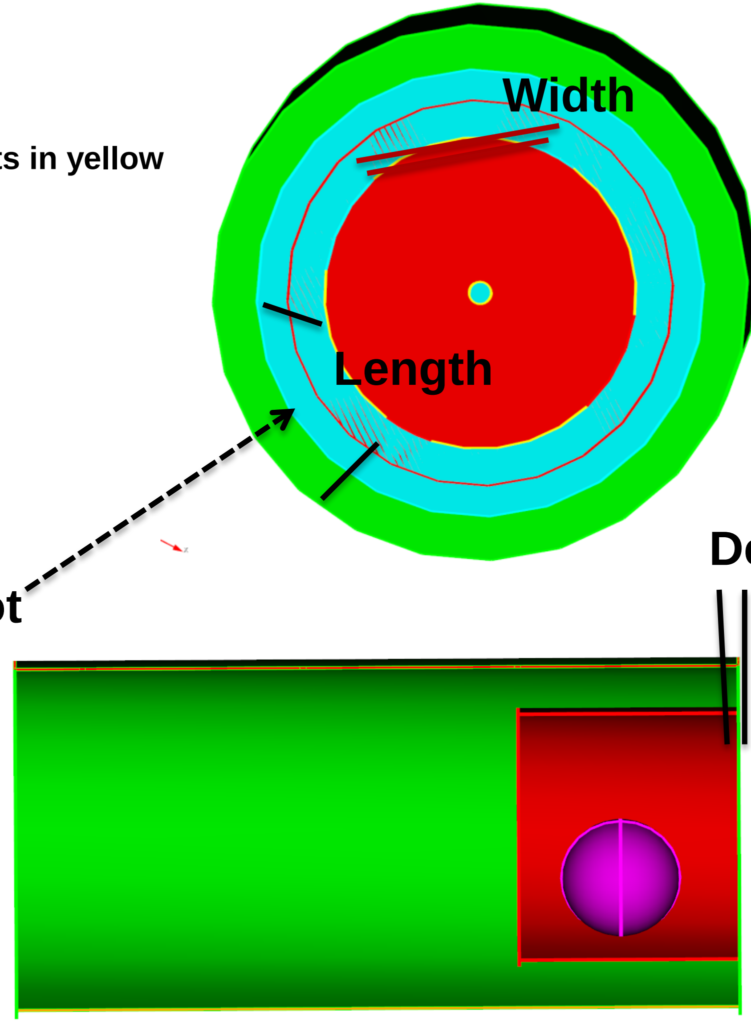
- **Based on research by Warne and Chen.**
  - **Slot is modeled by a wire (carrying magnetic current) whose effective radius depends of the depth and width of the slot.**
    - **Note the length of the slot >> depth, width**
  - **Incorporated into EIGER, EMPHASIS, and used by other investigators.**
  - **Validated**
    - **Compared to analytic and experimental results.**

EIGER Thin-Slot Formulation

- Key features
  - Integral equation for the exterior surface current and slot current (magnetic current)
  - Integral equation for the interior surface current and slot current (magnetic current).
  - Two contributions
    - Green's function
    - Non-Green's function
- Implications
  - The exterior unknowns do not interact with the interior unknowns.
  - Coupling of the exterior to the interior is through the slot contribution.
    - Matrix has blocks with zero elements – no coupling.

Thin-Slot Parameters





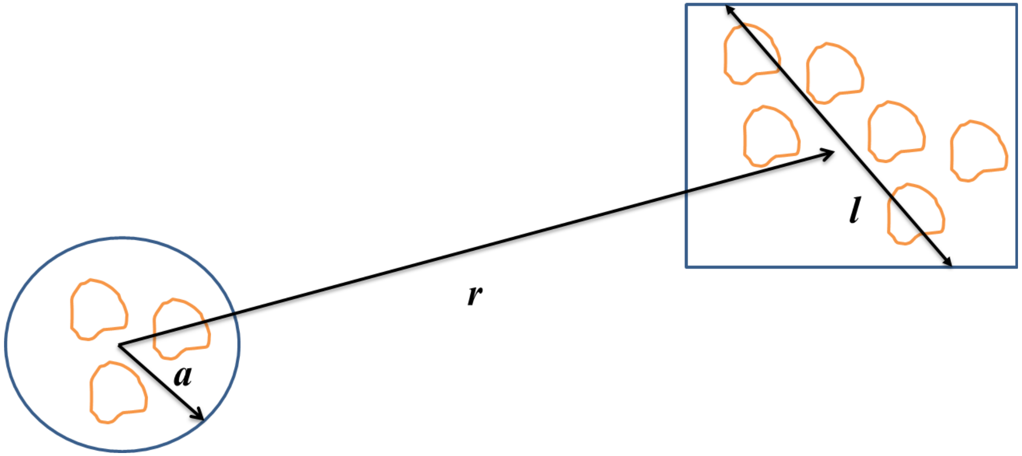
For most problems
Width, depth vary from .5 to 3mm

Compression Techniques

- **These are techniques that no longer store the full matrix but a lower rank version of the matrix.**

- **Based on work by Bucci and Francescetti**
  - **"On the Degrees of Freedom of Scattered Fields" IEEE AP, July 1989**

$$N_{dof} = \frac{4la}{r\lambda}$$



Compression Techniques

- **Fast Multipole Method (FMM)**
  - **Compression achieved through Green's function simplification:**
    - **Factorization**
    - **Use of the addition theorem**
    - **Diagonalization**
    - **Results in low-rank approximation of matrix blocks**

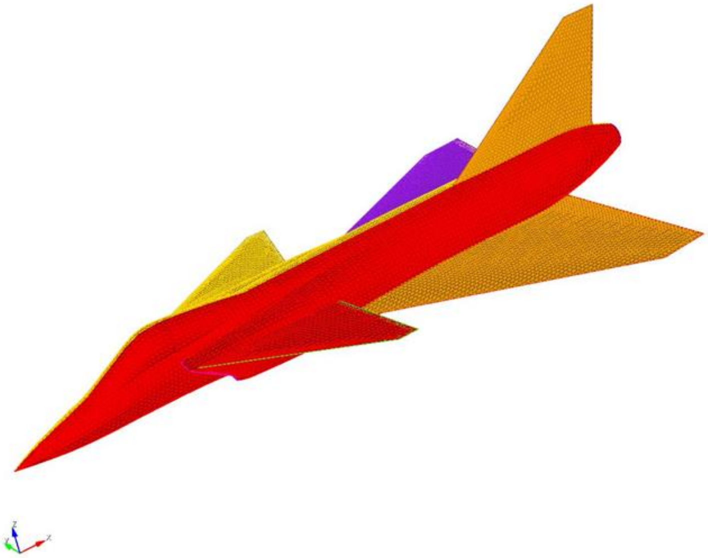
- **Adaptive Cross Approximation (ACA)**
  - **Compression achieved:**
    - **Low-rank approximation of matrix blocks.**
    - **Done on the fly**
      - **Compressed matrix blocks never fully populated.**
    - **Since the process only operates on matrix blocks it is independent of Green's function simplification.**

Compression Techniques

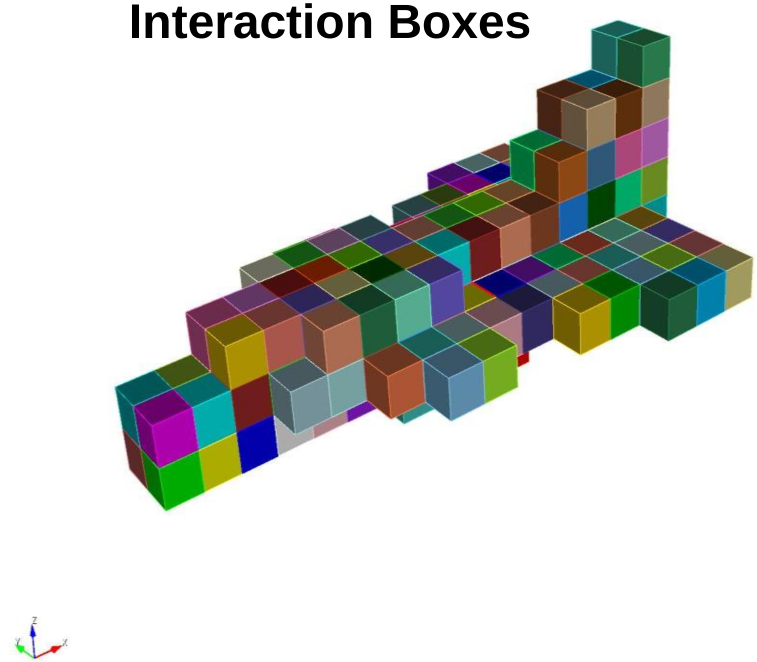
- **Identification of all matrix blocks**
  - **Discretized object (meshed) is encased in a oct-tree structure**

VFY 218

Meshed Object



Interaction Boxes



All compression techniques use this step in the solution process

ACA Matrix Compression

- Each box contains elements with current unknowns on the elements.
  - Can be compared to a 1-level fast multipole algorithm

- 2 boxes interact to form a matrix block.

- The distance between boxes, size of the boxes, and wavelength determine if a reduced or low-rank approximation can be used.
  - Not all blocks can be compressed.
    - Compression criterion :
      - Distance between the center of boxes > 2 * (box radius)

ACA Matrix Compression

- **The matrix** $\bar{\bar{Z}}$ **is given by:**

$$\bar{\bar{Z}} = \sum_{j=1}^{MOM\_blocks} Z_j^{mom} + \sum_{i=1}^{COM\_blocks} \tilde{Z}_i^{com}$$

MOM_Blocks – Moment method matrix blocks (full matrix blocks)

COM_Blocks – Compressed matrix blocks (low-rank approximation)

ACA Matrix Compression

- **Approximate matrix description:**

$$\tilde{Z}^{m\times n} = U^{m\times r} V^{r\times n} = \sum_{i=1}^{r} u_i^{m\times 1} v_i^{1\times n}$$

- **The key step is the determination of the sub-matrices *u* and *v*.**

Solution of the Compressed System

- **The matrix equation to be solved is :**

$$\bar{\bar{Z}}\,\bar{I} = \bar{V}$$

- **The matrix is not completely available but is stored as:**

$$\bar{\bar{Z}} = \sum_{j=1}^{MOM\_blocks} Z_j^{mom} + \sum_{i=1}^{COM\_blocks} \tilde{Z}_i^{com}$$

- **Therefore a iterative solution approach needs to be used.**
  - **Generalized Minimum residual method(GMRES)**
    - **Saad and Schultz 1986**
  - **Transpose Free Quasi Minimum Residual (TFQMR)**
    - **Freund 1993**

Solution of the Compressed System

- The Iterative solution technique of choice is the TFQMR method.
  - Based on heuristic numerical experiments performed on electromagnetic problems.
  - Extended for use on parallel platforms.

- On a parallel machine each processor does not have all the matrix blocks – they are partitioned on different processors for load balancing and memory balancing.
  - No processor can have more or less than one block than any other processor.
  - Processors have both MOM and COM blocks.

Solution of the Compressed System

Using the TFQMR Method

- **In all iterative methods a matrix vector product is needed during the solution process.**
  - **This is performed in parallel (each processor has a portion of the compressed and MOM blocks).**

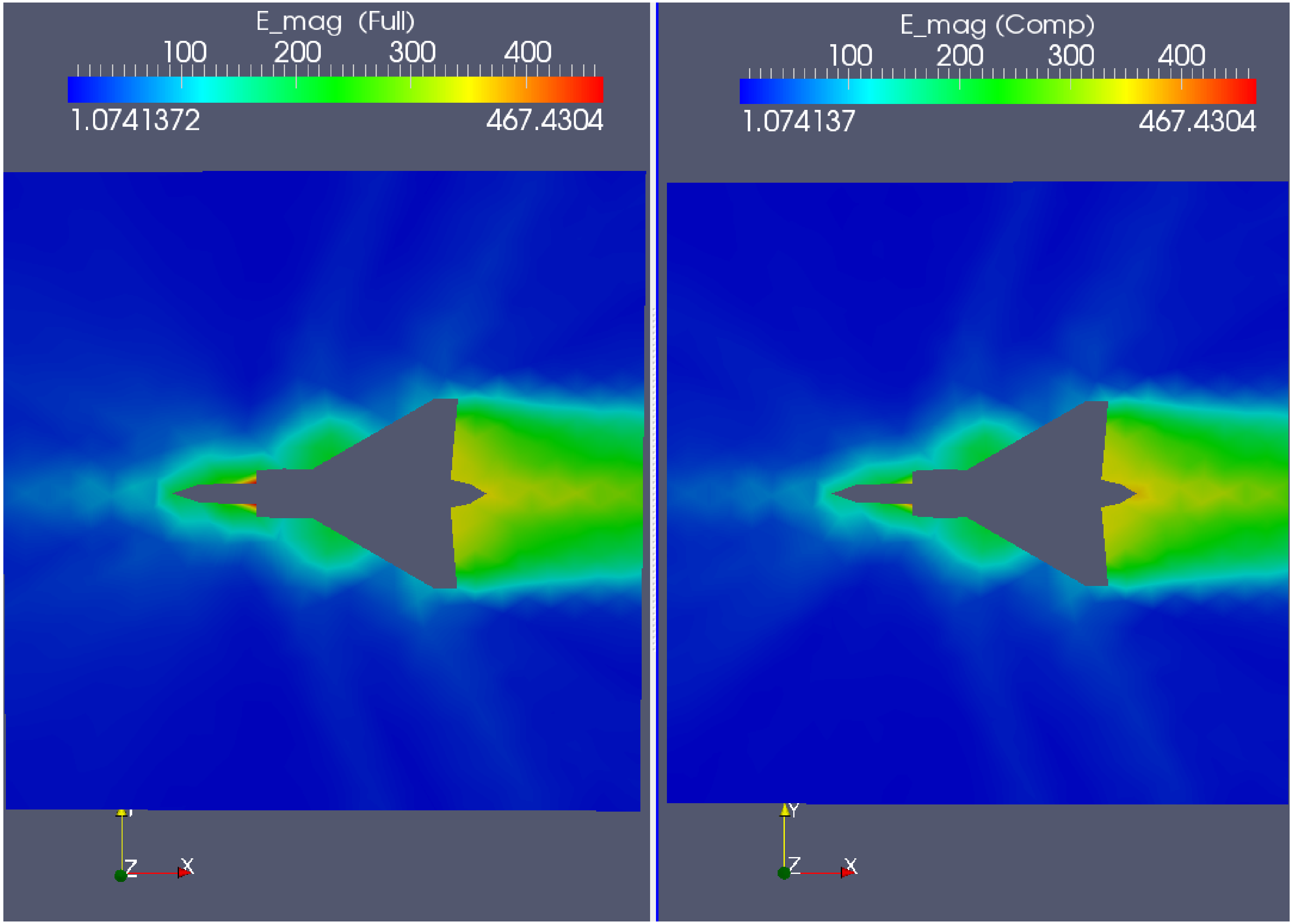
- **In the original algorithm (used here) the residual norm is not available.**
  - **However an estimate is computable.**
  - **The convergence curves show two values**
    - **The normalized initial residual norm**
    - **The estimate to the norm.**
- **A solution tolerance of 5 e-3 was used in all problems.**
  - **Will affect accuracy.**

VFY-218 Compression Results

- 15 meter long aircraft.
- Frequency 1 GHz
- Number of unknowns 934128
  - 2500 iterations
  - 256 Processors
  - 70,826 sec.
- Epsilon 4.e-02
- Memory
  - Full matrix 16 *(872) GBytes
  - Compressed 16*(19 + 7.7) GBytes
  - ~ 97 % compressed.

Compression Results VFY-218

Magnitude of the near field full and compressed matrix solution.



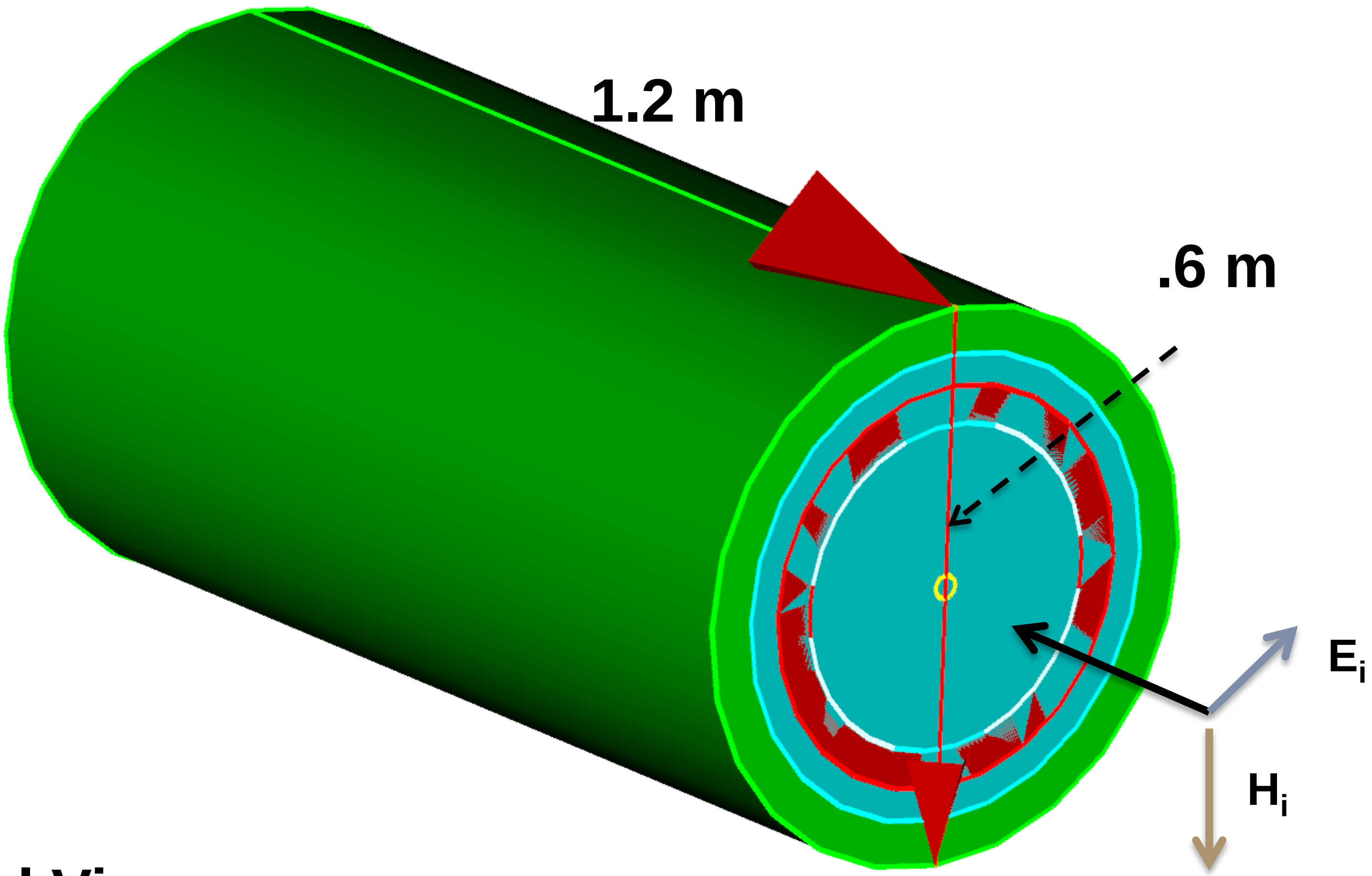
Compression applied to an object with slots

- Referred to as D_cavity.

- A number of different mesh densities considered.
  - Increases the useful upper frequency limit for the model.

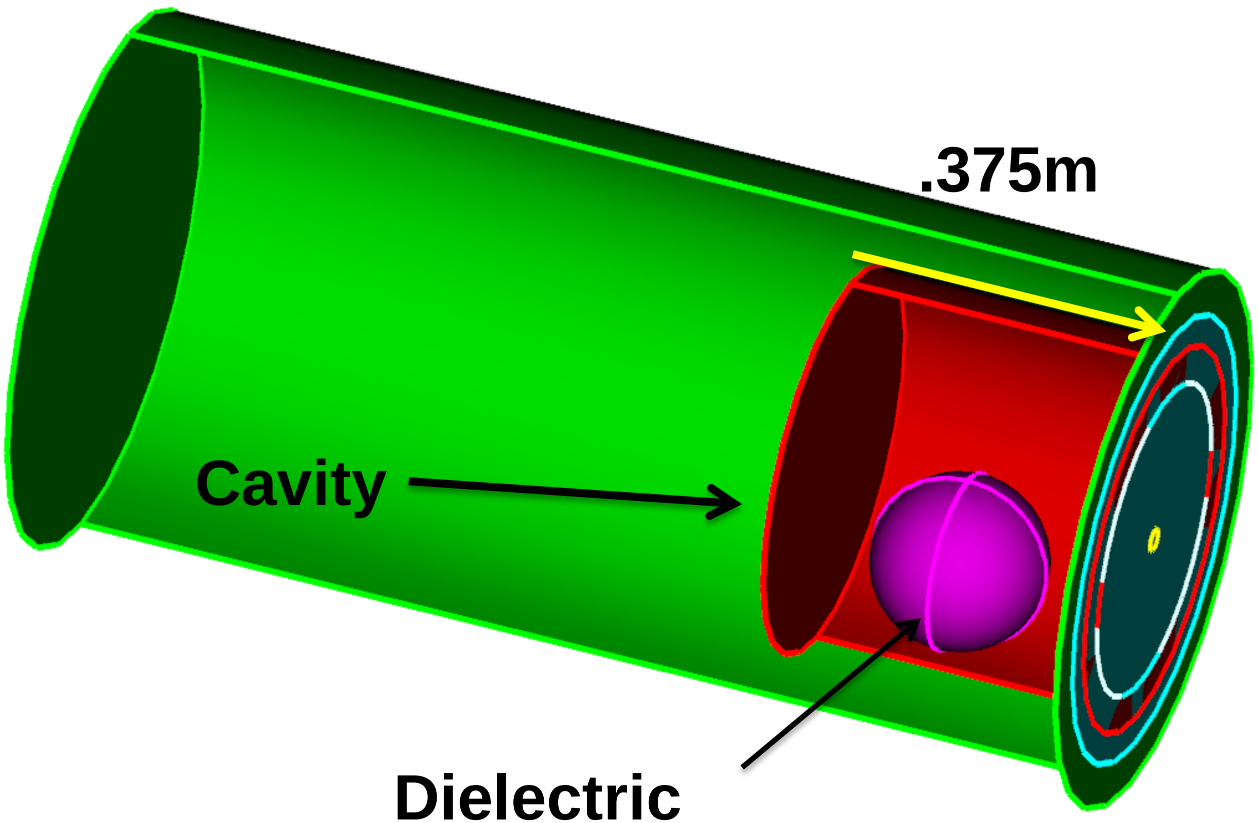
- Contains essential features to exercise the compression algorithm on an problem with slots.

Geometry D_cavity



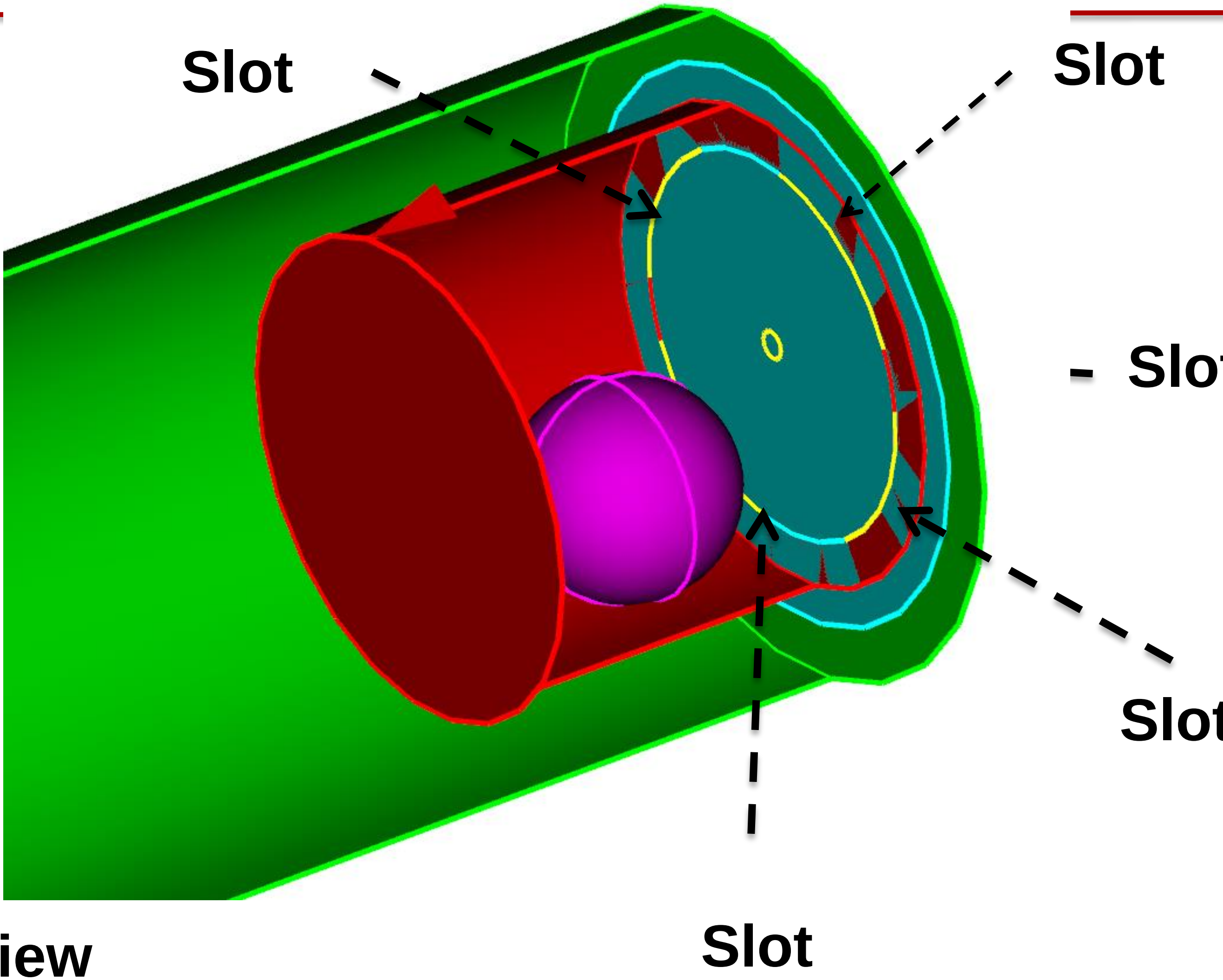
External View

Geometry D_cavity



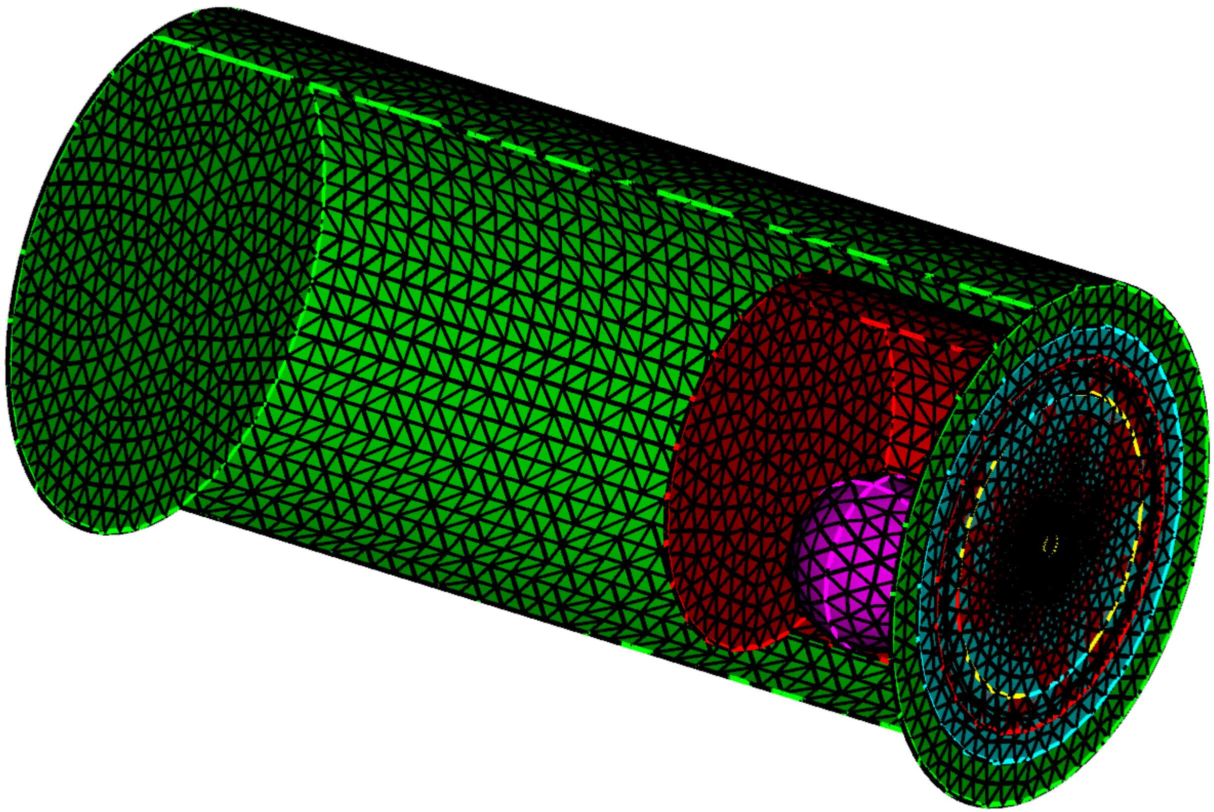
Internal View

Geometry D_cavity



Internal View

Geometry D_cavity with Mesh



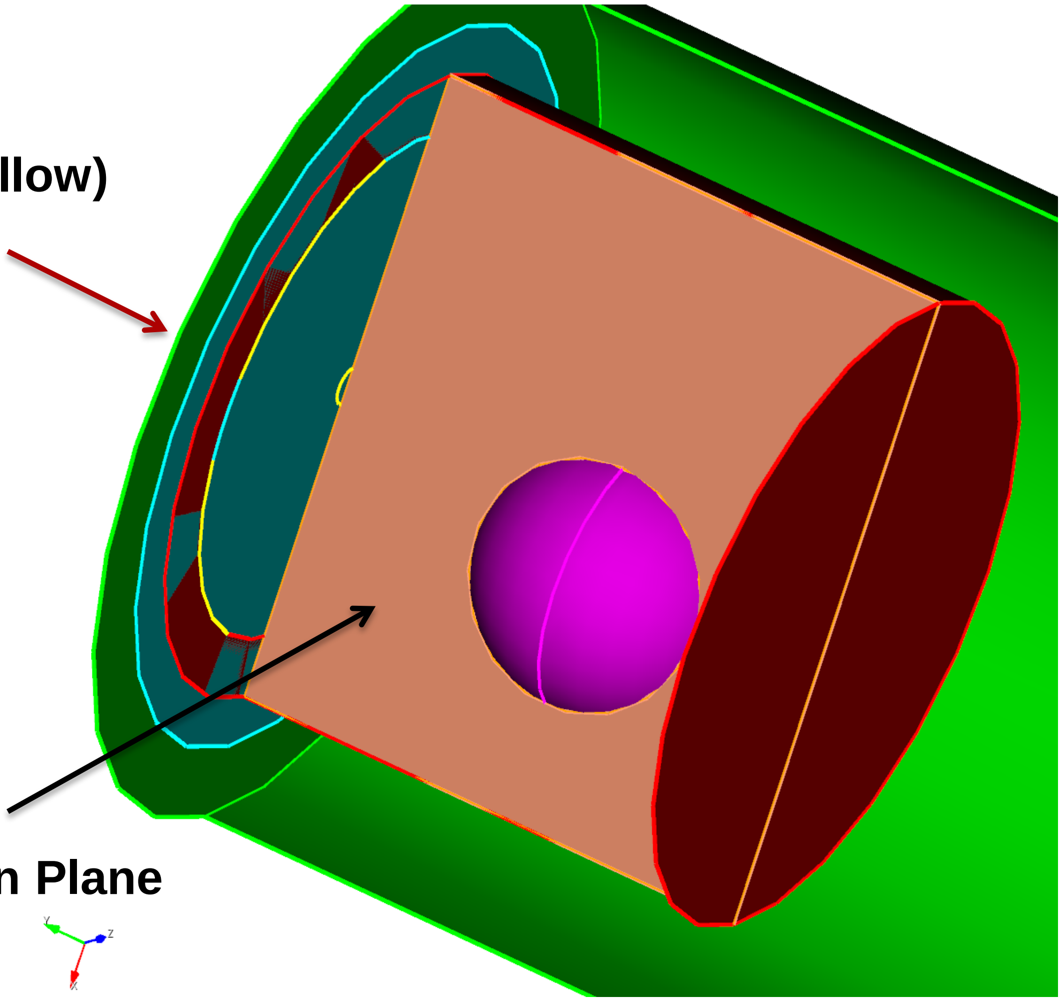
Mesh 1 – 10090 elements --- 15565 unknowns

Results

- **The magnitude of the scattered electric field will be considered.**
- **This field value will be calculated on planes both inside the cavity and outside the cavity.**
- **Because of the proximity of these observation points to the object these are near field quantities.**

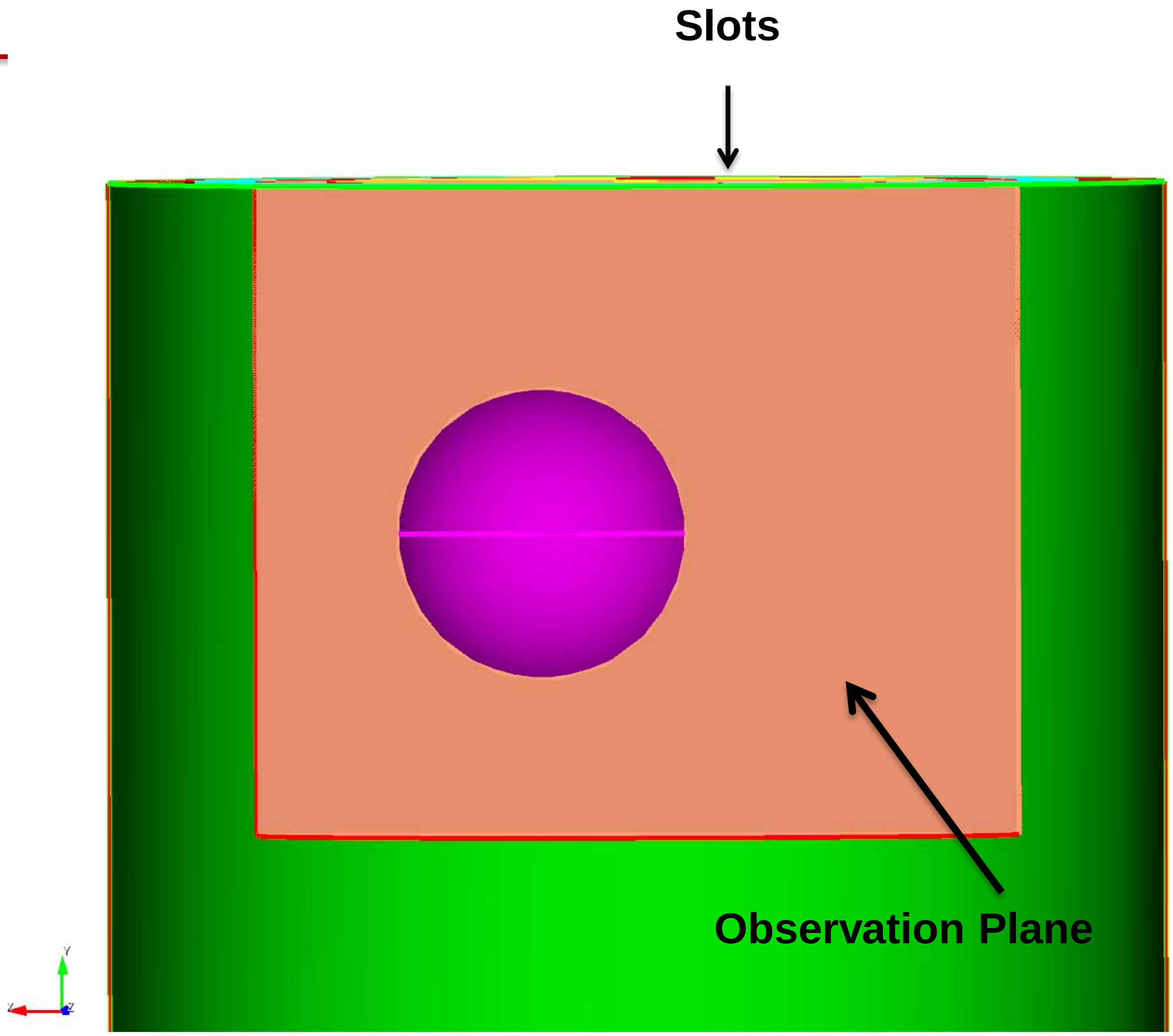
Data Results Observation Plane

Slots (yellow)



Observation Plane

Data Results Observation Plane

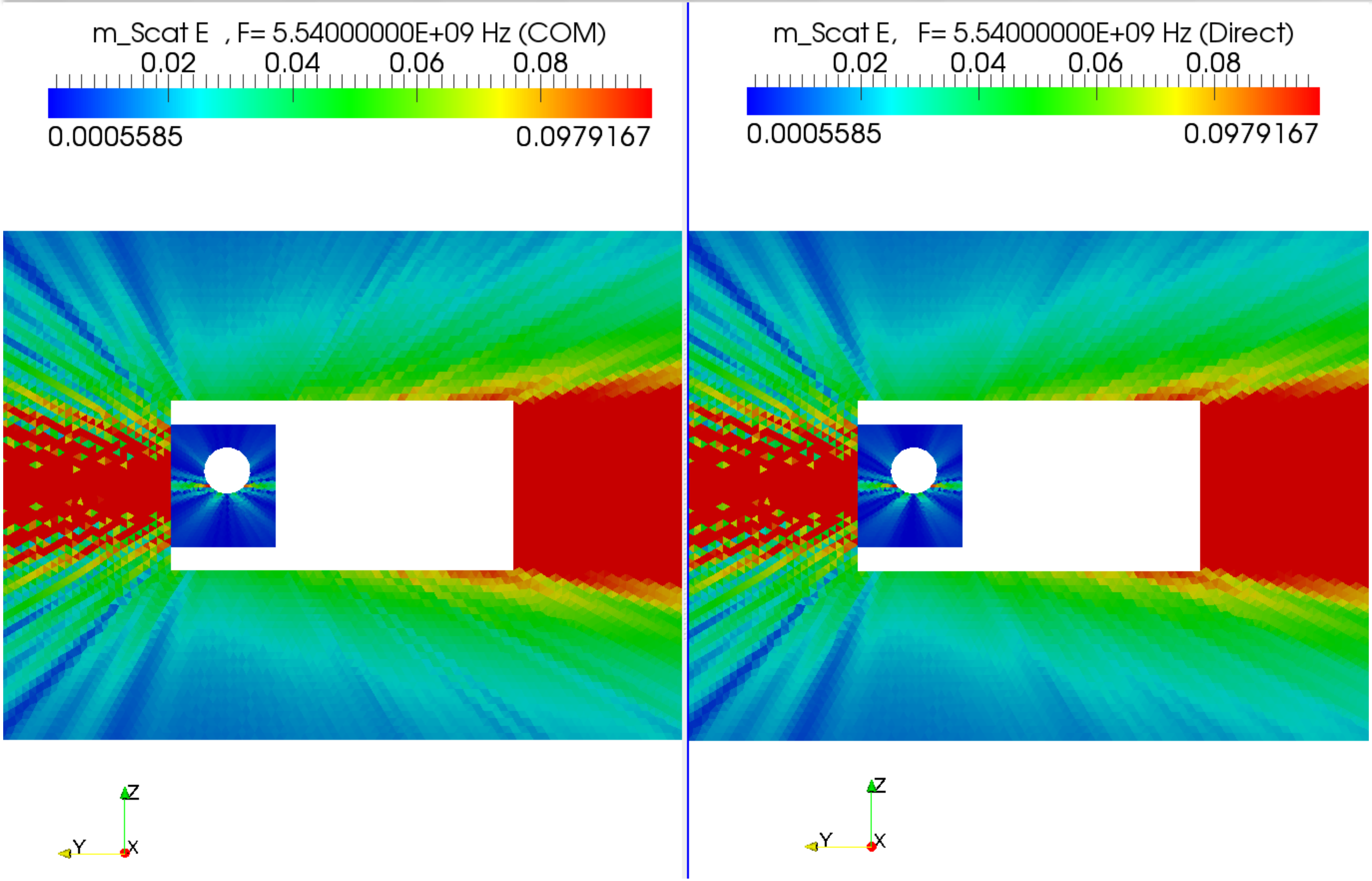


Results - Mesh 3 D_cavity

- **Object 1.2 m in length**
- **Frequency 5.5 GHz**
- **Number of Unknowns 247604**
- **Epsilon 3.1e-03**
- **Memory**
  - **Full matrix 16*(61) GBytes**
  - **Compressed 16*(36.8 + .2) Gbytes**
  - **~40% compressed.**

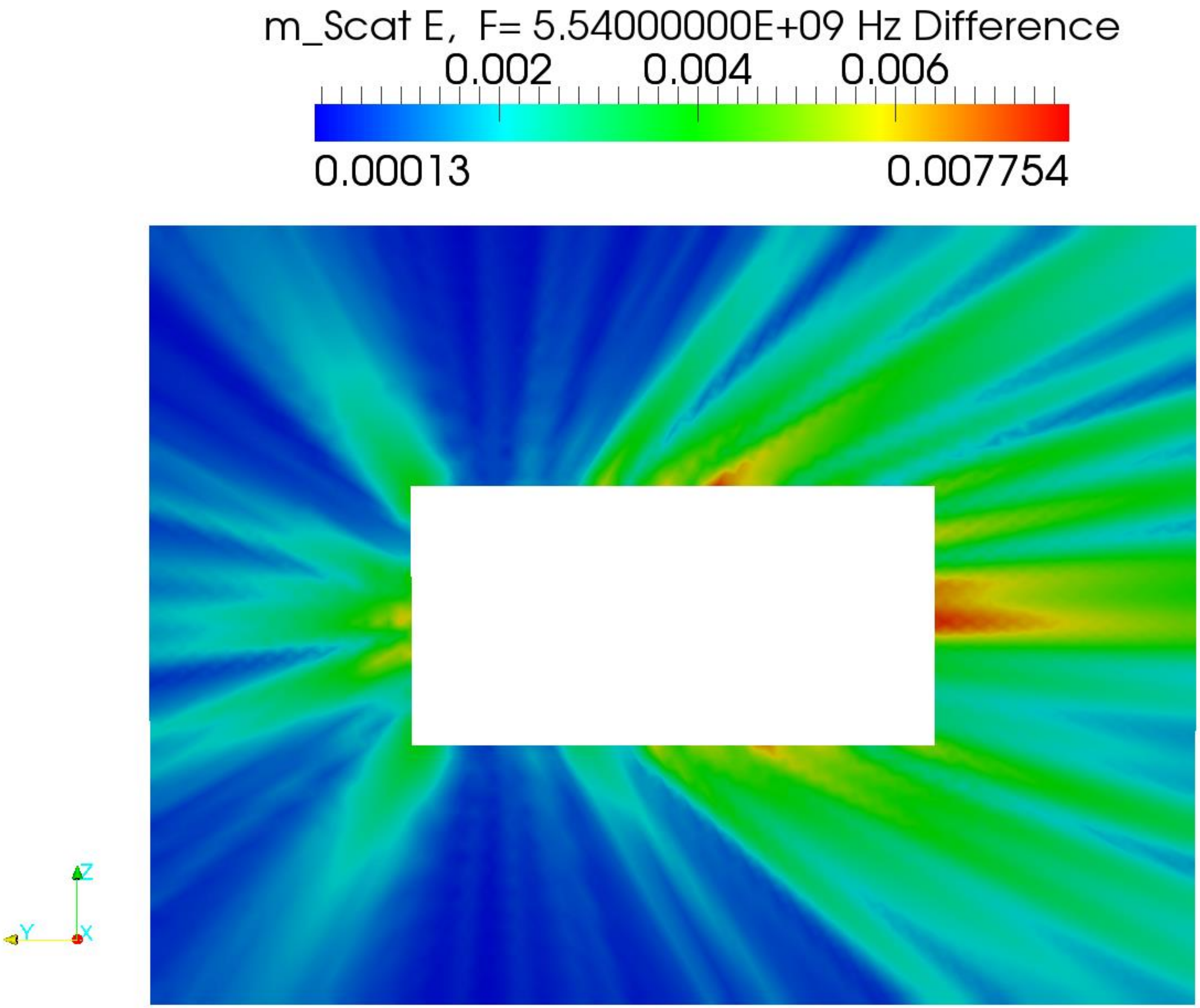
Results - Mesh 3 D_cavity

Magnitude of Scattered Field



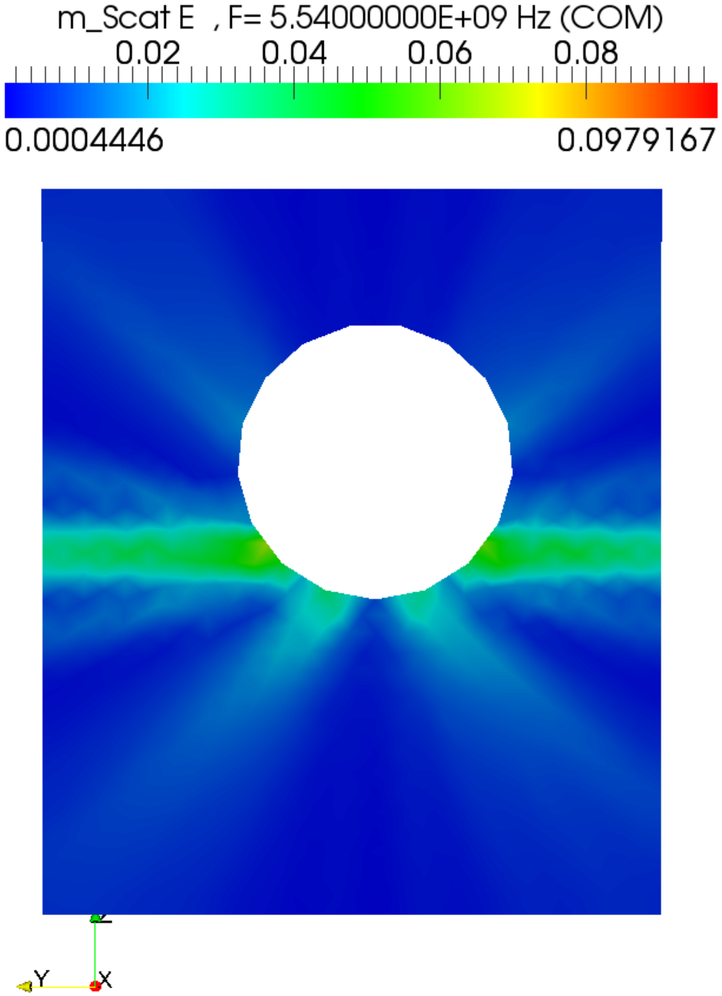
Results - Mesh 3 D_cavity

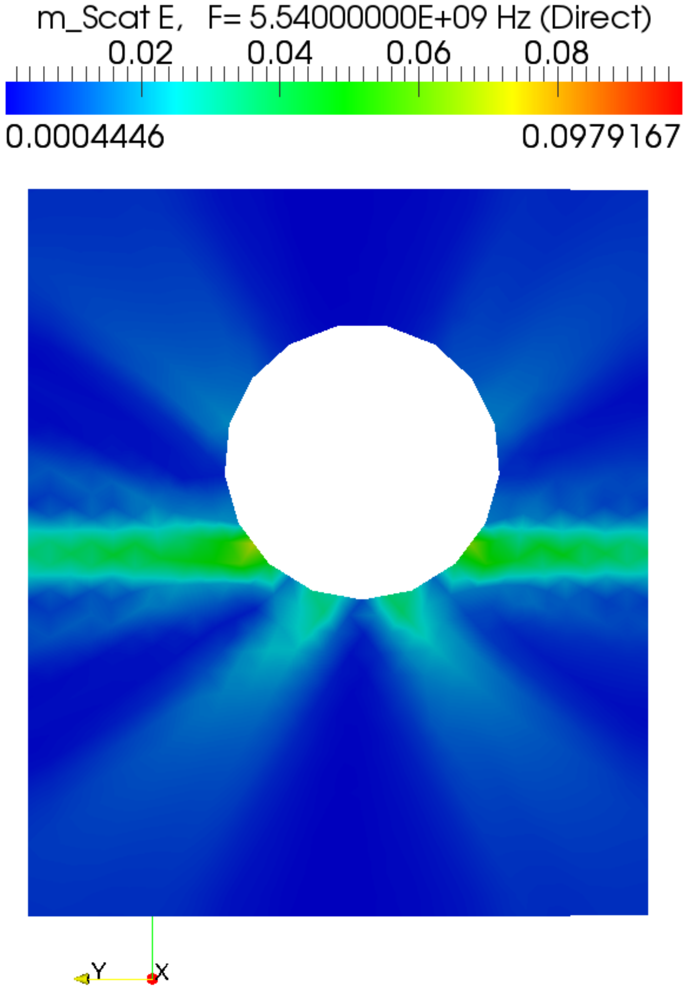
Magnitude of Scattered Field Difference between direct and compressed matrix solutions



Results - Mesh 3 D_cavity

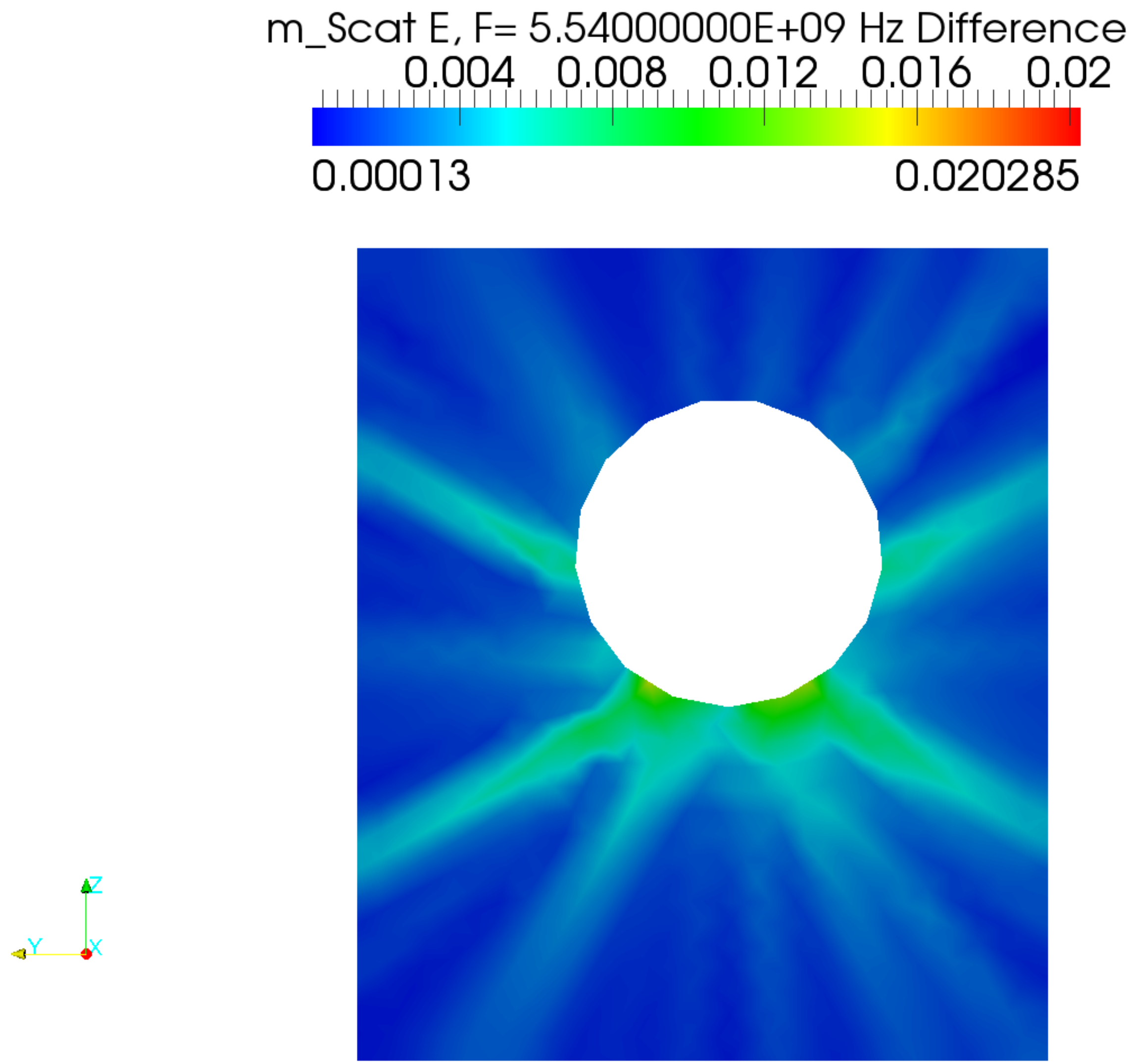
Magnitude of Scattered Field





Results - Mesh 3 D_cavity

Magnitude of Scattered Field Difference between direct and compressed matrix solutions



Error Norm

- **Definition**

$$2-norm=\frac{Sqrt(\sum_{po\text{int}s} abs(error\_x)^2+abs(error\_y)^2+abs(error\_z)^2)}{Sqrt(\sum_{po\text{int}s} abs(e\_x)^2+abs(e\_y)^2+abs(e\_z)^2)}$$

Error Norms

2-Norm

247604 Unknown Problem

Location	2-Norm
Interior_x	.23
Interior_z	.2
Exterior_x	5.33e-03
Extrerior_z	5.26e-03

Solution tolerance 5.e-03

Conclusions

- **The matrix compression has been successfully integrated in EIGER.**
  - **For parallel machines**
  - **With iterative solver**

- **The viability of the technique has been demonstrated on a diverse group of problems.**
  - **Exterior problems**
  - **Problems with external geometry connected through slots.**
    - **Uses the thin-slot formulation already integrated in EIGER**

Future Work - Compression

- **Improve the load balancing of the matrix:**
  - **For the MOM blocks, by the block size not just by block number.**
  - **Use preprocessing to generate block matrix structure.**

- **Improve solution time by reducing the iteration count**
  - **Preliminary work performed by Matt Bettencourt on preconditioning revealed:**
    - **Standard methods ILU, Diagonal preconditioning will fail**
    - **Use Sparse Approximate Inverse (SAI)**
    - **Applied it to the two smaller problems discussed earlier.**
    - **Defined the algorithm to implement and tested it in MATLAB.**

- **Continue testing on problems of interest to Sandia.**
  - **Verify and quantify errors for a robust implementation.**

Future Work

- **Implement alternative compression techniques**
  - **Fast Multipole Method (FMM)**
  - **Direct solve / ACA**

- **Implement cable models and interface to the EMPHASIS suite.**
  - **External field to pin voltage.**

- **Investigate hybrid techniques**
  - **High- frequency approximations with full wave solvers.**

- **Continue to validate the EMPHASIS suite**
  - **Comparisons to measurements.**

Future Work - Continued

- **1352 collaborates with Universities fro the advancement of our computational capabilities.**
  - **Contracts**
  - **Post-docs**
  - **Summer employment**

- **The codes developed in 1352 will be repackaged for Next Generation Computing Platforms (NGP).**

Matrix Compression Backup Slides

ACA Matrix Compression

Definitions

$Z(I_1,:)$ **Row 1 of matrix** Z

$Z(:,J_1)$ **Column 1 of matrix** Z

$$\|Z\|^2 = \|Z\|_F^2 = \sum_{i=1}^{m}\sum_{j=1}^{n}\left|z_{ij}\right|^2$$

Frobenius Norm squared of matrix Z

ACA Matrix Compression

Algorithm - Initialization

Compute the first row of the matrix. $Z(I_1,:)$

Find the maximum element of the row. $\max_j |Z(I_1 :, j)| = J_1$

Normalize the row by this element. $v_1 = Z(I_1,:) / Z(I_1, J_1)$

The vector u is defined. $u_1 = Z(:, J_1)$

The first contribution to the Frobenius Norm squared is calculated. $\left\|\tilde{Z}^1\right\|^2 = \|u_1\|^2 \|v_1\|^2$

Find the largest row value in the column J_1 – is different from the previous row used. $\max_i |Z(i :, J_1)| = I_2 \neq I_1$

ACA Matrix Compression

Algorithm – k'th Iteration

1)Calculate next row and compute approximate matrix row.

$$\tilde{R}(I_k,:) = Z(I_k,:) - \sum_{l=1}^{k-1} (u_l)_{I_k} v_l$$

2)Find the maximum element of the row.

$$\max_j \left|\tilde{R}(I_k, j)\right| = J_k$$

3)Normalize the row by this element.

$$v_k = \tilde{R}(I_k,:) / \tilde{R}(I_k, J_k)$$

4)Adjust approximate column and compute u_k.

$$\tilde{R}(:, J_k) = Z(:, J_k) - \sum_{l=1}^{k-1} (v_l)_{J_k} u_l$$

$$u_k = \tilde{R}(:, J_k)$$

5)Compute the update to the Frobenius Norm.

$$\left\|\tilde{Z}^{(k)}\right\|^2 = \left\|\tilde{Z}^{(k-1)}\right\|^2 + 2\sum_{j=1}^{k-1} \left|u_j^T u_k\right| \cdot \left|v_j^T v_k\right| + \left\|u_k\right\|^2 \left\|v_k\right\|^2$$

6)Find the next maximum row index.

$$\max_i \left|\tilde{R}(i, J_k)\right| = I_{k+1}$$

ACA Matrix Compression

Algorithm – Convergence

- **The test for convergence is (Step 5 in the previous slide) :**
  - **Epsilon chosen by the user**

$$\left\|u_k\right\| \cdot \left\|v_k\right\| \leq \varepsilon \left\|\tilde{Z}^{(k)}\right\|$$

- **The computation of a low-rank approximation to the matrix is complete.**
  - **Note that this was done by row and column – the full matrix was not computed and reduced.**
  - **The number of elements to store for this matrix is (n + m) x r, instead of m x n.**