Computational Science Research in Support of Petascale Electromagnetic Modeling

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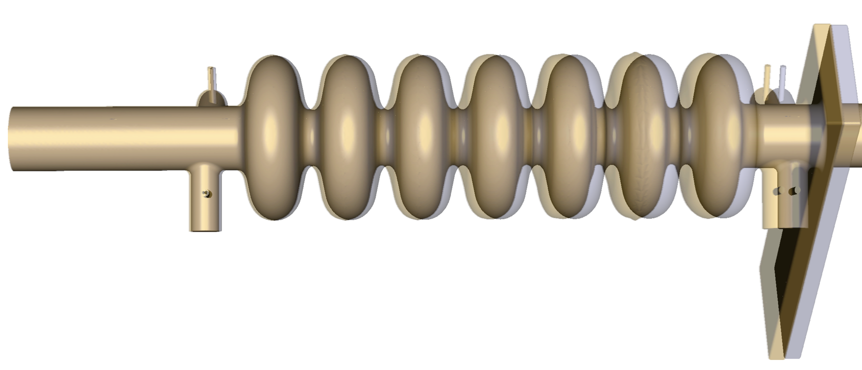
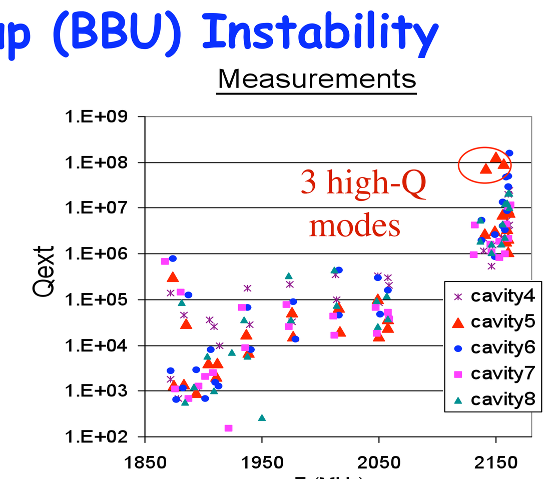
Computational Science Research was an essential component of the SciDAC-1 accelerator project and will play an even more vital role in the newly funded SciDAC-2 **Community Petascale Project for Accelerator Science and Simulation (ComPASS).** Current efforts in computer science and applied math in support of Petascale electromagnetic modeling for accelerator design and analysis focus on uncertainty quantification of accelerator cavity shape, mesh-based multi-level preconditioner for solving highly-indefinite linear systems, and adaptive refinement to improve beam simulation using a moving window. A summary of other computational science activities and plans for future work will also be presented.

Uncertainty Quantification of Cavity Shape

Accelerator Problem - CEBAF Beam-breakup (BBU) Instability





- Experiments showed 3 abnormally high Q modes in a high-gradient cavity
- Beam-breakup threshold current is significantly below design value
- Causes could not be identified experimentally

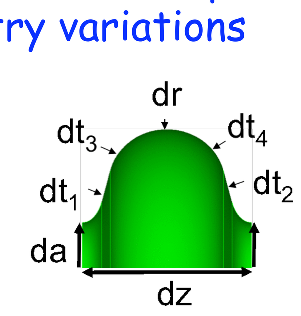
Solve the inverse problem to determine the deformed cavity shape

- Use measured RF parameters such as f, Q_{ext}, and field profile as inputs
- Parameterize shape deviations using pre-defined geometry variations
- Minimize weighted least square misfit

$$\underset{\mathbf{e}_j,k_j,\mathbf{d}}{\text{minimize}} \quad \sum_i \alpha \left(f_i - \bar{f}_i\right)^2 + \sum_i \beta \left(Q_i - \bar{Q}_i\right)^2$$

$$\text{subject to} \quad \mathbf{K}\mathbf{e}_j + ik_j\mathbf{W}\mathbf{e}_j - k_j^2\mathbf{M}\mathbf{e}_j = 0$$

$$\mathbf{e}_j^T\mathbf{M}\mathbf{e}_j = 1$$



SciDAC achievement - Using tools developed with TOPS

- Identified the main cause of BBU: *Cavity is 8 mm shorter than designed* and later confirmed by measurement
- Results explain the physics of the 3 abnormally high Q modes
- This **breakthrough** *only* possible through a **multidisciplinary collaboration** between physicists and computational scientists

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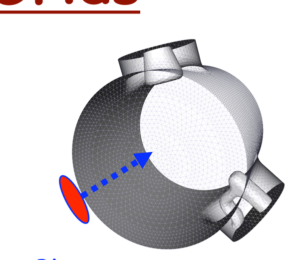
Moving Window for Unstructured Grids

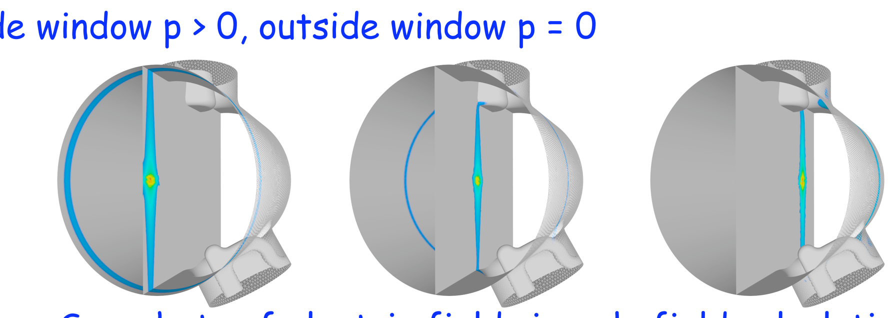
- Calculating short-range wakefield with short bunch requires high resolution in the beam region
- Moving window with adaptive refinement significantly reduces computational resources
- First moving window algorithms for **unstructured grids**



- Physics requirement:
  - Beam size ~300 microns
- Beampipe radius is 39 mm
- Estimated > 100 million tetrahedral elements

Using p-refinement

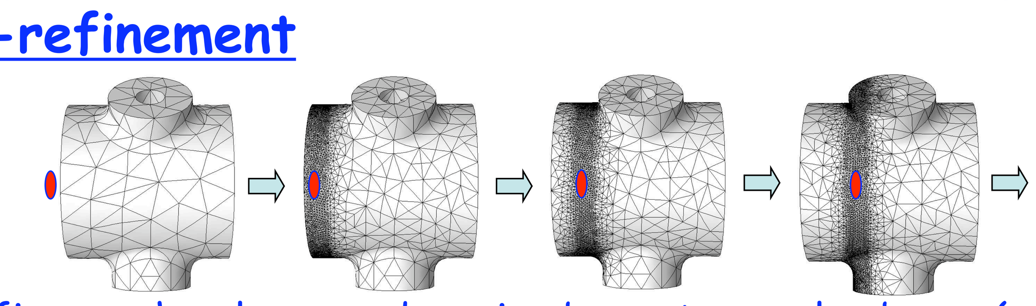
Inside window p > 0, outside window p = 0



- 800 micron beamsize
- 400 micron mesh size
- 13 million elements
- 5 windows in the run
- 1/10th of execution time
- 1/10th of memory usage

Snapshots of electric fields in wakefield calculations with moving window

Using h-refinement



- Refine mesh only around moving beam to resolve beam (collaborating with scientists at RPI/ITPAS)
- Transferring solution vectors from mesh to mesh uses the **new projection method** described in Slide 2 (**critical to control errors**)

See also: Poster by M Shephard, RPI/ITPAS, Curved Mesh Correction and Adaptation Tool to Improve COMPASS Electromagnetic Analysis

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Mesh-based Multilevel Preconditioner

Eigenvalue Problem:

Governing Equation: $\nabla \times \left(\frac{1}{\mu}\nabla \times \vec{\mathbf{E}}\right) - \varepsilon k^2 \vec{\mathbf{E}} = 0$

Finite element Discretization: $\vec{\mathbf{E}} = \sum_i x_i \vec{\mathbf{N}}_i$

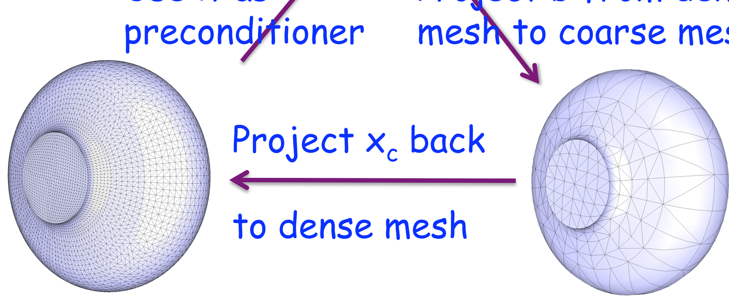
$\mathbf{K}\mathbf{x} = \mathbf{M}\mathbf{x}k^2 \qquad \mathbf{K}_{ij} = \left(\frac{1}{\mu}\nabla \times \vec{\mathbf{N}}_i, \nabla \times \vec{\mathbf{N}}_j\right)$ and $\mathbf{M}_{ij} = \left(\varepsilon \vec{\mathbf{N}}_i, \vec{\mathbf{N}}_j\right)$

Multilevel Preconditioner for the shifted linear system:

Solve (K-σM)x = b

Use it as preconditioner

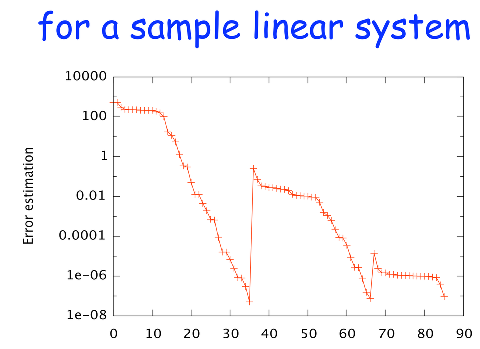
Project b from dense mesh to coarse mesh



Project x_c back to dense mesh

Solve a coarse version of $(K_c-\sigma M_c)x_c=b_c$

Convergence history of GMRES with MbMP for a sample linear system

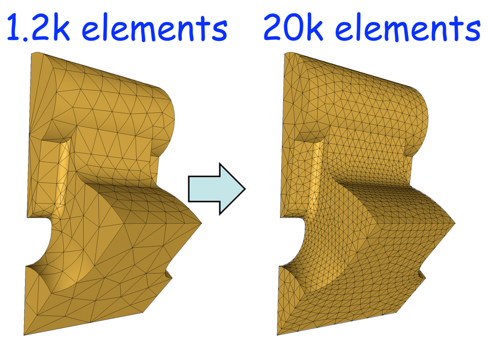


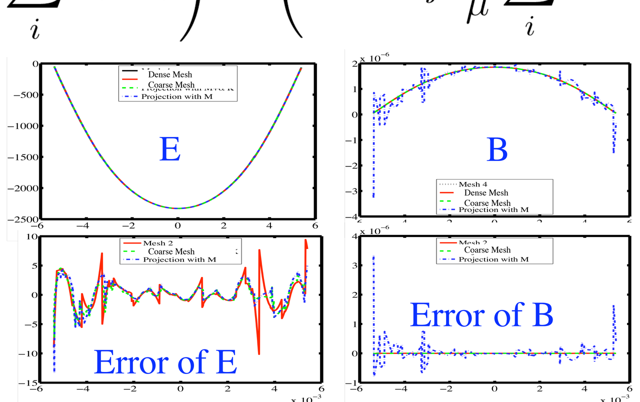
- The projection method is the **key** technique

New method to project an eigenvector from mesh a to mesh b:

$$(\mathbf{M} + \alpha\mathbf{K})\,\mathbf{x}^b = \left(\vec{\mathbf{N}}_j^b, \varepsilon \sum_i x_i^a \vec{\mathbf{N}}_i^a\right) + \alpha\left(\nabla \times \vec{\mathbf{N}}_j^b, \frac{1}{\mu}\sum_i x_i^a \nabla \times \vec{\mathbf{N}}_i^a\right)$$

1.2k elements 20k elements





- Balance errors of both E and B
- Keep the quality of the solution

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Other Activities and Future Directions

Other computational science advancements

- Overhauled application I/O with parallel-netcdf API (CScADs, NCCS)
- Improved solver scalability (NCCS)
- Replaced legacy communication pattern (NCCS)
- Deployed the algorithm for visualizing high-order tetrahedral elements

Future Work

- Search for more efficient algorithms for large-scale nonlinear eigenvalue problems emerged from accelerator modeling (TOPS)
- Continue exploring memory-efficient algorithms for solving large-scale indefinite linear systems
- Develop an efficient dynamic load balancing scheme for particle and field computations (CSCAPES, ITAPS)
- Implement moving window technique with combined hp -refinement for unstructured grids (ITAPS)
- Develop interactive parallel visualization (ISUV)

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SLAC Stanford Linear Accelerator Center, Menlo Park, CA :: Operated by Stanford University for the U.S. Dept. of Energy

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