Data Analysis and Visualization for Accelerator Modeling at Extreme-scale

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SLAC National Accelerator Laboratory

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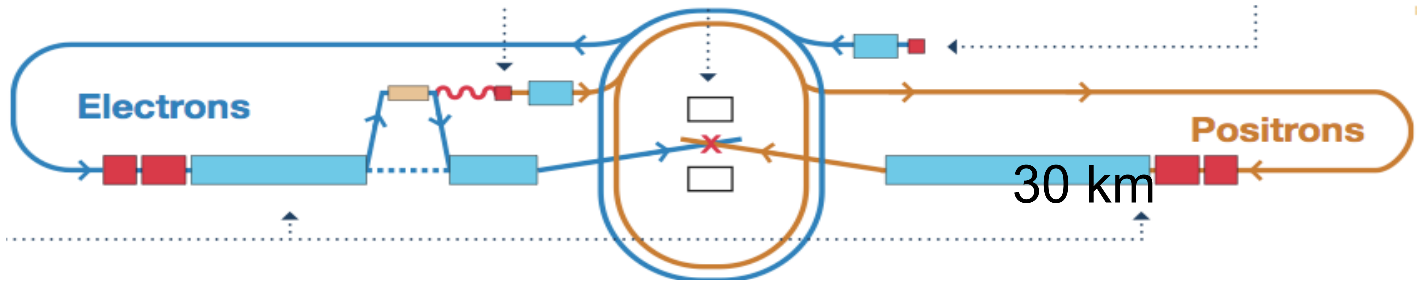
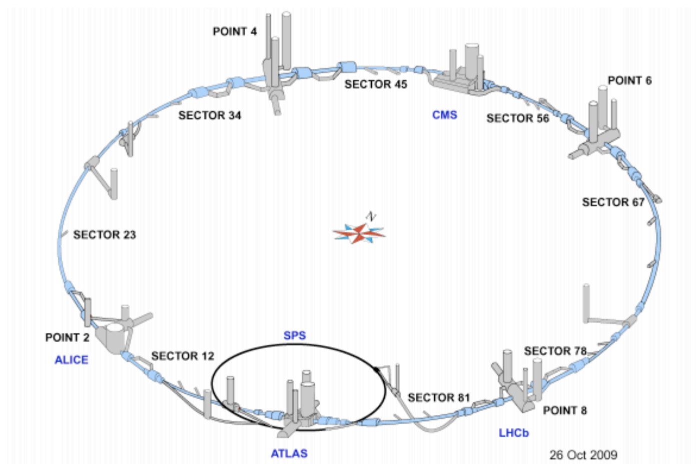
Advanced Computing for Accelerators

* Particle accelerators are **billion-dollar class facilities**
  – Proposed International Linear Collider: 6.75 billion dollars



30 km

  – Large Hadron Collider: 6.5 billion dollars



27 km

* Advanced computing enables **virtual prototyping**
  – **Cost savings** from design optimization through computing can be significant

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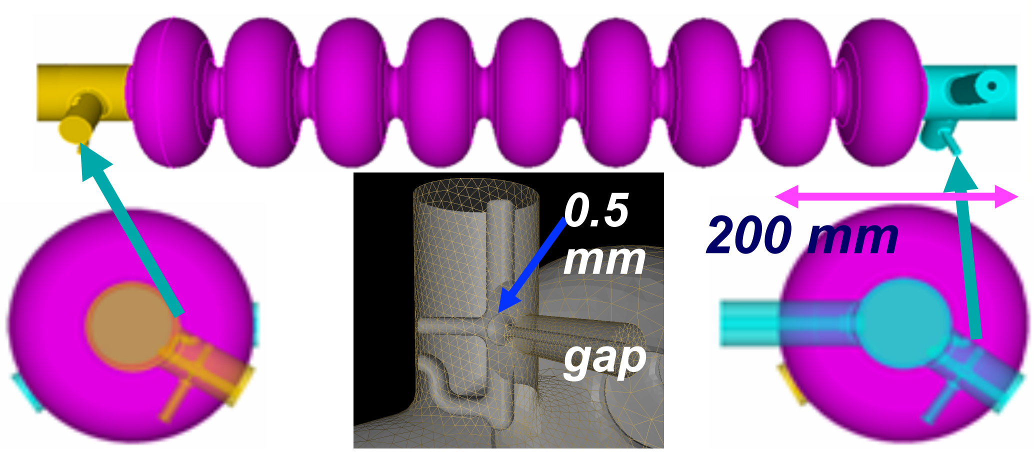
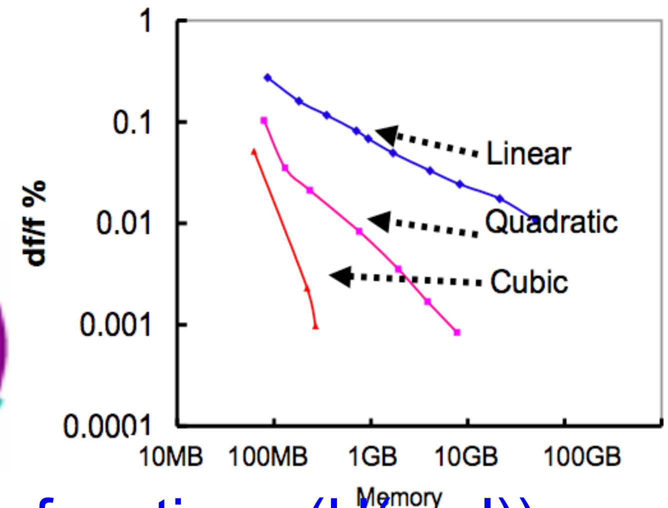
SciDAC for Accelerator Modeling

* ComPASS Accelerator Project (2007-2012) at SLAC has ongoing collaborations with
  - TOPS/LBL (Linear solvers and eigen-solvers)
    - E Ng, X Li, I Yamazaki
  - ITAPS/RPI, LLNL, Sandia (Parallel curvilinear meshing and adaptation)
    - Q Lu, M Shephard, L Diachin
  - Ultra-scale Visualization Institute/Sandia, UC Davis
    - K Mooreland, K Ma
  - ITAPS/CSCAPES/Sandia (Load balancing)
    - K Devine, E Boman

Finite Element Approach for High Fidelity Modeling

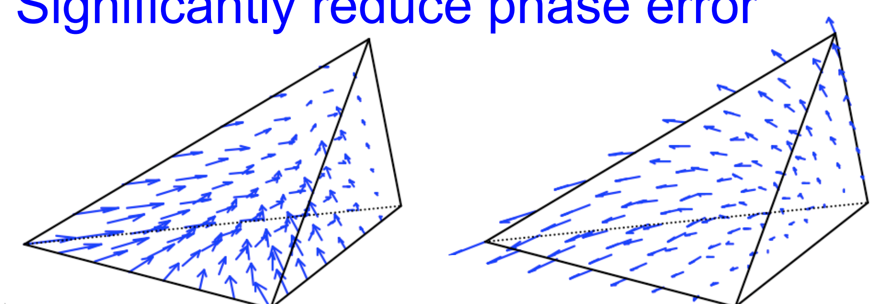
* Curvilinear tetrahedral elements:





* High-order hierarchical vector basis functions (H(curl))
  – Provide tangential continuity required by physics
  – Easily set the boundary conditions
  – Significantly reduce phase error

Entities	# of bases
Edge	p
Face	p(p-1)
Volume	p(p-1)(p-2)/2
Total	6E+4F+V



Shape functions

Parallel Finite Element Code Suite ***ACE3P***

Over more than a decade, SLAC has developed the conformal, higher-order, C++/MPI-based parallel finite-element suite of electromagnetic codes, under the supports of AST SciDAC1 and ComPASS SciDAC2 projects

	ACE3P Modules	**– Accelerator physics application**
***Frequency Domain*:**	**Omega3P**	**– Eigensolver (nonlinear, damping)**
	S3P	**– S-Parameter**
***Time Domain*:**	**T3P**	**– Wakefields and Transients**
***Particle Tracking*:**	**Track3P**	**– Multipacting and Dark Current**
EM Particle-in-cell	**Pic3P**	**– RF gun simulation**

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

Aiming for the Virtual Prototyping of accelerator structures

INCITE Award for Accelerator Modeling

* INCITE Award: Petascale Computing for Tera-eV Accelerators (2008-2010)
  - ORNL (Jaguar / Lens / Hpss)
  - Kitware (for ParaView visualization and analysis software)
  - Center for Scalable Application Development Software (CScADS)

- **Provide major computing resources and supports for efficiently using them in tackling challenging accelerator modeling problems**

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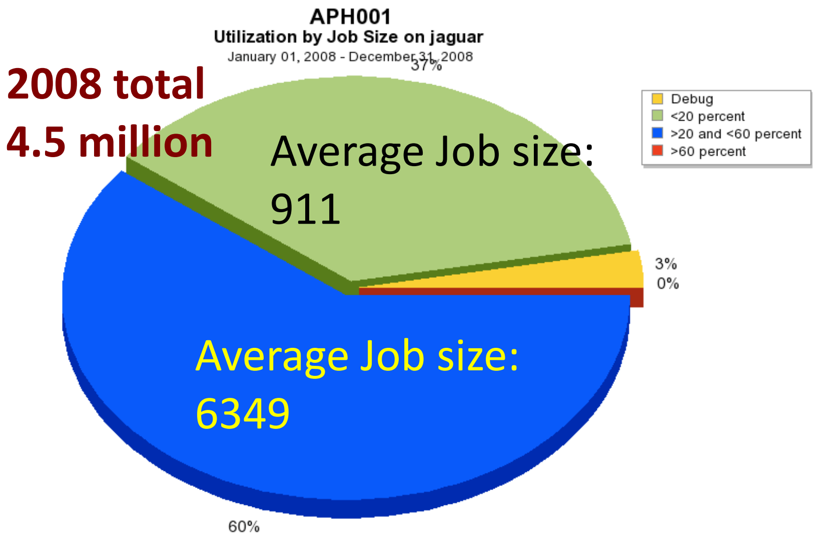
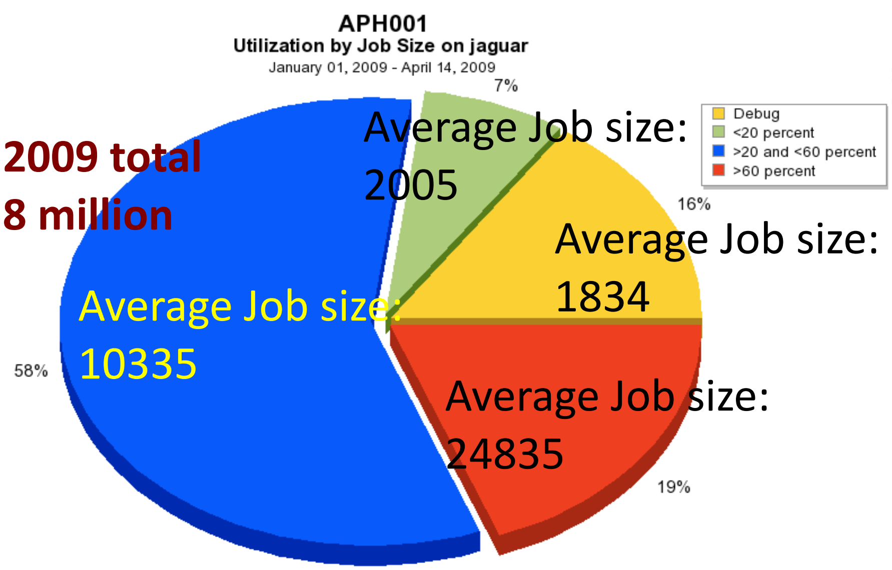
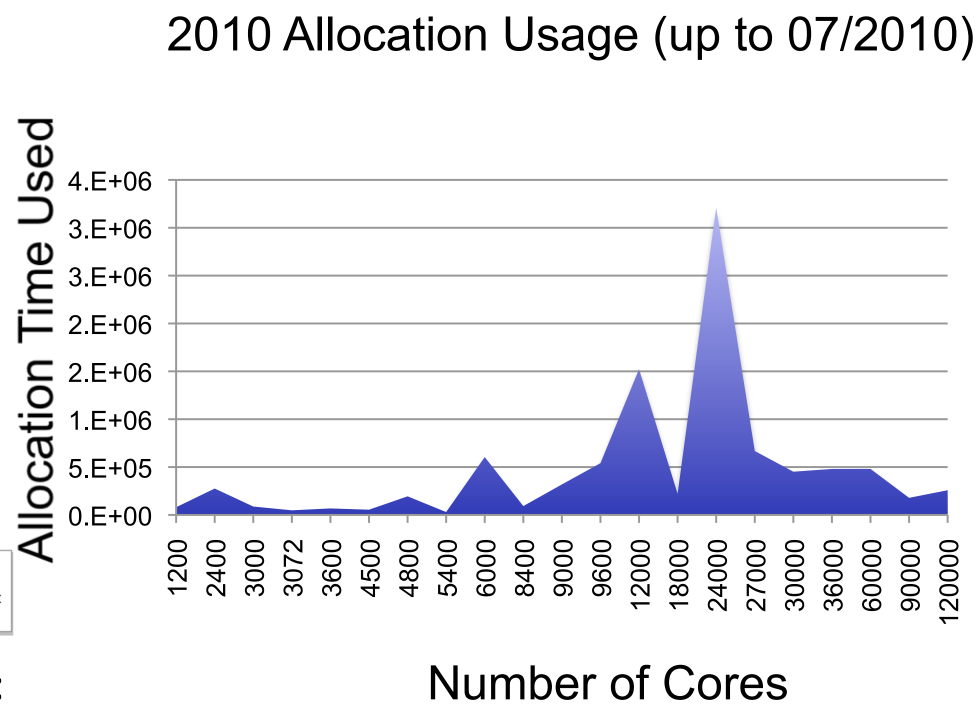
SLAC's INCITE Allocation Usage at NCCS





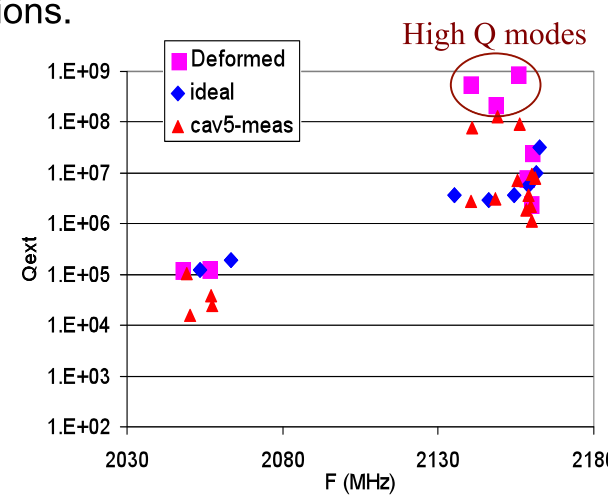
2010 total 12 million



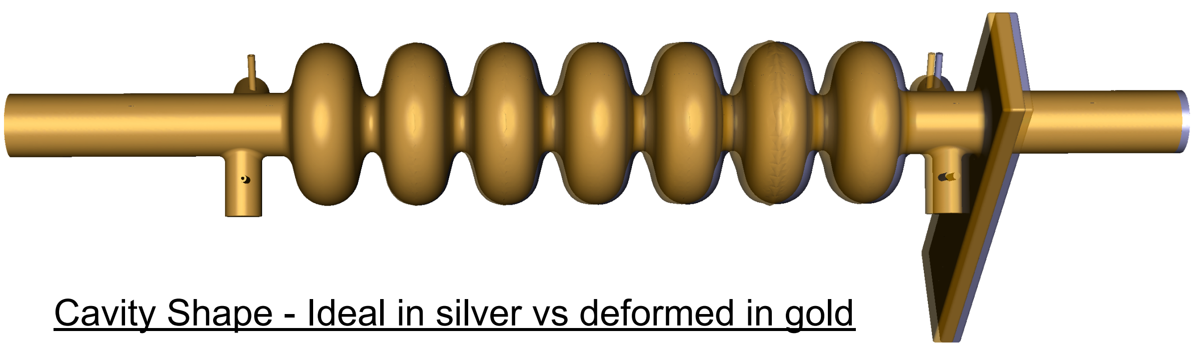
- ~60% of total time is used with 10% to 50% of the total resources (22k cores to 120k cores)

Solving CEBAF BBU Using Shape Uncertainty Quantification Method

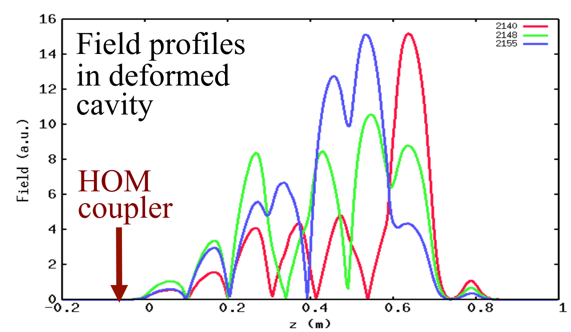
SciDAC Success as a Collaboration between Accelerator Simulation, Computational Science and Experiment – Beam Breakup (BBU) instabilities at well below the designed beam current were observed in the CEBAF12 GeV upgrade of the Jefferson Lab (TJNAF) in which Higher Order Modes (HOM) with exceptionally *high* quality factor (Q) were measured. Using the shape uncertainty quantification tool developed under SciDAC, the problem was found to be a deformation of the cavity shape due to fabrication errors. This discovery was achieved as a team effort between SLAC, TOPS, and JLab which underscores the importance of the SciDAC multidisciplinary approach in tacking challenging applications.



Method of Solution - Using the measured cavity parameters as inputs, the deformed cavity shape was recovered by solving the ***inverse*** problem through an optimization method. The calculations showed that the cavity was 8 mm shorter than designed, which was subsequently confirmed by measurements. The result explains why the troublesome modes have high Qs because in the deformed cavity, the fields shift away from the HOM coupler where they can be damped. This shows that quality control in cavity fabrication can play an important role in accelerator performance. .



Cavity Shape - Ideal in silver vs deformed in gold



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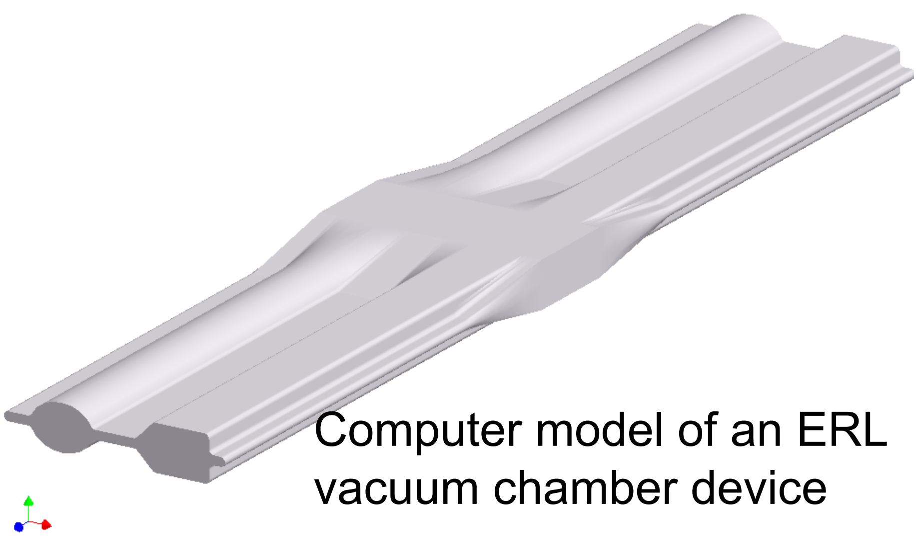
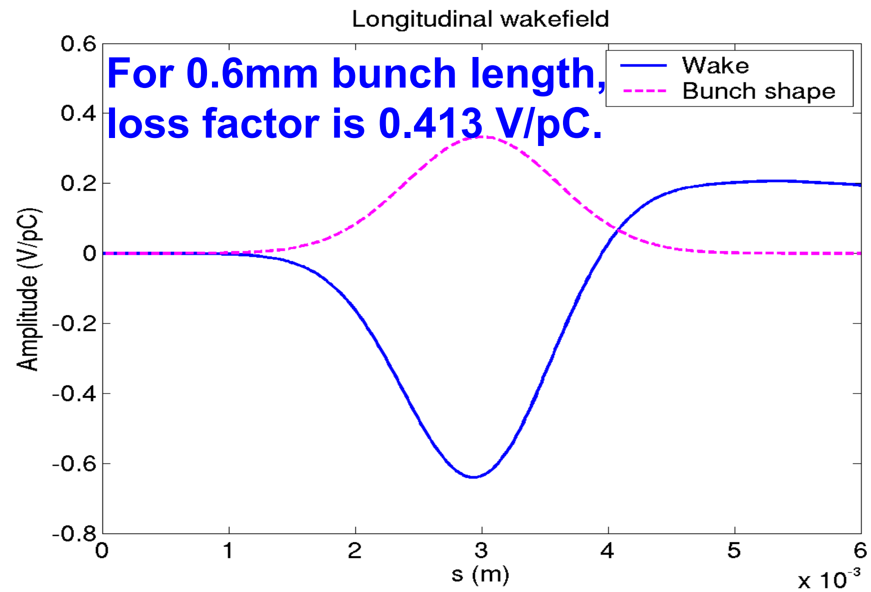
SLAC
TOPS Terascale Optimal PDE Simulations
Jefferson Lab

Wakefields in Cornell ERL Vacuum Chamber

* Energy Recovery Linac (ERL) Aluminum Vacuum Chamber
* Moving window with online mesh refinement; 18000 cores with ~5 hours on Jaguarpf at ORNL
* Not possible without algorithmic advance and INCITE-scale resources for calculating wakefields of such a short bunch



Computer model of an ERL vacuum chamber device



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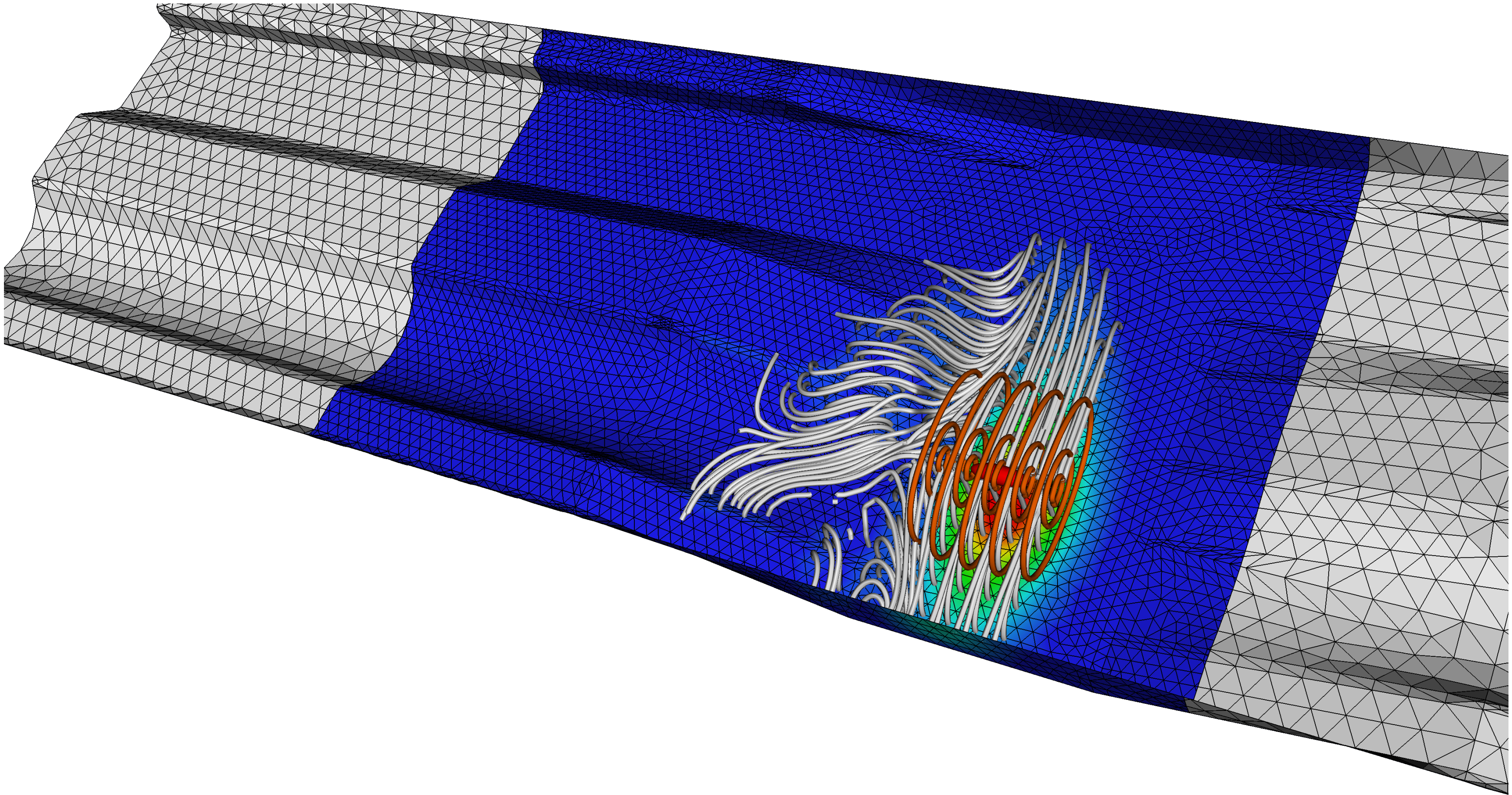
Movie of Wakefields in ERL Vacuum Chamber



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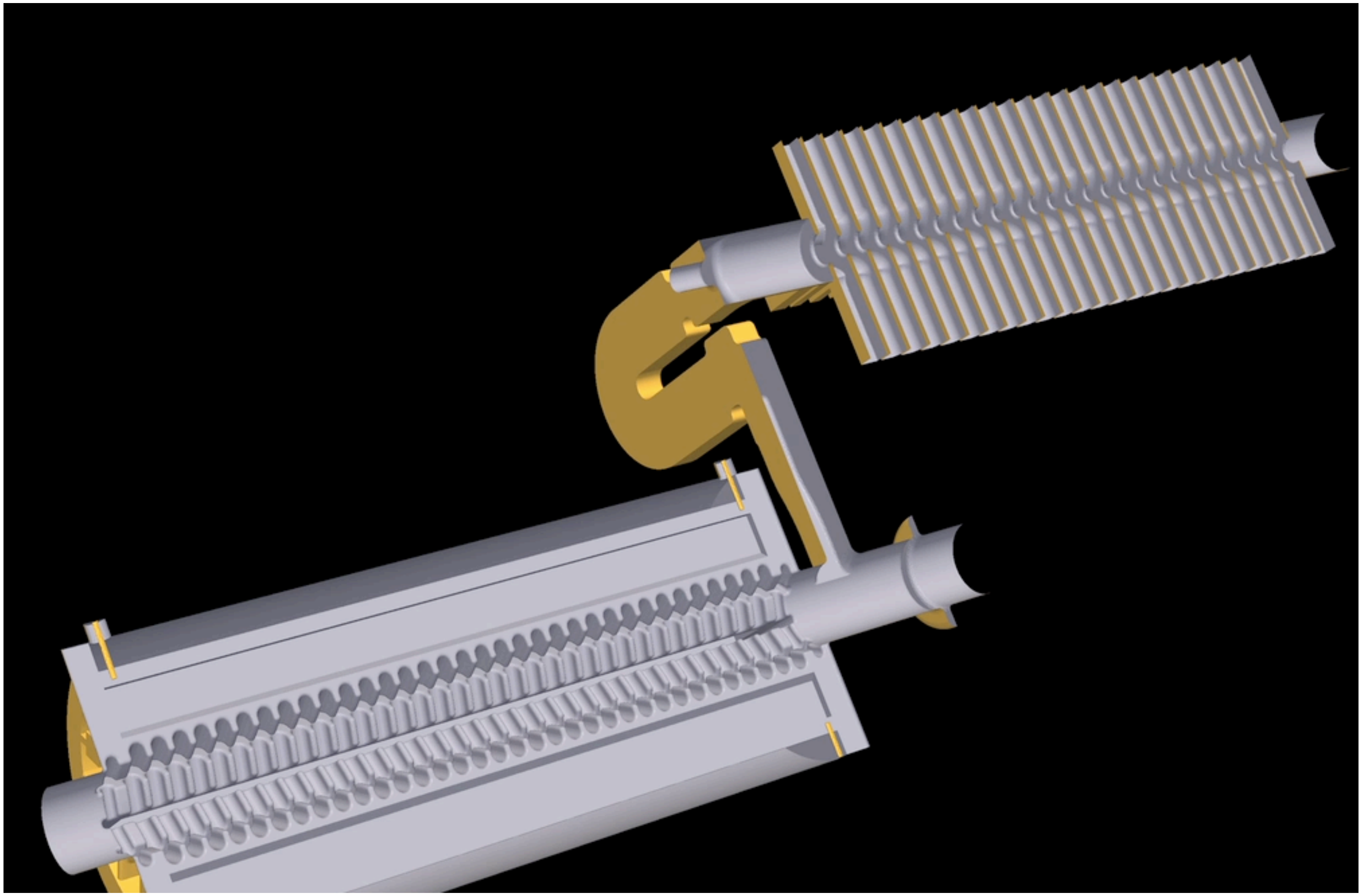
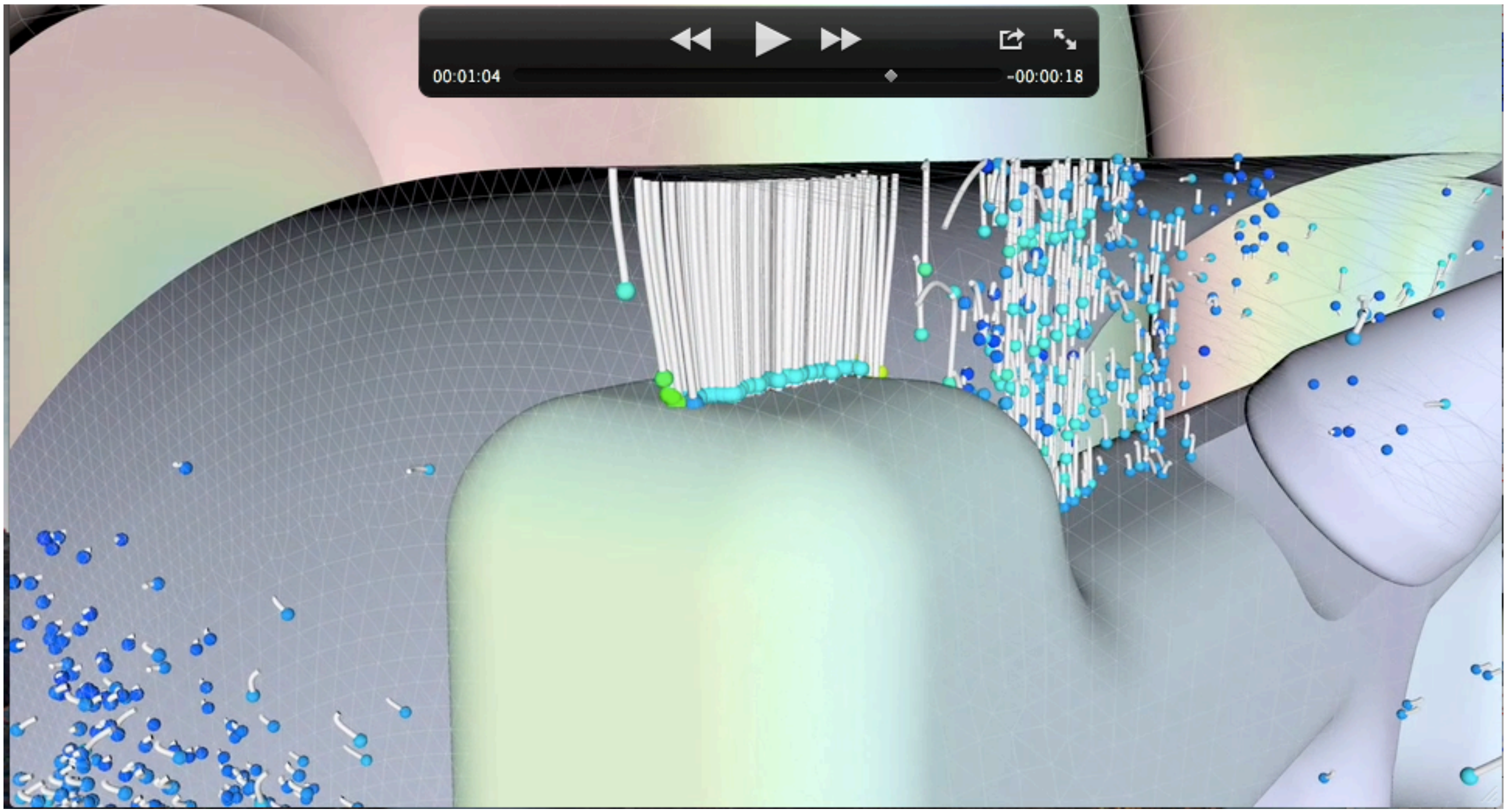
Electromagnetic Fields in Complicated Geometry



Visualizing Fields and Particles on Mesh



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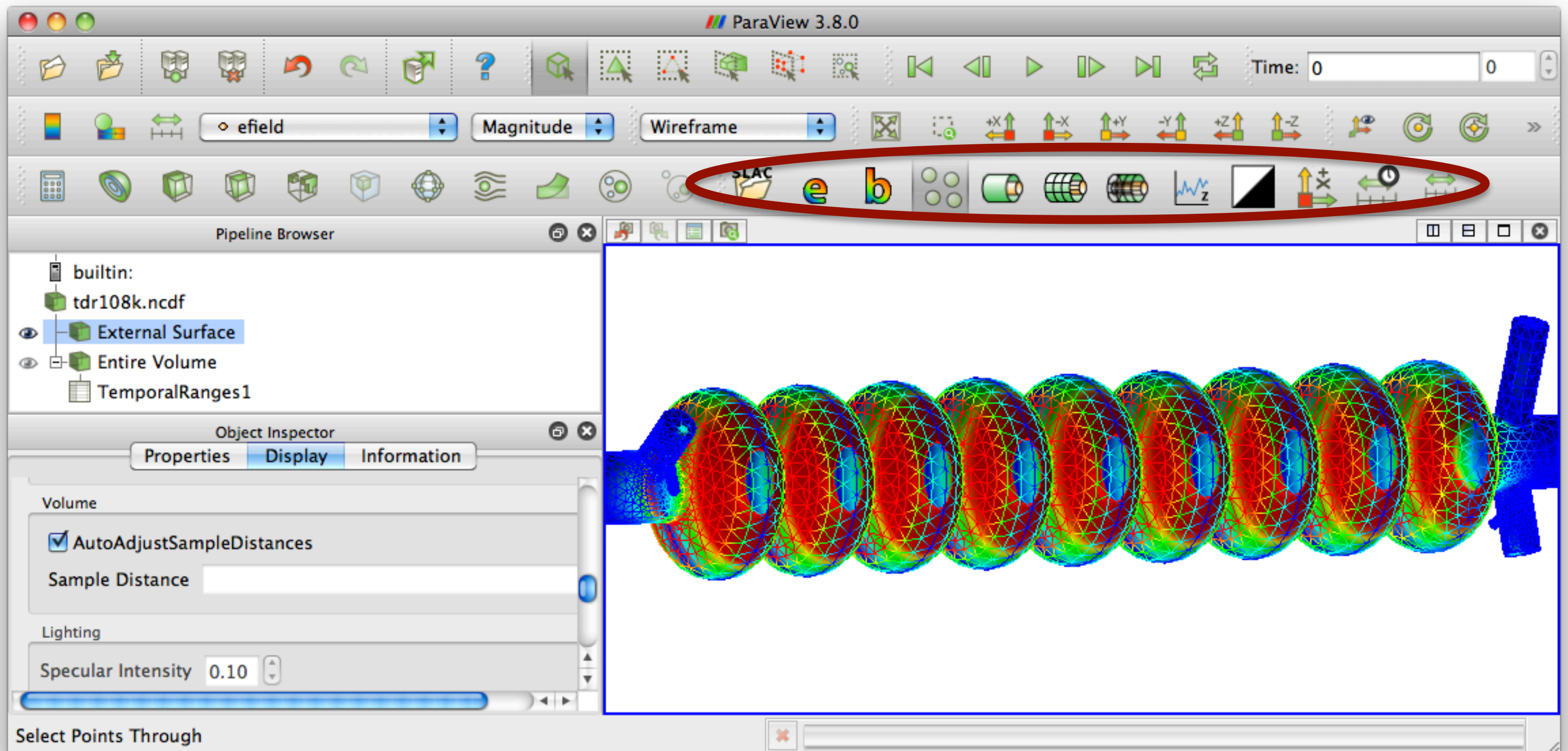
Data Analysis And Visualization for Accelerator Modeling at SLAC

* Collaborators
  – K Mooreland (UltraVis/Sandia), K Ma (UltraVis/UC Davis), Berk Geveci, Utkarsh Ayachit, Andy Bauer (Kitware)
* Current Status
  – Using ParaView
  – With Accelerator Toolbox developed
* Datasets
  – Unstructured mesh, fields, and particles
  – Typically, 7.5GB per snapshot, with 2000 snapshots for a movie

Accelerator Toolbox Plugin for ParaView

* Readers for tetrahedral meshes, electromagnetic fields, and particles in netcdf format
* A few commonly-used functionalities on the toolbar
* Developed with Sandia and Kitware (different supports)



Needs in Data Analysis And Visualization

* Dataset size keeps increasing
* More user-friendliness of paraview runs on computing centers (NERSC, ALCF, LCF) for community users
  - Easy to run in parallel
  - Able to open local display (for the performance purpose) on batch-queue computing
* More supports for visualizing high-order finite-elements
  - Better viewing of the geometry from high-order mesh elements
  - Better viewing of the fields from high-order basis functions
* Explorative or In-Situ visualization at exa-scale computing (beyond petascale)
  - Showing overall things but able to automatically identify the interesting parts and showing zoom-in view
  - Visualize resulting data while the simulation is running to avoid a large amount of IO

Facilitate Parallel Visualization

* ParaView has client-server mode and server can be executed in parallel
* Nontrivial for average Joe to use it
* Require many tweaks and tricks from both developers and computing center personnel to be able to run paraview in parallel on **lens** cluster (ORNL's viz cluster).
* ParaView not officially supported yet for Euclid (NERSC's data analysis computer)

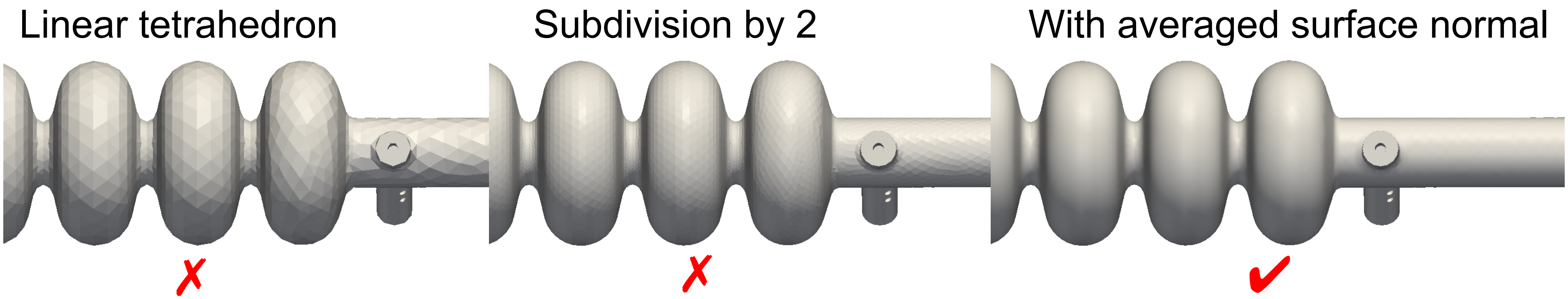
* Need support for computational accelerator community
  – CW09: 15 users/institutions
  – CW10: 29 users, http://www-conf.slac.stanford.edu/CW10
  – our NERSC repo m349: ~50 users

Need Remote Visualization

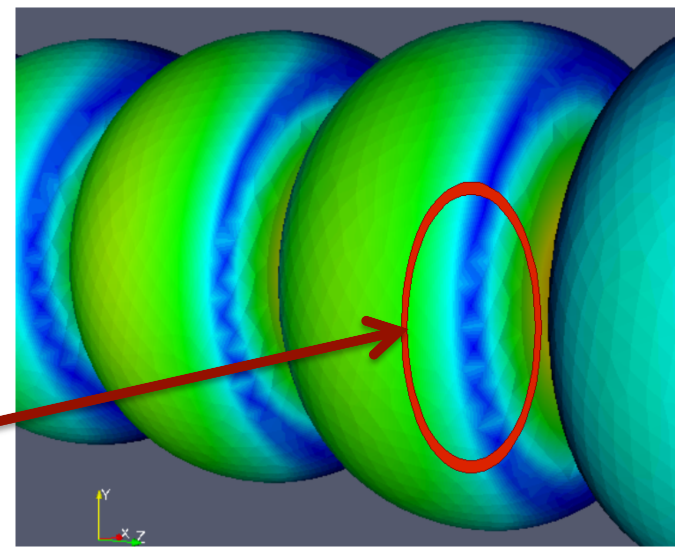
* Viz clusters are different to computing clusters
* Hardware acceleration of rendering relies on access to local X display
* X forwarding put the burden on the network and client computer
* Open local display
  – NX (?), or Mesa (?), or other ways

Enable Visualization of High-Order Elements

* We use curvilinear elements (2nd order 10 point tetrahedron)



* We use higher-order basis functions (p=2,3,4, or 5) and basis functions are on edges, faces, and volume of the tetrahedral elements
  * Current practice: compute fields at vertices
  * OpenGL use linear interpolation to assign colors that leads to artifacts
  * How can we visualize the true fields?



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Explorative or In-Situ Visualization at Exa-scale

* 10^{14} Elements, 10^{15} DOFs for simulating a whole module in a proposed linear collider (identified at DOE Extreme-scale Workshop for HEP, SLAC, 2008)

* Dataset will be too large to see all the details
  – Need explorative visualization technology to
  – Show overall things but able to automatically detect the interesting features and have zoom-in views
    • Strong field regions, High curvature zone, particle-concentrating zone, …
* Dataset will be too large to write into files and read in later in a separate visualization process
  – Visualize resulting data while the simulation is running

Thank you

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