Plans and Progress in HPC

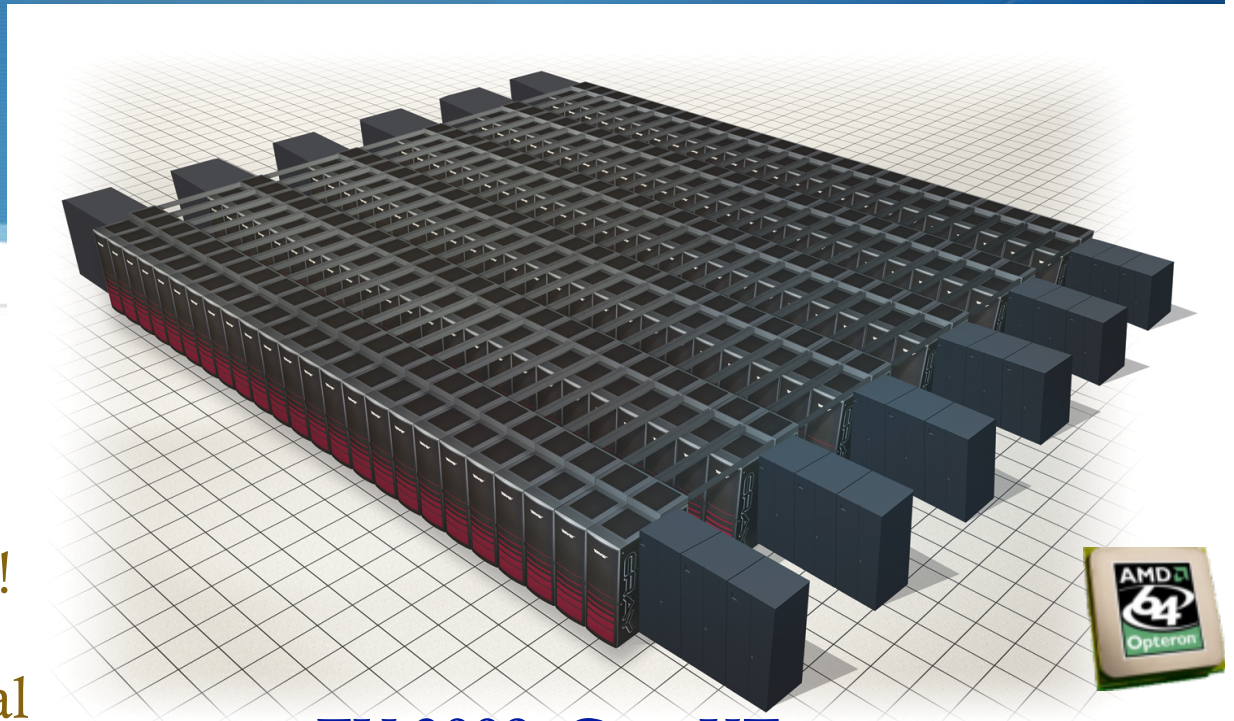## GPSC All Hands Meeting

3/29/2008
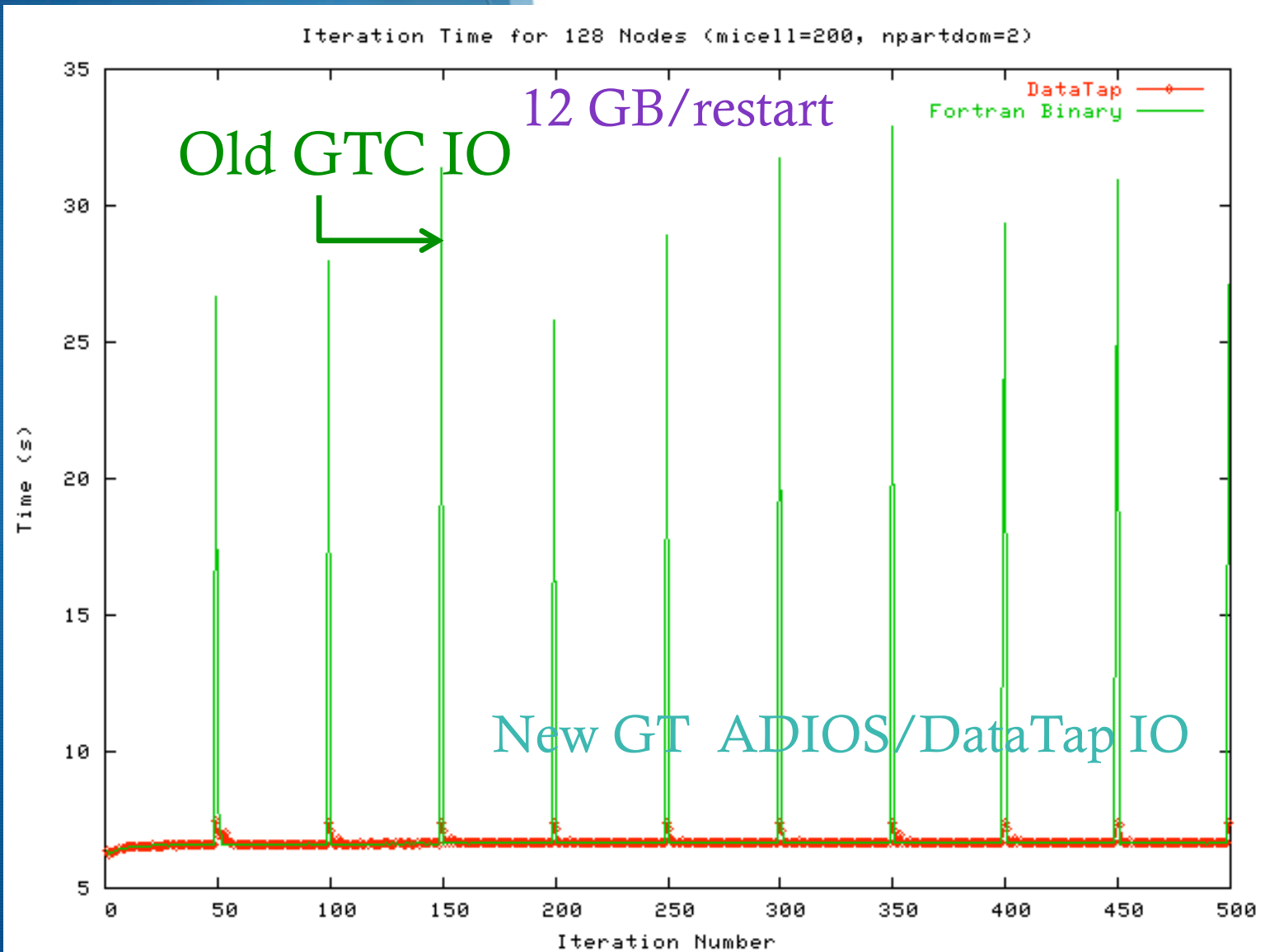
S. Klasky, S. Ethier, C. Jin

1 Petaflops System - Cray

- 1 Petaflops system

- 37 Gigaflops processor

- Over 27K quad-core processors. ~88K cores!

- 2 GB/core; 223 TB total

- 240 GB/s disk bandwidth

- 7.5 MW system power

- Liquid cooled

- FY 2009: Cray XT

IO Progress & Plans

Iteration Time for 128 Nodes (micell=200, npartdom=2)

12 GB/restart

Old GTC IO

New GT ADIOS/DataTap IO

DataTap
Fortran Binary

Time (s)

Iteration Number

ADIOS

- Projected September 1 release of ADIOS at NCCS.

- Through benchmarking of ADIOS into initial test codes : GTC (2 versions), XGC1, Chimera, S3D with
  - MPI-IO method, Fortran IO, MPI-AIO, MPI-CIO, DataTap, Dart
  - Already see 25GB/sec with MPI-IO ADIOS method

ORNL Work 2008

- Finish ADIOS integration into GTC framework IO modules.

- Start looking at Analysis routines.

- Dashboard analysis features.

- Dashboard collaborative features (see Klasky CPES talk).

- Place provenance collection system and PAPI information on dashboard from workflow automation.

Dashboard movie

Created using **Wink**

New Dashboard Features

- Select a shot by searching list or entering shot number
- Drop from both tree and notice tooltip and different background color to differentiate between shots
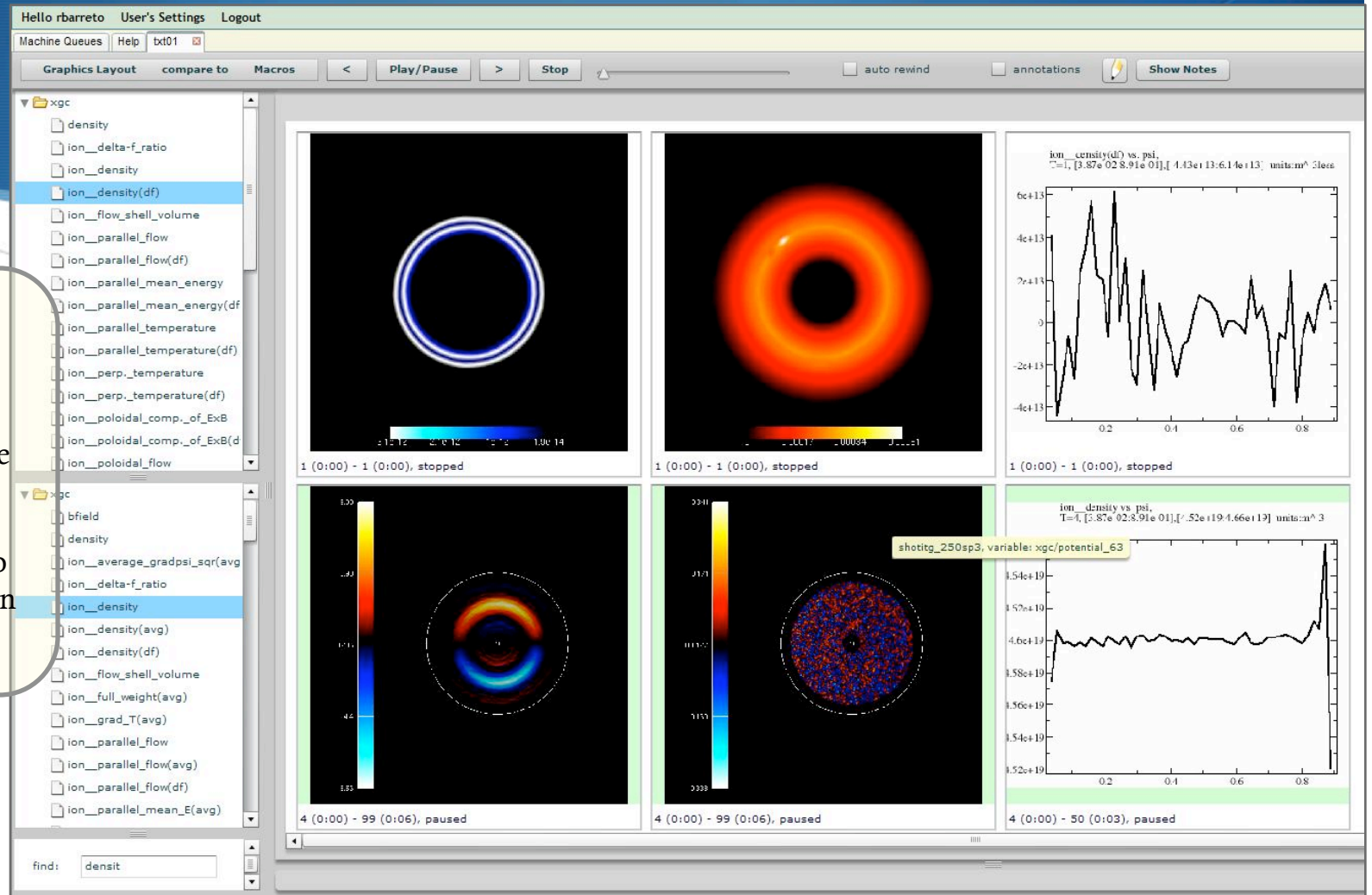
Compare shots

New Dashboard Features

New Dashboard Features

Performance characterization integrated in the dashboard along with the provenance information.
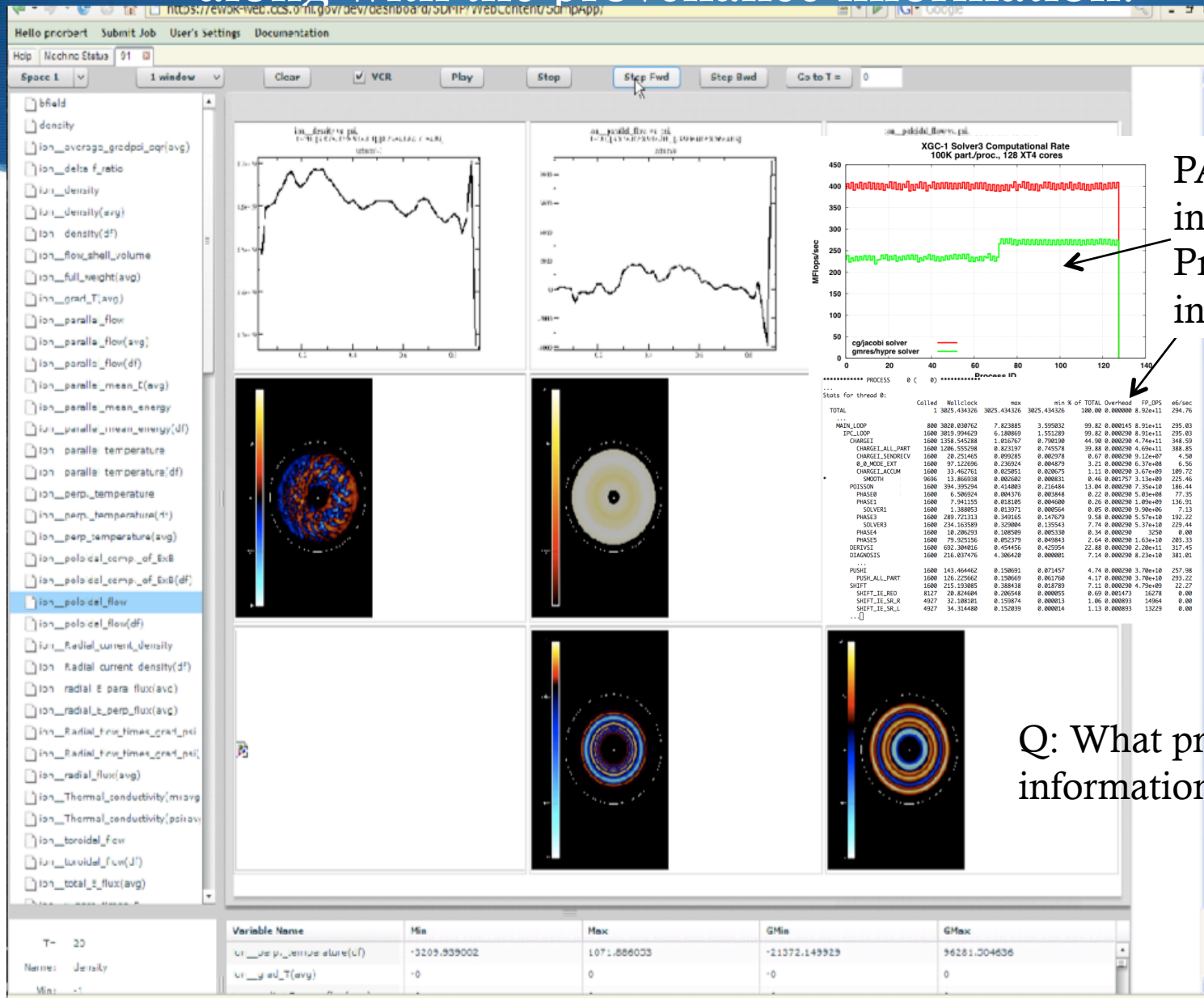
PAPI information
Provenance information

Q: What provenance information to keep?

Machine monitoring.

Eventual hooks into MDS+ for

Interactive Plotting on the dashboard

- Prototype web browser-based flash application with VisTrails (http://vistrails.sci.utah.edu/index.php/Main_Page) on server.
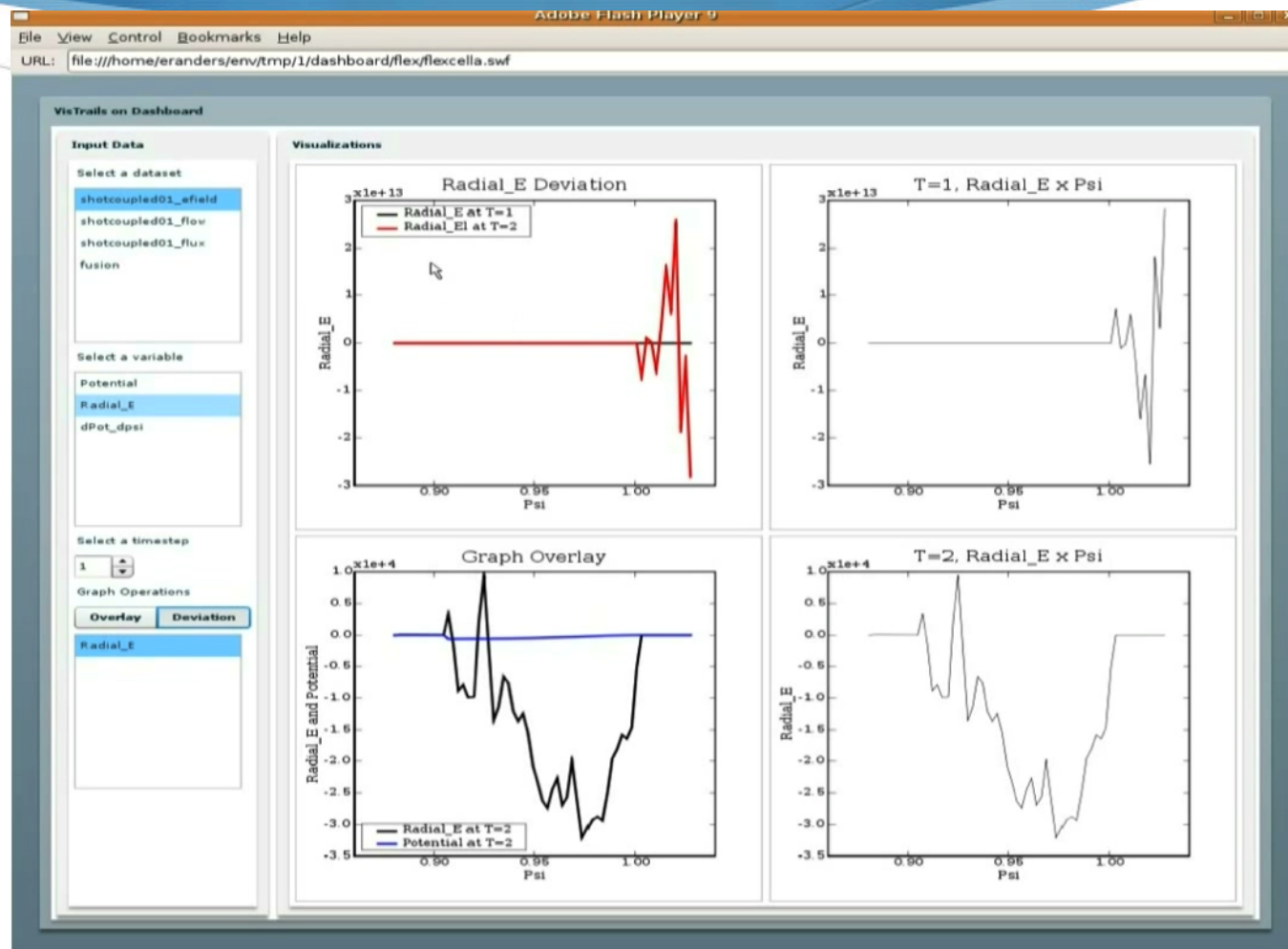
Dashboard Post processing.

Still need.

- Try to incorporate Ma's visualization into Dashboard environment for scaling GTC users.

- How to make GTC a more community code.

Performance Optimization work

- Update and tune OpenMP thread-based parallelism.

- Identify regions in the code where SSE3 vectorization can exploited.

- Optimizations for electron dynamics sub-cycling.
  - For a run with kinetic electrons most of the time is spent in the sub-cycling steps during which the electrons are moved (push phase) and then sent to the processor holding their location in space (shift phase).
  - This last step is particularly time-consuming since the electrons move fast and far.
  - We have now eliminated the shift step during the sub-cycling and do only the push steps.
  - A modified shift is then called only once at the end of sub-cycling, resulting in significant speed-up of the code (N. Wichmann).

Performance Optimization work

- We will test the benefits of process placement at large scale on Jaguar since it has shown to lead to a 30% performance improvement on Blue Gene L, at large concurrencies (8192 cores).

- We will look into one-sided communication routines when available on Jaguar.

- Use vectorized functions from ACML.

- IO is being optimized by using ADIOS.

- Test different solvers in PETSc, including multigrid solvers, for simulations of large devices.