Monitoring simulations and processing data on the fly with workflows

Norbert Podhorszki

Roselyne Tchoua, Scott Klasky

OLCF/NICS Spring
Cray XT5 Hex-core Workshop
May 2010

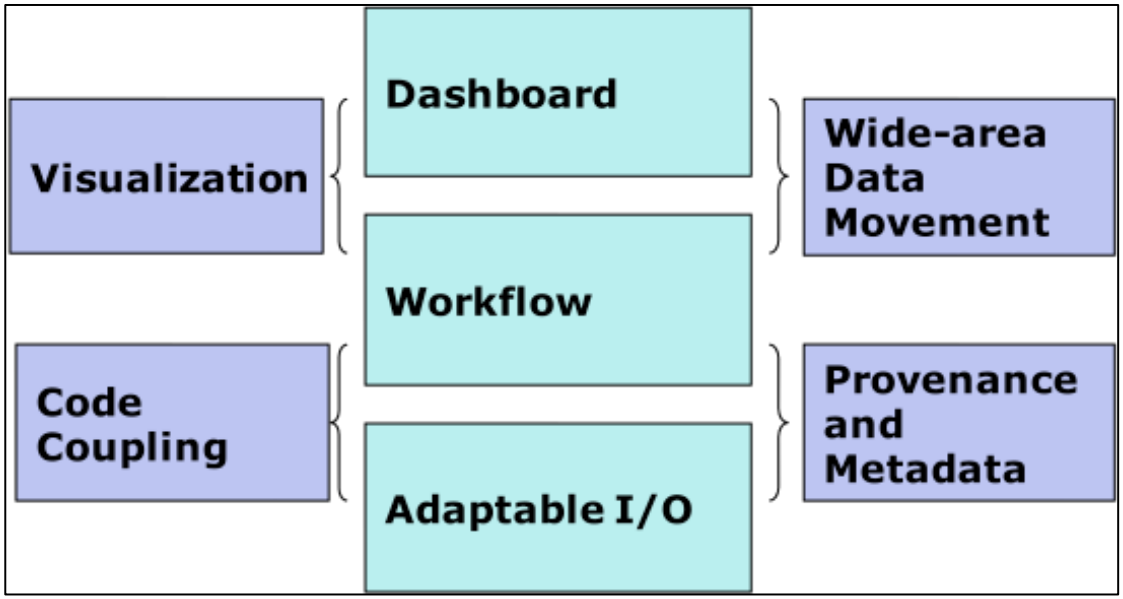
Outline

- Framework for Integrated End-To-End Scientific Data Management Technologies and Applications (FIESTA)
- Monitoring a simulation
- Coupling codes with workflows
- eSimMon Dashboard
- Future plans

OAK RIDGE National Laboratory

FIESTA: Framework for Integrated End-to-end SDM Technologies and Applications

Goal: Accelerate the scientific discovery process by developing middleware and dashboard that allow users to generate fast metadata-rich I/O, and then perform the mundane tasks needed to present scientists with meaningful results.

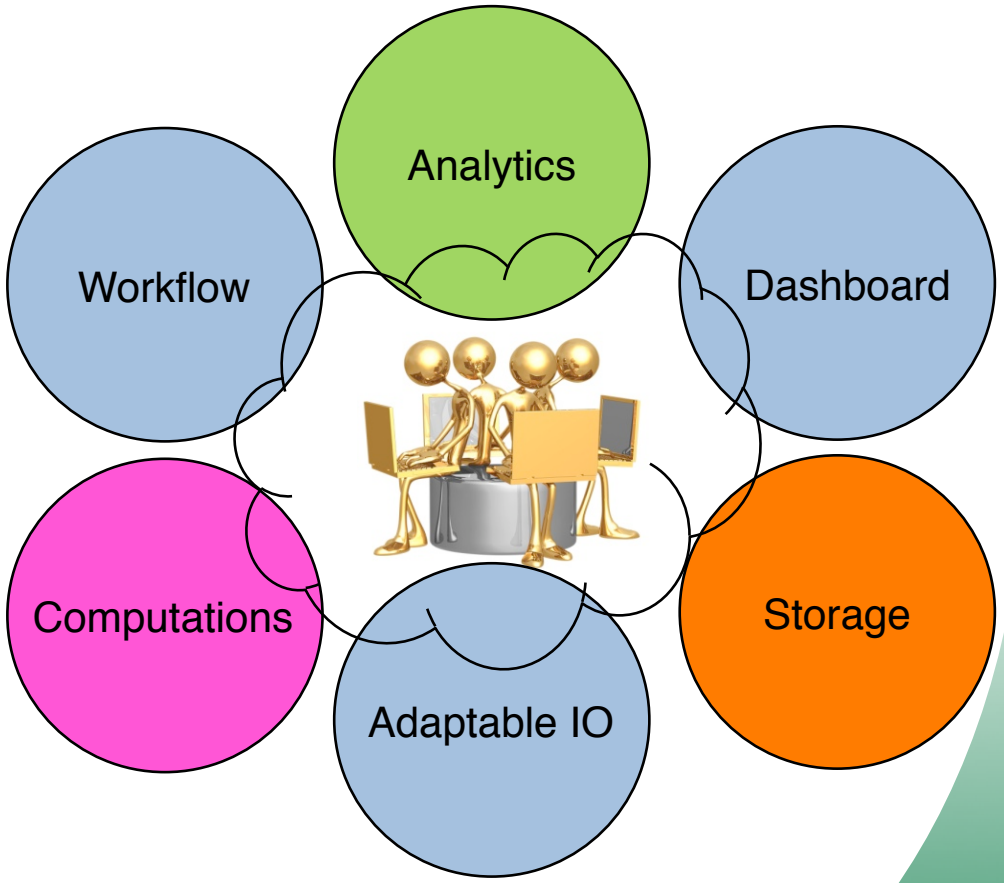


OAK RIDGE National Laboratory

FIESTA: Framework for Integrated End-to-end SDM Technologies and Applications

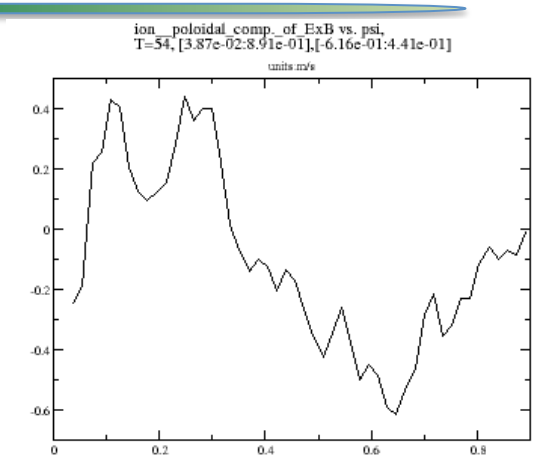
Main Components:

- The eSimMon dashboard provides access to simulation results, metadata and data storage and analytics tools
- Kepler workflow orchestrates parallel tasks on multiple computer platforms and feeds the dashboard with a multitude of output
- ADIOS provides portable, metadata-rich, fast, adaptable IO

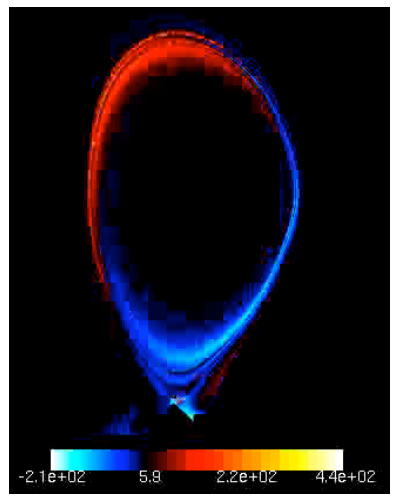


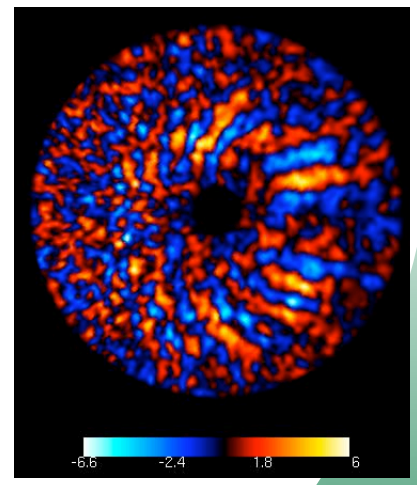
Monitoring a simulation + archiving (XGC1)

- 1D diagnostics NetCDF files
  - Transfer files to e2e system on-the-fly
  - Generate plots using grace library
  - Archive NetCDF files at the end of simulation



- 2D diagnostics (ADIOS-BP files)
  - Transfer to e2e system
  - Convert to HDF5 format
  - Start up AVS/Express service
  - Generate images with AVS/Express
  - Archive HDF5 files in large chunks to HPSS





- Generate movies from the images

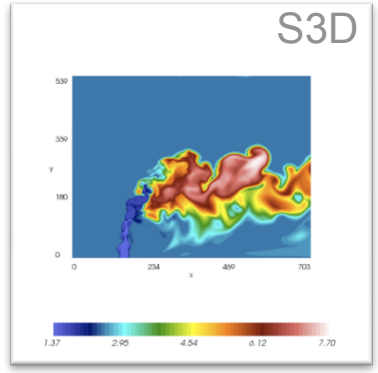
CPES
Center for Plasma Edge Simulation

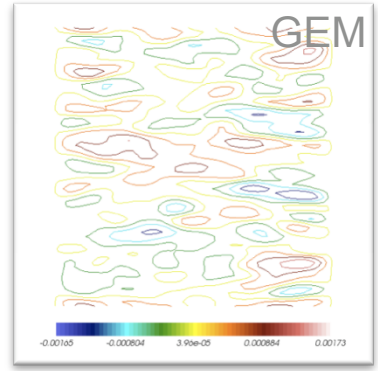
OAK RIDGE National Laboratory

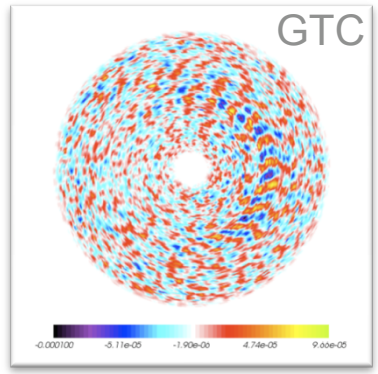
SHOW SWF…

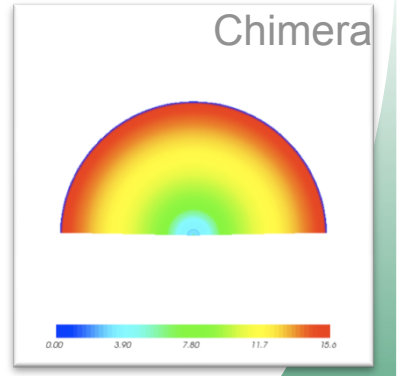
plotter: our tool for quick 1D/2D plots

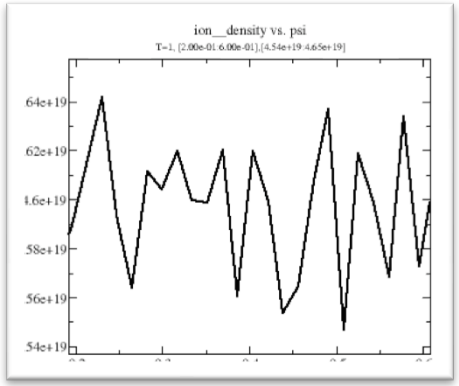
- reads ADIOS BP/NetCDF/HDF5 arrays
  - any slice from any multi-dimensional array
- Use xmgrace to make X-Y plots
- Use VTK for 2D graphics
- We use this tool to generate lots of plots at once and in parallel

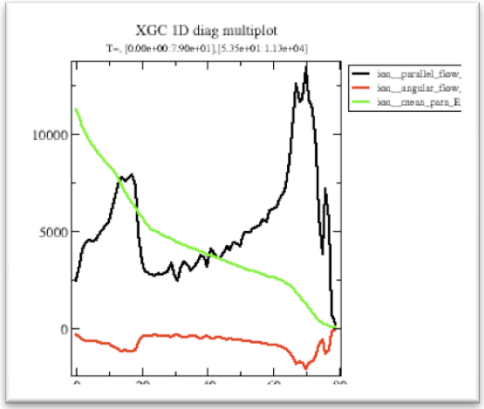


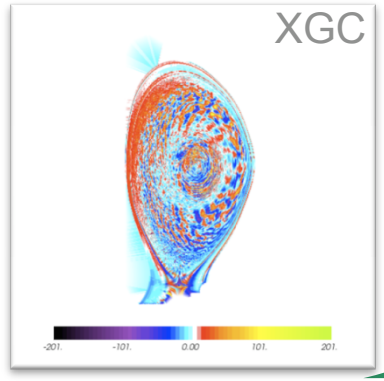








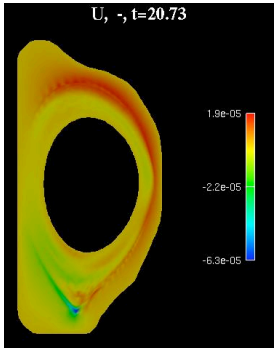


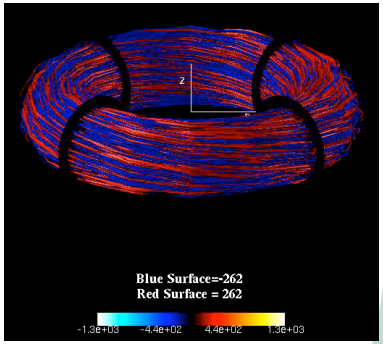


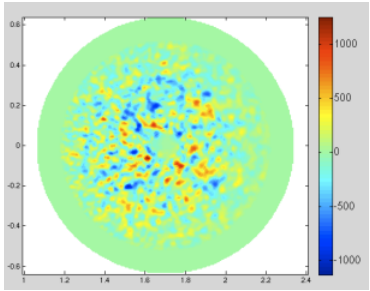
OAK RIDGE National Laboratory

for more generic viz…

- we use AVS in current workflows
  - run as service
  - e.g. M3D hexagonal mesh, 3D XGC
- working on to use VisIt
  - e.g. Pixie3D 3D viz, AMR codes, etc.
- can run Matlab scripts
- can run whatever is provided by others

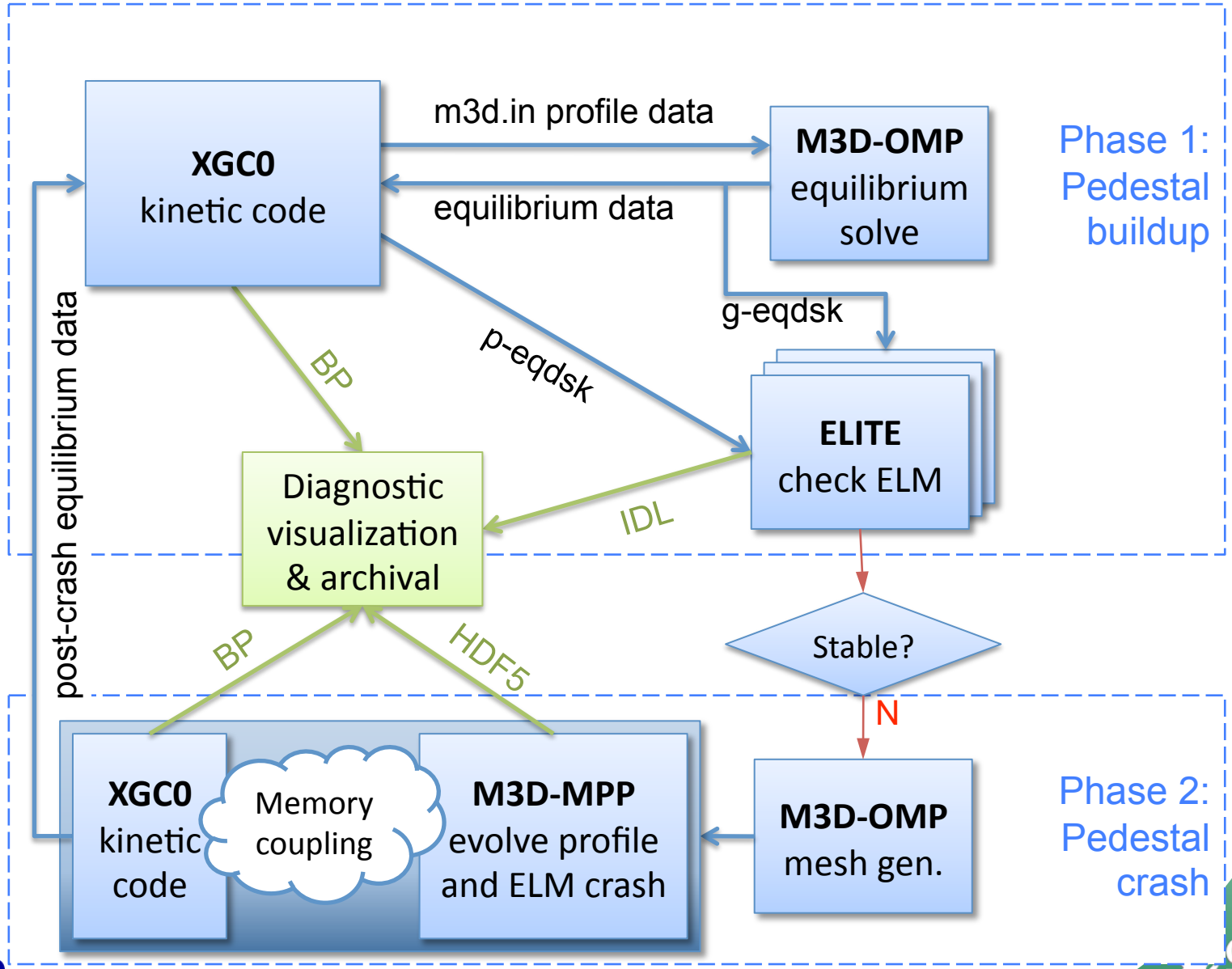






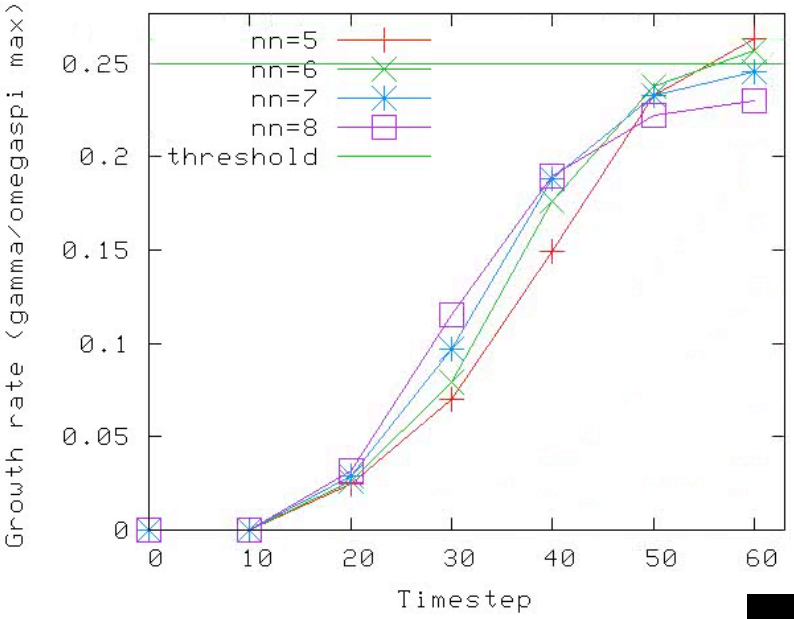
OAK RIDGE National Laboratory

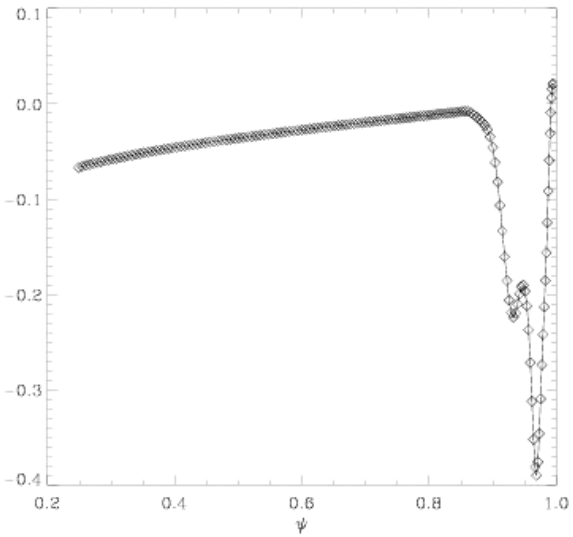
A scientific problem-solving process: Coupling Fusion codes

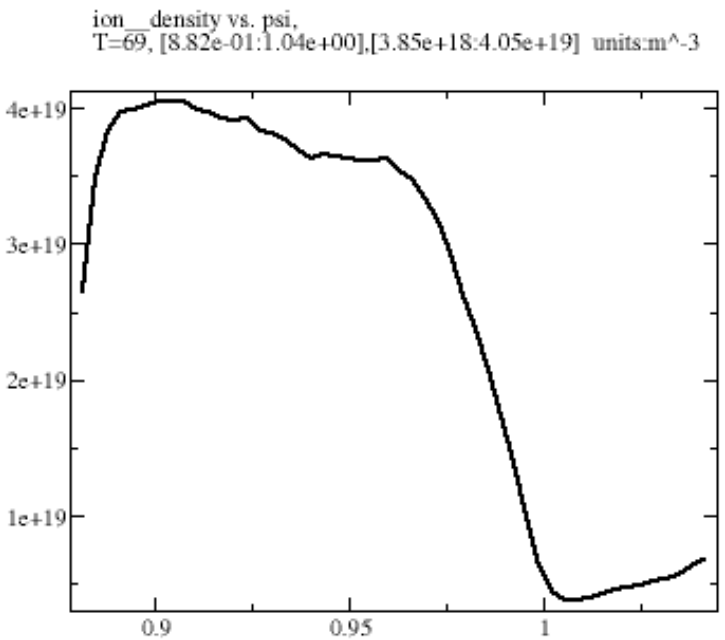


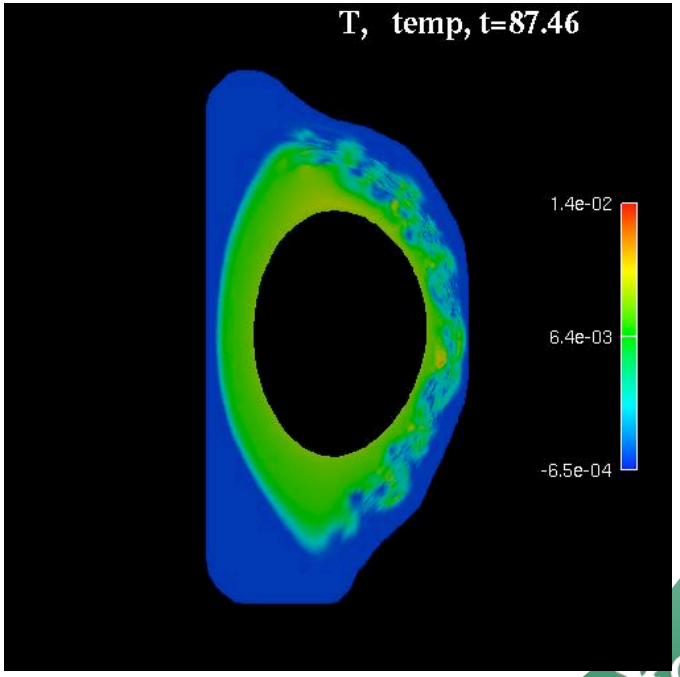
CPES
Center for Plasma Edge Simulation

Oak Ridge National Laboratory



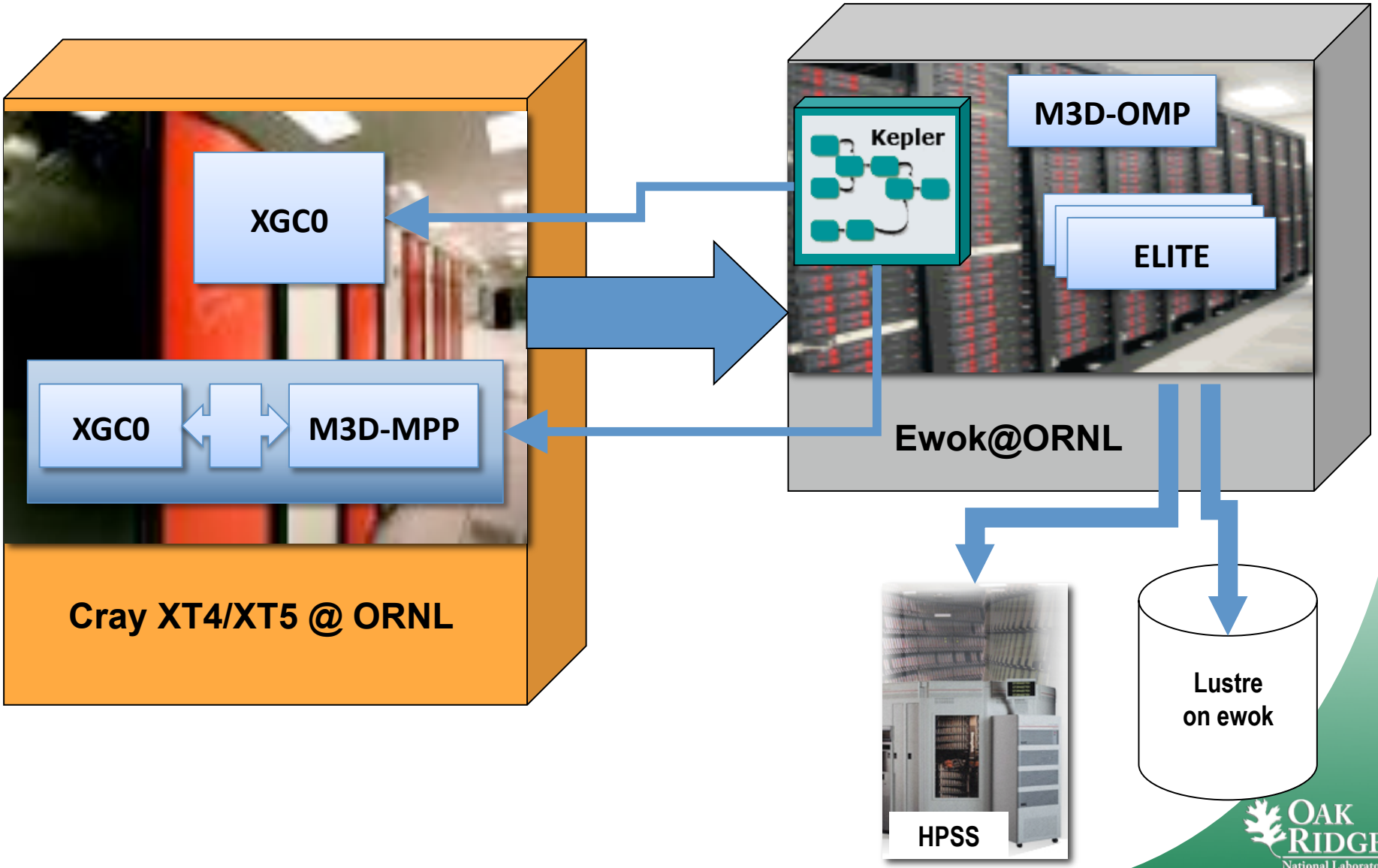






OAK RIDGE National Laboratory

Schematic view of components



Scientific Workflows

- Workflow management systems help in the *construction* and *automation* of scientific problem-solving processes that include executable sequences of components and data flows.
- It aims to solve scientific data integration, analysis, management, visualization tasks
  - by combining resources and services and orchestrating complex data flow patterns in a distributed environment
- in plainer English: do hard and/or messy stuff, and make it look easy.

OAK RIDGE National Laboratory

Kepler scientific workflow system

- Combination of data management, integration, analysis, and visualization steps
- The Kepler project is a cross-project collaboration to develop open source tools for Scientific Workflows:
  - Kepler/CORE: Development of a Comprehensive, Open, Reliable, and Extensible Scientific Workflow Infrastructure
  - SEEK: Science Environment for Ecological Knowledge
  - **SDM Center/SPA: SDM Center/Scientific Process Automation**
  - Ptolemy II: Heterogeneous Modeling and Design
  - GEON: Cyberinfrastructure for the Geosciences
  - ROADNet: Real-time Observatories, Applications, and Data Management Network
  - EOL: Encyclopedia of Life
  - Resurgence
  - CIPRes: CyberInfrastructure for Phylogenetic Research
  - REAP: Realtime Environment for Analytical Processing

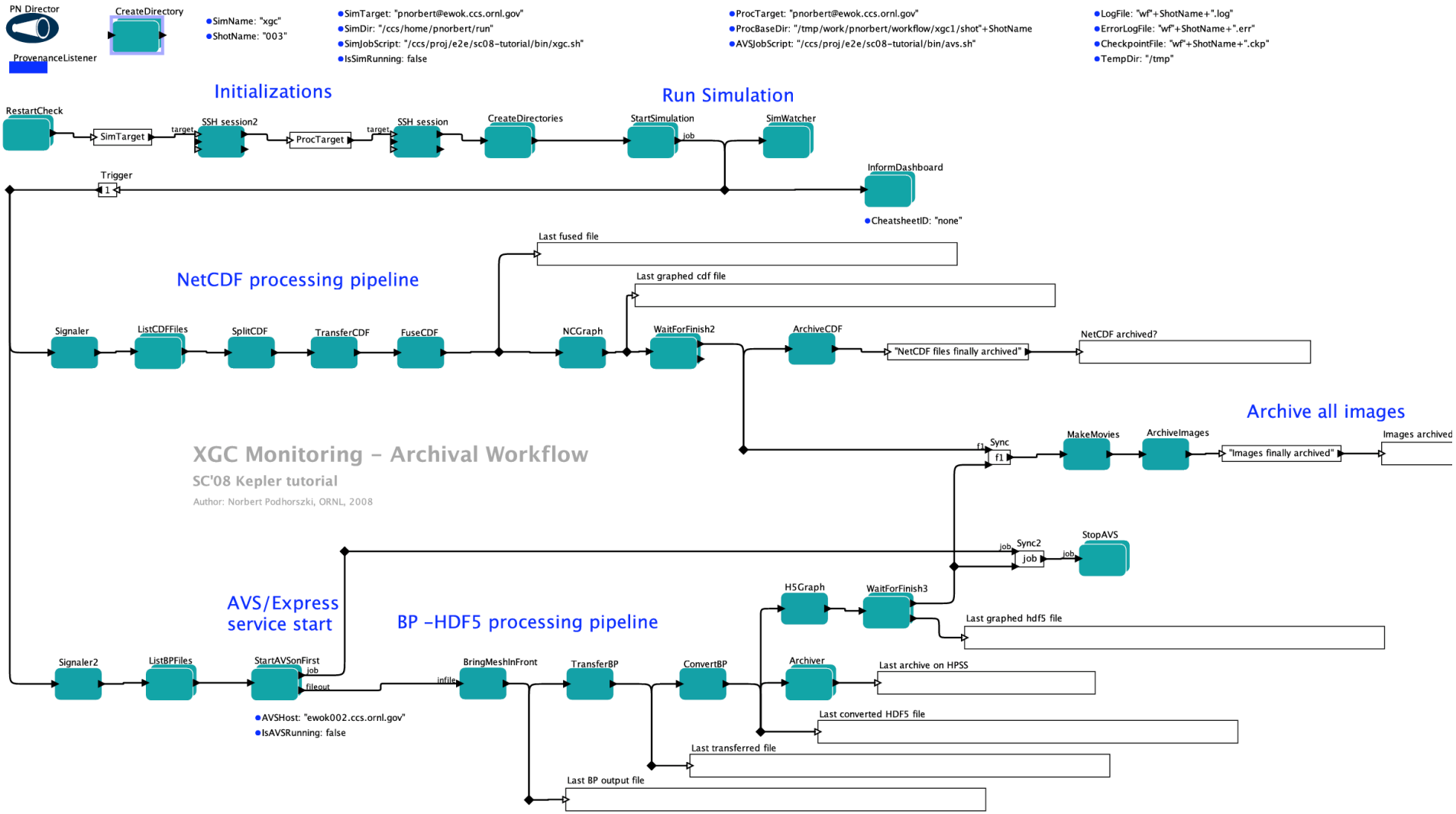
kepler-project.org

Kepler automation for code coupling, monitoring, and archiving.

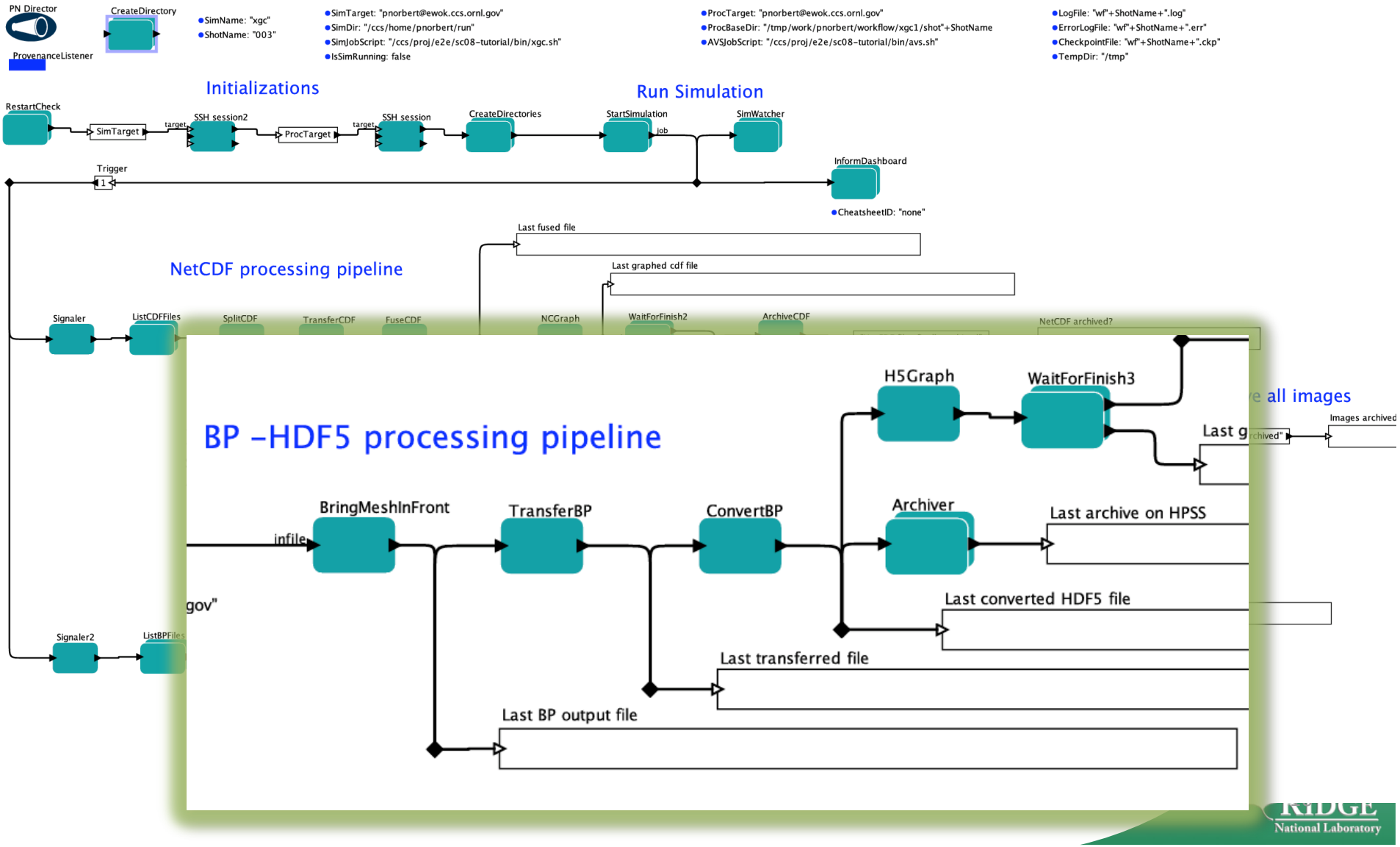
- We in SDM Center / CPES have extended Kepler with
  - Remote operations through SSH
    - deals with one time passwords
  - Job control (PBS, LoadLeveler, SGE, Condor)
  - Checkpointing to enable workflow restarts
  - Provenance Recorder (who did what in the workflow)
  - Generic actors to watch a simulation; tar to HPSS; execute remote operations with logging, error checking, etc.
- We have created workflows that are used daily at OLCF

OAK RIDGE National Laboratory

Activity of the XGC workflow



Activity of the XGC workflow



Monitoring Job: rst24 - Windows Internet Explorer

https://ewok-web2.ccs.ornl.gov/userspages/jobMonitoring.php?job=rst24&machine=ewok&colname=pnorbert&jobstate=old

Shot: rst24 | Graphics Layout | compare to | analysis | Macros

- calculator
- edit plot
- statitistical analysis
  - Descriptive Stats
  - Correlation
    - Auto Correlation
    - Cross Correlation
    - Partial Correlation
    - Covariance
  - FFT
- VisTrails Medleys

Annotate movies

5 (0:00) - 5 (0:00), stopped

9 (0:00) - 9 (0:00), stopped

xgc/ion__density vs. psi

xgc/ion__density vs psi,
T=1, [0.009:0.89], [5.95e+19:9.53e+19]

Download

If you have a question, please send an email to srm@lbl.gov

User information

UserID: rbarreto

Email Address: barreto@ornl.gov

Phone Number: 8652417552

Options

All Variables | All Time Steps | Single Dataset

Total Data Size: 6.66MB

Remote Target Absolute Path:

Remote Target Host Name:

Continue

Taking electronic notes on XGC1 shot rst 24. This is Norbert's shot. It tests restart shot
It has a new color map for most eD images.
I am building a screen shot for a conference talk on May 18th in Baltimore.

Calculator

Analysis name:

OAK RIDGE National Laboratory

Monitoring Job: 011 - Mozilla Firefox

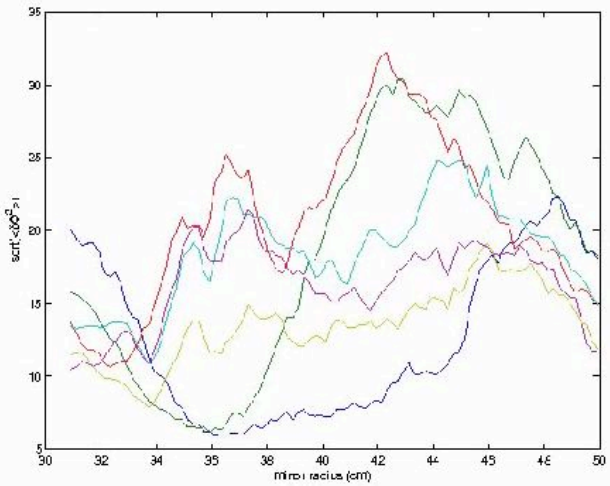
File Edit View History Bookmarks Tools Help

https://esimmon.ccs.ornl.gov/userspages/jobMonitoring.php?job=011&machine=ewok&colname=rbarreto&jobstate=old

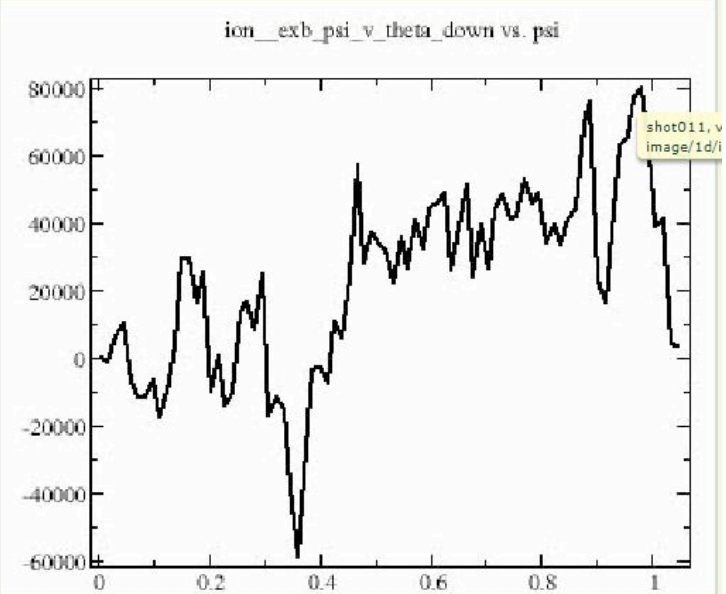
Main Page - Machine Monitoring | Monitoring Job: 011

Shot: 011 | Graphics Layout | Compare to | Analysis | Macros | TXT Show | global

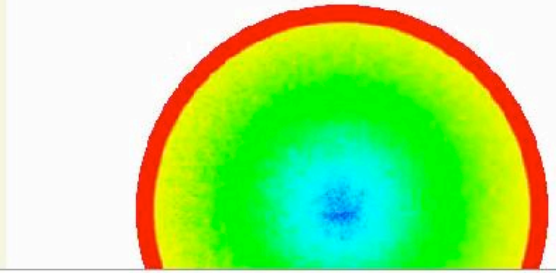
- image
- jobs
  - shku
- log
- txt

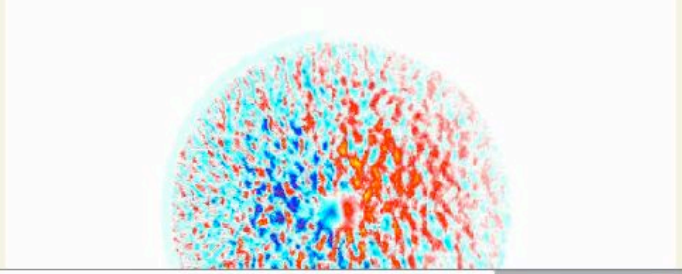


0 (0:00) - 1 (0:00), stopped



0 (0:00) - 1 (0:00), stopped





find:

Vector Graphics

OAK RIDGE National Laboratory

Collaboration

- Can see the collaborators' jobs
- Add notes to movies
- Run own analysis on data

Collaborators' Running | Collaborators' Old | Search Collaborators' ... | Add/Remove Collabor...

Collaborator	Machine	JobID	Shot#	Date	Notes
f9m	ewok	demo1	demo1	Wed Jan 9 16:06:44 EST 2008	
pankin	franklin	6505115	XGC-A23.1	Wed May 5 15:19:46 GMT-05:00 2010	
shku	jaguar	j28	j28	Fri Sep 12 13:50:33 EDT 2008	10 MW heating, 100K ptl per proc, same as f95_2
shku	jaguarpf	pf29	pf29	Thu Apr 16 20:42:56 EDT 2009	100MW heating case -- restart pf 28
shku	jaguarpf	82204	pf28	Sun Apr 12 14:16:36 2009	100MW heating case -- restart pf24
shku	jaguarpf	pf24	pf24	Tue Apr 7 14:32:35 EDT 2009	100MW heating case based on pf23 parameter
shku	franklin	f97	f97	Fri Sep 12 13:54:14 EDT 2008	10MW Heating, cyclone something Wrong
julianc	jaguar	815073	ttf_p2long1	Thu Apr 1 16:24:48 GMT-05:00 2010	24-hour run of XGC0/M3D in-memory coupling for the TTF case. XGC0 code slows down dramatically during the run and halts after 25000 time steps with a memory error due to particle load imbalance.
shku	jaguarpf	76966	pf23	Thu Mar 26 14:09:26 2009	50MW heating case -- heating bug exist
shku	jaguarpf	79807	pf27	Fri Apr 3 19:34:16 2009	50MW heating case -- restart pf23
sklasky	jaguar	98131	6260701	Tue Jun 26 10:54:36 2007	98131
julianc	jaguar	135438	012	Fri Sep 28 17:49:18 2007	Click to edit note or right click to delete job.

Plans

- ESimMon
  - Make a stand-alone release (1.0 in 2010)
  - API to allow simulation monitoring without workflows
- Workflows
  - Kepler 2.0 is coming out soon
  - Monitor long running simulations (weeks)
    - Use Grid Certificates (GSI infrastructure) to access Jaguar from Ewok

OAK RIDGE National Laboratory

Conclusions

- End-to-end Task is here to help to automate common data management tasks
- Scientific workflows can be used to
  - monitor simulations
  - develop complex problem-solving processes

- Contacts: pnorbert@ornl.gov, klasky@ornl.gov, tchoua@ornl.gov