Scientific Workflow Management

CCSM Software Engineering Working Group Session

6/19/2008

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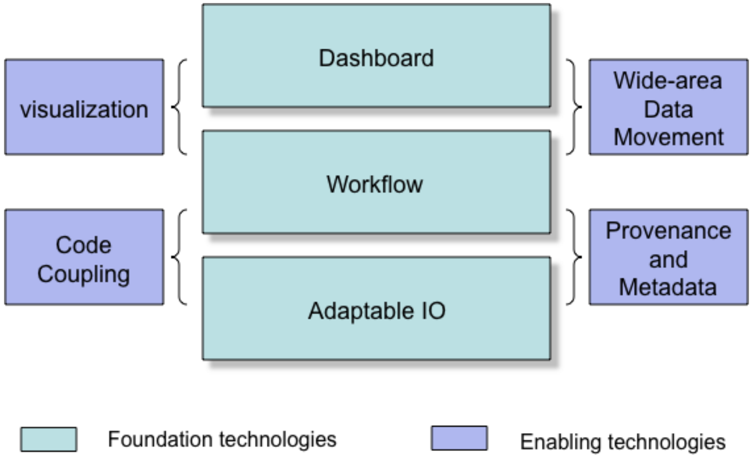
Outline

- ADIOS.
- Workflow.
  - What is a workflow
  - What advantages over python.
  - Monitoring workflow.
  - Coupling workflow.
  - Movie.
  - Marriage of ADIOS + workflow.
  - Napkin drawing of climate workflow.
- Dashboard.
- Conclusions.

End to End Computing at ORNL

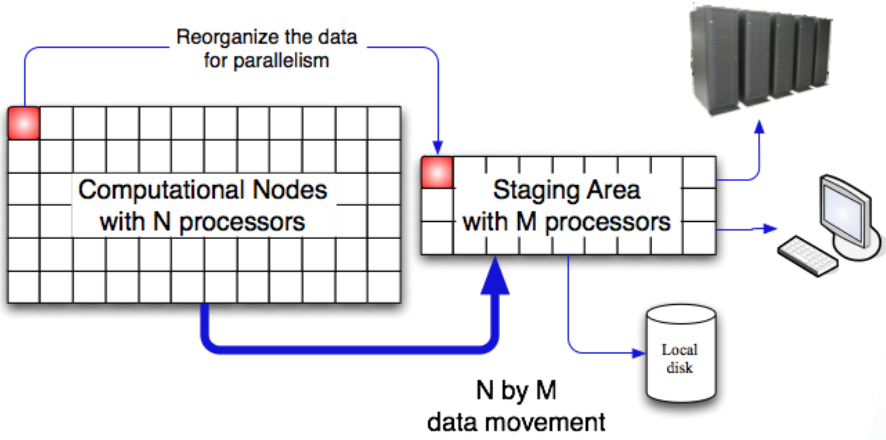
- Combines
  - Petascale Applications.
  - Petascale I/O techniques.
  - Workflow Automation.
  - Provenance capturing system.
  - Dashboards for real-time monitoring/controlling of simulations, and creating social spaces for scientists.



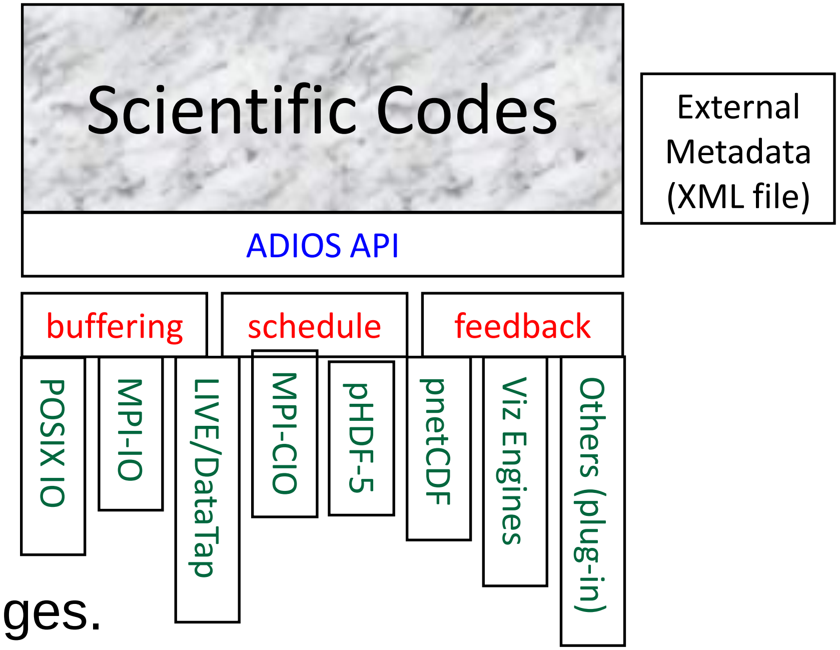
- **Approach**: place highly annotated, fast, easy-to-use I/O methods in the code, which can be monitored and controlled, have a workflow engine record all of the information, visualize this on a dashboard, move desired data to user's site, and have everything reported to a database.

ADIOS Overview – Design Goals

- ADIOS is an I/O componentization, which allows us to
  - Abstract the API from the IO implementation.
  - Switch from synchronous to asynchronous I/O at runtime.
  - Change from real-time visualization to fast I/O at runtime.
- Combines.
  - **Fast** I/O routines.
  - **Easy** to use.
  - **Scalable** architecture (100s cores) millions of procs.
  - **QoS.**
  - Metadata rich output.
  - Visualization applied during simulations.
  - Analysis, compression techniques applied during simulations.
  - Provenance tracking.


Reorganize the data for parallelism
Computational Nodes with N processors
Staging Area with M processors
Local disk
N by M data movement

ADIOS Overview



Scientific Codes

External Metadata (XML file)

ADIOS API

buffering

schedule

feedback

POSIX IO

MPI-IO

LIVE/DataTap

MPI-CIO

pHDF-5

pnetCDF

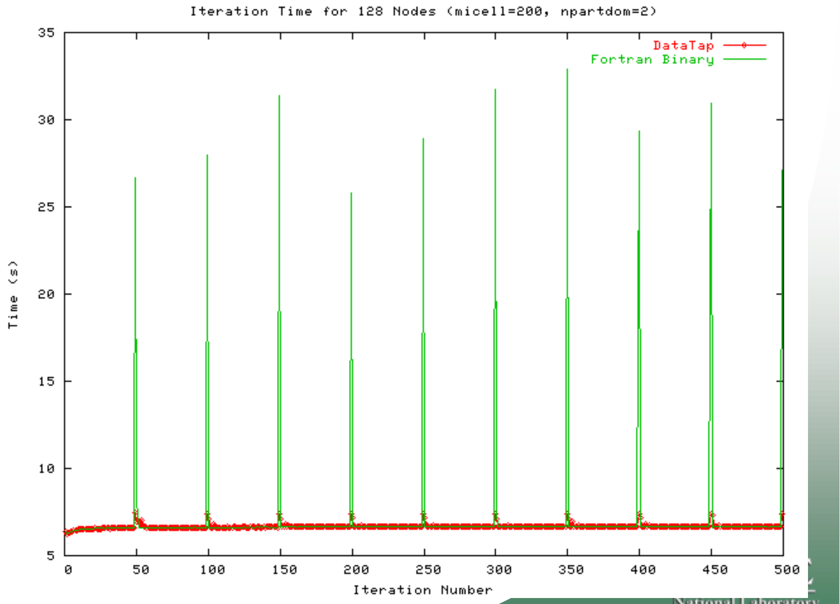
Viz Engines

Others (plug-in)

- Overview
  - Allows plug-ins for different I/O implementations.
  - Abstracts the API from the method used for I/O.
- Simple API, almost as easy as F90 write statement.
- Both synchronous and asynchronous transports supported without code changes.
- Best practices/optimize IO routines for all supported transports “for free”
- Componentization.
  - Don’t worry about IO implementation.
  - Components for IO transport methods, buffering, scheduling, and eventually feedback mechanisms.
- Change I/O method by changing XML file only, with metadata inside.
- Will support strong-coupling (code-code) in the future using a shared global memory address space

Initial ADIOS performance.

- MPI-I/O method.
  - GTC and GTS codes have achieved over 25 GB/sec on Cray XT at ORNL.
    - 30GB diagnostic files every 3 minutes, 1.2 TB restart files every 30 minutes, 300MB other diagnostic files every 3 minutes.
  - Chimera code speed up by 6.5% (overall time).
- DART: <2% overhead for writing 2 TB/hour with XGC code.
- DataTap vs. Posix
  - 1 file per process (Posix).
  - 5 secs for GTC computation.
  - ~25 seconds for Posix I/O
  - ~4 seconds with DataTap



EFFIS is a marriage between Keplerand ADIOS and the dashboard.

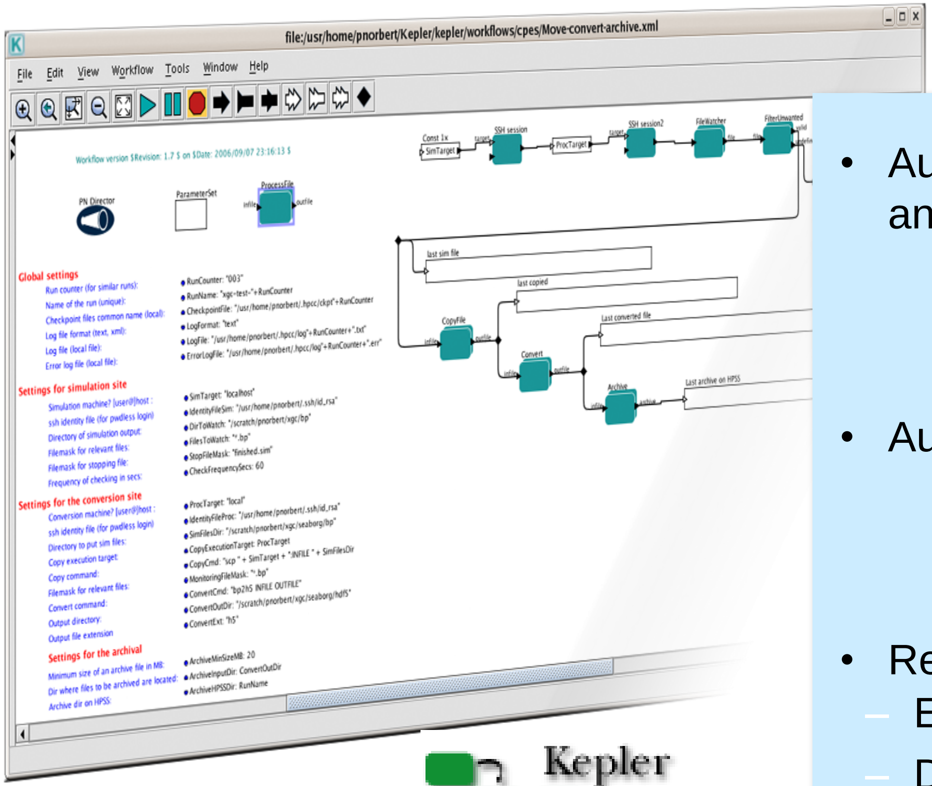
- ADIOS is being modified to send the I/O (and coupling) metadata from the compute nodes over to Kepler.
  - We send the file information(including the path).
  - We send the metadata that is contained.
    - Variables, + other annotations.
  - We can send commands to inform Kepler what to do.
- The information is NOT sent if there is no one listening; i.e. not dependent on Kepler).
- The information is saved in a database.

What is the Kepler Workflow Framework?

Kepler is a proven DOE technology from the SDM center for orchestrating scientific workflows, which aid construction and automation of scientific problem-solving processes.

- **Kepler workflow framework**
  - **Captures provenance information for**
    - Data provenance (Where did my data come from?)
    - Data movement and data replication (*e.g.*, during code coupling)
    - Tar files stored on HPSS (at NERSC or ORNL)
    - Workflow actions saved in log files for user debugging
  - **Is more powerful than Python scripts**
    - Allows pipeline-parallel processing with ease
    - Allows work to continue even if some scripts/components fail
    - Allows checkpoint/restart of the workflow
    - Easy to modify workflow for a continuously changing group of scientists
  - **Provides an excellent connection to databases**
    - Allows for easy queries of shots from coupled simulations
    - Large SDM effort to save provenance data into database

Workflow automation needs in Center for Plasma Edge Simulation



file:/usr/home/pnorbert/Kepler/kepler/workflows/cpes/Move-convert-archive.xml

Workflow version $Revision: 1.7 $ on $Date: 2006/09/07 23:16:13 $

Global settings

Run counter (for similar runs):	RunCounter: "003"
Name of the run (unique):	RunName: "xgc-test-"+RunCounter
Checkpoint files common name (local):	CheckpointFile: "/usr/home/pnorbert/.hpcc/ckpt"+RunCounter
Log file format (text, xml):	LogFormat: "text"
Log file (local file):	LogFile: "/usr/home/pnorbert/.hpcc/log"+RunCounter+".txt"
Error log file (local file):	ErrorLogFile: "/usr/home/pnorbert/.hpcc/log"+RunCounter+".err"

Settings for simulation site

Simulation machine? [user@]host :	SimTarget: "localhost"
ssh identity file (for pwdless login)	IdentityFileSim: "/usr/home/pnorbert/.ssh/id_rsa"
Directory of simulation output:	DirToWatch: "/scratch/pnorbert/xgc/bp"
Filemask for relevant files:	FilesToWatch: "*.bp"
Filemask for stopping file:	StopFileMask: "finished.sim"
Frequency of checking in secs:	CheckFrequencySecs: 60

Settings for the conversion site

Conversion machine? [user@]host :	ProcTarget: "local"
ssh identity file (for pwdless login)	IdentityFileProc: "/usr/home/pnorbert/.ssh/id_rsa"
Directory to put sim files:	SimFilesDir: "/scratch/pnorbert/xgc/seaborg/bp"
Copy execution target:	CopyExecutionTarget: ProcTarget
Copy command:	CopyCmd: "scp " + SimTarget + ":INFILE " + SimFilesDir
Filemask for relevant files:	MonitoringFileMask: "*.bp"
Convert command:	ConvertCmd: "bp2h5 INFILE OUTFILE"
Output directory:	ConvertOutDir: "/scratch/pnorbert/xgc/seaborg/hdf5"
Output file extension	ConvertExt: "h5"

Settings for the archival

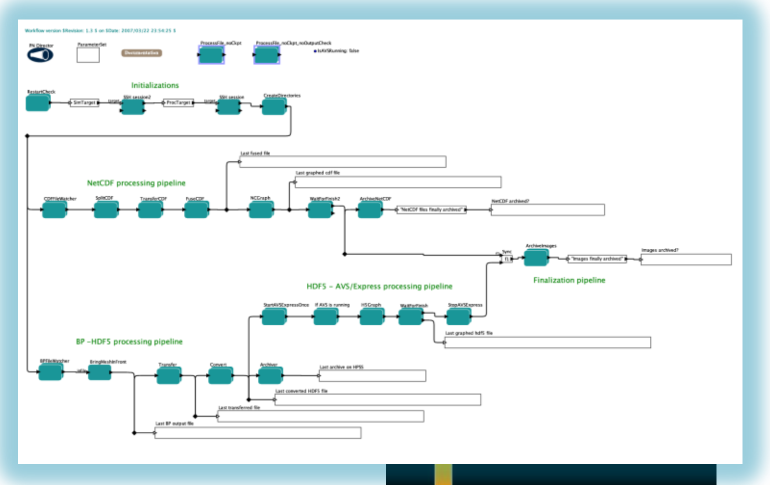
Minimum size of an archive file in MB:	ArchiveMinSizeMB: 20
Dir where files to be archived are located:	ArchiveInputDir: ConvertOutDir
Archive dir on HPSS:	ArchiveHPSSDir: RunName

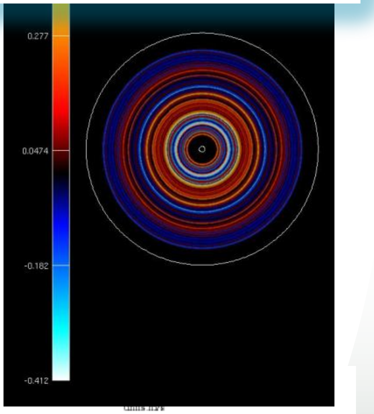
Kepler

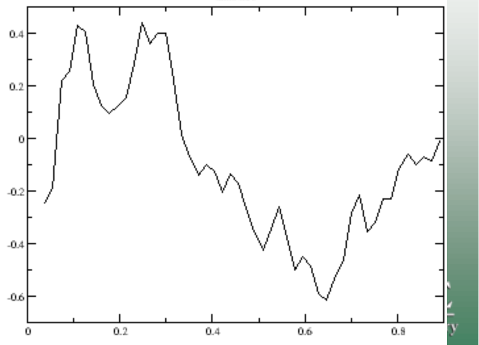
- Automate the data processing pipeline and simulation monitoring
  - Transfer of simulation output to remote machine
  - Execution of conversion routines
  - Image creation, data archiving, dynamic monitoring
- Automate the code coupling pipeline
  - Run simulation on a large supercomputer
  - Check linear stability on another machine
  - Re-run simulation if needed
- Requirements for petascale computing
  - Easy to use
  - Dashboard front-end
  - Dynamic monitoring
  - Parallel processing
  - Robustness
  - Configurability

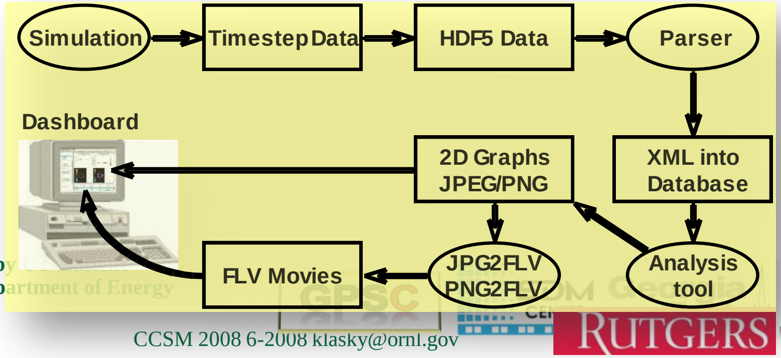
Workflows for monitoring a simulation

- NetCDF files
  - Transfer files to e2e system on-the-fly
  - Generateimages using grace library
  - ArchiveNetCDF files at the end of simulation
- Binary files from ADIOS
  - Transfer to e2e system using *bbcp*
  - Convert to HDF5 format
  - Generateimages with AVS/Express (running as service)
  - Archive HDF5 files in large chunks to HPSS
- Record Provenance information for everything!

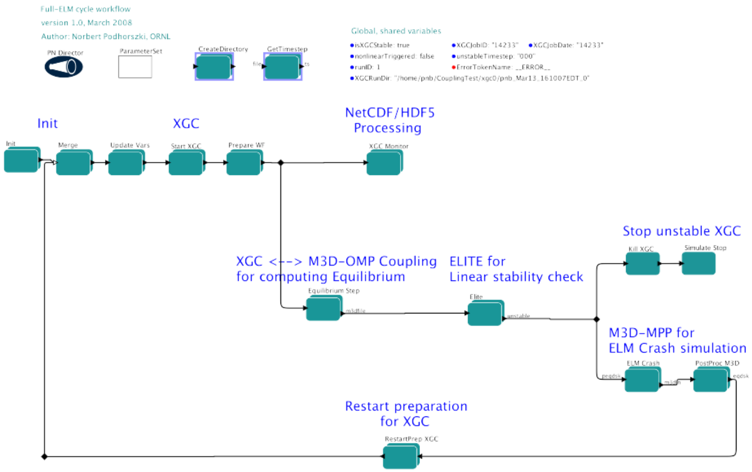








Coupling Fusion codes for Full ELM, multi-cycles

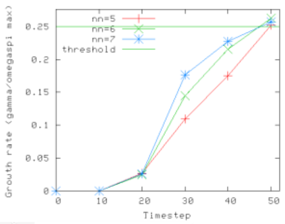


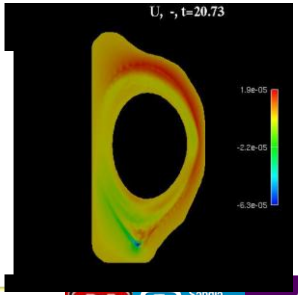
Full-ELM cycle workflow
version 1.0, March 2008
Author: Norbert Podhorszki, ORNL

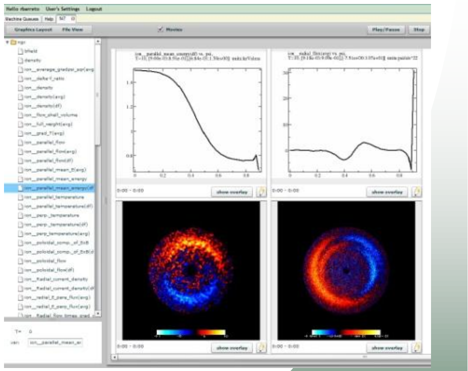
Global, shared variables

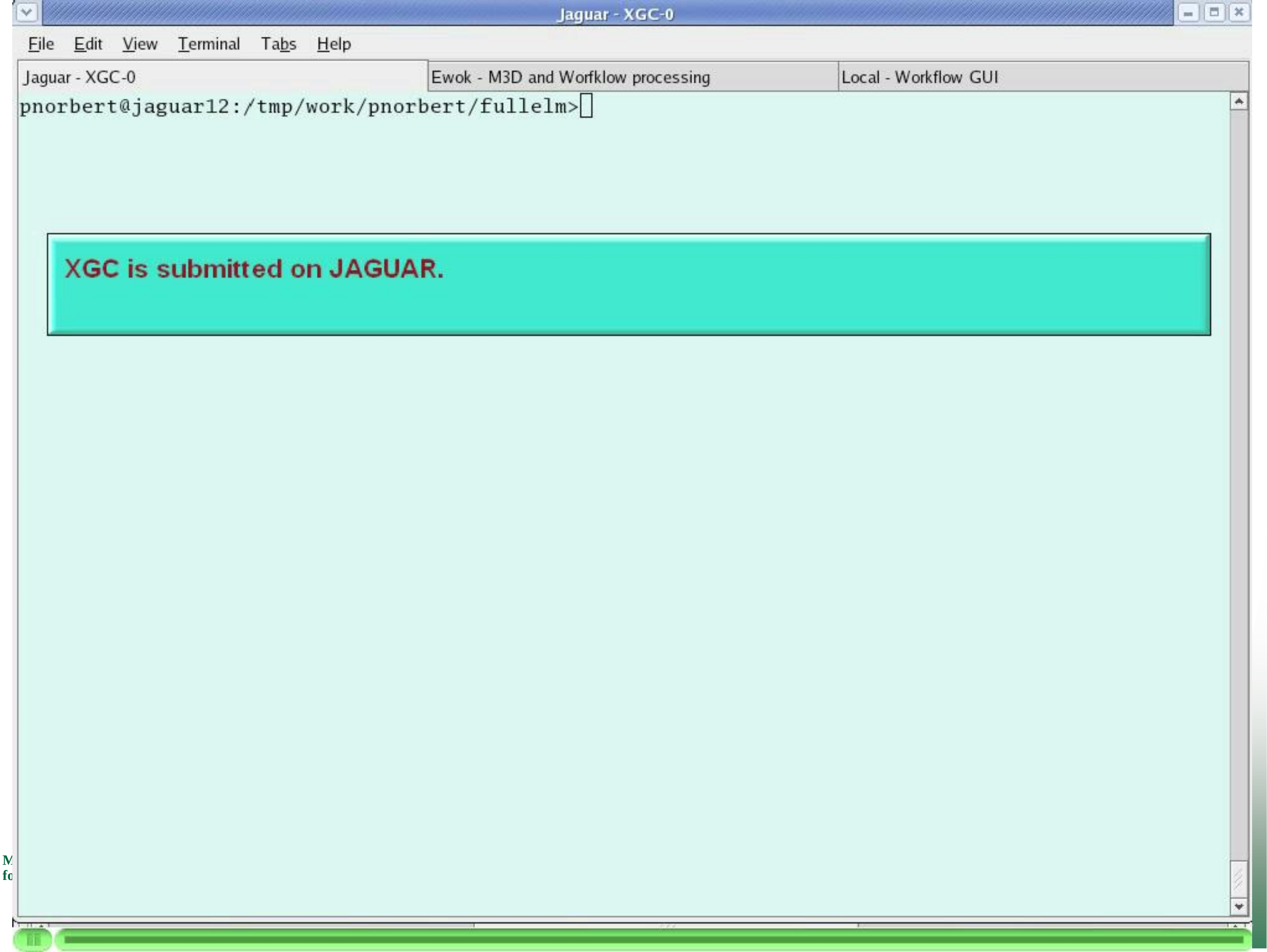
- isXGCStable: true
- nonlinearTriggered: false
- runID: 1
- XGCRunDir: "/home/pnb/CouplingTest/xgc0/pnb_Mar13_161007EDT_0"
- XGCJobID: "14233"
- unstableTimestep: "000"
- ErrorTokenName: __ERROR__
- XGCJobDate: "14233"

- Run XGC until ELMS are unstable
- M3D coupling data from XGC
  - Transfer to end-to-end system
  - Execute M3D: compute new equilibrium
  - Transfer back the new equilibrium to XGC
  - Execute ELITE: compute growth rate, test linear stability
  - Execute M3D-MPP: to study unstable states (ELM crash)
  - Restart XGC with new “helaled” equilibrium from M3D-MPP







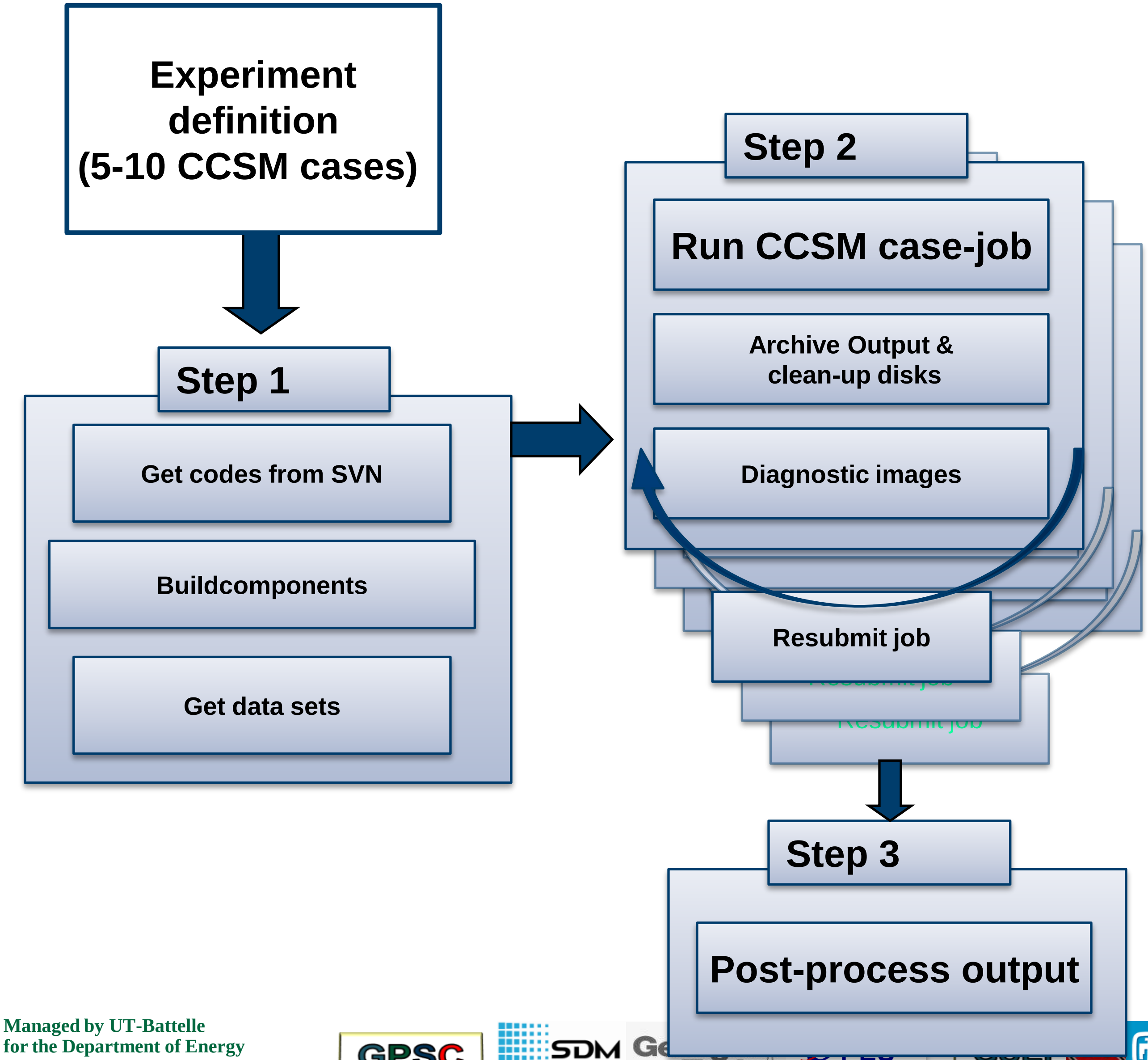


```
pnorbert@jaguar12:/tmp/work/pnorbert/fullelm>
```

XGC is submitted on JAGUAR.

M
fo

Climate workflow



Experiment definition (5-10 CCSM cases)

Step 1

Get codes from SVN

Buildcomponents

Get data sets

Step 2

Run CCSM case-job

Archive Output & clean-up disks

Diagnostic images

Resubmit job

Step 3

Post-process output

Running CCSM cases

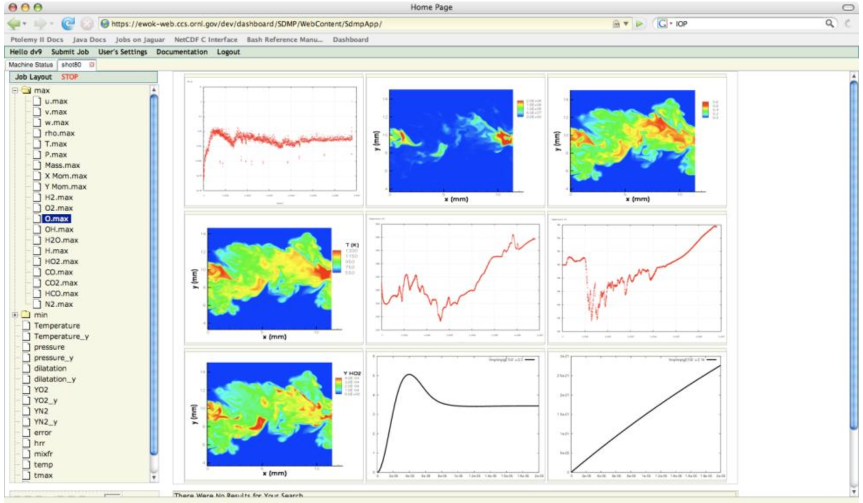
- Run an ensemble of several cases at once
  - ✓ one case consists of many jobs executed repetitively
- Run jobs at NCCS and other resource
  - ✓ one-time-password access from outside
- Archive output on the fly to HPSS while the job is running
- Make images from diagnostic output on the fly and put on the dashboard
  - ✓ to monitor the current status of each case

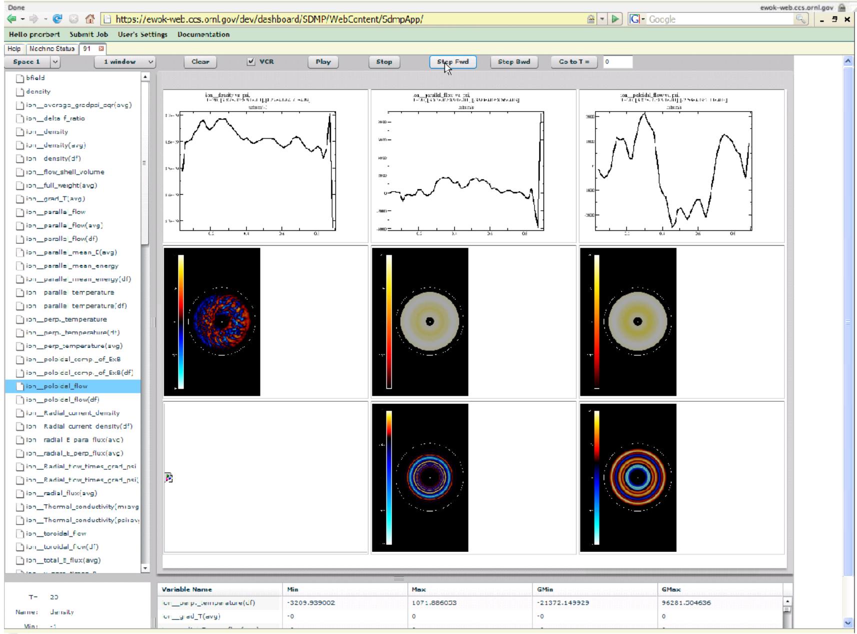
Design Criteria for the Dashboard

- Goal: provide users an easy way over the web to dynamically monitor simulation progress, to view images and movies, to perform basic analysis, and to move files to their site
- New design criteria for FSP codes on leadership class computers
  - Must support very large and small data, in a scalable fashion
- New security with One Time Passwords
  - Unrealistic to think that we can monitor jobs via one type of data output
  - Unrealistic to think that we can move data from a large parallel disk to user space
- Data management must be incorporated into the design
  - Database back-end is as important as front-end
  - Provenance display is very important to monitor long-running jobs
- Must be able to monitor computers/jobs from all resources
- Need to plug-in new visualization routines into the display
- Need to plug-in new analysis routines into the system
- Need to collaborate via shared space
- Make it robust by using enterprise web-2 technologies

Dashboard: Simulation Monitoring

- A basic browser-based visualization tool
- Local interaction for graphs/visualizations
- Server used for data manipulation, extraction
- Server used for more complex analysis
- Allows for pan and zoom locally
- Asynchronously queries
- MySQL for database support




ewok-web.ccs.ornl.gov
https://ewok-web.ccs.ornl.gov/dev/dashboard/SDMP/WebContent/SdmpApp/
Google
Hello prcrbert
Submit Job
User's Settings
Documentation
Help
Machine Status
91
Space 1
1 window
Clear
VCR
Play
Stop
Step Fwd
Step Bwd
Go to T =
0
bfield
density
ion__average_gradpsi_sqr(avg)
ion__delta_f_ratio
ion__density
ion__density(avg)
ion__density(df)
ion__flow_shell_volume
ion__full_weight(avg)
ion__grad_T(avg)
ion__parallel_flow
ion__parallel_flow(avg)
ion__parallel_flow(df)
ion__parallel_mean_E(avg)
ion__parallel_mean_energy
ion__parallel_mean_energy(df)
ion__parallel_temperature
ion__parallel_temperature(df)
ion__perp_temperature
ion__perp_temperature(df)
ion__perp_temperature(avg)
ion__poloidal_comp_of_ExB
ion__poloidal_comp_of_ExB(df)
ion__poloidal_flow
ion__poloidal_flow(df)
ion__Radial_current_density
ion__Radial_current_density(df)
ion__radial_E_para_flux(avg)
ion__radial_E_perp_flux(avg)
ion__Radial_flow_times_grad_psi
ion__Radial_flow_times_grad_psi
ion__radial_flux(avg)
ion__Thermal_conductivity(m avg
ion__Thermal_conductivity(psi av
ion__toroidal_flow
ion__toroidal_flow(df)
ion__total_E_flux(avg)

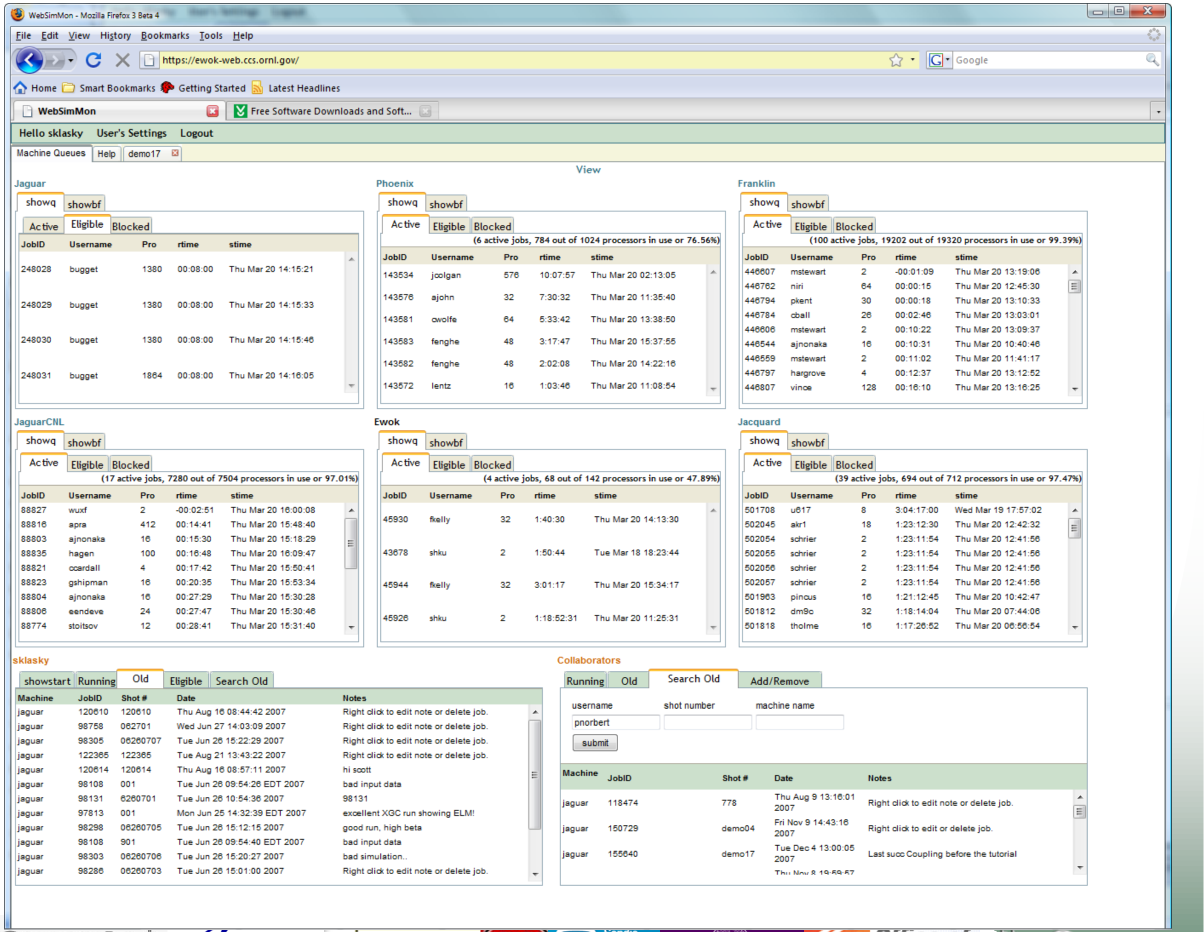
T= 20
Name: density
Min: -1

Variable Name	Min	Max	GMin	GMax
ion__perp_temperature(df)	-3209.939002	1071.886033	-21372.149929	96281.504636
ion__grad_T(avg)	-0	0	-0	0

Dashboard: Job Monitoring

Monitors machines, simulations and DB

- Secure login with OTP
- Job submission and kill
- Search old jobs
- See collaborators jobs
- Annotations/Notes
- Text display/movies



https://ewok-web.ccs.ornl.gov/

Jaguar

JobID	Username	Pro	rtime	stime
248028	bugget	1380	00:08:00	Thu Mar 20 14:15:21
248029	bugget	1380	00:08:00	Thu Mar 20 14:15:33
248030	bugget	1380	00:08:00	Thu Mar 20 14:15:46
248031	bugget	1864	00:08:00	Thu Mar 20 14:16:05

Phoenix

(6 active jobs, 784 out of 1024 processors in use or 76.56%)

JobID	Username	Pro	rtime	stime
143534	jcolgan	576	10:07:57	Thu Mar 20 02:13:05
143576	ajohn	32	7:30:32	Thu Mar 20 11:35:40
143581	cwolfe	64	5:33:42	Thu Mar 20 13:38:50
143583	fenghe	48	3:17:47	Thu Mar 20 15:37:55
143582	fenghe	48	2:02:08	Thu Mar 20 14:22:16
143572	lentz	16	1:03:46	Thu Mar 20 11:08:54

Franklin

(100 active jobs, 19202 out of 19320 processors in use or 99.39%)

JobID	Username	Pro	rtime	stime
446607	mstewart	2	-00:01:09	Thu Mar 20 13:19:06
446762	niri	64	00:00:15	Thu Mar 20 12:45:30
446794	pkent	30	00:00:18	Thu Mar 20 13:10:33
446784	cball	26	00:02:46	Thu Mar 20 13:03:01
446606	mstewart	2	00:10:22	Thu Mar 20 13:09:37
446544	ajnonaka	16	00:10:31	Thu Mar 20 10:40:46
446559	mstewart	2	00:11:02	Thu Mar 20 11:41:17
446797	hargrove	4	00:12:37	Thu Mar 20 13:12:52
446807	vince	128	00:16:10	Thu Mar 20 13:16:25

JaguarCNL

(17 active jobs, 7280 out of 7504 processors in use or 97.01%)

JobID	Username	Pro	rtime	stime
88827	wuxf	2	-00:02:51	Thu Mar 20 16:00:08
88816	apra	412	00:14:41	Thu Mar 20 15:48:40
88803	ajnonaka	16	00:15:30	Thu Mar 20 15:18:29
88835	hagen	100	00:16:48	Thu Mar 20 16:09:47
88821	ccardall	4	00:17:42	Thu Mar 20 15:50:41
88823	gshipman	16	00:20:35	Thu Mar 20 15:53:34
88804	ajnonaka	16	00:27:29	Thu Mar 20 15:30:28
88806	eendeve	24	00:27:47	Thu Mar 20 15:30:46
88774	stoitsov	12	00:28:41	Thu Mar 20 15:31:40

Ewok

(4 active jobs, 68 out of 142 processors in use or 47.89%)

JobID	Username	Pro	rtime	stime
45930	fkelly	32	1:40:30	Thu Mar 20 14:13:30
43678	shku	2	1:50:44	Tue Mar 18 18:23:44
45944	fkelly	32	3:01:17	Thu Mar 20 15:34:17
45926	shku	2	1:18:52:31	Thu Mar 20 11:25:31

Jacquard

(39 active jobs, 694 out of 712 processors in use or 97.47%)

JobID	Username	Pro	rtime	stime
501708	u617	8	3:04:17:00	Wed Mar 19 17:57:02
502045	akr1	18	1:23:12:30	Thu Mar 20 12:42:32
502054	schrier	2	1:23:11:54	Thu Mar 20 12:41:56
502055	schrier	2	1:23:11:54	Thu Mar 20 12:41:56
502056	schrier	2	1:23:11:54	Thu Mar 20 12:41:56
502057	schrier	2	1:23:11:54	Thu Mar 20 12:41:56
501963	pincus	16	1:21:12:45	Thu Mar 20 10:42:47
501812	dm9c	32	1:18:14:04	Thu Mar 20 07:44:06
501818	tholme	16	1:17:26:52	Thu Mar 20 06:56:54

sklasky

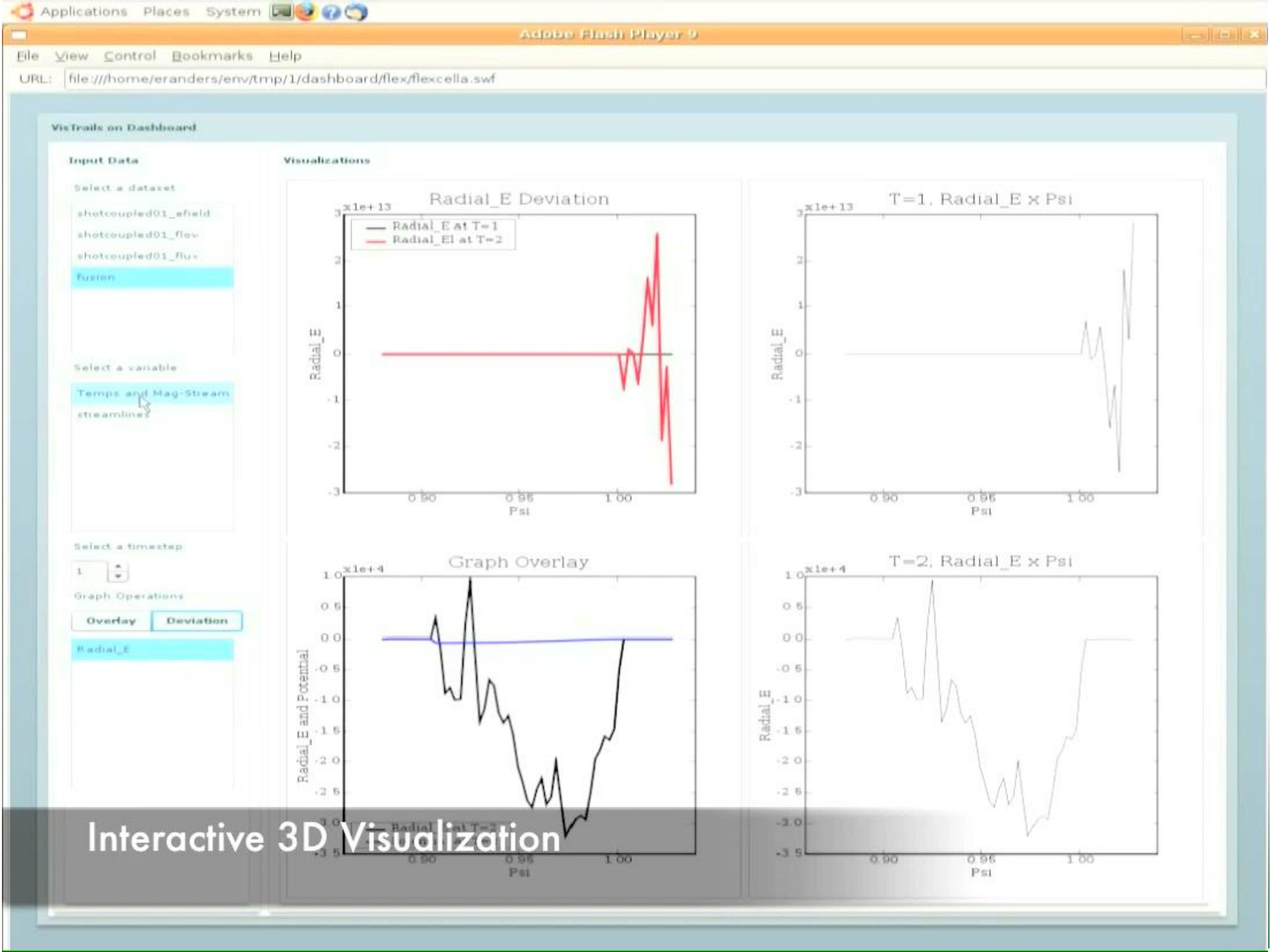
Machine	JobID	Shot #	Date	Notes
jaguar	120610	120610	Thu Aug 16 08:44:42 2007	Right click to edit note or delete job.
jaguar	98758	062701	Wed Jun 27 14:03:09 2007	Right click to edit note or delete job.
jaguar	98305	06260707	Tue Jun 26 15:22:29 2007	Right click to edit note or delete job.
jaguar	122365	122365	Tue Aug 21 13:43:22 2007	Right click to edit note or delete job.
jaguar	120614	120614	Thu Aug 16 08:57:11 2007	hi scott
jaguar	98108	001	Tue Jun 26 09:54:26 EDT 2007	bad input data
jaguar	98131	6260701	Tue Jun 26 10:54:36 2007	98131
jaguar	97813	001	Mon Jun 25 14:32:39 EDT 2007	excellent XGC run showing ELM!
jaguar	98298	06260705	Tue Jun 26 15:12:15 2007	good run, high beta
jaguar	98108	901	Tue Jun 26 09:54:40 EDT 2007	bad input data
jaguar	98303	06260706	Tue Jun 26 15:20:27 2007	bad simulation..
jaguar	98286	06260703	Tue Jun 26 15:01:00 2007	Right click to edit note or delete job.

Collaborators

username: pnorbert
shot number:
machine name:

Machine	JobID	Shot #	Date	Notes
jaguar	118474	778	Thu Aug 9 13:16:01 2007	Right click to edit note or delete job.
jaguar	150729	demo04	Fri Nov 9 14:43:16 2007	Right click to edit or delete job.
jaguar	155640	demo17	Tue Dec 4 13:00:05 2007	Last succ Coupling before the tutorial
			Thu Nov 8 19:59:57	

Dashboard movie



Interactive 3D Visualization

Collaborative Analysis Features

- Basic analysis on dashboard will feature
  - Calculator for simple math, done in Python
  - Hooks into "R" for pre-set functions
  - Ability to save the analysis into a new function
  - 2d and time history plots (initial version)
  - Full 3d plots (in future version)
- Advanced analysis will contain
  - Parallel backend to VisIT server, VisTrails, Parallel R, and custom MPI/C/F90 code
  - We will allow users to place executable code into the dashboard
- In progress: a portable dashboard!

Conclusions

- ADIOS is an I/O componentization.
  - ADIOS is being integrated integrated into Kepler.
  - Achieved over 20 GB/sec for several codes on Jaguar.
  - Used daily by CPES researchers.
  - Can change IO implementations at runtime.
  - Metadata is contained in XML file.
- Kepler is used daily for
  - Monitoring CPES simulations on Jaguar/Franklin/ewok.
  - Runs with 24 hour jobs, on large number of processors.
- Dashboard uses enterprise (LAMP) technology.