

Plans and Progress in HPC

GPSC All Hands Meeting

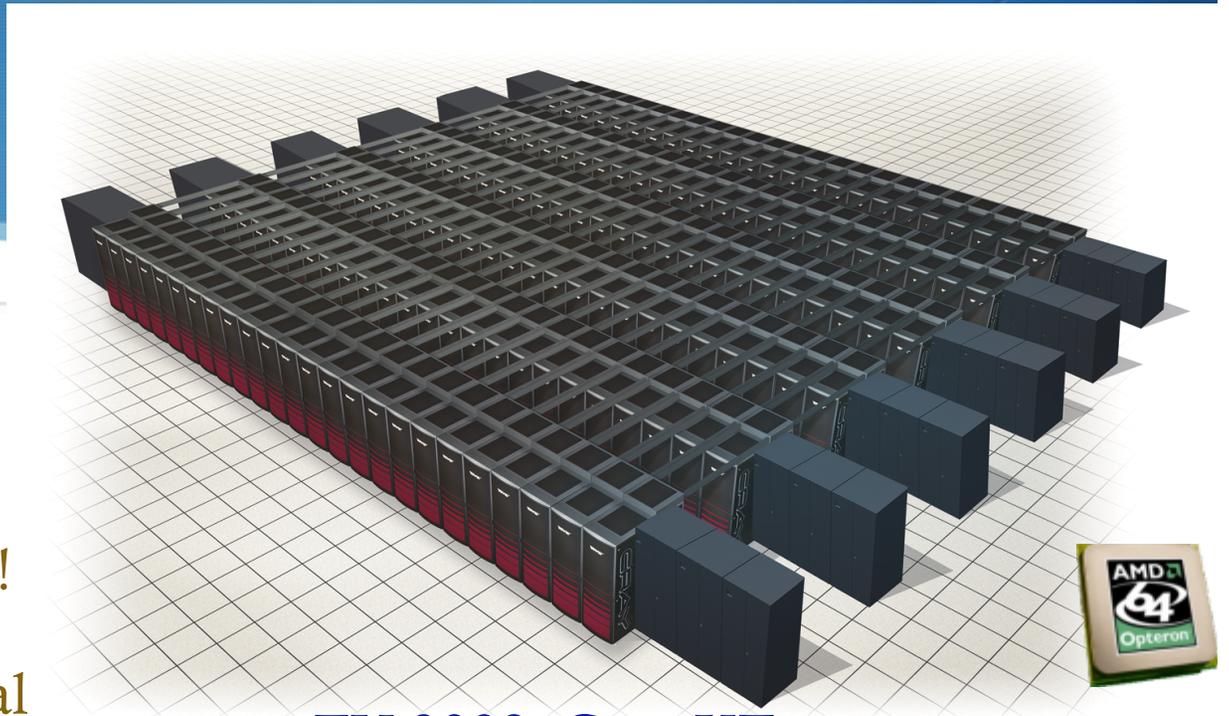
3/29/2008

S. Klasky, S. Ethier, C. Jin



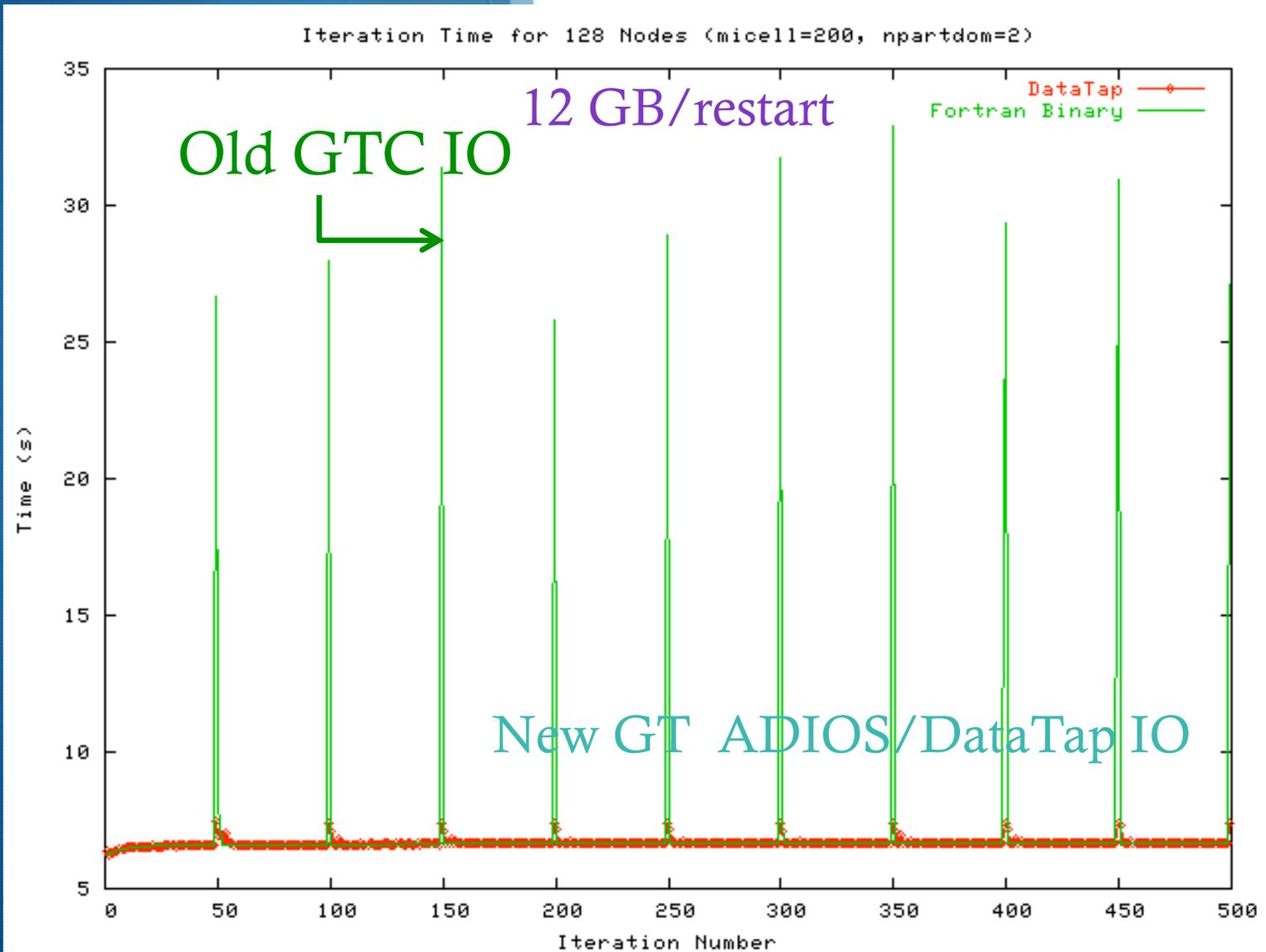
1 Petaflops System - Cray

- 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



1 FY 2009: Cray XT

IO Progress & Plans



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.

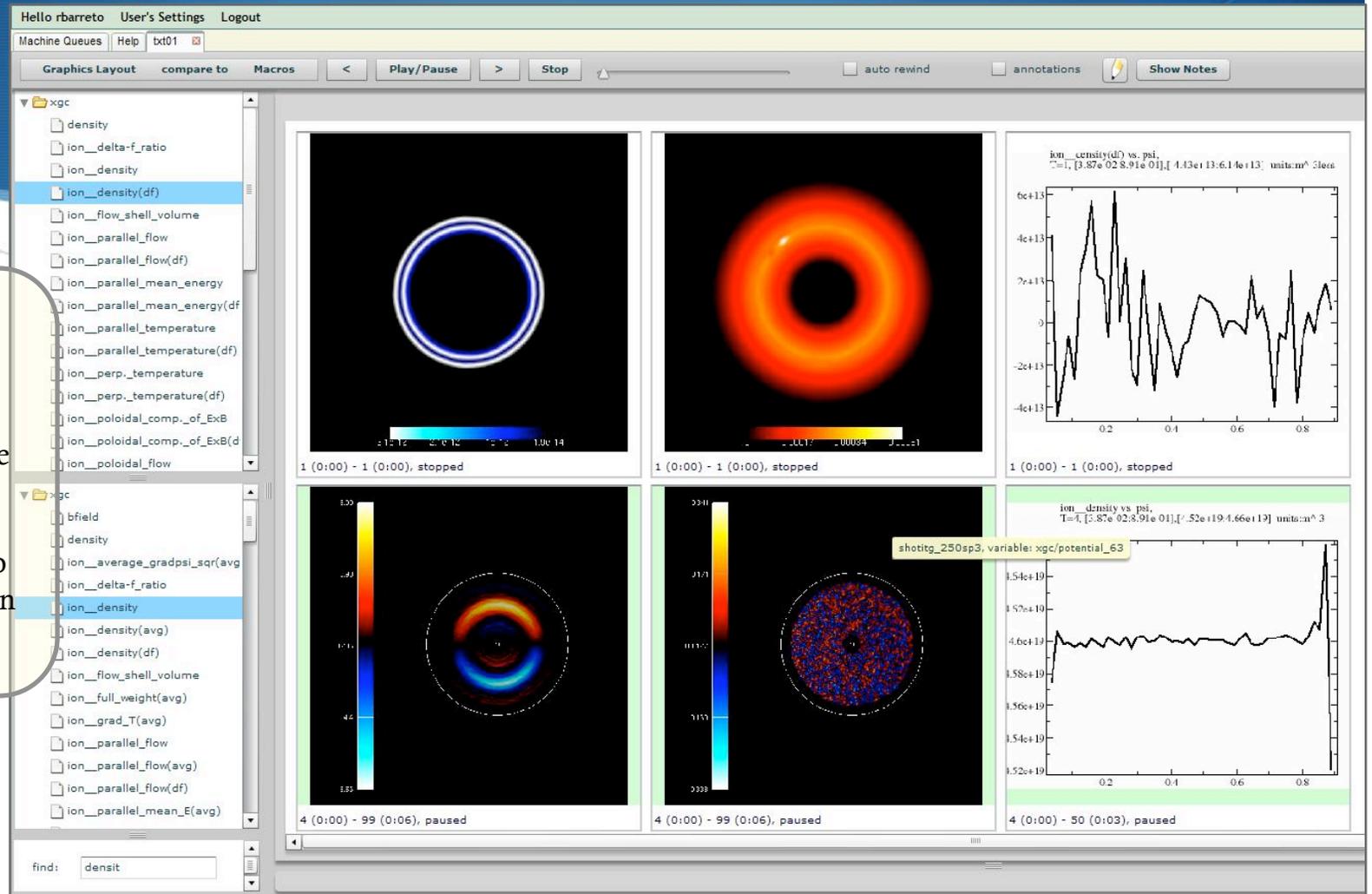
Dashboard movie



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

Hello rbarreto User's Settings Logout

Machine Queues Help txt01

Graphics Layout compare to Macros < Play/Pause > Stop auto rewind annotations Show Notes

ion_parallel_flow(df)
ion_parallel_mean_energy
ion_parallel_mean_energy(df)
ion_parallel_temperature
ion_parallel_temperature(df)
ion_perp_temperature
ion_perp_temperature(df)
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_flow_times_grad_f
ion_Radial_flow_times_grad_f(df)
ion_toroidal_flow
ion_toroidal_flow(df)
ion_v_para_times_B
ion_v_para_times_B(df)
potential
T_par
T_perp
v_ExB-R
v_ExB-Z
v_par

txt

xgc

fort.used.eq
input
output.out
xgcs

Find in text view

```
&sml_param
sml_machine=0 ! 0 circular, 1:D3D,
sml_node_file='cyclon4_coarse.1.node'
sml_ele_file='cyclon4_coarse.1.ele'
sml_bfollow_file=' !'cyclon4.bf'

sml_special=0 ! 0: normal simulation, 1: single particle simulation
sml_dt=5.00D-3 ! delta-t for one time step - unit of toroidal transit time.
sml_mstep=20000 ! totoal time step
sml_deltaf=1 ! delta-f simulation switch - incomplete
sml_turb_efield=1
sml_electron_on=0
sml_nphi_total=4
sml_canonical_maxwell=0 ! cononical maxwellian initial loading switch - incomplete
sml_bounce=2 ! Particle motion boundary condition
! 1 for edge simulation (including open field line region)
! 2 for core simulation (excluding open field line region)

sml_limiter=0 ! Limiter on/off
sml_fem_matrix=1
sml_inpsi=0.10 ! inner boundary of simulation - unit of eq_x_psi
sml_outpsi=0.90 ! outer boundary of simulation - unit of eq_x_psi
sml_dwdt_exb_only=1
sml_push_mode=1
sml_pc_order=3
sml_restart_write_period=9000
sml_restart=0
sml_initial_deltaf_noise=1D-10
sml_mode_select_on=0
sml_mode_select_n=23
sml_deltaf_f0_mode=-1
sml_zero_inner_bd=1
sml_f0_1_Ln=2.20D0
sml_f0_1_Lt=6.9D0
sml_guess_table_size=1900
sml_no_00_efield=1
sml_input_file_dir='/lustre/scratch/shku/XGC-1/inputs/'

&ptl_param
ptl_mass=2D0 ! 1 for hydrogen, 2 for deutron
ptl_charge=1D0 ! ion charge
ptl_num=1000 ! number of particle for simulation
```

Find

Find what:
simulation

Find

Basic find function

Drag text files from the tree

find:

New Dashboard Features

The dashboard interface includes a top navigation bar with "Hello rbarreto", "User's Settings", and "Logout". Below this is a browser-like header with "Machine Queues", "Help", and "txt01". A control bar contains "Graphics Layout", "compare to", "Macros", and playback controls: "<", "Play/Pause", ">", "Stop", "auto rewind", "annotations", and "Show Notes".

On the left, a sidebar lists variables: "xgc/density", "xgc/ion__density", "xgc/ion__density(df)", "xgc/ion__Radial_current_density", and "xgc/ion__Radial_current_density(df)".

The main plot area displays "ion_parallel_flow vs. psi, T=1, [3.87e-02:8.91e-01],[-5.03e+02:5.04e+02] units:m/s3less". The plot shows a black oscillating line and a blue line. A red circle highlights a point on the black line, with a green "Annotate movies" label next to it. Below the plot, it says "1 (0:00) - 1 (0:00), stopped".

An "Annotate Movie" dialog box is open on the right, featuring a toolbar with various shapes and a text tool. It includes input fields for "Apply annotation from timestep 1 to timestep 1 Last timestep=1", "Undo Add", "Erase All", "Help", "Save Annotation", "Delete Annotations", and "Close".

At the bottom, a note-taking area contains the text: "Take notes for this shots and save them in the dashboard database. I like those two, they look like the're each other upside down. (Saved on space 2)".

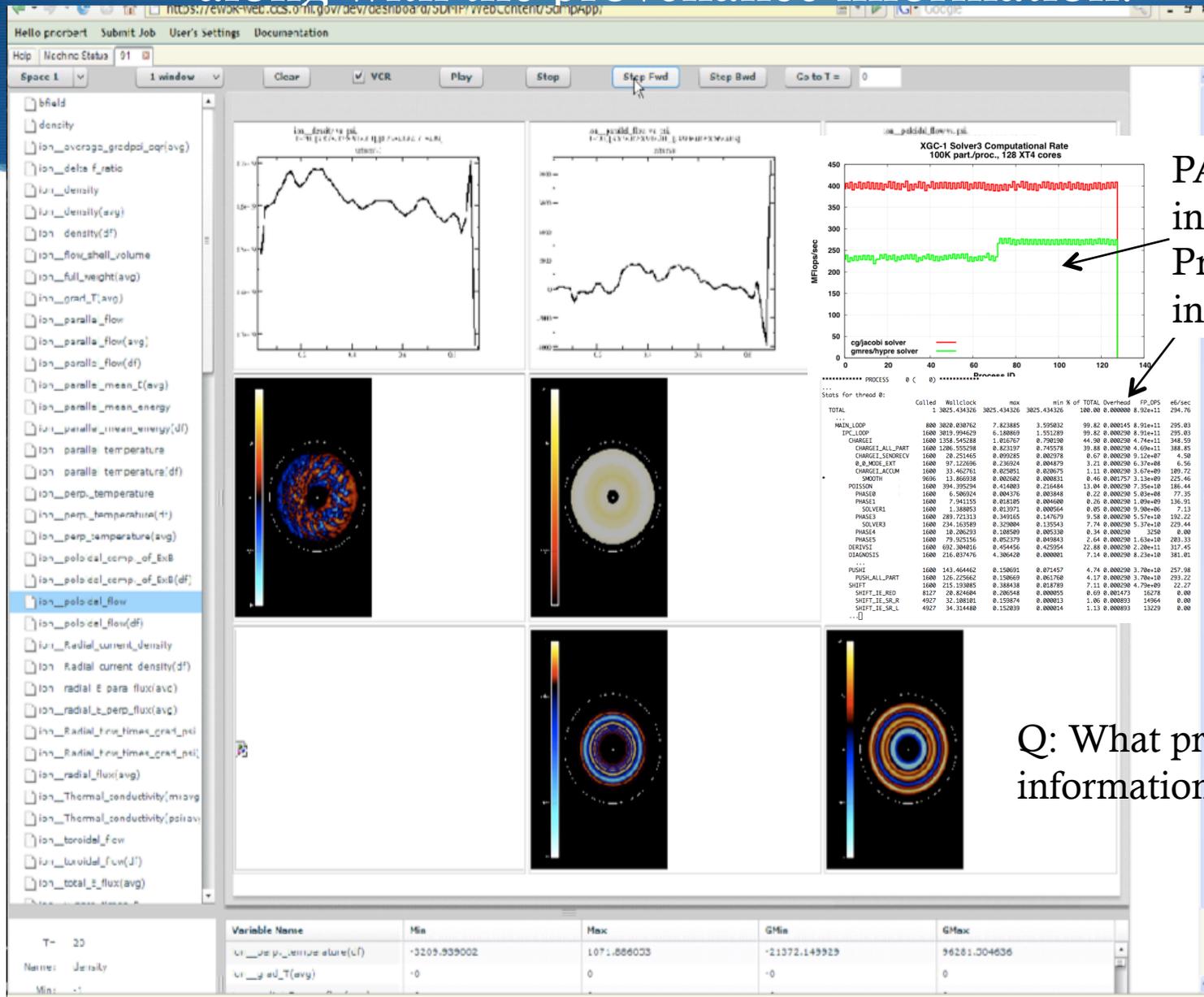
The bottom of the interface has a search bar with "density" entered, a font selector set to "Verdana", a size selector set to "10", and a "Save" button.

Search for a variable

Annotate movies

e-scratch book

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



PAPI
information
Provenance
information

Q: What provenance information to keep?

Machine monitoring.

WebSimMon - Mozilla Firefox 3 Beta 4

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

WebSimMon

Hello sklasky User's Settings Logout

Machine Queues Help demo17

View

Jaguar

showq showbf

Active Eligible Blocked

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

showq showbf

Active Eligible Blocked

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

JobID	Username	Pro	rtime	stime
143534	joogan	576	10:07:57	Thu Mar 20 02:13:05
143576	ajohn	32	7:30:32	Thu Mar 20 11:35:40
143581	owolfe	64	5:33:42	Thu Mar 20 13:38:50
143593	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

showq showbf

Active Eligible Blocked

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

JobID	Username	Pro	rtime	stime
446807	mstewart	2	-00:01:09	Thu Mar 20 13:19:06
446782	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
446806	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

showq showbf

Active Eligible Blocked

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

JobID	Username	Pro	rtime	stime
88827	wuof	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	coardall	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	stoltsov	12	00:28:41	Thu Mar 20 15:31:40

Ewok

showq showbf

Active Eligible Blocked

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

JobID	Username	Pro	rtime	stime
46930	fkelly	32	1:40:30	Thu Mar 20 14:13:30
43878	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

showq showbf

Active Eligible Blocked

(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	alr1	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	1:21:12:46	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

showstart Running Old Eligible Search Old

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	06260708	Tue Jun 26 15:20:27 2007	bad simulation..
Jaguar	98288	06260703	Tue Jun 26 15:01:00 2007	Right click to edit note or delete job.

Collaborators

Running Old Search Old Add/Remove

username shot number machine name

pnorbert

submit

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

Eventual hooks into MDS+ for

The screenshot displays the MDS+ software interface, which is used for data visualization and analysis. The interface includes a top menu bar with options like "Graphics Layout", "compare to", "Macros", "Play/Pause", "Stop", "auto rewind", "auto play", "annotations", and "Hide Notes".

On the left side, there is a file browser showing a directory structure with folders "elite", "m3d", and "xgc". Below this is a list of data series, with "ion__density(df)" selected. At the bottom left, there is a search bar labeled "find:".

The main area contains several plots:

- Top-left: A line plot titled "ion__density(z) vs psi" showing a decreasing trend. The y-axis ranges from 0 to 4e+19. The x-axis ranges from 0.9 to 1.02.
- Top-center: A 2D density plot titled "density, n=61.51" showing a ring-like structure with a color scale from 0 to 1e+00.
- Top-right: A line plot titled "ion__perp__temperature(z, psi)" showing a decreasing trend. The y-axis ranges from 0 to 1.2. The x-axis ranges from 0.9 to 1.02. A red circle highlights a region labeled "Strange problem".
- Bottom-left: A line plot titled "ion__density(z) vs psi" showing a noisy signal. The y-axis ranges from 0 to 2e+19. The x-axis ranges from 0.9 to 1.02.
- Bottom-center: A line plot titled "ion__density(z) vs psi" showing a smooth curve. The y-axis ranges from 0 to 2e+19. The x-axis ranges from 0.9 to 1.02.
- Bottom-right: A line plot titled "ion__density(z, psi)" showing a decreasing trend. The y-axis ranges from 0 to 4e+19. The x-axis ranges from 0.9 to 1.02.

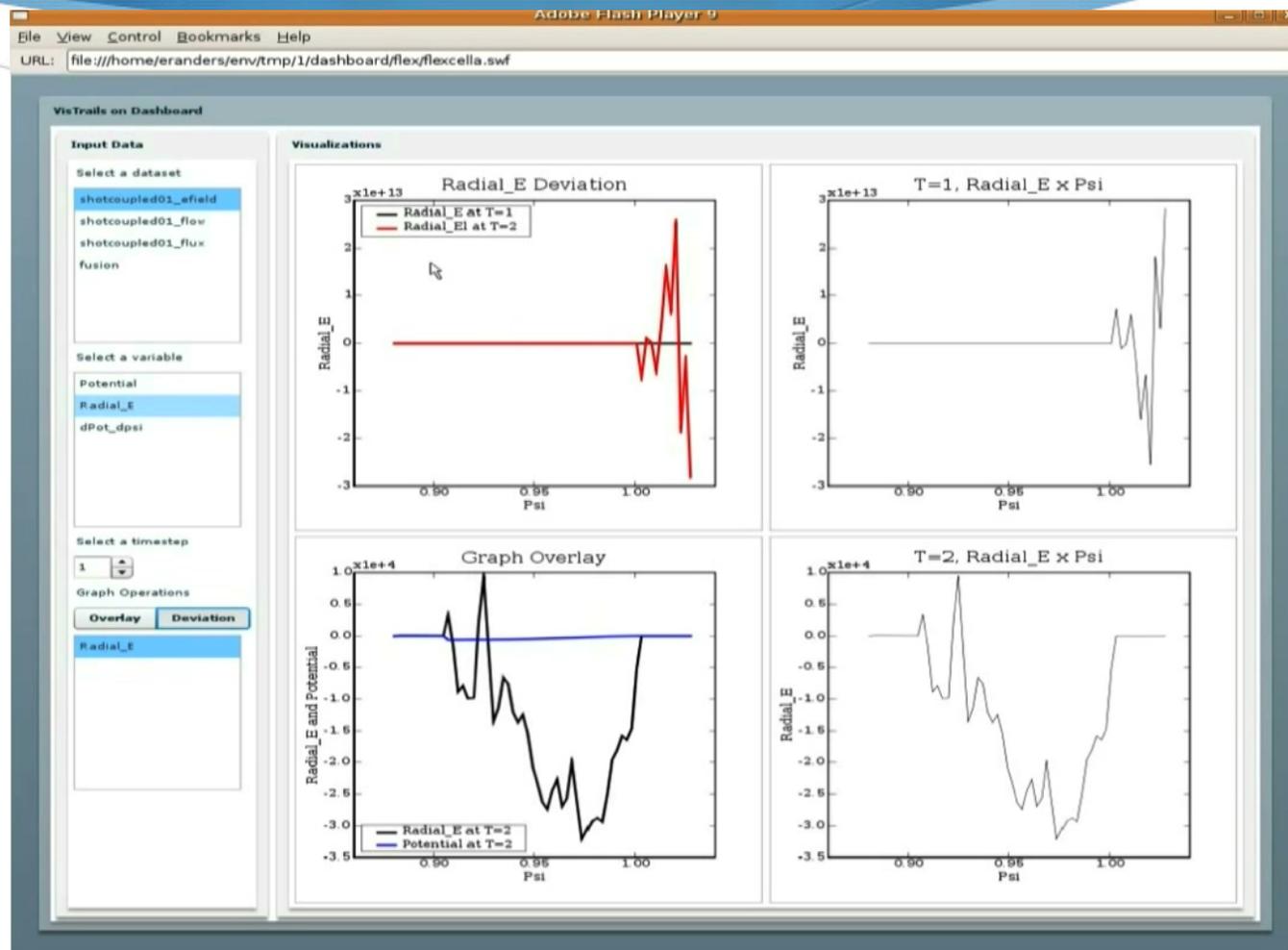
A central dialog box titled "MDS+ data" is open, containing the following fields:

- username: sklasky
- machine: NSTX
- shot: 94754
- signal: [empty]
- all
- Get button

At the bottom of the interface, there is a text area with the text "Compare the two runs... Lower panel on the left is a different run...". Below this is a font selection dropdown set to "Verdana", a size dropdown set to "10", and a "Save" button.

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 be 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.