Code Coupling: Pedestal-ELM Cycle

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CPES-CEMM Joint Meeting, Boulder CO,
March 30, 2008

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Research participants

- Gunyoung Park, NYU
  - *XGC0 kinetic code development*
- Julian Cummings, Caltech
  - *QA Testing, Convergence tests*
- Scott Klasky and Roselyne Barreto, ORNL
  - *Data visualization and Dashboard development*
- Norbert Podhorszki, UC Davis
  - *Kepler workflow development and testing*
- Linda Sugiyama, MIT; Hank Strauss, NYU
  - *M3D code development and expertise*
- Phil Snyder, General Atomics
  - *ELITE code development and expertise*
- Alexey Pankin, Lehigh University
  - *XGC - NIMROD Coupling*
- C.S. Chang, NYU: Principal Investigator
- R. Samtaney, Coordinator

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Talk outline

- Motivations for kinetic-MHD code coupling
- Description of code coupling scenario and operation
- Discussion of Kepler workflow automation activities
- Data movement and visualizations for sample run
- Conclusions and future work

Kinetic <–> MHD coupling in a nutshell

- Overarching goal is to model edge pedestal buildup (kinetic model) followed by ELM crash (MHD model)
- As kinetic code proceeds, we must determine when the pedestal pressure and current density profiles become MHD unstable
- Then switch control to MHD model for nonlinear evolution of ELM and “healing” of MHD equilibrium
- Ideally, we then restart/rerun kinetic code based upon the new equilibrium and continue the cycle
- Process of alternating control should be automated

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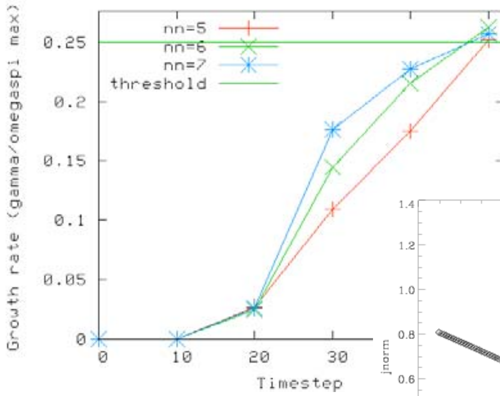
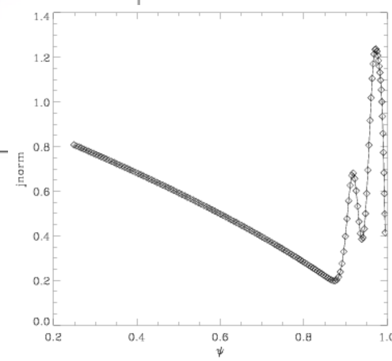
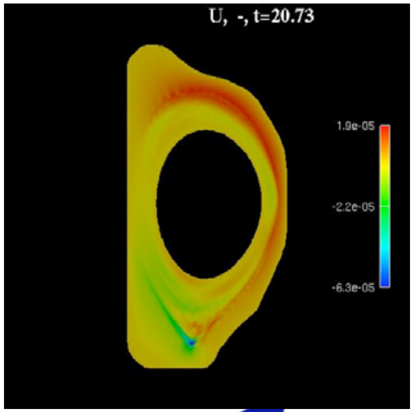
Coupling Fusion codes for Full ELM, multi-cycles

- **Run XGC until unstable conditions**
- **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 equilibrium from M3D-MPP*







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Basic code coupling scenario

- Four different simulation codes in use
  - *XGC0: kinetic simulation of edge plasma, including neoclassical transport with ion-electron-neutral dynamics*
  - *M3D-OMP: MHD analysis code, produces equilibrium & mesh*
  - *ELITE: ideal MHD linear stability analysis code*
  - *M3D-MPP: parallel two-fluid nonlinear MHD initial value code*
  - *DEGAS-2 : atomic physics -not discussed in this talk*
- MHD codes accept plasma profile data (n,T,j) from kinetic code, use eqdsk file for magnetic equilibrium
- M3D-OMP generates hi-res equilibrium for ELITE linear analysis and mesh for M3D-MPP nonlinear simulation
  - *EFIT eq. 65x65, ELITE eq. 140x200, M3D-MPP mesh 40x200*
- If ELM is linearly unstable, M3D-MPP run is launched

Details of code coupling scenario

- XGC0 code run on Cray XT3, initialized with *geqdsk*
- XGC0 periodically writes profile data *m3d.in* and *peqdsk*
  - *Plasma profile, equilibrium data transferred to Infiniband cluster*
- M3D-OMP reads *m3d.in* and eqdsk data, performs equilibrium solve, and writes high-res *eqdsk* file
- ELITE does linear stability check on *eqdsk* and *peqdsk*
  - *Linear growth rate of sample mode compared to* $\omega_{*pi}/2$ *threshold*
  - *Kepler enables simultaneous runs to obtain converged growth rates for several toroidal mode numbers across the spectrum*
- If stable, return updated *eqdsk* data file to XGC0
- If unstable, stop XGC0 and do nonlinear M3D-MPP run
  - *Requires one-step M3D-OMP run to produce M3D meshfile*

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User's view of scientific workflow

- User launches XGC simulation on production computing platform (e.g., *jaguar*) as usual via PBS script
- User then initiates workflow via shell script (or GUI)
- Workflow monitors simulation output, requests post-processing & visualization, and directs any code coupling
  - *Migrate binpack *.bp files and NetCDF *.cdf files to ewok*
  - *Run bp2h5 utility to convert binpack files to portable HDF5*
  - *HDF5 files can be input to AVS service for data visualization*
  - *NetCDF time history data files "split" to recover newest time slices since last monitoring update, then migrated and "fused"*
  - *NetCDF data is imaged with ncgraph utility or can be monitored*
  - *All data and images archived into HPSS at simulation end*

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Kepler workflow basics

- Open-source, actor-oriented framework using Java
  - *Actors encapsulate parameterized actions*
  - *Communicate via input and output data ports*
- Computations performed by flow of control
  - *No call-and-return semantics*
  - *Tokens passed from one actor to the next trigger actions*
- Several key advantages for scientific workflows
  - *Supports parallel-pipeline processing (sync or async)*
  - *Not restricted to web service or computing grid applications*
  - *Open-source development of customized actors*

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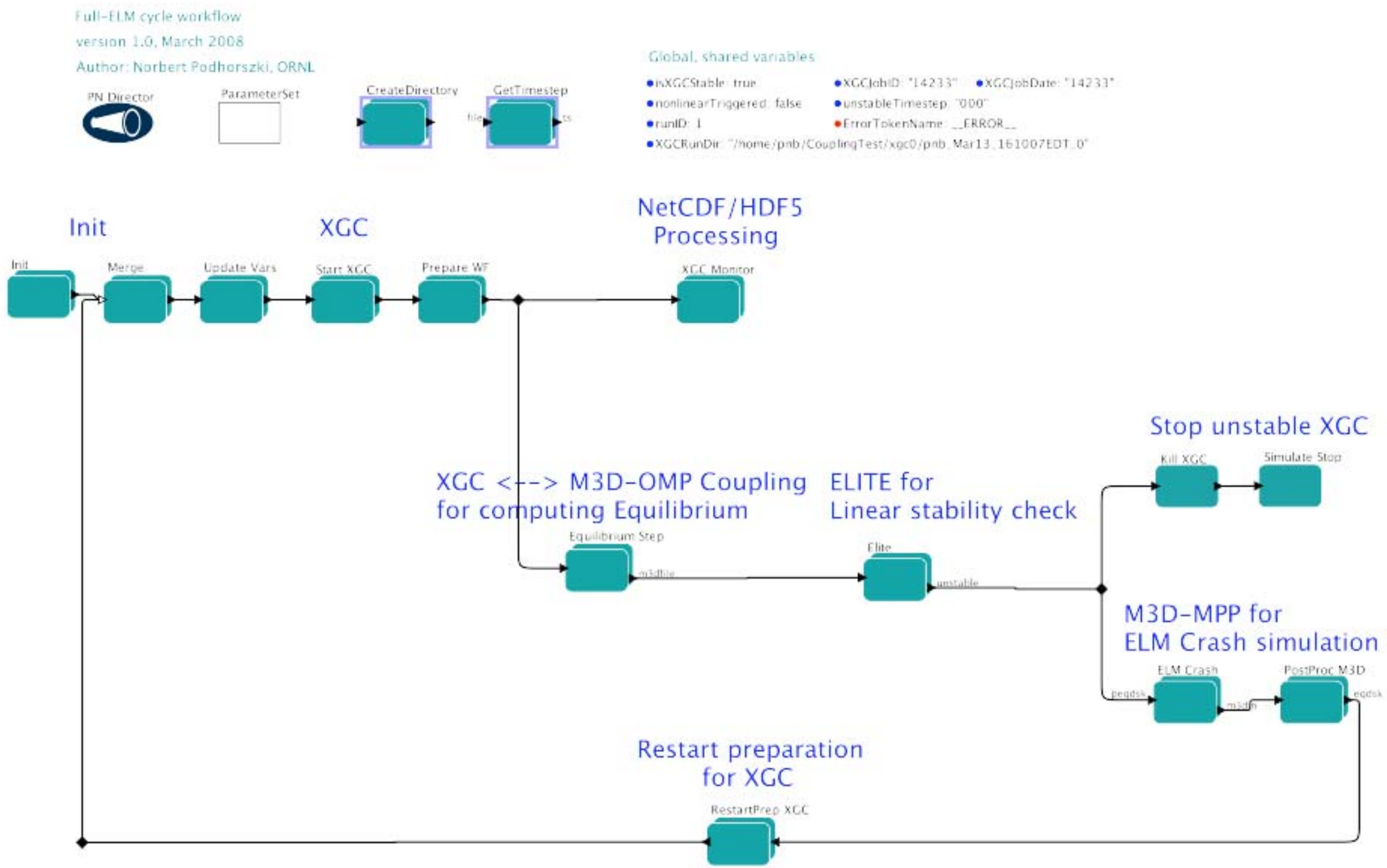
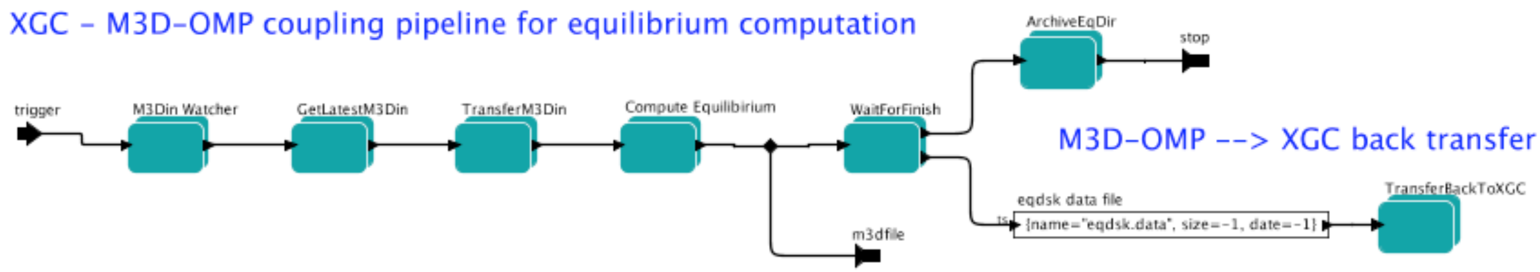
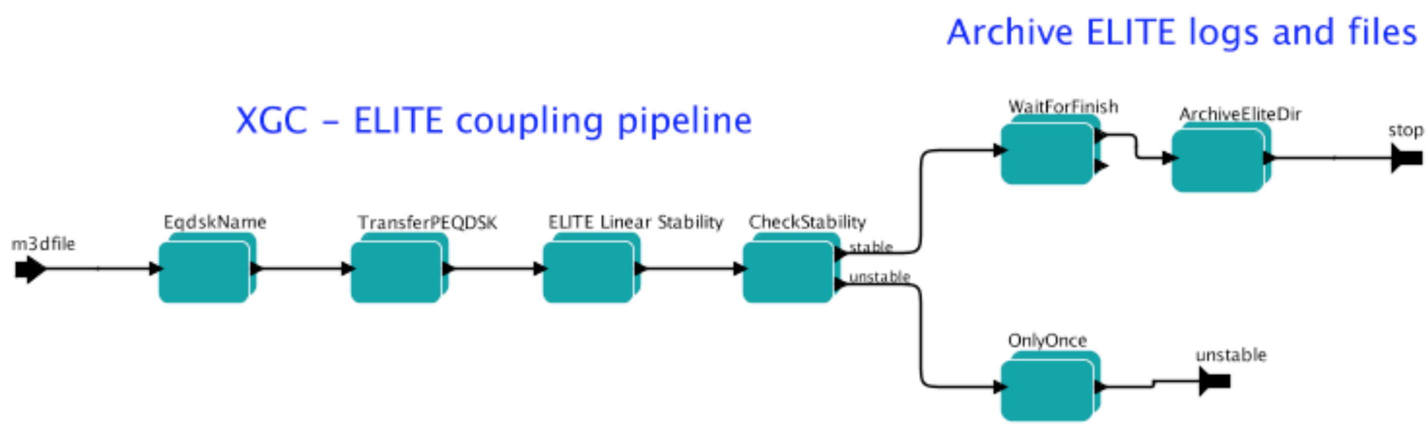
CPES Coupling workflow



Kepler graphical workflow (cont'd)





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Running the Kepler scientific workflow

- Kepler is Java-based framework and uses the JRE
  - *User must load jre module on ewok for workflow use*
- Create “workflow” dir in lustre disk area on ewok
  - *Contains all transferred and post-processed simulation files*
- Launch XGC0 job on jaguar with PBS script as usual
  - *XGC0 uses input parameters to indicate MHD coupling*
- Run shell script from */ccs/proj/fus011/Workflows* area
  - *Script command: start-workflow.sh <shot#> <jobid>*
  - *Script logs in to specific ewok node to process files and launch M3D codes as needed (user passcode required)*
  - *Separate scripts exist for just code monitoring or for coupling*
- Then, go to ewok (or Dashboard!) and view results

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Sample run of code coupling workflow

- Basic XGC0 simulation of edge pedestal buildup
- Input data drawn largely from DIII-D shot analysis
  - *Initial equilibrium from EFIT analysis of shot 096333*
  - *Model profiles for initial plasma density and temperature*
- XGC0 run parameters
  - *320,000 ion particles run on 128 cores of Cray XT4*
  - *Set to run for 100 ion toroidal transit periods in 50,000 steps*
  - *Simple neutron physics model with 0.985 recycling rate*
  - *One dump of plasma profiles and eqdsk update in each ion toroidal transit time*
- Equivalent uncoupled run takes ~75 minutes on jaguar
- Full ELM cycle simulation takes 2-3 hours wall clock time on the combined jaguar-ewok system

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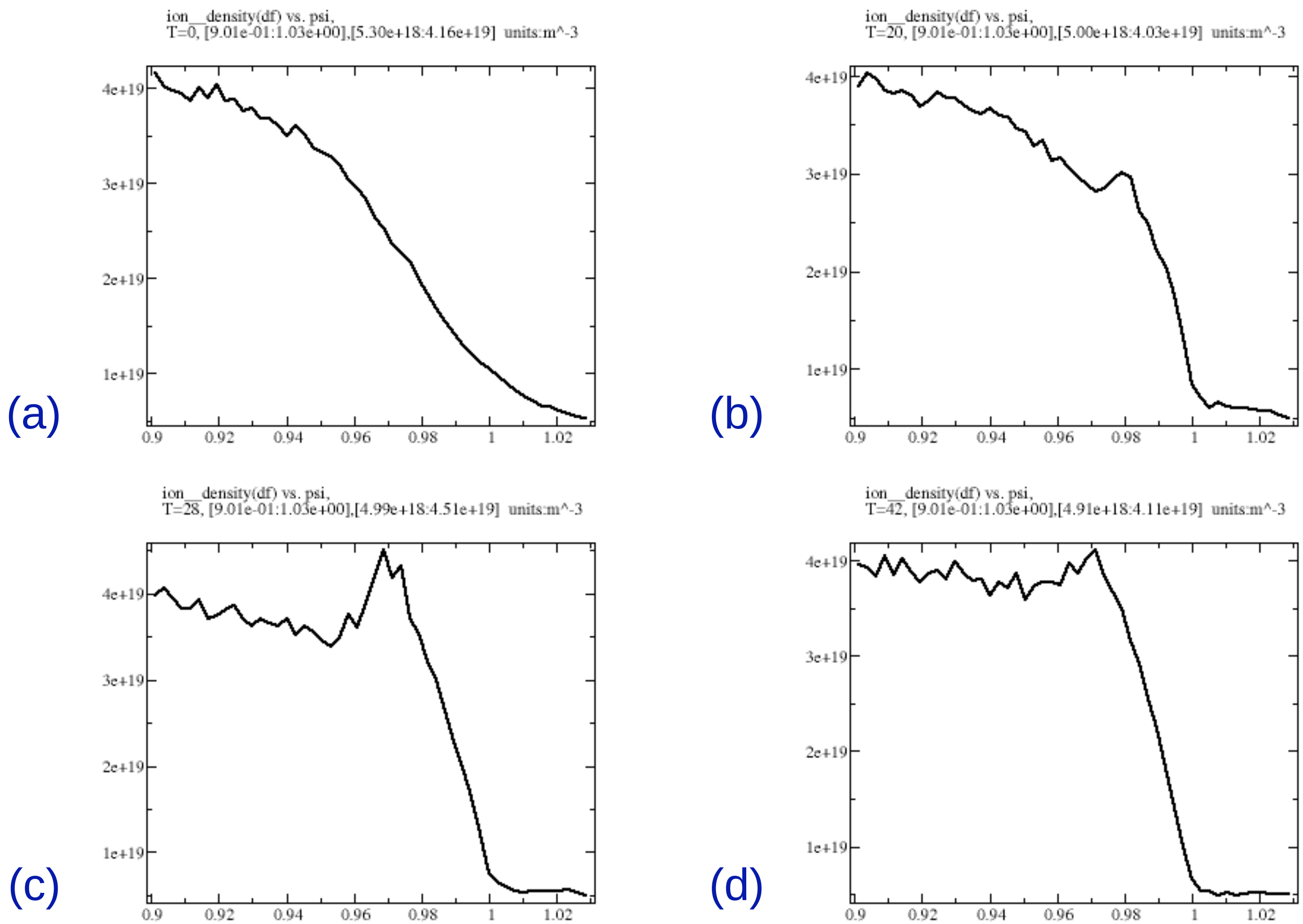
Edge pedestal buildup



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Data movement: XGC0 and M3D-OMP

- XGC0 writes *m3d_<ts>.in* files with (n,T,j) profile data
  - *Here <ts> represents the timestep or dump number*
- Kepler actor looks for most recent dump file
  - *Migrated from Cray XT3 to Infiniband cluster, renamed m3d.in*
- Kepler runs serial M3D-OMP code to update eqdsk
  - *Kepler is provided with M3D-OMP input file for “eq only” run*
  - *Initial run starts from same EFIT equilibrium data as XGC0*
  - *Subsequent runs update from the previous eqdsk file*
- Kepler actor transfers updated eqdsk back to XGC0
  - *XGC0 rereads equilibrium data in each coupling phase*
- Output from each M3D-OMP run saved in subdirectory

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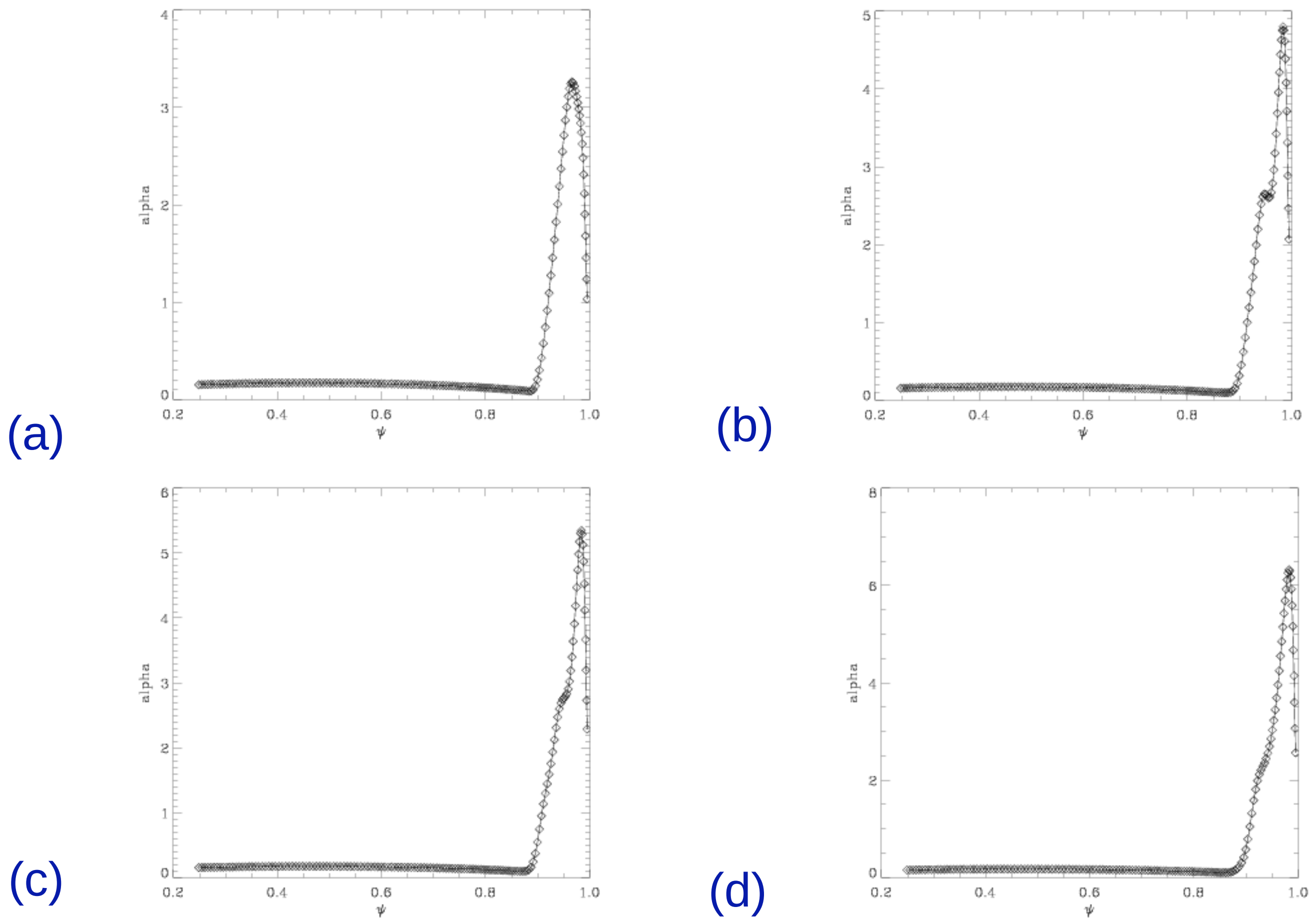
Data movement and visualization: ELITE

- ELITE run for linear stability check has several inputs
  - *High-resolution equilibrium data copied from M3D-OMP run*
  - *Plasma density data in peqdsk format transferred from XGC0*
  - *ELITE input file controls grid resolution, modes of interest, etc.*
- After each M3D-OMP run, Kepler gathers inputs, runs serial ELITE code, and monitors and graphs results
  - *ELITE run has 3 phases: eq solve, vacuum bc, eigenvalue*
  - *Kepler scans results of each phase, logs possible problems*
    - *Example: ELITE results may indicate eigenmode not resolved*
  - *Growth rate is collected, compared with stability threshold*
  - *Kepler plots ELITE output variables using IDL script*
- Output from each ELITE run saved in subdirectory

ELITE output: normalized pressure gradient



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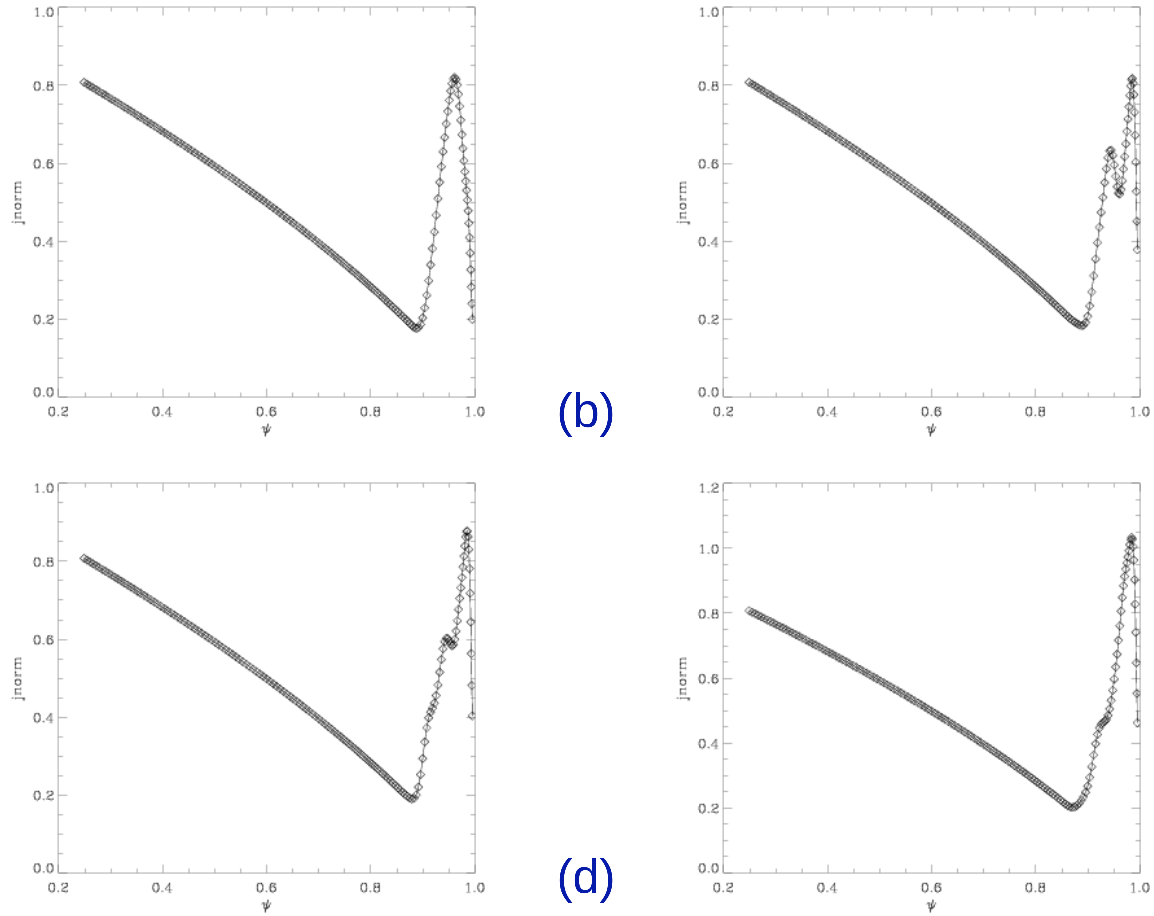
ELITE output: normalized plasma current



(a) (b)

(c) (d)

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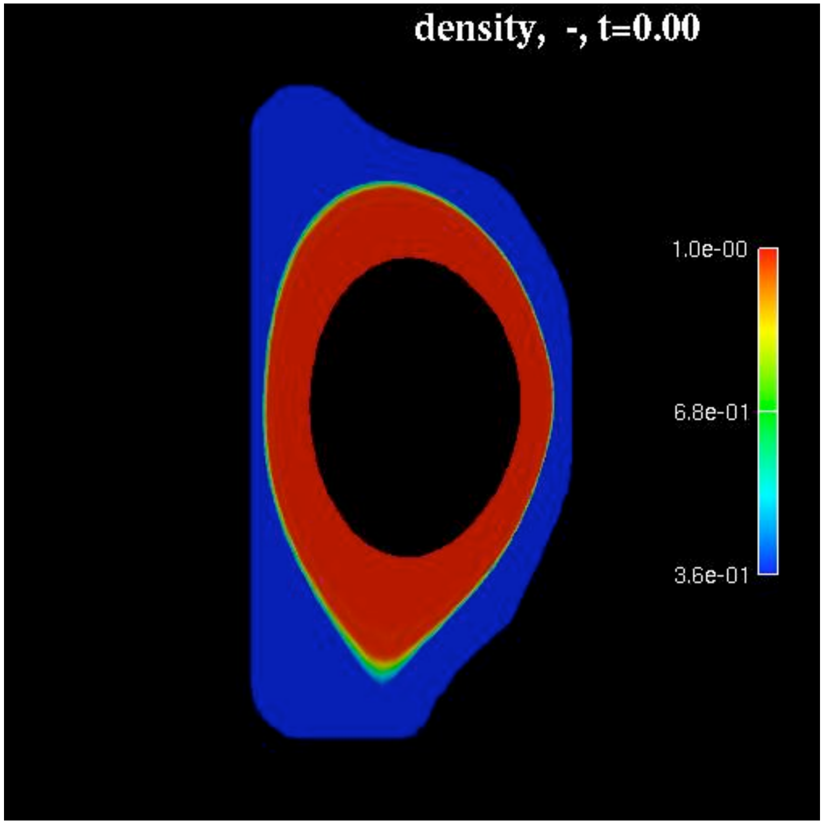
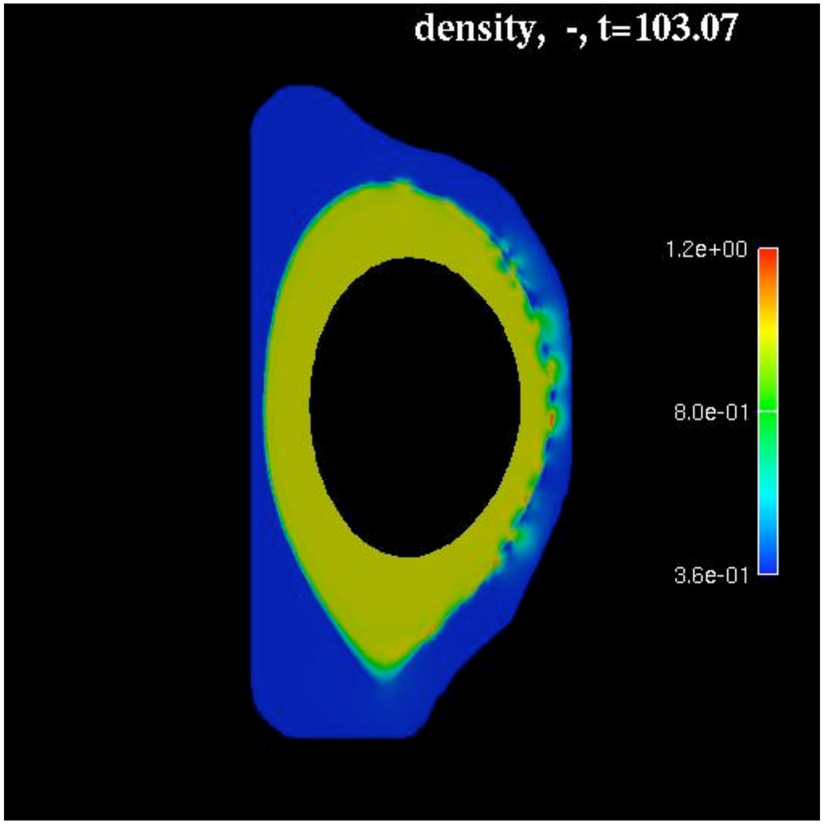
Data Movement and Visualization: M3D-MPP

- If ELITE returns *unstable*, Kepler launches M3D-MPP
  - *Prepare: run one step with M3D-OMP, write meshfile omp.out*
  - *Run: submit 128-process batch job on cluster with omp.out and input parameters file for nonlinear ELM simulation*
  - *Typical run has 16 poloidal planes with toroidal period = 3*
- M3D-MPP produces periodic output in HDF5 format
- AVS/Express module used to plot output variables
  - *Visualization routines made available as a service*
  - *Kepler launches service to listen for plotting requests*
  - *Simple Python script extracts data and requests plots*
  - *Resulting images organized within shot output directory*
- Resulting data and images are archived using HPSS

M3D-MPP: plasma density





Time given in units of the Alfvén period

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ORNL Dashboard tool

- Monitor computational resources and simulations within a standard web browser
  - *Secure login using one-time-password token*
  - *View job queues on various ORNL and NERSC machines*
  - *Access current and archived runs, plus those of collaborators*
  - *Each run offers list of output variables for plotting*
- Graphical display utilizes Flash animation
  - *Plots update on-the-fly as new data is discovered*
  - *View of dashboard can be recorded for later playback*
  - *Flash capabilities include display of 3d visualizations*
- Provenance information

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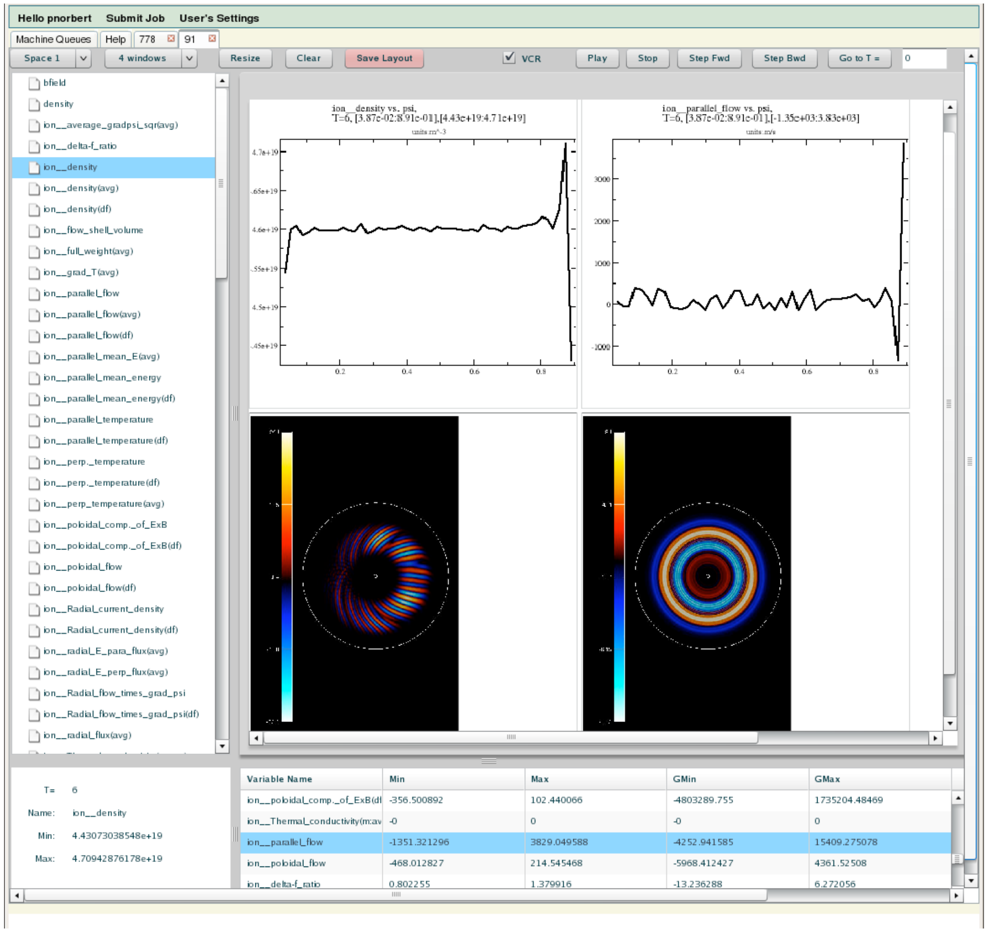
Monitoring XGC output on Dashboard



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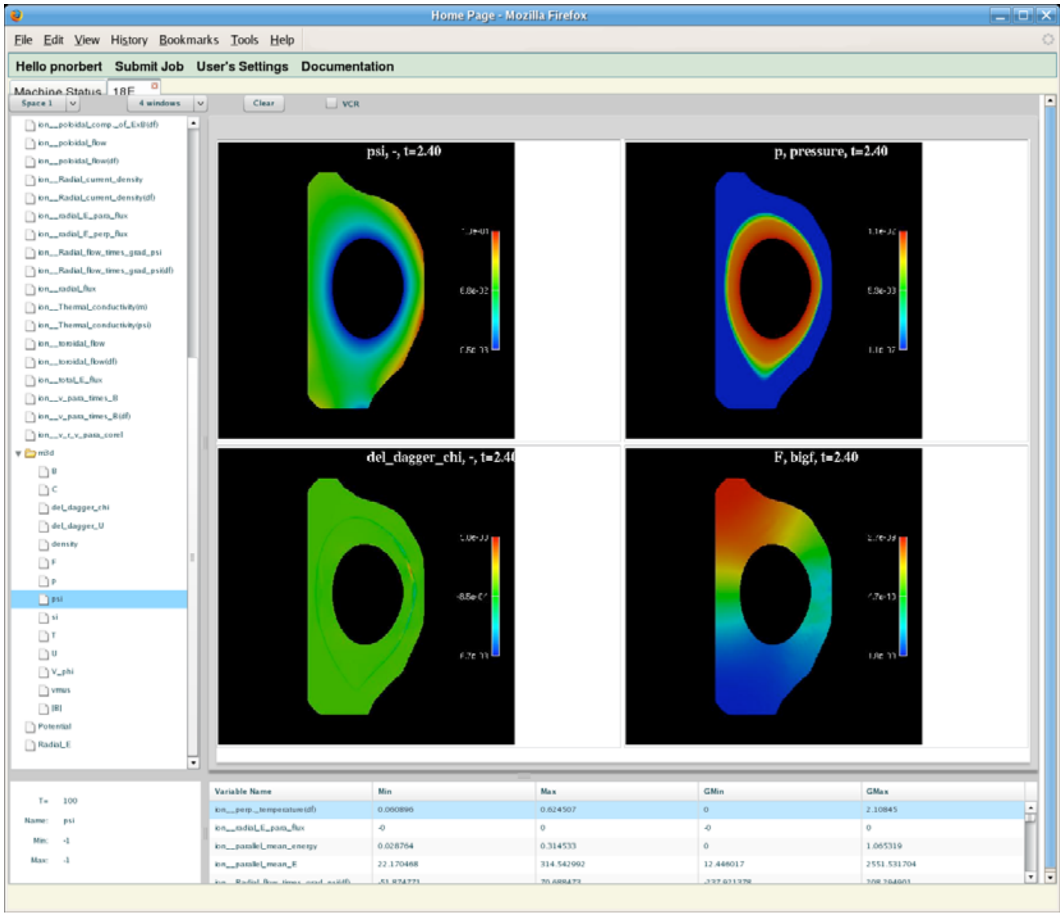
Monitoring M3D-MPP output on Dashboard



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Next steps for code coupling workflow

- Improvements for M3D-MPP
  - *Automatic detection of quasi steady-state (n,T,j) profiles*
  - *Transfer of "healed" equilibrium back to XGC0 code*
- Attempt multiple ELM cycles by restarting XGC0
- Extend workflow designs to accommodate alternate MHD equilibrium and stability analysis codes
  - *TEQ module in XGC0 along with ELITE stability check and nonlinear ELM simulation with NIMROD*
- Enhance use of simulation metadata within workflow
  - *Provenance tracking for a simulation database*
  - *Improved interaction with the ORNL Dashboard tool*
- Verification of coupling results
  - *Convergence tests have been planned*

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