Verification and Validation of Petascale Simulation of Turbulent Transport in Fusion Plasmas

NCCS USERS MEETING

PI: Pat Diamond, UCSD

4/17/2008

Co Pis:
Z. Lin (UC Irvine)
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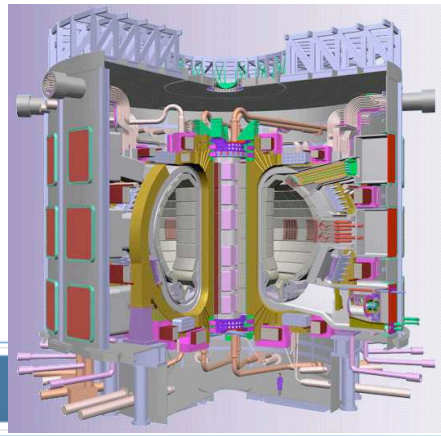
S. Klasky (ORNL)
S. Ethier (PPPL).

Participated by 3 fusion SciDACs: GPS-TTBP, GSEP, & CPES

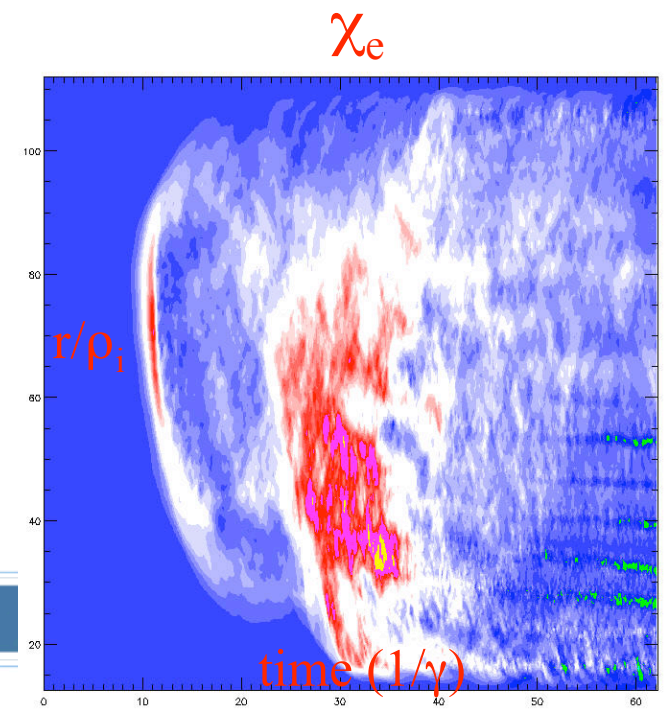
Overview of our INCITE Project

- Understanding turbulent transport is one of the most important scientific challenges in fusion experiments such as ITER.
- Direct comparisons of turbulence simulation with measurement become feasible thanks to remarkable progress in simulation and petascale computers.
- We study three critical issues in fusion core and edge plasmas: heat transport, momentum transport, energetic particle transport
- Benchmark between GTC & XGC for verifications
- Synthetic diagnostics developed for validations.
- This INCITE supports three SciDAC projects
  - GPS-TTBP (PI: P. H. Diamond, UCSD)
  - GSEP (PI: Z. Lin, UCI)
  - CPES, Proto-FSP (PI: C-S. Chang, NYU)



GTC Simulation of Momentum & Electron Heat Transport

- Our INCITE will study physics of momentum transport and origin of intrinsic rotation in ITER plasmas.
  - Plasma rotation can quench macroscopic instability and suppress microscopic turbulence for a transition to high confinement regime
- A probable origin is turbulence driven by Collisionless Trapped Electron Mode (CTEM).
- CTEM turbulence is difficult for simulation due to strong wave-particle interaction & fast electron motion.
- Initial GTC simulations of CTEM observed
  - Spectral cascade & spatial spreading
- Our INCITE studies key non-diffusive processes
  - Electron dynamics: granulation in velocity space
  - Spectral transfer: multi-scale interaction
  - Spatial spreading: non-locality
- Supported by SciDAC GPS-TTBP

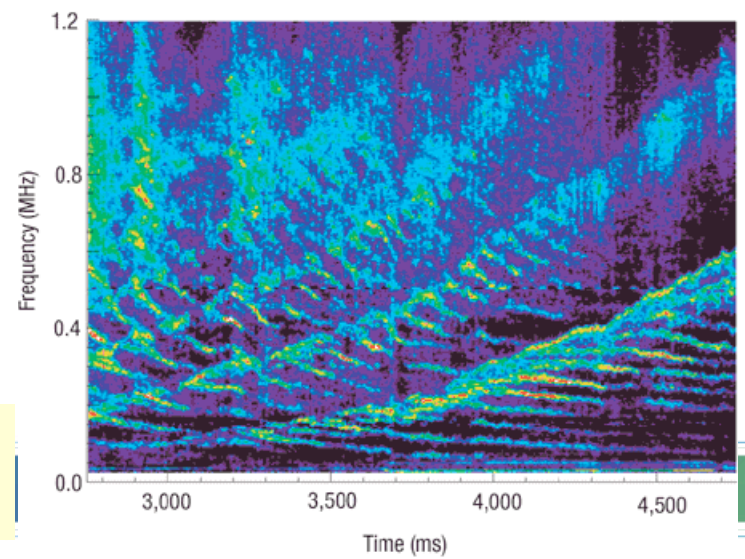


Some CS Challenges

- We want <5% overhead for I/O. (Jin, Lofstead)
  - 55GB at 20GB/sec = 2.75 seconds to write.
  - Can only write data every 60 seconds (every 3 time steps).
- Particle data needs to be saved as 5D mesh.
  - (96 x 1200 x 128) x (100 x 10) * 4 bytes = 55 GB
- Scalar data will be about 2TB/run.
- Total amount of data = (107+2)TB * 4 = 438 TB.
- Time to move to/from tape/run = 109TB/300MB/sec= 4.4 days
  - Looking at streaming techniques for data analysis.
- Still working with physics community for synthetic diagnostics for post processing. (**Requires experimental data from MDS+).**
- Need to monitor run for failures (1.5days/run).
- Need to get better performance (vectorization). (N. Wichmann)

GTC Simulation of Energetic Particle Transport

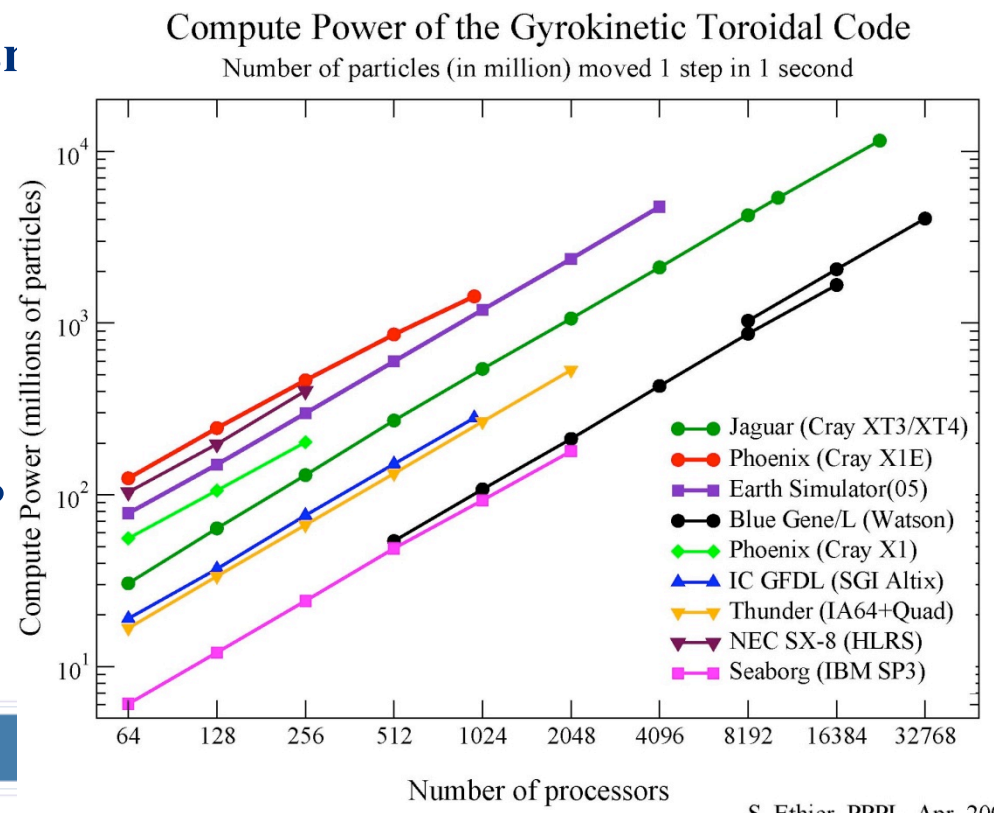
- Confinement of energetic α-particle produced by fusion is critical for heating plasmas in ITER.
- Energetic particle (EP) drives unstable Alfven modes, such as toroidal Alfven eigenmode (TAE), which in turn induces rapid loss of EP.
- EP turbulence and transport requires kinetic turbulence simulation
  - Kinetic effects of thermal plasmas important for damping Alfven modes
  - Nonlinear interaction of many Alfven modes leads to EP turbulence in ITER
  - EP turbulence could couple with microturbulence driven by thermal plasmas
- Initial GTC simulations observed TAE modes excited by spatial gradient of EP density
- Our INCITE is 1st fully kinetic EP simulations
- Supported by SciDAC GSEP: *Center for Gyrokinetic Simulation of Energetic Particle and Transport*



Spectrum of Alfvén eigenmodes in DIII-D [Nazikian et al, PRL06]

GTC Status: State-of-the-Art

- Gyrokinetic toroidal code (GTC) [*Z. Lin et al, Science 1998*] is a particle-in-cell code for simulation of turbulence and transport in fusion plasmas
- GTC physics modules: kinetic electron, electromagnetic turbulence, multi-species, general geometry, collision operator, guiding center Hamiltonian
- GTC global field-aligned mesh; Parallel elliptic solvers via PETSc
- MPI/OpenMP multilevel parallelisı
- Comprehensive analysis package
- Key code for GPS-TTBP & GSEP
- Part of NERSC benchmark suite
- Part of ORNL pioneer application
- Developed by GPS-TTBP & GSEP projects & maintained at UCI



S. Ethier, PPPL, Apr. 2007

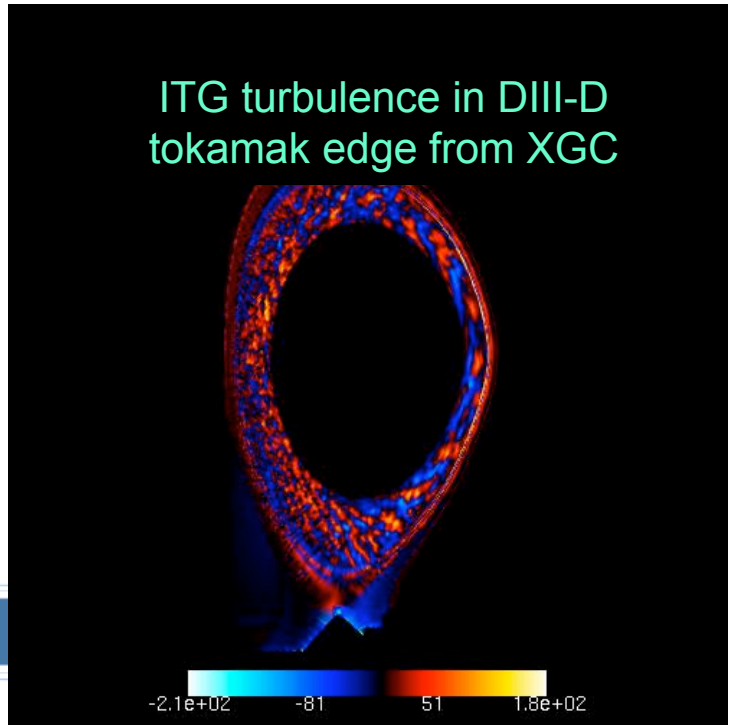
GTC Plan: More Powerful Computer →Better Physics

- Formulate new physics modules: full-f ion, profile evolution
- Sustain parallelization for 100,000+ cores; optimize for multi-core computer
- Implement advanced computational tools: ADIOS, workflow & dashboard
- Develop synthetic diagnostics for validation; Better version control & integration

simulation	Computer	procs	TF	Particles	tsteps	Publication
1998	Cray T3E NERSC	10^2	10^{-1}	10^8	10^4	Zonal flow physics (Science, 1998)
2002	IBM SP NERSC	10^3	10^0	10^9	10^4	Transport size scaling (PRL, 2002)
2007	Cray XT3 ORNL	10^4	10^2	10^{10}	10^4	Electron turbulence (PRL, 2007)
2008	Cray XT4 ORNL/NERSC	10^4	10^2	10^{10}	10^5	Electron transport in ITER Momentum transport
2009	Cray XT5 ORNL	10^5	10^3	10^{11}	10^5	Energetic particle transport
201?	?	10^6?	10^4	10^{12}	10^5	Core-edge coupling

XGC global Simulation of Tokamak Edge Transport

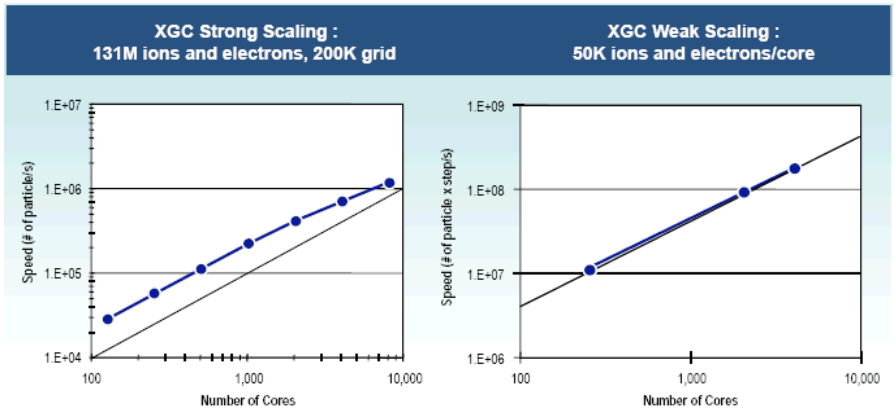
- Understanding the tokamak edge transport is a critical issue for ITER physics:
  - A significant portion of the tokamak confinement is determined at the edge (H-mode pedestal).
  - Edge pedestal height is a key boundary condition for core transport.
  - Edge rotation propagates into core, affecting the core confinement/stability
- Plasma edge is highly kinetic, but there has been no kinetic turbulence code prior to XGC: Difficult problem due to wall-loss, non-Maxwellian ions and strong mean-flow interactions with turbulence. A full-f gyrokinetic code is needed.
- Full-f XGC code has successfully simulated the gyrokinetic Ion Temperature Gradient (ITG) turbulence in the entire edge for the first time.
- Full-f XGC observed surprising existence of ITG turbulence in the edge pedestal region: ITG can be a significant edge transport source
- XGC-GTC coupling may predict plasma transport in the whole core-edge
- Supported by SciDAC Proto-FSP CPES

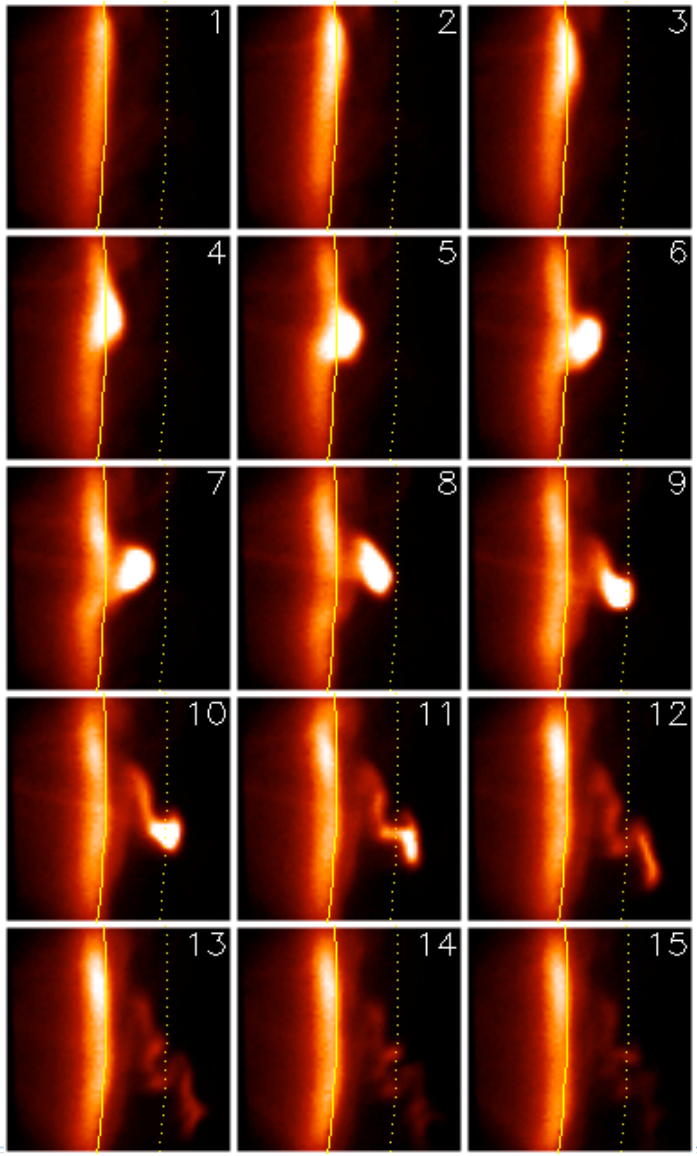


XGC shows excellent HPC scaling

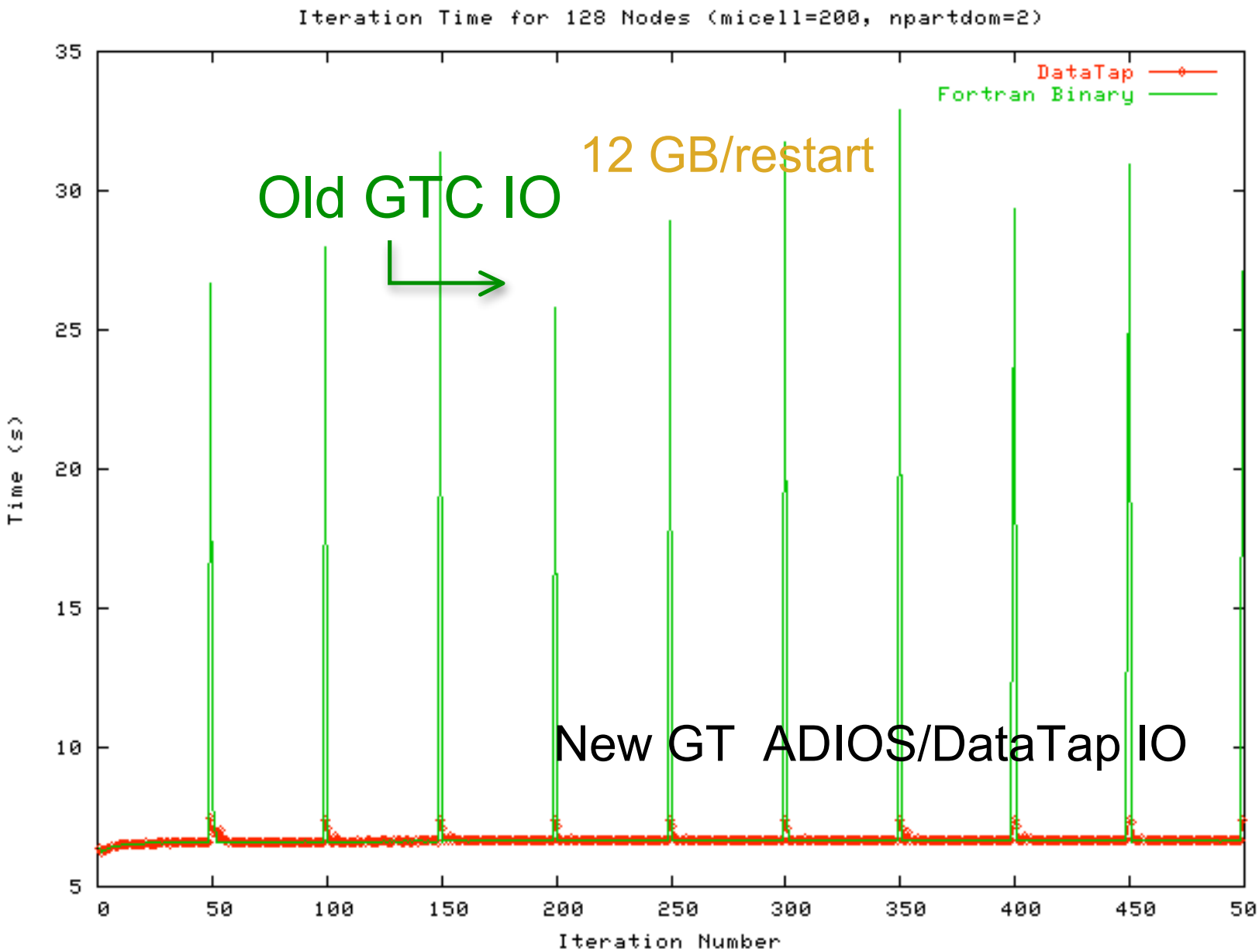
- Since XGC is a full-function code, it demands much more HPC resource than a perturbed-function code (factor of ~1,000).
- Peta-scale+ computing can enable prediction for the whole device transport for ITER and future fusion reactors, in coupling with GTC
- During 2008 campaign, XGC plans to simulate the ITG-driven blobby transport in the DIIID and C-Mod edge plasmas, which has been experimentally known to be the major transport mechanism at the tokamak edge. Study on the edge momentum source and wall load is to be included.

  Jaguar requirement: 20,000 processors X 20 hrs X 7 runs = 2.8M hrs





ADIOS IO



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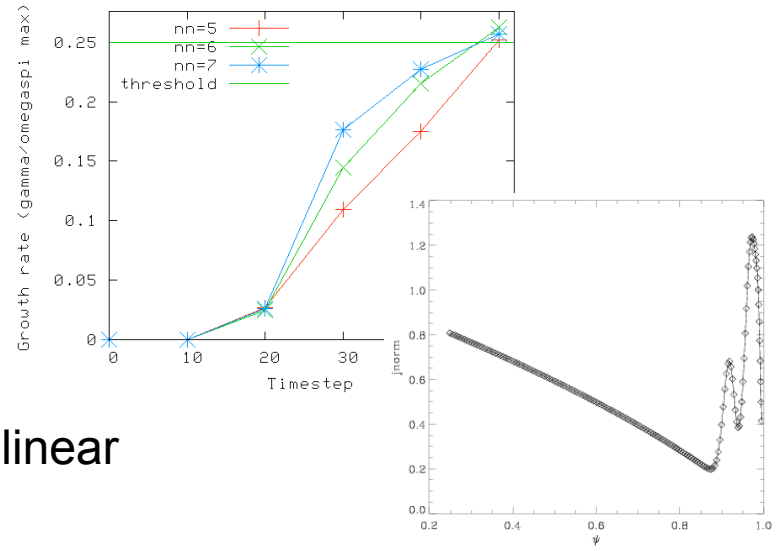
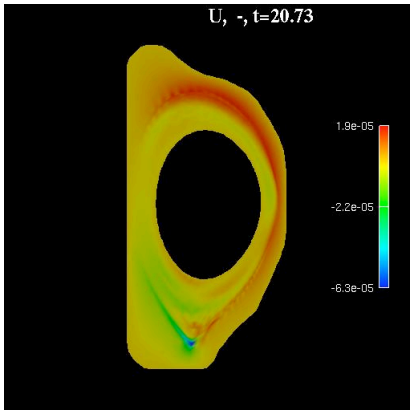
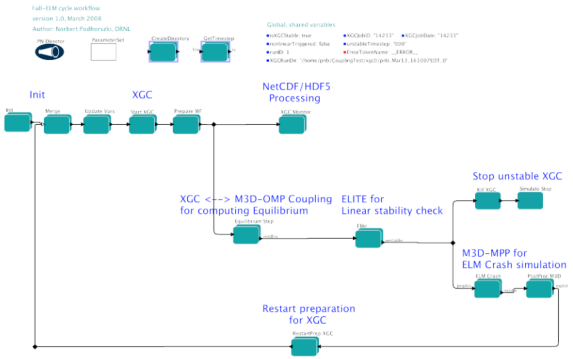
Kepler: Coupling Fusion codes for Full ELM, multi-cycles

- **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

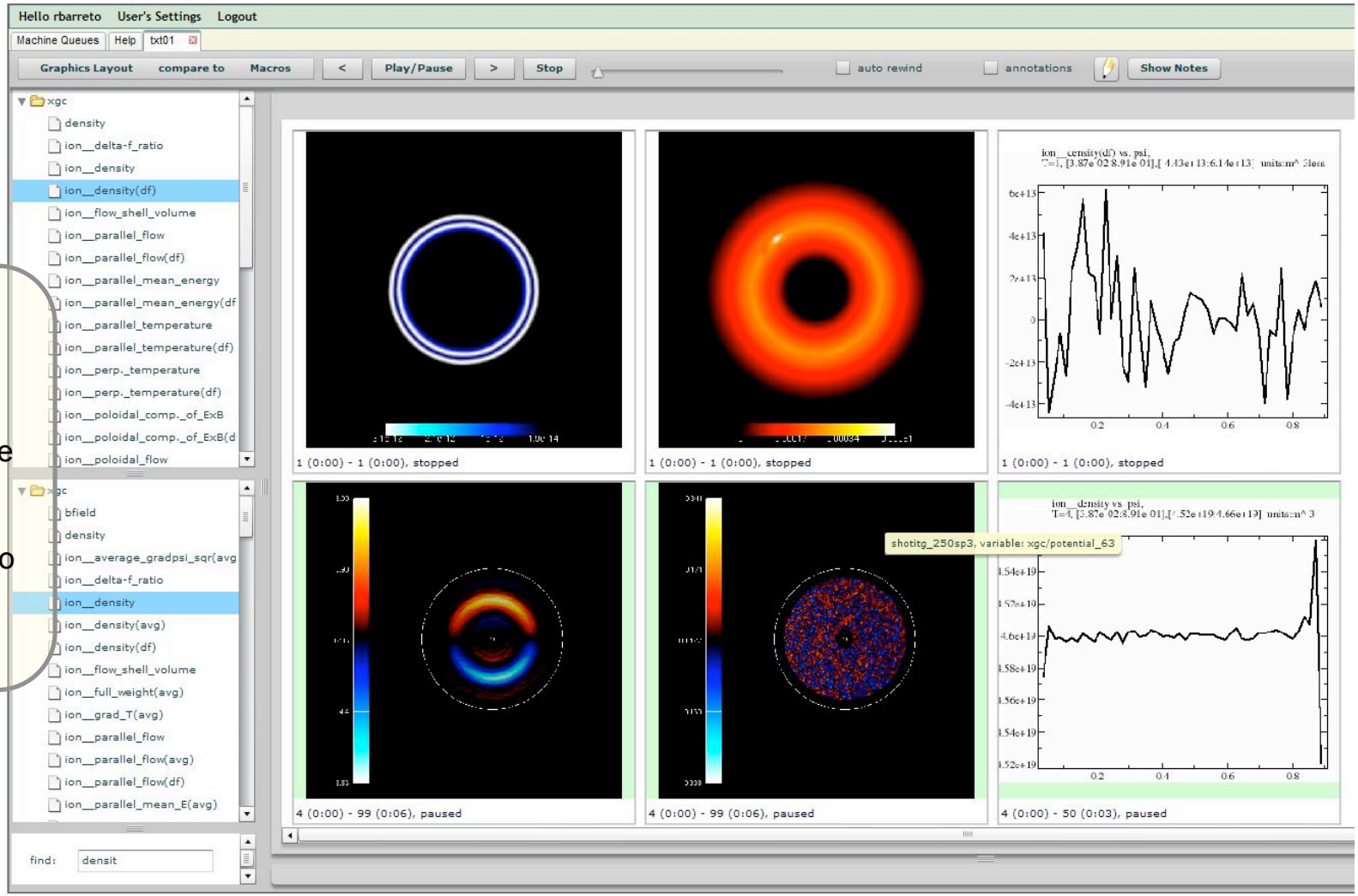






Dashboard to Monitor/Analyze results

- 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