SciDAC Proto-FSP

Center for Plasma Edge Simulation

C-S Chang (Lead PI),

Courant Institute of Mathematical Science, NYU

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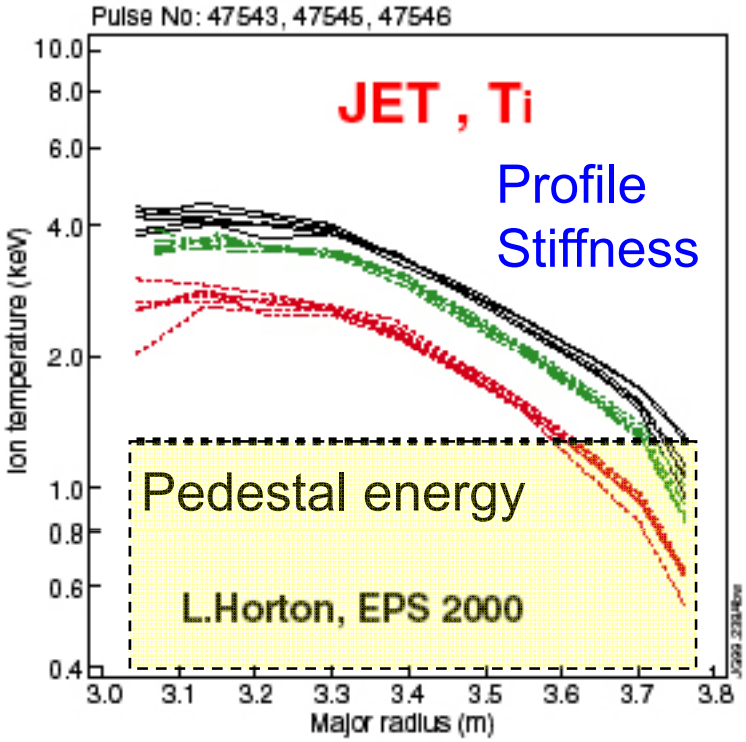
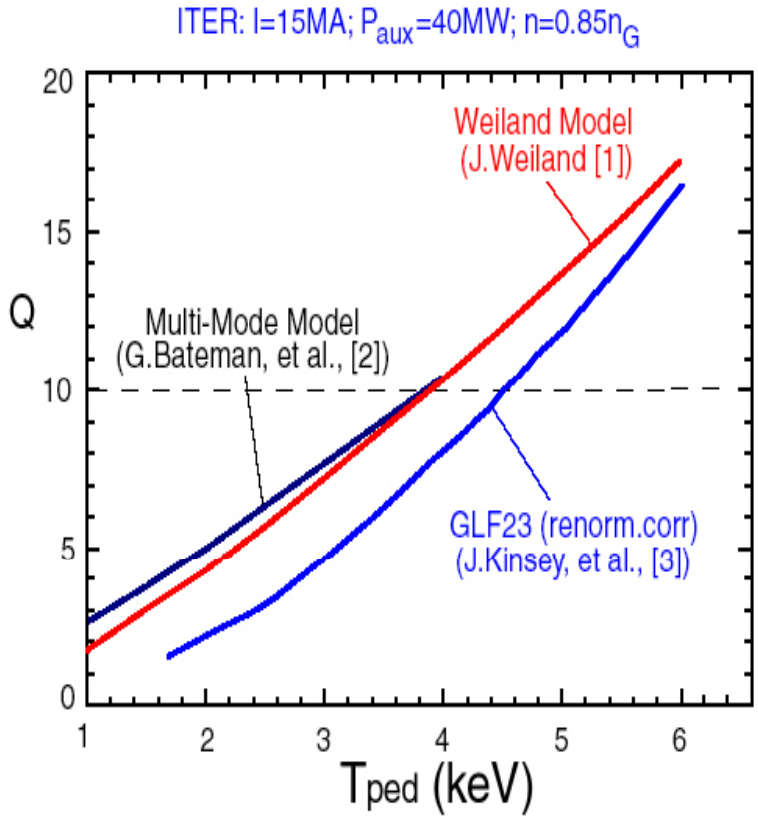
Fusion performance in ITER critically depends on pedestal height – achieve T_{ped}> 4-5 keV?





Fusion merit: $N_i \tau_E T_i \propto H^{3.2} B^{3.5}/q^3$

Edge Localized Mode Instability damages wall.

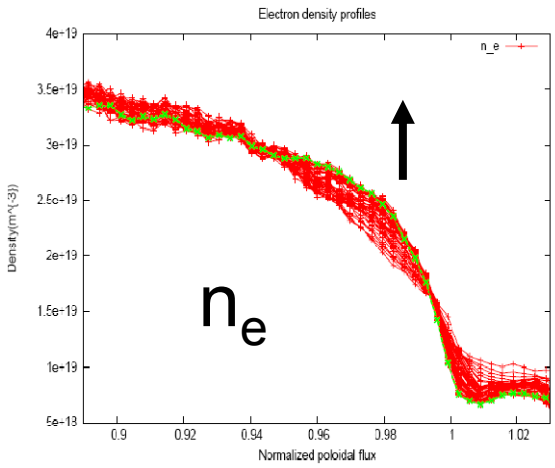
Edge physics (unknown)

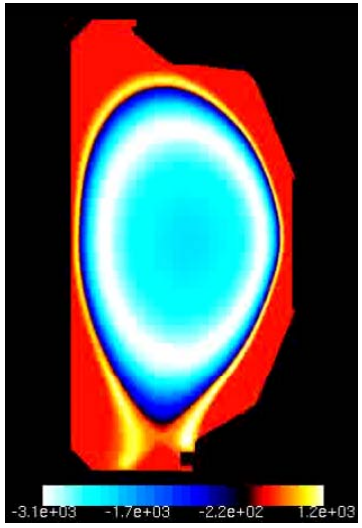
Multi physics in edge requires an integrated simulation framework now (μs–s, 0.1mm–10m)

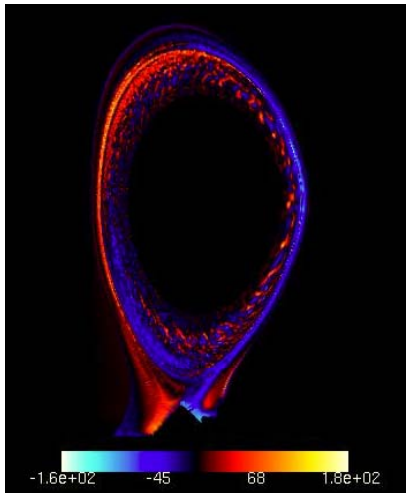
1. Equilibrium evolution with B_o-reconstruction (10^{-3} – 10^{-1} s, mm – 10 m)
2. Radial electric field response (10^{-5} s, mm – m)
3. turbulence physics (10^{-5} - 10^{-4} s, mm-cm)
4. MHD physics (~10^{-6}s, cm – 10 m): stability check, ELM crash
5. Neutral transport (10^{-05} – 10^{-7} s, mm – 10 m)
6. Atomic physics (<<< 10^{-7} s, <<< mm)

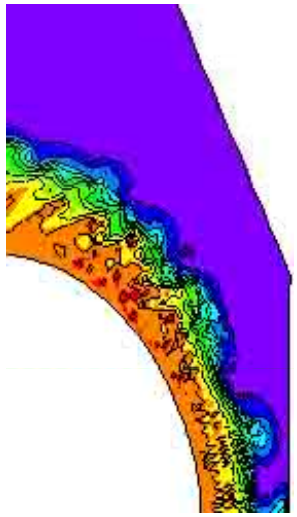
Two new full-f kinetic codes are under development to include1,2,3 and 5 for two separate time scales (but with overlapping of 2).

- Closed and open magnetic field lines with X-point
- Large flux expansion ratio and shaped wall
- Non-thermal-equilibrium plasma (sources and sinks)



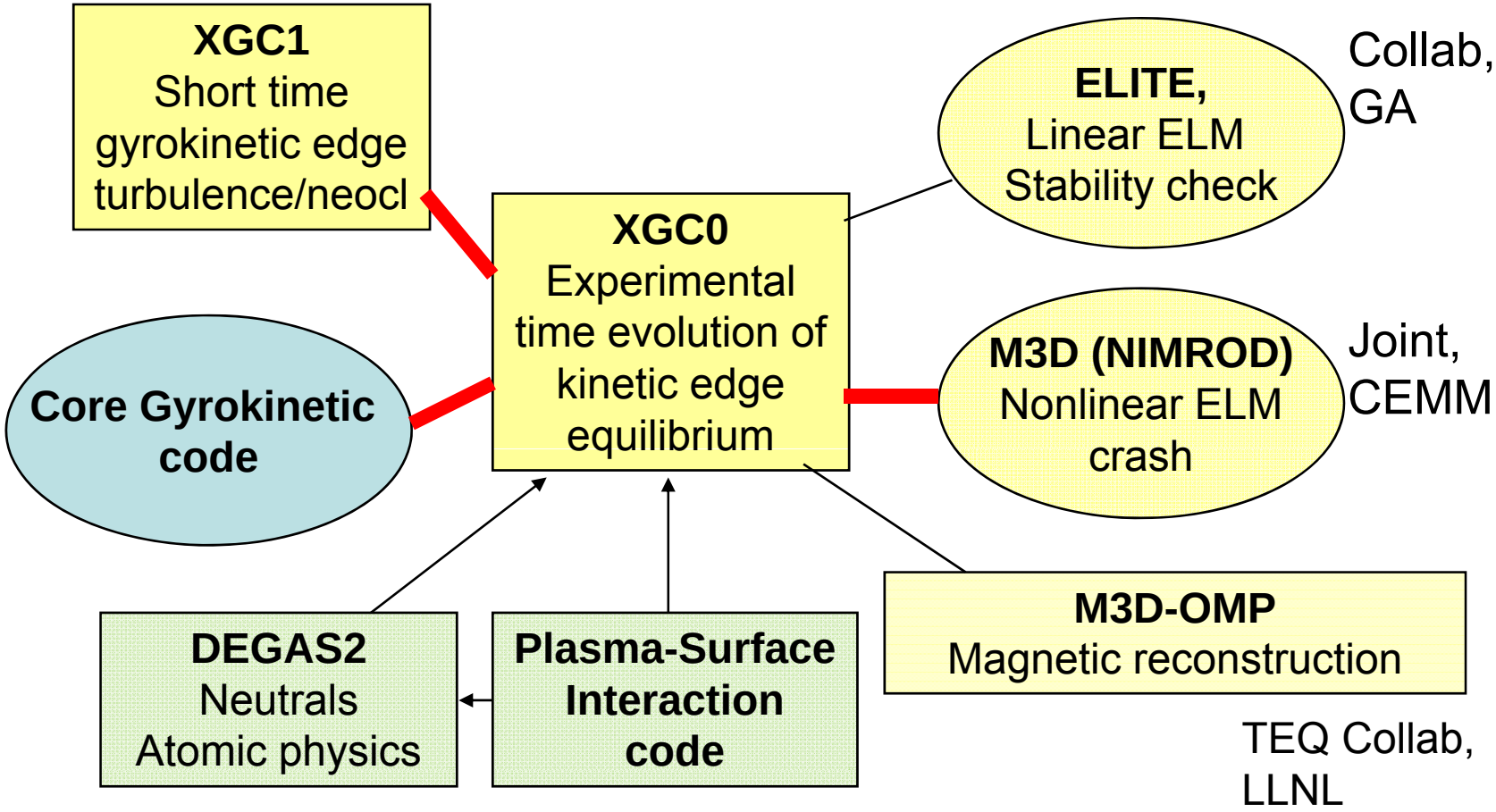




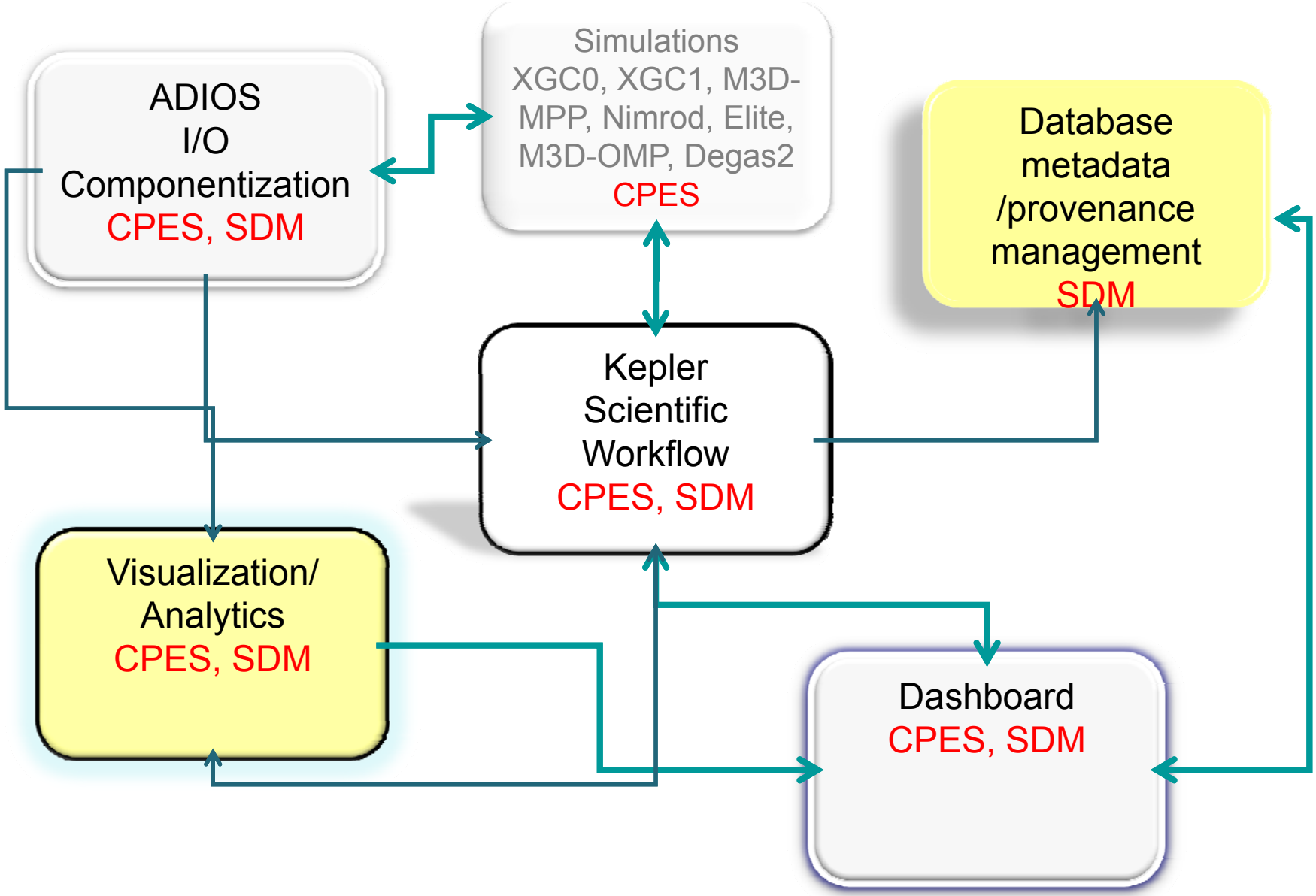


End-to-end Framework for Fusion Integrated Simulation (EFFIS)

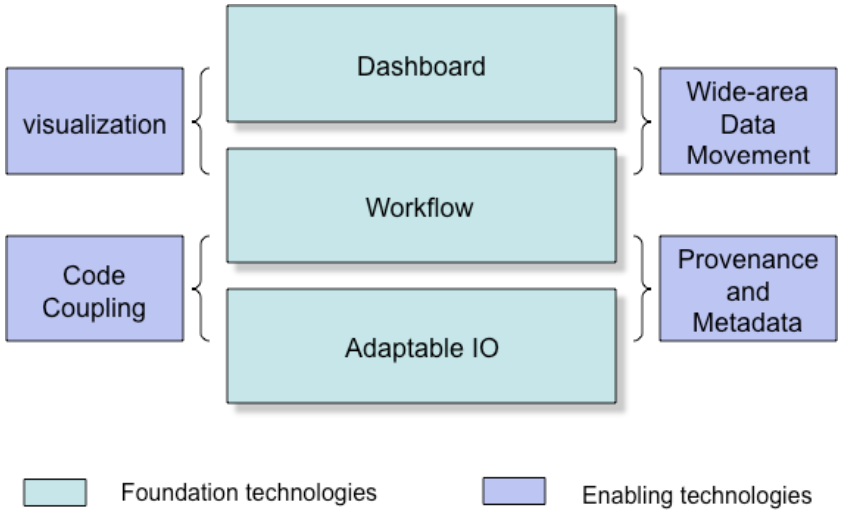
is at work for multiple ELM cycles



It's all about the Data Management



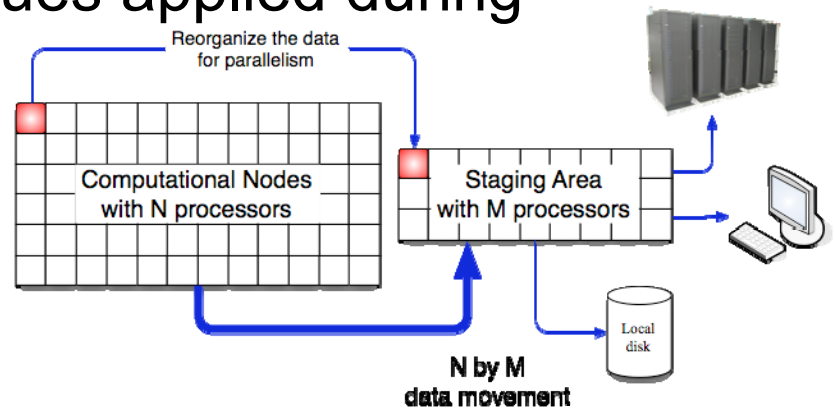
It's all about the Science→ The Data!



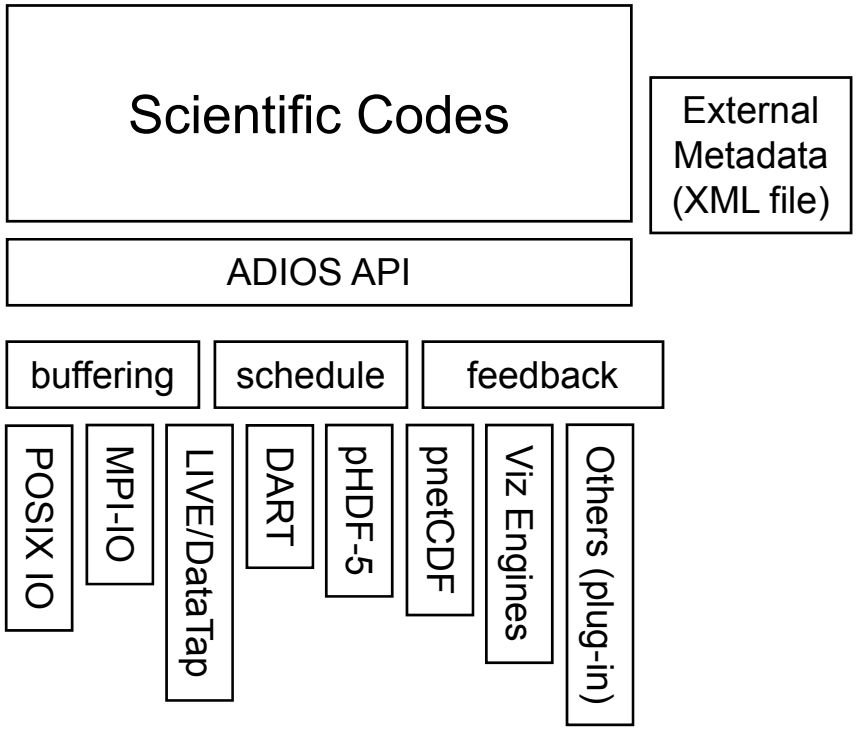
- Combines
  - Petascale Applications.
  - Petascale I/O techniques.
  - Workflow Automation.
  - Provenance capturing system.
  - Dashboards for real-time monitoring/controlling of simulations, and creating social spaces for scientists.
- Basic Idea: place highly annotated fast, easy to use I/O methods in the code, which can be monitored, and controlled, have a workflow engine record all of the information, visualize this on a dashboard. Have everything report to a database.
- Remember: It's all about the science!

ADIOS Overview – Design Goals

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



ADIOS Architecture



Combines
High performance I/O.
In-Situ Visualization.
Real-time analytics.

- Simple API for Fortran and C nearly as simple as Fortran standard IO for both read and write
- Both synchronous and asynchronous transports supported without code changes. Change IO method by changing XML file only!
- Free hooks into visualization and workflow systems through the data flows.
- Optimized IO implementations provided for each transport method (e.g., MPI-IO, pHDF-5, pnetCDF, etc.)
- Binary, tagged format provided by default (including support for data paths and attributes).

What is the Kepler Workflow Framework?

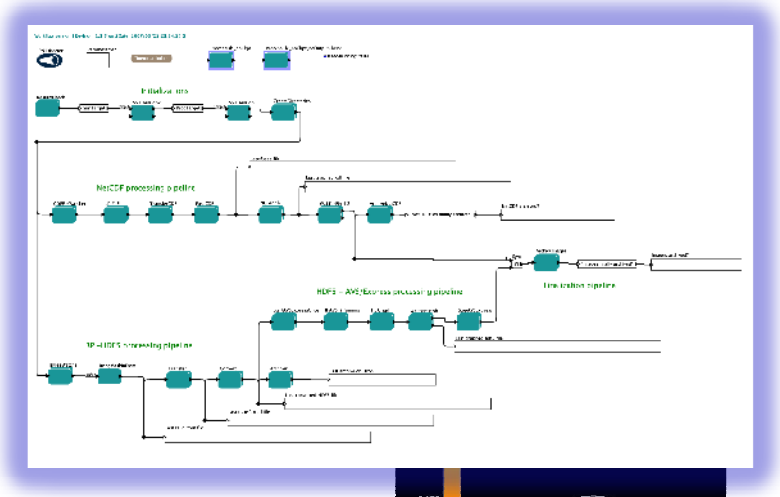
- Workflow framework.
  - **Kepler is a proven DOE technology for orchestrating scientific workflows which help in the construction and automation** of scientific problem-solving processes.
  - **Captures provenance information for**
    - Data provenance. (Where did my data come from).
    - Data movement, data replication. (during code coupling).
    - Which files are in which tar files on HPSS (NERSC/ORNL).
    - Helps users debug by saving log files.
  - **More powerful than python scripts**.
    - Allows you to do pipeline-parallel with ease!
    - Allows you to continue working even if some scripts/components fails.
    - Allows you to checkpoint/restart the workflow!
    - Makes it easy to modify the workflow for a continuously changing group of scientists.
  - **Excellent Connection to databases**.
    - Allows for easy queries of shots from coupled simulations.
    - **Large SDM effort to save provenance data into DB**.

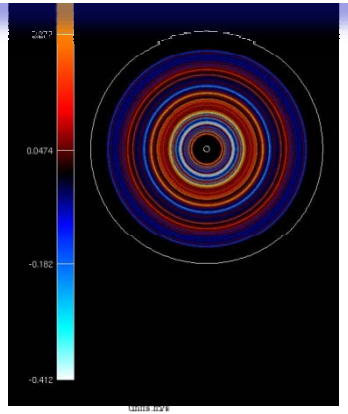
Workflow Automation.

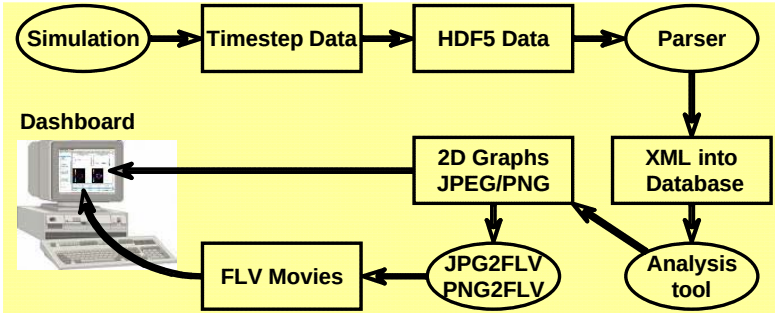
- XGC0, M3D-OMP, Elite, M3D-MPP (Nimrod)
- XGC1 monitoring.
- M3D monitoring.
- Workflow Automation template propagating into other projects.
  - Astrophysics
  - Combustion
  - Fusion SciDAC GPSC
  - Fusion GSEP
  - EU-ITER fusion (Euforis)

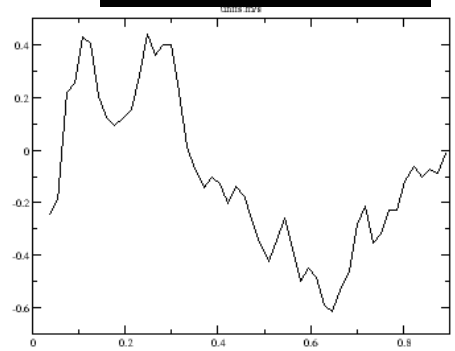
Workflows for monitoring a simulation

- 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
  - Generate images with AVS/Express (running as service)
  - Archive HDF5 files in large chunks to HPSS
- Record Provenance information for everything!



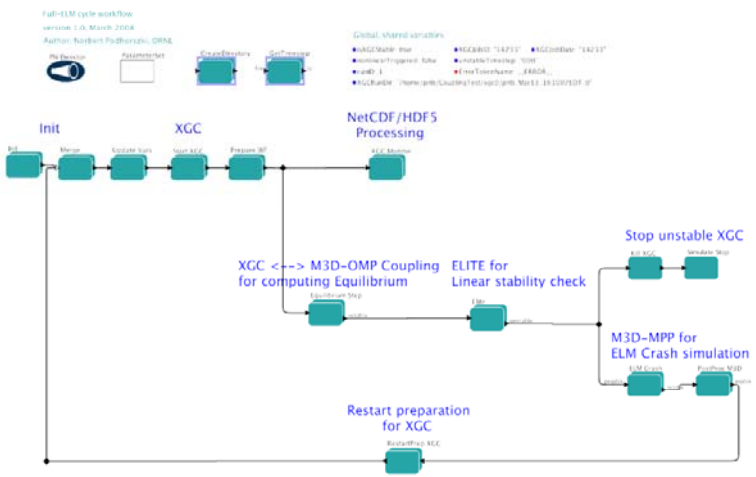


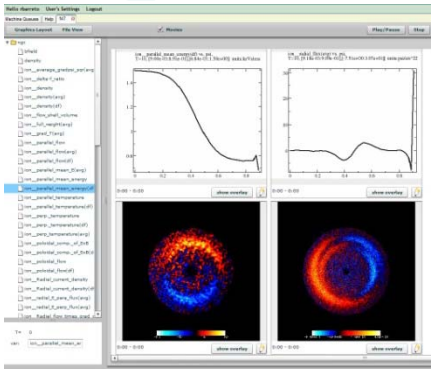


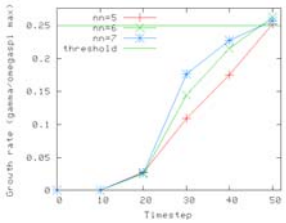


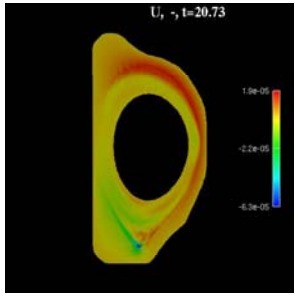
Coupling Fusion codes for Full ELM, multi-cycles

- 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



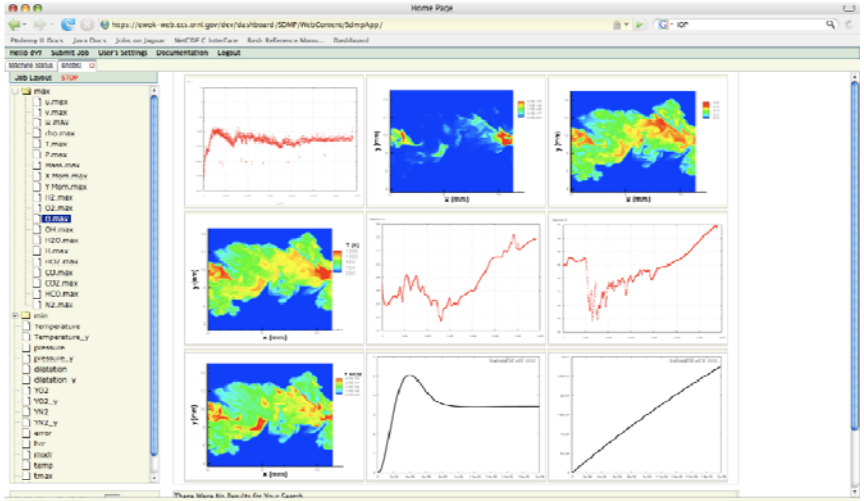


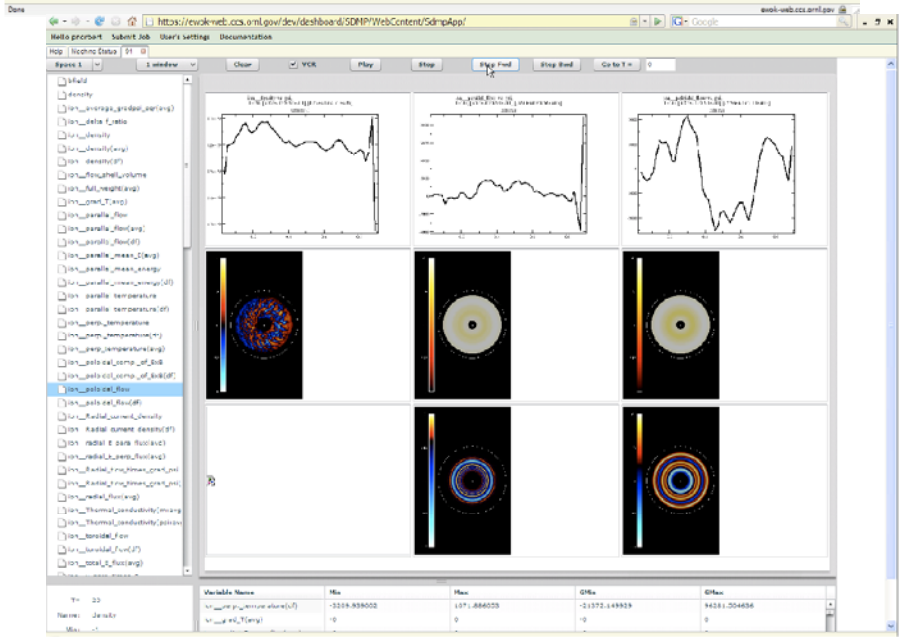




ORNL/CPES/SDM Dashboard.

- Designing a basic browser-based visualization tool.
- Local interaction for line graphs, 2D slices, particles
- Server used for data maniupulation, extraction
- Server used for more complex visualizations
- “Google maps” for your data.
- Allows for pan and zoom locally
- Asynchronously queries
- MySQL for database support.
  - It’s all about the data management !
- First Dashboard featured methods to only look at simulation movies.
  - Now moving into interacting with data.

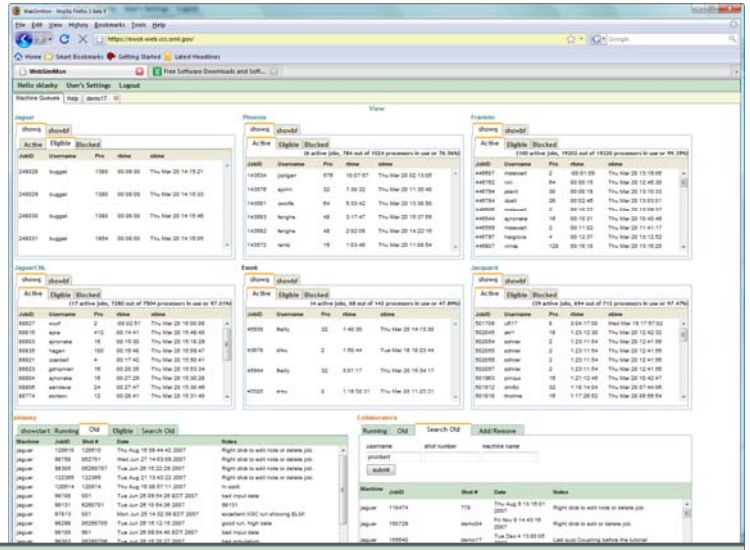


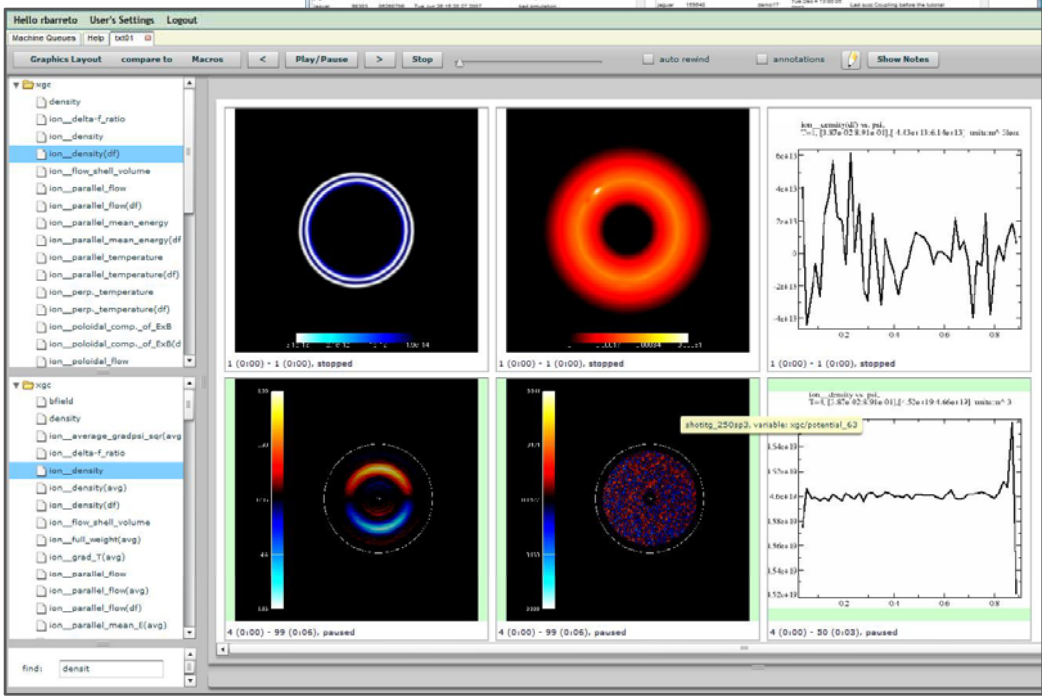


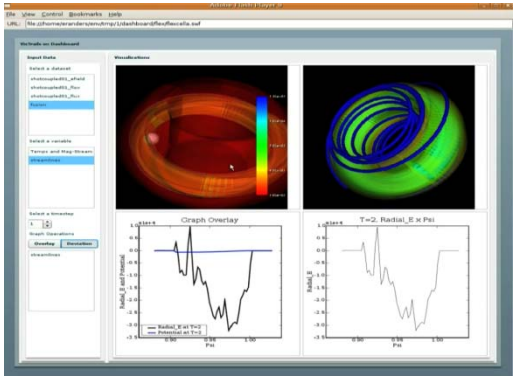
Dashboard

Monitors machines, simulations and DB

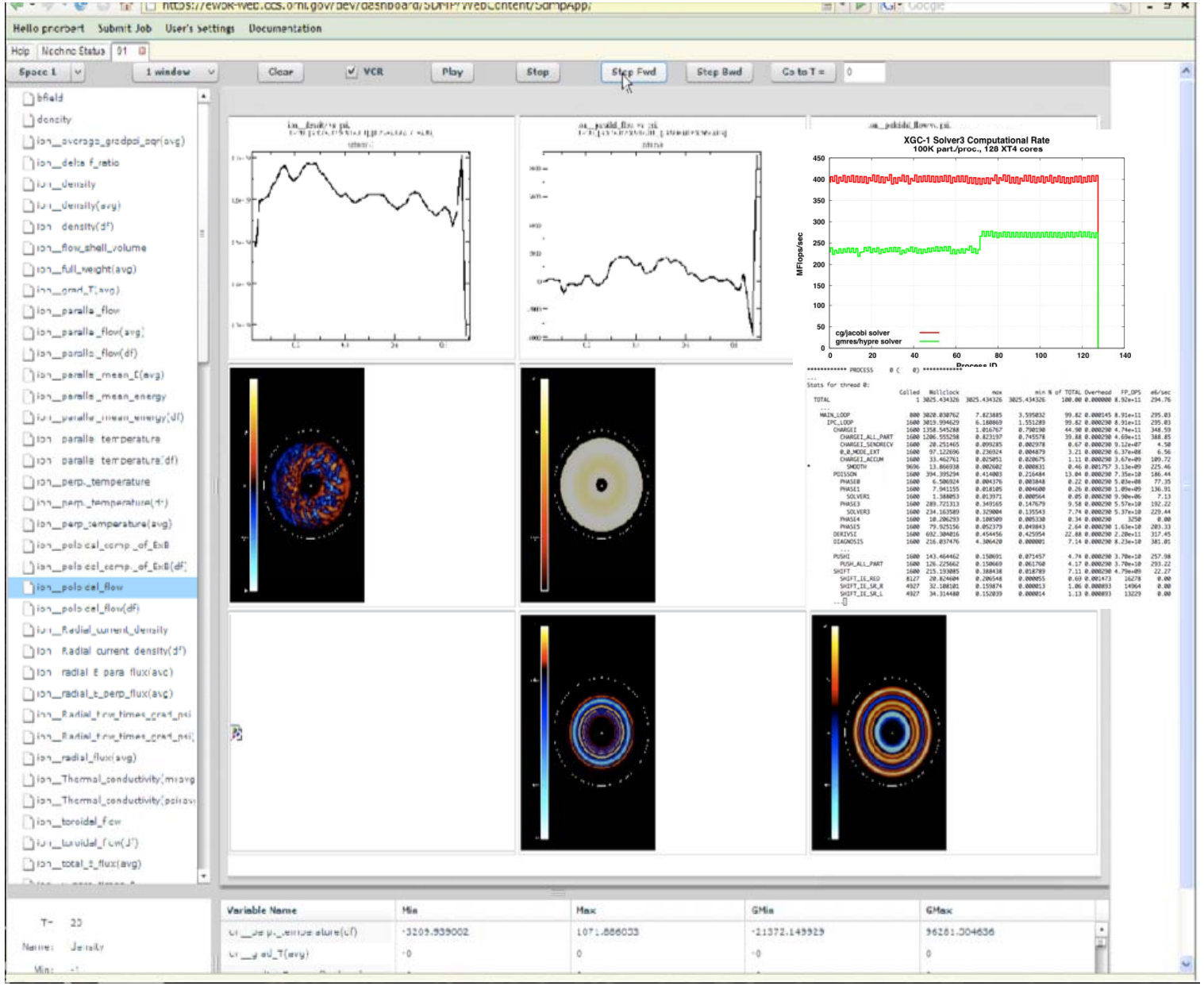
- Secure login
- Job submission and kill
- Search old jobs
- See collaborators jobs
- Annotations/Notes.
- Text display/movies.







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



User experiences with workflow and coupling

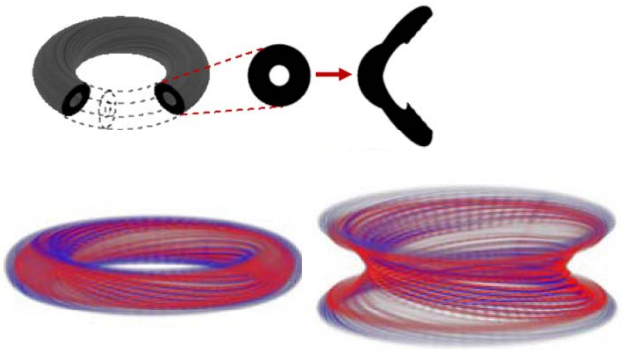
- Once tested & debugged, workflow scripts worked well
  - Monitoring is convenient and produces nice archive of results
  - Workflow produces logfiles, allowing user to review tasks that occurred during code coupling procedure and outcomes
- Basic code coupling scenario is now well tested
  - Improvements made to solver in M3D-OMP to produce higher-resolution equilibrium for ELITE stability analysis
  - Worked with ELITE developers to tune input parameters
  - Added output of peqdsk with density data to XGC0
  - Worked with M3D-MPP users to tune input parameters and improve code stability during nonlinear ELM simulation
- Full ELM cycle simulation takes 2-3 hours wallclock
- Complaints will only strengthen/harden our workflow/dashboard!

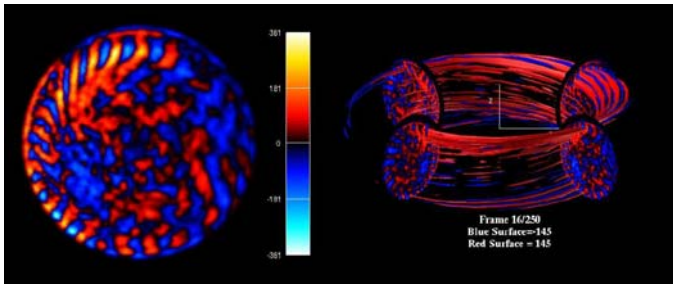
WAN Data Movement.

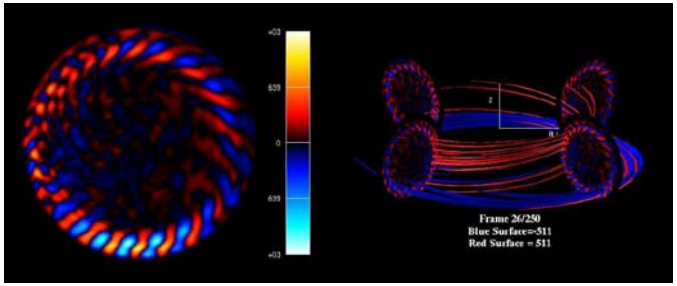
- On the dashboard, we keep track of the provenance.
- Users can point to a variable from a CPES simulation on the dashboard, and download the “raw” data to another mahcine.
- SRM-light manages all of the possible failures of moving the large data from one location to another.
  - Network failures
  - Disk failures (not enough disk space).

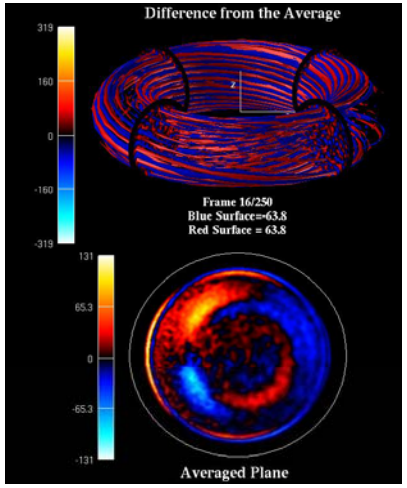
CPES Visualization

Shape Aware Visualization:
Interior wall view of 3D simulation

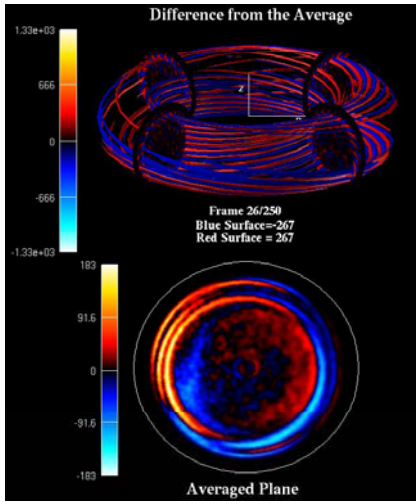


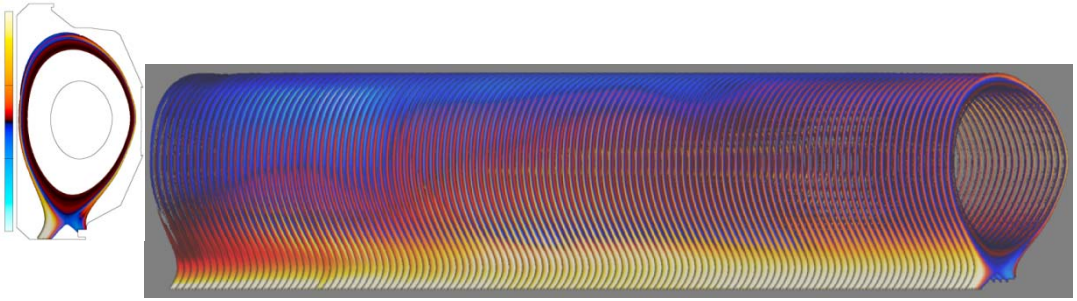






Average plane View:--average is subtracted from all planes





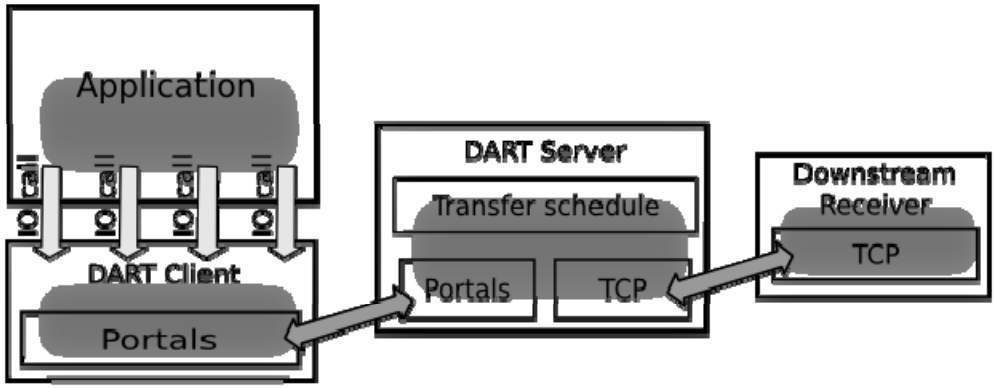
"Curtain Rod" View of 2D edge simulation

EFFIS Summary

- ✓ Physics Objects
- ✓ ADIOS
  - ✓ High Speed I/O.
  - ✓ DART is showing amazing low I/O overhead for IO
- ✓ Kepler workflow Automation.
  - ✓ Complex code coupling made easy
- ✓ Dashboard
  - ✓ Easy to use interface to monitor and annotate complex simulations.

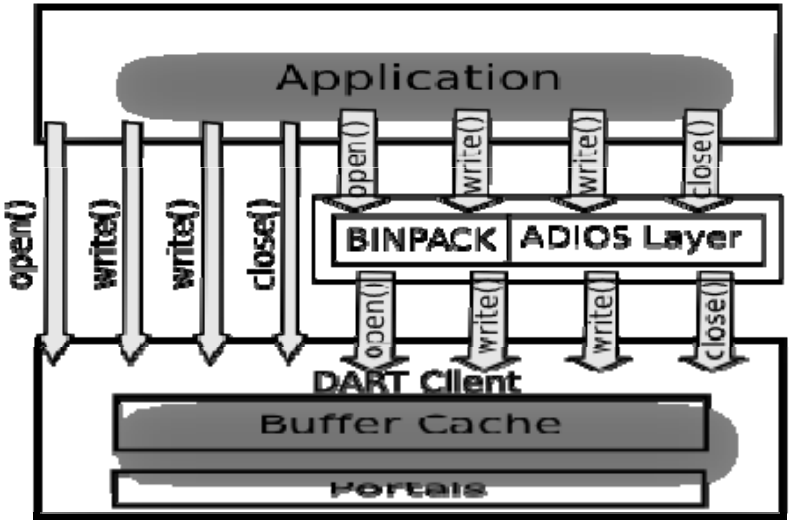
Technology transfer to other projects and fields are already in progress.

Asynchronous Data Transfer for CPES Simulations



- **XGC1 simulation on 1k nodes**
  - **transferred 380GB, in 3000sec with 5 sec spent in I/O - ~0.2% overhead**

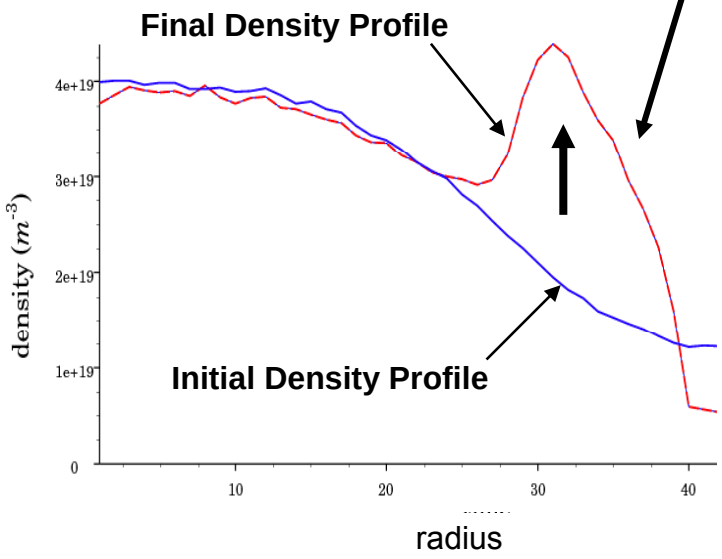
- DART Asynchronous IO Substrate
  - Objectives
    - Minimize IO time & overheads
    - Maximize data throughput
    - Minimize latency of data transfers
  - Approach
    - Asynchronously schedule IO operations to overlap with computations
    - Dynamically manage buffering and mapping of IO to service nodes
    - Build on RDMA and Portals



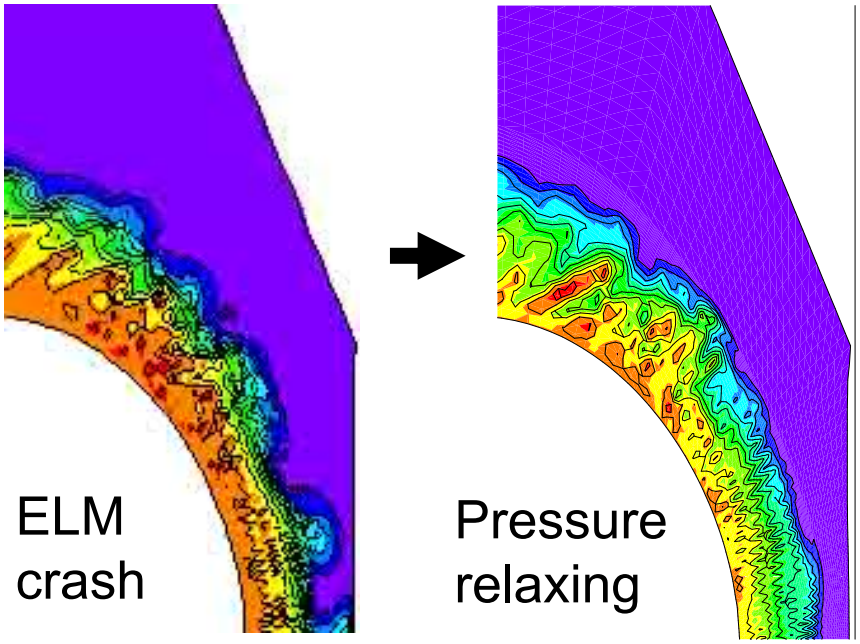
Coupled XGC0-MHD simulation of ELM cycle In EFFIS

Linear stability check (M3D-linear, Elite)

Pedestal buildup by XGC0



ELM crash by M3D (Nimrod)



Long term CPES Physics Goals

Through as much first principles simulations as possible, obtain predictive capability of

- L-H transition
- Pedestal growth and ELM cycle
- ELM control
- Edge rotation source
- Scrape-off and divertor physics (with impurities)
- Wall heat load
- Core-edge transport coupling (fluxes, pedestal height and rotation boundary condition)
- RF antenna effect on edge plasma
- Effect of core events on edge and heat load

Scientific Results reported at 2007 PSACI-PAC

XGC1 edge gyrokinetic code (full-f, 5D)

A full-f kinetic solution of plasma equilibrium across the separatrix (pedestal top to scrape-off), for the first time.

- Large scale convective cell with strong ExB sheared flow has been observed in the whole edge plasma, which may be related to turbulence suppression in H-mode.
- Strong edge rotation source has been observed, which can propagate inward by turbulence pinching (Hahm's analytic theory)

Electrostatic turbulence capability is under verification

XGC0 edge kinetic equilibrium code (mature)

- Full-f ions, electrons, neutrals, conserving collisions
- Verification reported at 2007 US-EU Transport Task Force Workshop
- Existing J_{Boot} formula works unless the density pedestal is very steep.
- Successfully simulated the density drop by Resonance Magnetic Perturbation (RMP), for the first time

GTC and GEM: preparatory exploration of edge turbulence.

PIC Noise problem is solved (reset, collisions)

Plasma surface interaction data are beginning to emerge

Long time kinetic simulation in XGC0

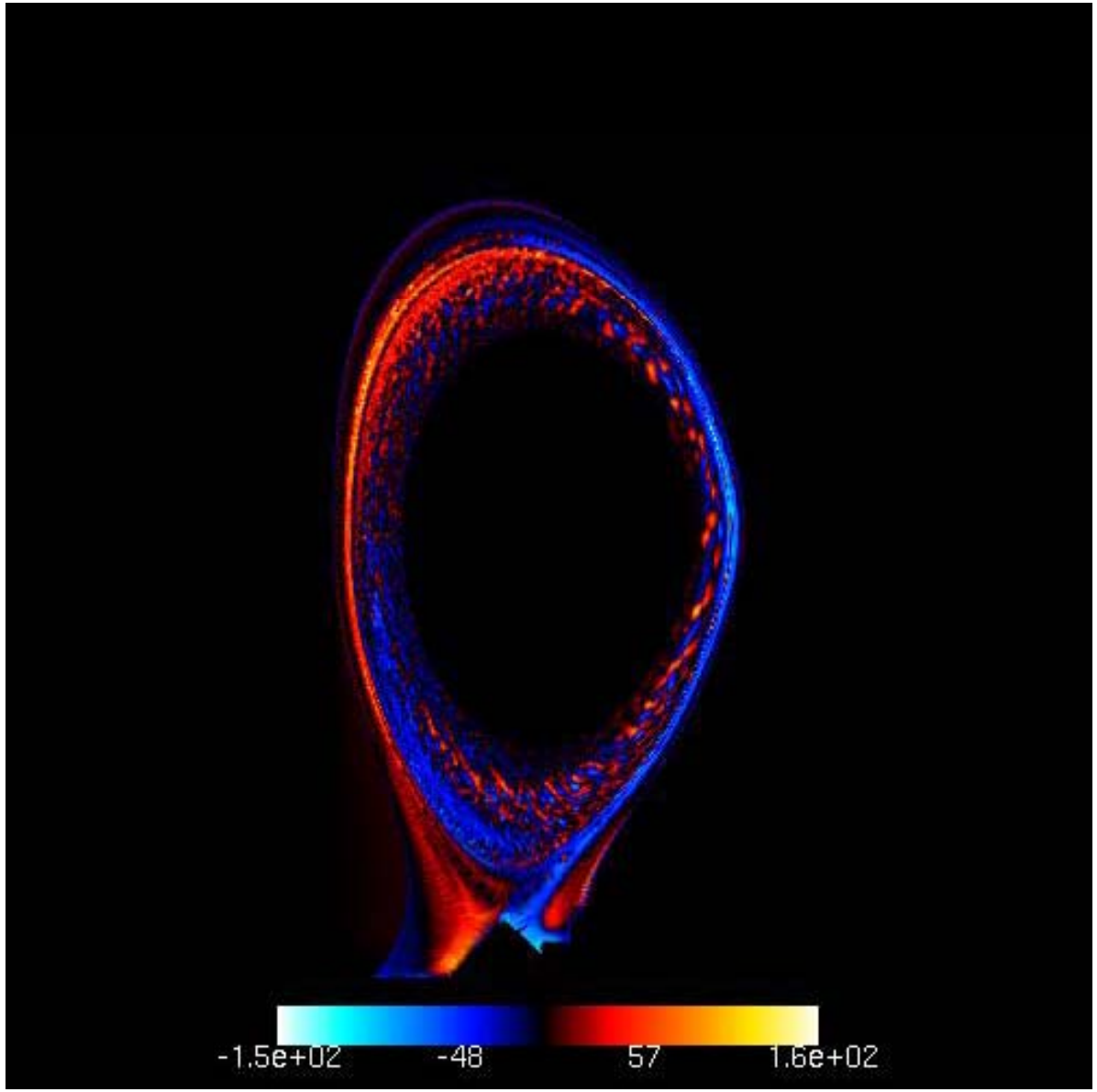
We have built (and demonstrated) our full-f gyrokinetic edge code XGC1 which can include the equilibrium kinetic physics [PoP, June 2008]. However, under the present computing capability, it is not reasonable to perform experimental time scale profile evolution in a gyrokinetic simulation.

We take a reduced kinetic model approach in XGC0 for the long time equilibrium evolution of plasma profiles.

- Evaluate the turbulence transport flux in XGC1
- Evolve the profile for Δt in the kinetic equilibrium code XGC0
- E_r and toroidal flow will be evaluated consistently with the profile evolution
- Evaluate again the turbulence transport flux in XGC1 using the new profile information, and repeat
- This is a stable "weak" coupling scheme, but the convergence with Δt is to be studied. The most efficient time marching scheme is to be investigated.

- At the present time, we use empirical diffusion coefficients (D, χ_e, χ_i), either validated by experiment or qualified by a turbulence code.

XGC1 finds that ITG turbulence exists globally in the whole pedestal when η_i >~ 3 at pedestal top.



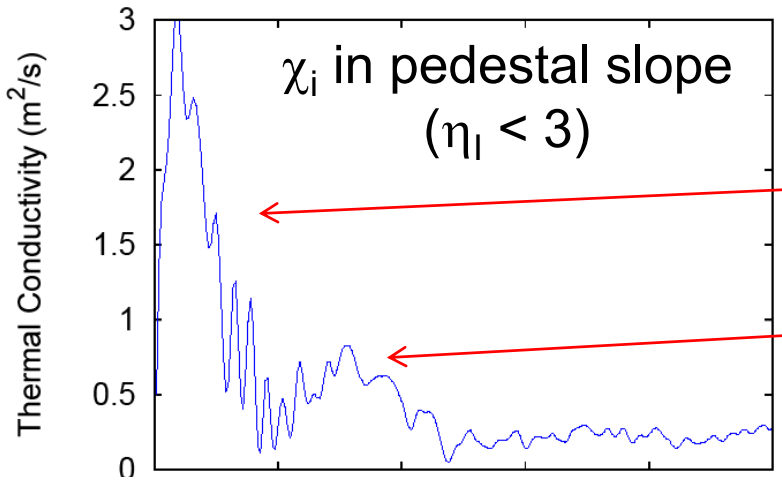
Movie of ITG turbulence in the real geometry (DIII-D) pedestal.

Full-f ions and adiabatic electron response to turbulence is used, while the background steady state is found from full-f electrons.

Zonal flows are assumed to be absent in the scrape-off region.

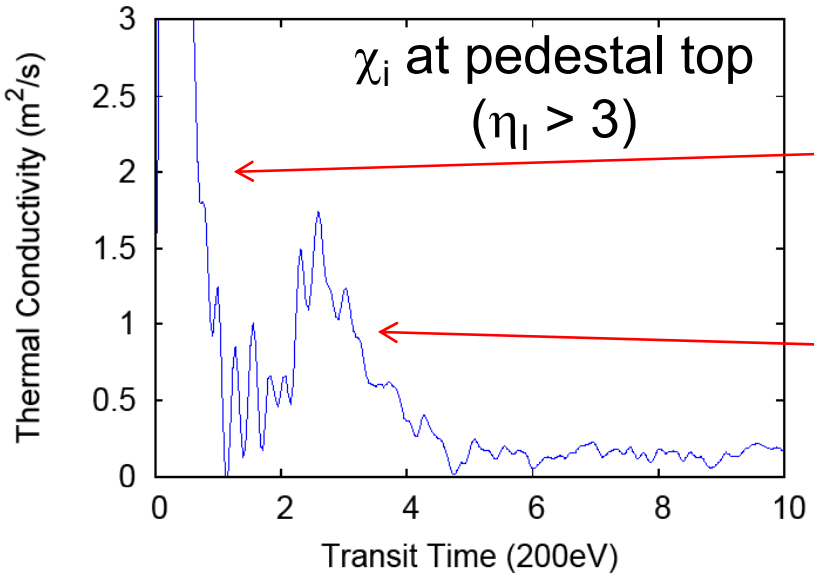
Ion thermal conductivity behavior in time

- Collisionless
- 3.2 billion particles (3,500 particles per node)



Neoclassical settling down

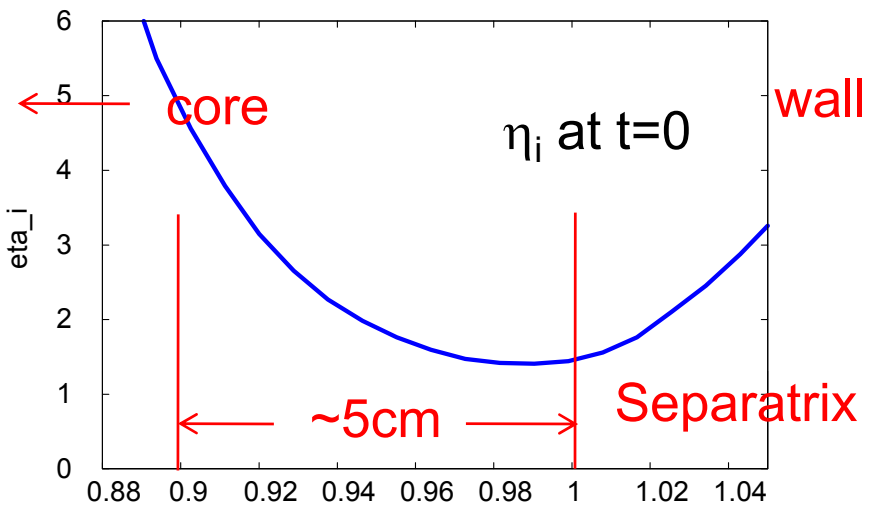
ITG growth and settling down

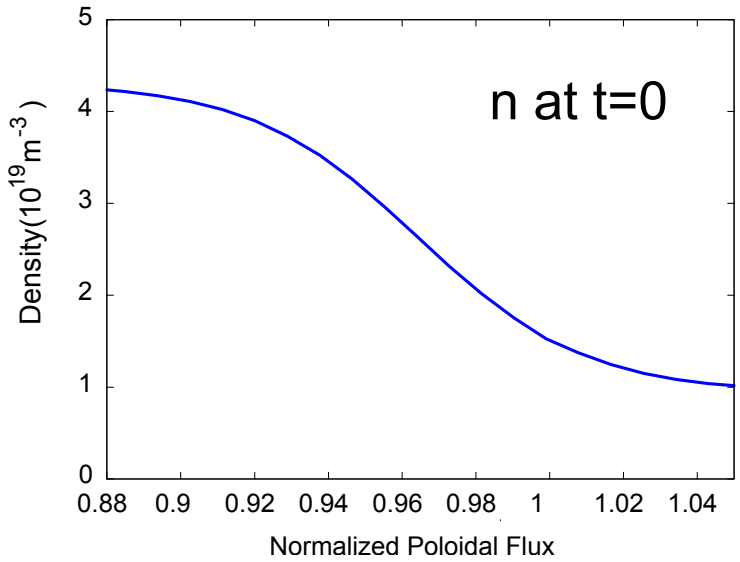


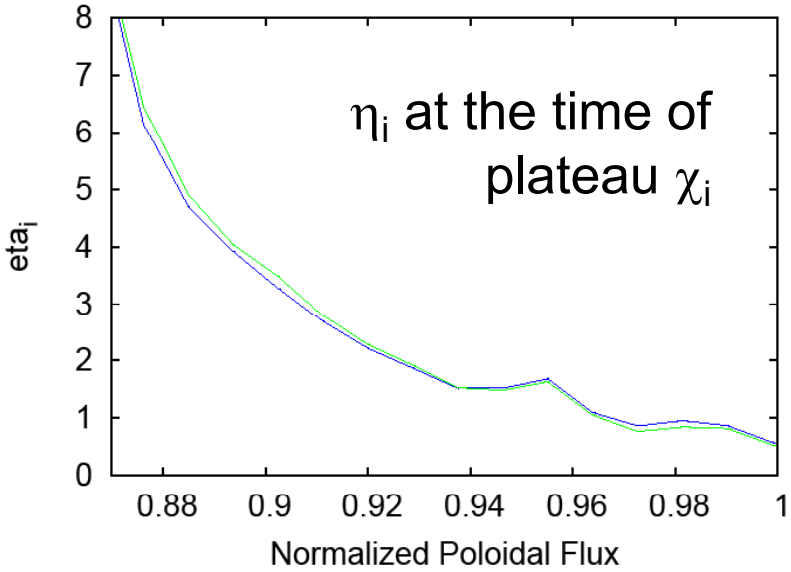
Neoclassical settling down

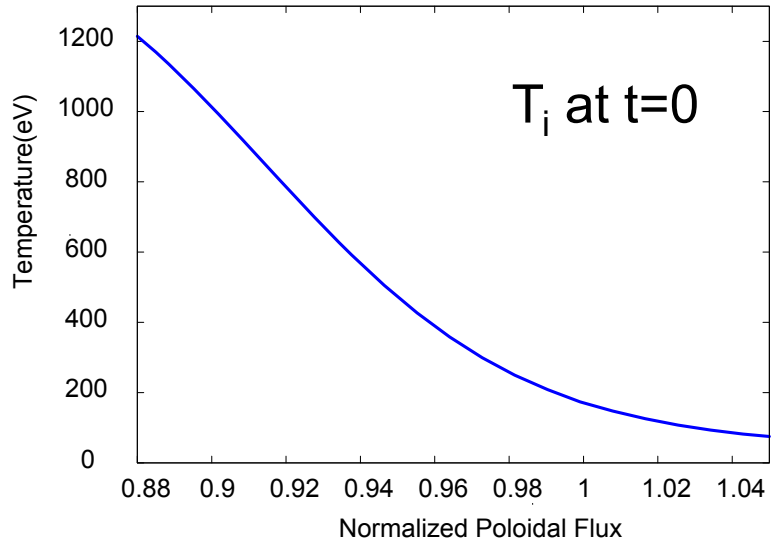
ITG growth and settling down

Plasma profiles

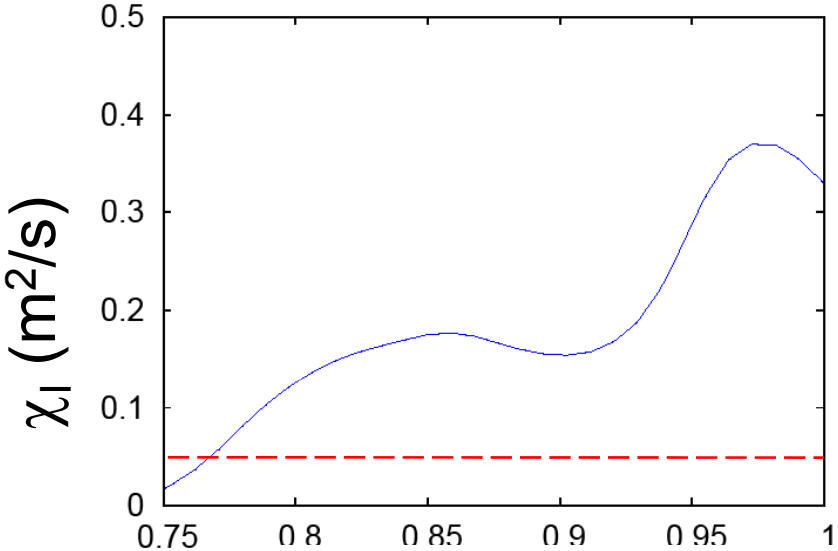




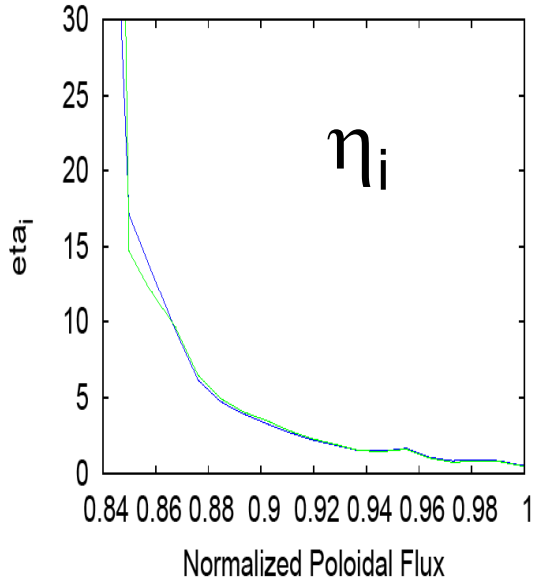




Ion thermal conductivity distribution in radius

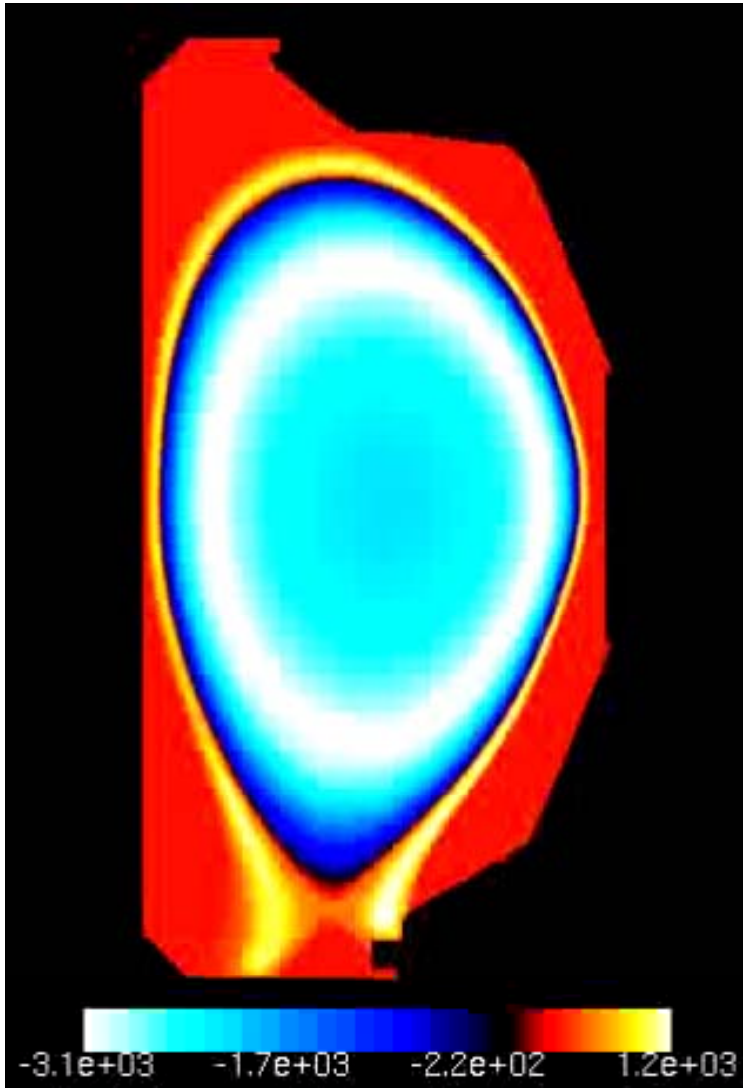


Noise level



We ran a case with η_i being kept below 1.5 at all radii, χ_I went down to noise level (~0.05 m^2/s)

GAM oscillations in the edge pedestal



- Nonlocal GAM oscillations over the whole pedestal
- $\omega_* \sim \omega_{GAM}$
- Nonlocal spread of turbulence energy by GAM is to be investigated.

Movie of Axisymmetric, flux surface averaged potential dynamics

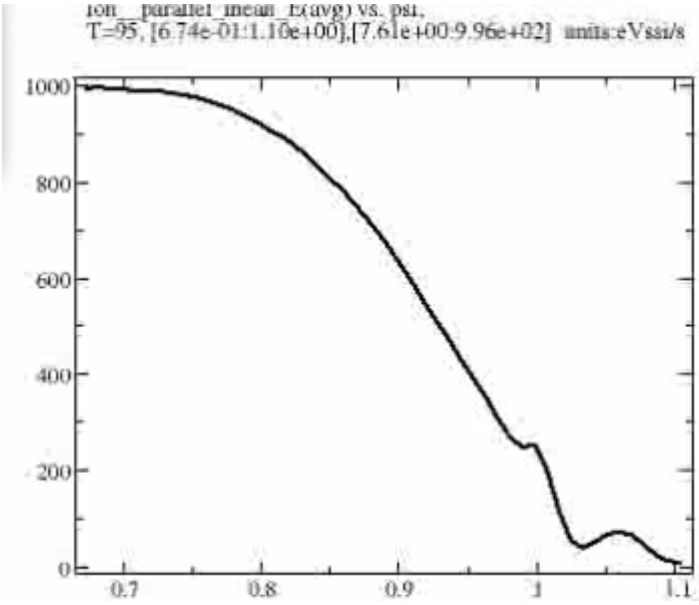
New Physics in the new territory:
A localized turbulence concept questionable in edge.

- Nonlocal interaction of edge kinetic physics with turbulence
  - Nonlocal GAM interaction with turbulence
  - Finite orbit-width mixing of turbulent energy
  - Interaction of nonlocal turbulence energy with strong equilibrium gradient through the finite orbit-width
  - Easier mean field generation and interaction
  - Sensitive response of squeezed neoclassical polarization dynamics to mean field
  - Easier distortion from the conventional neoclassical pressure isotropy → Turbulence-neoclassical Reynolds stress and radial momentum transport

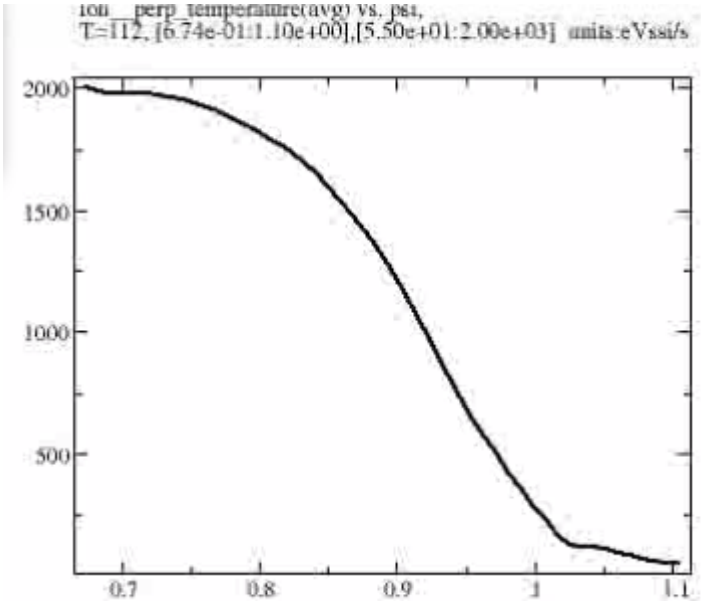
  Radial turbulence dynamics is compressed into these non-local kinetic range
- Magnetic separatrix seems to play a compressional role → blob penetration through separatrix wall by non-adiabatic electron respose?

Preliminary evidence for mean flow interaction across the separatrix

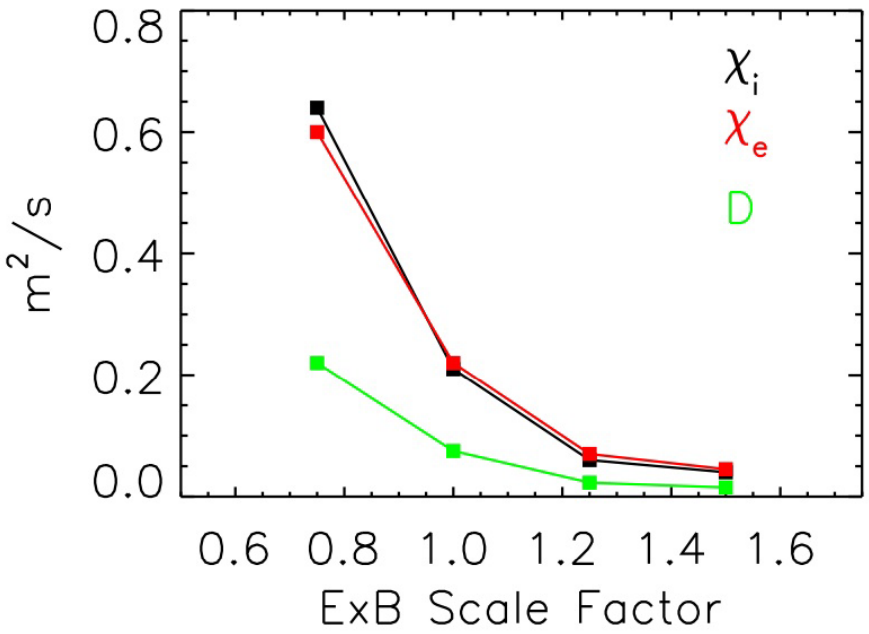
Ion parallel kinetic energy



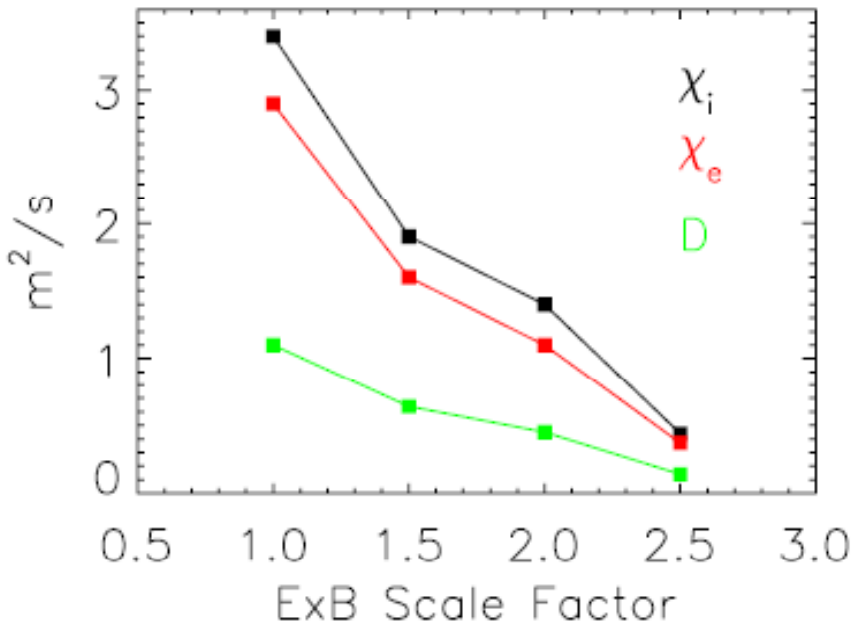
Ion perpendicular kinetic energy



Manually coupled GEM-XGC0 simulation of finite beta turbulence in an edge-like pedestal



Electrostatic transport coefficients versus scaled shearing rate.



Electromagnetic transport coefficients versus scaled shearing rate.

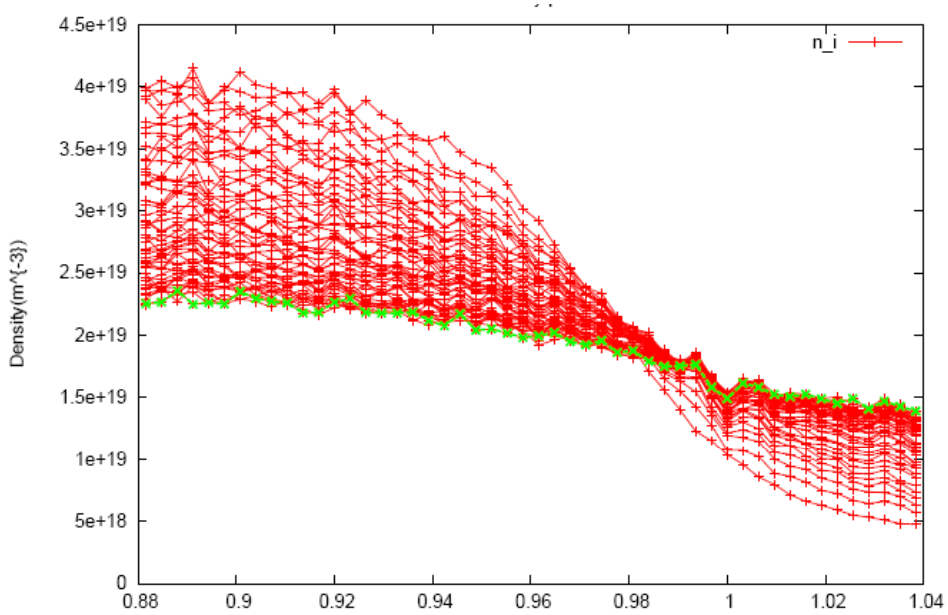
A scale factor of one corresponds to the shearing rate determined by XGC0.

Manually coupled GEM-XGC0 simulation of finite beta turbulence in an edge-like pedestal

1. Build up a mild edge pedestal in XGC0 (using DIII-D geometry) with a small anomalous χ_I, χ_e, and D until a reasonably acceptable profile shape is reached, then stop.
2. Export the n, T_i, T_e, E_r, q profiles and the flux surface shape information to GEM electromagnetic delta-f turbulence code
3. GEM uses analytic Miller geometry to create the pedestal with similar profiles and flux surface shape, but without the separatrix.
4. The GEM calculated turbulent transport coefficients are imported back into XGC0 and watch further pedestal behavior.

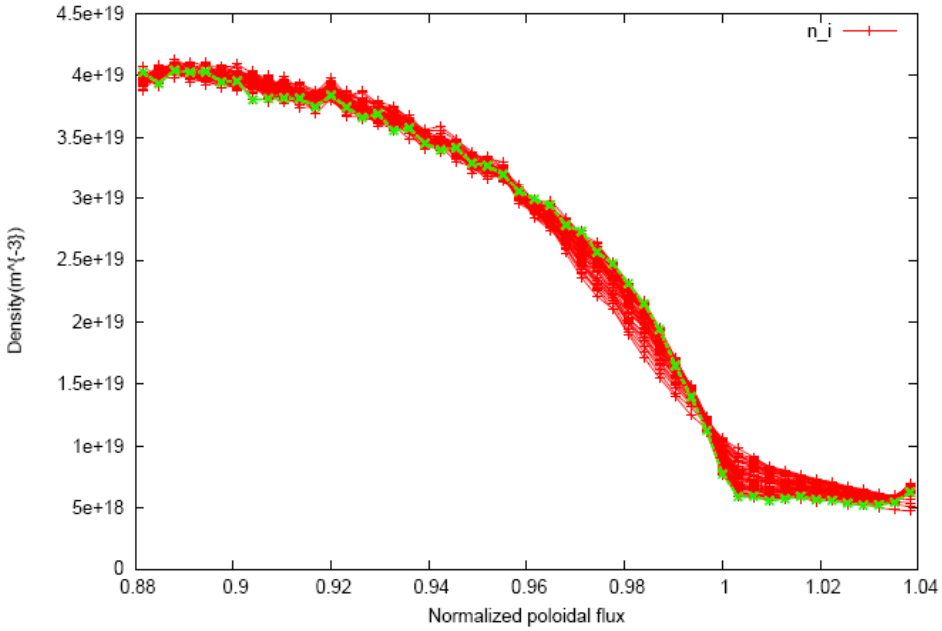
- **Electromagnetic** turbulent transport coefficients could not support the pedestal → Over estimated transport coefficients
- **Electrostatic** turbulent transport coefficient gave a healthy pedestal buildup to an experimental level.

Density pedestal behavior in XGC0 using the GEM-evaluated Electromagnetic diffusion coefficient.



Density pedestal behavior in XGC0 using the GEM-evaluated Electrostatic diffusion coefficient.

6MW of heat flux from core and 100% neutral recycling is used.



Manually coupled GEM-XGC0 simulation of finite beta turbulence in an edge-like pedestal (3)

Electromagnetic turbulence contains more complete physics than the electrostatic turbulence does.

Then why does the electrostatic estimate give a better result?
Is this an indication that the separatrix alters the turbulent transport physics significantly?

The answer is to be found by importing the GEM split weight kinetic electron technique into XGC1 (summer 2008 plan).

A cross verification with GTC is needed.

Roles of Applied Math in CPES

- "Service role"
  - Incorporating already mature techniques and software, developed for general users, into CPES codes
  - Natural and primary type of applied math contribution in CPES and throughout FSP & SciDAC, e.g., for CPES:
    - algebraic multigrid in potential and potential-like solves
    - higher-order temporal integration for particle dynamics
    - construction of conservative, nonnegative velocity pdfs from particles
  - As a result, the kernels of CPES are near state-of-art for most tasks, in terms of software: Triangle, Zoltan, PETSc, hypre, etc.
- Physics-driven research innovation
  - Finding original research directions from challenges that arise solely because of CPES collaborations
  - This part is increasing, as mutual understanding develops
    - integral-equation based evaluation of Rosenbluth potentials
    - accuracy and stability vs. complexity tradeoffs in code coupling
    - projective temporal integration for multiscale problems
  - CPES may benefit from a higher-level integration of components, or even reformulation of mathematical models, e.g., skipping the mesh in particle codes through kernel-free fast multipole methods

Applied math accomplishments, plans

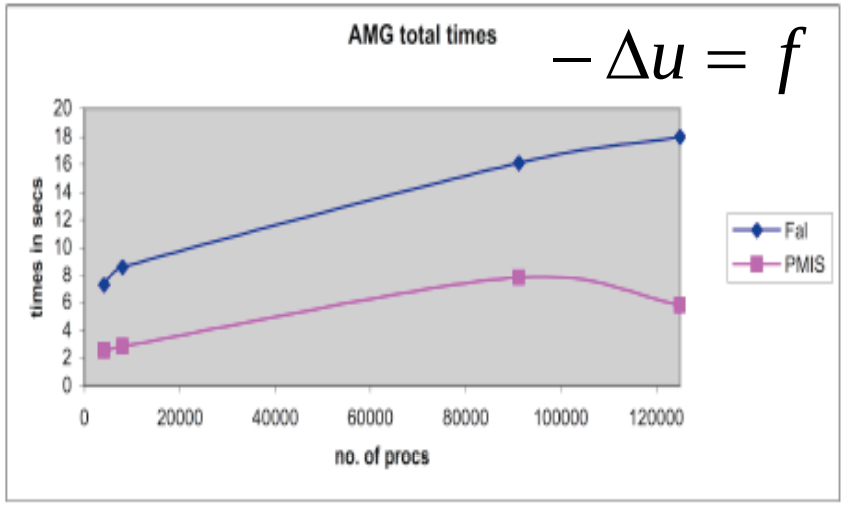
- Unstructured (poloidal crossplane) grid generation
- Potential solves
  - grid-based
  - fast multipole method (FMM)-based
- Time integration of multirate problems
  - conventional single-model (R-K, Adams-based P-C, implicit)
  - multiscale model (projective integration)
- Conversion between representations and data structures
  - particles to conservative, nonnegative probability density functions
  - mapping of particles to grid elements
  - accurate electric fields from potentials on unstructured meshes
- Code verification by means of manufactured solutions
- Multiscale coupling of equilibrium evolution and turbulent transport
- Efficiency algorithms on advanced-architecture computers

Solvers *are* scaling:

algebraic multigrid (AMG) on BG/L (hypre)

- **Algebraic multigrid a key algorithmic technology**
  - **Discrete operator defined for finest grid by the application, itself, *and* for many recursively derived levels with successively fewer degrees of freedom, for solver purposes**
  - **Unlike geometric multigrid, AMG not restricted to problems with "natural" coarsenings derived from grid alone**
- **Optimality (cost per cycle) intimately tied to the ability to coarsen aggressively**
- **Convergence scalability (number of cycles) and parallel efficiency also sensitive to rate of coarsening**

- **While much research and development remains, multigrid will clearly be practical at BG/P-scale concurrency**



7-pt Laplacian, total execution time, AMG-CG, total problem size ~2 billion

Figure shows weak scaling result for AMG out to 120K processors, with one 25×25×25block per processor (up to 1.875B dofs)

U. M. Yang, LLNL

CPES Physics Research Roadmap, Schedule, Achievement

	Pre-CPES	2006	2007	2008	2009	2010
Edge Kinetic code	XGC0, Full-f ions with 1D E_r solver	**XGC1, Full-f ions & electrons, 2D solver (E_r, E_θ) + 1D solver parallel to B**	**XGC1, Full-f, electrostatic turbulence in the entire edge**		XGC2, full-f E&M edge Turbulence code	
			XGC0-MHD ELM cycle			Develop coupling to core code
			Enhance XGC0 with Electrons,	**Multiscale XGC0-XGC1 coupling**	Develop Multiscale XGC0-XGC2 Integration framework	
		DEGAS2 into XGC, update atomic data →				
Physics	First 1D neoclassical ion edge solution, with pedestal buildup by neutrals	**First 2D neoclassical kinetic solution in the entire edge**	**Edge E_r & Rotation. Nonlinear ELM**	**Electrostatic turbulence and L-H transition**	**• RMP & ripple**	
				Study pedestal-ELM cycle with concurrent turbulence transport		E&M turbulence, Core-edge coupled physics

What is the science enabled by maximum number of CPUs used, efficiency?

1. We have used up to 16,384 processor cores and up to 3.3B particles to enable the first gyrokinetic turbulence simulation in the real geometry edge.
2. Routine test runs use 8,000 cores and 1B particles.
3. Efficiency was about 7% in early 2007 (XGC1 is a particle code).

How much did XGC1 use the high performance computing time?

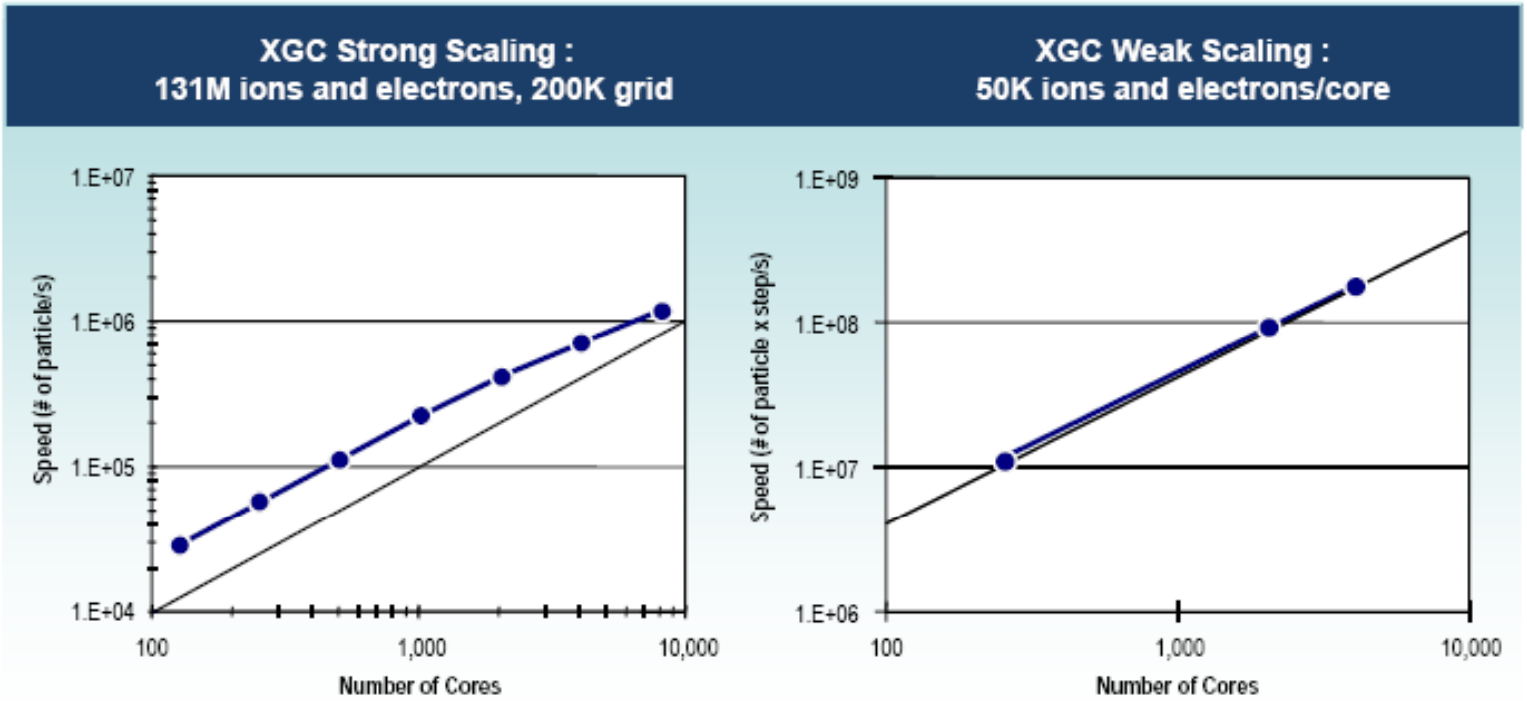
In the last 12 months period, XGC1 used ~ 2M XT4 hours on Jaguar and ~5M hrs on Franklin. Getting time has been a struggle.

Since XGC1 is maturing, we expect factor 3-10 increase in HPC usage in the next 12 months period.

XGC edge particle code shows excellent HPC scaling

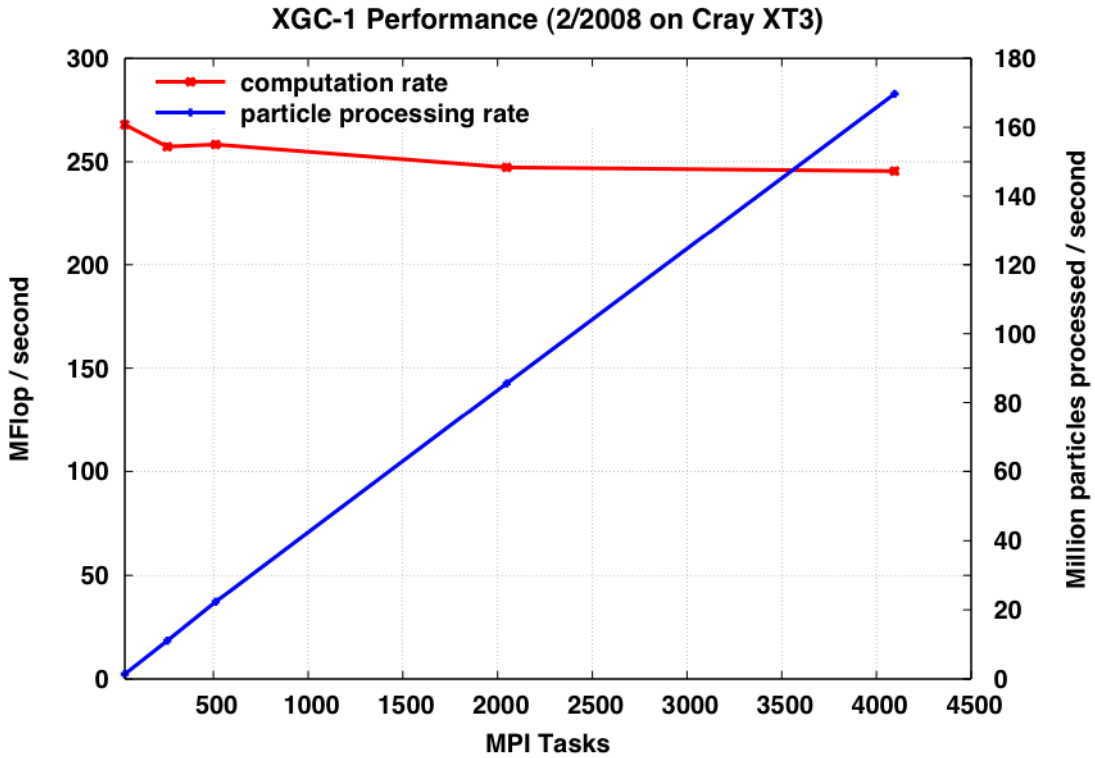
- Since XGC is a full-function code, it demands much more HPC resource than a perturbed-function code (factor of >100).
- Office of Science ‘s computing plan can enable simulation for the whole edge physics in ITER.

Jaguar requirement for one run: 20,000 processors X 20 hrs =0.4 M hrs



Spring 2007

Recent PERI analysis of XGC1 HPC performance



XGC1 performance data from recent benchmark experiments on the Cray XT3 at Oak Ridge National Laboratory. Performance scalability is excellent when keeping the number of particles per MPI task fixed as the number of tasks increases.

Education and Training in CPES

5 postdocs and 17 gradate students
(+ 3 foreign students)

- 17 graduate students; 6 in physics, 9 in computer science, and 2 in applied mathematics.
- 5 postocs; 2 in physics and 3 in computer sciences

CPES Meetings since last PSACI review

- 2007 Fall meeting: December 3-5, ORNL
- 2008 Spring meeting: March 29-30, Boulder, CO

Dissemination of CPES research

Conferences/workshops represented by PI in a year: 12

Summary

- We are in schedule (some items are ahead of schedule)
- XGC0 is becoming mature. Active experimental validation is in progress
- XGC1 has produced electrostatic ITG turbulence in real geometry edge, will move into electromagnetic regime soon.
- HPC availability to XGC1 is essential for further progress.
- Active collaborations with other centers are essential.
- Validation activities with domestic and international collaborators will expand (presently DIII-D, NSTX, JET; to include CMOD and ITPA-ITER).