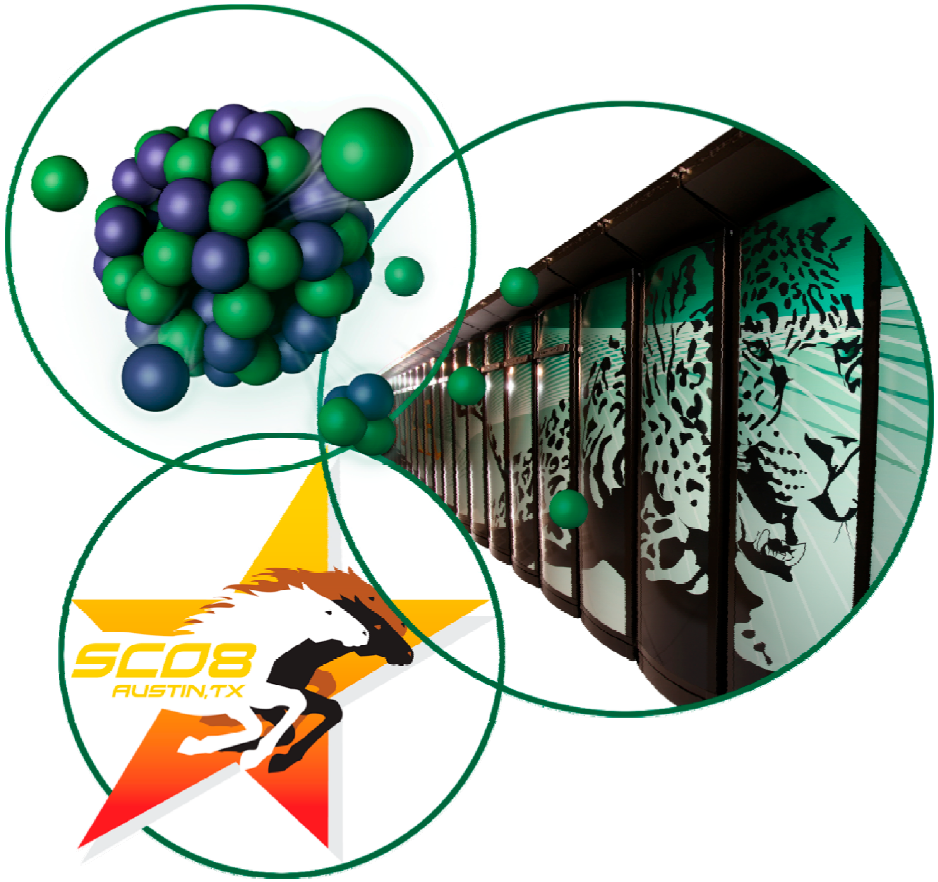
CPES: Toward a First-Principles Integrated Simulation of Tokamak Edge Plasmas



Presented by

Scott A. Klasky

Scientific Computing
National Center for Computational Sciences

On behalf of

SciDAC FSP Prototype
Center for Plasma Edge Simulation

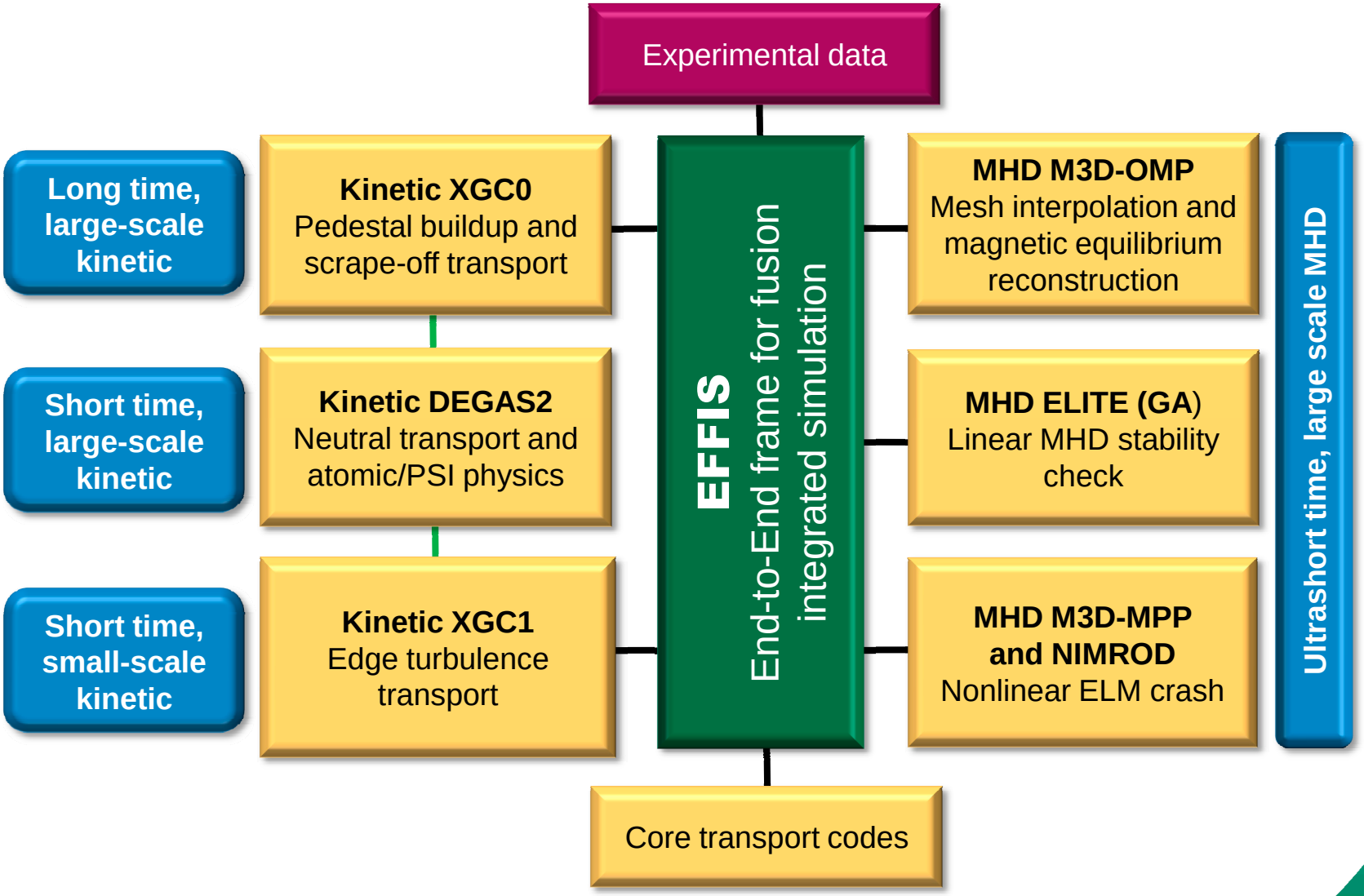
CPES
A collaborative effort by

- Three SciDAC enabling technology centers and institutes
  - SDM (A. Shoshani)
  - TOPS (D. Keyes)
  - PERI (P. Worley)
- One DOE-OASCR laboratory
  - CMCL (L. Greengard)
- Two SciDAC fusion centers
  - GPS-TTBP (Z. Lin, T.S. Hahm, P. Diamond consultant)
  - CEMM (H. Strauss, L. Sugiyama)
- Three national laboratories, 11 universities, and 1 private-sector institution
  - PPPL, ORNL, LBNL
  - Caltech, Colorado, Columbia, Georgia Tech, Lehigh, MIT, NYU, Rutgers, UCI, UC−Davis, Auburn
  - Hinton Associates

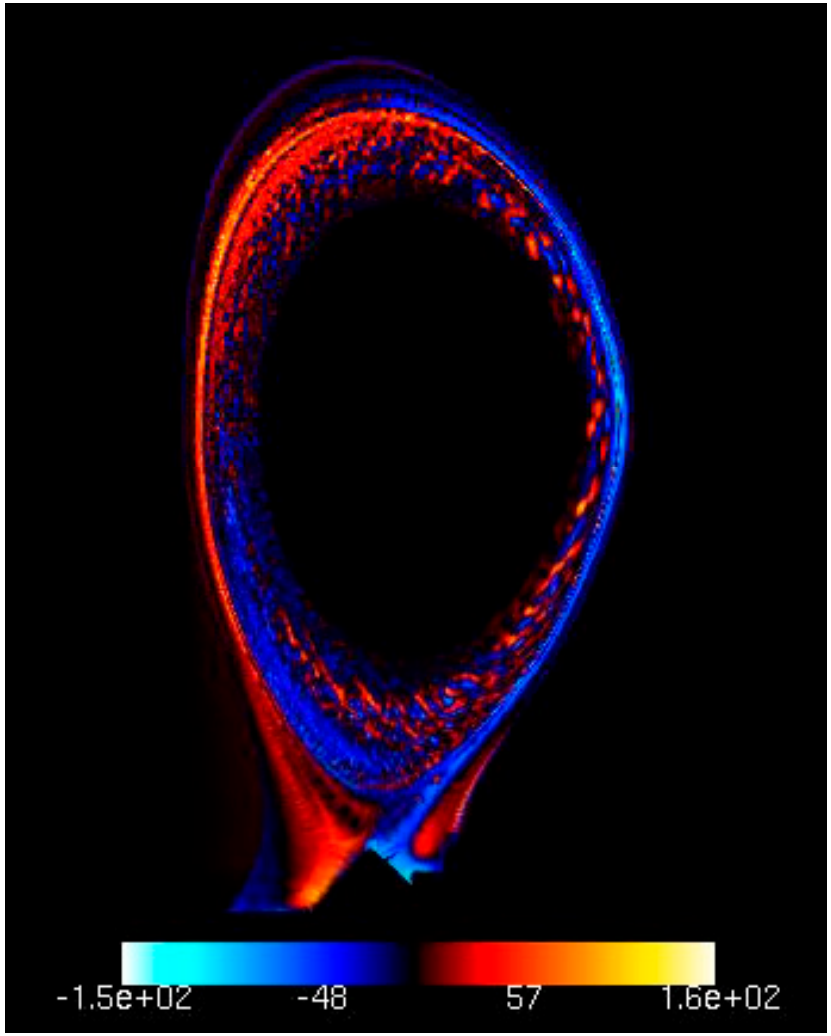
Executive summary of the XGC codes

- Particle-in-cell with 5D Lagrangian equation of motion
- Full-f (conventional PIC) ion, electron, and neutral particles
- Numerical edge geometry (realistic X-point and wall)
- Particle-momentum-energy-conserving collisions
- Heat, particle, and momentum flux from core plasma
- Neutral Monte Carlo particles with wall recycling
- Excellent scalability with number of processors
- XGC1 and XGC0
  - XGC1 for edge turbulence (together with neoclassical background)
  - XGC0 for equilibrium evolution: 1D radial grid; reduction in grid and particle number, and enhancement in Δt leads to $>10^3$ reduction in computing time.

Multiscale edge physics simulation in CPES



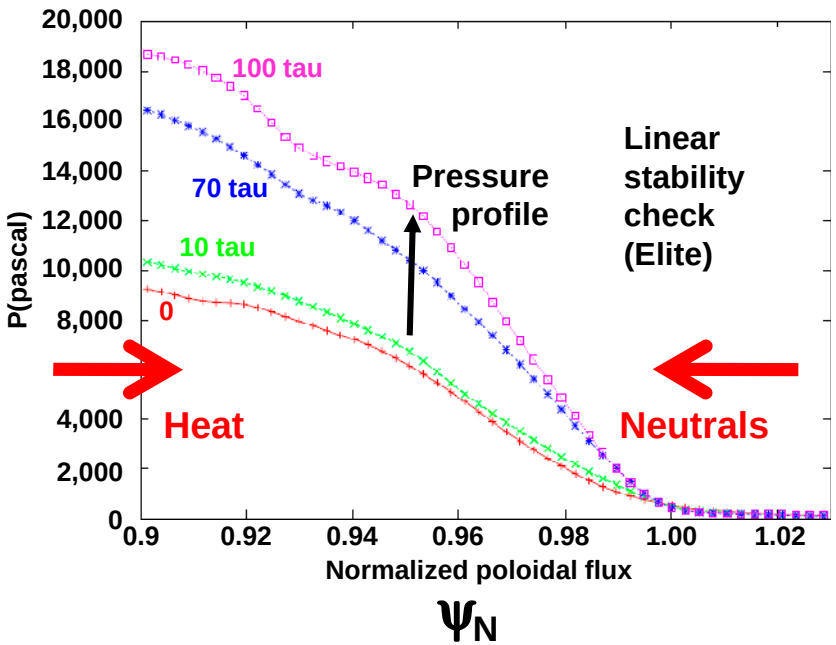
Full-f XGC1 finds ITG turbulence in the pretransition L-mode pedestal



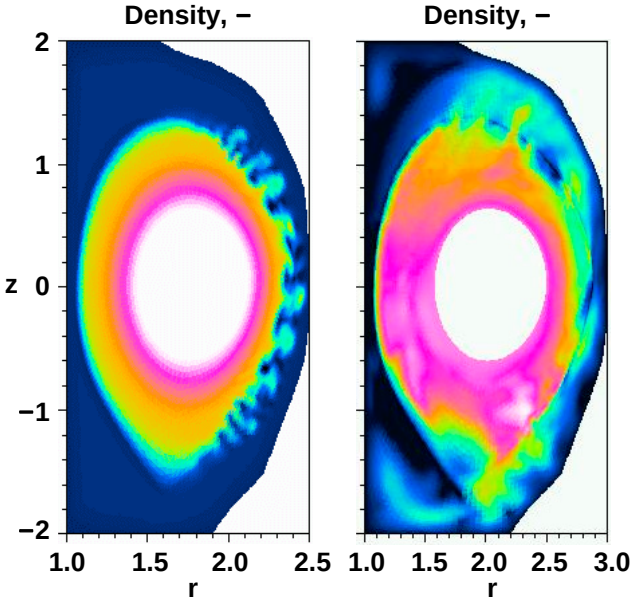
- Real geometry (DIII-D)
- Full-f ions and adiabatic electron response to turbulence, initialized with a quasi-steady state obtained from full-f electrons
- 3.2B particles on 8,192 cores for ~10 hours

Coupled XGC0-Elite-M3D simulation of ELM cycle in automated EFFIS

Pedestal buildup in XGC0 with B-reconstruction by M3D-omp



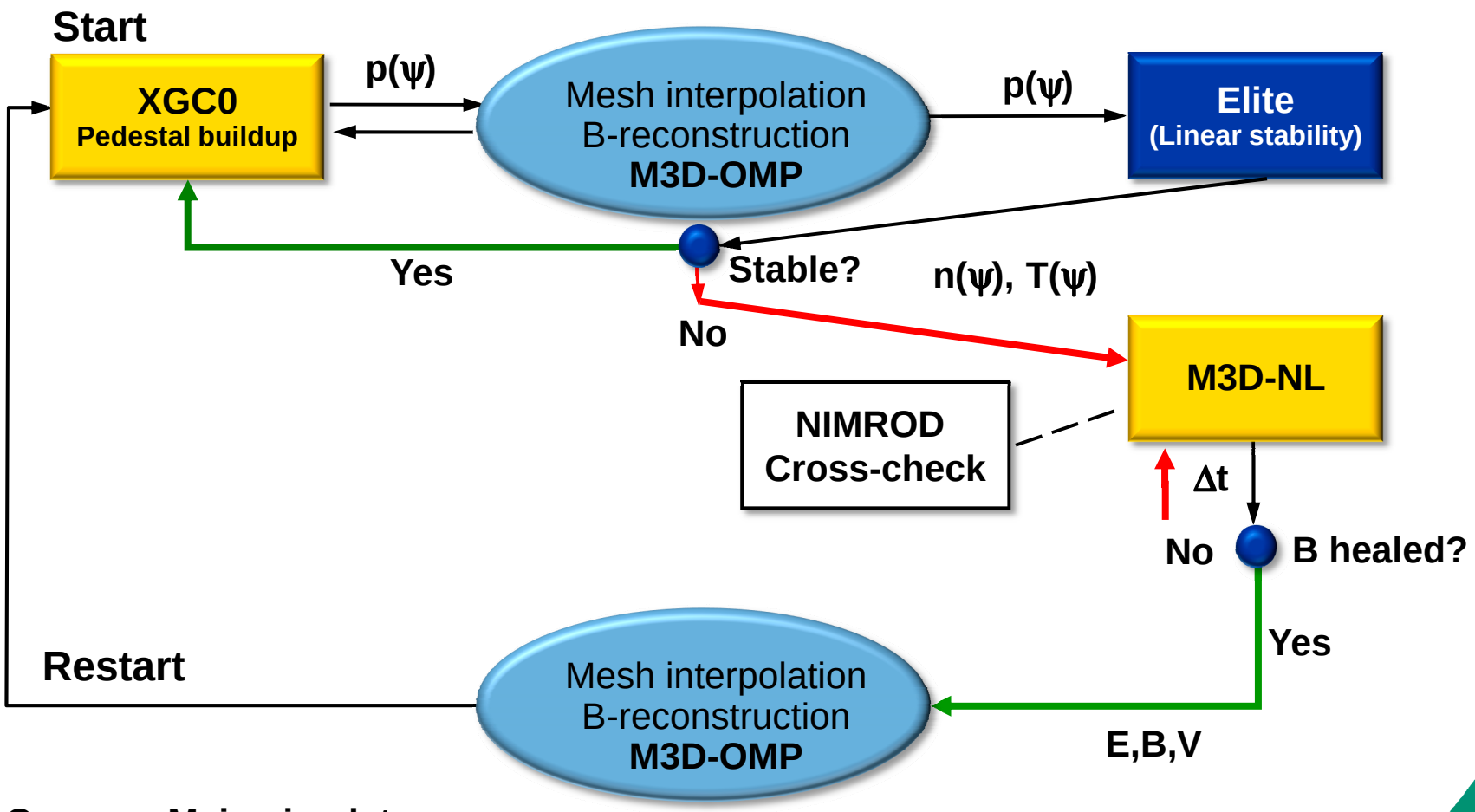
ELM density crash to relaxation in resistive M3D



T=76 saturation

T = 496 relaxation

Current EFFIS automated workflow between XGC0, M3D-OMP, Elite and M3D-MPP



Orange : Main simulator

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 and electrons, 2D solver (E_r, E_θ) + 1D solver parallel to B

XGC1, Full-f, electrostatic turbulence in the entire edge

XGC0-MHD ELM cycle

XGC2, full-f E&M edge turbulence code

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 and rotation, nonlinear ELM

Electrostatic turbulence and L-H transition

RMP and ripple

Study pedestal-ELM cycle with concurrent turbulent transport

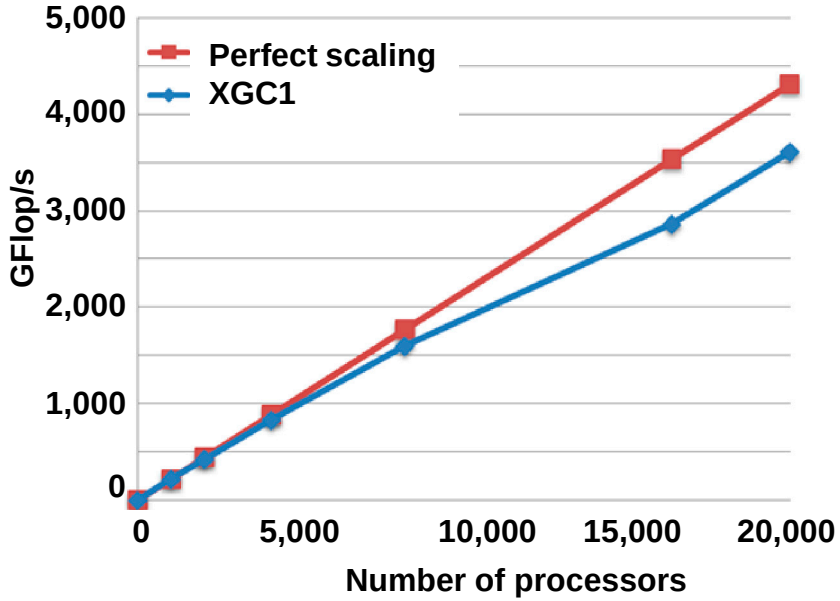
E&M turbulence, core-edge coupled physics

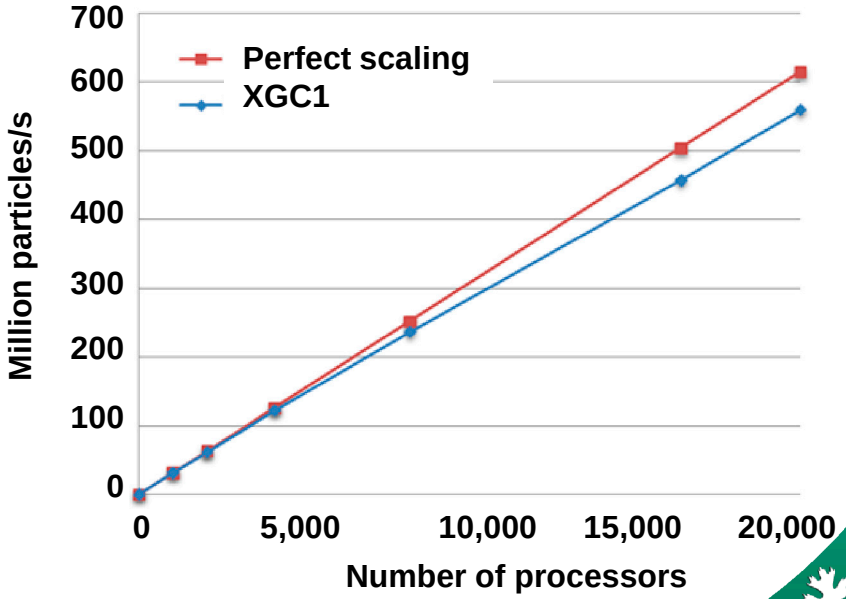
Oak Ridge National Laboratory

XGC1 edge particle code shows excellent HPC scaling

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

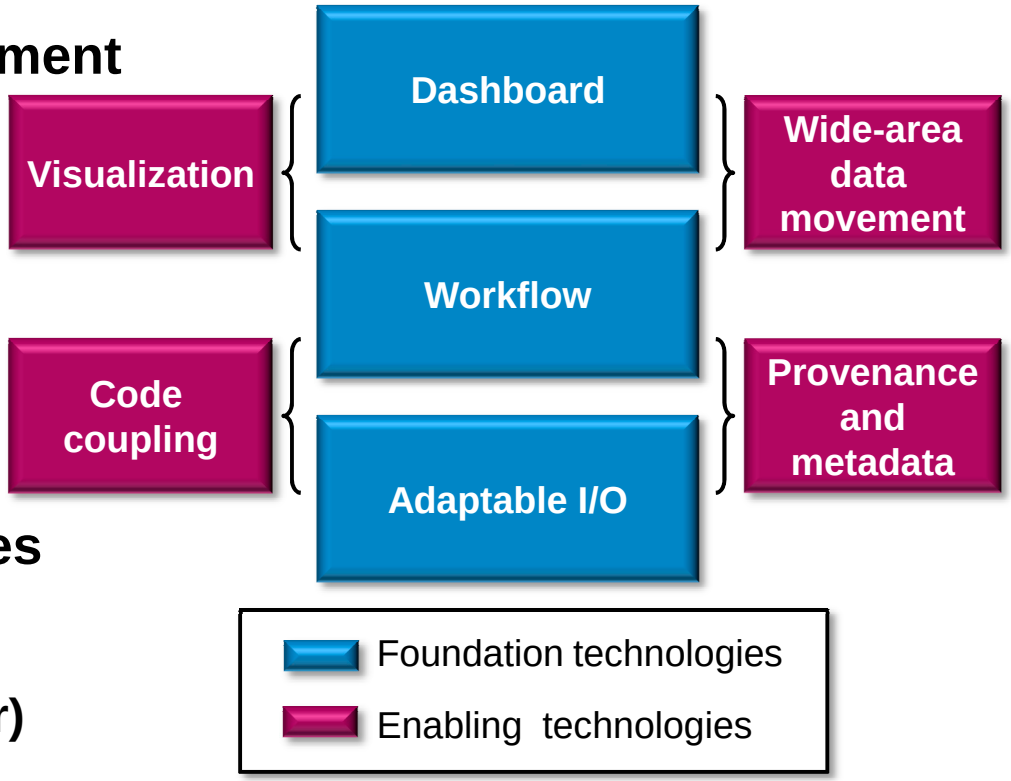
Weak scaling graph of XGC1 Jaguar, 100K ptl/proc, core full-f simulation





EFFIS: End-to-end framework for fusion integrated simulation

- From Scientific Data Management (SDM) Center*
  - Workflow engine – Kepler
  - Provenance support
  - Wide-area data movement
- From universities
  - Code coupling (Rutgers)
  - Visualization (Rutgers)
- Newly developed technologies
  - Adaptable I/O (ADIOS) (with Georgia Tech)
  - Dashboard (with SDM Center)

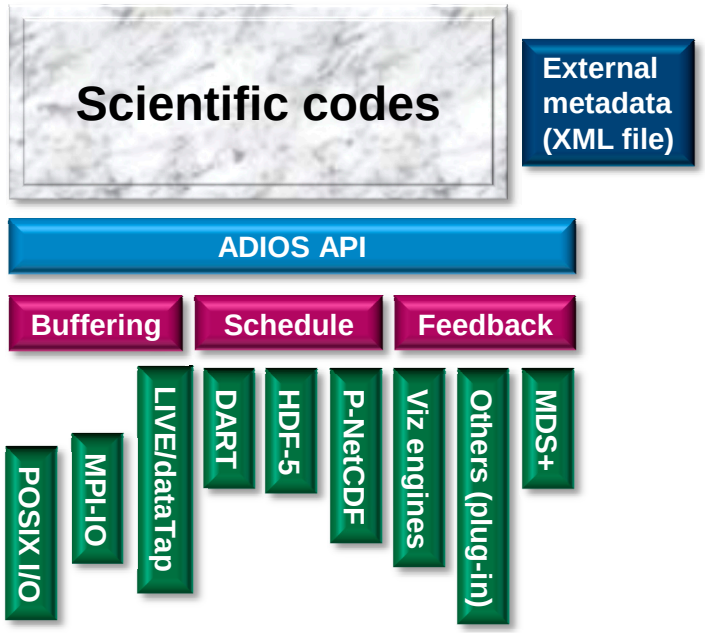


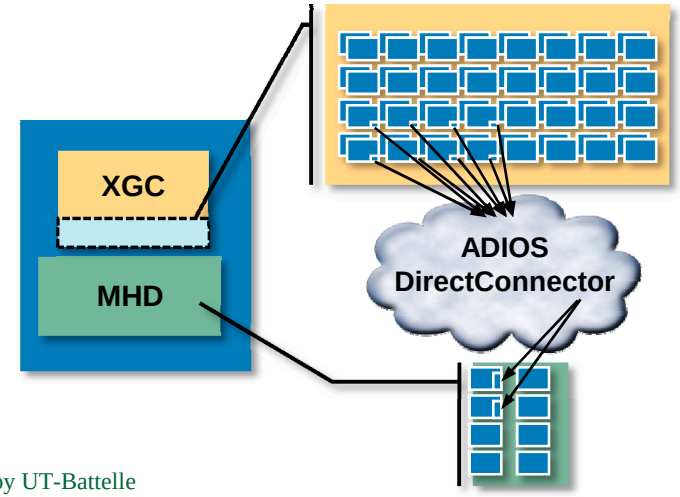
Approach: Place highly annotated, fast, easy-to-use I/O methods in the code, which can be monitored and controlled; have a workflow engine record all of the information; visualize this on a dashboard; move desired data to the user's site; and have everything reported to a database

* Institutions involved: LBNL, NCSU, ORNL, SDSC, UC-Davis, U. Utah

ADIOS: Adaptable I/O System

- 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
- Componentization
  - No need to worry about I/O implementation
  - Components for I/O transport methods, buffering, scheduling, and eventually feedback mechanisms
- Change I/O method by changing XML file only!



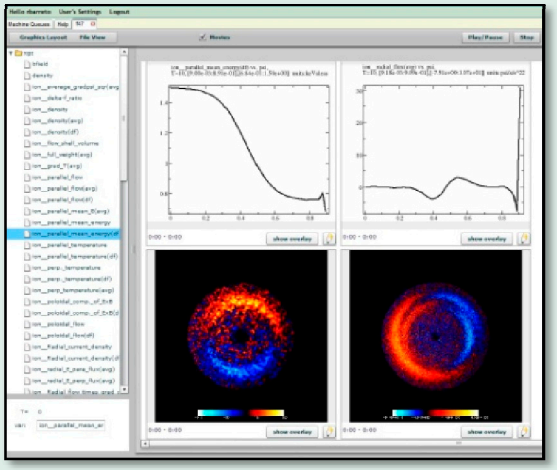


- ADIOS DirectConnect leverages the existing file-based code coupling
- Provides optimizations for the M-to-N array remapping

Monitoring and coupling fusion codes with Kepler workflow engine for full ELM, multicycles

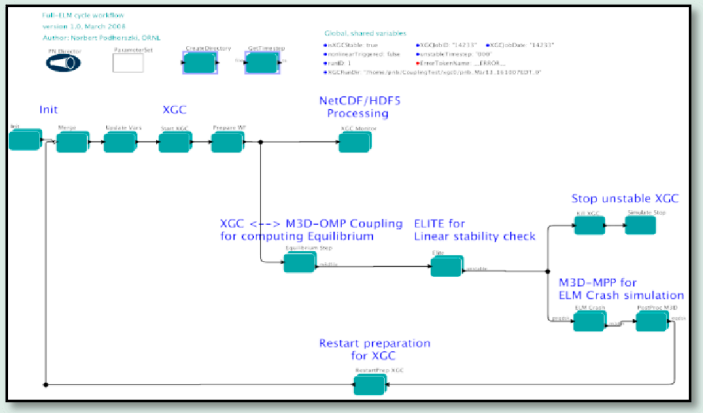
Monitoring

- NetCDF files
  - Transfer files to e2e system on the fly
  - Generate images using Grace library
  - Archive NetCDF files at 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



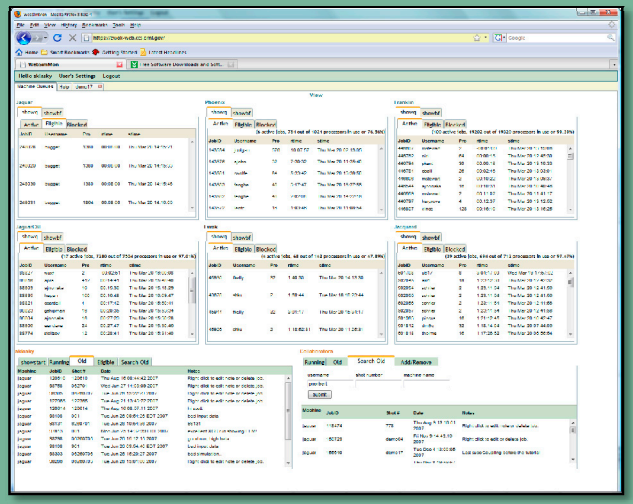
Coupling

- Run XGC until ELMs are unstable
- M3D coupling with XG
  - Transfer profile data to end-to-end system
  - Run M3D-OMP: Compute new equilibrium
  - Transfer the new equilibrium back to XGC
  - Execute ELITE: Compute growth rate; test linear MHD stability
  - Execute M3D-MPP: Study unstable states (ELM crash)
  - Restart XGC with new “healed” equilibrium from M3D-MPP



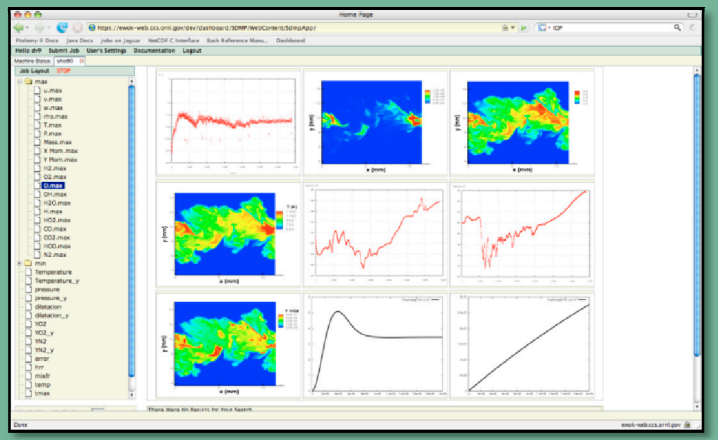
Dashboard: Simulation and job monitoring

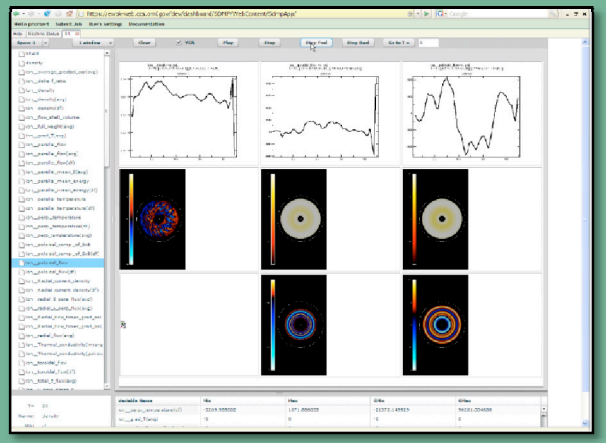
- A basic browser-based visualization tool
- Local interaction for graphs/visualizations
- Server used for data manipulation, extraction
- Server used for more complex analysis
- Allows for pan and zoom locally
- Asynchronous queries
- MySQL for database support



Job monitoring

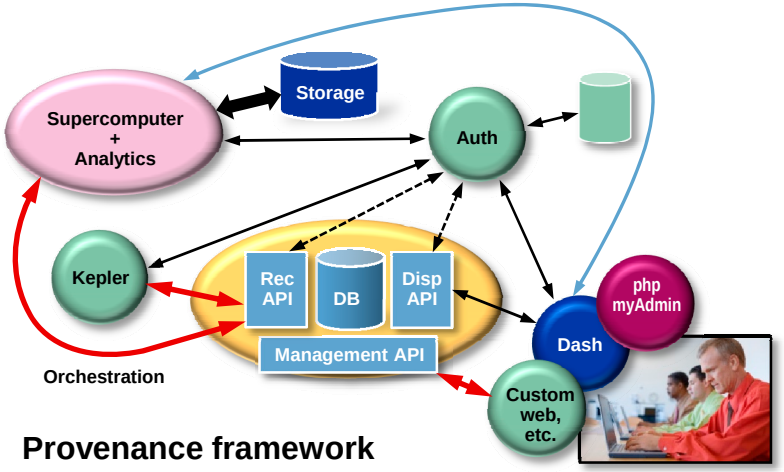
Simulation monitoring





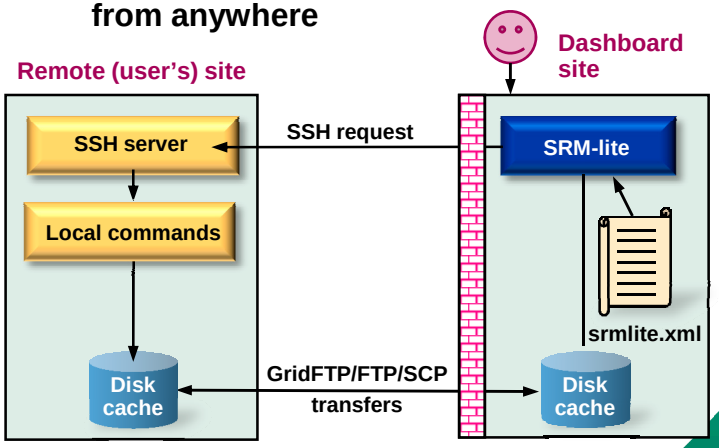
Provenance + data movement

- **Process provenance**
  - The steps performed in the workflow, the progress through the workflow control flow, etc.
- **Data provenance**
  - History and lineage of each data item associated with the actual simulation (inputs, outputs, intermediate states, etc.)
- **Workflow provenance**
  - History of the workflow evolution and structure
- **System provenance**
  - Machine and environment information
  - Compilation history of the codes
  - Information about the libraries
  - Source code
  - Run-time environment settings



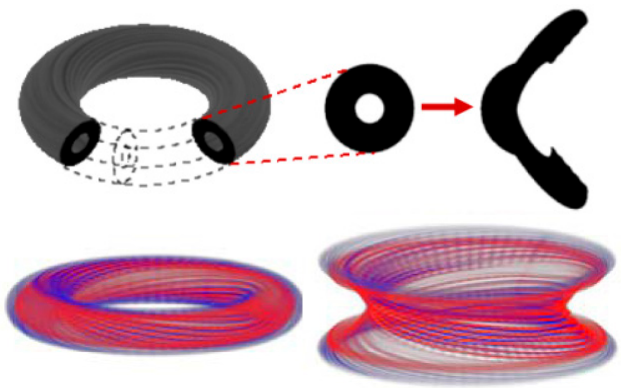
Provenance framework

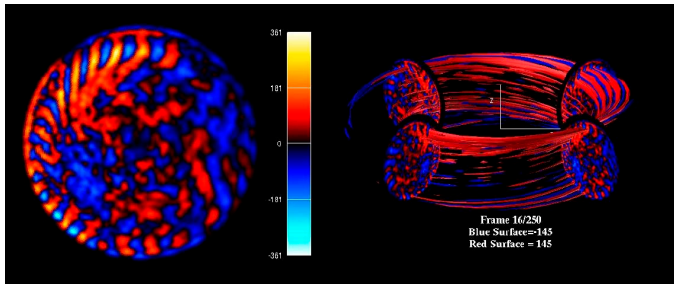
- **Data movement**
  - Given an OTP firewall at one site, where local files resides
  - Need a client program that "pushes" file to users, which …
- **Automates movement of multiple files**
  - Concurrent transfers: Utilize bandwith
  - Using various transfer protocols
  - Support entire directory transfers
  - Recover from midtransfer interruptions
- **Can be invoked from Dashboard**
  - Show what files are to be transferred
  - Provide asynchronous service—user can log out of Dashboard
- **Has a way to show transfer progress asynchronously**
  - Support monitoring from anywhere

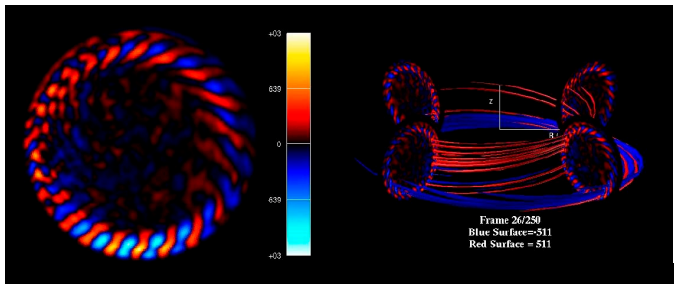


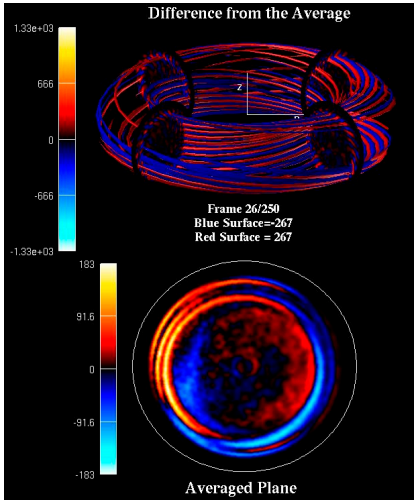
CPES visualization techniques

Shape-aware visualization:
Interior wall view of 3D simulation

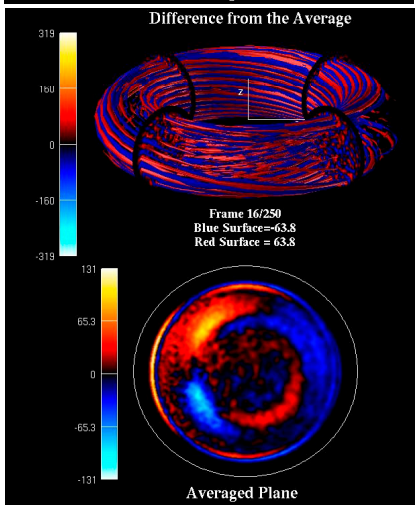




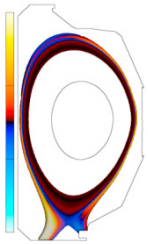


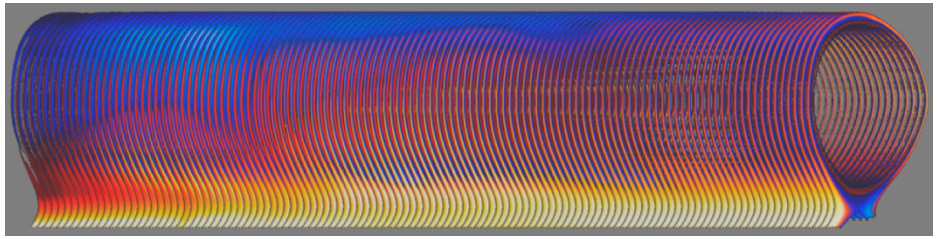


Average-plane view: Average is subtracted from all planes



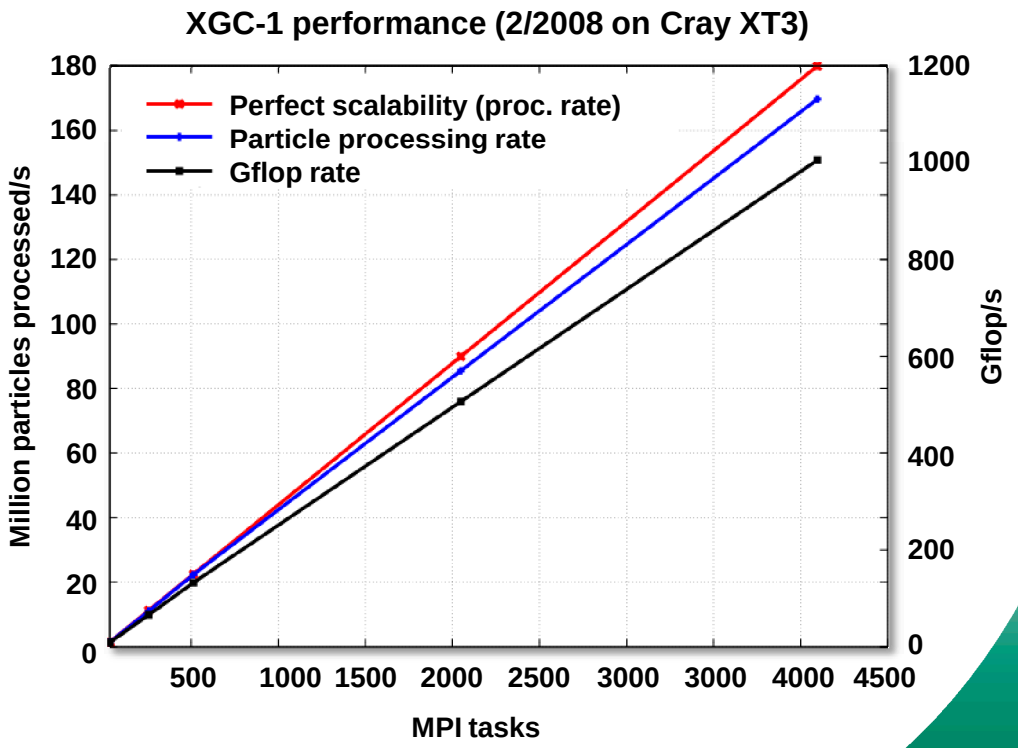
"Curtain rod" view of 2D edge simulation





XGC1 performance on the Cray XT

- As a result of the computer science team's effort, XGC1 runs on a large number of processors
  - Specifically, our I/O makes it possible to work around any I/O scaling issues and run on large (>12K) numbers of processors!
- Performance engineering discovered some bottlenecks and optimized XGC1
- EFFIS enables CPES researchers to work together on
  - Performance engineering
  - Fast I/O
  - Monitoring long-running jobs



CPES external collaborations

- **Domestic**
  - Code collaboration: General Atomics (Elite, EFIT), LLNL (TEQ)
  - Experimental collaboration: NSTX, DIII-D, C-Mod
- **International**
  - ITPA-ITER, JET, EUFORIA, KSTAR, Max Planck-Garching
- **Other proto-FSPs**
  - Facet-CPES: Core-edge coupling between kinetic codes, memory−memory data coupling
  - SWIM-CPES: XGC-RF in plasma state to provide distribution function information to AORSA, Kepler workflow
- **Other government-funded centers**
  - NSF PetaApps: “Supernova Simulation with Chimera”
  - ASCR: “Data Discovery from Petascale Combustion Science Simulations”

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