Gyrokinetic Particle Simulation of Fusion Plasmas

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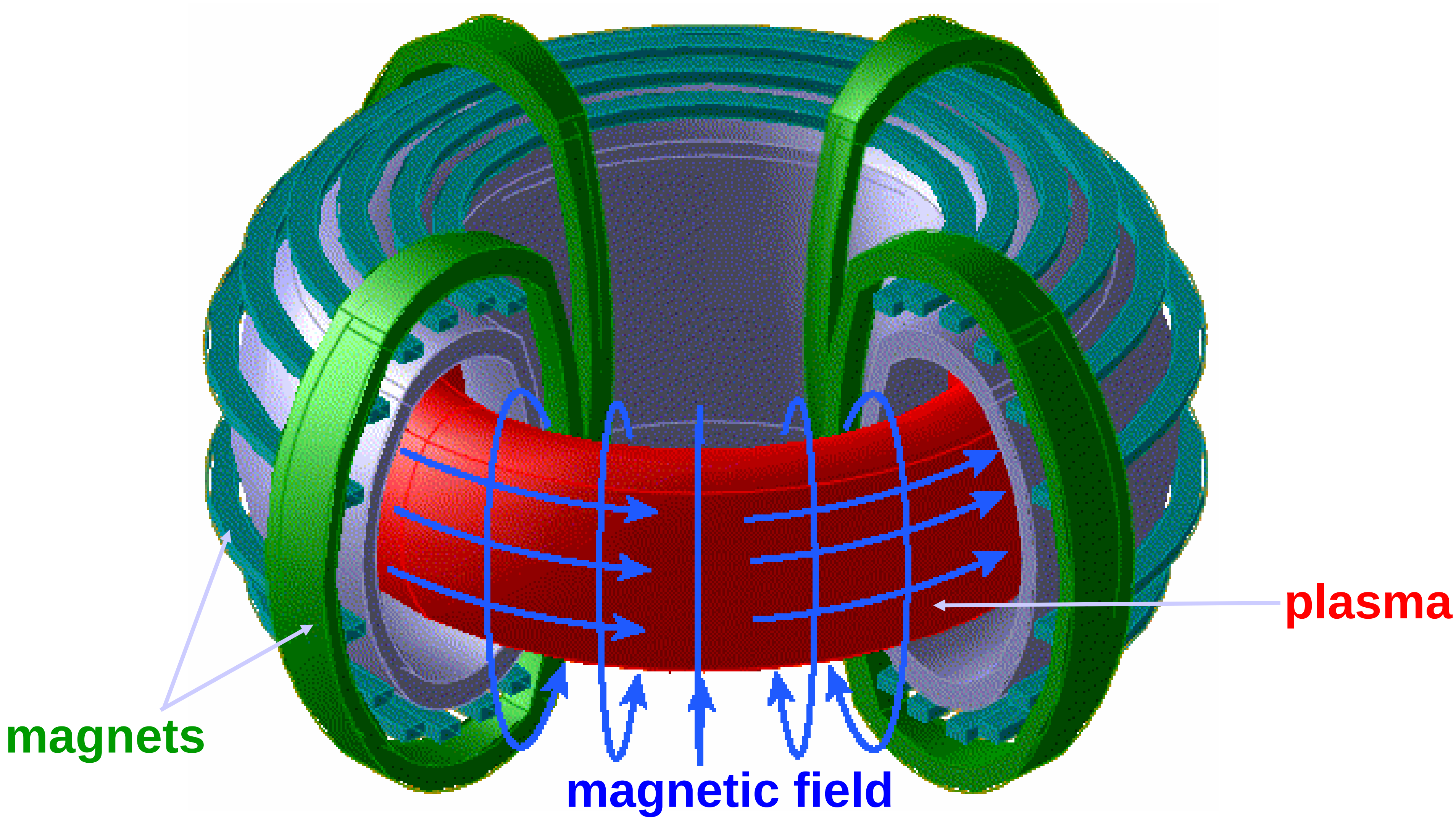
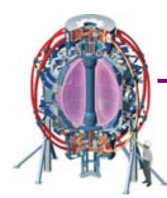
The Sun in a bottle: confining 100-million degree plasma with magnetic fields

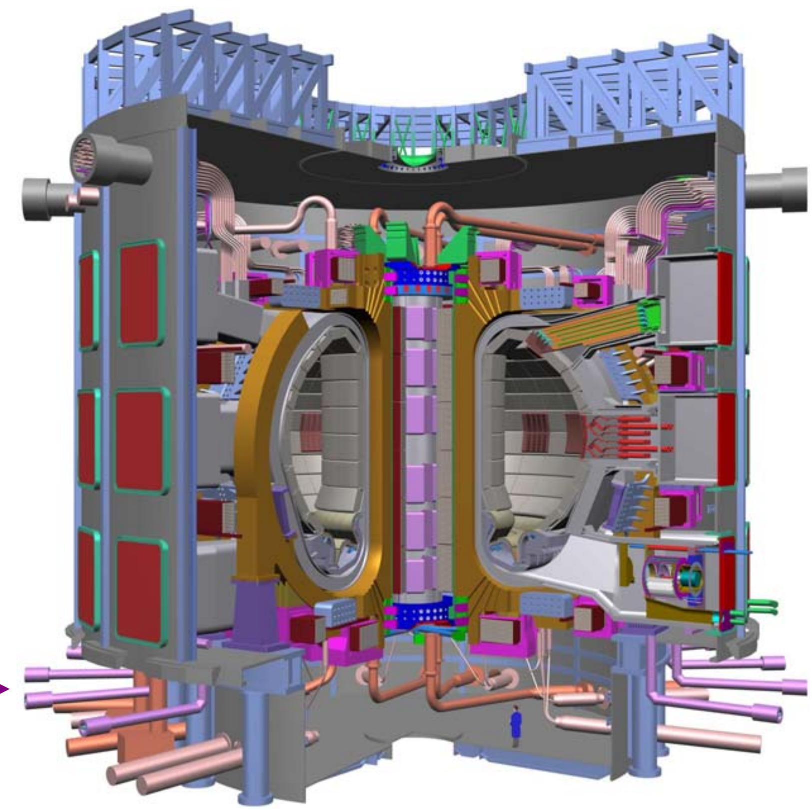


The petascale challenge of simulating magnetic confinement fusion experiments

- What would make us very happy: a comprehensive kinetic simulation of the ITER experiment at all time and spatial scales with wall effects, MHD, heating,etc.
- The reality: currently need at least 4 levels of codes to treat this multiscale physics.



NSTX



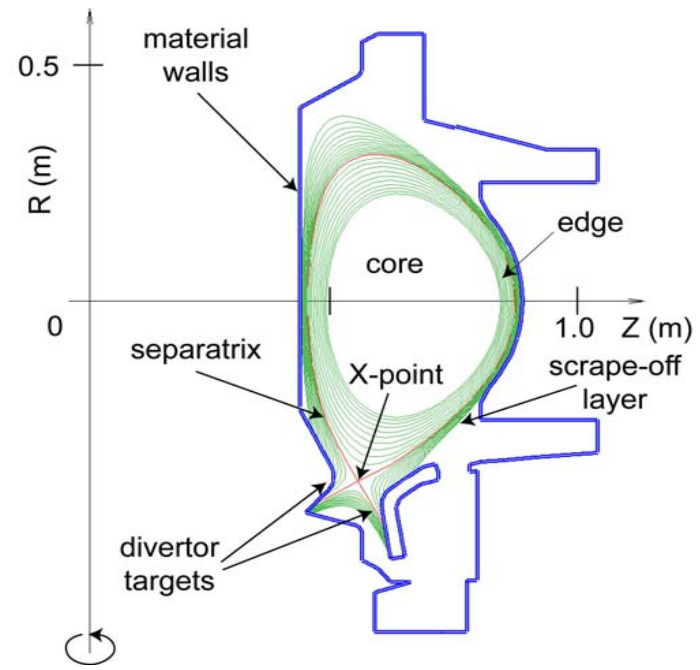
ITER

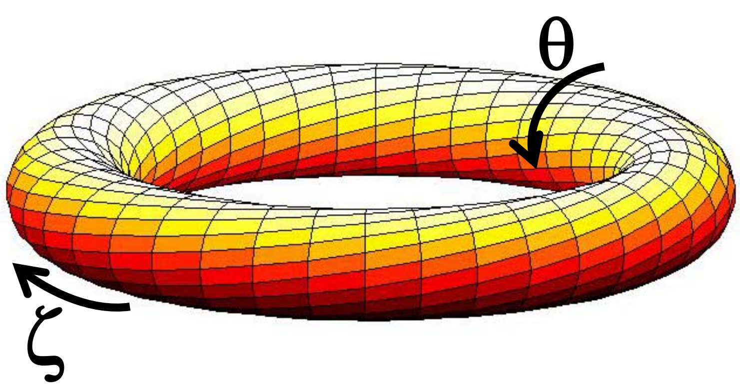
GPSC

CPES
Center for Plasma Edge Simulation

The Projects

- SciDAC Center for Gyrokinetic Particle Simulation of Turbulent Transport in Burning Plasmas (GPSC)
  - PPPL (lead P.I. W.W. Lee), Columbia, Colorado, ORNL, UC-Irvine, UCLA, UC-Davis, UT-Knoxville
  - Focus on **core** turbulence and transport
- FSP Center for Plasma Edge Simulation (CPES)
  - NYU (lead P.I. C.S. Chang), Caltech, GA, LBNL, Lehigh, UC-Irvine, Colorado, ORNL, MIT, Rutgers, PPPL, Utah, UT-Knoxville
  - Focus on **edge** region, all the way to the device wall
  - Coupling between 3D MHD code (stability calculation), 3D particle code for turbulence and neoclassical transport (XGC), and neutral recycling physics code (DEGAS 2)

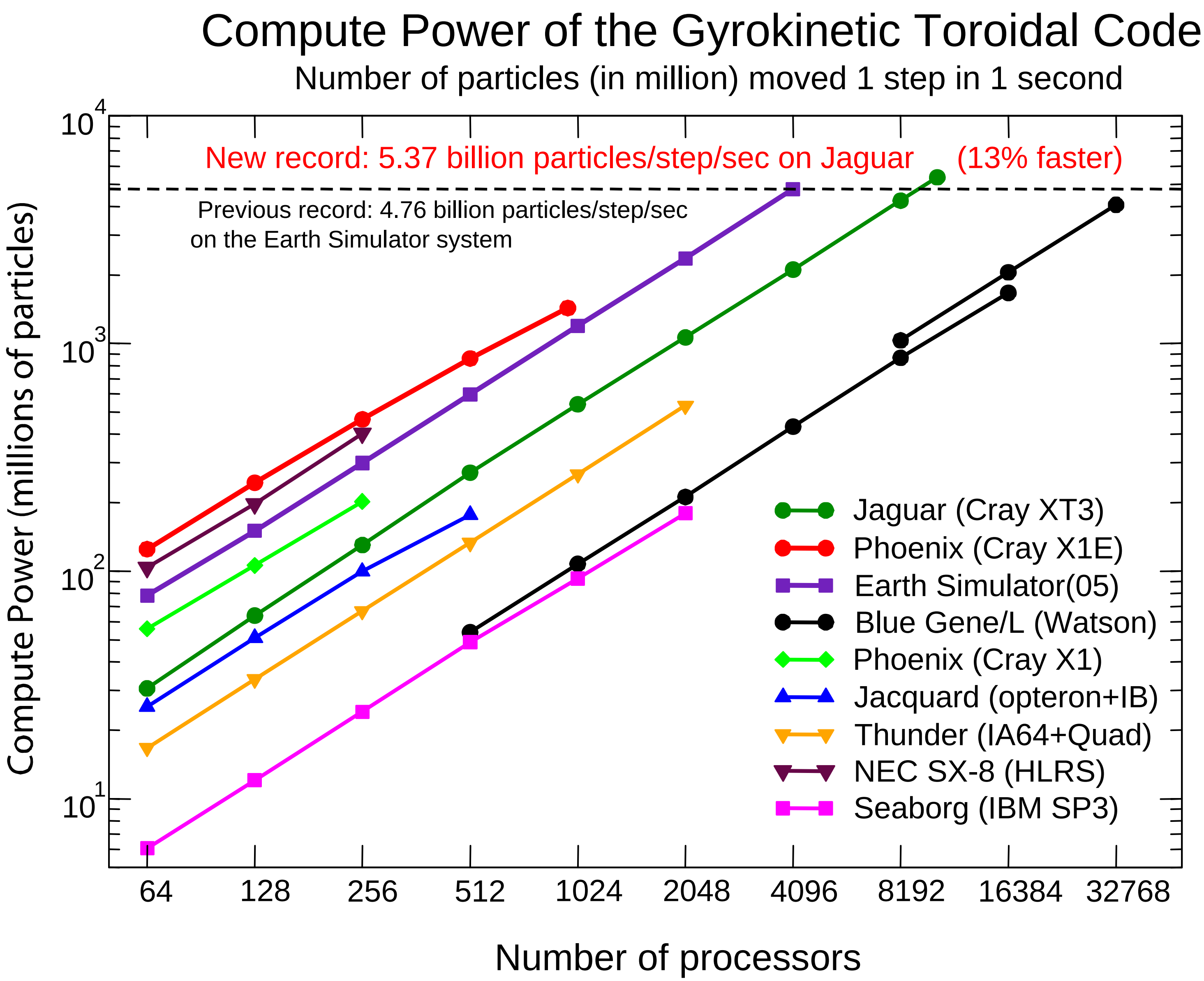




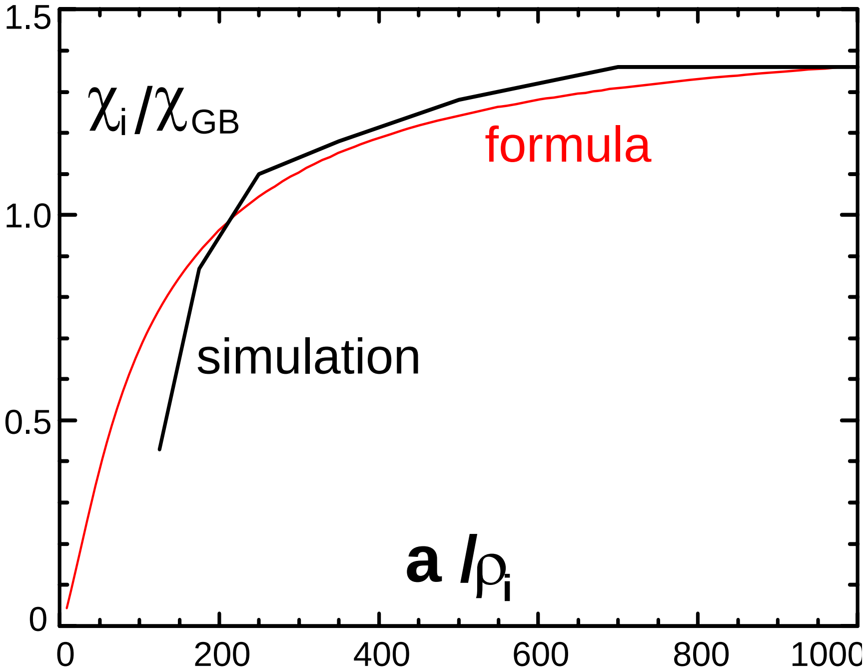
GPSC gyrokinetic PIC codes used for studying microturbulence in plasma core

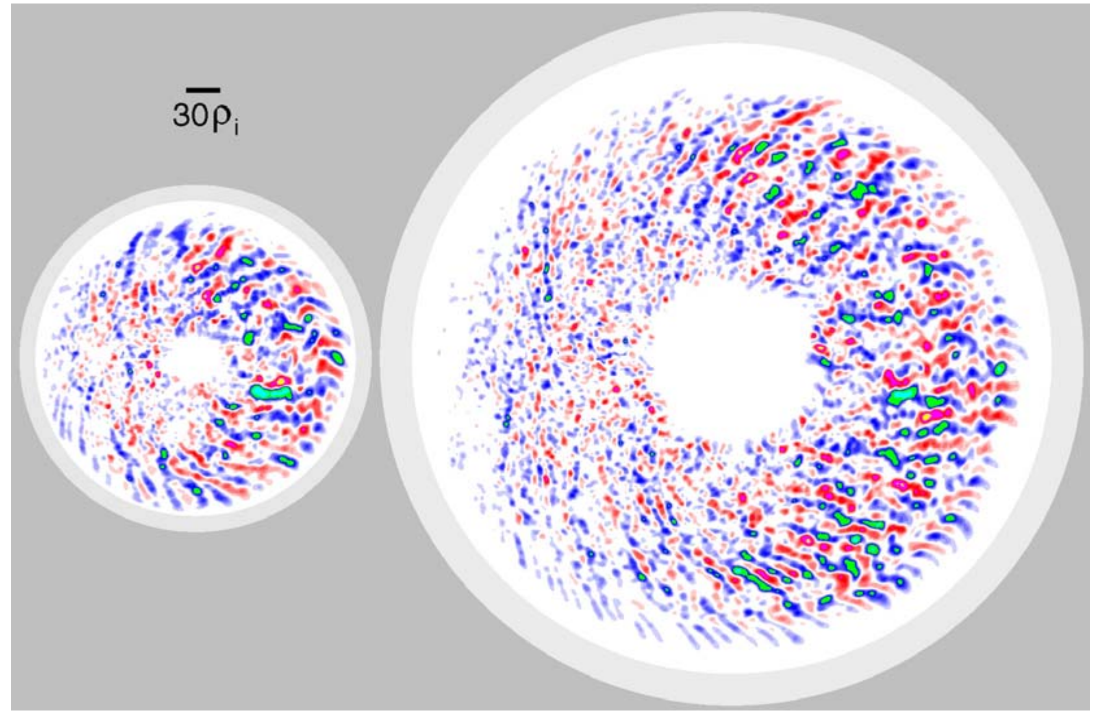
- GTC (Z. Lin et al., Science 281, p.1835, 1998)
  - Intrinsically global 3D nonlinear gyrokinetic PIC code
  - All calculations done in real space
  - Scales to > 10,000 processors
  - Delta-*f* method
  - Currently being upgraded to fully electromagnetic
- GEM (Y. Chen & S. Parker, JCP, in press 2006)
  - Fully electromagnetic nonlinear delta-*f* code
  - Split-weight scheme implementation of kinetic electrons
  - Multi-species
  - Uses Fourier decomposition of the fields in toroidal and poloidal directions (wedge code)

GTC performance and scaling



GTC Global code allows device-size scans: ITER-size simulations

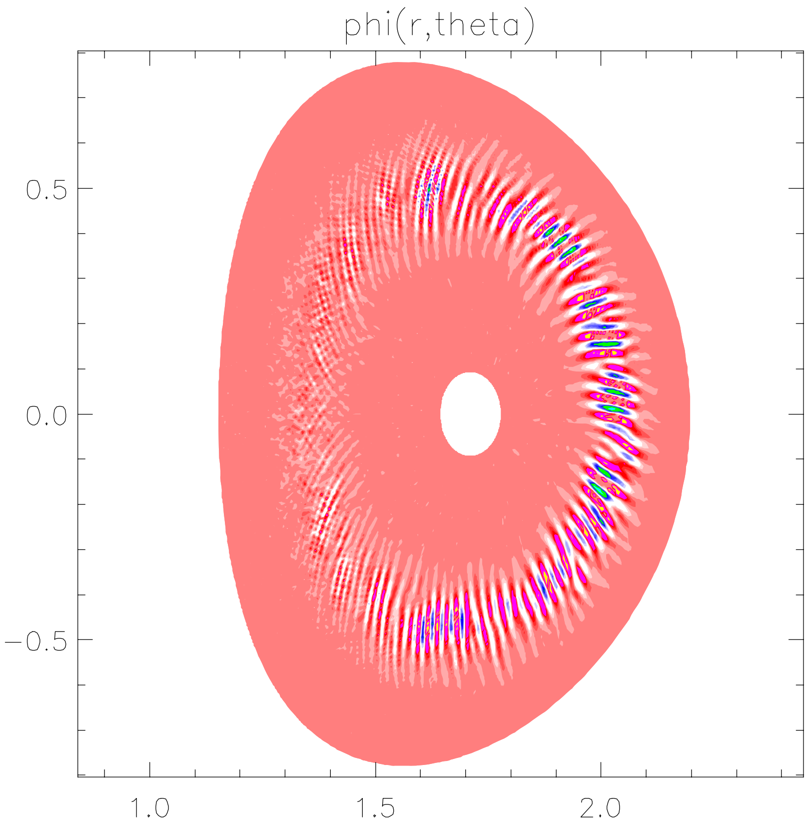




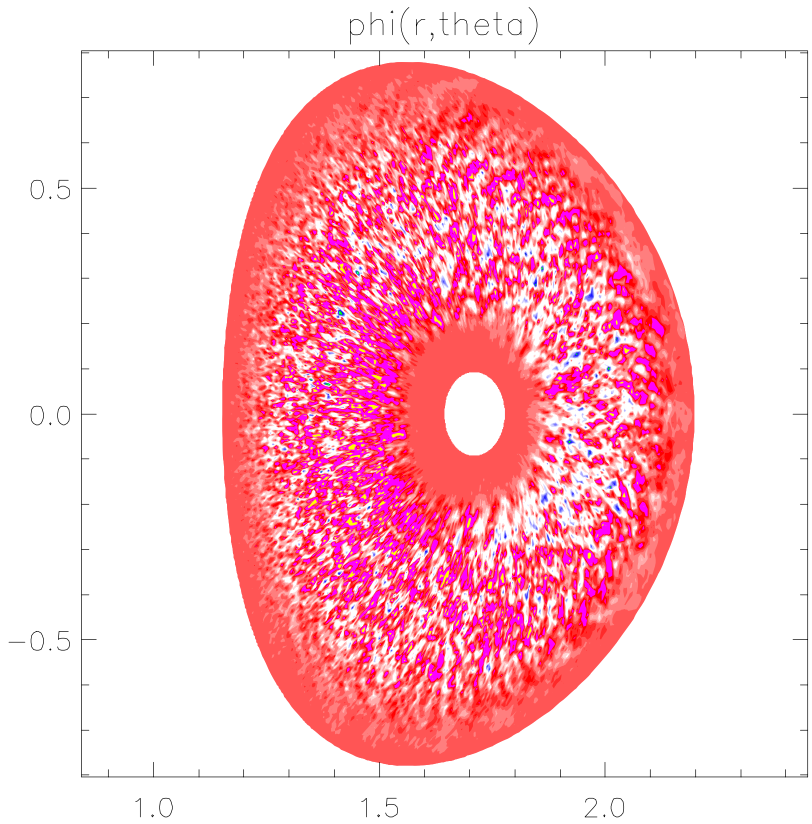
- Lead to important results showing that level of energy losses will roll over with size of device
- Good news for ITER!

Important physics unveiled by global effects: Turbulence spreading

early time



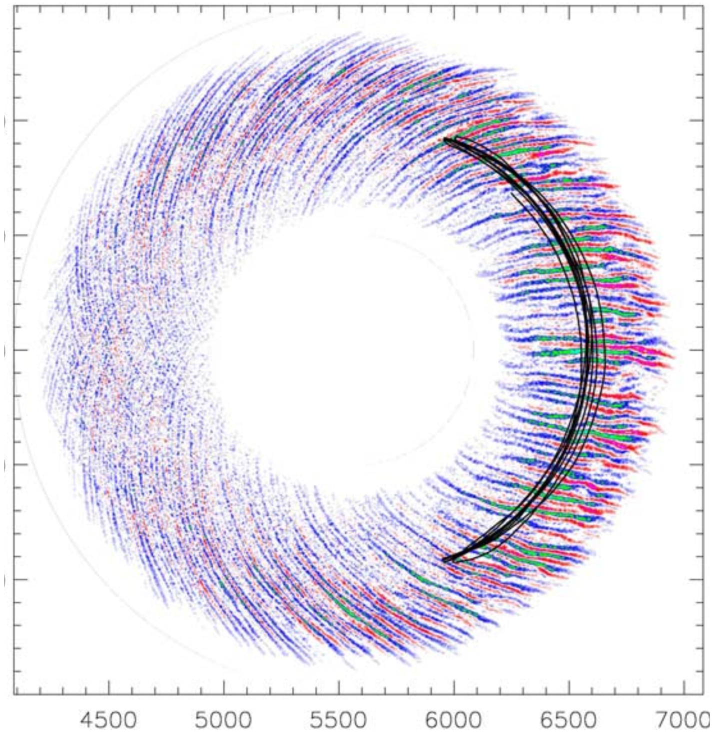
late time

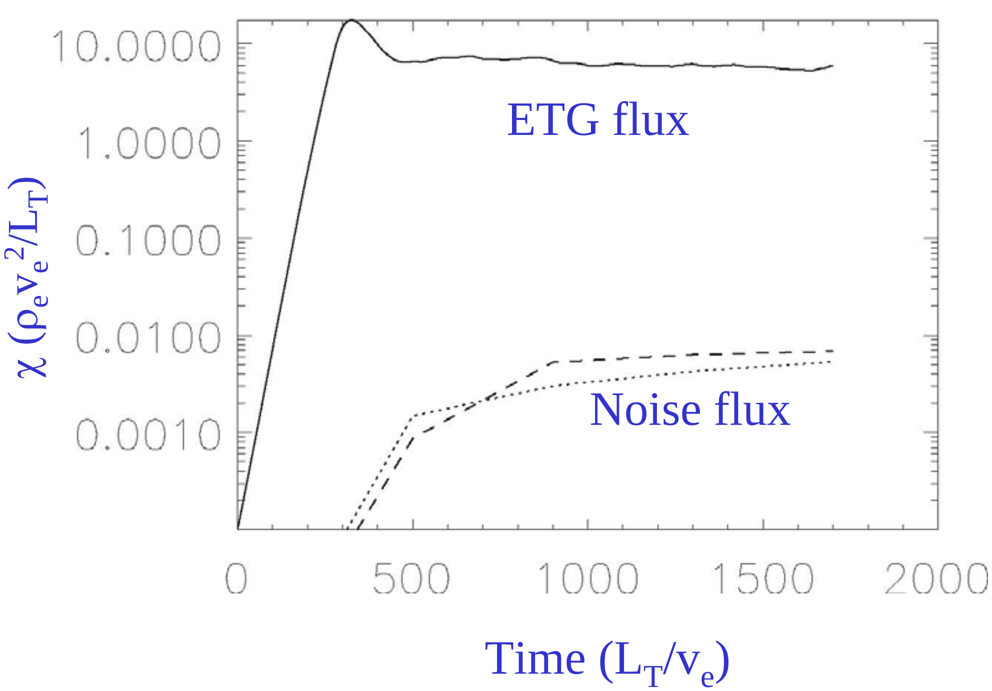


- Narrow region driving turbulence
- Turbulence spreads outside of driving region = global effect

Record size simulations on Jaguar shows convergence for ETG runs

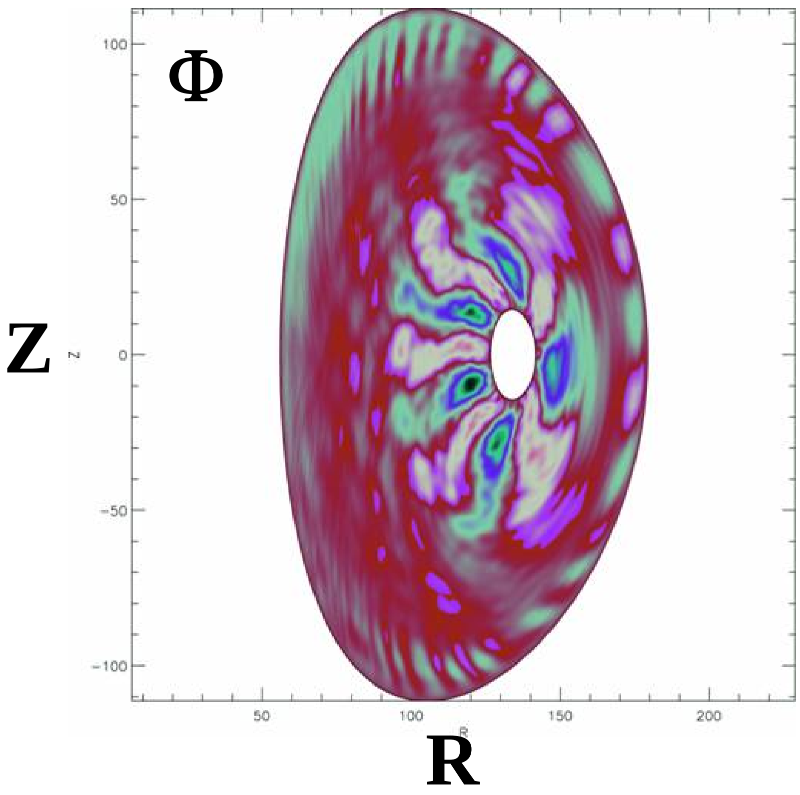
- Flux driven by particle noise is 1000 times smaller than ETG in global GTC simulation: noise does not affect ETG physics
- Convergence: consistent ETG c_e when using 200-2000 particles/cell
- GTC simulation calculates orbits of 40 billion particles, 10000 time steps using ORNL Cray XT3, 6400 compute cores (1.3 million cpu-ours)

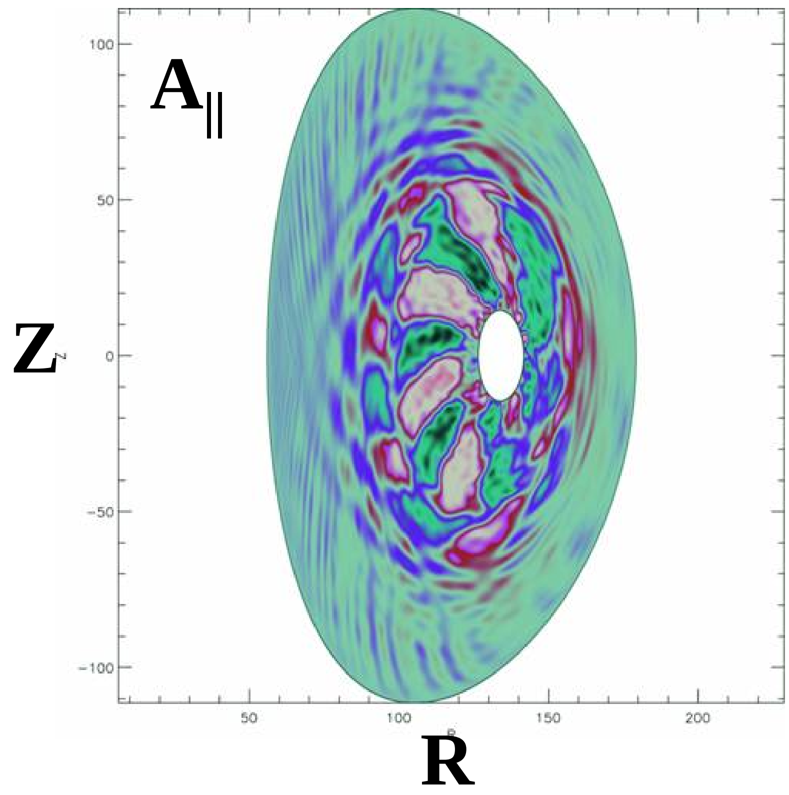




New electromagnetic simulations of NSTX experimental device with the GEM code

- Includes kinetic electrons and 3 ion species, nonlinear effects of KBM, microtearing, TEM, and ITG.
- Runs on Jaguar with 1024 cores





CPES particle code for studying edge transport

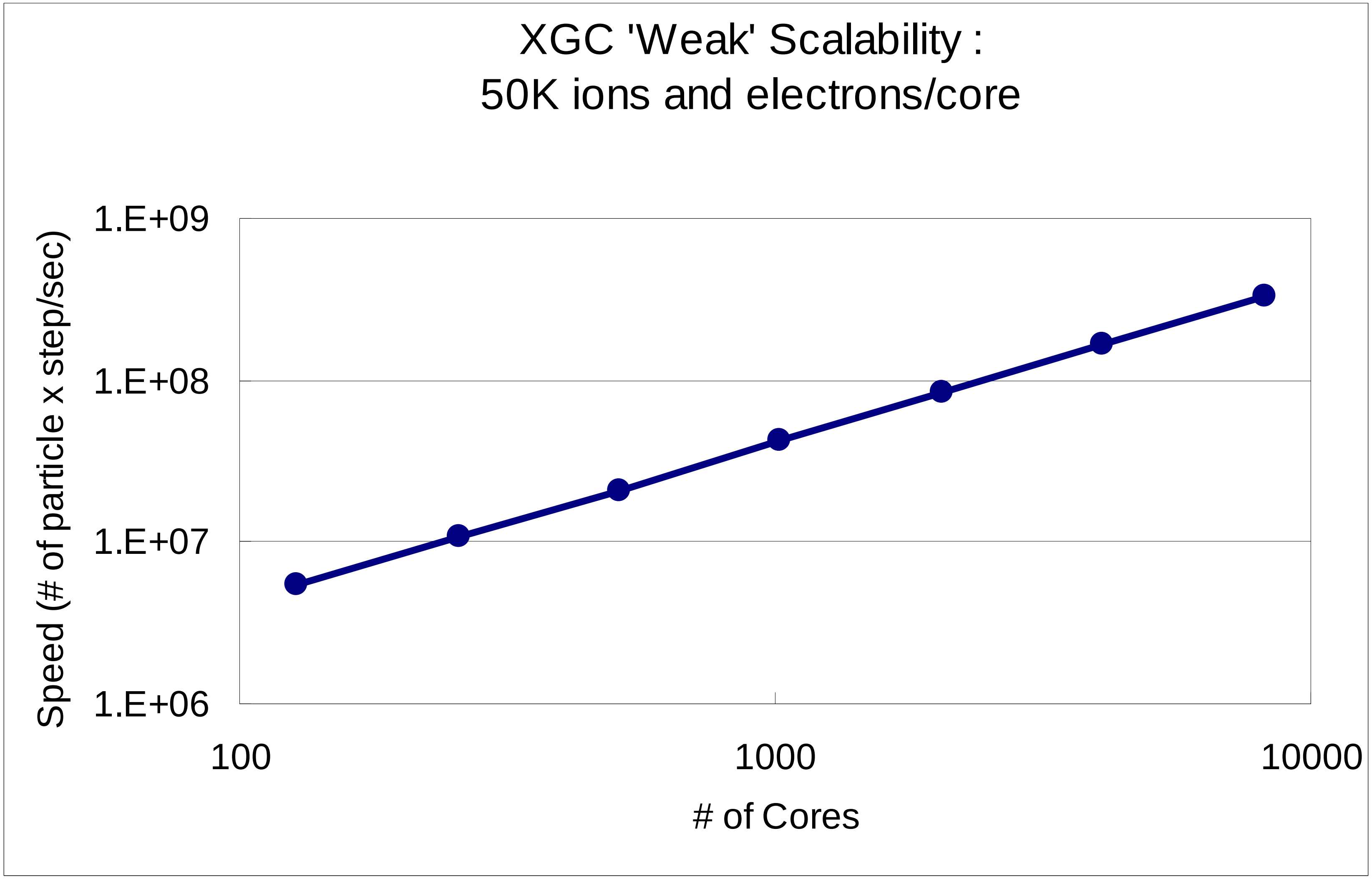
- XGC
  - Particle-in-cell
  - 5D (3D real space + 2D v-space)
  - Conserving plasma collisions
  - Full-*f* ions, electrons, and neutrals (recycling)
  - Neoclassical and turbulence integrated together
  - Realistic magnetic geometry containing X-point
  - Heat flux from core
  - PETSc library for Poisson solver
  - Particle source from neutral ionization

XGC roadmap

Full-f neoclassical ion root code (**XGC-0**)	Buildup of pedestal along ion root by neutral ionization.
Full-f ion-electron electrostatic code (**XGC-1**) -Whole edge	Neoclassical solution
	Turbulence solution
	Study L-H transition
	Multi-scale simulation of pedestal growth in H-mode
XGC-MHD Coupling for pedestal-ELM cycle	
Full-f electromagnetic code (XGC-2)	

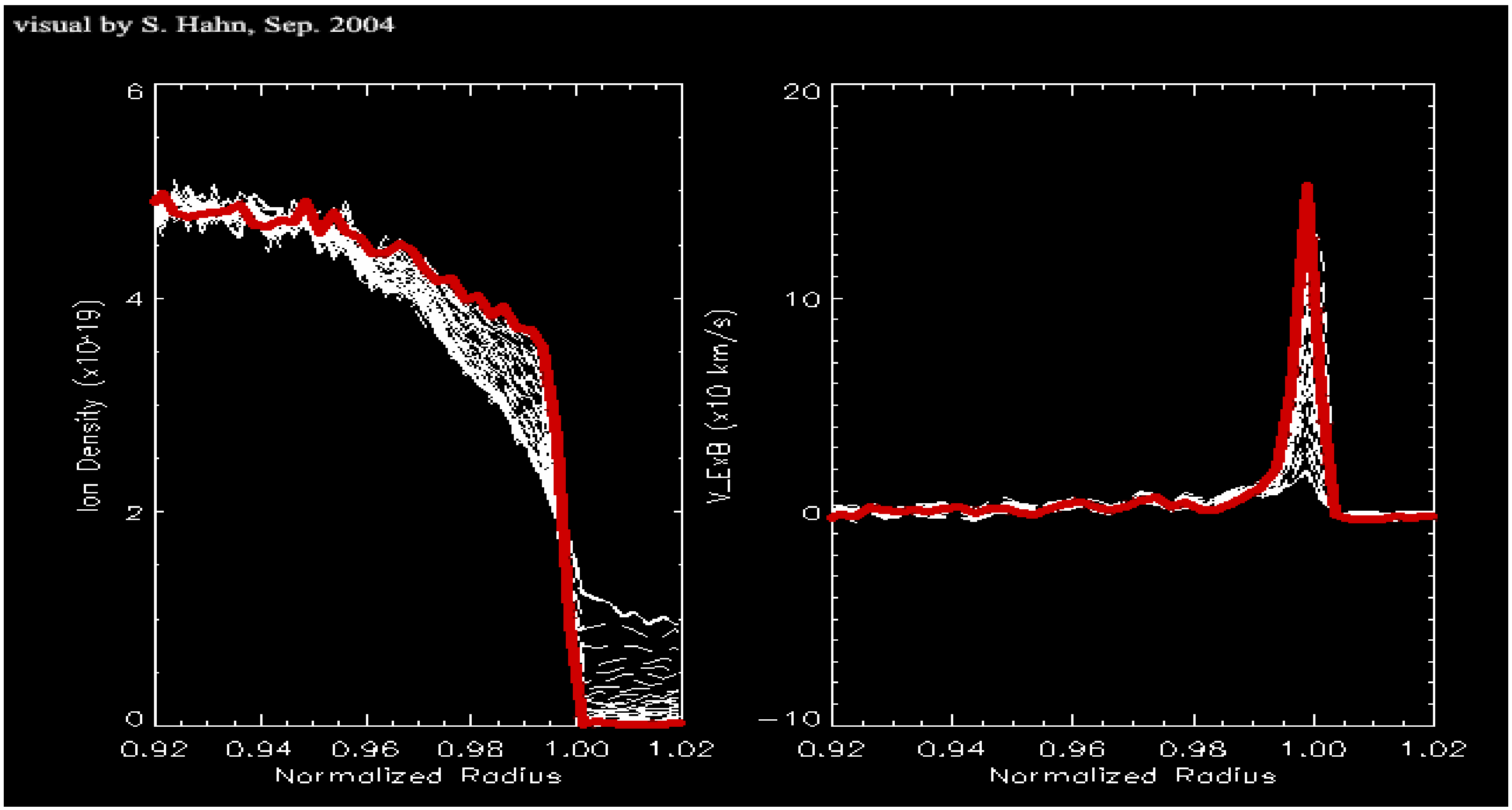
Black: Achieved, **Blue: in progress**, Red: to be developed

XGC performance and scaling



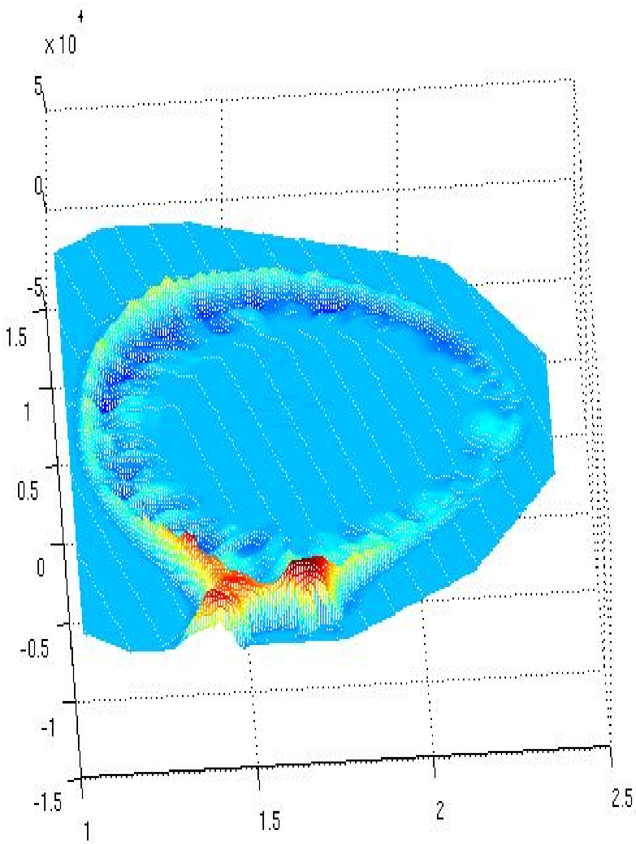
Edge transport with XGC code

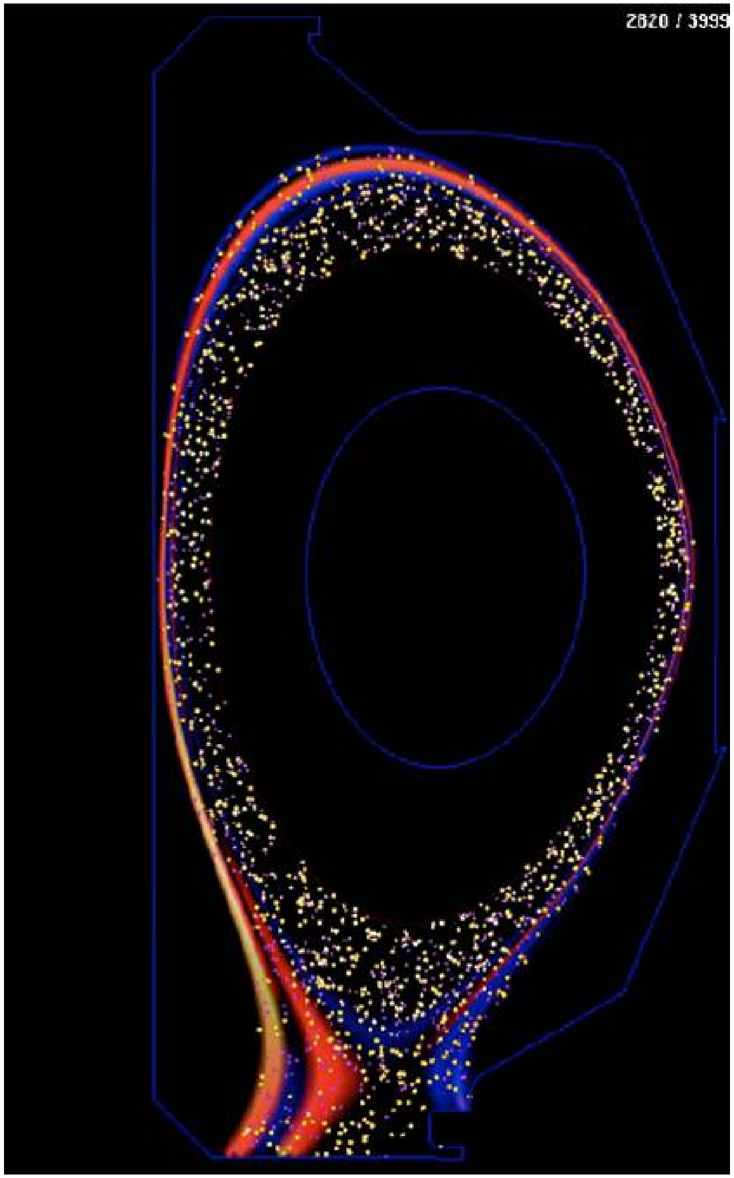
- Study "L" and "H" confinement modes in tokamaks
- Involves device wall effects



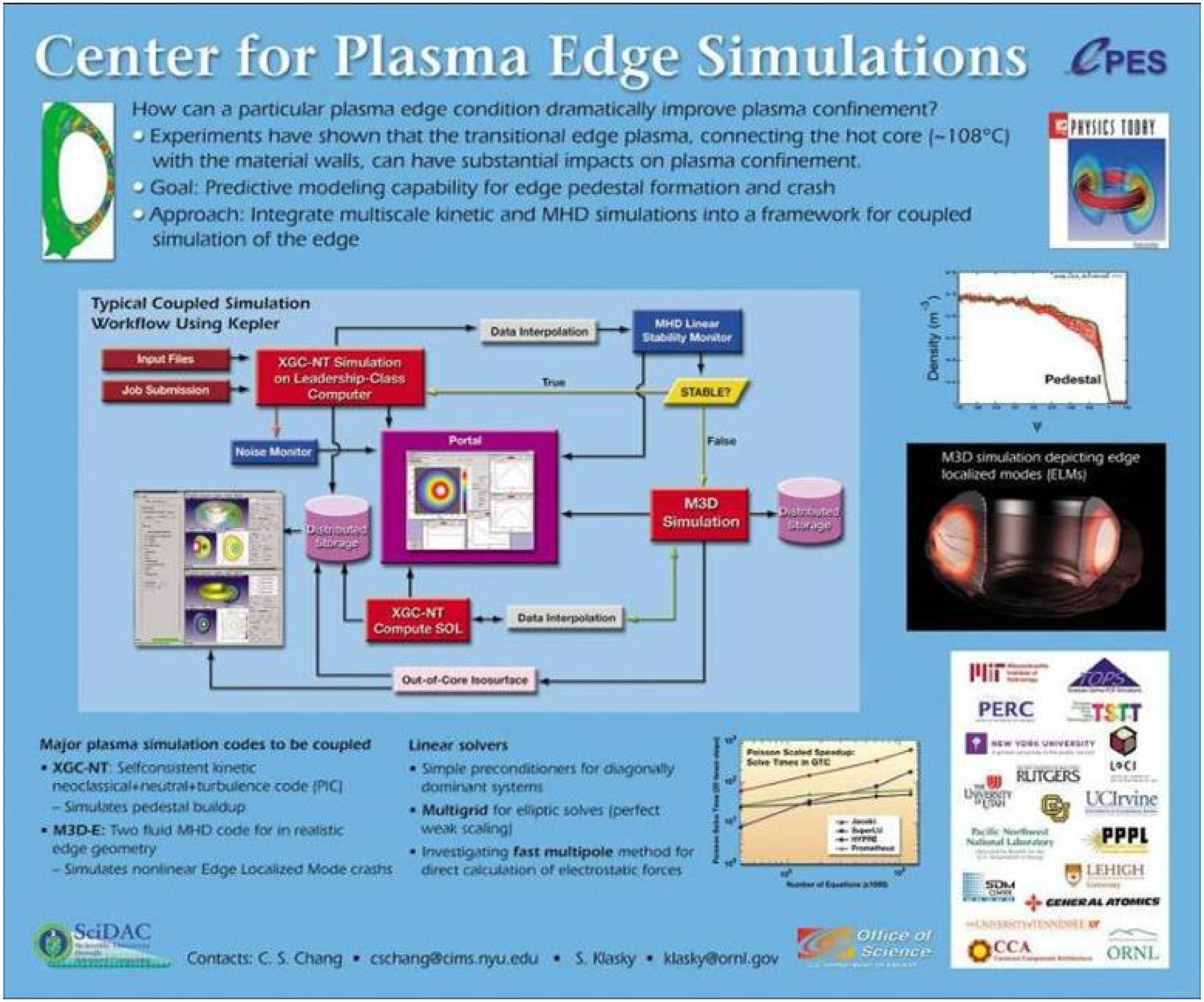
XGC-1 simulation on Jaguar: Turbulence+neoclassical

- Correct electron mass
- Formation of a negative potential layer just inside the separatrix ⇒ **H-mode layer**

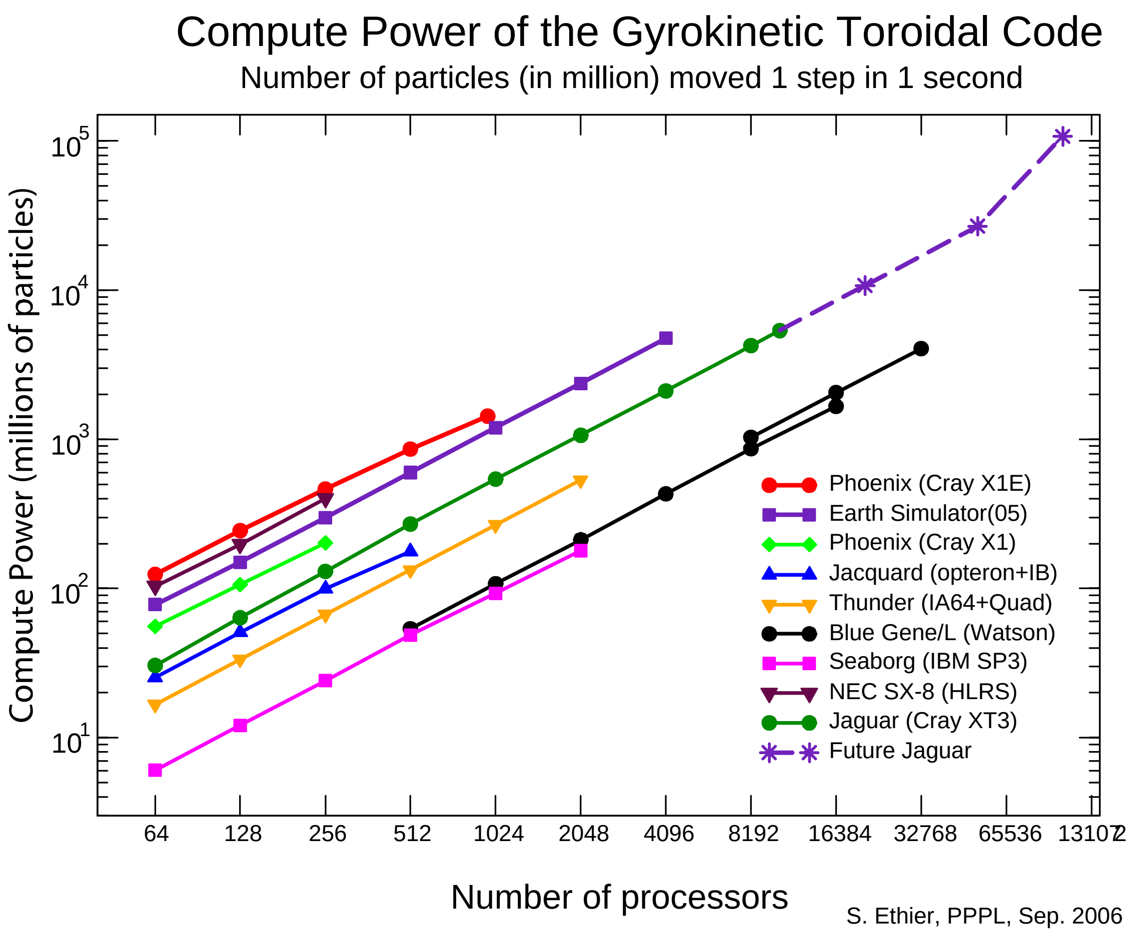




Strong computer science component in both projects but especially CPES Edge project



Well on the road to petascale…
as far as the processors are concerned



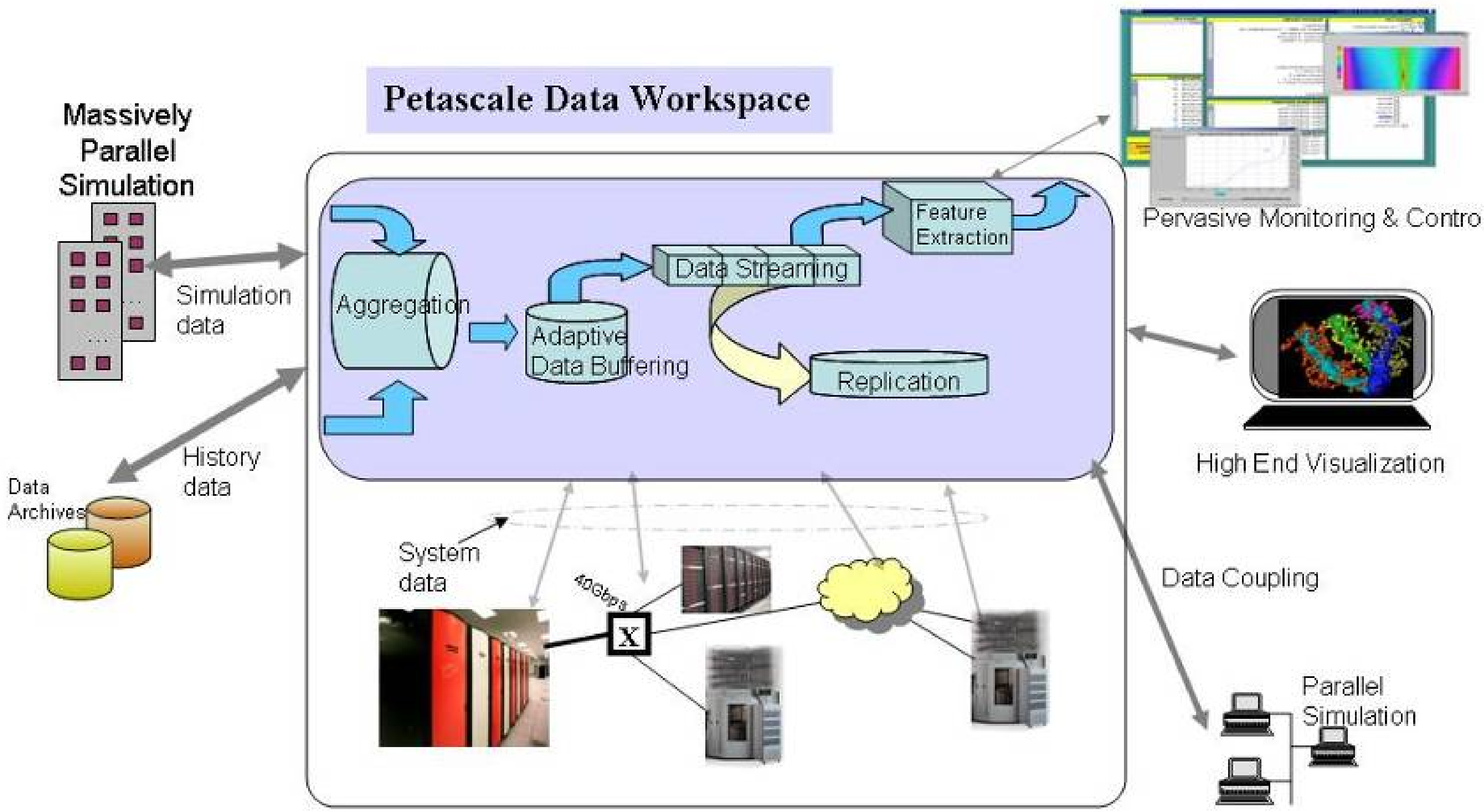
But what about I/O and all the generated data???

Data Management & Visualization Challenges

- Data-management challenge in some scientific areas already exceeding compute-power challenge in needed resources
- Automated Workflow Environment:
  - Tera- to Peta-bytes of data to be moved *automatically* from simulations to analysis codes
  - Feature Detection/Tracking to harvest scientific information -- impossible to understand without new data mining techniques
- Parallel I/O Development and Support - define portable, efficient standard with interoperability between parallel and non-parallel I/O
  - Massively parallel I/O systems needed since storage capacity growing faster than bandwidth and access times
- Real-time data visualization and analysis to enable "steering" of long-running simulations

- Work lead by NCCS end-to-end task lead Scott Klasky

Automated data workflow for on-the-fly data analysis and visualization

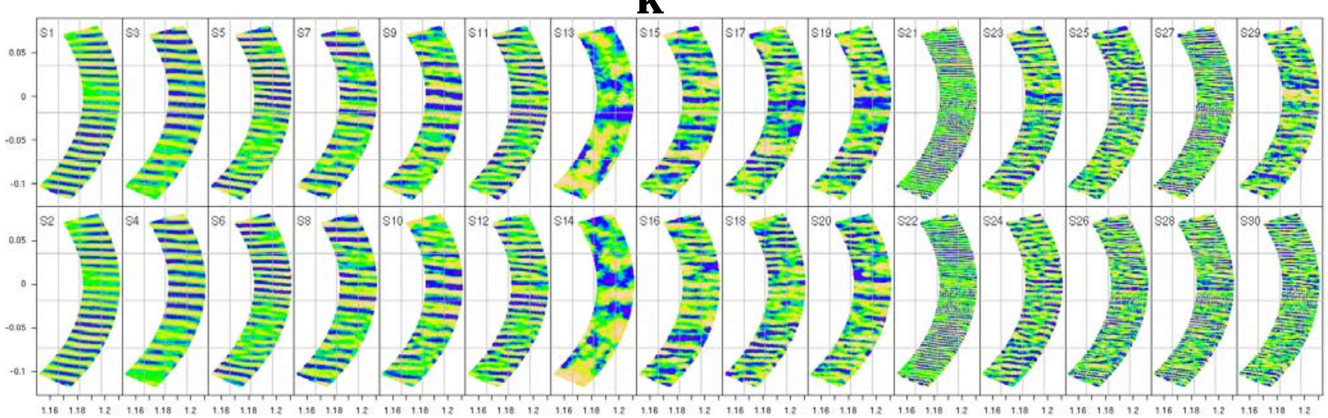


Advanced analysis of raw data

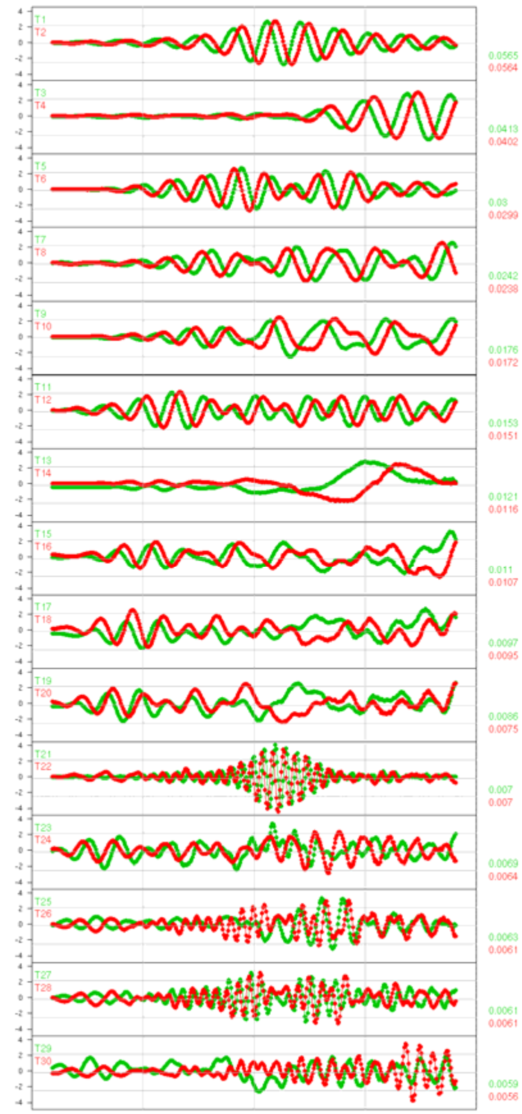
- Principal Component Analysis (PCA) or Single Value Decomposition (SVD)
- Statistical decomposition of time-varying simulation data (e.g. electrostatic potential)
- Decomposition shows transitions between wave components in time

$$f(X_t) = S_0 + \tau_{1t} S_1 + \ldots + \tau_{kt} S_k + E_t$$

$\mathbf{S_k}$



$\boldsymbol{\tau_k}$



George Ostrouchov of the *Statistics and Data Sciences Group*, CSM ORNL

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Need for petaflops and beyond…

- Fully electromagnetic runs with multiple ion species and kinetic electrons for ITER-size devices.
- Going further in coupling turbulence codes with MHD and transport scale codes.
- Simulate interaction with device walls.
- and much more…