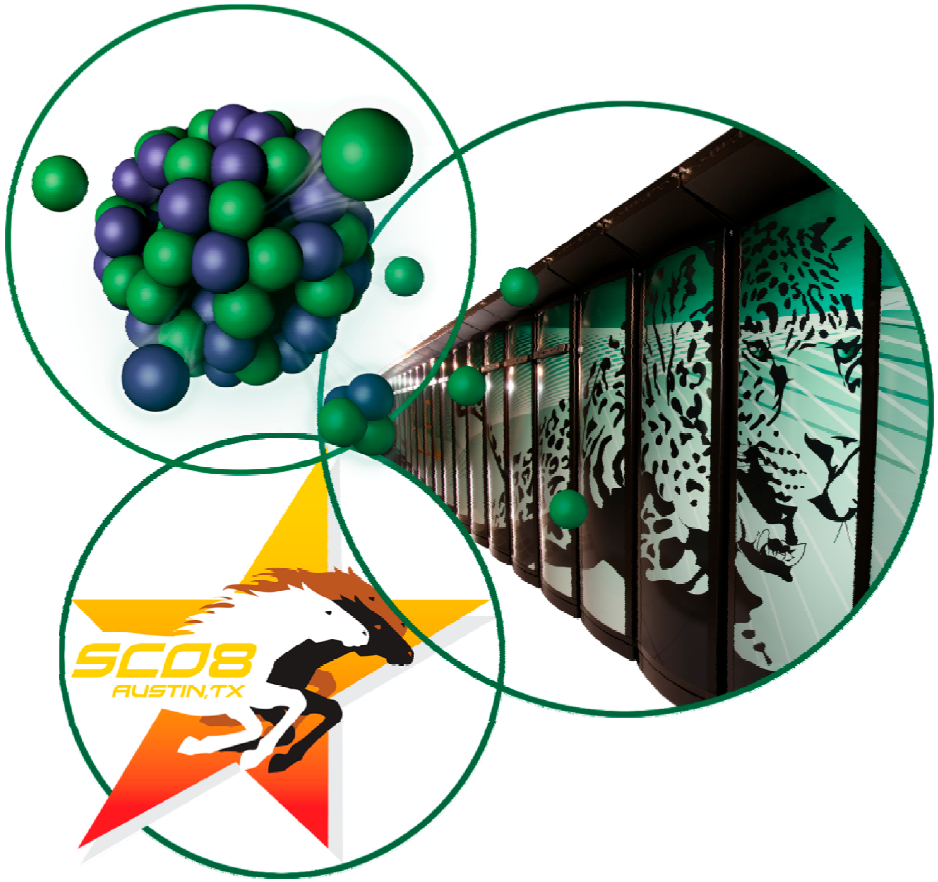
Gyrokinetic Particle Simulations of Fusion Plasmas



Presented by

Scott A. Klasky

Scientific Computing
National Center for Computational Sciences

UCSD: P. Diamond
UCI: Z. Lin, Y. Xiao
PPPL: S. Ethier, W. Wang

Near-term priorities

Priority: 1
ITER

The Facility: ITER is and international collaboration to build the first fusion science experiment capable of producing a self-sustaining fusion reaction, called a "burning plasma." It is the next essential and critical step on the path toward demonstrating the scientific and technological feasibility of fusion energy.

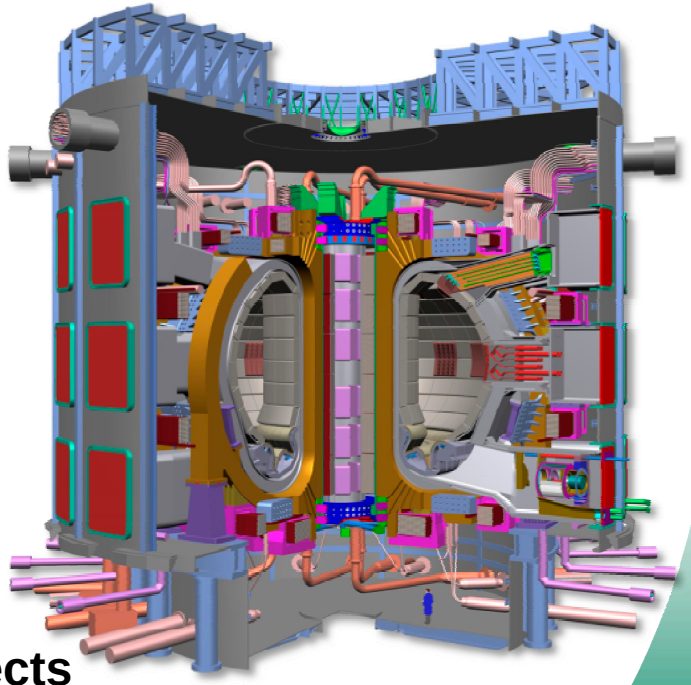
Priority: 2
UltraScale Scientific Computing Capability (USSCC)

The Facility: The USSCC, located at multiple sites, will increase by a factor of 100 the computing capability available to support open (as opposed to classified) scientific research—reducing from years to days the time required to simulate complex systems, such as the chemistry of a combustion engine, or weather and climate—and providing much finer resolution.

November 2003

Overview of this fusion INCITE project (FUS17)

- Understanding turbulent transport is one of the most important scientific challenges in fusion experiments such as ITER
- Large-scale, first-principles simulation has emerged as a powerful tool to study turbulent transport in fusion plasmas, complementing theory and experiment
- Direct comparisons of turbulence simulation with measurement become feasible thanks to remarkable progress in simulation and availability of petascale computer
- We study three critical issues in fusion core and edge plasmas: heat transport, momentum transport, and energetic particle transport
- Benchmark between **GTC** and **XGC** for verifications
- Synthetic diagnostics developed for validations
- This INCITE project 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 and electron heat transport

- **Plasma rotation can quench macroscopic instability and suppress microscopic turbulence for a transition to high confinement regime**
- **Our INCITE project will study physics of momentum transport and origin of intrinsic rotation in ITER plasmas**

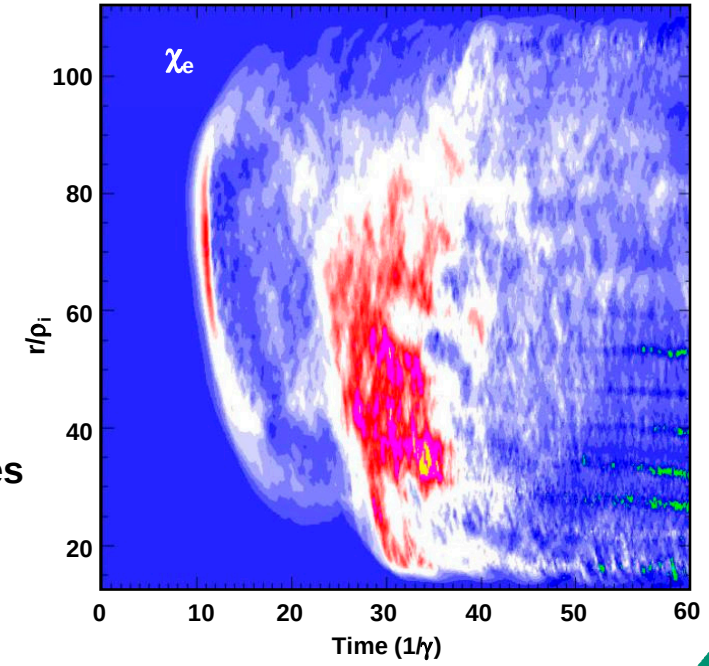
  I. Holod and Z. Lin, "Gyrokinetic particle simulations of toroidal momentum transport," *Phys. Plasmas* **15**, 092302 (2008)

  C-S. Chang and S. Ku, "Spontaneous rotation sources in a quiescent tokamak edge plasma," *Phys. Plasmas* **15**, 062510 (2008)

  P. H. Diamond, invited talk, "Physics of non-diffusive turbulent transport of momentum and the origins of spontaneous rotation in tokamaks," Paper TH/1-1, the 21th International Conference on Plasma Physics and Controlled Nuclear Fusion Research, October 13−18, 2008, Geneva, Switzerland

  P. H. Diamond, invited talk, "Anti-friction, homogenization and angular momentum transport in tokamaks, planets and the solar tachocline," 35th European Physical Society Conference on Plasma Physics, June 9−13, 2008, Crete, Greece

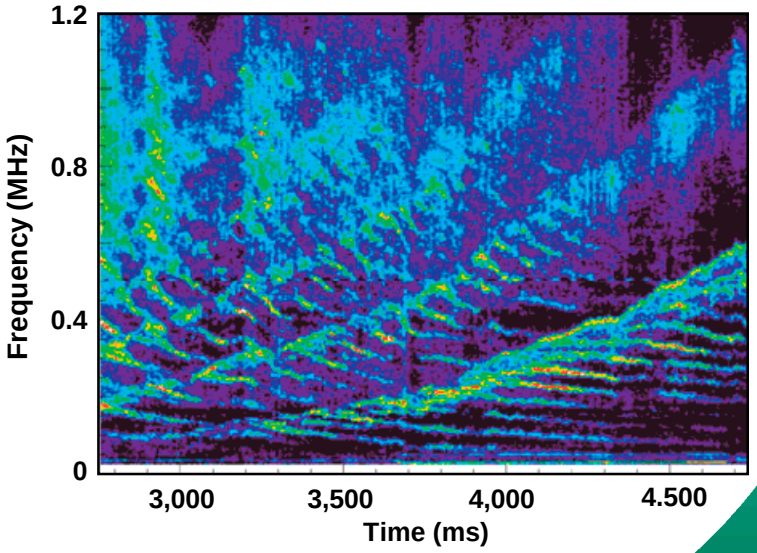
- **Electron turbulent transport is of current interest in fusion research; a probable origin is turbulence driven by collisionless trapped electron mode (CTEM)**
- **CTEM turbulence is difficult for simulation due to strong wave-particle interaction and fast electron motion**
- **Initial gyrokinetic toroidal code (GTC) simulations of CTEM observed**
  - **Spectral cascade and spatial spreading**
- **Our INCITE project studies key non-diffusive processes**
  - **Electron dynamics: granulation in velocity space**
  - **Spectral transfer: multiscale interaction**
  - **Spatial spreading: non-locality**
- **Supported by SciDAC GPS-TTBP**



GTC simulation of energetic particle transport

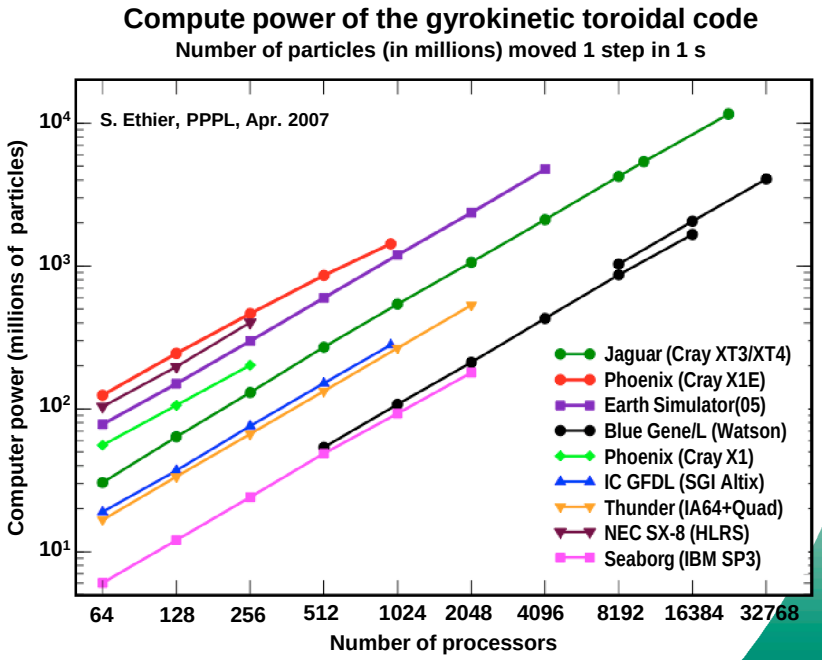
- **Confinement of energetic α-particle produced by fusion is critical for heating plasmas in ITER**

  W. Zhang, Z. Lin, and L. Chen, "Transport of energetic particles by microturbulence in magnetized plasmas," *Phys. Rev. Lett*. **101**, 095001 (2008)
- **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 require 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 project is first fully kinetic EP simulation**
- **Supported by SciDAC GSEP: *Center for Gyrokinetic Simulation of Energetic Particle Turbulence and Transport***



GTC status: State of the art

- **GTC is a particle-in-cell code for simulation of turbulence and transport in fusion plasmas** (Z. Lin et al., "Turbulent transport reduction by zonal flows: Massively parallel simulations," *Science* **281**, 1835 [1998])
- **GTC physics modules: kinetic electron, electromagnetic turbulence, multispecies, general geometry, collision operator, guiding center Hamiltonian**
- **GTC global field-aligned mesh; parallel elliptic solvers via PETSc**
- **MPI/OpenMP multilevel parallelism**
- **Comprehensive analysis package**
- **Key code for GPS-TTBP and GSEP**
- **Part of NERSC benchmark suite**
- **Part of ORNL pioneer application**
- **Developed by GPS-TTBP and GSEP projects and maintained at UCI**

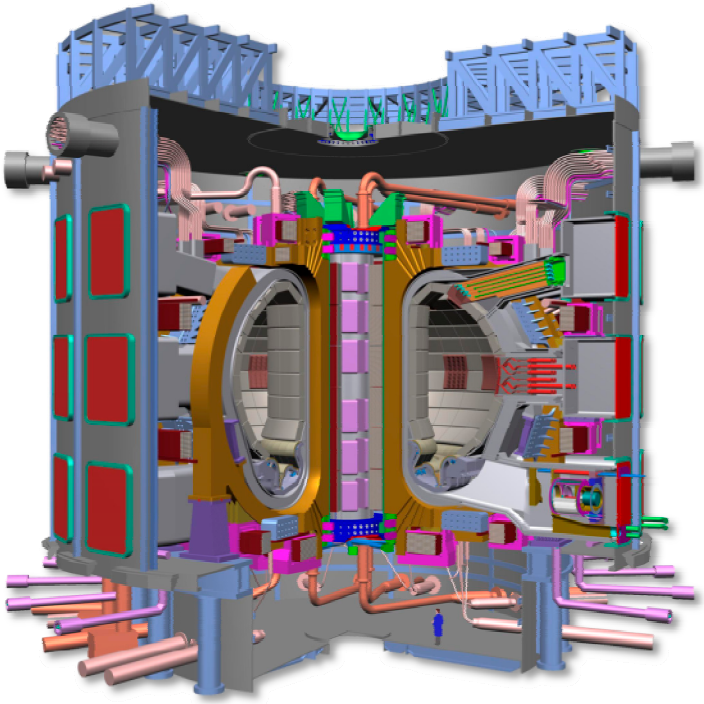


GTC plan: More powerful computer ⇒ better physics

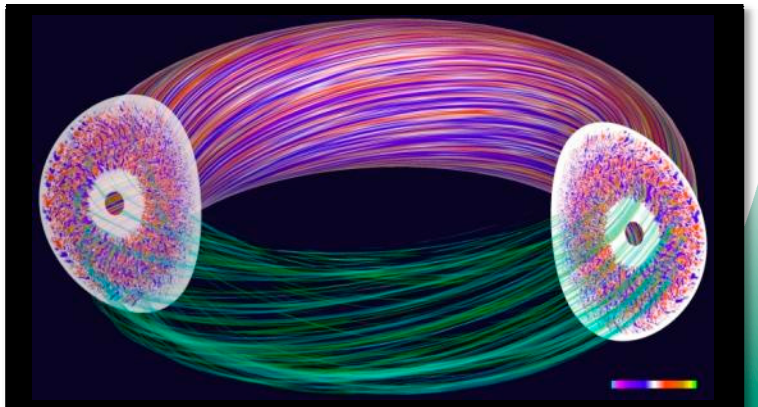
- Formulate new physics modules: full-f ion, profile evolution
- Sustain parallelization for 100,000+ cores; optimize for multicore computer
- Implement advanced computational tools: ADIOS, workflow, and dashboard
- Develop synthetic diagnostics for validation; better version control and integration

GTC simulation	Computer name	PE# used	Speed (TF)	Particle #	Time steps	Physics discovery (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 (*Phys. Rev. Lett.* 2002)
2007	Cray XT3 ORNL	10^4	10^2	10^{10}	10^4	Electron turbulence (*Phys. Rev. Lett.* 2007)
2008	Cray XT4 ORNL/NERSC	10^4	10^2	10^{10}	10^5	Electron transport in ITER EP and momentum transport (*Phys. Rev. Lett. 2008*)
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

ITER is a donut-shaped device based on the tokamak magnetic confinement concept



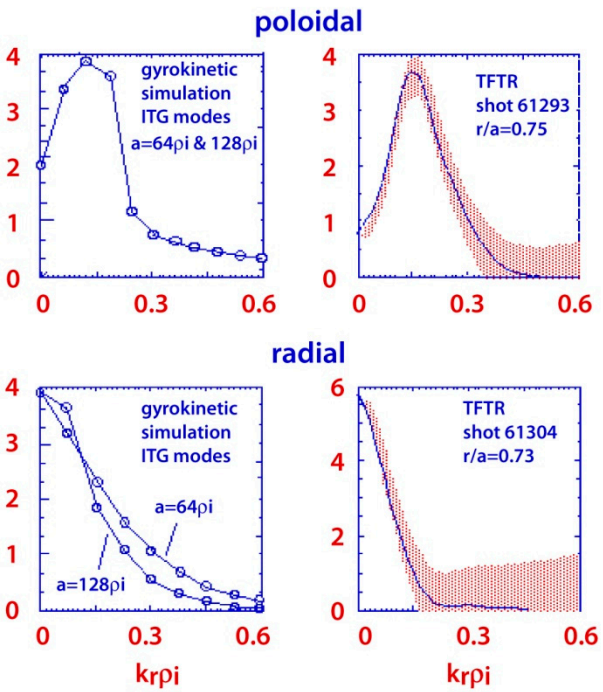
- Parameters
  - Plasma major radius 6.2 m
  - Plasma minor radius 2.0 m
  - Ion gyroradius 2.0 mm
  - Electron skin depth 0.5 mm
- ITER is a dramatic step from today's 10 MW for 1 s with gain ~1 to 500 MW for 400 s with gain ~10
- ITER is the last step before a demonstration power plant, DEMO—a device of similar size and field, but with 2500 MW continuous operation with gain >30
- ITER is an international project to be built in France with US, EU, PRC, Japan, ROK, India, Russia as partners
- The first plasma is scheduled for 2016



Visualization by Klasky, Wang, Ethier

First microturbulence simulation on MPP platforms

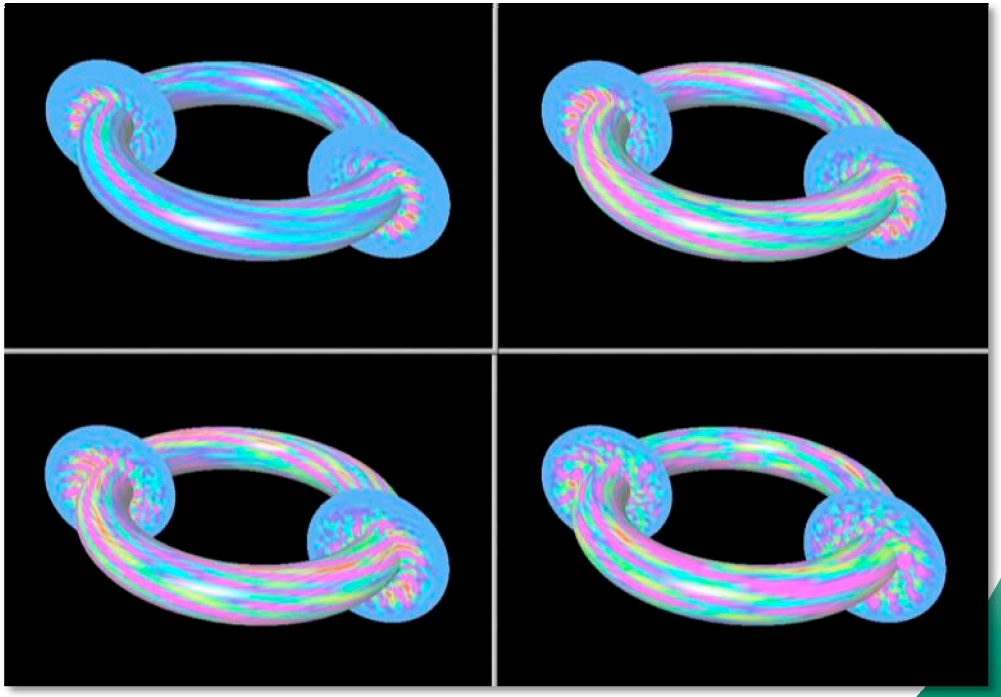
Turbulent spectra in simulation and experiment: $S(k_r)$ and $S(k_\theta)$ in arbitrary units



$\chi_i \propto 1/(k_\perp \rho_s)^2 (\rho_s/a)(cT_e/eB)$ -- Bohm vs. Gyro-Bohm

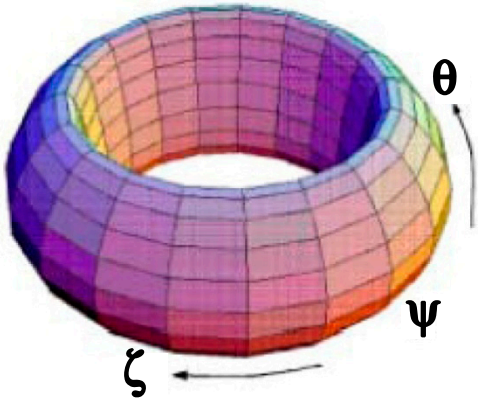
- R. Fonck, et al., TFTR BES measurement, *Phys. Rev. Lett.* **70**, 3736 (1993)
- S. Parker, W. Lee, and R. Santoro, Gyrokinetic Particle Simulation, *Phys. Rev. Lett.* **71**, 2042 (1993)

- **These simulations and experimental observations established the fact that ion temperature gradient (ITG) drift instabilities are one of the main causes for turbulent transport in tokamaks**
- **Using 1 million particles for minor radius, (a)/gyroradius (ρ) = 64 - 128 on C_{90} at NERSC**

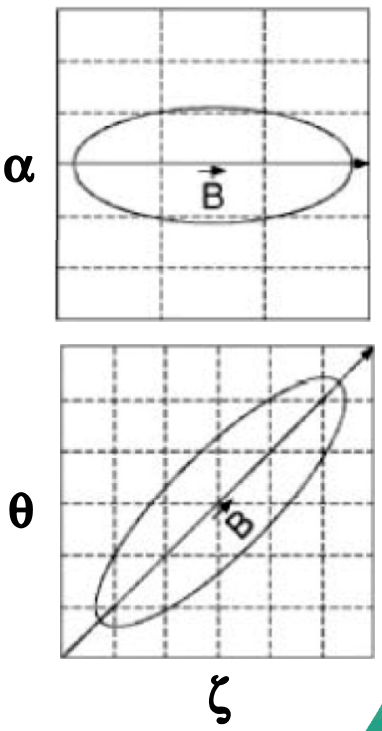


S. Parker, W. Lee, R. Santoro 1993

Global gyrokinetic toroidal particle-in-cell codes



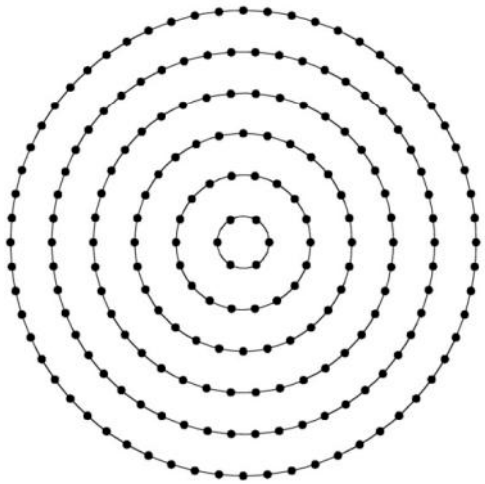
- **Turbulence code with circular cross-section GTC** (Z. Lin et al., *Science* [1998])
- **Magnetic coordinates (ψ,θ,ζ)** (Boozer 1981)
- **Guiding center Hamiltonian** (Boozer 1982; White and Chance 1984)
- **Non-spectral Poisson solver** (Lin and Lee 1995)
- **Global field-line coordinates: (ψ,α,ζ) $\alpha = \theta - \zeta/q$**
  - **Microinstavility wavelength: $\lambda_\perp \propto \rho\lambda_{||} \propto qR$**
  - **With field-line coordinates: grid # $N \propto \alpha^2$: minor radius, $\Delta\zeta \propto R$**
  - **Without field-line coordinates: grid # $N \propto \alpha^3$, $\Delta\zeta \propto \rho$**
  - **Larger time step: no high $k_{||}$ modes**
- **Collisions: e-i, i-i, and e-e**
- **W. Wang, Neoclassical transport code in general geometry: GTC-NEO (2004)**
- **S. Ethier et al., Optimized GTC, *J. Phys.*: *Conf. Series* 16, 1 (2005)**
- **W. Wang et al., Shaped plasmas code in general geometry: GTC-S, *Phys. Plasmas* 13, 092505 (2006)**



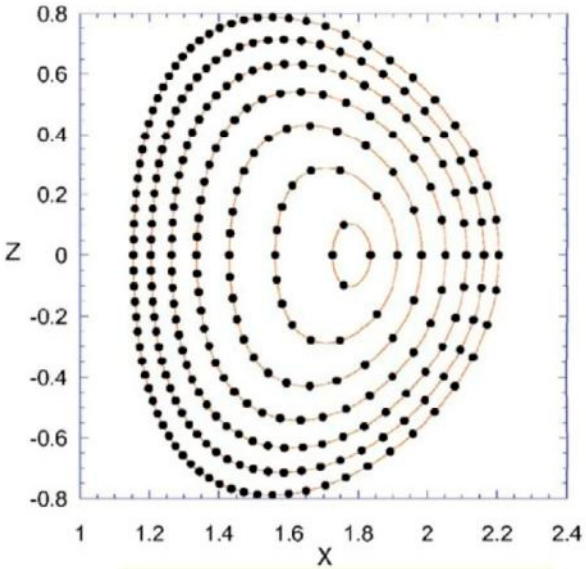
New grid for GTS follows change in gyroradius with temperature profile

- Local gyroradius proportional to temperature $\rho \propto \sqrt{T}$
- Evenly spaced radial grid in new ρ coordinate where

$$\frac{d\rho}{dr} = \sqrt{T_c/T_i(r)}$$



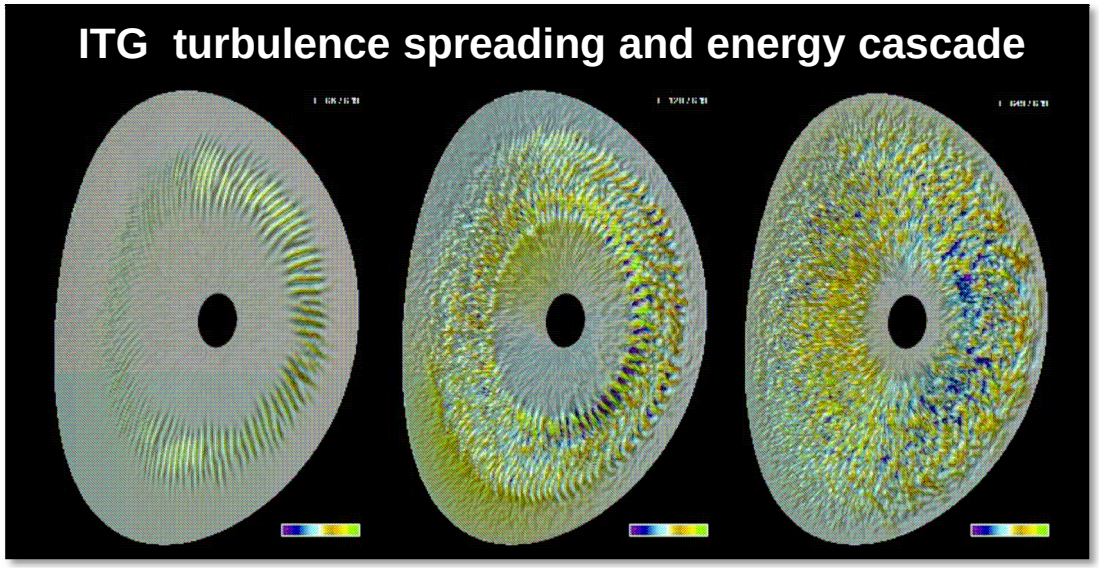
Original GTC circular grid with flat temperature

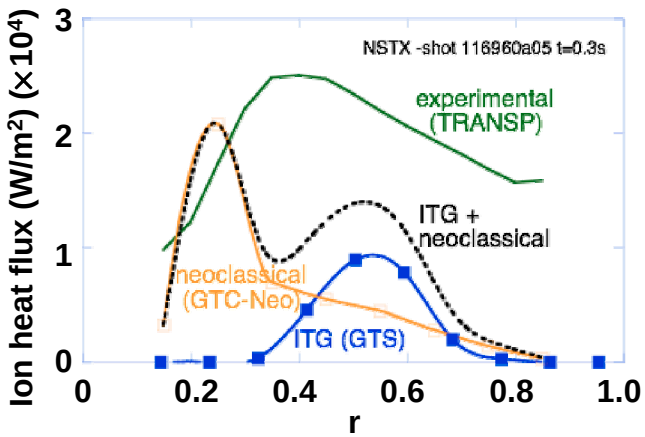


New GTC-S follows (r)

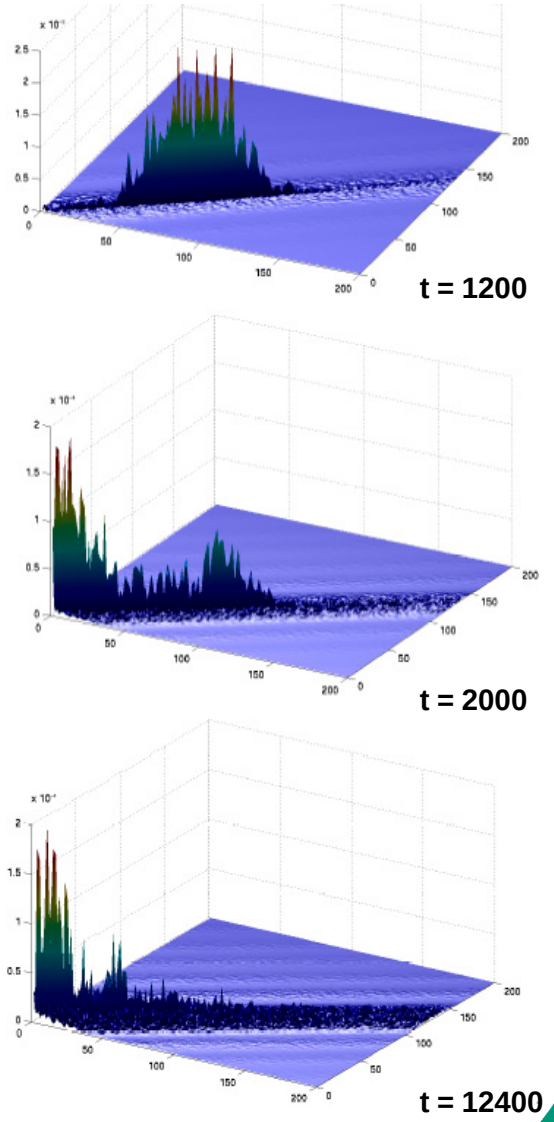
Verification and validation using GTC-S on MPP platforms (2006)

- Global turbulence dynamics in shaped plasmas
- Interfaced with TRANSP and JSOLVER and ESC



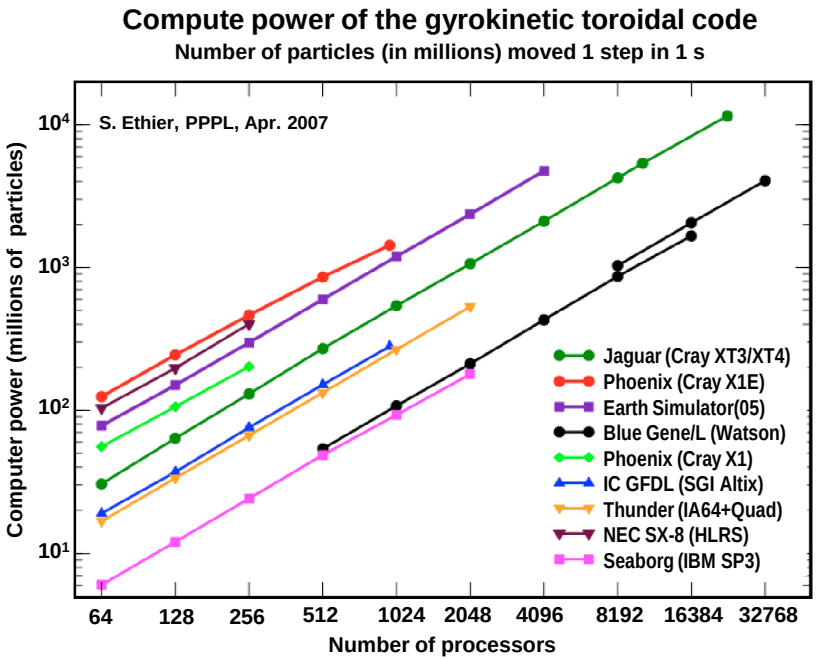


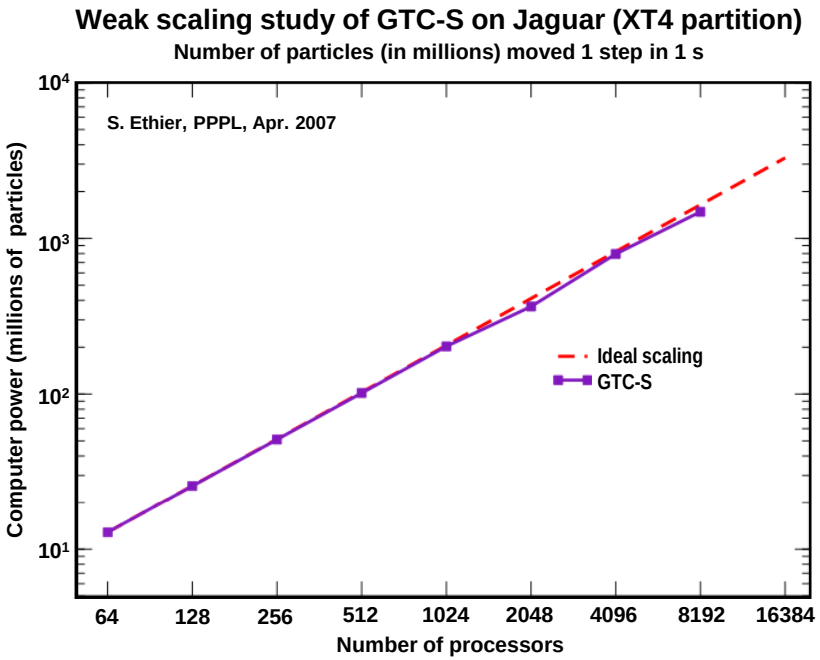
Comparison with NSTX plasmas



W. Wang et al. 2006

Gyrokinetic PIC codes are most suitable for MPP platforms



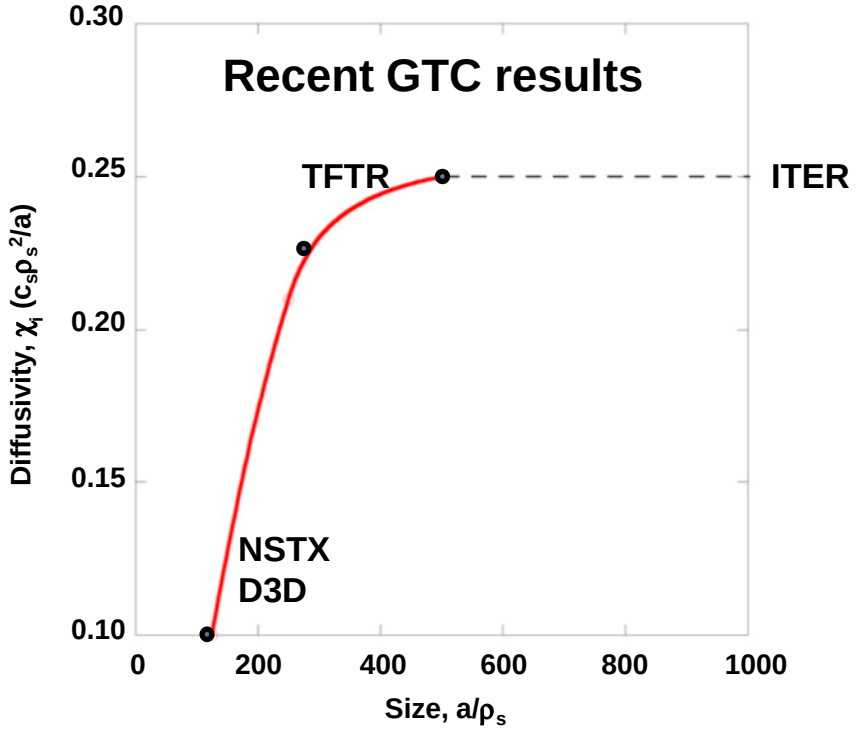


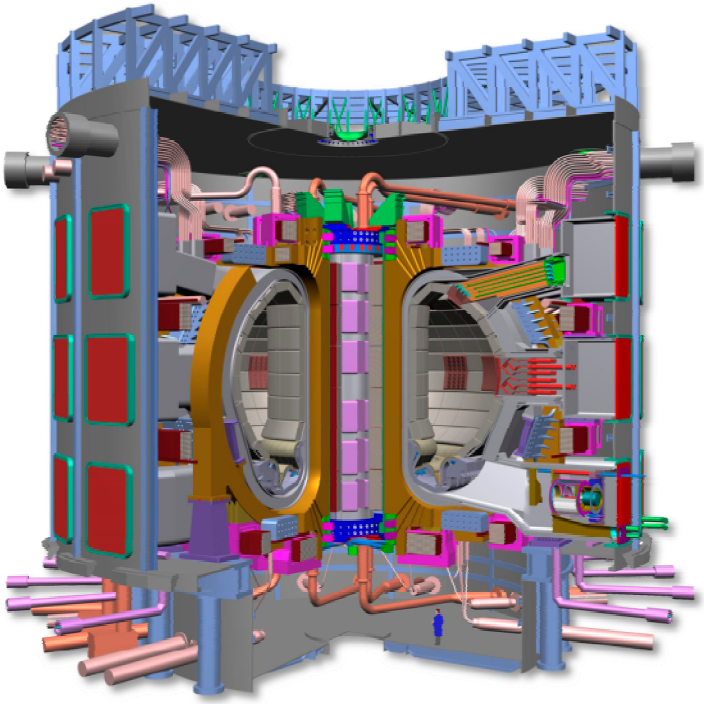
- **GTC is very portable, scalable, and efficient on both cache-based and vector-parallel MPPs**
- **20 TF/s performance has been achieved with 74 billion particles on Jaguar (ORNL) with 22,976 cores and 2.8 times faster than with 32,786 BG/L cores**

- **Participation of GTC-S in Joule applications and 250 TF campaign at ORNL**
- **20 TF/s performance has been achieved with 74 billion particles on Jaguar (ORNL) with 22,976 cores and 2.8 times faster than with 32,786 BG/L cores**

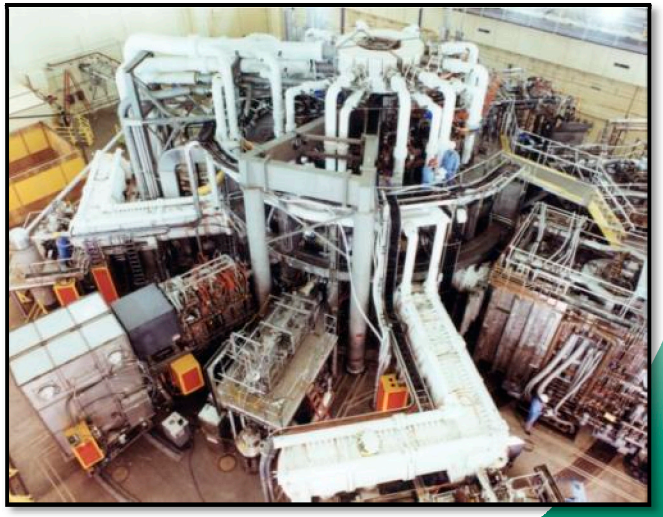
S. Ethier 2007

Petaflop computing is needed to understand scaling trend for ITER

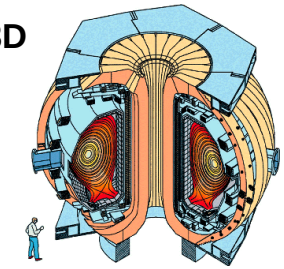




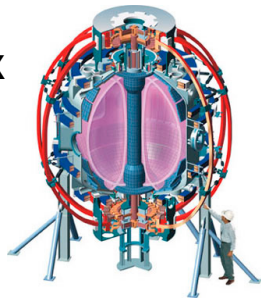
TFTR



D3D

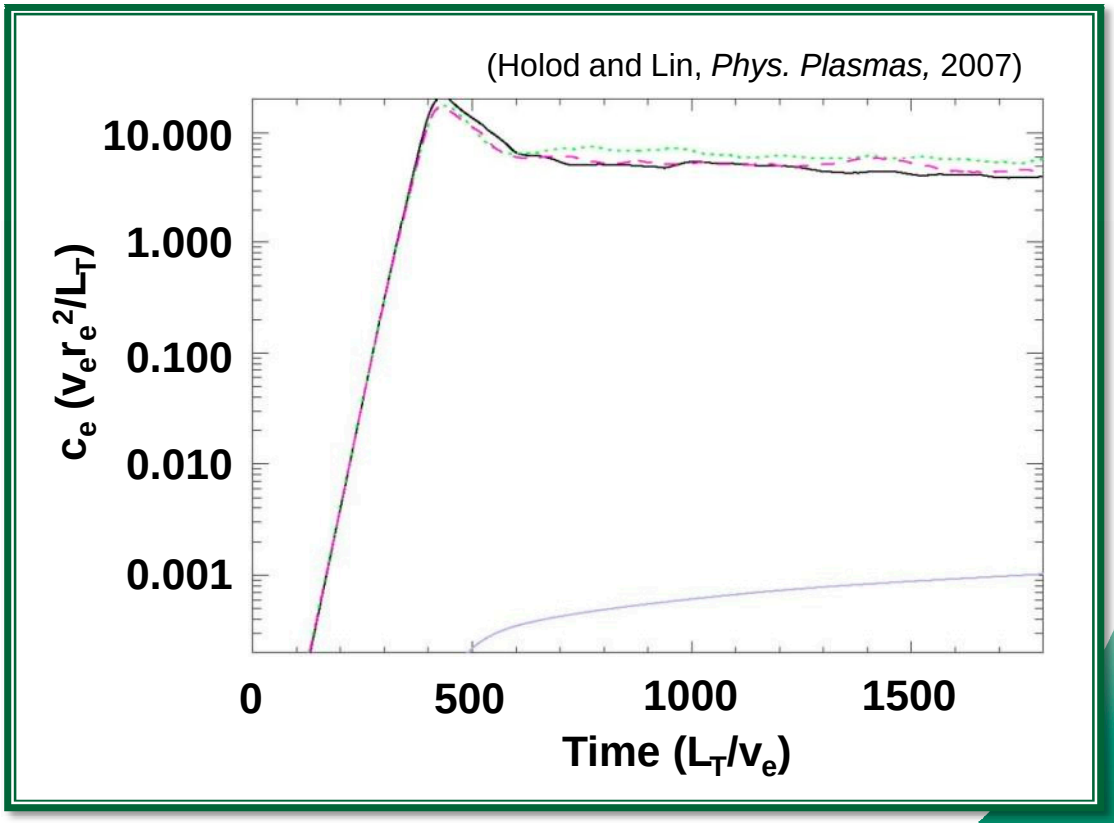


NSTX



GTC nonlinear convergence in ETG simulation

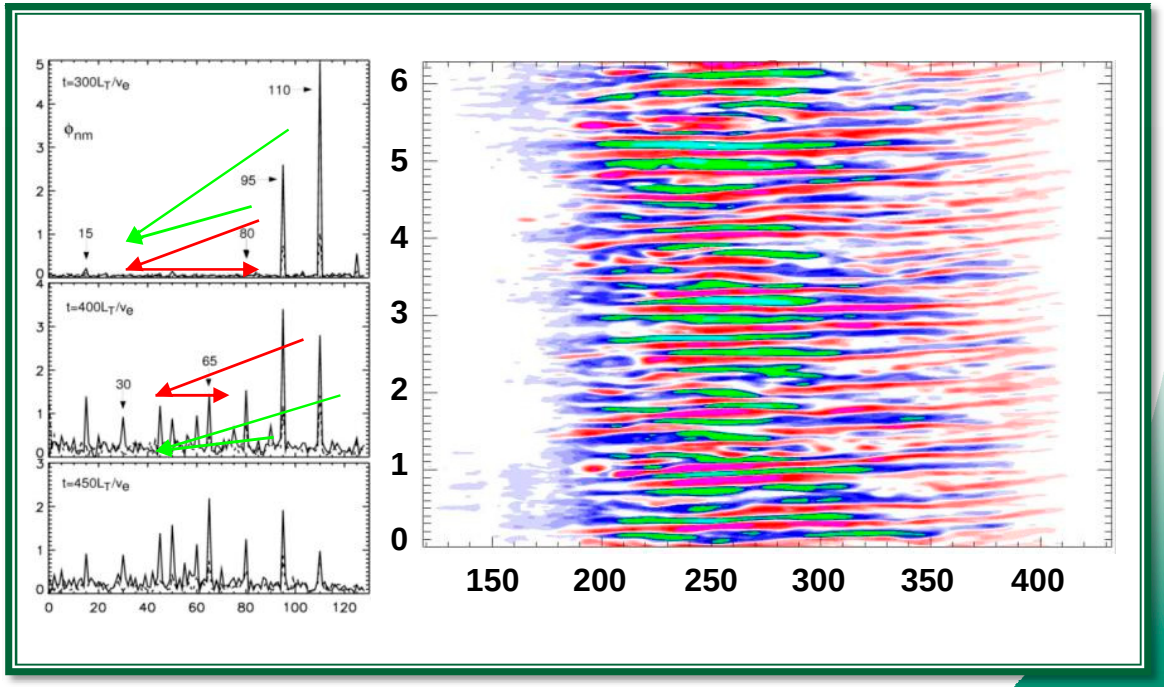
- Convergence from 400 to 2000 particles per cell
  - Cyclone weak case: $R/L_T = 5.3$, $s = 0.78$, $q = 1.4$, $a/r_e = 500$, $g \sim w_r/4$
- Noise-driven flux is 4000 times smaller than electron temperature gradient (ETG)−driven flux
- Noise spectrum in ETG simulation measured. Noise-driven flux calculated and measured; both in good agreement
- ORNL Cray XT4, 6400 PE, 4×10^{10} particles



Saturation and transport mechanisms in ETG turbulence

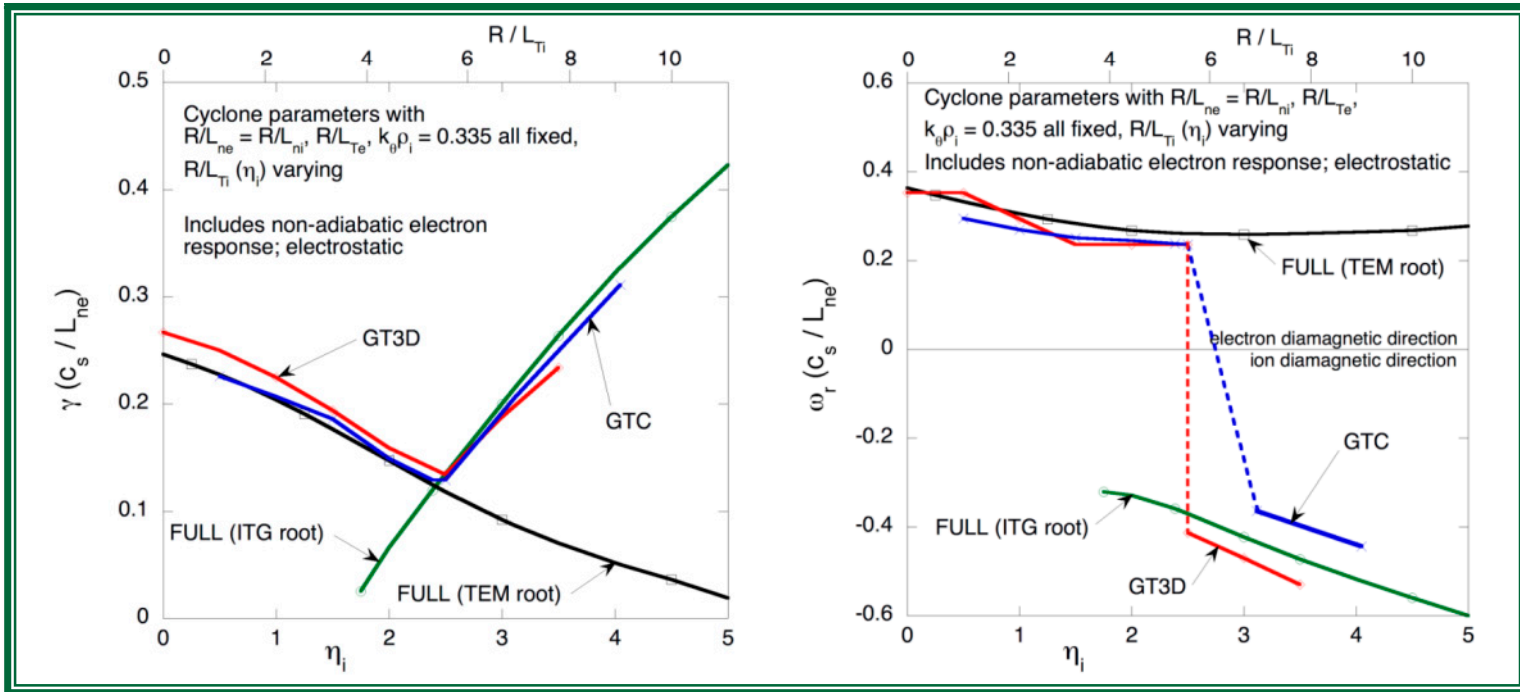
- **Global simulations using GTC find that electron temperature gradient (ETG) instability saturates via nonlinear toroidal coupling, which transfers energy successively from unstable modes to damped modes preferentially with lower toroidal mode numbers** (Z. Lin, L. Chen, and F. Zonca, *Phys. Plasmas* **12**, 056125 [2005]; L. Chen, F. Zonca, and Z. Lin, *Plasma Phys. Contr. Fusion* **47**, B71 [2005])

- **Comprehensive analysis of large data set from GTC simulations finds that stochastic wave-particle decorrelation is the dominant mechanism responsible for electron heat transport driven by ETG turbulence with extended radial streamers** (Z. Lin et al., *Phys. Rev. Lett.* **99,** 265003 [2007])



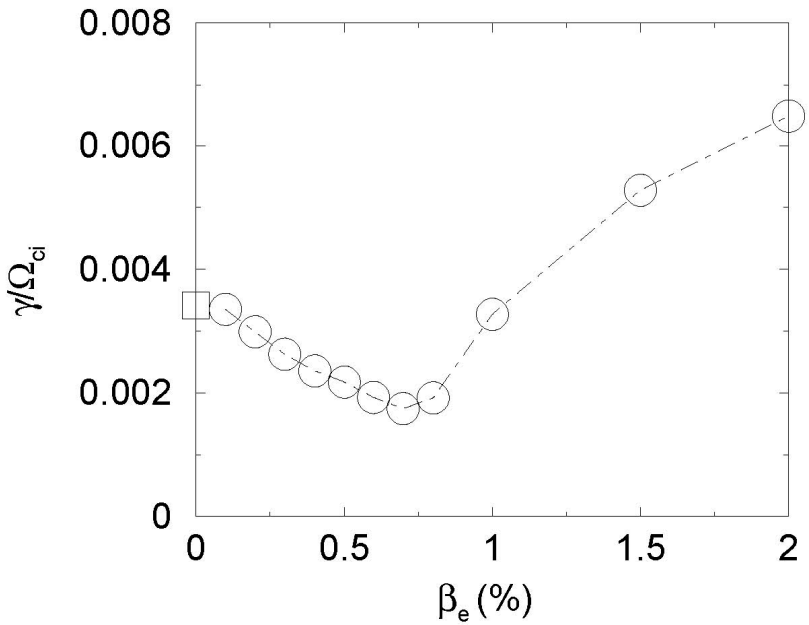
Global GTC simulation with kinetic electrons

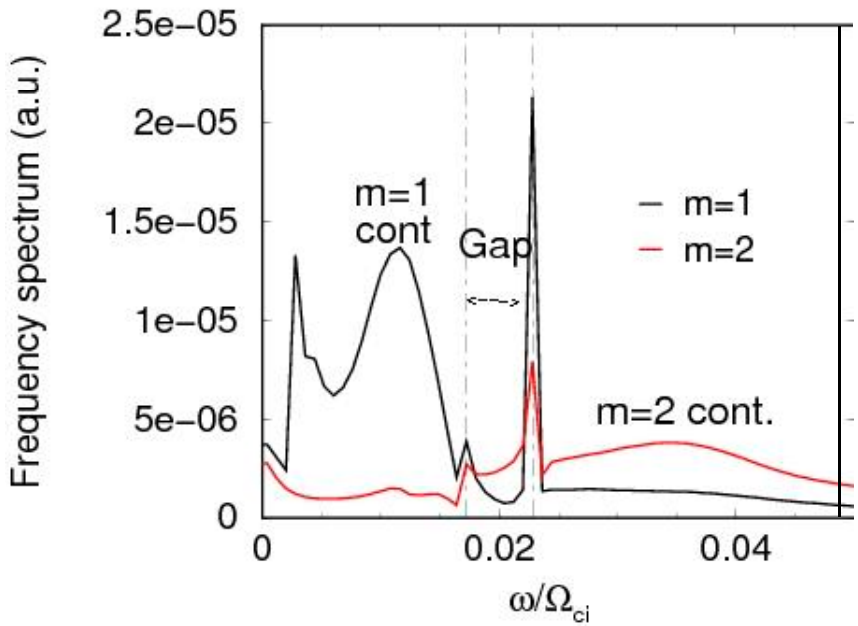
- **Electron response expanded using $\varepsilon = (m_e/m_i)^{1/2}$** (Z. Lin and L. Chen, *Phys. Plasmas* [2001])
- **Approximation: re scales; no inductive $\delta E_{\|}$ ($k_{\|} = 0$)**
- **Model treats rigorously all other $k_{\|} = 0$ modes: electrostatic δE, magnetic δB, zonal flows/fields, all ideal and resistive MHD modes**
- **Model optimal for drift and Alfvenic turbulence on ρ_i scales**
- **Electrostatic ITG/CTEM benchmark** (G. Rewoldt, Z. Lin, and Y. Idomura, *Computer Physics Communications* [2007])



GTC electromagnetic simulation

- **Global GTC electromagnetic simulations demonstrate finite-β stabilization of ITG and excitation of KBM/AITG, Alfven wave propagation in tokamak, continuum damping via phase mixing, and existence of toroidal frequency gap** (Y. Nishimura, Z. Lin, and W. Wang, *Phys. Plasmas* 2007)
- **New science: Nonlinear evolution of micro-meso multiple scales turbulence of toroidal Alfenvic eigenmodes driven by energetic particles using fully self-consistent, global, gyrokinetic GTC simulations**

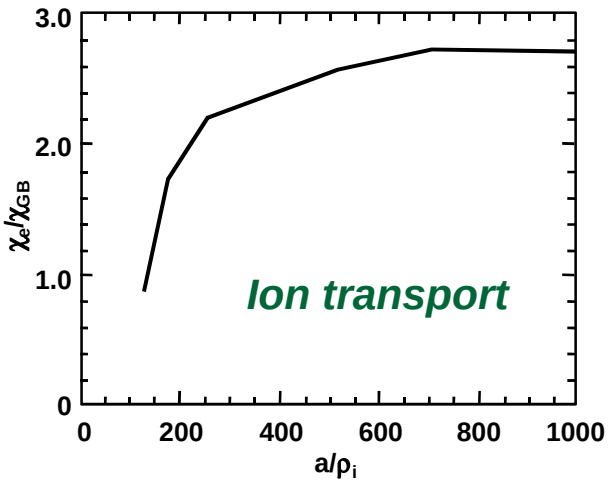


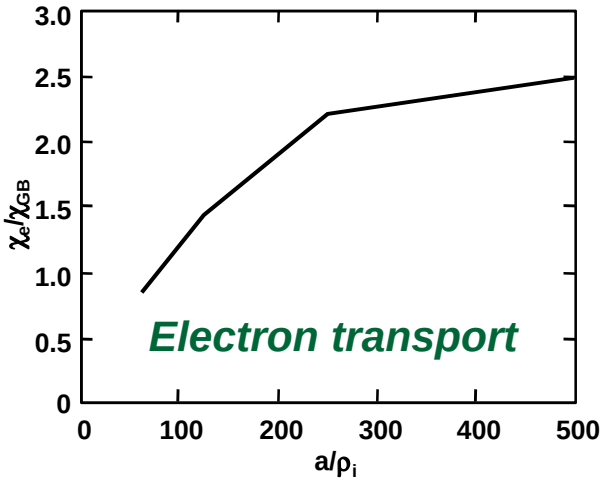


GTC early application: Electron microturbulence in fusion plasma

- "Scientific discovery" transition to favorable scaling of confinement for both ions and electrons now observed in simulations for ITER plasmas
- Electron transport less understood but more important in ITER because fusion products first heat the electrons
- Simulation of electron turbulence is more demanding due to shorter timescales and smaller spatial scales
- Recent GTC simulation of electron turbulence used 28,000 cores for 42 hours in a dedicated run on Jaguar at ORNL producing 60 TB of data currently being analyzed. This run pushes 15 billion particles for 4800 major time cycles

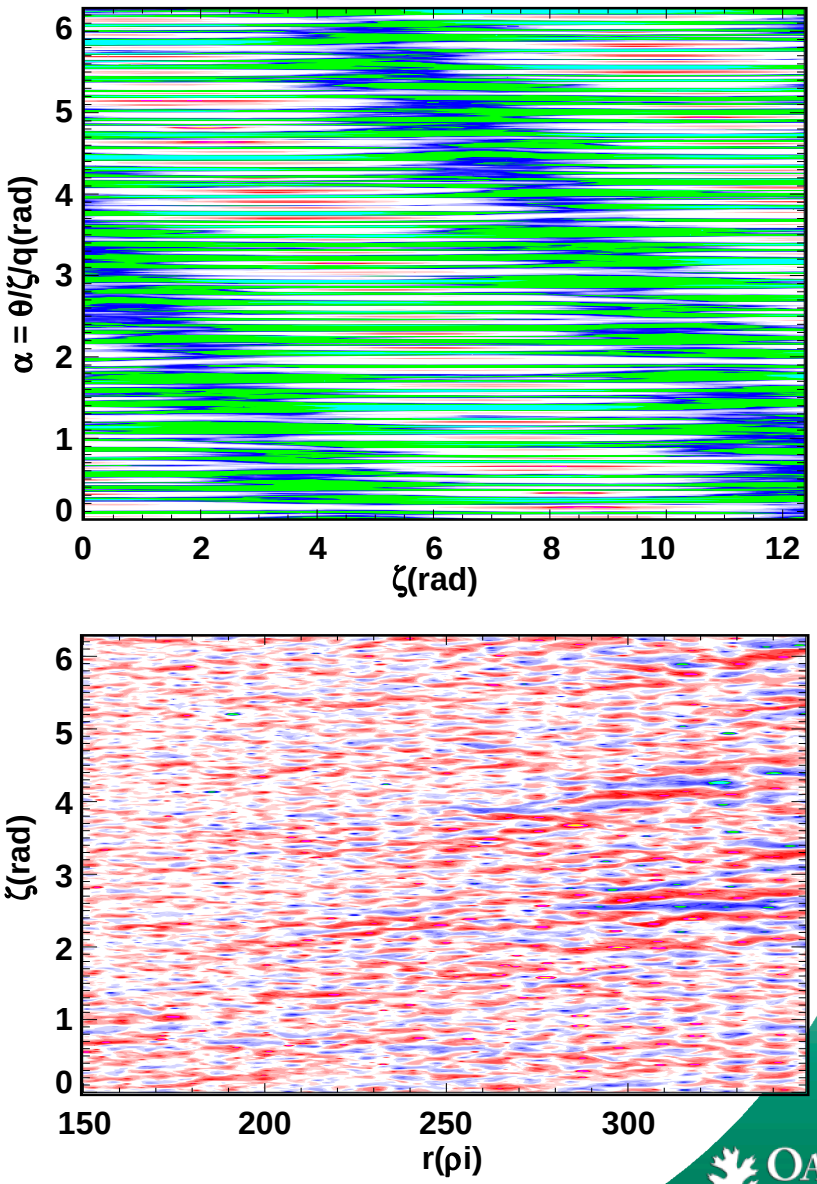
Good news for ITER!





GTC electron microturbulence structure

- Three-dimensional fluid data analysis provides critical information to characterize microturbulence, such as radial eddy size, eddy autocorrelation time
- Flux surface electrostatic potential demonstrates a ballooning structure
- Radial turbulence eddies have average size ~5 ion gyroradius



Computer science challenges of GTC early application

- Run on 93% of Jaguar (28,000 cores) for 42 hours with only 5 node drops
- Apply multilevel parallelism, MPI+OpenMP: 7168 MPI processes between the nodes and each QuadCore opening 4 OpenMP threads; this parallelism is suitable for multiple-core supercomputer
- Produce 60 TB data for post analysis with writing speed of 20 GB/s; the file I/O accounts for only 3% of total running time (ADIOS, Klasky)

Contact

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Near-Term Priorities

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ITER

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November 2003

OAK RIDGE National Laboratory