Extreme Scale Computing with the Fusion Particle Code XGC1

Presented by

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On Behalf of
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Plasma Edge Simulation (CPES)

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CPES

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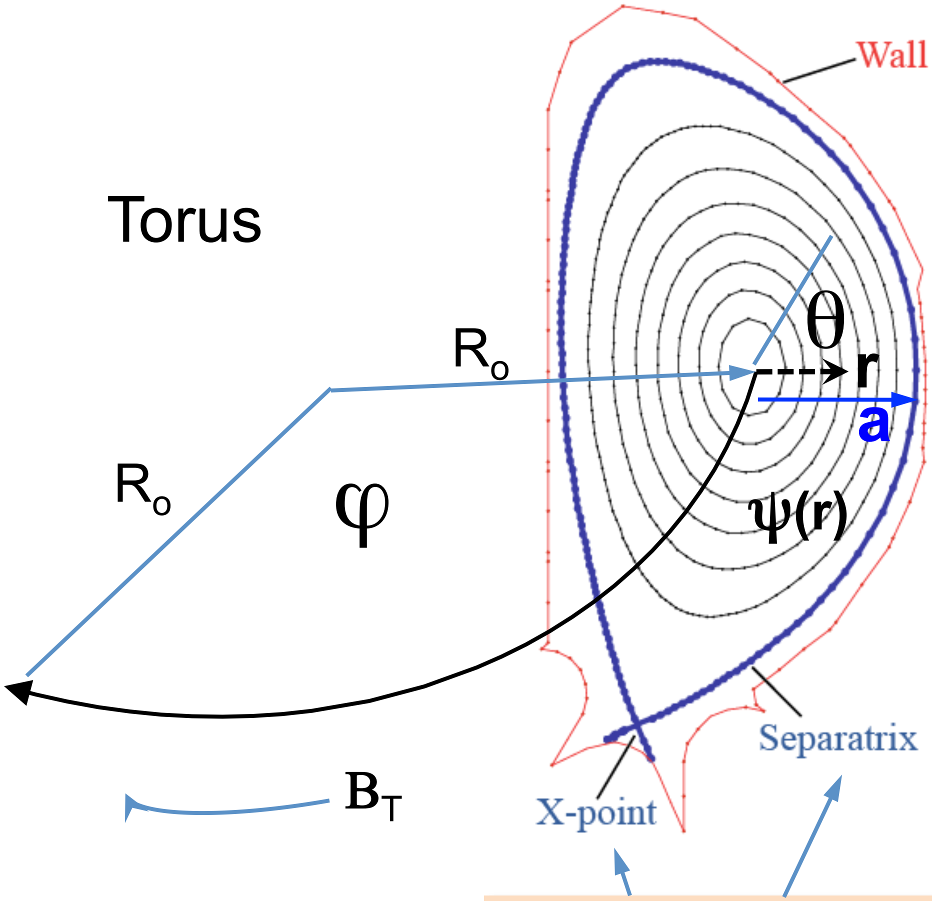
SDM CENTER OLCF Oak Ridge Leadership Computing Facility CPES Center for Plasma Edge Simulation TOPS Terascale Optimal PDE Simulations ADIOS

Introduction

- Tokamak fusion plasma is a gaseous system of charged particles (D^+, T^+ and e^-) that flow along strong magnetic field lines in a torus (called magnetic confinement)
- When D^+ and T^+ ions are hot enough (>10 keV), they fuse together to form α particles (energetic He^{2+}) and release 14 MeV neutrons ($E = \Delta m c^2$)
- Energy from 14 MeV neutrons is used for electricity generation
- Tokamak plasma is subject to
  – Collisional transport enhanced by an inhomogeneous toroidal magnetic field (neoclassical transport)
  – Microscale turbulences and slow loss of plasma
  – Macroscale instabilities and fast loss of plasma
- Assuming that the macroscale instabilities (item 3) are controlled in a fusion reactor

Our simulation performs item 1 and 2 in full-function multiscale in realistic diverted geometry.

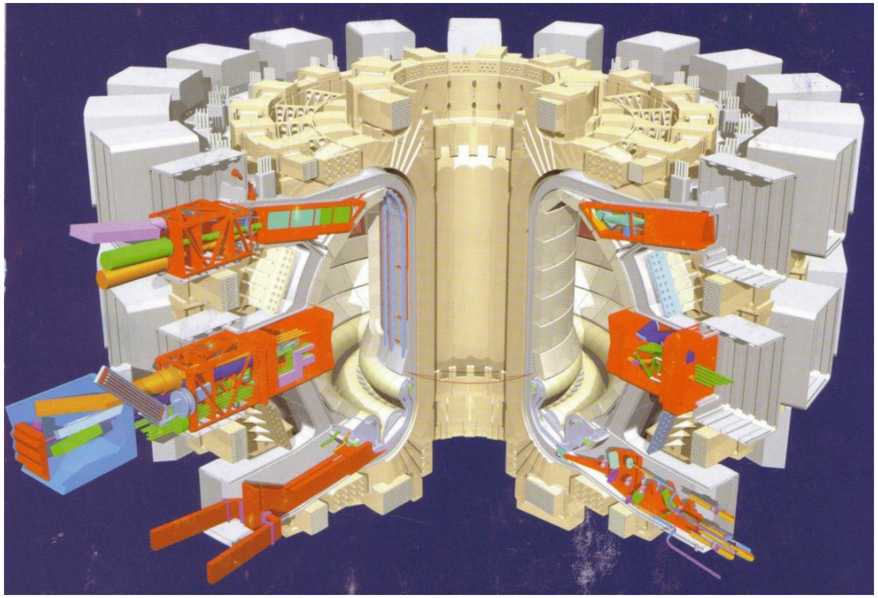
Tokamak geometry



Difficult to simulate: XGC is unique.

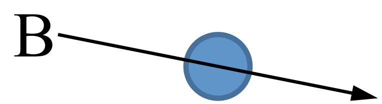
Poloidal cross-section (poloidal plane) at a constant toroidal angle

Poloidal magnetic flux label ψ (r): 1 at r/a = 1; 0 at r/a = 0



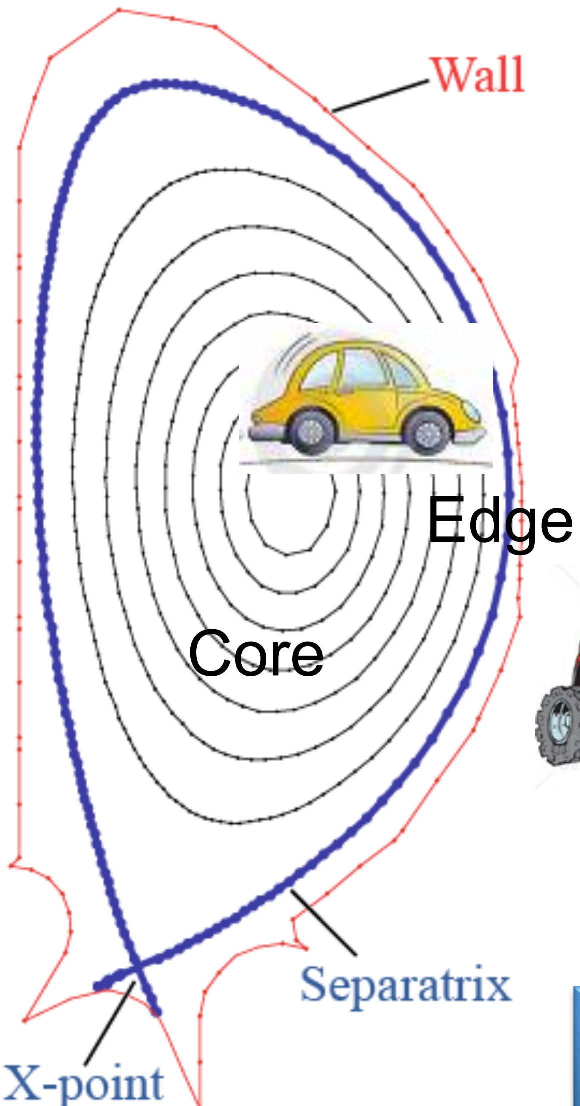
Gyrokinetic particle simulation of fusion plasma

- **Gyrokinetic:** Reduce 6D (x,y,z,v1,v2,v3) to 5D ($x,y,z,v_{||},v_{\perp}$) by assuming that the gyrofrequency is much faster and that the gyroradius is much shorter than the interesting physics scale



- **Particle-in-cell approach:** Solve the marker particle dynamics in 5D space, and solve the Maxwell's equations on 3D position grid
  - Optimal for leadership-class computing (larger device or higher resolution physics → bigger grid → larger # particles → larger # cores)
    - Because particle # per core is limited by memory size
  - Reduced memory requirement via random v-space sampling
  - Statistical particle noise 1/sqrt(N) → smoothing or large enough N (convergence and sensitivity studies are needed)
  - Full-function simulation is needed for solving the background and turbulence dynamics together, and for handling the edge plasma

Difficulty of the whole volume simulation



Higher fidelity physics needs whole volume simulation in full-function: many experimental evidences exist for critical nonlocal core-edge interactions

Magnetic separatrix is a singular surface for core codes which use the easy-to-handle "magnetic" coordinate system

Thus all the gyrokinetic codes stay in the core

- **At a safe distance inside the magnetic separatrix surface**
- **Delta-f perturbed simulation is used in the core**

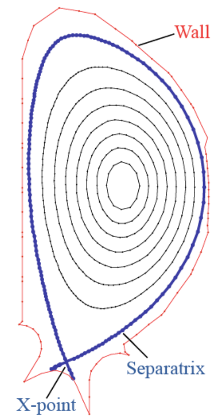
XGC on cylindrical grid is the only kinetic code capable of the whole-volume simulation in full-function.

Understanding the edge-core interaction is critical for fusion

- 30 years of experiments find that the edge plasma condition has a direct influence on the core fusion plasma condition
  - At a much faster information transmission speed than a plasma heat transport speed
    - Overall $\Delta_r T_i$ profile is "stiff," with the core $\Delta_r T_i$ responding to the edge plasma within only several milliseconds, while the plasma heat transport time scale is 10^2 slower
- ITER operation assumes this experimental finding, but an agreeable physics understanding does not exist
- Whole-volume first-principles full-function modeling of background and turbulence dynamics HPC is needed

XGC1 gyrokinetic PIC code
(typically on 30K–220K cores, 1–10 wall-clock days)

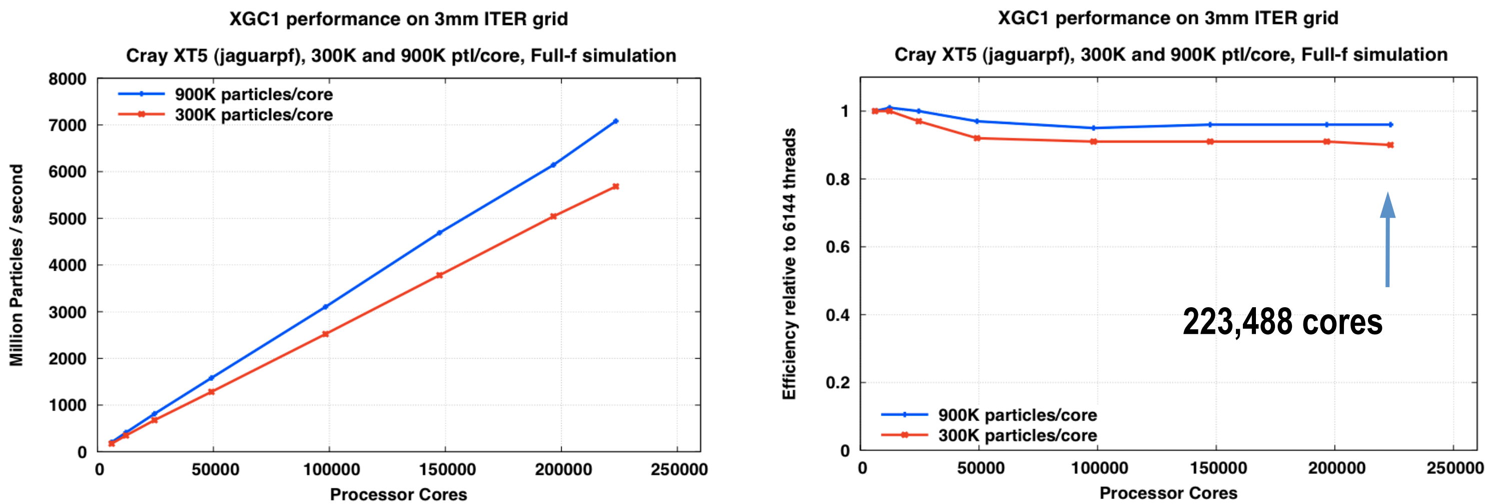
XGC1: full-function (full-f), X-point included Gyrokinetic Code in realistic tokamak geometry across magnetic separatrix surface



- **Spatial simulation domain:** Whole tokamak plasma volume with realistic tokamak edge geometry and Dirichlet wall boundary condition (grounded wall)
- **Unstructured triangular grid:** Particles advance in cylindrical coordinate. Field solver on B-following grid
- **Capability in hand:** Electrostatic turbulence **without scale-separation from mean plasma (ion) dynamics**, with heat source and conserving Coulomb collisions
  - Full-f ions and full-f electrons (for axisymmetric solution)
  - Full-f ions and adiabatic electrons (for turbulent solution)
  - Delta-f ions (for verification against other delta-f simulations)
- **Capability under development: Full-function electromagnetic turbulence**
  - Current electromangetic capability: delta-f

XGC1 scales efficiently to the maximal number of Jaguar cores

12 cores per node, 2 MPI processes per node



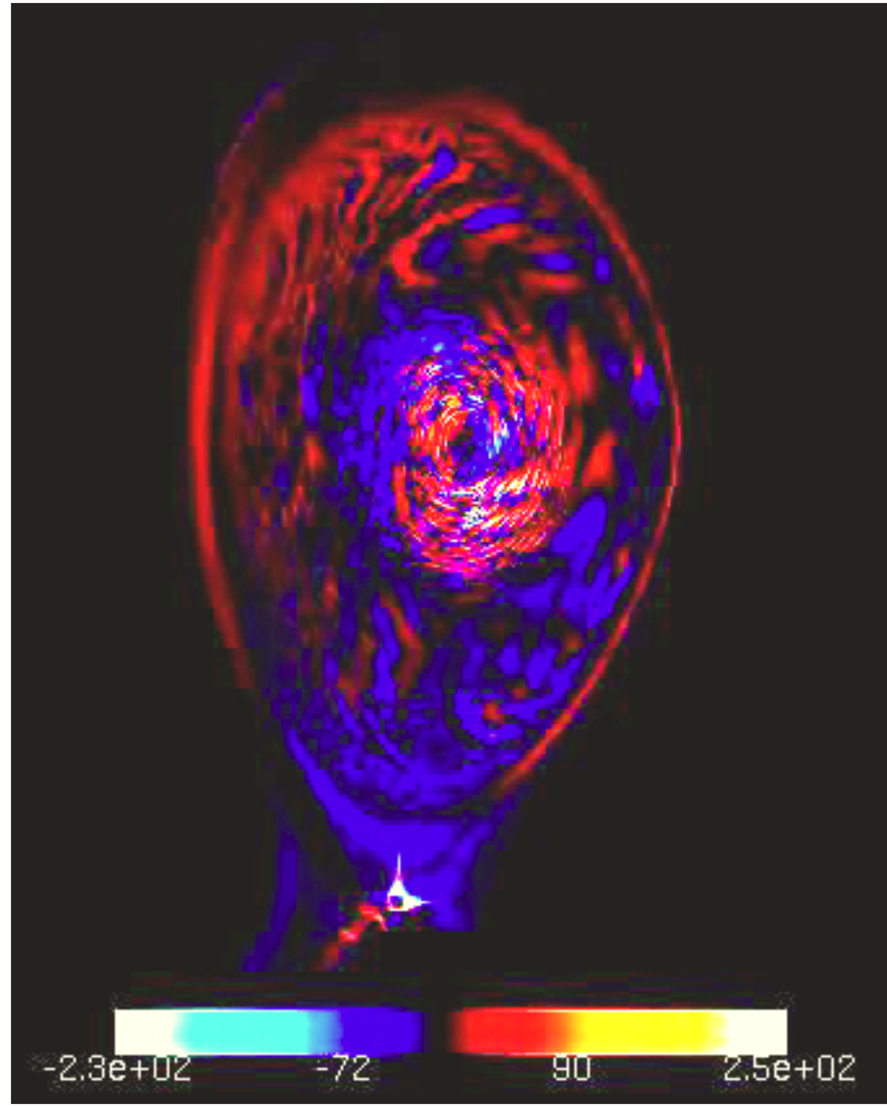
- 900K particles per thread problem is more computationally intensive than 300K problem, which leads to ~20% higher particle push rate
- Performance scaling is excellent for both problems

CY10 Average Job Size and Utilization by Job Size Bins (Jan. 1 – June 27, 2010)

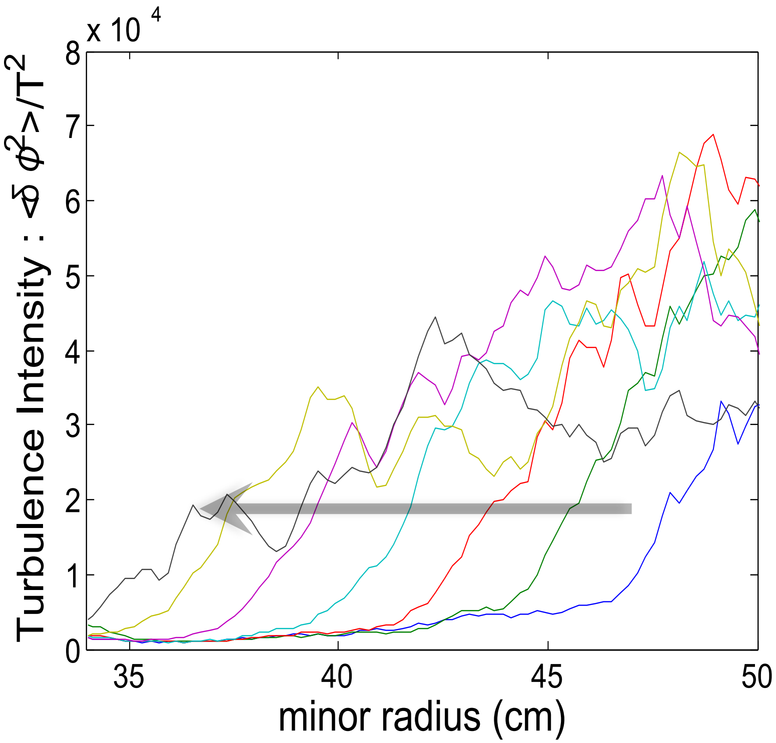
	Average Job Size in Cores	Utilization in Core-Hours
Jobs requesting <20% of the available resources	3,079	8,446,978
Jobs requesting between 20% and 60% of the available resources	66,474	3,042,575
Jobs requesting >60% of the available resources	170,304	14,311,232

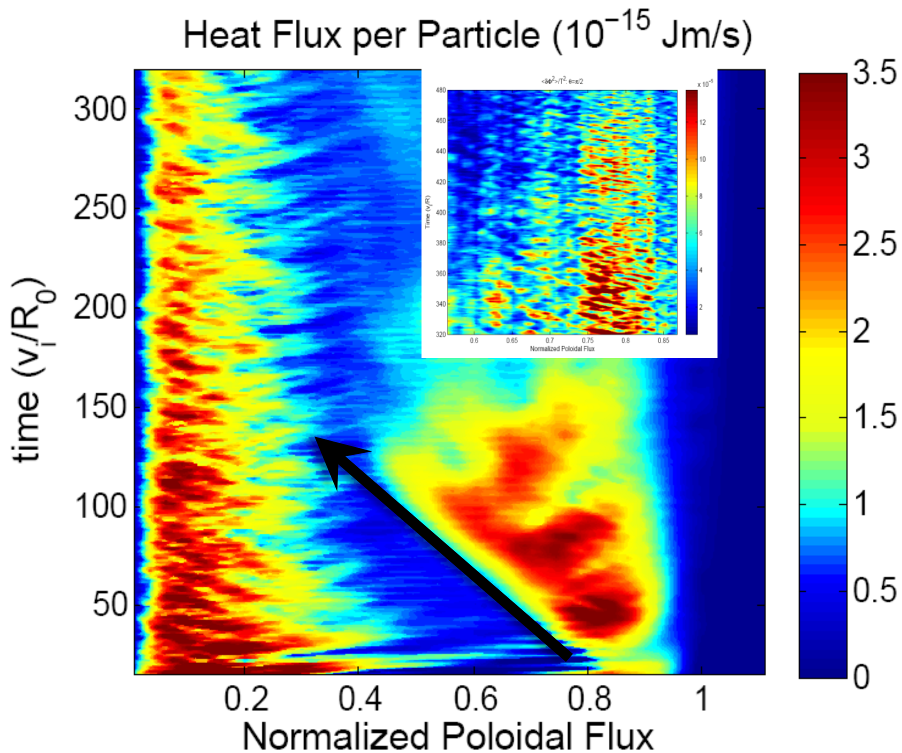
Whole-volume, full-f ITG simulation for DIII-D

- ITG (ion temperature gradient) driven turbulence is the most robust and fundamental microturbulence in a tokamak plasma
- Includes diverted edge geometry and magnetic axis
- Realistic Dirichlet BD condition $\Phi = 0$ on conducting wall
- Heat source in the central core
- This type of simulation is possible only on extreme HPCs will push the edge of future HPC
- Several new scientific discoveries have emerged



Edge turbulence propagates deep into the core and self-organizes the global temperature profile to criticality (SOC)



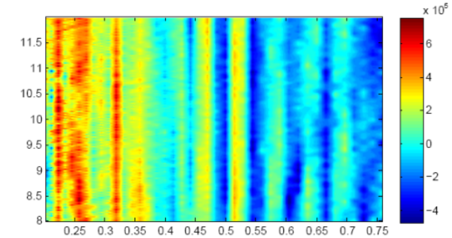


As edge turbulence arrives, local turbulence is aroused/modified and induces adequate heat flux to yield self-organized criticality.

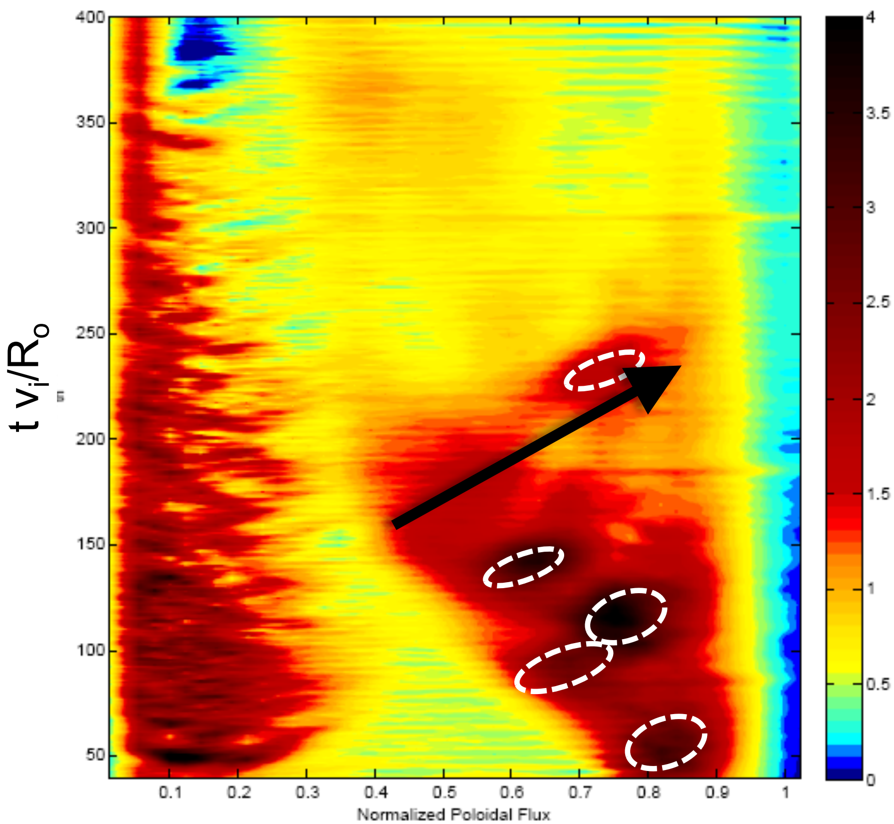
Textbook type of turbulence interaction with self-organized ExB shearing dynamics is observed

Turbulence propagation and heat burst settle down to quasi-steady SOC (avalanching) state in ~3–5 ms

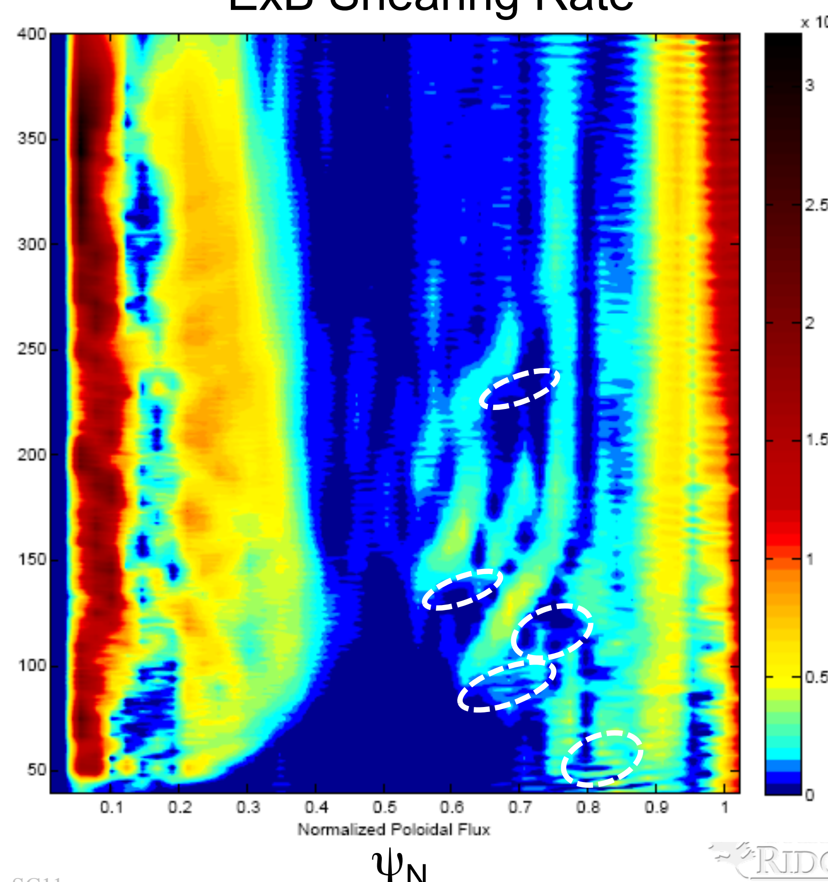
Experimental core-edge interaction time



Heat Flux

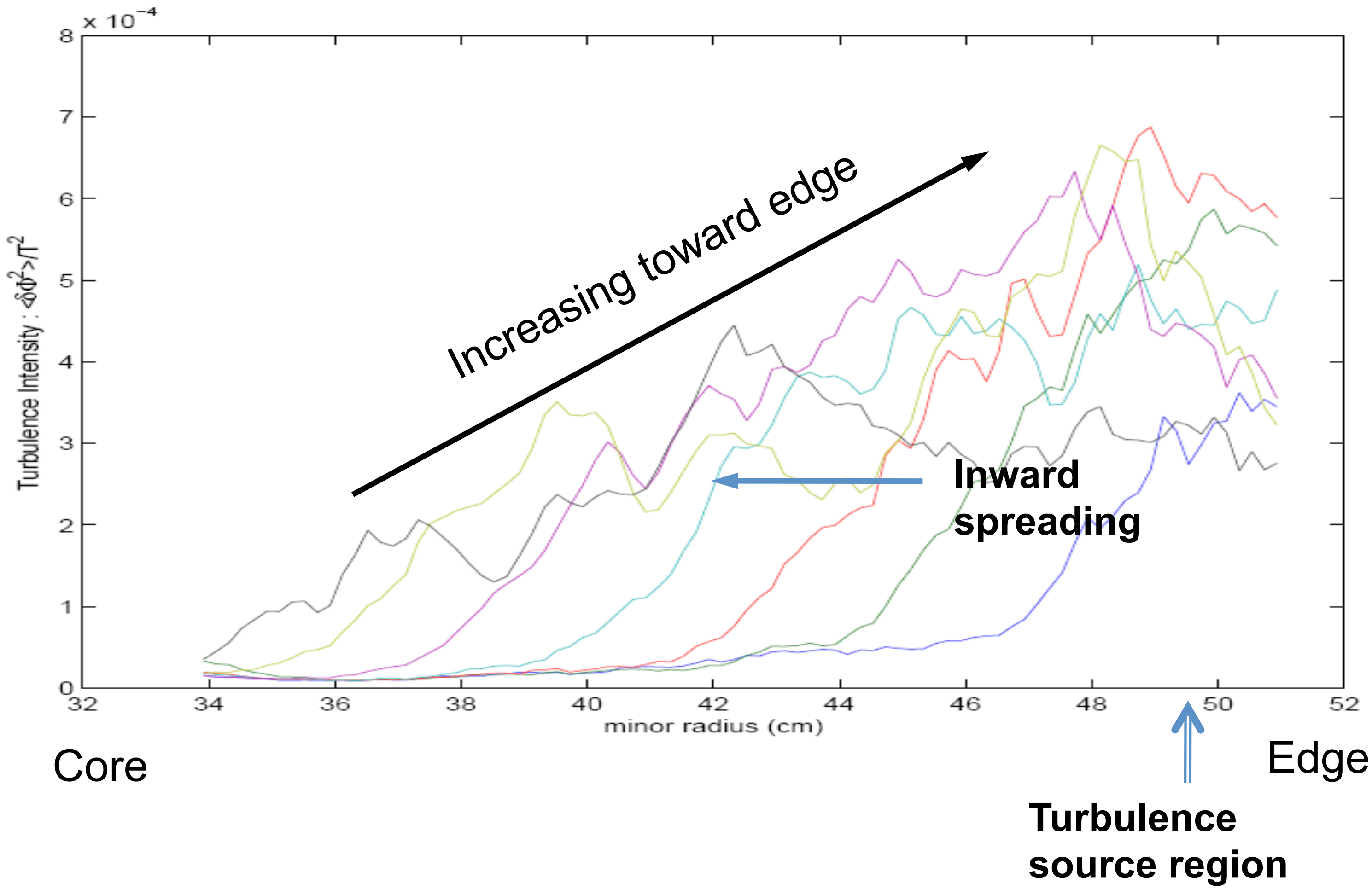


ExB Shearing Rate



Self-organized δΦ2/T2 increases toward the edge

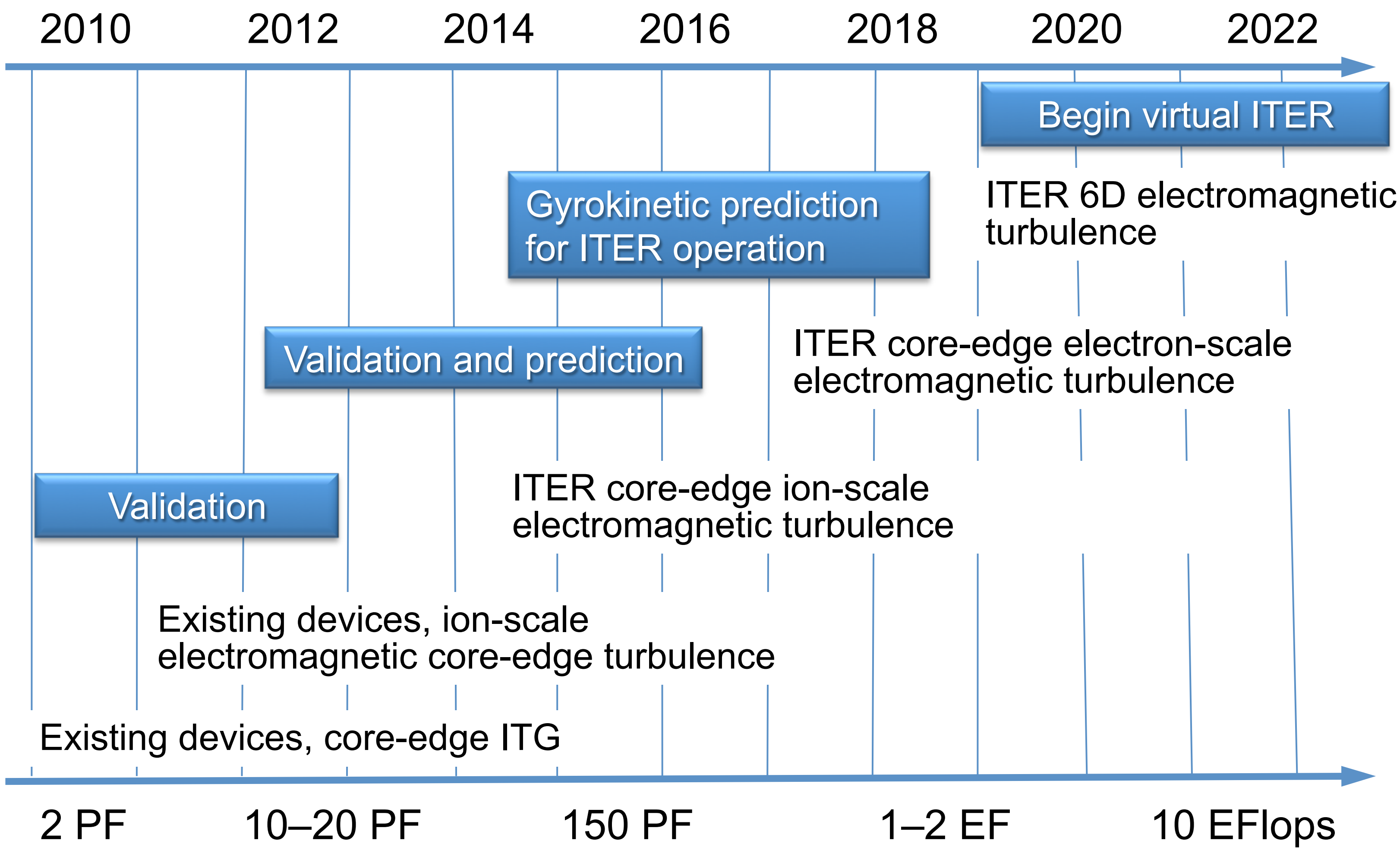
Seen in experiments, but unexplained for 30 years



Looking forward to exascale simulation

- Lack of computing power has been forcing us to study the 6D Vlasov plasma system in the reduced 5D system, restricting the kinetic simulation validity to << gyrofrequency and ≥ gyroradius
- On exascale HPC, the dream of a 6D whole-volume tokamak simulation can be realized but highly challenging: requires close co-design with computer science and applied mathematics
  - Implicit time-marching to avoid CFL trouble with Alfven waves
  - How well can we localize the computation?
  - Efficient in-memory data staging and data analysis
  - Resiliency and fault tolerance?
  - Concurrency issue: dynamics load balancing?
  - How much can we improve I/O?
  - Flexibility to unknown new hardware and programming models

XGC1 roadmap to exascale (1 day run-target)



Conclusion

- **XGC1 is a new generation fusion particle code, efficiently scaling to the maximal number of Jaguarpf cores**
  - Unlike other existing gyrokinetic codes, XGC1 simulates the whole-volume tokamak in realistic diverted magnetic field geometry in full-function (as opposed to the perturbative delta-f)
  - XGC1 performs multiscale background and turbulence dynamics in a single framework
  - XGC1 has already made several scientific discoveries
- **For a higher degree first-principles multiscale tokamak modeling in XGC1, more extreme-scale HPC is needed**
  - XGC1 is getting ready for next-generation HPC with state-of-the-art computational and applied math technologies
- **If an exascale HPC is available in the future, fusion particle code can make a quantum jump into the formidable 6D tokamak physics simulation. An efficient co-design is a necessity**

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