Fusion Plasma Science from Large Scale ab initio XGC1 Simulation

C.S. Chang[1,a], S. Ku[1], R. Hager[1], J. Lang[1], S. Janhunen[1], S. Ethier[1], S. Parker[2], Y. Chen[2], W. Wan[2], M. Greenwald[3], G. Tynan[4], A. Kritz[5], and the EPSI Team[6]

[1]Princeton Plasma Physics Laboratory, [2]U. colorado, [3]MIT, [4]UCSD, [5]Lehigh U., **[6]SciDAC-3 Center for Edge Physics Simulation**

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Outline

- SciDAC Institute Collaboration
- What Science are we studying in EPSI?
- The Fusion Edge Gyrokinetic Code XGC1
- Example Achievements
- Future Direction toward Exa-Scale
- Conclusion and Discussion

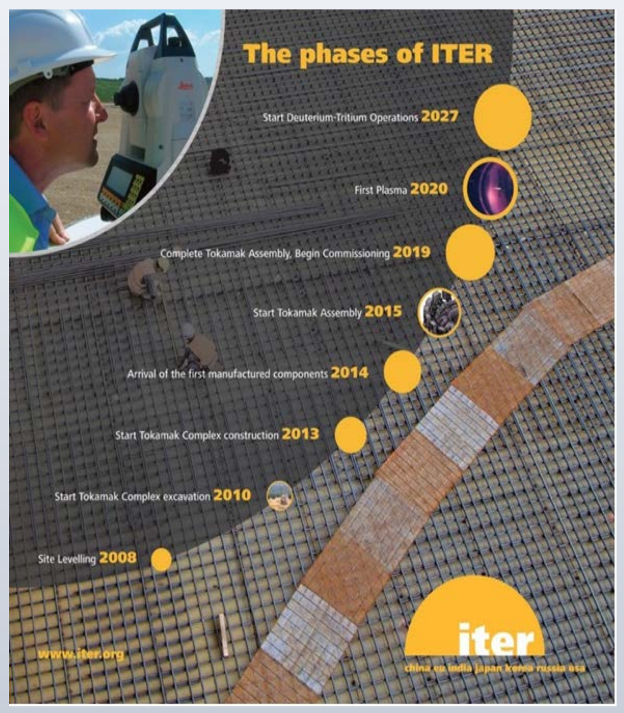
Institute Collaboration

- Fusion edge has a challenging multiscale self-organization problem:
  - The more powerful the computer is, the more ab initio physics we can simulate.
- Inherently requires a close collaboration and innovation with ASCR scientists: *e.g.,*
  - ✧ Development of Adios and DataSpaces
  - ✧ Improvement of Solvers and Algorithm
  - ✧ Improvement of Meshing
  - ✧ Enhancement of Code Performance on LCFs
  - ✧ Perform UQ on extreme scale simulation

EPSI-Supported Liaisons with SciDAC Institutes

FASTMath	QUEST	SDAVE	SUPER
M. Adams M. Shephard	R. Moser	S. Klasky M. Parashar	P. Worley Ed D'Azevedo

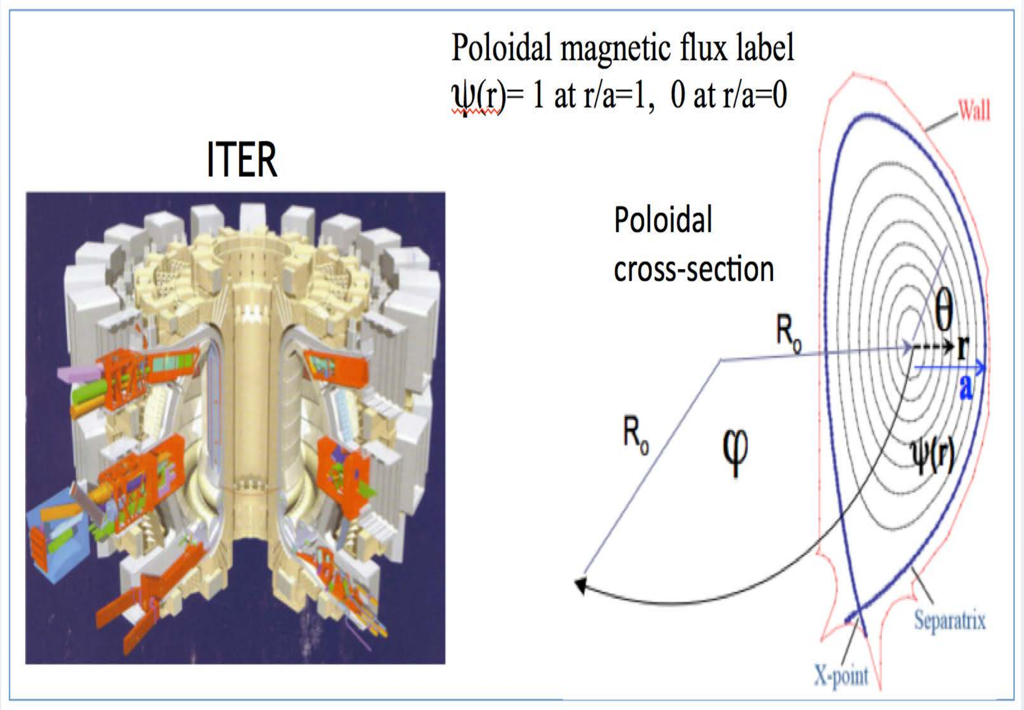
ITER schedule is well-aligned with exascale roadmap



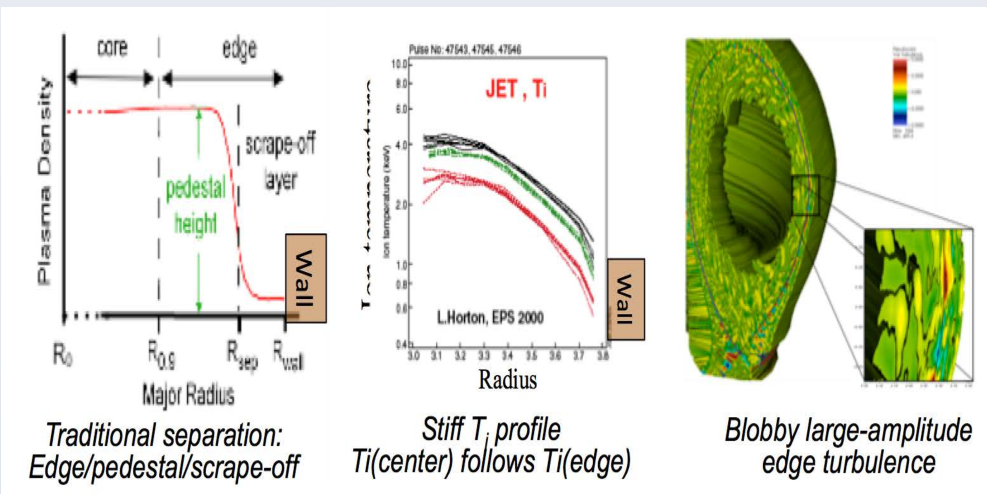
Future: Exa-scale whole-device simulation of fusion reactor ab initio

Present:
- Extreme scale Plasma physics simulation.
- More compute power → more physics.

Tokamak Geometry



What science are we studying?



- Found experimentally that edge plasma self-organizes into a steep pedestal shape (H-mode).

→ Smaller & cheaper tokamak, by allowing a hot plasma at plasma edge

- Why does the H-mode occur?
- Property of a pedestal plasma?
- Edge plasma physics is a challenging issue: Plasma and turbulence across steep gradient, and in direct/indirect contact with material wall.
  - **non-equilibrium thermodynamics ≠** Maxwellian
    - →Must solve kinetic equation.
  - Large amplitude nonlinear coherent turbulence, "blobs," interact with background plasma and neutral particles in multiscale.

The XGC1 approach

- Solve the non-equilibrium, multiscale problem in the whole plasma volume using **ab initio kinetic** equations (Vlasov eq. with Fokker-Planck collisions)
- Simulate **realistic physics**, magnetic **X-point, odd wall shape, sources and sinks, atomic physics**

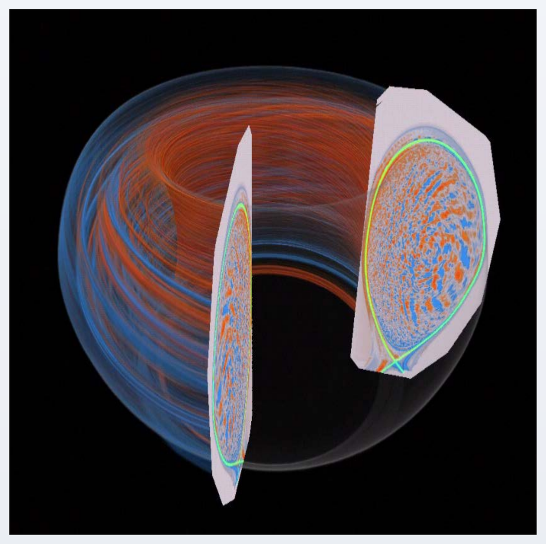
→We choose the particle-in-cell approach
- **✧More stable to CFL than PDE approach**
- **✧Lower memory requirement than a PDE approach in higher dimensional space**
- **✧Easier to parallelize**
- **✧Easier to handle the plasma wall interaction**

→Inherently expensive: physics is limited by compute-power

- The PDE E&M field solver: ~ 5% compute time

Whole-volume simulation achieved in 2009

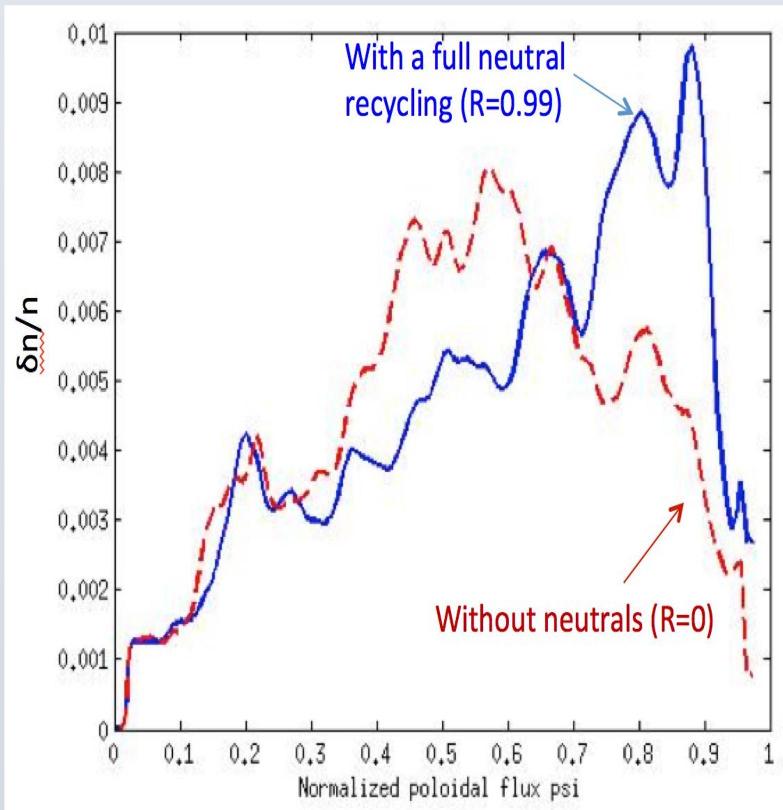
ASCR Joule Metric: ASCR scientists enabled XGC1 to scale linearly to Maximal JaguarPF (~1.5 pF)



- For the first time, whole volume a tokamak plasma was simulated to quasi-steady turbulence saturation
  - In realistic diverted geometry
  - Ion turbulence, background plasma dynamics, and neutral particle recycling.
- Multiple new physics found, and propagated through out the fusion community
  - 15 International invited Talks
  - 14 Journal publications

Earlier discovery example

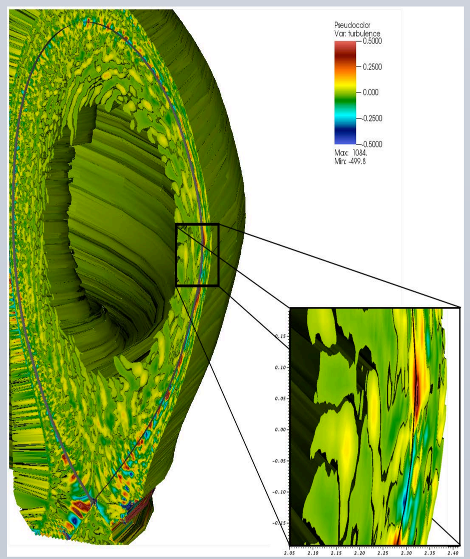
Experiments claims, for over 30 years, that a good wall-conditioning is a prerequisite to H-mode transition.
- XGC1 discovered that the less neutrals from wall lowers the turbulence intensity in edge



Recent Breakthrough

Heterogeneous Titan, under ASCR collaboration, allowed addition of kinetic electrons to XGC1: requires much faster HPCs → ab initio simulation of "blobs" for the first time through 2013-2014 INCITE, **using up to 88% CPU-GPU Titan (16,384 nodes~20pF)**

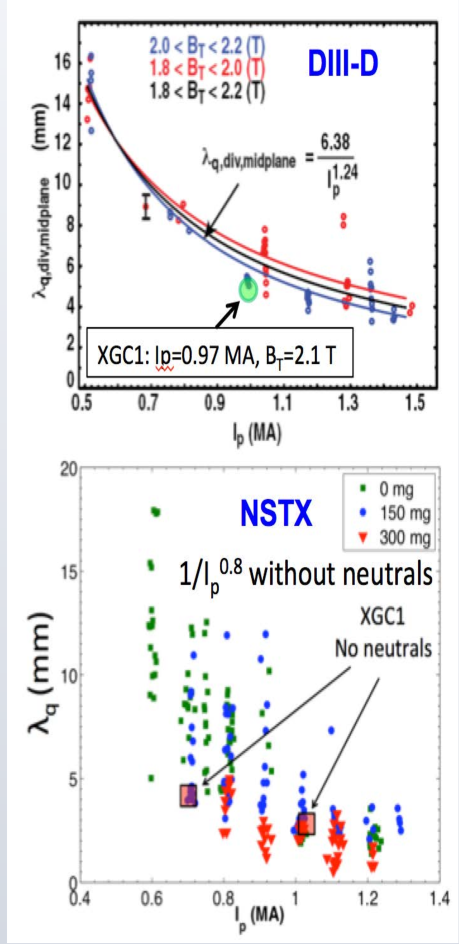
Experiments shows edge turbulence is "blobby"
- Large amplitude density and potential blobs (~50%)
- Theorists could only use simple models to explain how the blobs could occur.
- OLCF Featured Highlight, in 2/2014



Visualization by D. Pugmire

Several international invited talks already including 2014 IAEA Fusion Energy Conference

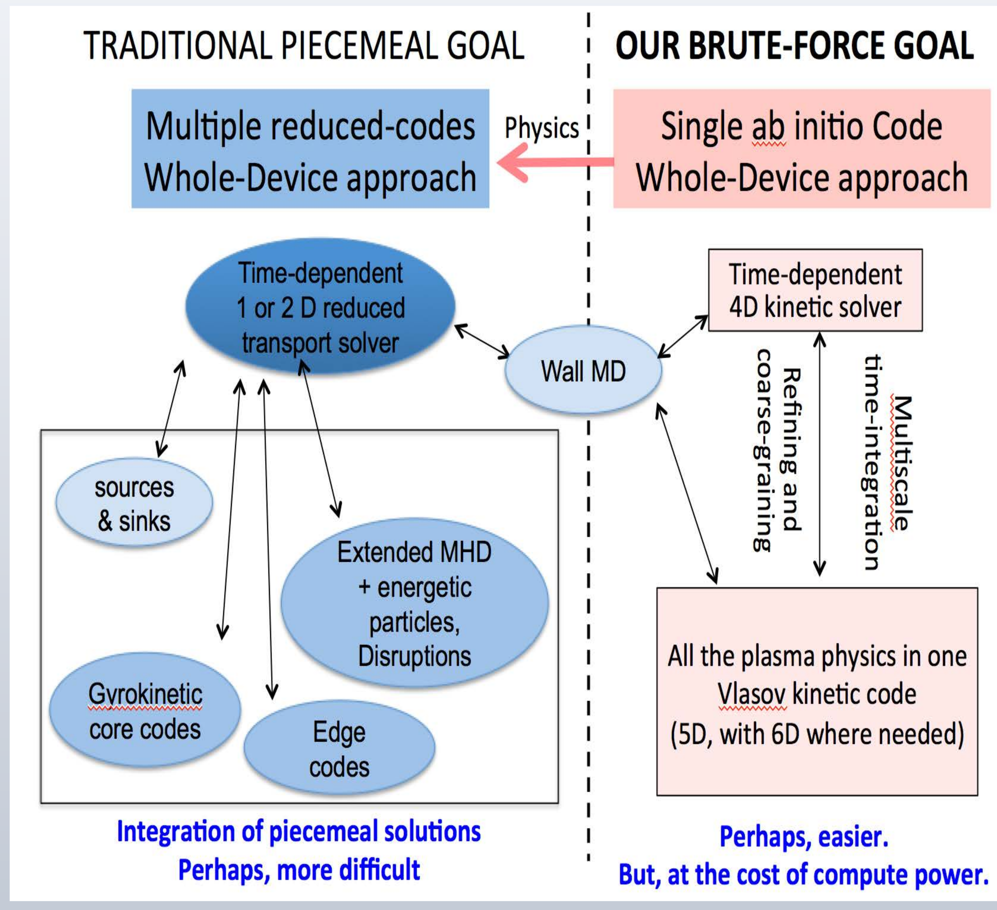
XGC1 tries to predict divertor heatload



- ITER's divertor heatload width $\lambda_{q,mid}$ would be ~1 mm (when mapped back to outboard midplane), if extrapolated from the present devices $\propto 1/I_p$.
- However, we do not fully understand what sets the heat load width.
- A huge question: Will the simple extrapolation to ITER valid?
- $\lambda_{q,mid}$ from XGC1 agrees with experiments on the present tokamaks.
- Broadening of $\lambda_{q,mid}$ by blobs (width >1cm) has been found to be insignificant in the present machines.
- Will the blobs saturate the $1/I_p$ scaling when $1/I_p$ becomes ~ 1mm?

Simulations are in progress to add more numerical points to validate predictability.

Ultimate Goal: Ab initio Numerical Fusion Reactor



Enough Compute Power for the Goal?

- Present: ~10 pF, Future: ~1 exa F → **100X**
- Code could become ~5X faster from the combined hardware (e.g., host-integrated accelerators) and algorithm improvements

→500X effective compute power

- DIII-D → ITER: requires 10X compute power for the same physics
- Thus, we could include **50X** more physics in the ITER simulation on exascale computers than what we do now on the present devices
- By 2018, with **10X** compute power on Coral, we could include **5X** more physics in ITER simulation than what we do now on the present devices.