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Harnessing OLCF HPCs for
High-fidelity Simulation of Tokamak Edge Plasma Transport

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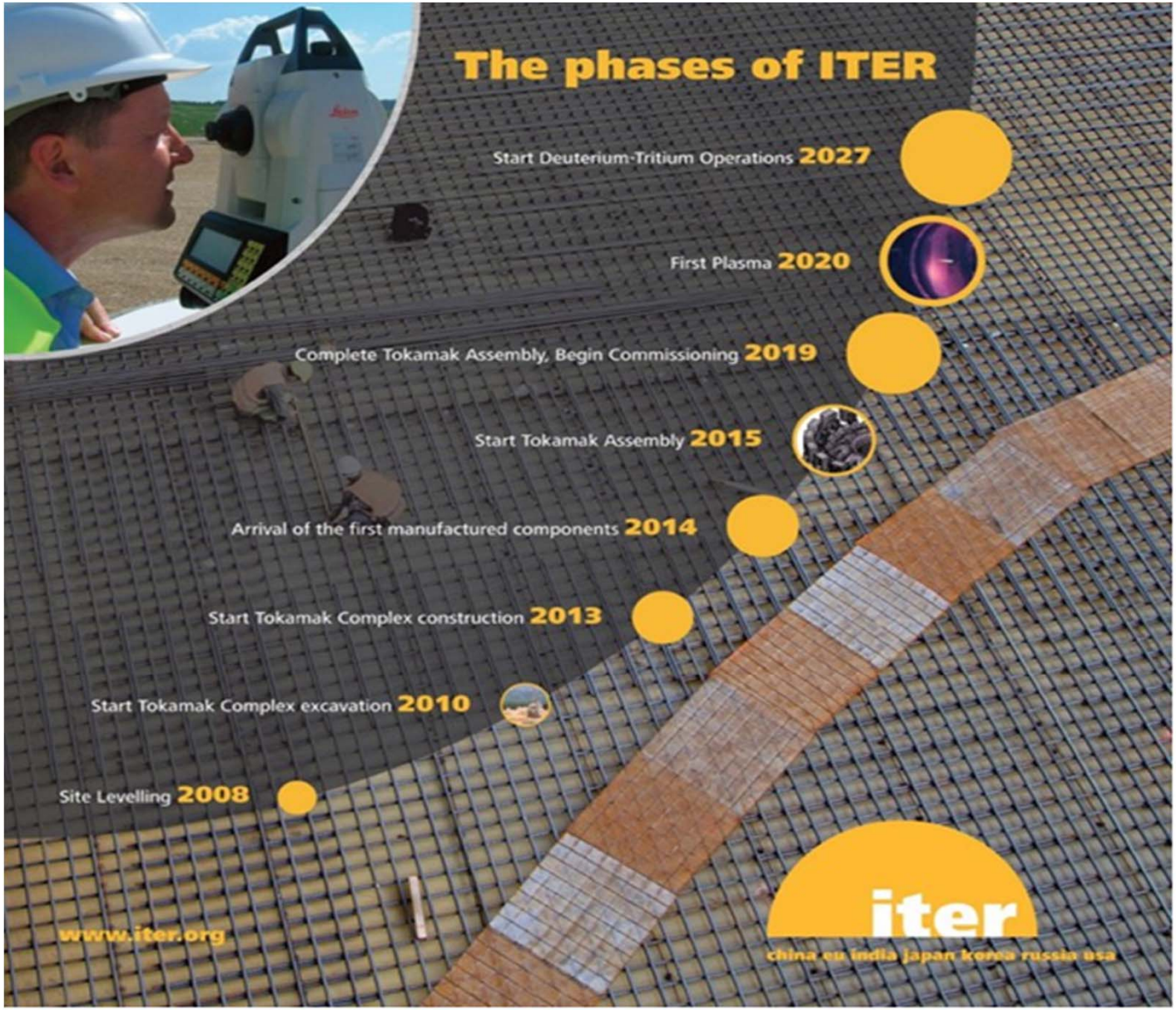
For
SciDAC-3 Center for Edge Physics Simulation

EPSi
Edge Physics Simulation

Outline

- What Science are we studying in the SciDAC EPSI?
- The Fusion Edge Gyrokinetic code XGC1
- Example achievements as OLCF user
- Future direction toward exa-scale
- Conclusion and Discussion

ITER schedule is well-aligned with Exascale Computing plan

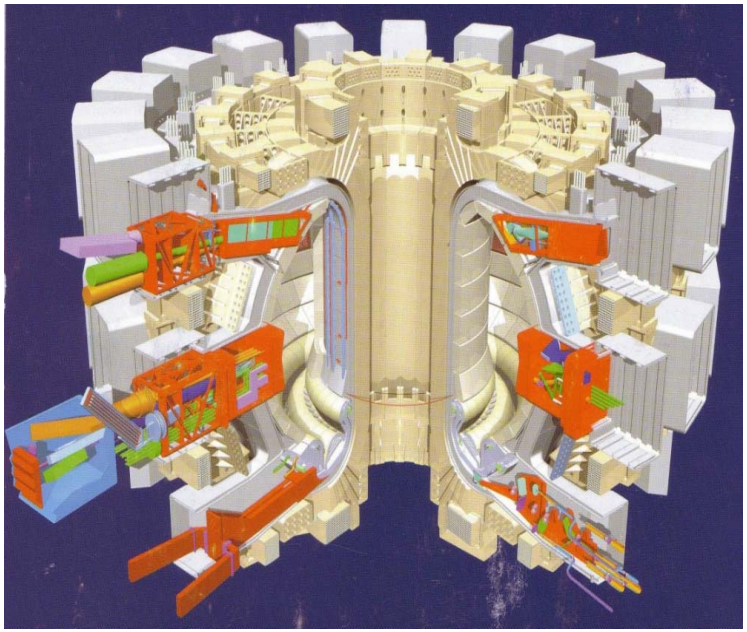


Future: Exa-scale whole-device simulation of burning plasma ab initio

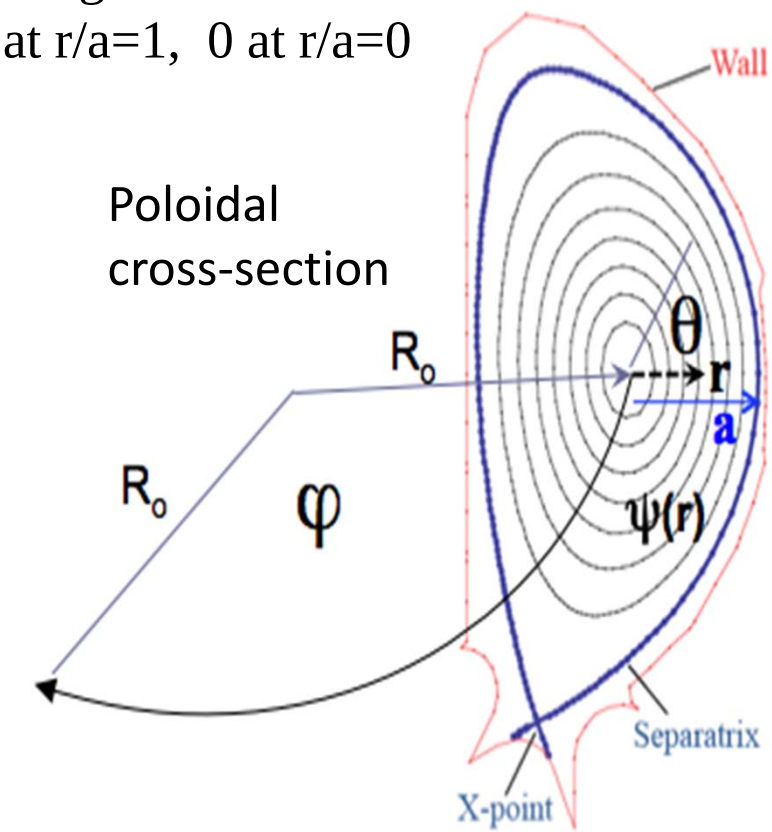
Present:
- Extreme scale Plasma physics simulation.
- Higher compute power → more physics.

“Toroidal” Tokamak Geometry

ITER

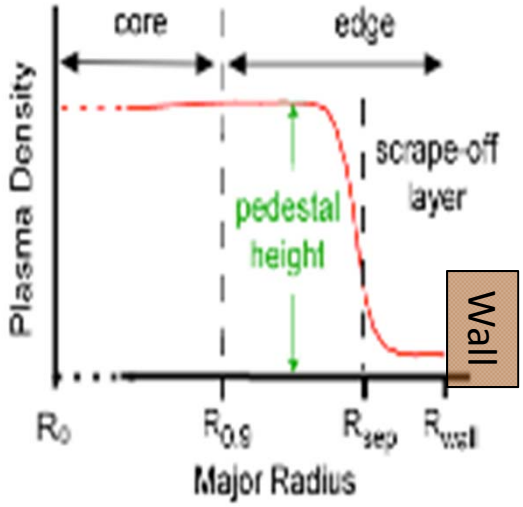


Poloidal magnetic flux label
$\psi(r)$= 1 at r/a=1, 0 at r/a=0

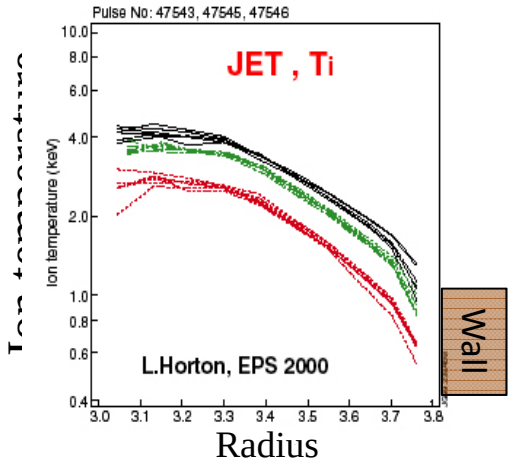


Torus, not a straight cylinder: plasma sees **inhomogeneous** physical space (magnetic field) → complicates **physics** (& **math)** through **magnetic mirroring, curvature drift, ballooning, toroidal mode coupling, etc**.

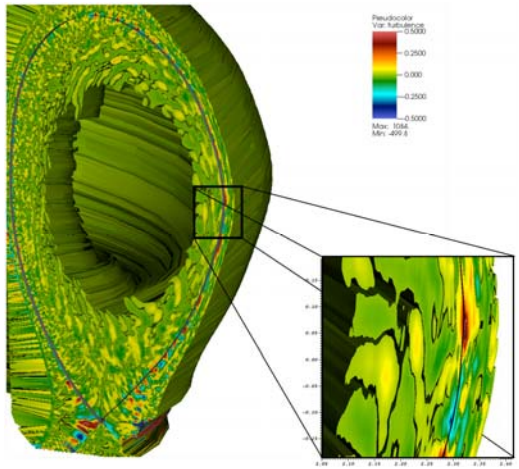
What science are we studying?



Traditional separation: Edge pedestal



Stiff T_i profile
Ti(center) follows Ti(edge)



Blobby large-amplitude edge turbulence

- 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 such a pedestal plasma?
- Edge plasma physics is a challenging issue: Plasma and turbulence are across steep gradient, and in direct/indirect contact with material wall.
  - **non-equilibrium thermodynamics** and non-Maxwellian
    → The "fluid closure" becomes a difficult issue.
  - Large amplitude nonlinear coherent turbulence, "blobs," interact with background plasma and neutral particle dynamics in multiscale.

The Strategy

- Solve the non-equilibrium, multiscale problem in the whole plasma volume using brute-force **first-principles kinetic** equation
  - ✧ Other fusion researchers couple piecemeal physics→ integrated simulation
- Simulate **realistic physics**; ab initio kinetic plasmas including magnetic **X-point, odd wall shape, sources and sinks (atomic physics)**

→ **We choose the Lagrangian ODE scheme (particle-in-cell, Monte-Carlo):**

- ✧ **More stable to CFL instability than a PDF approach**
- ✧ **Lower memory requirement than a PDF approach in higher dimensional space**
- ✧ **Easier to parallelize**
- ✧ **Easier to handle the plasma wall interaction**

→ **Inherently expensive: physics is limited by compute-power**

- ✧ **The more powerful the computer becomes, the more complete physics our simulation can contain.**

EPSI and Computational Scientists

- Fusion edge has a challenging multiscale self-organization problem:
  - The bigger the computer is, the more physics we can simulate.
  - Must utilize extreme scale HPCs for first-principles understanding.
- 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
  - ✧ How to perform UQ on extreme scale simulation

EPSI-Supported Liaisons with SciDAC-3 Institutes

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

The XGC1 code: Innovation & Improvement

- Particle-In-Cell
- Unstructured triangular grid
- Augmented by v-space grid approaches wherever advantageous

- **5D gyrokinetic equation**
  - **ODE**

    Time advance of physics characteristic on cylindrical coordinate system
  - **Finite difference**

    Integro-differential Fokker-Planck collision operator discretized on retangular v-space grid
  - **PDEs (PETSc)**

    Maxwell's equations on unstructured triangular configuration-space grid

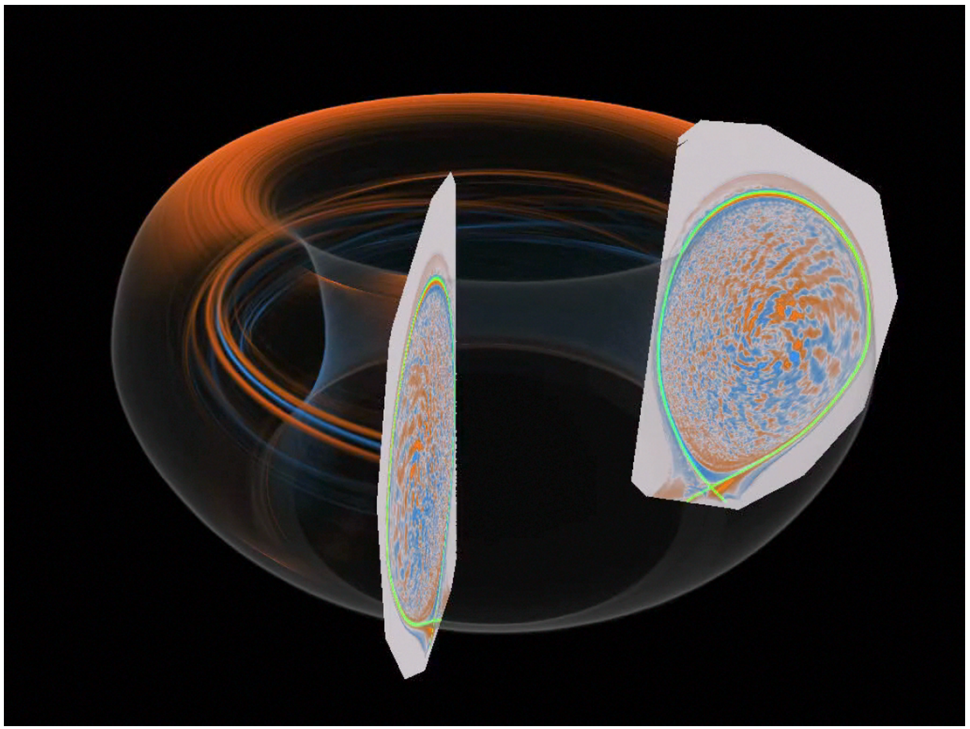
- **The usual interpolation issue exists**
  - Marker particles to unstructured triangular configuration-space grid
  - Marker particles to structured velocity-space grid

- Portability emphasized: Avoid commercial or machine-specific software

Earlier Example: Ion Turbulence in XGC1 on Jaguar

FY2009 ASCR Joule Metric, led by D. Kothe, using 119,808 Jaguar/XT5 cores (~1.5pF)

- For the first time, whole volume DIII-D tokamak plasma was simulated to quasi-steady turbulence saturation:
  - Without artificial boundaries
  - In realistic diverted geometry
  - Included physics: ion turbulence (ITG*), background plasma dynamics, and neutral particle recycling together
- Multiple new physics found, and propagated to fusion community
  - 15 International invited Talks
  - 14 Journal publications
  - Some essential discoveries are now taken for granted.



Simulation by S. Ku, Visualization by K. Ma

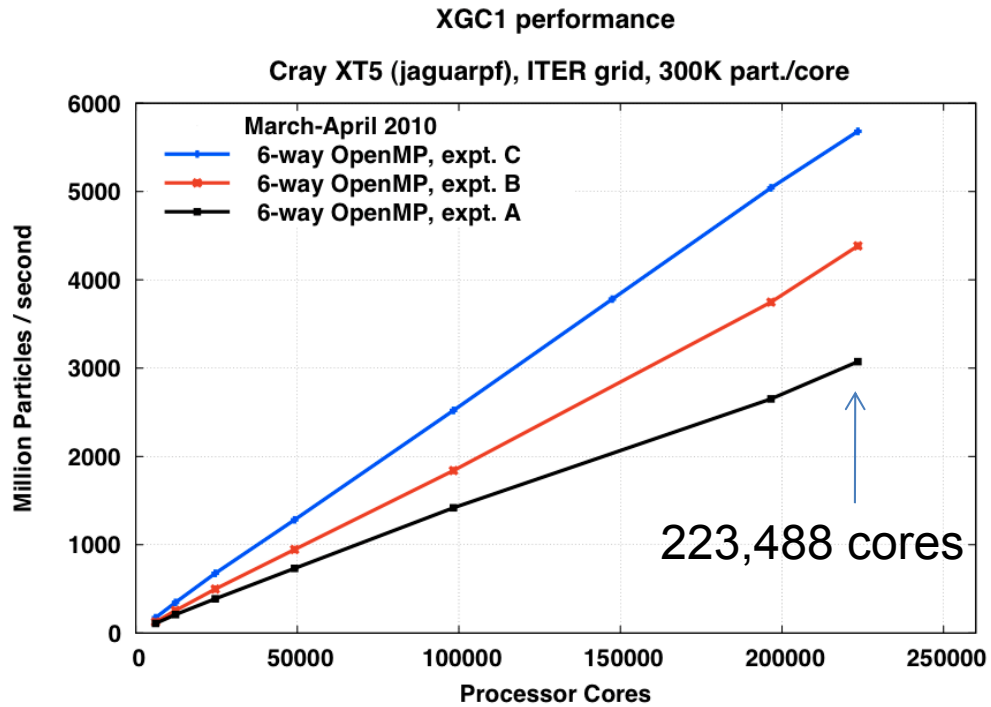
Large scale turbulence in the whole volume DIII-D geometry

*ITG (Ion Temperature Gradient) driven turbulence is the most robust turbulence in tokamak plasma

Enabling Technology, then: XG1 performance on Jaguar/XT5 doubled in less than a year by 3/2010

- **4X speed up of particle time integration by R-K + Adams-Bashforth-Moulton**
- **Nonlinear collision solver**
- **Multi-dimensional domain decomposition**
- **Dynamic load balancing**
- **Geometric hashing and Hilbert space filling curve particle search algorithm**
- **OpenMP parallelization**
- **Optimized MPI communication**
- **Optimized spline interpolation, …**

300K particles/thread, 12 cores per node, 2 MPI processes per node



Plotting number of particles processed per timestep per wallclock second.

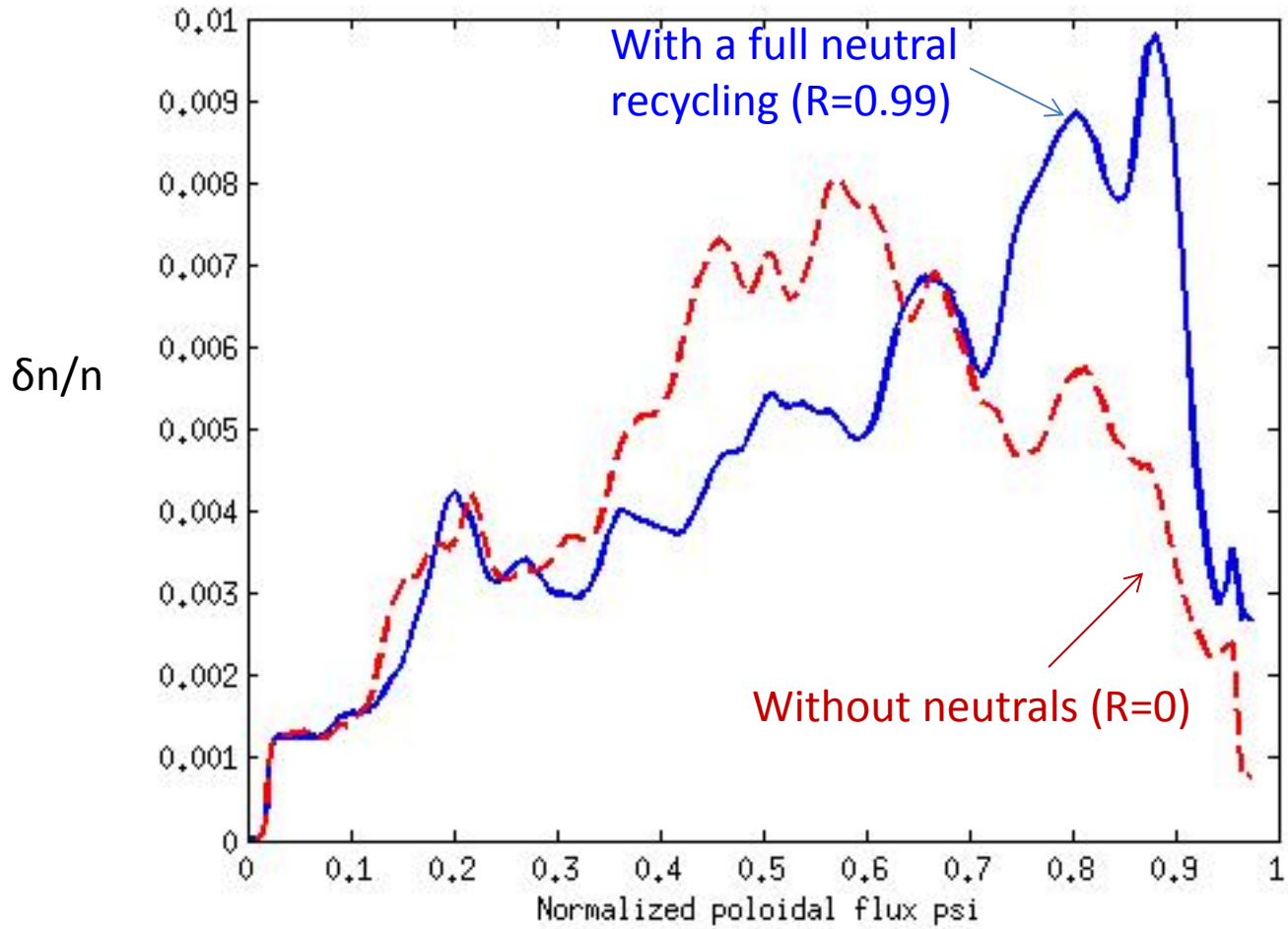
<u>Expt. A</u>: May, 2009 version of XGC1

<u>Expt. B</u>: + a more efficient search technique for locating particle position in grid; removing array syntax within OpenMP-parallelized loops that was degrading OpenMP performance; thread-safe random number generation

<u>Expt. C</u>: + spline interpolation optimizations (March, 2010)

Mystery: Good wall-conditioning (less neutrals) in fusion devices yields better edge plasma.

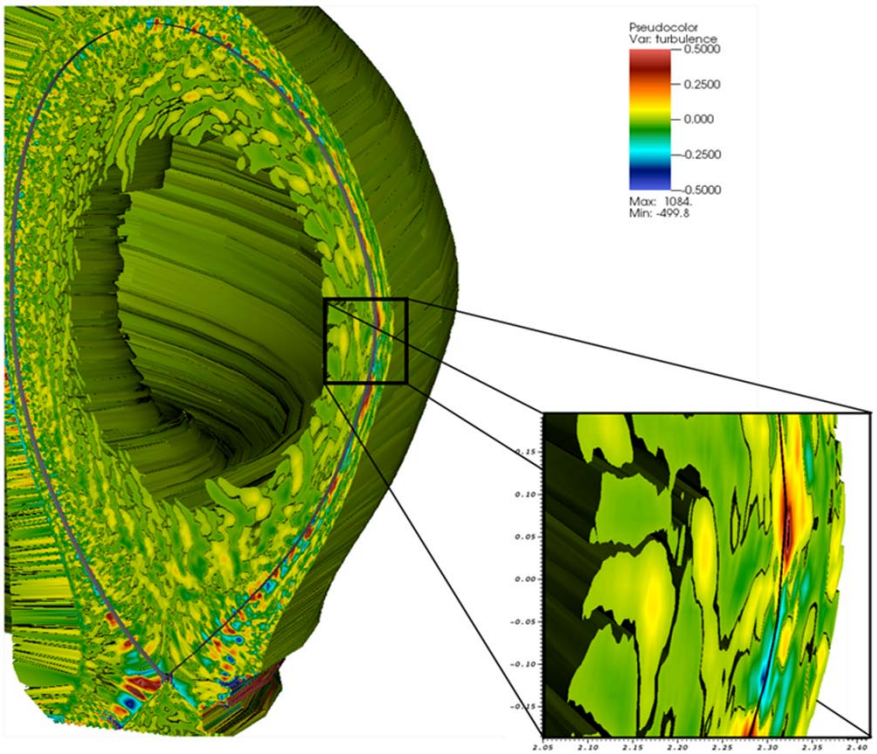
XGC1 finds that neutral atomic physics enhances edge turbulence level [to be submitted to Physics of Plasmas]: we are still publishing from old OLCF success, using NERSC HPCs.



Recent Example: Combining Kinetic Ions and Electrons in XGC1 on Titan

2013-2014 INCITE, using up to ~90% maximal heterogeneous Titan (16,384 nodes~20pF)

- Experiments: edge turbulence is in "blobby" form.
  - Large amplitude density and potential blobs (~50%)
  - In the past, theorists could only use simple models to explain how such blobs could occur.
  - **Requires kinetic ions and electrons in non-thermal state**
  - **Electron simulation consumes much more compute time**
- For the first time, XGC1 has simulated the "blobby" edge
  - Ab initio understanding of blobs
  - In Realistic diverted geometry
  - OLCF Featured Highlight, 2/2014
  - Several international invited talks [(e.g., IAEA-Fusion Energy Conf.]

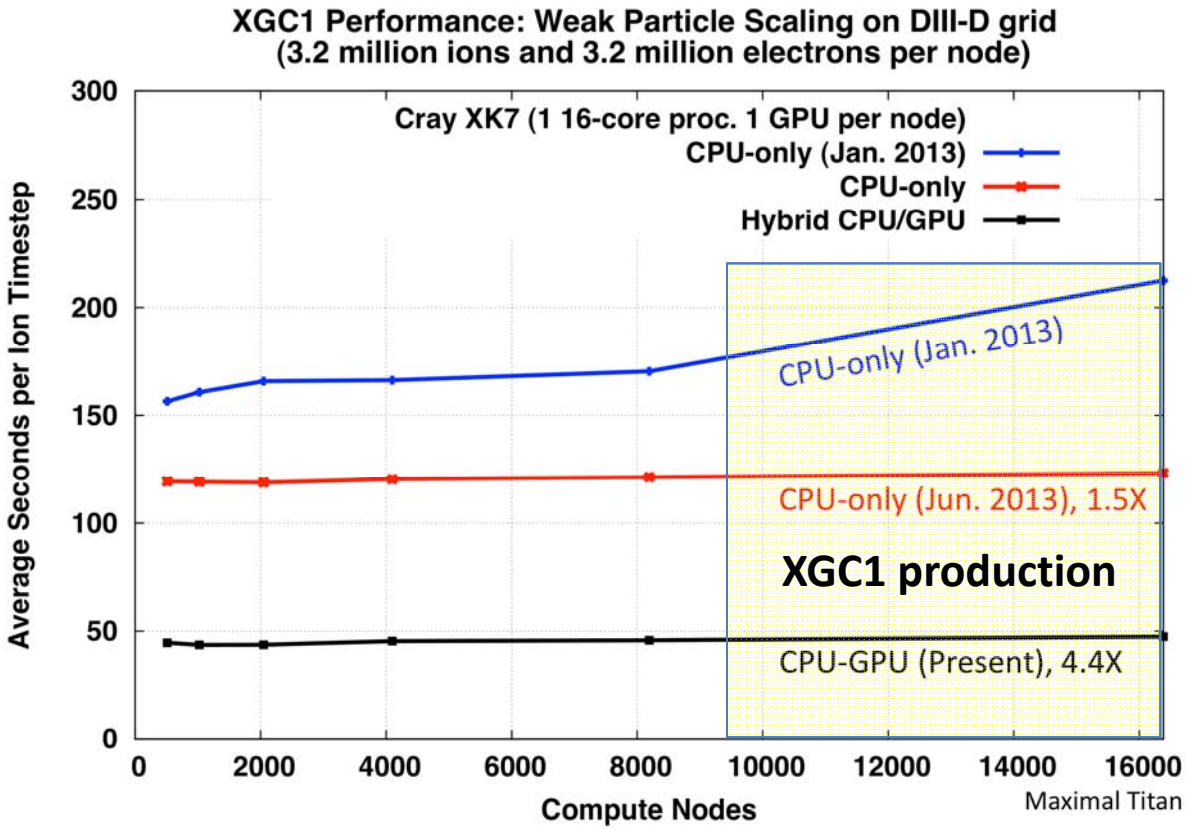


Simulation by S. Ku, Visualization by D. Pugmire

Gyrokinetic simulation of edge blobs in DIII-D plasma

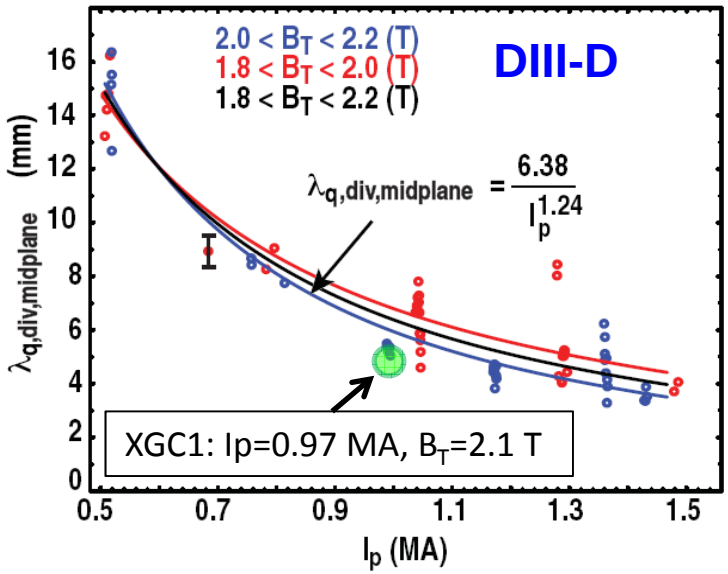
XGC1's performance has been enhanced to take full advantage of heterogeneous Titan

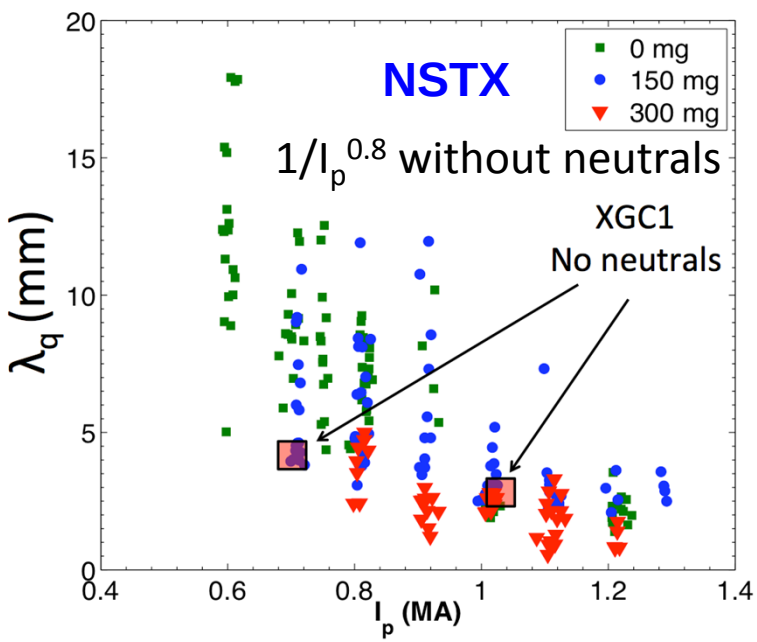
- Performance enhancement on new hardware/software HPC architectures
- Mathematical and computational algorithm improvement
- Extreme scale real-time data management



ASCR and OLCF team sped up XGC1 by 4.4X in <10 months, to enable the ab initio "blobby" turbulence simulation for the first time.

XGC1 tries to predict divertor heat load width





- ITER's divertor heatload width $\lambda_{q,mid}$ would be ~1 mm (when mapped back to outboard midplane), if extrapolated simply 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 experimental values from both DIII-D and NSTX.
- Broadening of $\lambda_{q,mid}$ by blobs (width >1cm) is found to be insignificant in both machines.
- Will the blobs saturate the $1/I_p$ scaling when $1/I_p$ becomes ~ 1mm?

In progress: Add more simulation points to validate predictability.

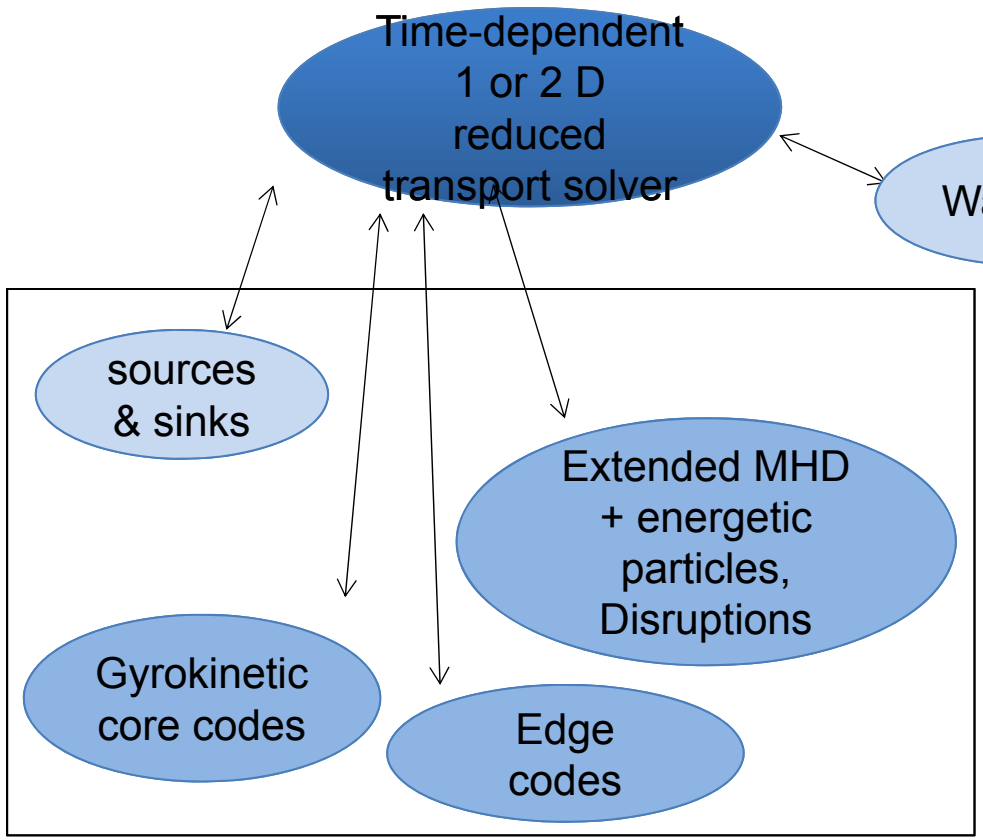
TRADITIONAL PIECEMEAL GOAL

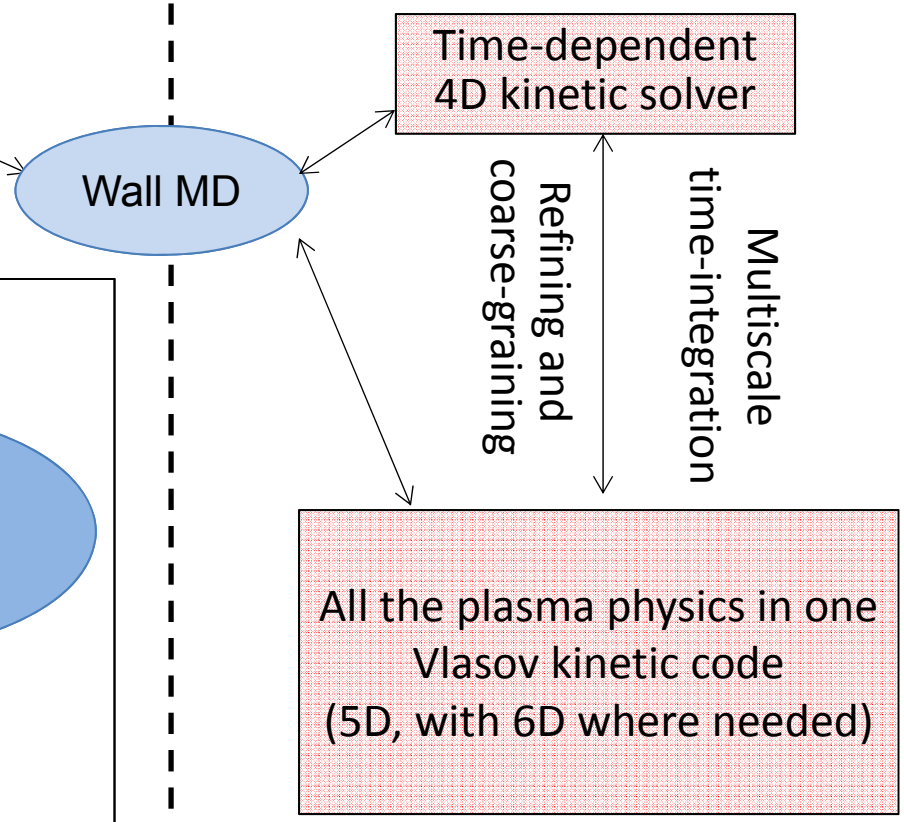
OUR BRUTE-FORCE GOAL

Multiple reduced-codes
Whole-Device approach

Physics

Single ab initio Code
Whole-Device approach





Integration of piecemeal solutions
Perhaps, more difficult

Perhaps, easier.
But, at the cost of compute power.

Will we have enough compute power to achieve such a goal in 10 years?

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

→ 500X 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
  - Electron scale turbulence modes in edge (sub mm grid compared to mm grids). Core region could still be on ion scale grid.
  - Ion gyromotion can be resolved: nonlinear heating source physics
  - MHD time-scale modes can be included
  - Kinetic-kinetic multiscale time integration technique could prolong the ab initio simulation from 10 ms to ~10s time scale
    - Under development using Adios, DataSpaces, and math technologies
- By 2018, with **10X** compute power, we could include **5X** more physics in ITER simulation: great for more complete ITER edge physics.

Conclusion and Discussion*

- Fusion has a challenging multiscale self-organization problem
  - Must rely on extreme scale HPCs for first-principles understanding.
  - Can help improve the traditional community approach: integration of piecemeal solutions
- The ab initio code XGC1 has been developed to be a modern portable code that can efficiently utilize the heterogeneous Titan (and other LCFs) to its maximal capability
  - Highly fruitful collaboration with OLCF Liaison, backed by our SciDAC-3 EPSI members and Institute liaisons
  - Many new basic physics have been discovered
- The more powerful the HPC becomes, the more complete physics XGC1 can model
- Our long term goal is aligned well with the CORAL procurement plan and the exa-scale plan: to include the whole physics in a single ab initio code.

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