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Challenges in First-Principles Multiscale Simulation of Fusion Plasma

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for
The Edge Physics Simulation Team

EPSi
Edge Physics Simulation

Outline

- Introduction
- What Science are we studying in the SciDAC EPSI?
- The Fusion Edge Gyrokinetic code XGC1
- A representative collaborative achievement: Performance Engineering
- A representative collaborative challenge: multiscale time integration

EPSI and Instute Liaisons

- Fusion edge has a challenging multiscale self-organization problem to solve: Must utilize extreme scale HPCs for first-principles understanding.
- Our problem inherently requires a close collaboration & innovation with ASCR scientists

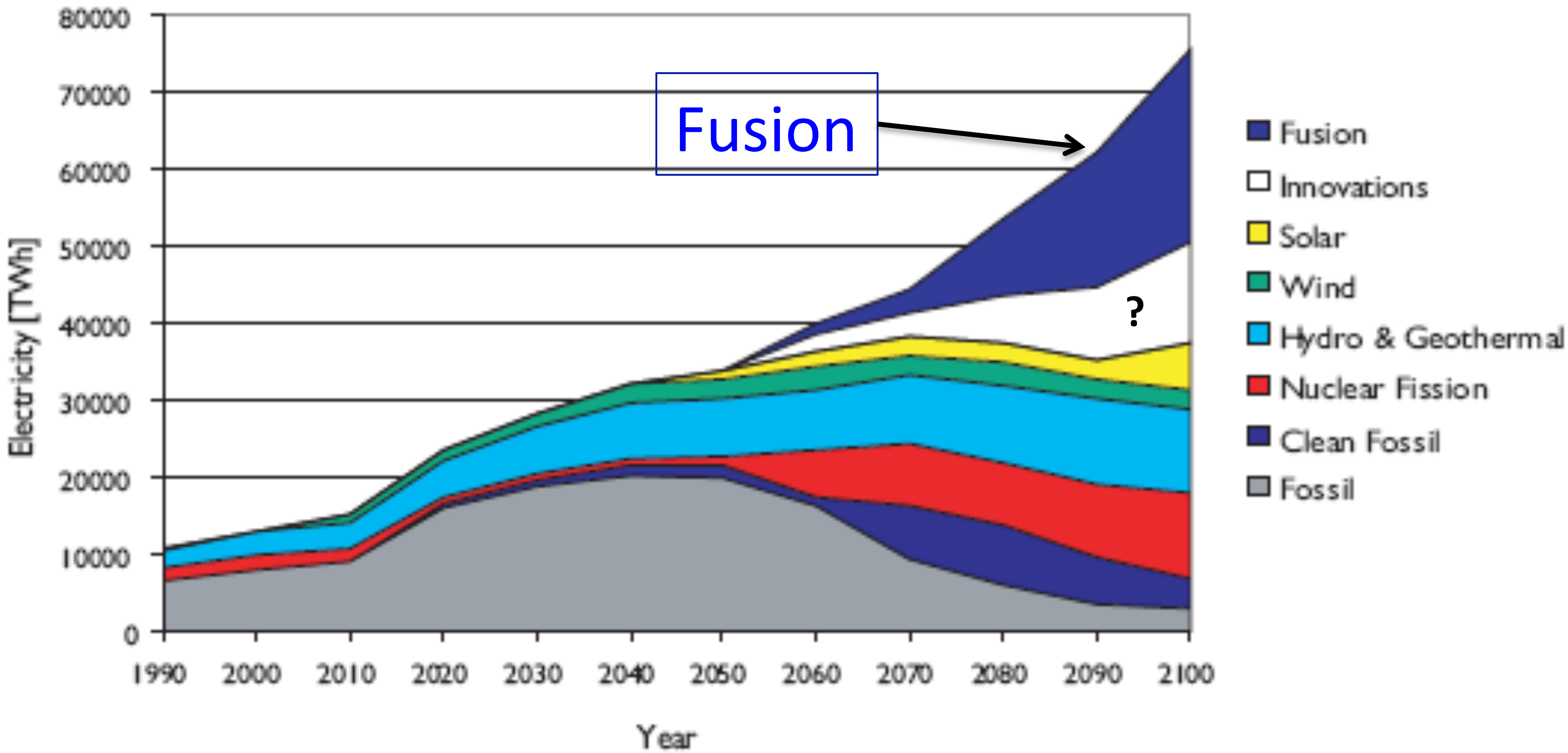
  → e.g., Development of Adios (including DataSpaces and eSiMon)

EPSI-Supported Liaisons with SciDAC-3 Institutes

FASTMath	QUEST	SDAVE	SUPER
M. Adams M. Shephard	R. Moser	S. Klasky M. Parashar	P. Worley

Environmentally safe energy scenario for the world electricity up to the year 2100

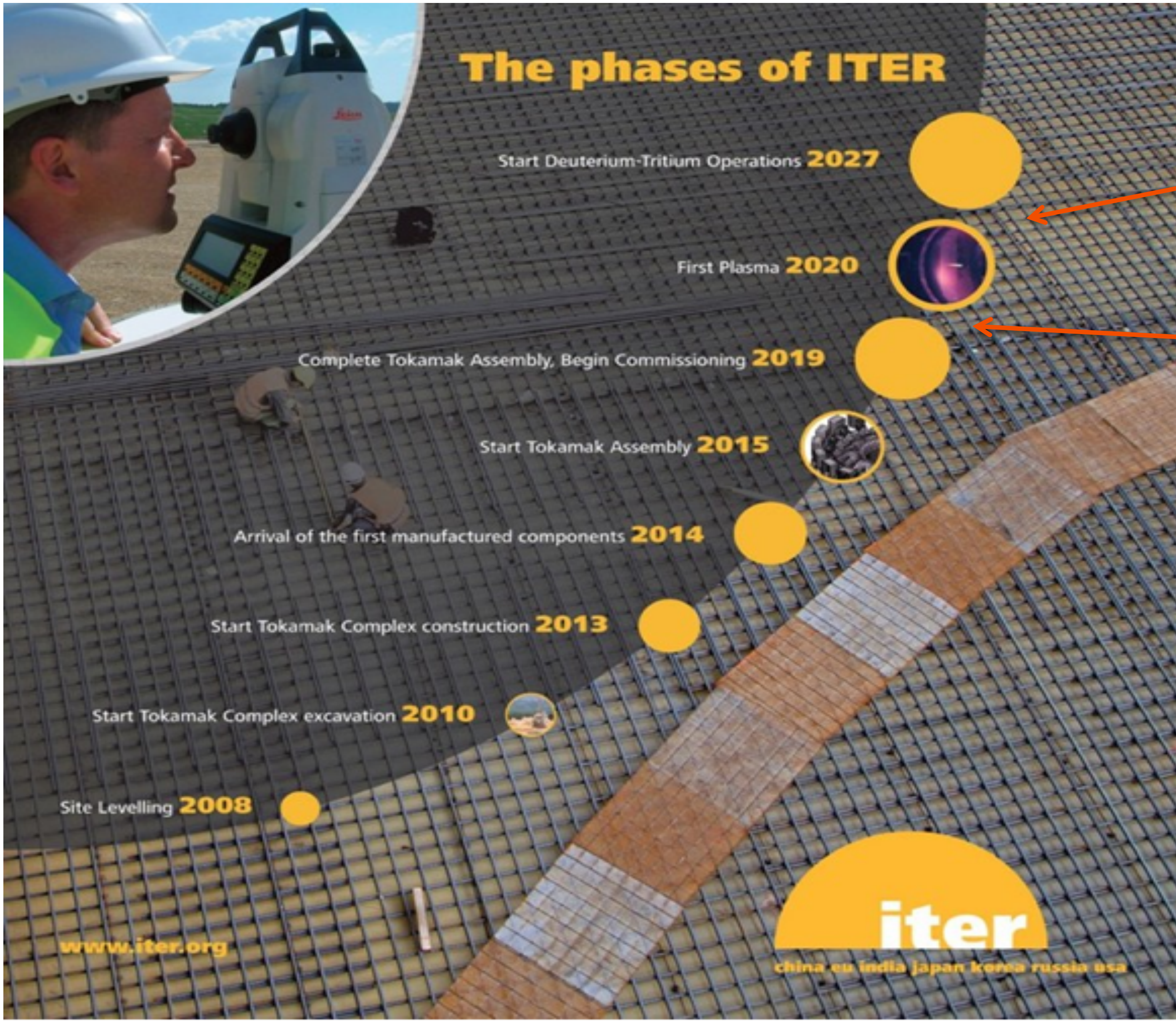
(Source: the Research Institute of Innovative Technology for the Earth, Tokyo)



With all the resources being considered optimistically, we are still short significantly by 2100!

Fusion science is an extremely high payoff research.

ITER Phases are well-aligned with the US Exascale Computing Phases



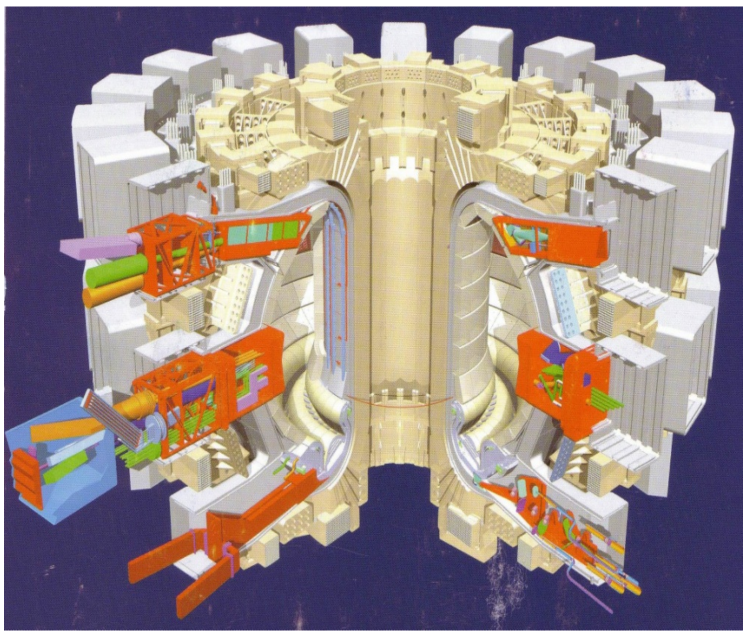
Burning plasma simulation

Plasma physics simulation

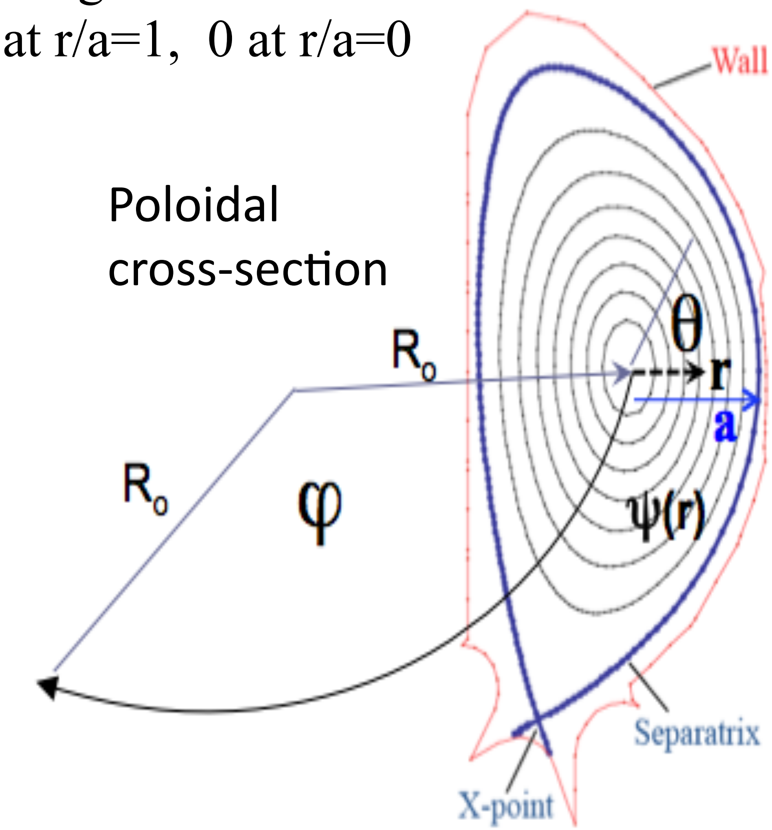
"Toroidal" tokamak Geometry

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

ITER

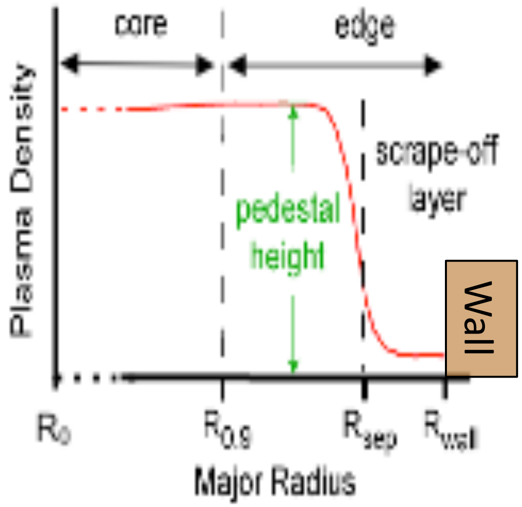


Poloidal
cross-section

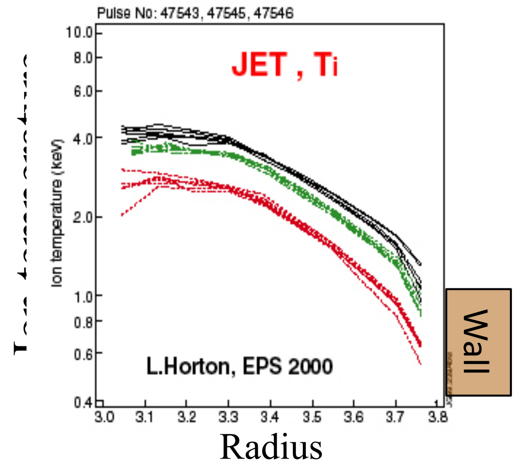


Torus, not a straight cylinder: plasma sees **inhomogeneous** physical space (magnetic field) → complicates **physics** (& **math)** through **magnetic mirroring, curvature drift, ballooning, toroidal mode coupling**, **etc**.

What science are we studying?



Plasma edge region



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

MAST
A. Kirk
2012

Edge localized instabilities could destroy pedestal and damage wall.

- Edge plasma self-organizes into a steep pedestal shape (H-mode).
  → Smaller & cheaper tokamak, by allowing a hot plasma at plasma edge
- When the edge pedestal becomes too steep, plasma instability appears.

- Edge plasma physics is a challenging issue: Plasma and turbulence are across steep gradient, and in direct and indirect contact with material wall.
  → **non-equilibrium thermodynamics** and non-Maxwellian
  → Outside the fluid approximation regime

The Strategy

- Solve the non-equilibrium, multiscale problem from **first-principles kinetic** equation
- Simulate **realistic device**; including magnetic **X-point, sources and sinks**
- We choose a scheme stable to the multiscale dynamics
  - Multiscale dynamics: Large scale variation of electric field and background profile could severly violate CFL condition if 5D PDE scheme is used.
- The scheme should also easily handle the odd edge shape

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

→**Solve the whole muti-scale problem together**

→**Inherently expensive**

The XGC1 code

- ODE based Particle-In-Cell approach on configuration space grid
  - Uses **unstructured triangular grid**
- Aided by v-space grid approaches wherever advantageous
- **5D gyrokinetic equations**
  - **ODE**

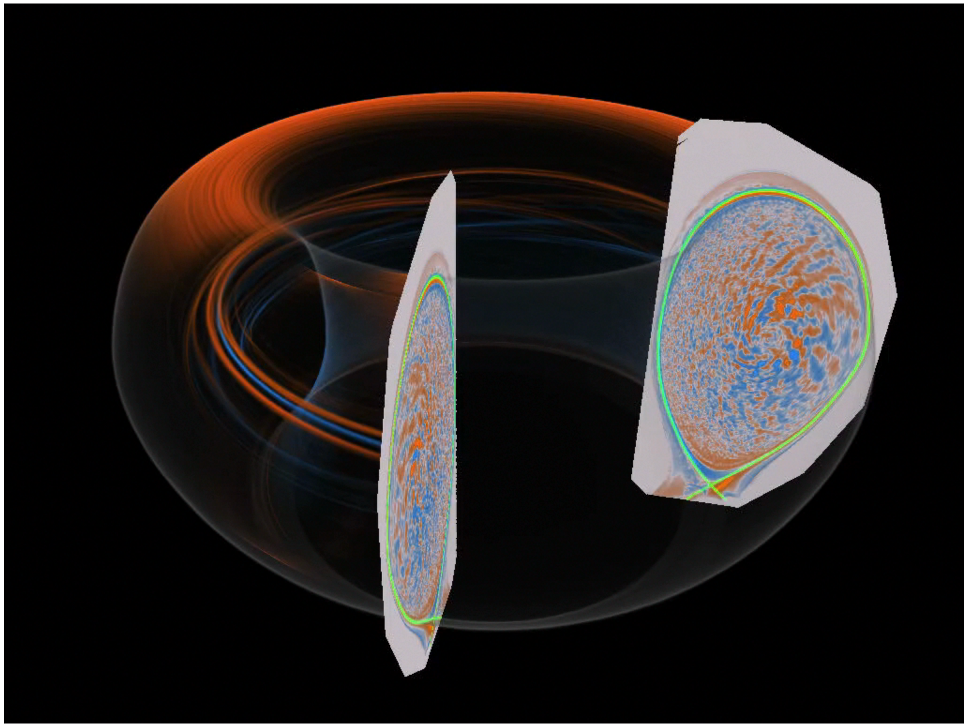
    Time advance of marker particles
  - **Finite difference**

    Partial integro-differential Fokker-Planck collision operator discretized on retangular v-space grid
  - **PDE (PETSc)**

    Maxwell's equations on unstructured triangular x-space grid
- **The usual interpolation issue exists**
  - Marker particles to unstructured triangular **x**-space grid
  - Marker particles to structured retangular **v**-space grid

XGC1 is studying all the critical edge physics

- We normally simulate the whole volume with a coarse grained mesh in the core to capture the large scale turbulence (ITG*) interaction between core and edge.
  - When we confine the simulation to the edge, by placing a core-edge boundary, the turbulence solution gets distorted.
- Use a realistic BD condition for torus: $\Phi=\Phi_w$ on the wall.



Simulation by S. Ku, Visualization by K. Ma

Large scale turbulence in the whole volume simulation in DIII-D geometry

*ITG: Ion Temperature Gradient driven turbuence

Further Development of XGC1, the challenges, and the necessity for Institue Collaborations

- **Electromagnetic turbulence capability, requiring more accurate calculation of turbulent electrical current and denser toroidal grid**
  - More # particles → requiring more # compute nodes: **SUPER**
  - Higher accuracy particle-mesh interpolation: **FASTMath**
  - Increased solver cost → more scalabile solver: **FASTMath**
  - Optimized parallel unstructured meshing: **FASTMath**
  - Higher degree uncertainty quantification & validation: **QUEST**
  - More efficient large-scale in-memory data management: **SDAV**
  - More sophiticated visualization: **SDAV**
- **Multi-scale time advance to prolong XGC1 simulation to experimental edge evolution time scale**
  - In memory coupling between coarse and fine grained executables: **SDAV**
  - Performance optimization with two executables sharing node memory: **SUPER**
  - Time step, stability, stiffness, bifurcuation: **FASTMath**
  - More complex UQ: **QUEST**

Collaboration example with Institutes: SUPER

Challenge: Using XGC1 on full-size heteroheneous Titan

Collaborating SciDAC Institue: SUPER

SUPER liaison: Patrick H. Worley, Oak Ridge National Laboratory

EPSi Science Team Lead for Performance: Worley (20%)

Other EPSI team members: D'Azevedo, Lang, Ku, Ethier, Chang

- The electron subcycling time-advance takes ~85% of computing time in XGC1, designed to be without external communication in each cycle
  - Ideal for occupying GPUs while most other routines occupy CPUs
  - Solver spends <5% of total computing time

Weak Scaling in Number of Particles

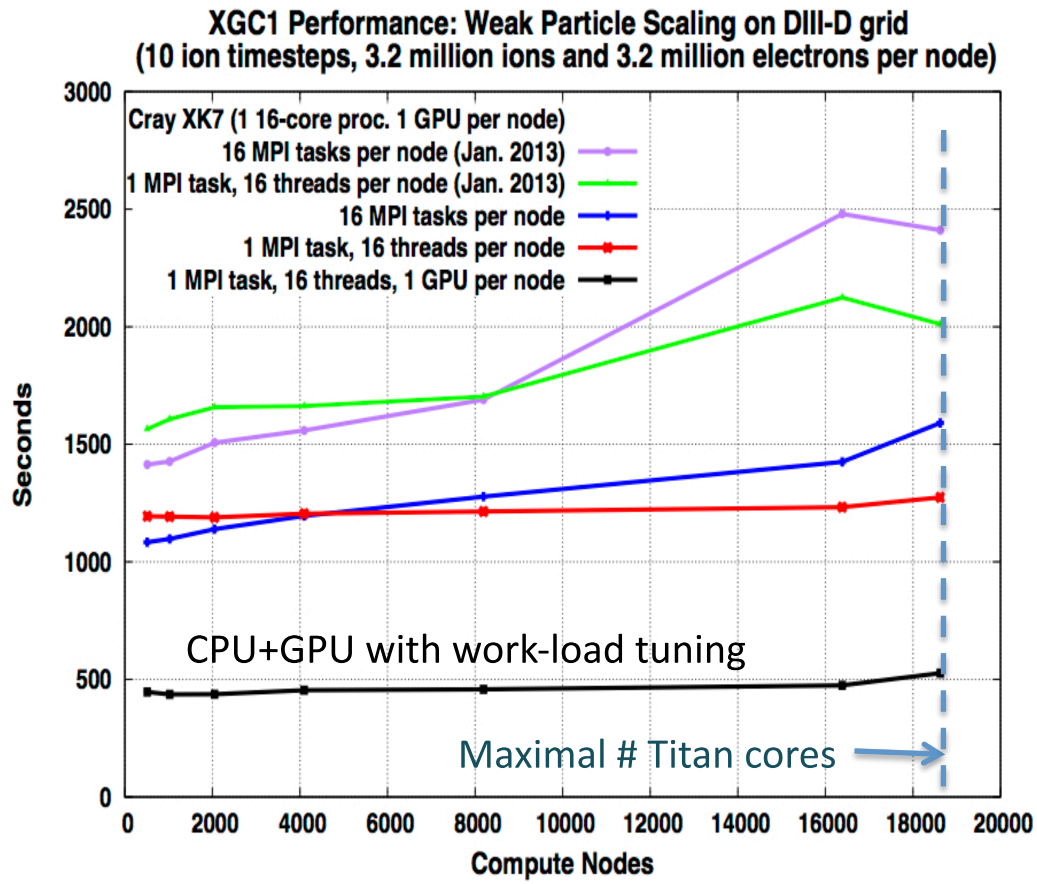
- Bigger problem size in XGC1 requires more number of particles.
  - XGC1 has not reached the weak-scale-breaking MPI communication limit.
- #Particles per grid-node is fixed → #Grid-nodes, thus #particles, in a compute-node is determined by memory → More #particles → more #compute-nodes
- We achieved efficient weak scaling of XGC1 to Maximal Titan capability

EPSI-SUPER Collaboration

- Optimization of
  - computational kernel,
  - OpenMP parallelism to allow effective use of 16 threads per task, and
  - MPI communication

  led to

  4X performance improvement and good weak scaling to full system size in 6 months.



- Work far from over
  - New science capabilities will change performance characteristics dramatically
  - Continuous diagnostics and performance engineering are required.
  - New SUPER tools and techniques should accelerate the process.

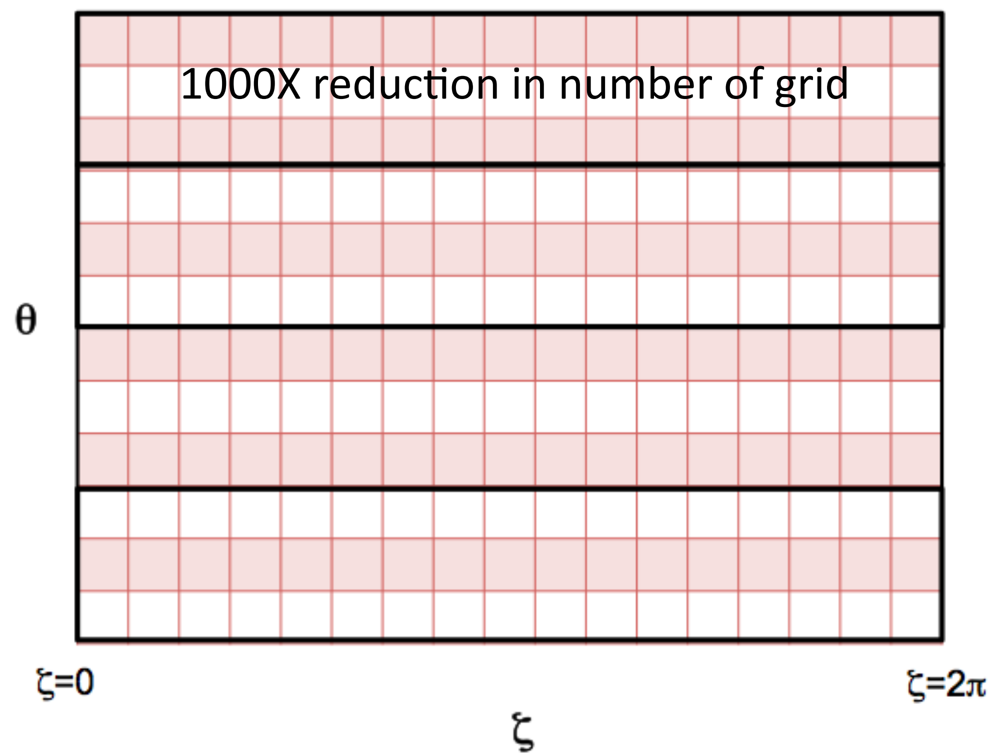
An Example Challenge in EPSI, requiring collaboration with all four Institutes+

Multi-scale Time Advancement

- Prolong the high fidelity simulation to experimental edge transport time scale
- Time consuming turbulence simulation may not be needed at all time steps
- Divide XGC1 in XGC^F(axisymmetric+turbulence) and XGC^C(axisymmetric)
- Use the Φ^F(turbulence) data in XGC^C, with updates as needed

Grid coarsening and refining for restricting and lifting

- Perform the computation of XGC^C and XGC^F at data source.
- Minimal loss of kinetic information in restricting and lifting.
  - Common (gyrokinetic) equations between fine and coarse grained systems

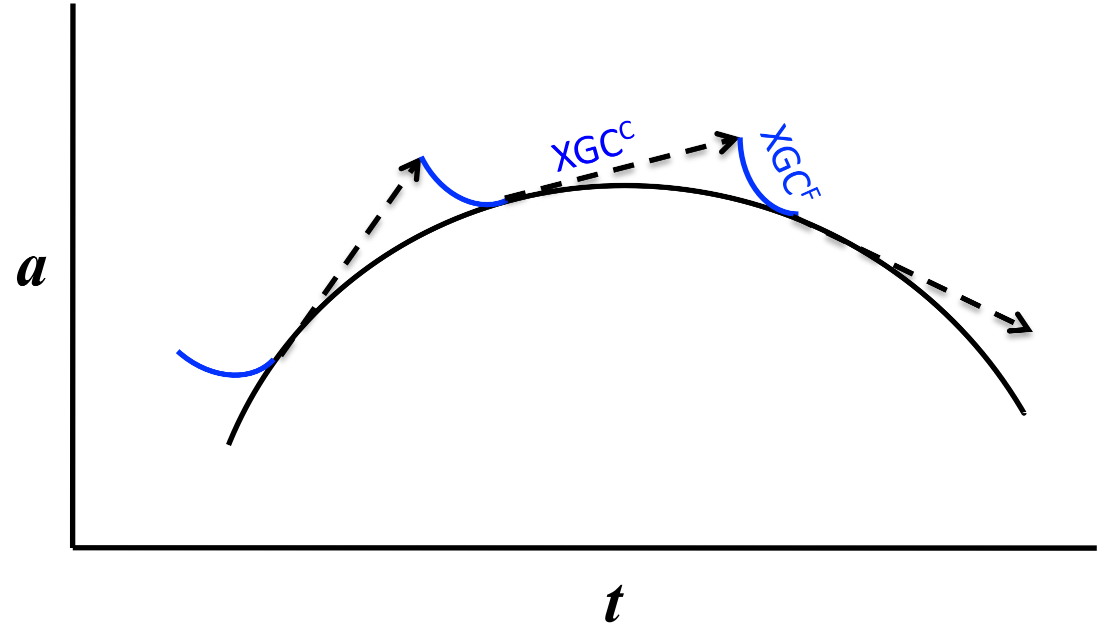


Questions to study

- Time steps ΔT^C and ΔT^F?
- Stability?
- Stiff profile?
- Solution bifurcation?

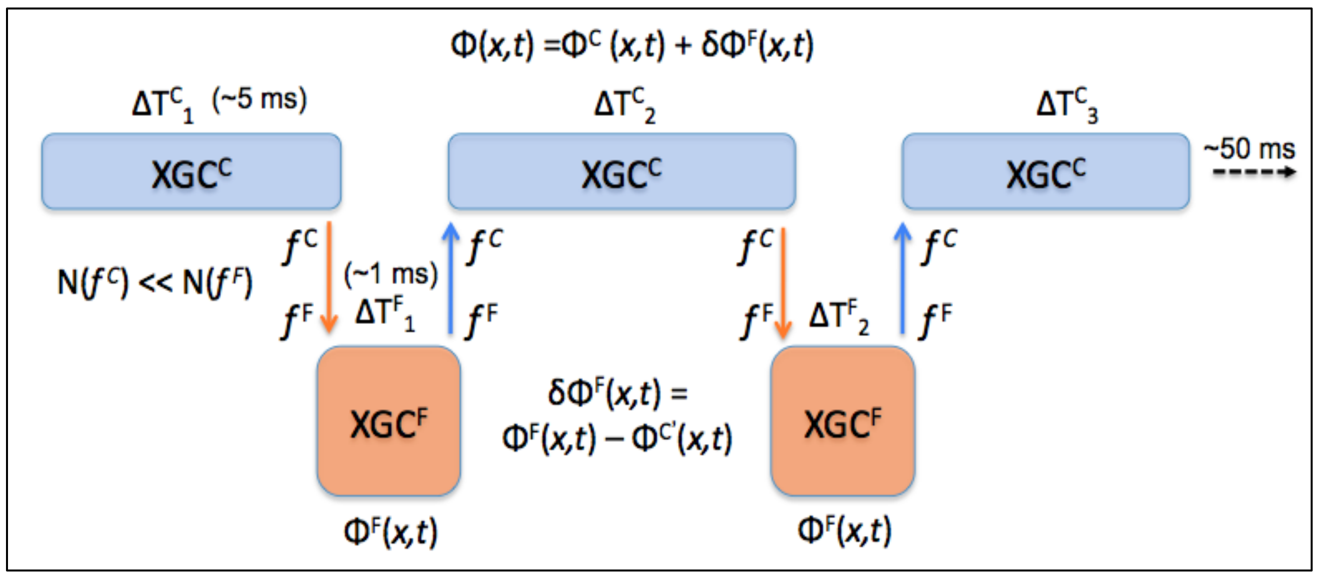
→Heavy usage of data management, math and analysis in-momory.

Collaboration with SUPER and QUEST is essential



$G^F(f^F, d)=0$
$G^C(f^C, D)=0$

$D=\Phi^F(x,t)$
Different from Heterogeneous Multiscale Method



Accomplishments

- Developed a detailed strategy for coarse/fine grain coupling through the electrostatic potential to encode turbulent information in the coarse grained simulation.
- Developed a coarse grained XGCa and demonstrated coupling with XGC1.
- Identified a strongly turbulent benchmark case to help guide the development of strategies for adaptive multi-scale advancement.

Challenges and near-term next steps

- Identify and understand appropriate measures of quality of the simulation and validate against fully resolved simulations to quantify the impact of the multi-scale approach on the physical fidelity.
- Strategies for physically correct sampling of particles when coupling the two codes to minimize the transitional effects, e.g., phase space density reconstruction and conditional sampling techniques.
- Consider the potential for spatial coarse graining by quantifying the local strength of the kinetic effects and adjust particle number accordingly.

Discussions

- Fusion has a challenging multiscale self-organization problem to solve: Must utilize extreme scale HPCs for first-principles understanding.
- Our code XGC1 can efficiently utilize the heterogeneous Titan to its maximal capability
- The more powerful the HPC is, the more complete physics XGC1 can model
- The problem inherently requires a close collaboration & innovation with ASCR scientists

  → e.g., Development of Adios (including DataSpaces, eSiMon)

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