Extreme Scale Computing of Fusion Phyiscs in the Center for Edge Physics Simulation

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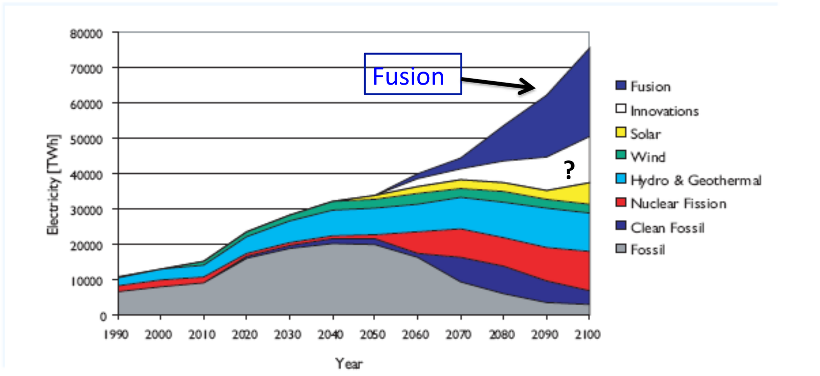
Outline

I. Introduction to Fusion

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!

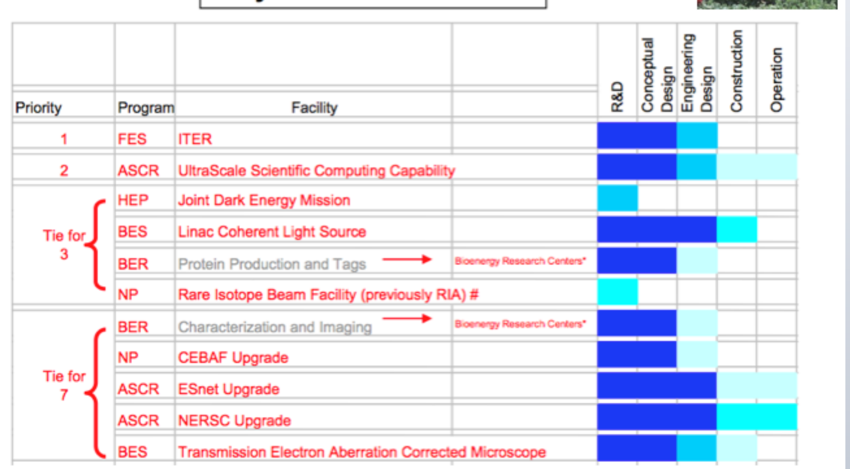
Fusion science is an extremely high payoff research.

Facilities for the Future of Science

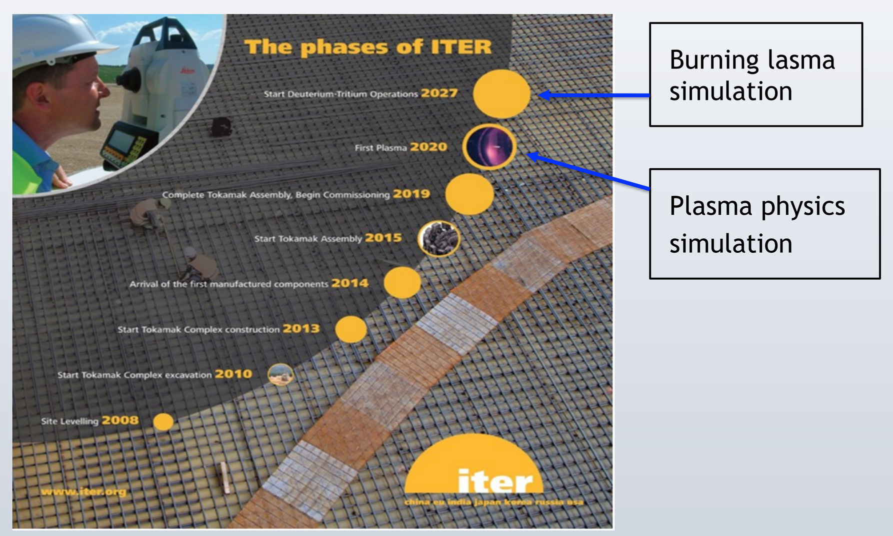
DOE Office of Science, 2003 & 2007

Status of Facilities in 20-Year Outlook

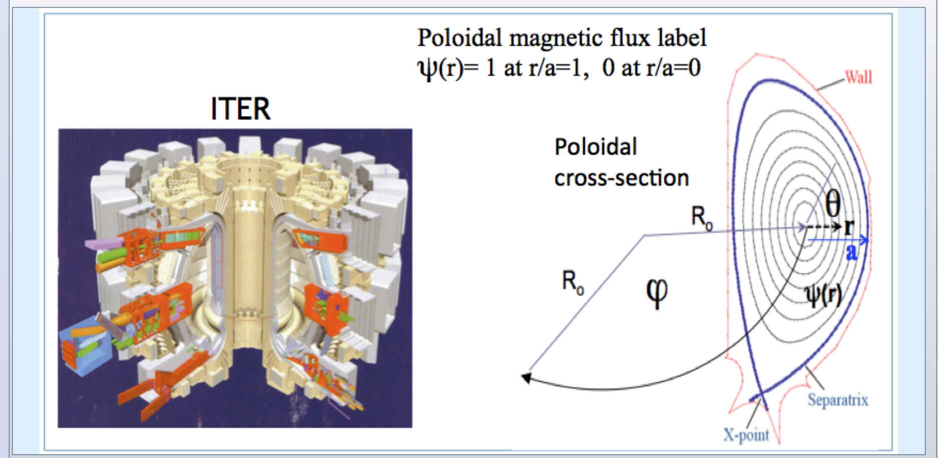
By the end of FY 2007



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

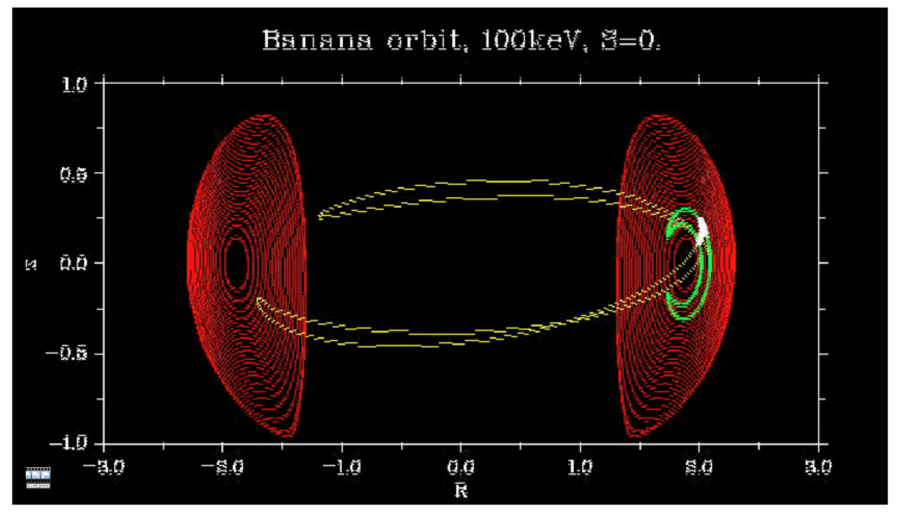


II. Introduction to Tokamak (a 3D Torus)



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

Many particles execute "banana" orbits, with large excursion across flux surfaces → Nonlocal radial mixing of physics

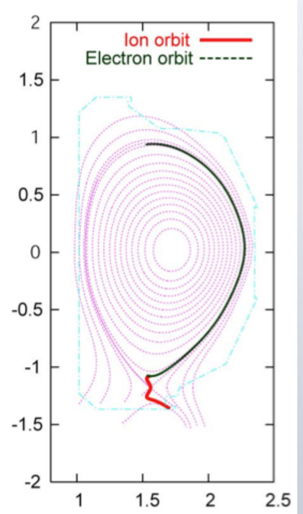


In the edge plasma, the degree of non-local orbit excursion can be extreme

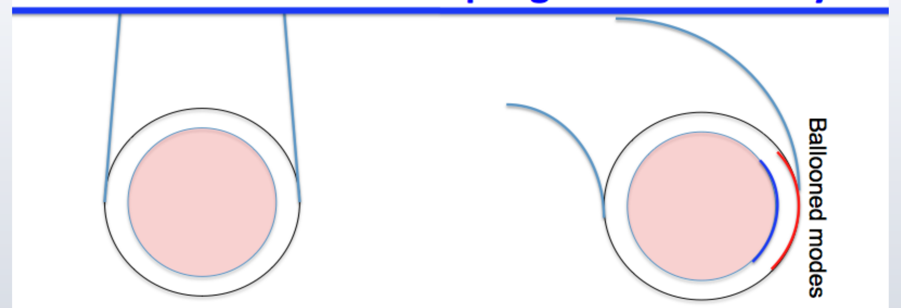
- Most of the edge particles are of banana type with large radial excursion
  - ~ L_p : gradient width of steep edge pedestal pressure
- Some particles even have such a large radial excursion that they are lost to divertor
- Radial turbulence de-correlation length is even wider

→**Non-equilibrium thermodynamics.**

Application of simplified math or simulation is difficult.



Nonlocal field-mode coupling from toroidicity

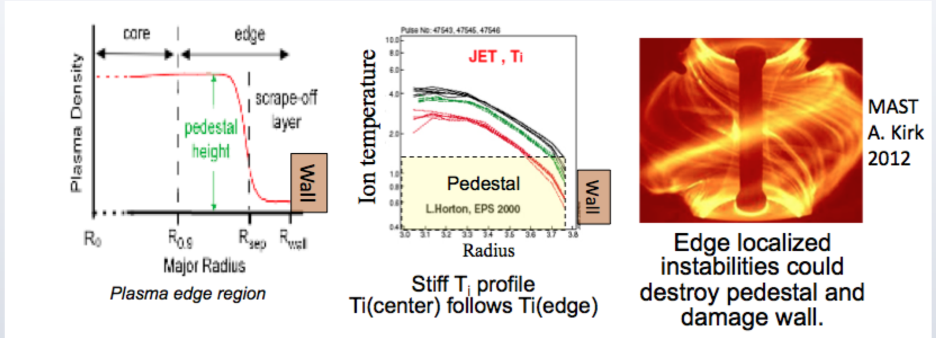


A conducting, straight cylindrical surface does not yield perturbation at inner surface ("shielding").

A conducting toroidal surface yields perturbation at inner surface ("incomplete shielding due to poloidal inhomogeneity").

Further affects nonlocal self-organization of fusion plasma
→Difficulty in math, V&V, UQ, etc.

III. What Science Are We Studying?

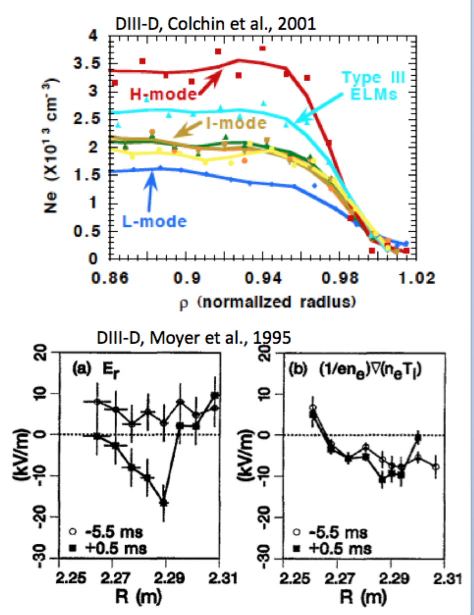


- Edge plasma self-organizes into a steep pedestal shape (H-mode).
  → Smaller & cheaper tokamak, by allowing a hot plasma at plasma edge
- Edge plasma physics is a challenging issue: Plasma contacts material wall. Particle orbits and turbulence are across magnetic separatrix.
  → non-equilibrium thermodynamics and non-Maxwellian
  → Outside of a fluid theory regime

An approach to solve PDE on a 5D-grid has been difficult.
Particle-in-cell approach → Extreme scale computing is necessary

Critial Edge Physics to Help ITER

- How does the pedestal grow?
- How does the core pressure grow together with edge pressure?
- What determines pedestal shape?
- How localized the heat load will be on divertor plate?
- How does the plasma fueled into core against gradient?
- Why is there a rotation source at edge and how does it propagate in?
- How are edge localized modes (ELMs) triggered and how to suppress them?
- What is the physics for bifurcation from L-mode E_r to H-mode E_r?
- What is the threshold $P_{L\to H}$?



The Strategy

- Solve the non-equilibrium problem from first-principles kinetic equation
- Simulate realistic device; including magnetic X-point, sources and sinks
- Avoid neglecting important effects
  – Toroidal mode coupling
  – Coupling of radial drift motions to turbulent field variations
  – Variation of background profile (free energy driver)
  (Neglect of these effects are called "local" approximation.)
- We choose a scheme stable to the multiscale dynamics
  – Multiscale dynamics: Orbital motions across a large scale fluctuation of the background field could severly violate CFL condition if 5D PDE
- The scheme should also easily handle the odd edge shape

→ **Lagrangian ODE scheme (particle-in-cell)**

Gyrokinetic simulation in 5D phase space

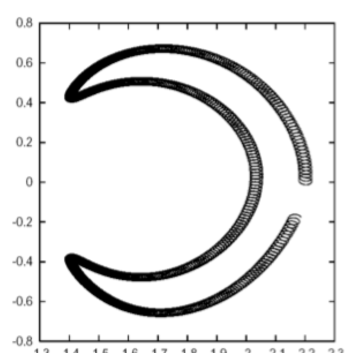
Vlasov equation is 6D (3D in **x** and 3D in **v**), requiring **exa-scale** computing for a tokamak plasma simulation

$$df/dt = \partial f/\partial t + \mathbf{v}\cdot\nabla f + e(\mathbf{E}+\mathbf{v}\times\mathbf{B})\cdot\partial f/\partial \mathbf{v} = C(f) + \text{Source} + \text{Sink}$$

Reduction of 6D to 5D by using a justifiable assumption: "Gyro motion is much faster than the time scale of interest"

→Analytical removal of the gyro-angle velocity variable α

→5D Gyrokinetic Eq.: 3D in **x** and 2D in **v**



[Freeman, Chen, Lee, Hahm, Brizard, Qin, Scott, Lin, Parker, Dimits, Catto, Dorland ...]

IV. The XGC1 code

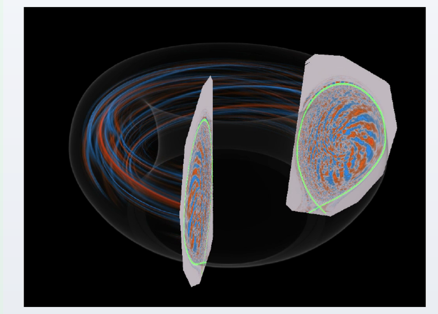
- ODE based Particle-In-Cell approach on configuration space grid
  – Uses unstructured triangular grid
- Aided by PDE and v-space grid approaches when advantageous
- **5D gyrokinetic equations**
  – ODE
    Time advancement of marker particles
  – Finite difference (PETSc)
    Partial integro-differential 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 containes all the basic physics compoents

- Gyrokinetic ions
- Drift-kinetic electrons: small gyroradius limit
- Monte-Carlo neutral particle with wall-recycling coefficients (DEGAS2 is built into XGC1)
- Multi-species impurity particles
- Plasma heating in the core
- Torque input in the core
- Fully non-linear Coulomb collisions (Fokker-Planck-Landau)
- Logical Debye-sheath: code determines wall sheath from ambipolar loss constraint.
- Reads in an experimental geometry and plasma data

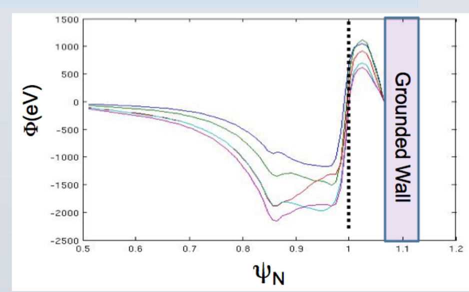
XGC1 is studying all the critical edge physics

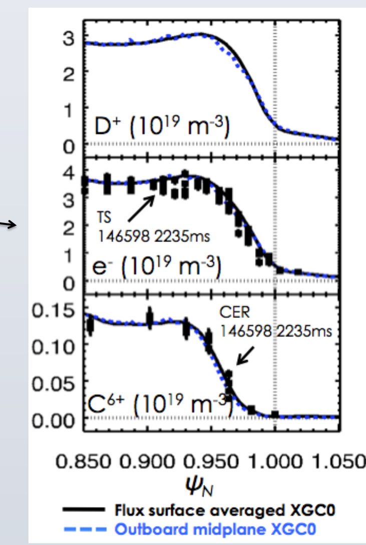
- We normally simulate the whole volume with a coarse grained mesh in the core to capture the large scale turbulence interaction between core and edge.
  – When we confine the simulation to the edge, by placing a core-edge boundary, the turbulence solution gets distorted.
- Use a realistic BD condition for torus: Φ=a on the wall.
- L-H transition is being studied.



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

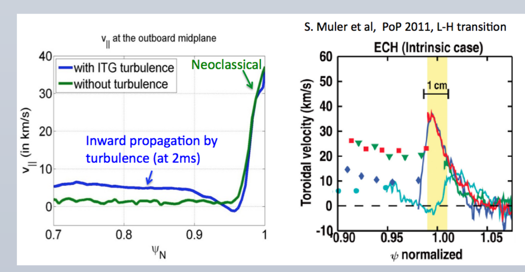
- Edge potential forms spontaneously and the edge pedestal grows, with ionization of wall-recycled neutrals.
- Inward pinch of cold particles found
- Agreement with experimental pedestal profile is excellent

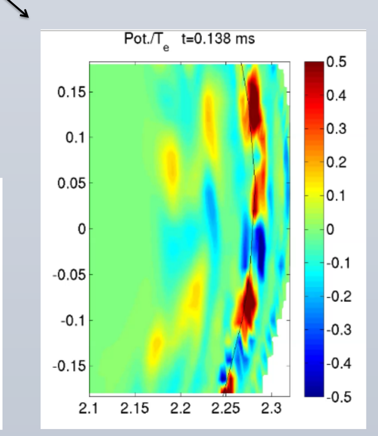




XGC1 has simulated for the first time the nonlinear coherent potential & density structures ("blobs") across separatrix at outside midplane

- Edge rotation soruce has been identified as a toroidicity effect, but the inward transport has been identified as turbulence effect.



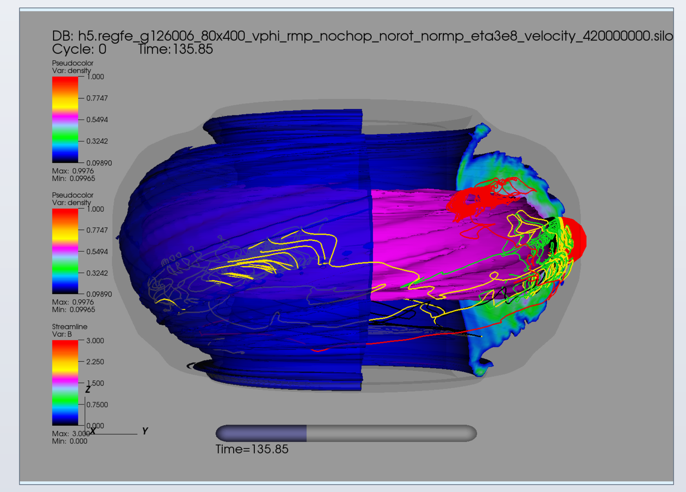


V. Further Development of XGC1 and Challenges

- **Electromagnetic turbulence capability**
  – XGC1 currently can handle perturbative electromagnetic turbulence in a thermal-equilibrium plasma background: called "delta-f" simulation
  – Edge plasma is in non-equilibrium state. The perturbative delta-f capability needs to be upgraded to "full-f."
  – Improving accuracy in the calculation of turbulent electrical current is the remaining challenge.
  – Needs support for parallel unstructured meshing
- **Enhancement in the accuracy of Edge Localized Mode simulations in an MHD code by allowing more proper closure terms, through a data coupling** (see next section).
- **Inclusion of 3D perturbed field penetration capability in XGC1 to understand the control of Edge Localized Modes**
  – We presently have this capability without turbulence
- **Verification of large scale code**
  – There is no other codes with the capability of XGC1 for cross-verification
  – Analytic solution is difficult due to nonliear self-organization nature
  – Even a manufactured solution is difficult due to the toroidal mode coupling
  – Verification in a simplified problem must be cleverly designed
- **Uncertainty quantification** of large scale code is a challenge
  – Cannot take the usual statistical approach on full scale code
  – Thus, UQ also requires a cleverly designed simplified problem set
- **Achieve good strong scaling to shortest length electromagnetic turbulence-physics grid in ITER** on a heterogeneous platform
  – A longer term challenge since we do not forsee immediate necessity for such a study
  – We need to take advantage of advancement in the programing languages
- **Prolongation of XGC1 simulation to experimental edge evolution time scale via a multi-scale time advance technique**
  – In memory coupling between coarse and fine grained kernels.
  – Strong collaboration among physics, applied mathematics, and data management scientists is a critical necessity
  – Must be supported by performace optimization experts
  – Uncertainty Quantification is another challenge

VI. Edge Localized Mode Simulation in M3D

- A large scale Edge Localized Mode (ELM) could make the pedestal crash and send the plasma energy to the material wall → Premature damage to wall, potentially severe under fusion-burning conditions
- Presently, a gyrokinetic code cannot simulate a large scale ELM
- Many observed properties of ELM crash can be explained with MHD
  – Addition of kinetic information could be important. Presently, two-fluid information is used, but edge plasma is kinetic.



- Figure shows an ELM instability event from M3D in a DIII-D plasma
  – Cut-plane view of density contours (blue-green-purple) shows large 'fingers' being expelled towards the wall at top and bottom.
    ○ Top and bottom have magnetic X-points that form near-Hamiltonian "homoclinic" tangles for small perturbations
  – Two 3D density contours (blue and purple) show helical striations along equilibrium magnetic field
  – Edge disturbances couple strongly to the plasma interior
  – Velocity streamlines (3 starting values near outer midplane) show instability motion and gradual development of coherent rotation

Plans and Challenges

- Full understanidng of ELMs requires coupling of MHD to particles, which have different physics and computational structures
  – Different time scales, velocities, electric field, etc.
  – Fluid-based MHD solutions are globally coupled, depend on boundary conditions - do not parallelize well on present systems! Particles have more local dynamics, parallelize well.
- Tight coupling (every few time steps) to resolve physics differences.
  – MHD code computes magnetic field **B**, passes to particle code
  – Particle code computes particle pressure tensor or current density for MHD momentum equations. Challenge: accurate calculation of small velocity moments from particles
  – Main challenge: How to couple codes efficiently on leadership class HPC between non-scalable and scalable codes?

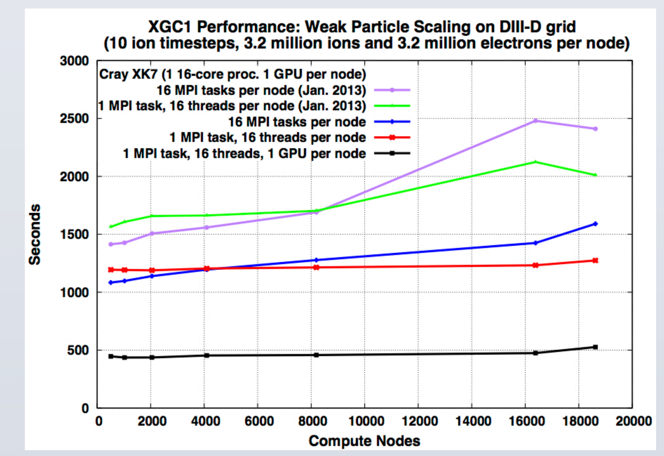
VII. An example Achievement: Performance Engineering

Challenge: Running XGC1's 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: E. D'Azevedo, J. Lang, S. Ku, S. Ethier

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

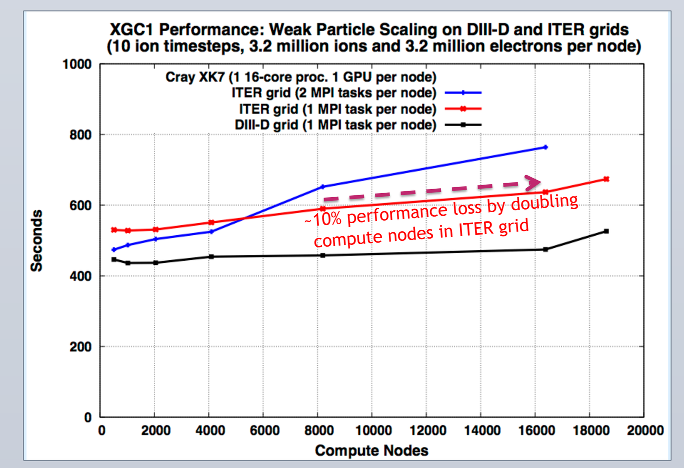
Weak Scaling in Number of Particles

- 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 #grid-nodes
- We achieved efficient weak scaling of XGC1 to Maximal Titan capability
- 4X performance enhancement in <1 year from CPU-only to GPU-CPU



Preliminary study on ITER

- For an efficient simulation of ITER physics, we need to use the heterogeneous Titan to its maximal capability
- For our coarse-grained physics simulation in the core, we have chosen 4X more number of grid points in ITER than DIII-D
- A reasonable preliminary scability has been achieved, even without a further optimization in the ITER grid → We expect improvement.



Plans for Further Performance enhancement

- Reduce MPI communication to GPUs by transporting scalar electrostatic potential, rather than 3D electric field vector
- 2D domain decomposition to partition grid and particles ("poloidal decomposition") instead of the current 1D domain decomposition.

Conclusion and Discussion

- We utilize leadership class computers (Titan and Hopper) to prouce science that has not been possible before
- Strong support by SciDAC Instiues and individusl ASCR scientists has been essential
  – The collaboration is anticipated to get even stonger as the science gets elevated to ITER level
- Developing an in-memory multiscale time advancement technique is a high pay-off challenge (see the other EPSI poster and an EPSI talk on Thursday)
  – Prolong the high fidelity simulation to experimental edge time scale (~50 ms)
  – Expensive turbulence simulation may not be needed at all time steps
  – Reset error accumulation at the same time
  – Centralized joint activity with Applied Math, Data Management, Performance Optimiztion, and UQ
- Verification and validation are challenging and emphasized.