SciDAC-PI Meeting, Sept. 10-12, Rockville, MD

Overview of the Fusion Edge Physics Simulation Project:

Subtitle: Challenges

EPSI
Edge Physics Simulation

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and
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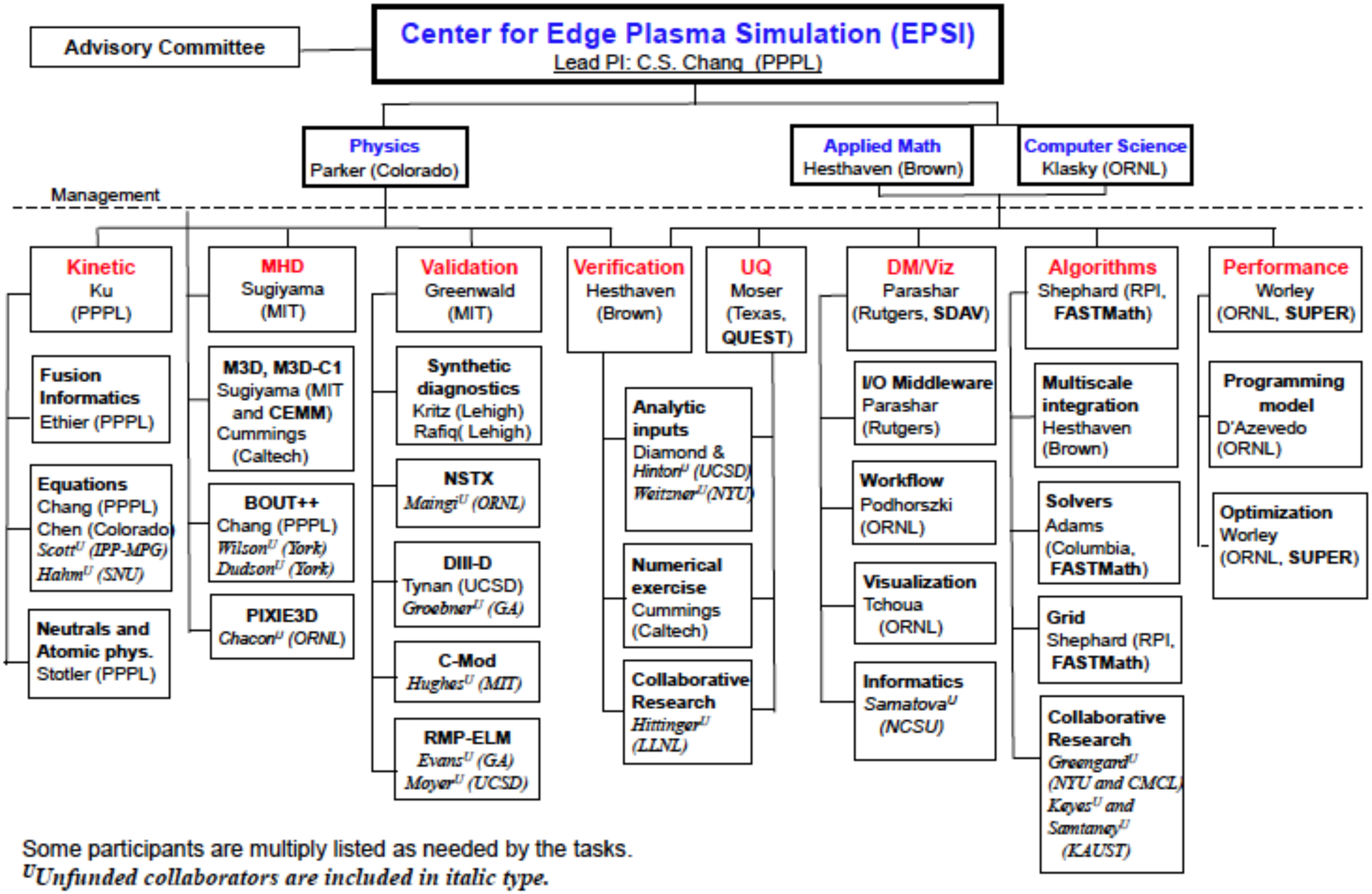


2 National Labs and 8 Universities: PPPL, ORNL;

Brown, Caltech, Colorado, MIT, Texas, UCSD, RPL, Rutgers

Outline

- Geometry
- Science
- XGC1 Fusion Edge Gyrokinetic code and challenges
- Challenges to ASCR community

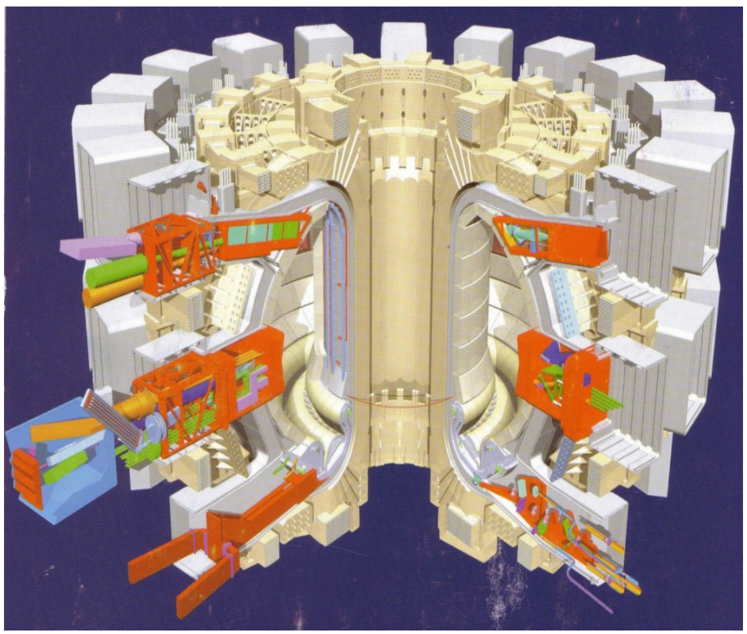
  Poster I
  - Algorithm and Applied Math
  - V & V, UQ
  - Code Performance

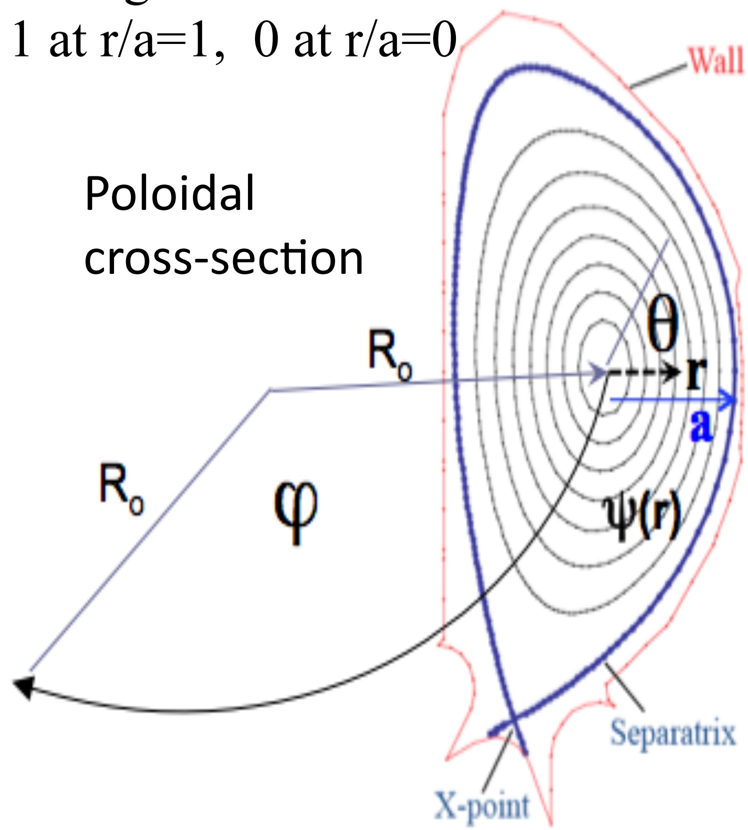
  Poster II
  - Computer Science
- Some examples
- Discussion

"Toroidal" tokamak Geometry

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

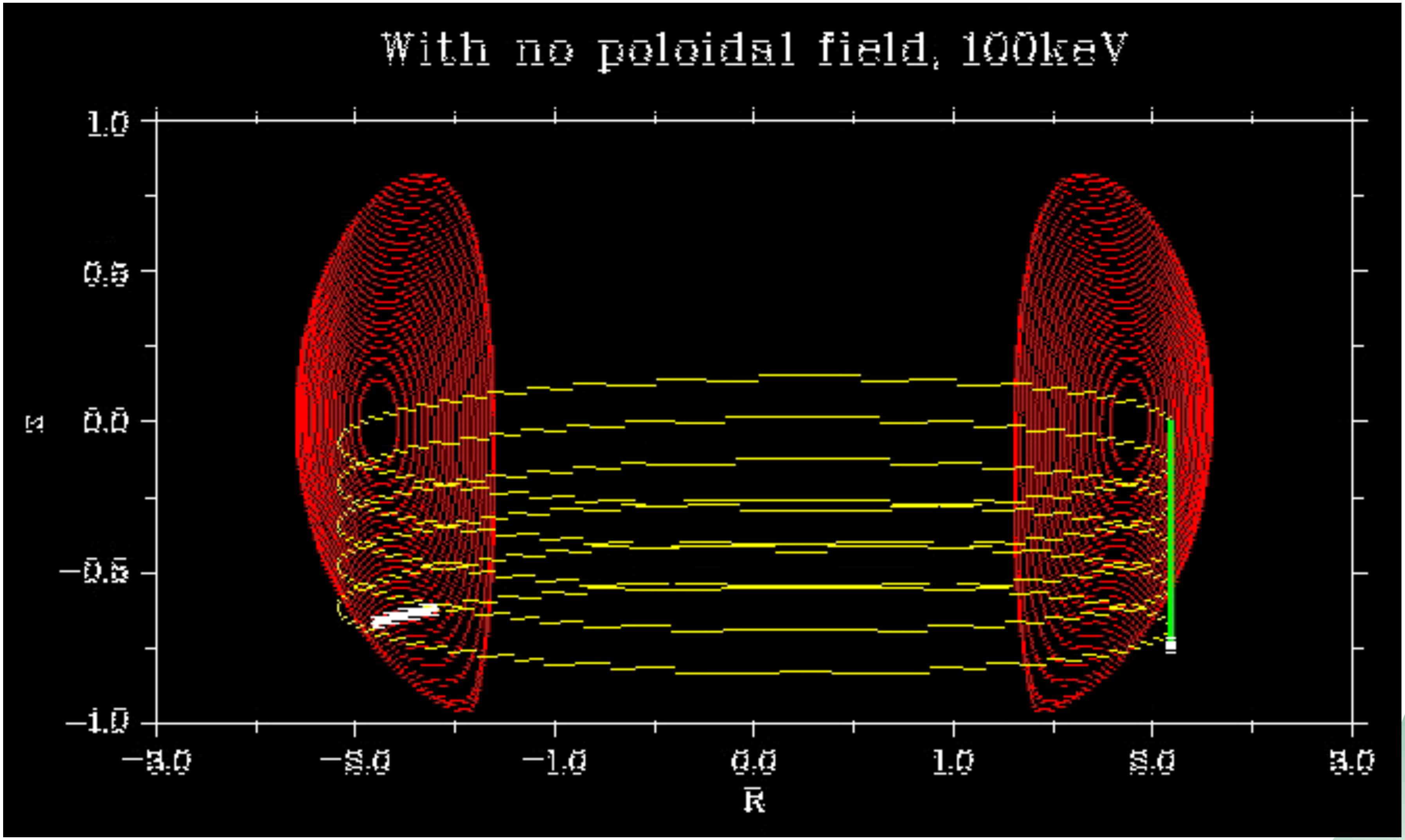
ITER



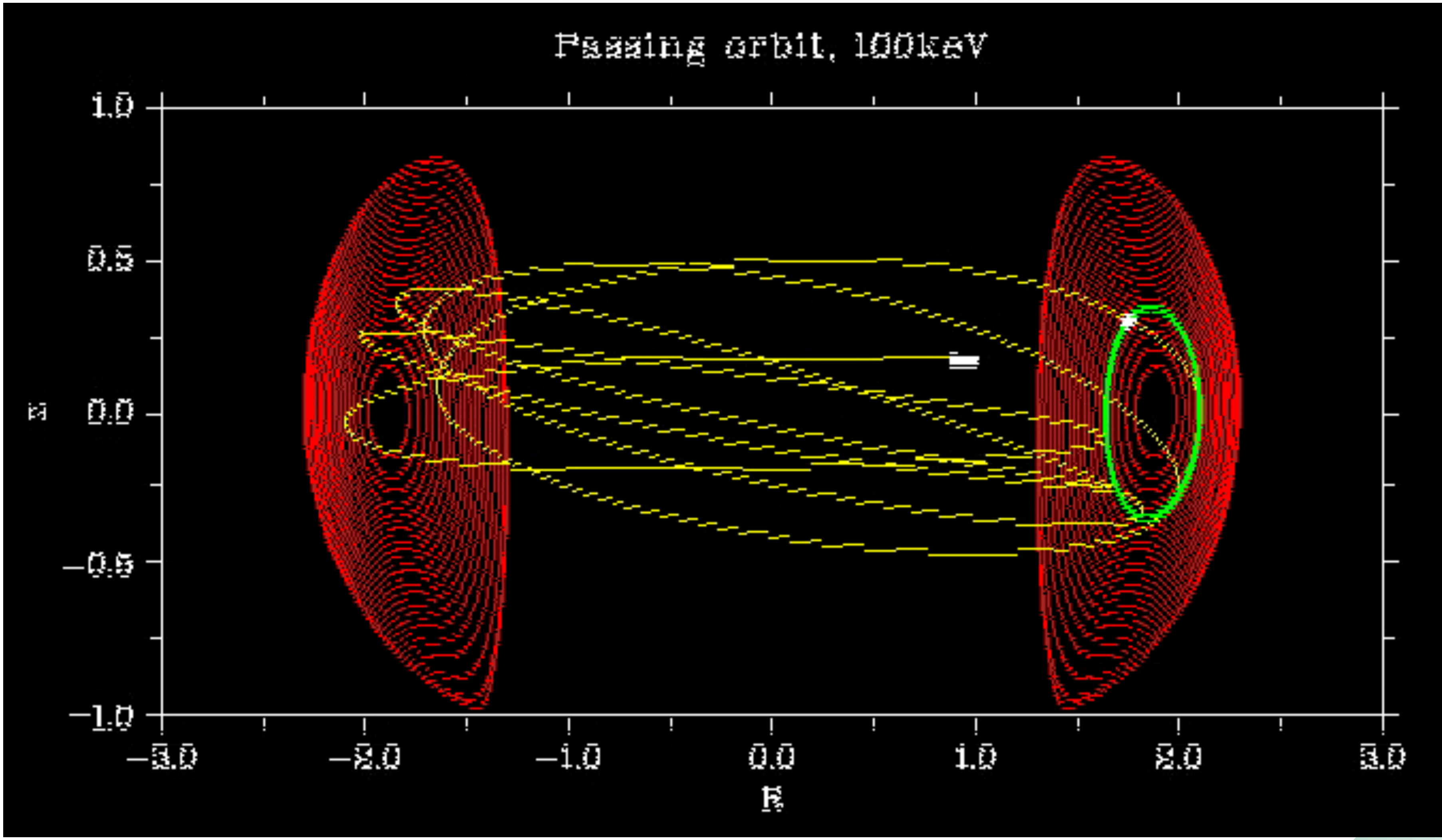


Torus, not a straight cylinder: plasma sees **inhomogeneous** physical space (magnetic field) → complicates physics & math through **magnetic mirroring, curvature drift, ballooning, toroidal mode coupling, etc**.

Tokamak confinement requires B_P



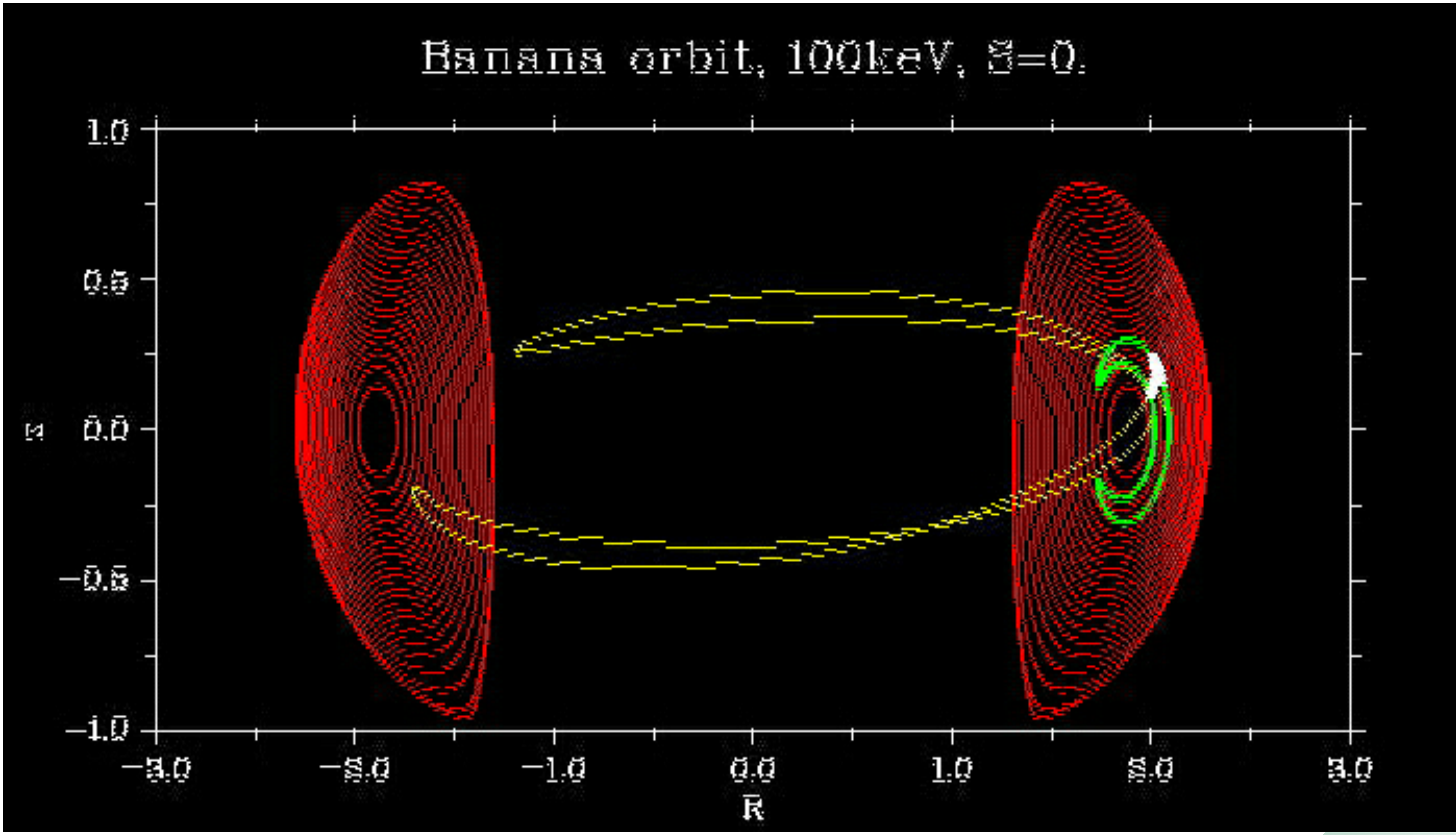
When adequate B_P (~0.1 B_T) is present, particle orbits are confined → Local physics?



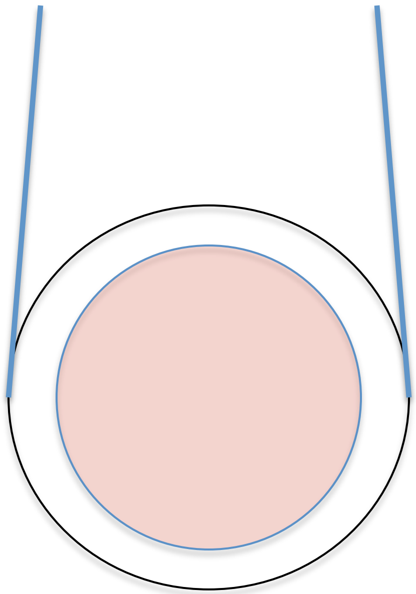
Many of the particles execute "banana" orbits

→ Nonlocal radial mixing by particles

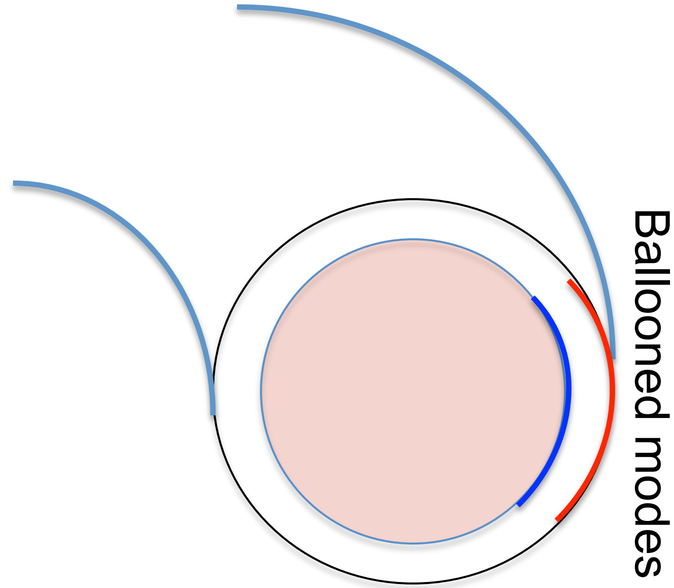
→ "Neoclassical transport" & "Neoclassical turbulence"



Nonlocal field coupling from toroidicity



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



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

(There exist other important nonlocal coupling sources.)
Nonlocal particle and field coupling
→Affects nonlocal self-organization of fusion plasma
→Creates difficulty in physics, math, V&V, UQ, etc.

What science are we studying?

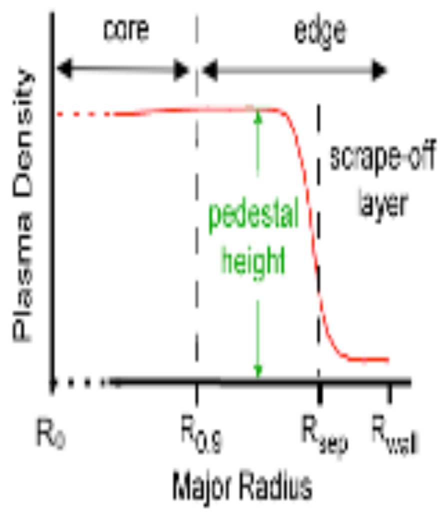
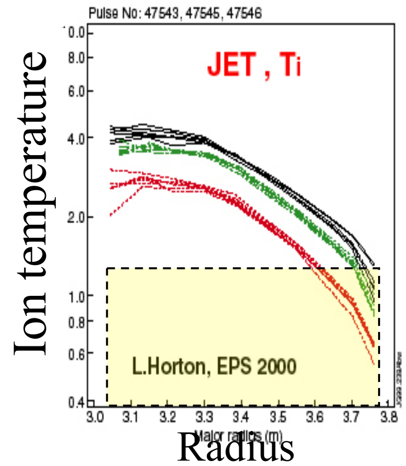
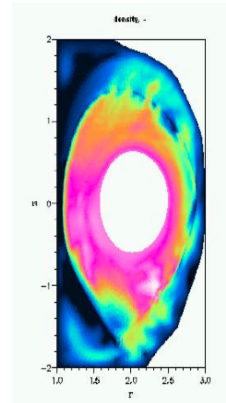


Figure .1a: Plasma edge region



Stiff T_i profile on edge pedestal



Edge localized instabilities could destroy pedestal and damage wall.

- Edge plasma self-organizes into a steep pedestal shape (H-mode). This made fusion to be possible with a cool edge in contact with wall.
- Edge physics is a challenging plasma theory issue, in contact with material wall and across magnetic separatrix → non-Maxwellian
- Solution is sensitive to both v- and x-space structures and dynamics

→Outside of a reduced (i.e., fluid) theory regime →
Particle-in-cell approach → Extreme scale computing is necessary

Gyrokinetic simulation in 5D phase space

Vlasov equation is 6D (3D in **x** and 3D in **v**), requiring

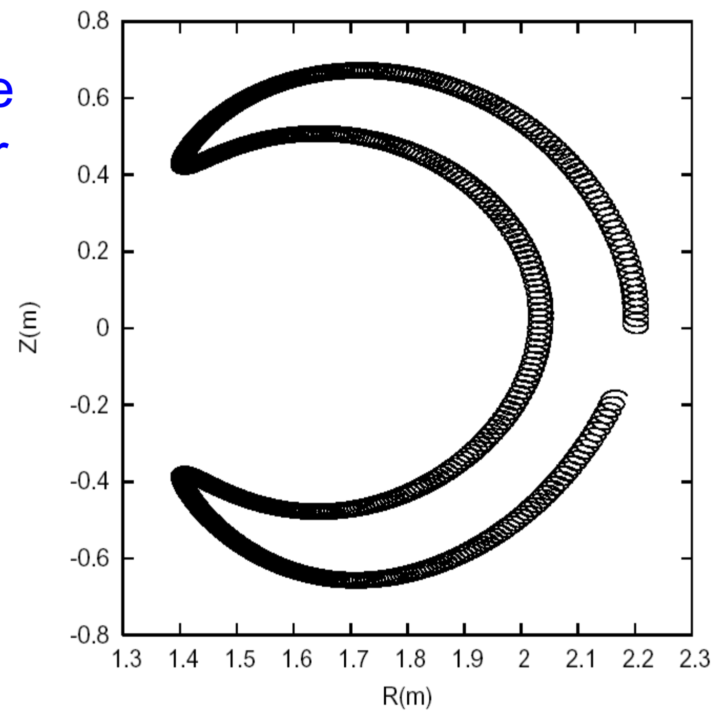
exa-scale computing for a tokamak simulation

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

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

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



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

The XGC1 code

- Electrostatic **5D gyrokinetic equations**
  - **ODE**

$$\frac{\partial f}{\partial t} + \frac{d\mathbf{X}}{dt}\cdot\frac{\partial f}{\partial \mathbf{X}} + \frac{du}{dt}\frac{\partial f}{\partial u} = C + \text{source} - \text{sink}$$

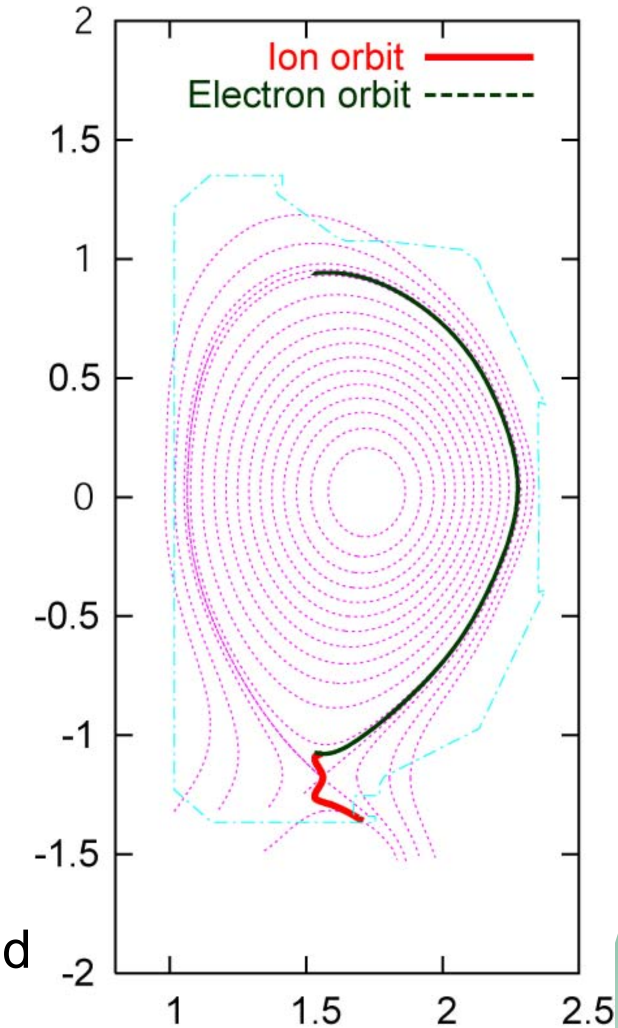
$$\frac{d\mathbf{X}}{dt} = \frac{1}{D}\left[u\hat{b} + \frac{u^2}{B}\nabla\times\hat{b} + \frac{\mathbf{B}\times(\mu\nabla B - \mathbf{E})}{B^2}\right]$$

$$\frac{du}{dt} = -\frac{1}{D}\left(\mathbf{B} + u\nabla\times\hat{b}\right)\cdot\left(\mu\nabla B - \mathbf{E}\right)$$

$$D = 1 + (u/B)\hat{b}\cdot\left(\nabla\times\hat{b}\right)$$

  - **PDE** Variable coeff.

$$-\nabla_\perp \frac{\rho_i^2}{\lambda_{Di}^2}\nabla_\perp\Phi = e(1-\nabla_\perp\rho_i^2\nabla_\perp)(\bar{n}_i - n_e),$$



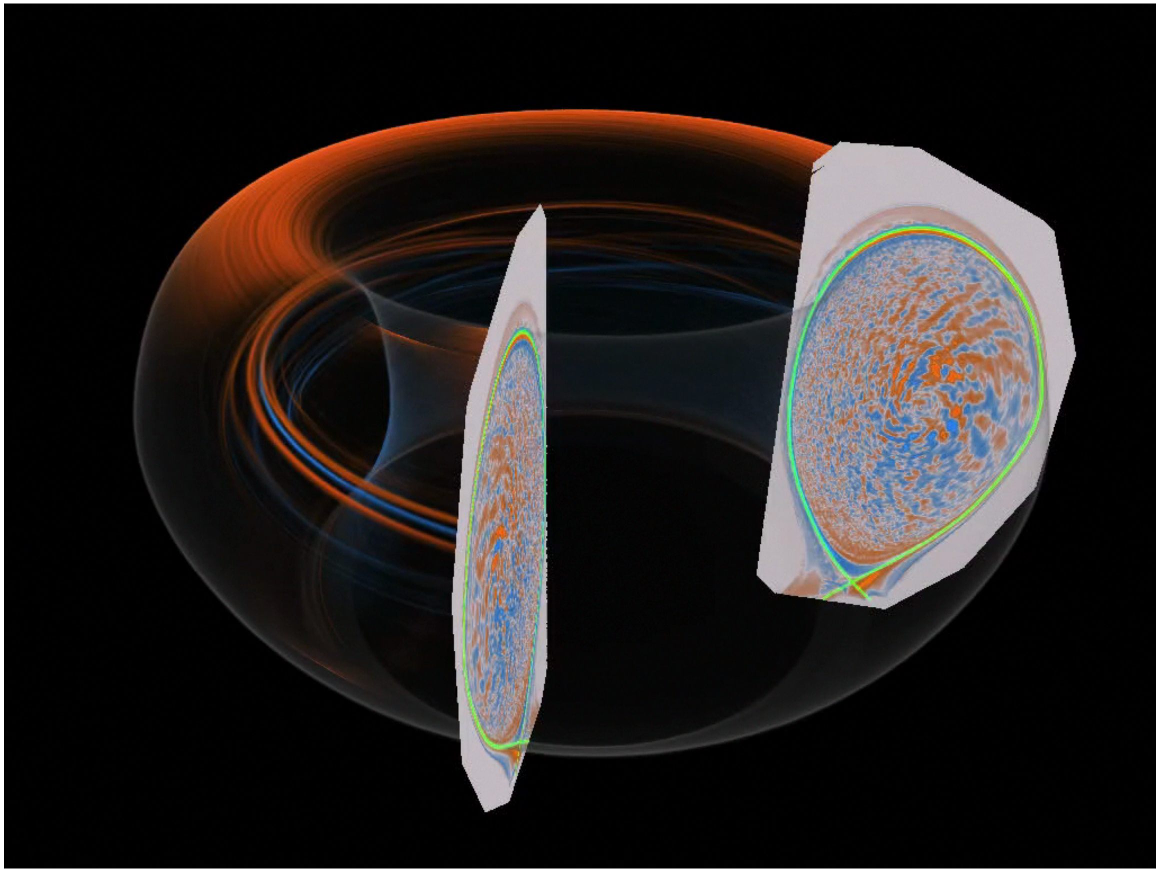
Orbit loss → total-f even in pedestal

- Particle-In-Cell approach, combined with 5D grid approach wherever advantageous
- To be improved to steep-gradient E&M eqns. (Hahm, Dimits, Scott, Brizard …)

Closer-to-reality global simulation in XGC1

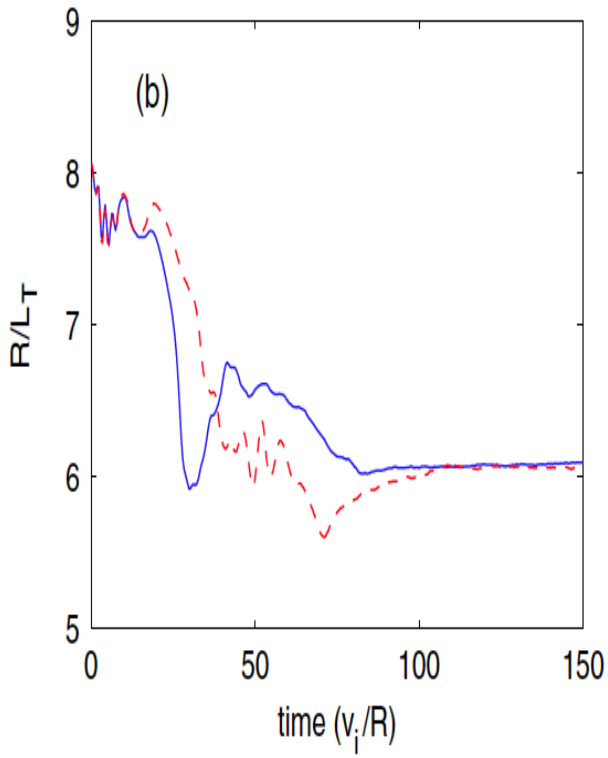
- Grounded wall potential is the only BD condition for solver
- Multiscale simulation (below gyro frequency)
- Low main-memory requirement (<0.5GB/core).

Global turbulence spreading (in 5D space)

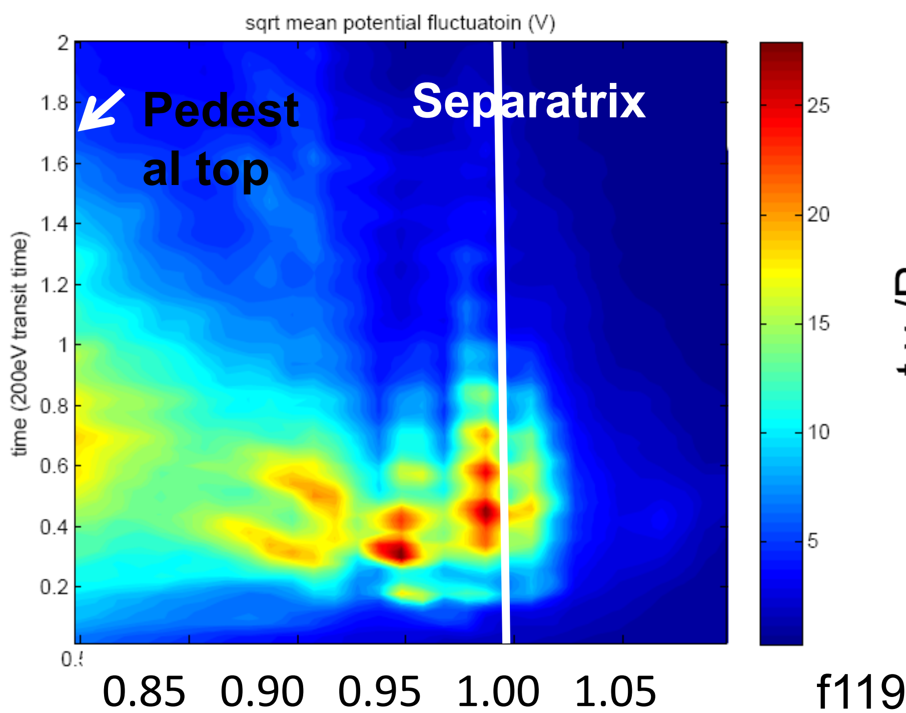


Simulation by S. Ku, Visualization by K. Ma

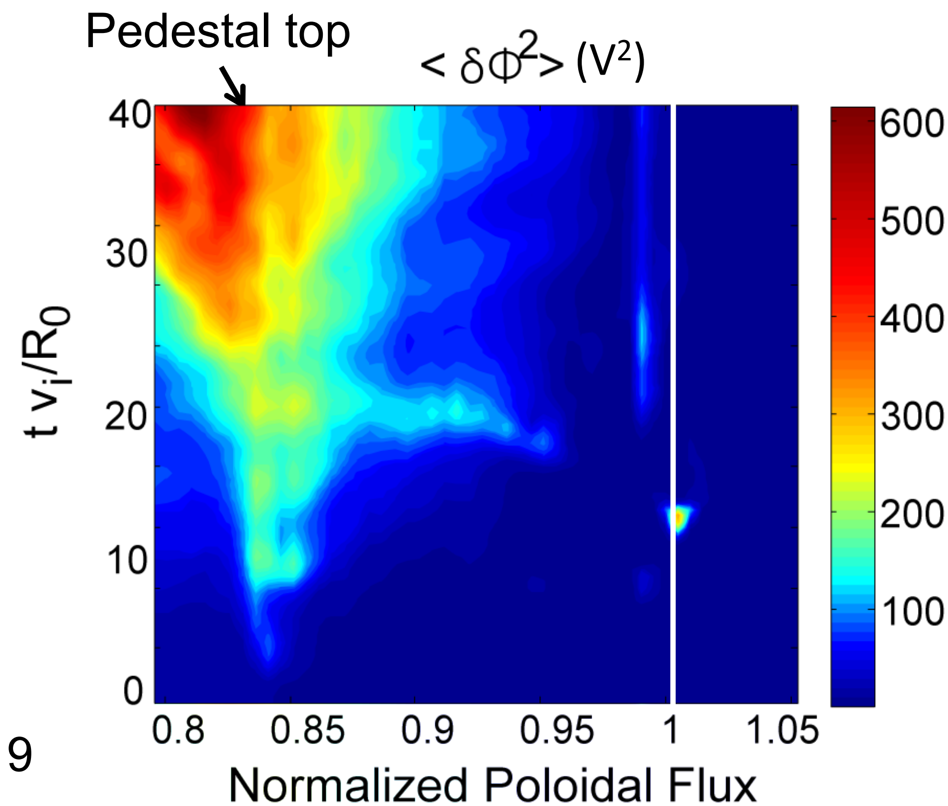
Initial T'(r) does not mean too much → UQ



Edge turbulence solution became different when we imposed an artificial core-side boundary.



Edge only simulation with an artificial BD condition at core-edge BD

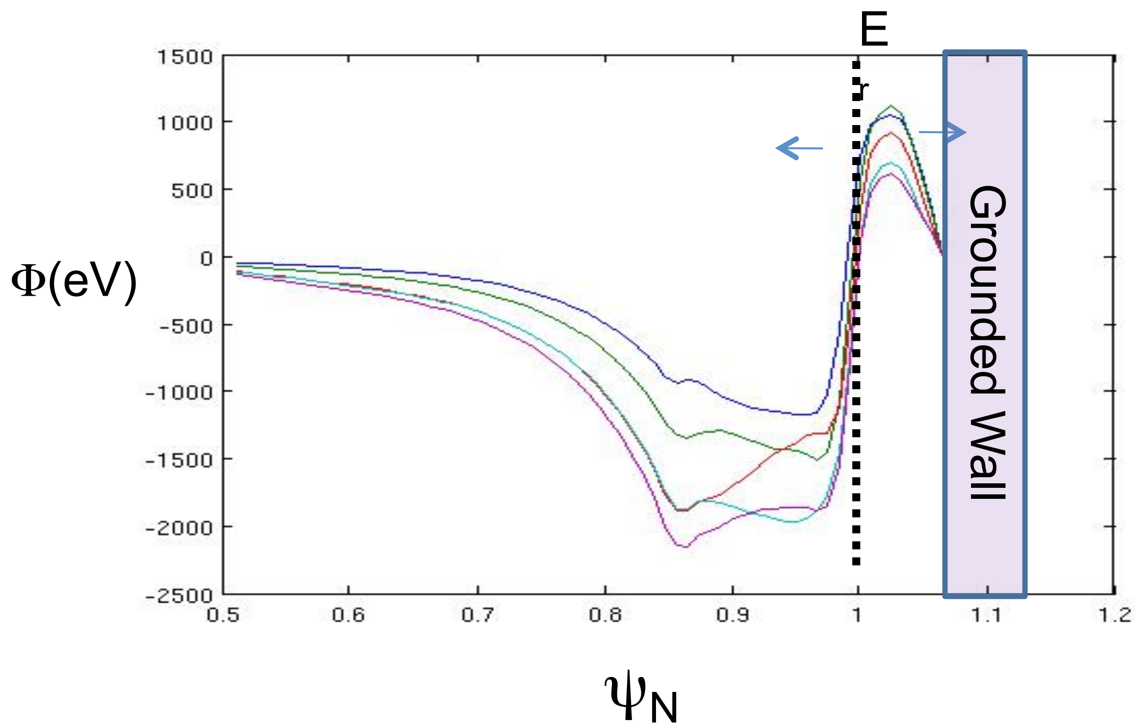


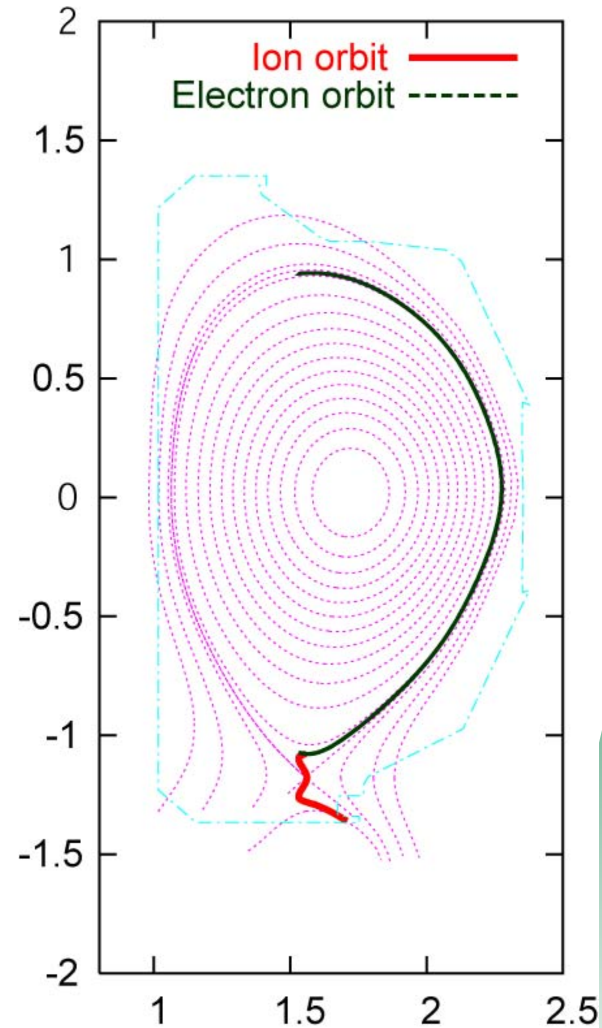
Core-edge simulation

Simulation by S. Ku

Edge potential-well formation

A robust H-mode feature, not understood previously.





Orbit loss → full-f even in pedestal

Physics Challenges (→ ASCR Challenges)

- Intrinsically multiscale physics, which are inseparable
  - Steep background profile, ion orbit excursion, electron dynamics, ion dynamics, neutral penetration, impurity particles, plasma-wall interaction, various micro instabilities and turbulence, MHD/Fluid type instabilities, scrape-off layer … **(10^{-4}m – m, 10^{-6}s – 10^{-2}s)**
  - Nonlinear self-organization among these multiscale components
  - Coupling of many scale-separated codes would be difficult.
- Requires higher order accuracy
- Complicated edge geometry with separatrix and wall
- Highly disparate electron and ion time-integration step size
- Experimental time scale simulation (~50ms for edge plasma)
  - An easier research, than the accuracy-improving research, would be to develop a self-consistent coarse-fine grained kinetic spatio-temporal integration: a high payoff research.

Challenges in Algorithm & Applied Math

- Complicated velocity-space physics and geometry
  → Particle-in-cell (PIC) with **unstructured triangular mesh**
  - Mesh generation (AMR to be tried later)
  - **Higher dimensional spatial domain decomposition**
  - **Particle search and scattering to mesh**
  - **Field interpolation to random particle positions (with Div B=0)**
- Multiscale self-organization on the same equations → accuracy
- Scalable solvers, as GPUs accelerate the particle time-advances
  - Improved scalability of the PETSc—Algebraic Multi Grid solver
  - FMM type Hierarchical solver for variable coefficient gyrokinetic elliptic operators (high pay-off research component)
- Implicit electron time advances in GPUs
  - Kinetic electron push in CPUs is ~10X more expensive from smaller Δt
- Optimization by combining-in the 5D grid technology
- Multiscale spatio-temporal integration of Kinetic PIC (subgrid modeling) (high pay-off research component)
  - Stability, accuracy, bifurcation, stiffness

Challenges in Computer Science

- Large scale Data Management: Handle I/O gracefully when each simulation time step produces over 1TB of data.
- Minimize Data Movement: Keep data in-memory and close to computation due to overheads associated with I/O and data movement.
- In-Situ Data Analytic: Perform data processing at data source and along the data path.
- Tight Data Coupling: Enable scalable memory-to-memory coupling for both inter and intra multiscale integration

→ In-situ/in-transit Data Management

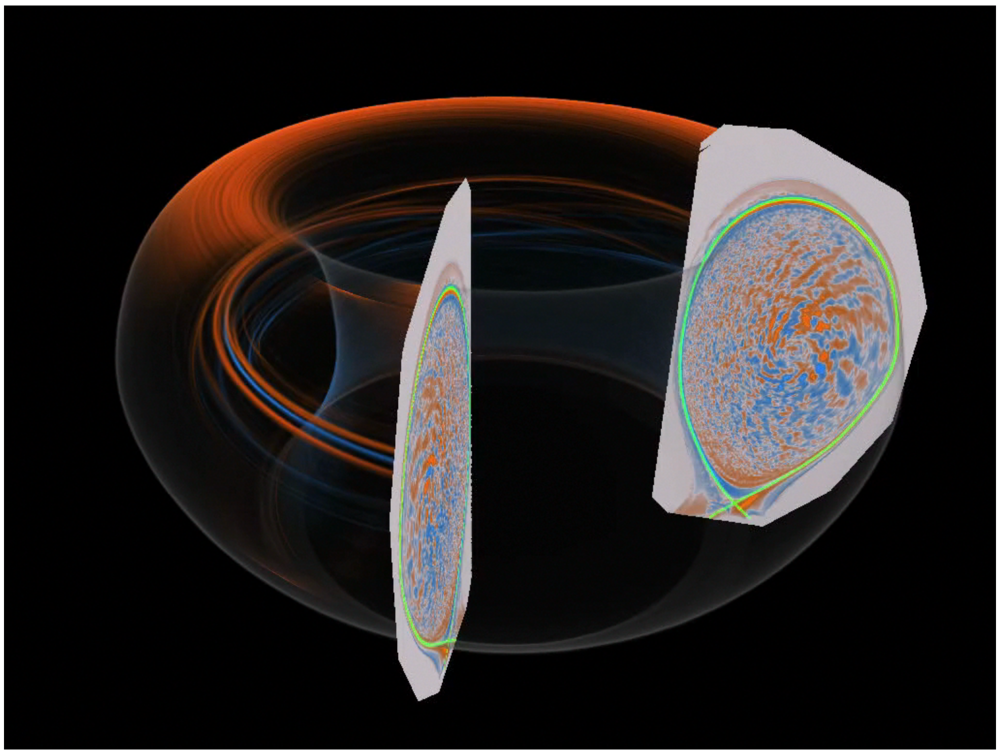
The **Adios** adaptable I/O system, **DataSpaces** data-staging substrate, and **eSiMon** dashboard have been conceived and developed under the previous CPES project, as part of the End-to-end Framework for Fusion Integrated Simulation (EFFIS).

Challenges in Verification, Validation & UQ

- **Large and comprehensive multiscale simulation brings up extra challenges to V&V and UQ.**
  - Multi variable physics observables are spread in 5D **x-v** space
    - at all heirarchical levels
    - in nonlinear self-organized states
  - Many runs of the whole model is not possible for conventional UQ
- **Validation metric needs to include all heirarchical level observables**
- **Verification**
  1. Study sub-models independently -- UQ
  2. Need innovation for the whole model: manufactured solution, …?
- **UQ**
  - UQ on a sub-model may not be related too well to the self-organized solution (a self-organized system has an ability to compensate)
  - Need to develop a smaller-size representative problem
  - Need to identify dominant and relevant uncertainties (2 step approach?)
  - …

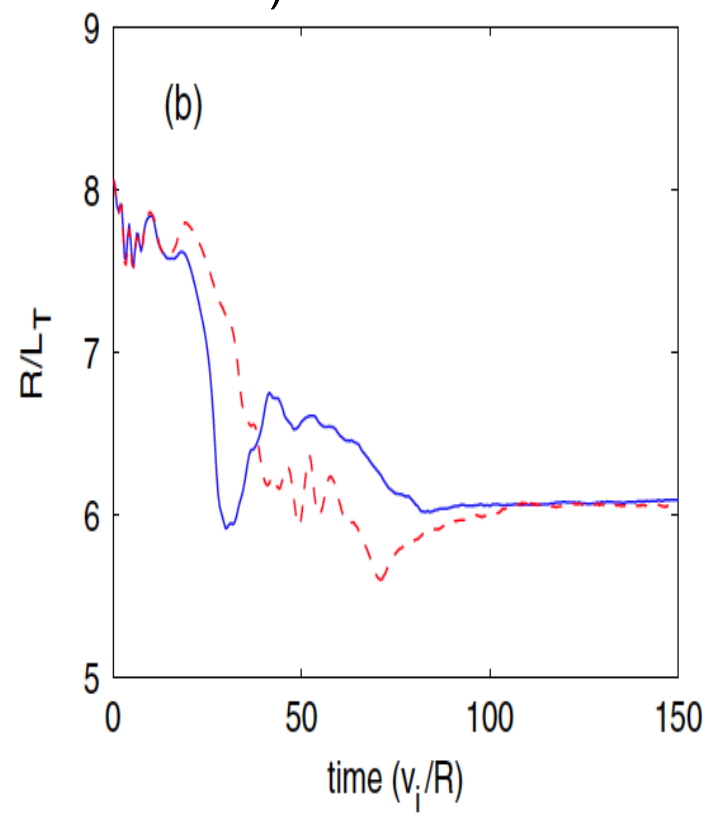
UQ on a self-organizing, extreme scale system may benefit from different types of innovative techniques

Self-organization among multi-physics



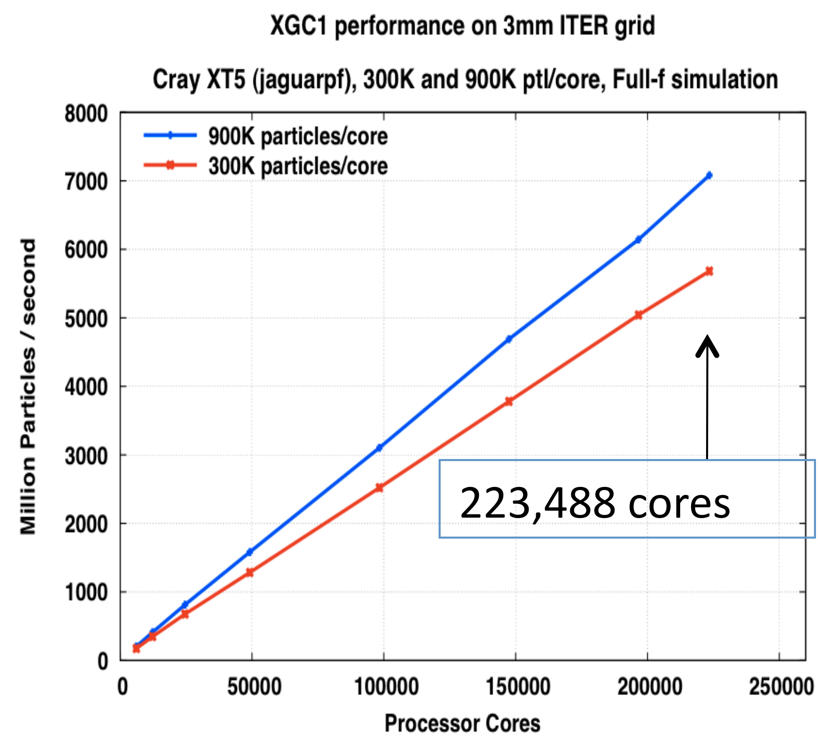
Simulation by S. Ku, Visualization by K. Ma

Initial T(r) does not mean too much → Can be removed from UQ data early on? (External control means more)



Challenges in Performance Engineering

- **Excellent performance and scalability on current generation of HPC platforms were achieved in the previous CPES project**
  - ASCR scientists played essential role
- **But,**
  - Computational, data and I/O requirements are increasing significantly
  - Target computer system architectures are changing rapidly
  - Increasing frequency of faults, …

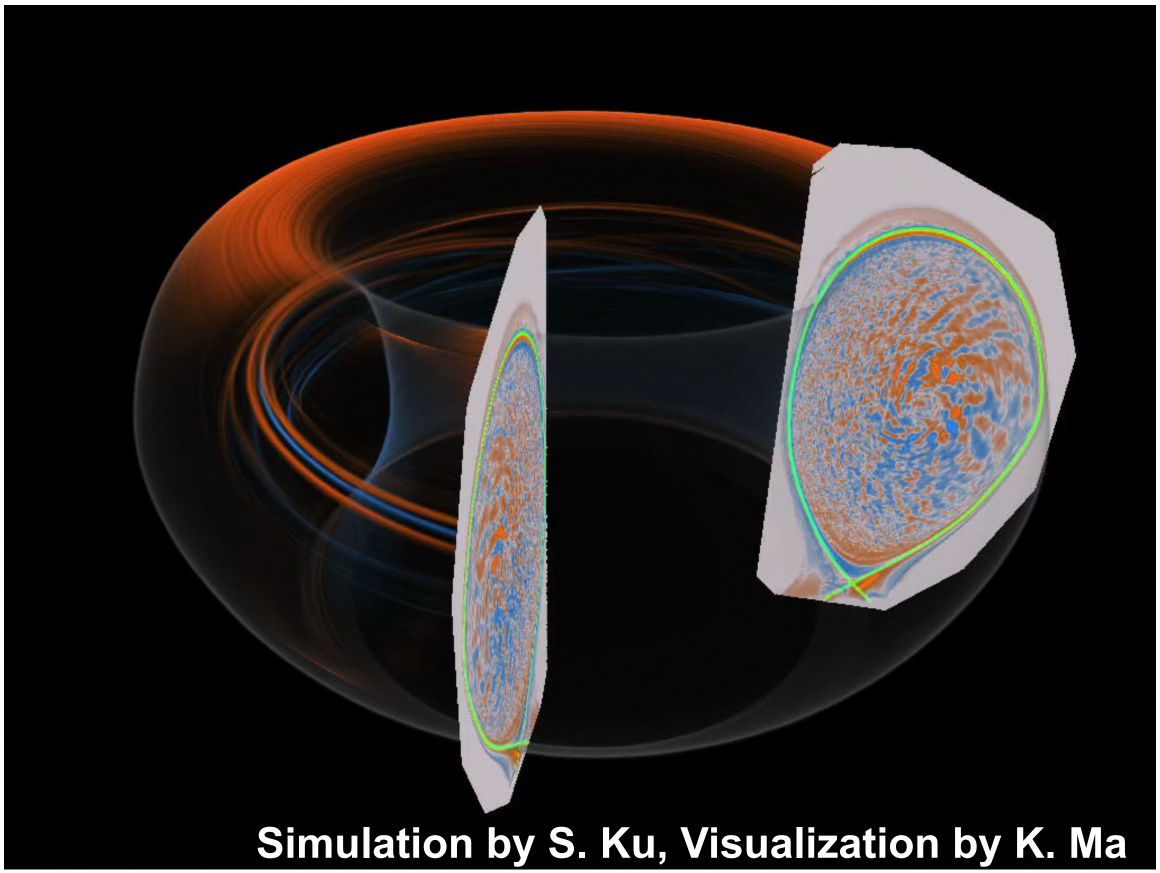


- **Initial porting of Fortran XGC1 to Titandev XK6 (16 core CPU + GPU per node): compare with Toedi XK6 (two 16 core CPUs); and with Hopper XE6 (using the same #cores)**
  1. **Un-optimized** CPU, **un-optimized** GPU → 2.2X acceleration relative to Toedi
  2. Optimized CPU (-fast option), **un-optimized** GPU → 1.4X relative to Toedi
  3. Most Recent: Optimized CPU, **un-optimized** GPU → 1.7X acceleration relative to Hopper
- **GPU optimization of XGC1 has begun! Expected to accelerate XGC1 further.**

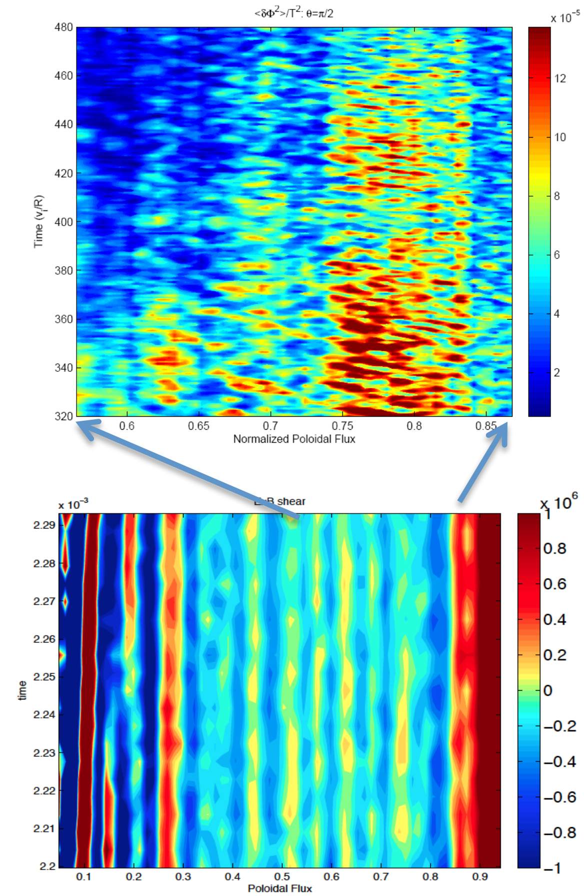
Informatics can reveal new scientific understanding

- **Fusion data informatics should be a closely coupled effort by physics, applied mathematics, UQ, and computer science**
- **Known and unknown patterns**

Global turbulence spreading (in 5D space)

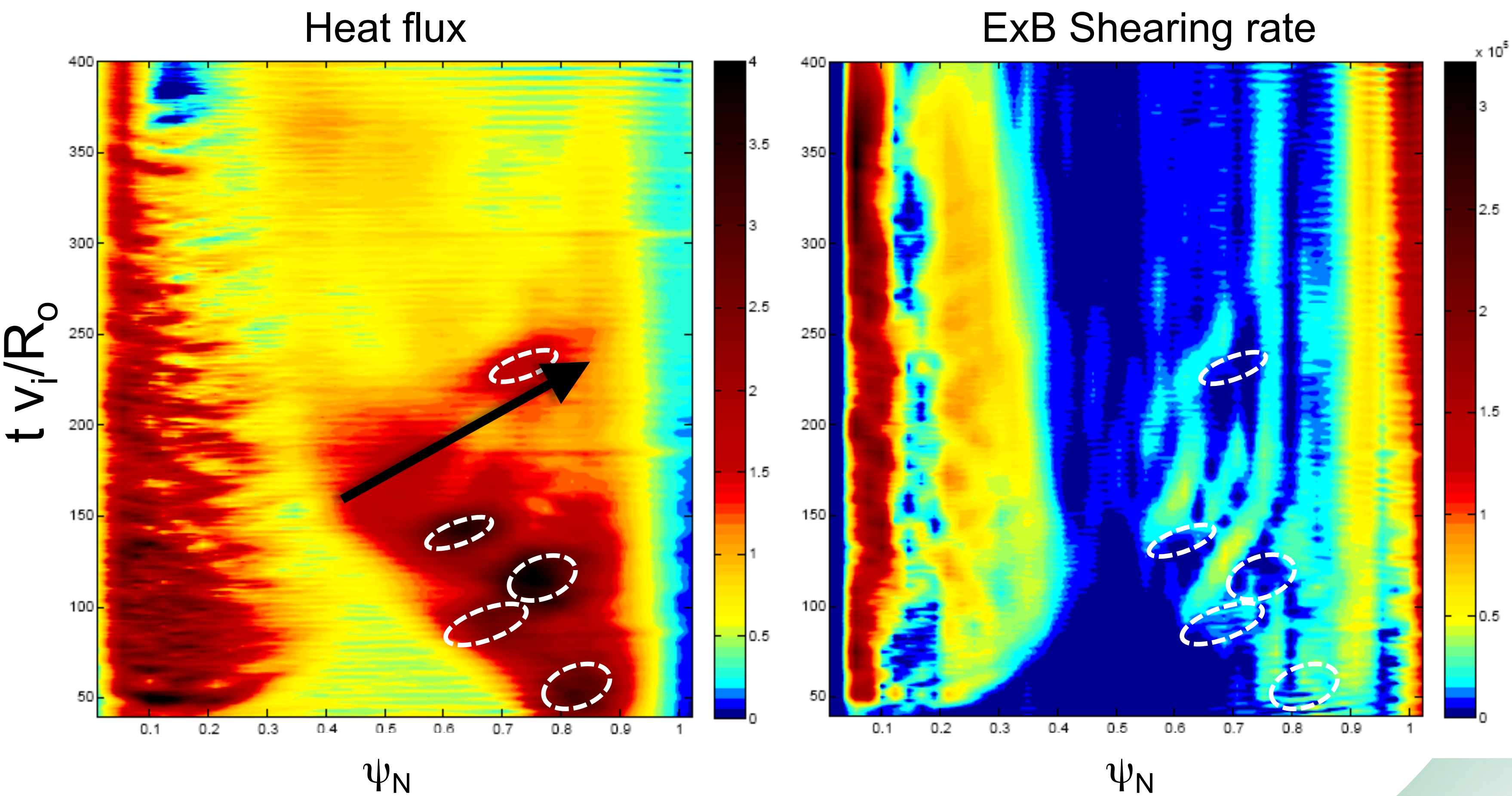


Non-local avalanches



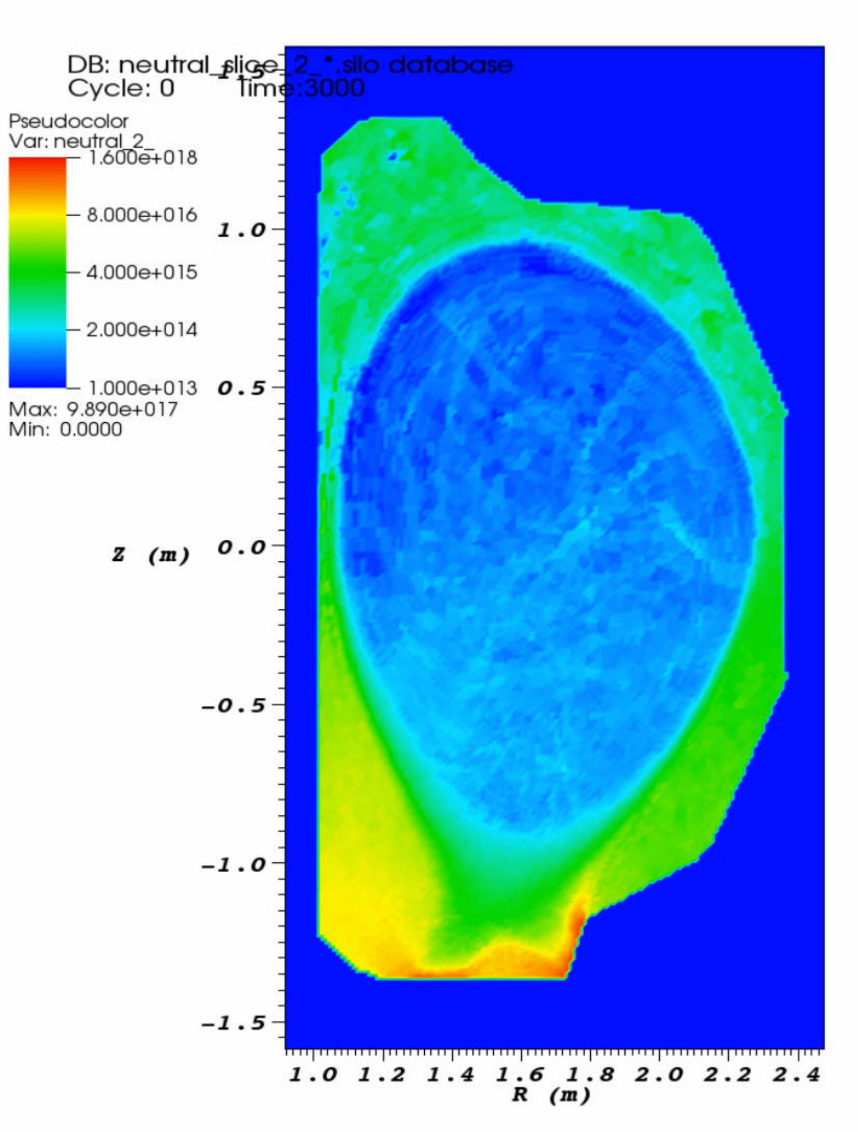
Self-organizing interaction between mean (ExB flow) and micro-scale (turbulence and heat flux) physics

Speed of non-local turbulence interaction (and bursty outward heat flux) is similar to the experimental observation.



Shot pf1-4
Simulation by S. Ku

Experimentally missing, but important, data
e.g., distribution of neutral particles



Neutral particle density distribution in realistic DIII-D edge geometry from XGC [simulation by Stotler].

Material interface-preserving mesh is important.

Connection with the “Plasma Surface Interactions” SciDAC is important for a higher fidelity edge physics.

Discussion

- **Fusion has a challenging multiscale self-organization problem to solve: Must utilize extreme scale HPCs**
- **During the previous SciDAC cycle, a first-principles multiscale gyrokinetic code XGC1 has been created**
  - Efficient scaling to the maximal Jaguarpf XT5 capability (>2 pf)
- **Initial GPU porting (Cuda Fortran) of XGC1 on Titandev shows a reasonable success.**
- **The more powerful the HPC will be in the future, the more complete physics XGC1 can model.**
- **The problem inherently requires a close collaboration & innovation with ASCR scientists**

  → e.g., Birth of Adios, DataSpaces, eSiMon … technologies
  - **Partnership with all four SciDAC-3 Institutes**

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