Solving the Multiscale Multi-Physics Puzzles in Tokamak Edge

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- *On behalf of the XGC team*
- *Funded by DOE FES & ASCR*
- *Computing resources provided by NERSC, OLCF and ALCF*

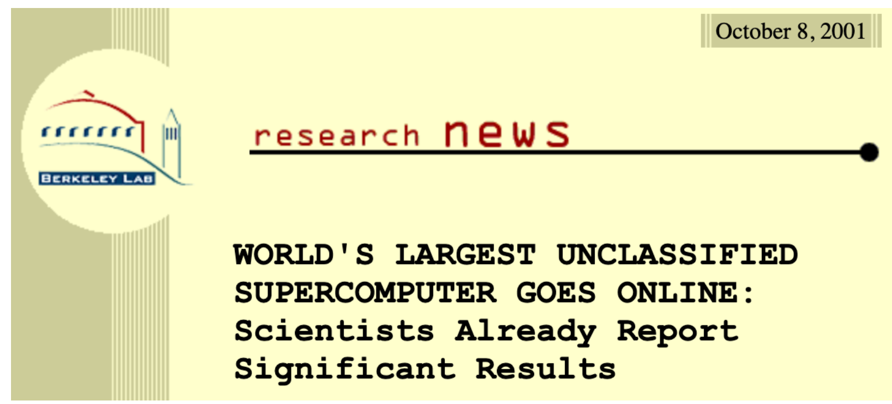
My research journey has been shaped by “50 years of NERSC” (1)

- I became a NERSC user in the CTRCC and NMFECC era
  - CTRCC: Controlled Thermonuclear Research Computer Center: (1974-1976, CDC7600, 36 megaflops/s)
  - NMFECC: National Magnetic Fusion Energy Computing Center (1976-1990)
  - I built my first “major” code on NMFECC computer in mid 80s.
- Until the launch of GSEABORG in 1999 (IBM Power3, 512 cores and 0.5GB/core), I was still mostly an analytic theorist
- When GSEABORG was installed in 1999, my concept of physics research changed in a transformative way.
  - I felt about what was coming in the computing world
  - I saw a way to crack out of the analytic theory cage. Nature is mostly governed by nonlinear multiscale multi-physics.
  - Tokamak boundary was one of the most severe examples.
- I recruited a few graduate students who were willing to start the “crazy” computational journey with me.

My research journey has been shaped by "50 years of NERSC" (2)

- We started building a multi-physics kinetic code XGC for tokamak boundary physics
  - All the kinetic codes were (still true mostly) taking the perturbative approach to save compute time, assuming scale separation
  - Since the whole plasma should be solved without scale-separation, instead of solving only the perturbed part (~1%), the required computing power is ~100x more expensive
  - I envisioned that the computing power would grow according to the Moor's law: I got lucky!

- With the launch of SEABORG I&II, my dream was becoming more realistic.
  - We completed the first multi-physics, parallelized kinetic code XGC0 using particle-in-cell technology,
  - which accurately followed the 3D plasma particle trajectories with a field solver in action at every timestep, thus the evolution of the background plasma, together with the MC neutral particle trajectories
  - in realistic tokamak edge geometry.



SEABORG I NEWS in 2001

My research journey has been shaped by "50 years of NERSC" (3)

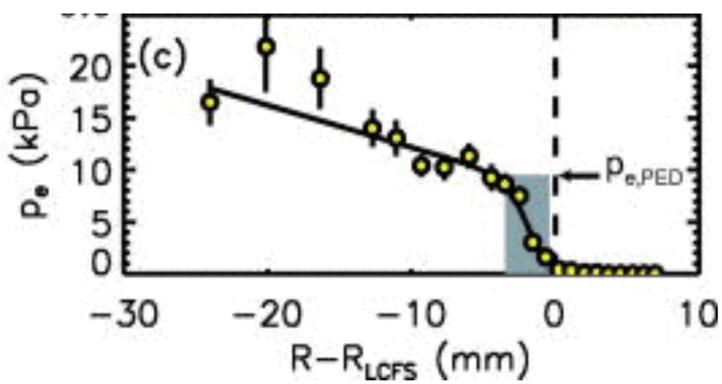
- For a few years in the early 2000s, FESAC subcommittee heavily emphasized the necessity for a multiscale multi-physics code to study the formidable tokamak edge physics problem
  - But such codes did not exist except XGC: a big credit to NERSC!!!!
- I was awarded with Proto-FSP and SciDAC 2, 3 and 4 centers
  - Our dream-team (applied mathematicians, computer scientists and performance engineers) developed XGC into a modern parallel code
- XGC has been getting tremendous help from consecutive NERSC NESAP programs ever since
- XGC became one of the largest INCITE award codes since 2007
- In 2009, XGC became the ASCR Joule Milestone code on Jaguar at ORNL; and Early Science Code for all the subsequent new computers at NCCS/OLCF
- In 2012, XGC became one of the first GPU codes on Titan
- In 2016, XGC became one of the ECP application and co-design codes (WDMApp and CoPA)
  - Became one of the most successful exascale codes on Frontier and Aurora
- XGC is now used by four FES SciDAC5s

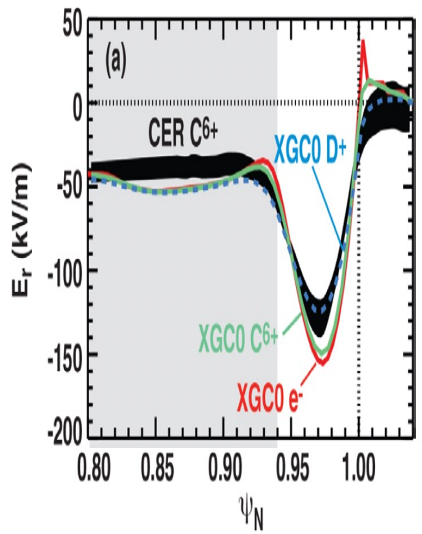
SciDAC Scientific Discovery through Advanced Computing

ECP EXASCALE COMPUTING PROJECT

kokkos

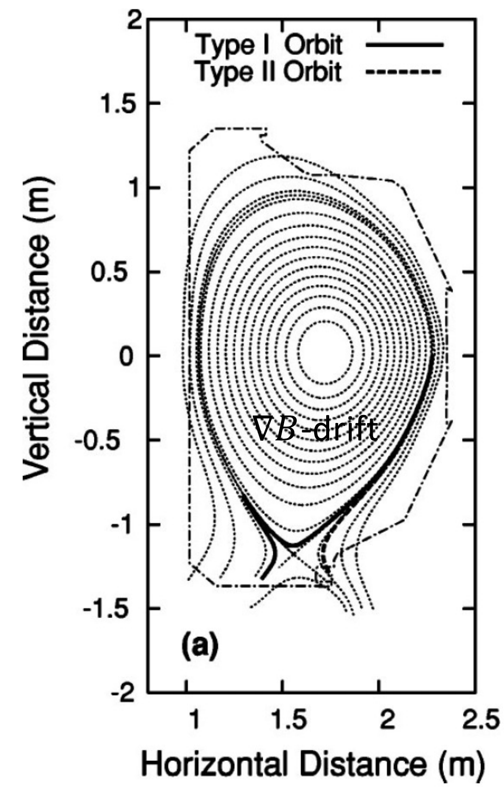
A baseline H-mode mystery was solved on SEABORG (2001-2008)



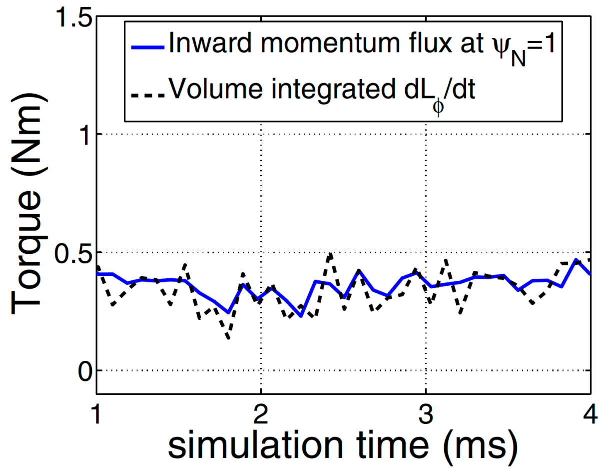


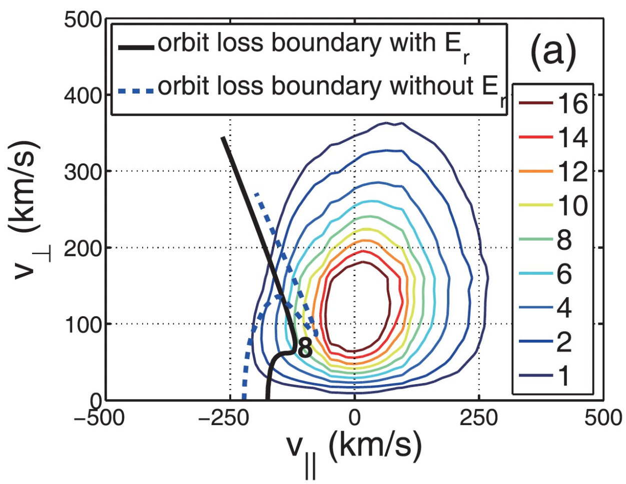
- Tokamak plasma spontaneously bifurcates into H-mode (high confinement mode)
  - allows an economical size reactor possible
- Negative electric field well was found to proceed the bifurcation and provide the ion transport barrier at edge
  - How it formed was a mystery
- XGC discovered the ion X-point orbit loss physics on SEABORG
  - One of the big theoretical discoveries in magnetic fusion

[Chang, Ku et al., Phys. Plasmas 2002, 2004]
[S. Ku, Chang et al., Phys. Plasmas 2004]



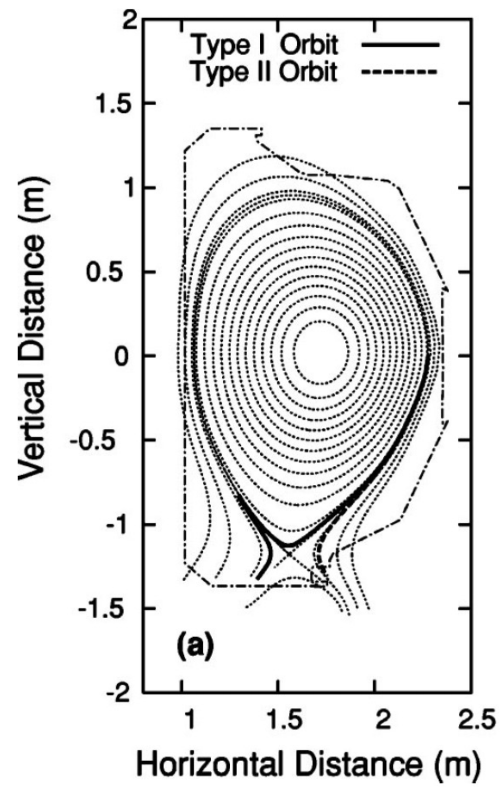
Source of core plasma rotation was identified on Hopper (2010-2015)



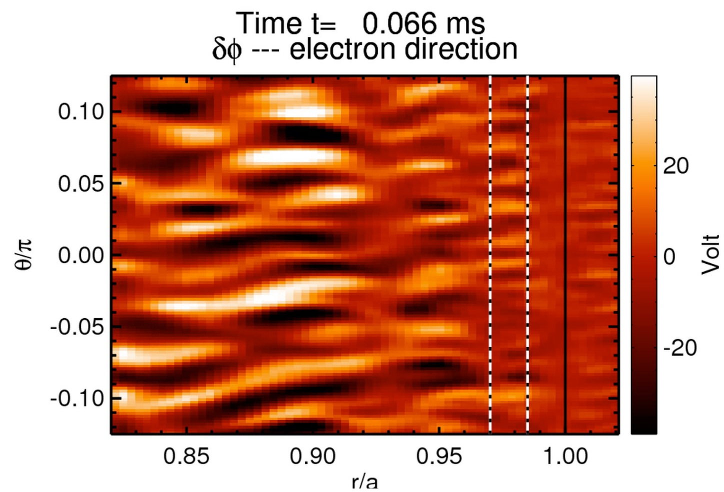


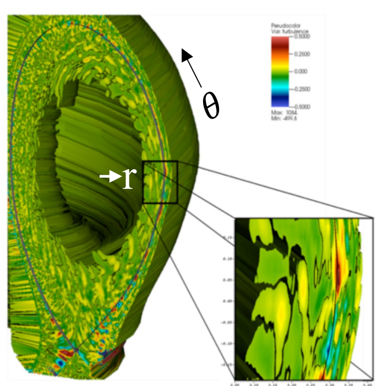
- Plasma rotation enhances reactor economy
  - by allowing better confinement and stability
- Plasma angular momentum was observed to increase in the core without an external injection
  - Momentum is conserved in the core plasma. Then how?
- XGC discovered that the momentum in core plasma is from the core-edge interaction
  - Agreed MIT experiments
  - Another significant theoretical discoveries

[Seo, Chang et al., Phys. Plasmas 2014]



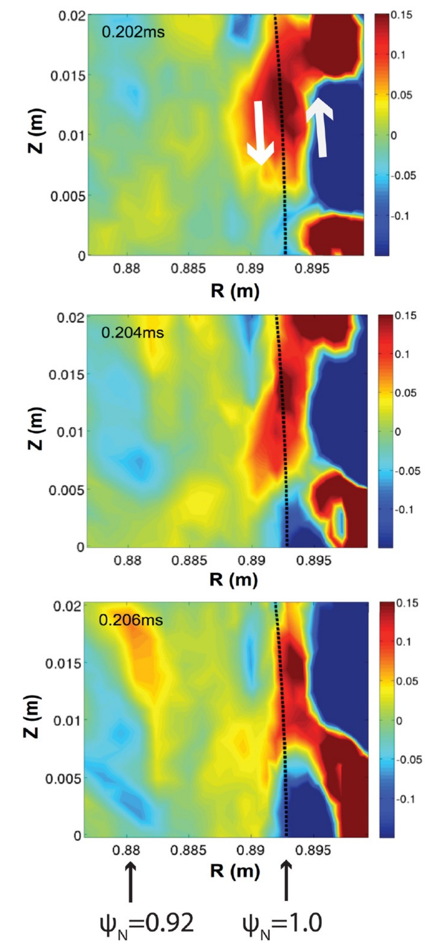
XGC then utilized OLCF's world #1 supercomputer Titan (2012-2019) to achieve the Low to High operation mode bifurcation (L-H bifurcation)





- Achieving L-H bifurcation is a necessary condition for ITER
  - First-principles understanding of the L-H bifurcation physics did not exist
- XGC found that L-H bifurcation is from multiscale self-organization
  - Reynolds stress transfers turbulence energy to small-scale sheared flow and starts the turbulence suppression
  - Global sheared flow from X-point orbit loss finishes up the bifurcation
  - Another hottest achievement

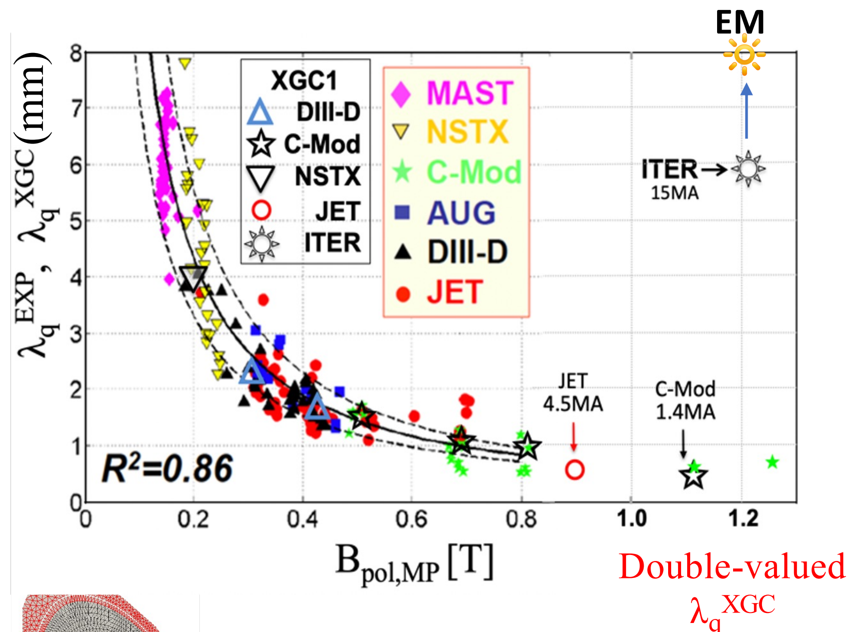
[Chang, Ku et al., Phys. Re. Lett. 2017]
[Ku, Chang et al., Phys. Plasmas 2018]

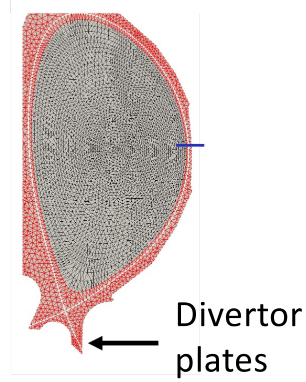


XGC continued to utilize extreme scale HPCs to predict turbulent widening of the exhaust heat-load on the divertor plates of ITER

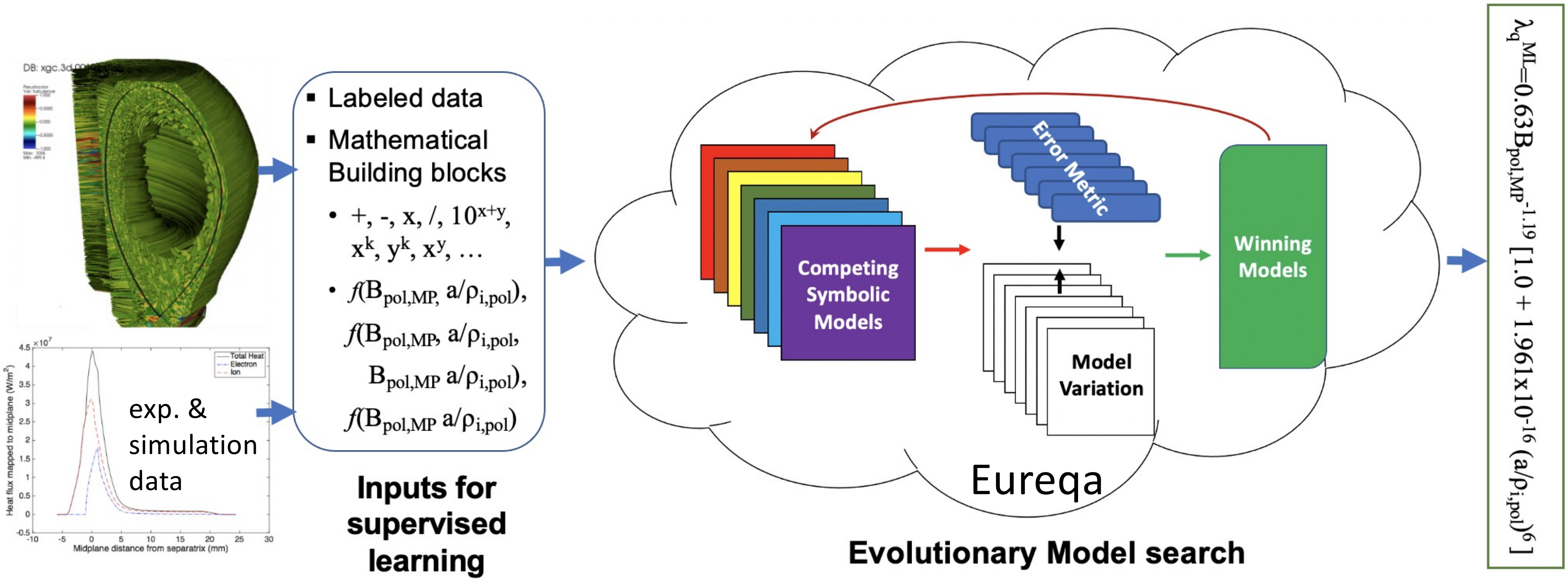
- One of a few biggest concerns for ITER was the damage to divertor plates by exhaust heat
  - Extremely narrow heat-load channel width
- XGC found that ITER edge is in a different physics regime from the present tokamaks
  - Exhaust heat-load width from XGC are validated at NERSC against present-day experimental data.
  - Strong e-directional edge turbulence due to high magnetic field and large size is making difference in ITER
- Turbulence spreads the heat-load width by 6x from the previous best estimate that was based on the simple data extrapolation → close to design value
  - A simple surrogate model has been created using AI
  - ITER operation can be much easier, if this prediction can be **validated**
  - ITER has already been accepting this discovery.

[Chang, Ku et al., Nucl. Fusion 2017]
[Chang, Ku et al., Phys. Plasmas 2021]





A physics-informed supervised AI program produced a simple surrogate model



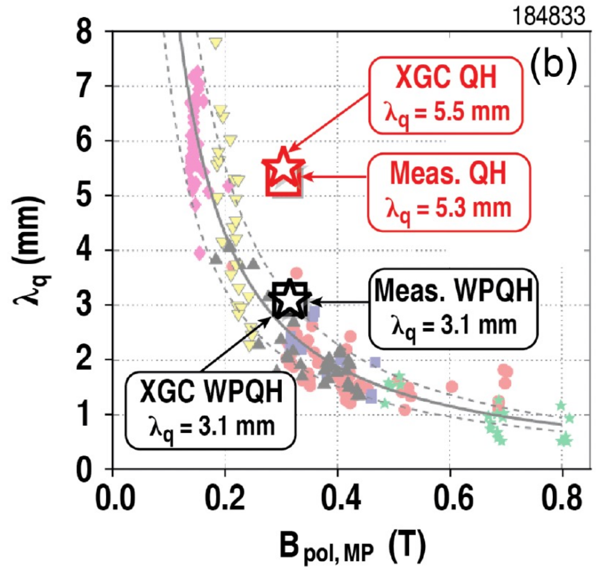
#An AI-powered modeling engine by Nutonian (https://www.nutonian.com/products/eureqa/); now acquired by DataRobot

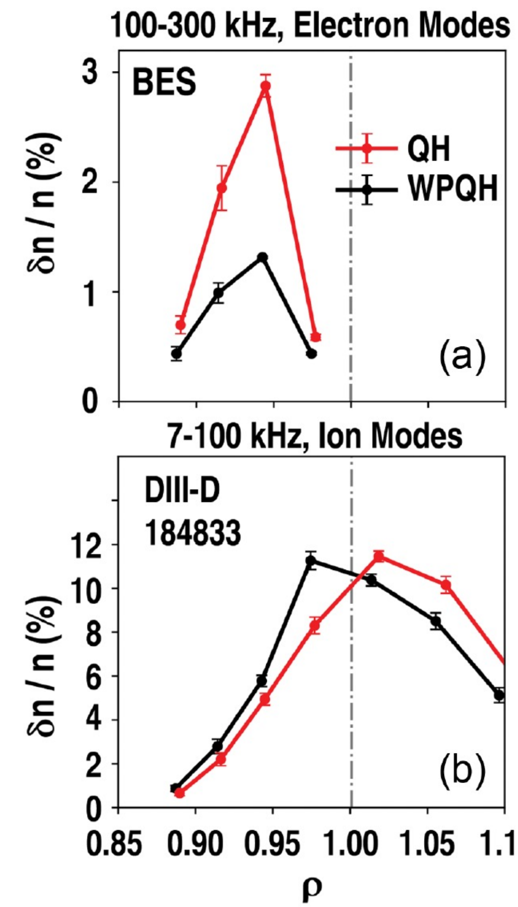
→ **"Simulation anchored machine learning"** [CS Chang et al., Phys. Plasmas 2021]

Turbulence widening of divertor heat-load width has now been validated

[Ernst, Ku, Chang et al., Phys. Rev. Lett. 2024]

- DIII-D tokamak has just confirmed the widening of divertor heat-load width λ_q when the electron-directional turbulence becomes stronger
- XGC simulations on **Perlmutter** agree with the experiments
- We now anticipated that ITER will operate at the design value of divertor heat-load width
  - A good example that ML from today's data is only an interpolation
  - Extrapolation to the future physics regime requires first-principles-based HPC simulation

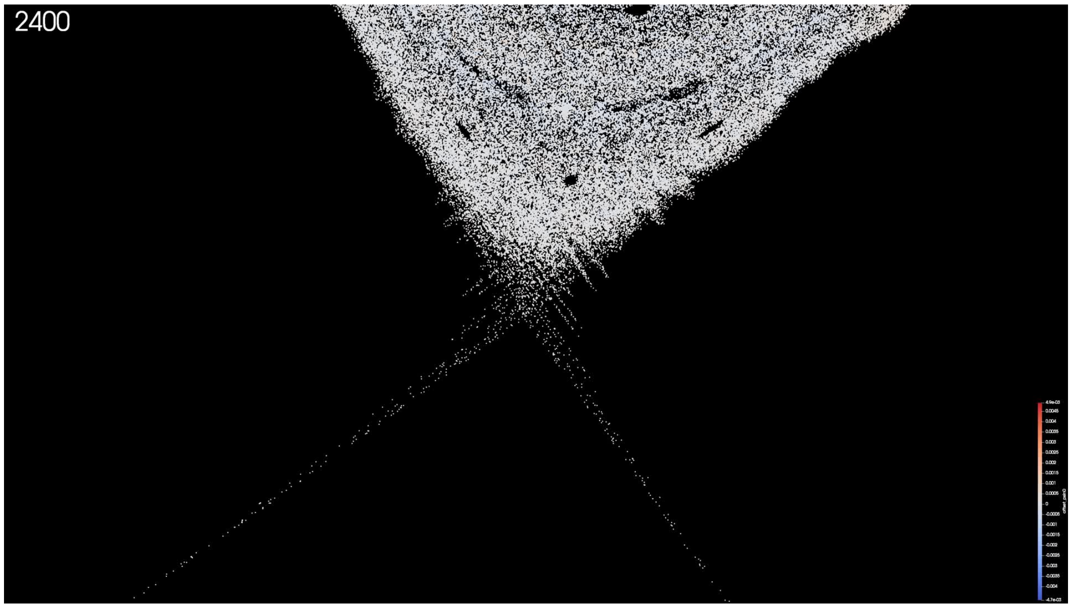




→ **Simulation-anchored ML/AI** *[Chang et al. Phys. Plasmas 2021]*

- Our surrogate model will become more accurate as more studies are performed on leadership class computers

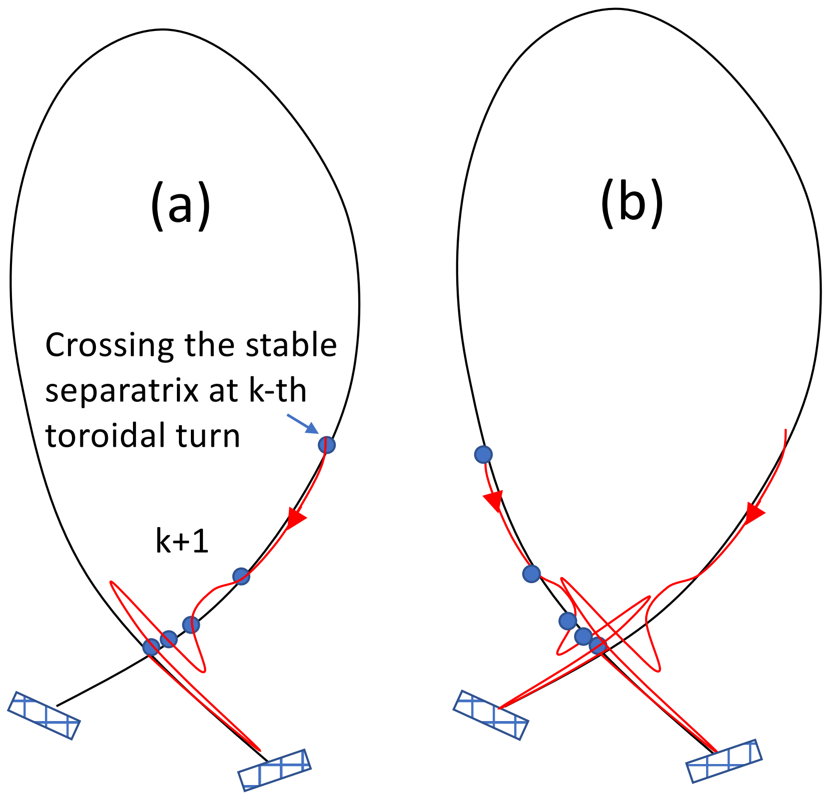
Perlmutter has a significant power: A capability computing in the NESAP program allowed us to make an unexpected discovery



Poincare puncture plot of magnetic field lines in DIII-D edge. Electromagnetic XGC discovers that the separatrix surface gets tangled up by the intrinsic turbulence, with thin and long lobes connecting the core electrons to the divertor electrons.

- Fusion researchers have assumed that the divertor magnetic separatrix surface provides the last confinement w/o extrinsic perturbation; i.e., external perturbation or MHD
- XGC already found in 2002 that the separatrix surface does not confine ions
  - The ion X-point orbit loss supports the essential H-mode edge pedestal
  - However, edge pedestal tends to become too steep and drives edge instabilities that destroy the divertor surface
- XGC has now discovered that, intrinsically, the separatrix surface does not confine the electrons either. *[Chang, Nucl. Fusion 2024, invited talk, IAEA-FEC2023]*
  - Divertor heat-load width becomes even wider in ITER
  - Edge pedestal slope can become milder if there is a heat sink around X-point, mitigating the dangerous edge instability

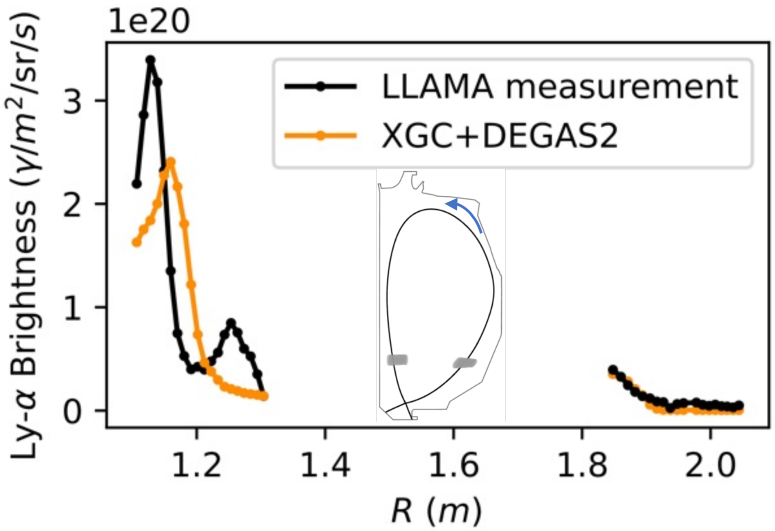
A cartoon picture introduction to homoclinic tangle



- Homoclinic tangle is formed due to magnetic-flux conservation upon perturbation of the separatrix B-field, which has a hyperbolic fixed point (= X-point)
- Tangled $\vec{B}$ avoids B-field crossing ($\nabla \cdot B = 0$): poloidal crossing at different toroidal locations
- For theoretical description of extrinsic homoclinic tangles driven by external field or MHD, see
  - T. E. Evans et al., *Contrib. Plasma Phys.* 44, 235 (2004)
  - A. Punjabi and A. Boozer, *Phys. Lett. A* 378, 2410 (2014), and others
- XGC now finds that the space-time fluctuating homoclinic tangle is an intrinsic property, at much finer scale.

First-principles based study of plasma fueling on Perlmutter

- Understanding plasma fueling by neutral particle ionization is an important subject in controlling the H-mode edge pedestal in ITER and, thus, sustaining the fusion burn
- Experiments unexpectedly observed that most of the refueling is on the inboard side, while most of the neutral particles are born on the outboard side
  - Any fueling control needs to be done inboard!
- Coupled XGC-DEGAS2 simulation result (orange line) qualitatively agrees with the strongly in-out asymmetric fueling measurement (black line) on DIII-D H-mode plasma 186414.
  - The in-out asymmetry is found to be caused by the neoclassical poloidal flow of scrape-off plasma



[Wilkie et al., Phys. Plasmas 24, Invited talks at IAEA-FEC2024 and APS-DPP2024]

DEGAS2 is a MC neutral particle transport and atomic physics code

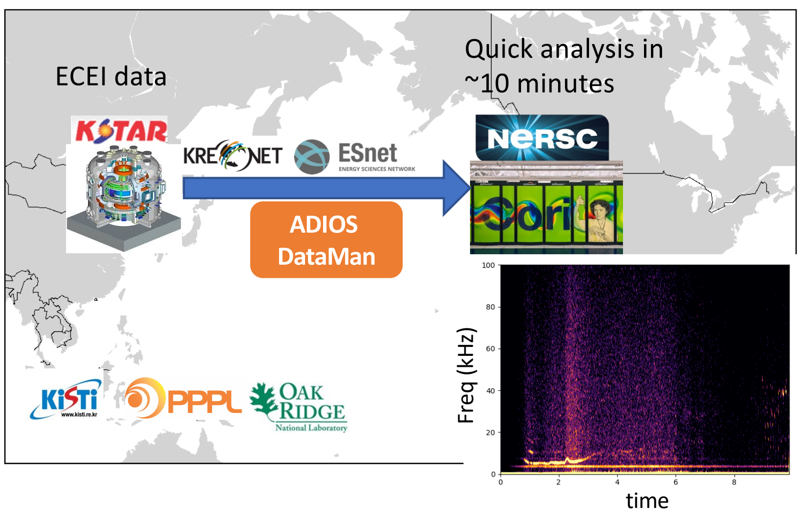
We established a baseline capability for Federated Data System on Cori: near-real time networked analysis of big KSTAR data (PPPL, ORNL, ESnet, NERSC, KSTAR, KISTI)

Objectives

- Federated Data System requires streaming data reduction (at data source) and streaming analyses/reduction on remote HPC
- Develop a streaming workflow framework, to enable near-real-time streaming analysis of KSTAR data on a US HPC
- Allow the framework to adopt ML/AI algorithms to enable adaptive near-real-time analysis on large data streams
- Utilize it for effective ITER collaboration by US researchers

Impact

- Created a framework to enable US fusion researchers to have broader and faster access to the KSTAR data, enabling
  - Faster analysis of data and quick steering of experiment
  - Faster and autonomous utilization of ML/AI algorithms for incoming data
  - Efficient utilization of US HPC for KSTAR collaboration
- Our streaming workflow framework can be utilized in a Federated Data Framework (e.g., magnetic fusion spoke in HPDF) for ITER collaboration



Accomplishments

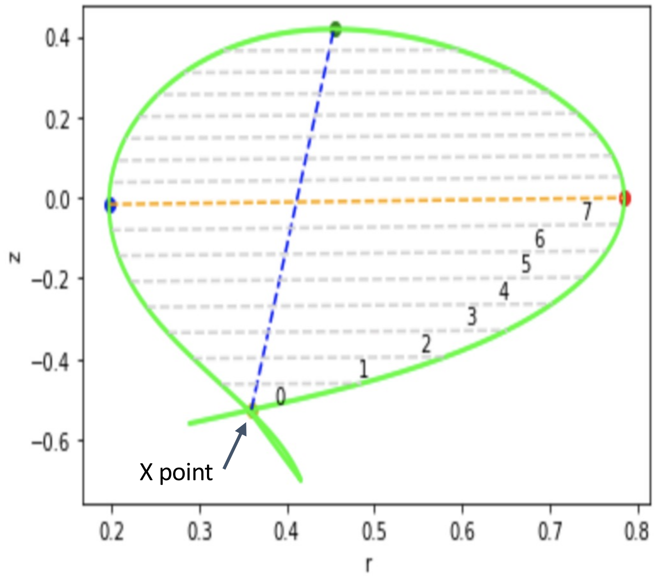
- **Created end-to-end Python framework DELTA[1], streams data using ADIOS DataMan over WAN (at rates > 4 Gbps), asynchronously processes on multiple workers with MPI multi-threading**
- **Applied to KSTAR streaming data to NERSC Cori. Reduces time for an ECEi analysis from 12 hours on single-process to 10 minutes on 6 Cori nodes.**
  - **Streaming analysis time will be further reduced if more nodes are used**
- **Implemented deep convolutional neural networks for working with multi-scale fusion data, e.g. ECEi, for recognizing events of interest.[2]**
- **Next step: Improve "adaptive" nature of data stream: adaptive, lossy compression at KSTAR source**

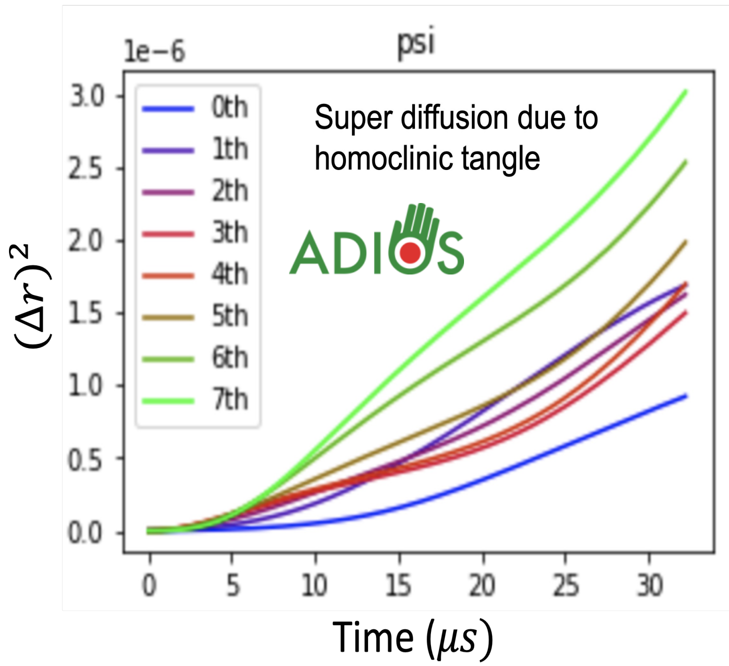
[Chang (PI), Klasky (Co-PI), **Kube, Churchill, Choi, Dart** et al, and **Korean collaborators**]

[1]http://github.com/rkube/delta
[2]R.M. Churchill et al, NeurIPS 2019

On Perlmutter, we have developed an in-transit evaluation workflow for the subgrid electron transport across the magnetic separatrix surface

- Homoclinic tangle lobes are subgrid phenomenon: electrons follow the lobe field lines
- Need to identify the electrons that cross the separatrix surface and follow them for transport calculation
- Trillions of particles cannot be post-processed, nor can be ID-tagged for time-dependent in-line transport calculations.
- Send asynchronously the identified particles to analysis/vis nodes for time-dependent transport calculations
  - Free up the simulation





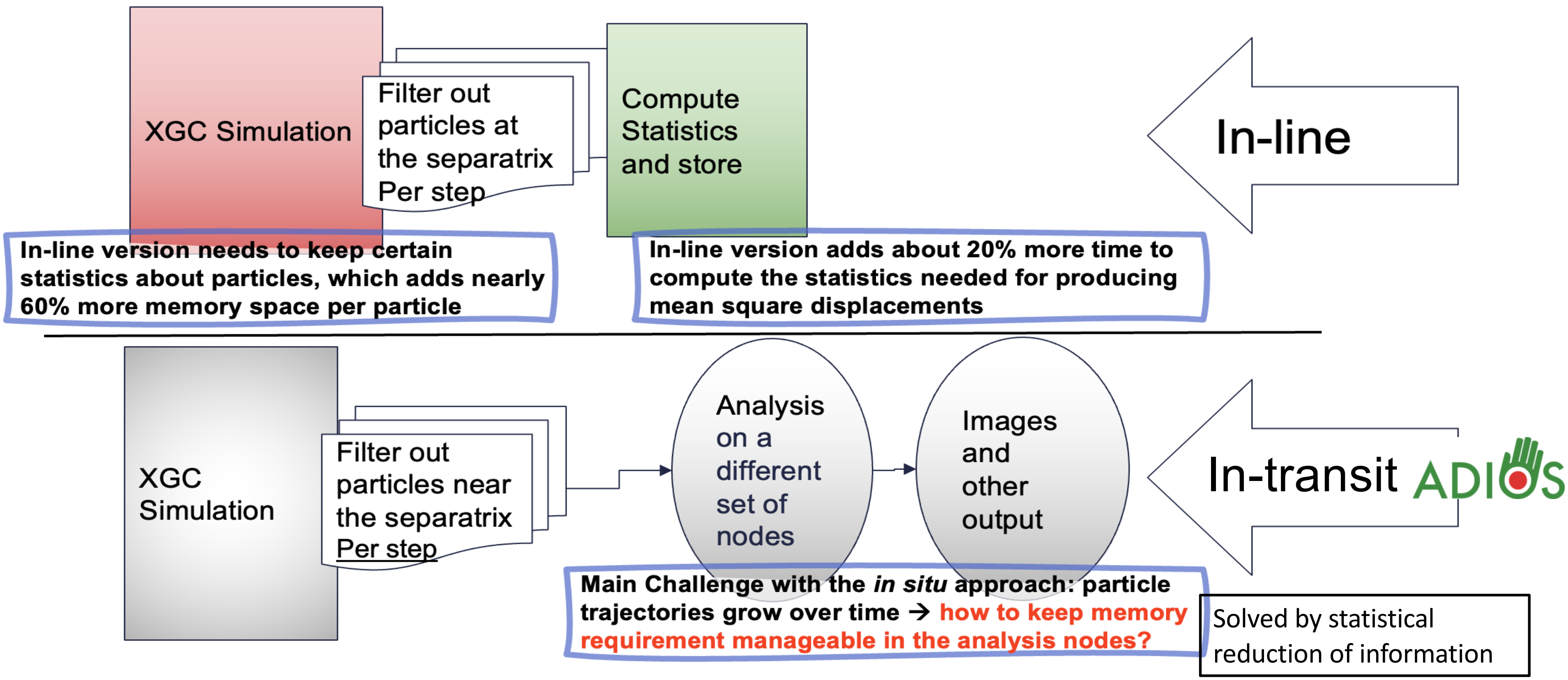
J. Gu, K. Wu, P. Lin (LBNL),
S. Ku, CS Chang, R. Hager (PPPL),
J. Choi (ORNL) *et al.*

[accepted for SSDBM24]

In-line vs in-transit workflows for subgrid particle transport analysis on Perlmutter

J. Gu, K. Wu, P. Lin (LBNL),
S. Ku, CS Chang, R. Hager (PPPL),
J. Choi (ORNL) *et al.*

Overview: In-line vs In-transit



Conclusion and Discussions

- My career path has been steered and shaped by "50 years of NERSC."
  - XGC kinetic code started on GSEABORG and SEBORG (1999-mid 2000s), and has been riding the rapid rise of NERSC's computing power. I was lucky, I had the right betting.
  - It became one of the most successful exascale codes and a multiple SciDAC-5 code.
- Three most dangerous events in ITER and future tokamak fusion reactors are
  - Plasma disruption: mostly core physics
  - Collapse of edge pedestal by edge localized mode (ELM) instability: edge physics
  - Melting of divertor surface material in a steady state energy production phase: edge physics
- We have made substantial first-principles-based understanding and improvement of the two edge issues.
  - They are subject to nonlinear, nonlocal, multi-scale self-organization of multiphysics
- XGC will continuously study the two edge physics problems to help commercialization
  - NERSC computers: basic physics research and validation on present-day tokamaks
  - Exascale computers: large scale predictive study for ITER or fusion pilot plants (FPP)
  - XGC could become a HPC digital twin and also produce predictive surrogate models.