Scientific Discovery in Fusion Edge Plasmas*

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and the SciDAC HBPS Team

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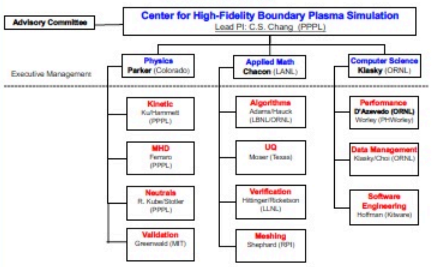
HBPS
High-fidelity Boundary Plasma Simulation

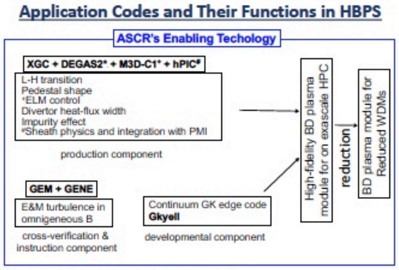
Partnership Center for High-fidelity Boundary Plasma Simulation (HBPS)

Goal: Utilize the SciDAC FES-ASCR collaborative framework to solve the difficult multiscale-multiphysics edge plasma physics problems on the most powerful HPCs, which have not been possible before.

HBPS Leaders



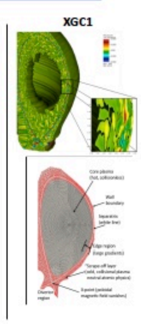
Application Codes and Their Functions in HBPS



*DEGAS2 is coupled into XGC as a subroutine.

Introduction to the main production code XGC

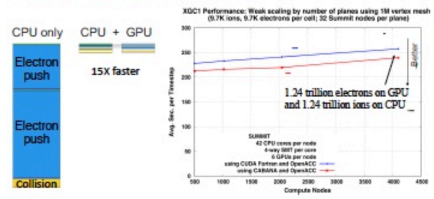
- **Particle-in-Cell, with added continuum technology**
- **In contact with material wall**
  - Far-from-equilibrium (non-Maxwellian)
  - Neutral recycling, impurity sputtering
- **Magnetic X-point and separatrix (one poloidal B winding→ infinite distance)**
  - Unconfined X-point orbit loss from pedestal
- **Multi-scale, multiphysics in space-time**
- **Unstructured triangular mesh**
- **PETSc (only ~2% of total computing time)**
- **Large simulation-size (≥10k particles per grid-vertex) per time-step → > trillion particles for ITER**
- **Total-f XGC has been developed to study this kind of plasma**
- **XGC is not only a SciDAC code, but also an ECP code**
- **Summit-ESP, Aurora-ESP, NESAP, and INCITE**



*Acknowledgement: Funding from DOE FES and ASCR. Computing resources provided via INCITE by OLCF and ALCF. Additional computing resource provided by NERSC.

XGC on Summit

- XGC utilizes Kokkos, a programming model written in C++
  - Fortran interface has been developed for XGC
- Single version XGC can be performance portable to different future architectures: Permutter, Aurora, Frontier



Example Scientific Discoveries Since Last SciDAC Meeting

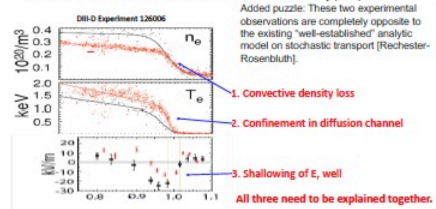
For the first time, the XGC code enabled total-f gyrokinetic simulation of RMP-neoclassical-turbulence-neutral interaction in diverted geometry

[R. Hager, 2019 APS-DPP Invited Talk, used 50% Theta]

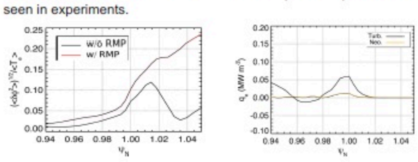
Two big puzzles seen in the experimental RMP-driven edge transport:

1. Why is there density pumpout?
2. How could an electron heat-barrier co-exist with density pumpout?

Added puzzle: These two experimental observations are completely opposite to the existing "well-established" analytic model on stochastic transport [Rechester-Rosenbluth].

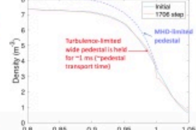


- Finds that micro-turbulence is responsible for the density pump-out in the M3D-C1 RMP field, not neoclassical as conjectured previously.
- Finds that the RMP-interacted turbulence preserves the electron heat barrier around $\Psi_N \approx 0.96$-0.98.
- Finds that the E_r-well shallows.
- Finds that the divertor heat-flux width widens by ~30% by RMPs, as seen in experiments.



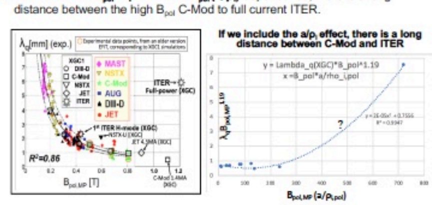
Answering the critical question on the (non)existence of pedestal in the target ITER plasma (used 60% Summit)

- ITER's goal of achieving 10-fold energy production relies on the existence of high enough edge pedestal (H-mode), as seen in today's tokamak experiments
  - There is a concern that, due to the much greater physical size of ITER, the background ExB flow may be too weak to shear away the edge turbulence
    - Edge turbulence could become too strong to support edge pedestal
  - We find the (electrostatic) turbulence self-organization with background slope keeps ITER's edge pedestal high



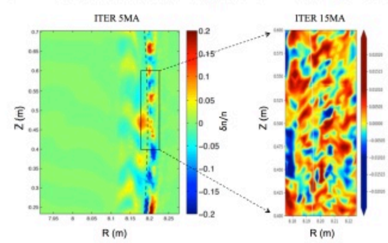
Further investigation of the ITER divertor heat-flux width

- The XGC-predicted divertor heat-flux width λ_q **has been well-validated**
- Why **λ_q(XGC, ITER) >6X wider** than λ_q(Eich)?
  - To check if it is a pure size (major radius, R) or B_{pol} effect, a lower B_{pol} ITER and a highest B_{pol} C-Mod case simulated → No is the answer.
- Community question: Why such a strong difference at similar B_{pol}?
- The suspect, "**ρ_i/a effect,**" remains: Texas [Kotschenreuther], PPPL [Chang]
  - **If we correct the B_{pol} dependence to $B_{pol}(a/\rho_i)$** dependence, there is a long distance between the high B_{pol} C-Mod to full current ITER.



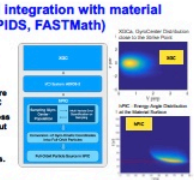
Evidence for different edge physics between higer and lower ρ_i/a values.

In all the higher ρ_i/a tokamaks, including low-current ITER, edge tubulence across the separatrix is blob type and the ExB shearing rate is high. In the high-current ITER, the turbulence is streamer type and the ExB shearing rate is low.



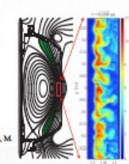
XGC-hPIC Coupling: enabling WDM integration with material codes (U. Illinois, PPPL, ORNL, RAPIDS, FASTMath)

- **Coupling via ADIOS-2/EFFIS**
- **hPIC (6D full-orbit PIC) allows to account for finite gyro-orbit effects near material surface, where a plasma sheath and a magnetic presheath are formed**
- **The 5D Gyro-Center distributions provided by the XGC code are converted into Full 6D distributions and fed in as input to hPIC**
- **hPIC provides the Energy-Angle distributions of the ions across the sheath before they impact on the surface, a necessary input for material codes evaluating sputtering and reflection of the plasma particles at the surface (e.g. Fractal-TRIDYN, etc.)**
- **Next Steps: Testing of coupled codes on HPC, porting to GPUs.**



Gkeyll: First Continuum 5D Gyrokinetic Simulations of Turbulence in Tokamak Model SOL

- XGC (PIC) only code with X-point now. Independent codes helpful to cross-check, explore new algorithms.
- Gkeyll can't handle X-point yet (hard). SOL tested.
- General geometry w/ X-point major goal next year.
- Collaborating with applied math team (C. Hauck & E. Endive, ORNL) on super-time-stepping / implicit methods.



Gkeyll core gyrokinetic team : A. Hakim (leader), N. Mandell, M. Francisquez (MIT), T. Bernard (GA), G. Hammett.
E. Shi, A. Hakim, G. Hammett, et al. JPP 2017, PoP 2019,
T. Bernard et al. PoP 2019

Applied Mathematics Developments for the High-Fidelity Boundary Plasma Simulation SciDAC Center

HBPS
High-fidelity Boundary Plasma Simulation

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C. S. Chang (HBPS PI, PPPL)

Abstract / Motivation

The main goal of the **Partnership Center for High-fidelity Boundary Plasma Simulation** is to enhance our suite of advanced high-fidelity kinetic simulation codes running on extreme-scale computers to address the physics challenges arising in the boundary region of magnetically confined plasmas. This work is essential to understand existing tokamak experiments and confidently predicting ITER operation and performance.

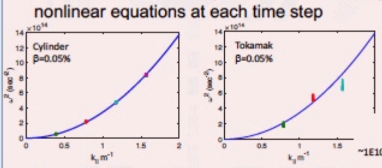
The Applied Mathematics component of this project is critical to achieve this goal, and is organized around a few core organizing principles:

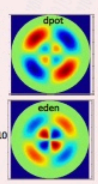
- **Solvers and Algorithms**: To enhance the performance and capabilities of the physics codes by improved meshing and solution algorithms.
- **Particle Compression and Remapping**: To efficiently use computational resources by improving the accuracy of the discretizations for a given set of resources
- **Verification and Uncertainty Quantification**: To demonstrate correctness, optimally sample input parameter space, maximize information retrieval from physics simulations, and provide bounds of confidence.

Solvers and Algorithms

Particle-in-cell EM GK solvers: fully implicit algorithms

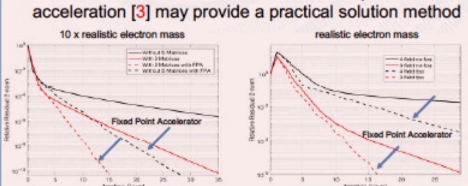
- **Goal**: to extend XGC to include electromagnetic field evolution
- Electromagnetic gyrokinetic Particle-in-Cell (PIC) methods suffer from numerical difficulties (severe time step constraints or the Ampere cancellation problem)
- Fully implicit PIC [1,2] does not have these difficulties, but requires an efficient way to solve the resulting system of nonlinear equations at each time step





Top: Dispersion relation for low-wavenumber Alfven modes, demonstrating the absence of cancellation issues. Right: Snapshots of electrostatic potential and electron density.

- Preconditioned Picard iterations with fixed-point acceleration [3] may provide a practical solution method



$E_\| \rightarrow \mathcal{S}E_\|$ $\qquad$ $T_e\nabla_\| n_e \rightarrow T_e\nabla_\|^2 j_\|/e$

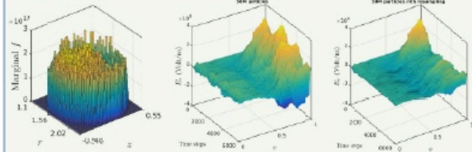
- Particle/grid interactions are accounted for with a directional smoothing operator on parallel electric field
- Further improvements by eliminating the continuity equation, putting a Laplacian on pressure term to mimic nonlocality of particle moment deposition

Particle compression and remapping

- **Goal**: efficiently compress and resample particle distribution function (PDF) for
  1) variance reduction (noise control),
  2) dynamic load balancing,
  3) checkpoint-restart.
- We have been exploring **two approaches**:

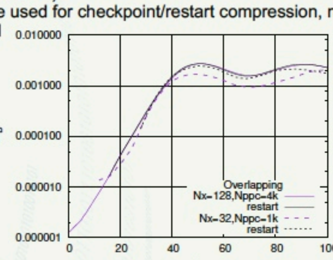
Moment-Preserving Constrained Resampling [6]

- Binning approach with weight reconstruction by constrained minimization (with moments) of weight correction



Machine-Learning PDF reconstruction [5]

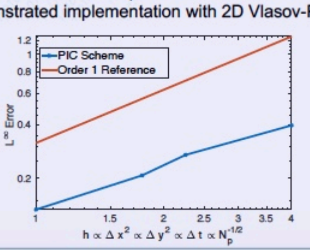
- Fit Gaussian Mixtures from particles
- Gaussians feature universal approximation property
- Low-noise particle resampling available (quiet start)
- Conserves first three moments (mass, momenta, temperatures)
- Can be used for checkpoint/restart compression, noise control



ML restart applied to electromagnetic Weibel instability, demonstrating improved nonlinear performance with fewer particles

Verification

- Seek rigorous verification methodology for particle-in-cell solutions to the Vlasov-Poisson equation.
- Employ **Method of Manufactured Solutions.**
- We have expanded and corrected previous work [6] in two important ways:
  1) Fixed conceptual issue that failed to identify errors in field-particle coupling
  2) Extended to multiple dimensions
- Demonstrated implementation with 2D Vlasov-Poisson



Uncertainty Quantification

UQ Challenges

- UQ requires sampling parameter space ➔ need many solutions with different inputs
- Two primary challenges for HBPS:

1. Computational cost of high-fidelity (HF) models
2. Governing equations have chaotic solutions (gradients difficult to compute, QoIs contaminated by finite-time avg.)

UQ Approach

- Leverage **Multifidelity Monte Carlo (MFMC) methods** to reduce number of high-fidelity solves
- Develop extensions to tailor MFMC to reduce number of high fidelity model evaluations and estimate impact of averaging error

Model Correlation Bound Estimates in MFMC

- Seek to combine low-order and high-order models to give unbiased estimator with lowest possible variance

Peherstorfer, Willcox & Gunzburger (PWG)* MFMC Approach

$$\hat{s} = \overline{q}^{(1)}_{m_1} + \sum_{i=2}^{k} \alpha_i \left(\overline{q}^{(i)}_{m_i} - \overline{q}^{(i)}_{m_{i-1}} \right) \quad \text{where} \quad \overline{q}^{(i)}_{m} = \frac{1}{m}\sum_{j=1}^{m} q^{(i)}(\mathbf{z}_j)$$

- Optimal numbers of samples m_i and weights α_i determined based on correlation between models

MLMC Estimator Variance Reduction

$$\frac{\mathrm{Var}[\hat{s}]}{\mathrm{Var}[\overline{q}^{(1)}_{n}]} = \left(\sum_{i=1}^{k} \sqrt{\frac{w_i}{w_1}\left(\rho^2_{1,i} - \rho^2_{1,i+1}\right)} \right)^2$$

ω_i Model complexity
$\rho_{1,i}$ Model correlation

- Developed *a priori* (w/o HF) estimation bounds for $\rho_{1,2}$ with noise and discretization errors, and **extended it to chaotic systems [7]**

$$u_t + \nabla^4 u + \nabla^2 u + \frac{1}{2}|\nabla u|^2 = 0$$

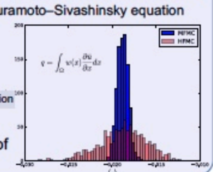
Kuramoto–Sivashinsky equation

$$\rho_{1,2} \geq \left(1 + \frac{\gamma^2}{1-\gamma^2} + \frac{\beta_1^2 + \beta_2^2}{(1-\gamma)^2} + \frac{\beta_1^2\beta_2^2}{(1-\gamma)^4} \right)^{-1/2}$$

$\beta_j = \sigma_{\epsilon,j}/\sigma_q$ is the sampling uncertainty standard deviation

Estimating β_j requires estimates of sampling errors,

- MFMC reduced std. dev. by a factor of 4 with NO HF sims. (savings of 16x).



Next Steps

- **Solvers**: Finalize preconditioner developments. Comparisons with other iterative methods, including Jacobian-Free Newton-Krylov. Benchmark simulations of ion temperature gradient/kinetic ballooning instabilities and microtearing modes
- **Particle remapping**: port ML strategy to XGC, extend to treat particle collisions
- **Verification**: proof theorem to avoid computation of error in PDF by focusing on fields/moments only (large complexity reduction and speedup), extend to ES GK PIC
- **UQ**: Developing ideas to further reduce required high fidelity simulations. Testing error bounds and MFMC on particle-in-cell application. Planning deployment of techniques for boundary physics applications

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