SciDAC PI Meeting, July 26-18, 2019

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

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and the HBPS Team

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ALCF
• HBPS team leaders and the project OV
• The XGC gyrokinetic code
  – Performance enhancement
• Example scientific discoveries last year
  – Turbulence interaction with external magnetic perturbation
  – Further investigation of ITER’s divertor heat-flux width
• Getting ready for WDM integration
• Collaboration with FASTMath and RAPIDS
  – FASTMath: M. Shephard, J. Hittinger
  – RAPIDS: S. Klasky, W. Hoffman
• Conclusion and discussion

+Funding provided by US DOE FES and ASCR via SciDAC-4
*Computational resources provided by INCITE (OLCF, ALCF) and NERSC
**Center for High-fidelity Boundary Plasma Simulation**

(High-fidelity gyrokinetic simulation of the global BD plasma)

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**ASCR’s Enabling Technology**

- **Production Component**
  - XGC + DEGAS2* + M3D-C1† + hPIC#
    - L-H transition
    - Pedestal shape
    - ELM control
    - Divertor heat-flux width
    - Neutral particles and Impurities
      - Sheath physics and integration with PMI
- **Developmental Component**
  - GEM + GENE
    - E&M turbulence in omnigeneous B
    - Cross-verification & instruction component
  - Continuum GK edge code
    - Gkeyll
    - Developmental component

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*DEGAS2 is coupled into XGC as a subroutine.*
The XGC Gyrokinetic Code

• 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 compute time if done right)
• 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
XGC performs well on world #1 Summit

[E. D’Azevedo, A. Scheinberg, P. Worley, S. Ku, R. Hager, S. Slattery]

- XGC utilizes Kokkos for “future proofing,” a programming model written in C++
  - Fortran interface has been developed for XGC via Cabana particle library
- Single version XGC can be performance portable not only to Summit and KNL, but also to different future architectures: Permutter, Aurora, Frontier

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**CPU only**

**CPU + GPU**

Asynchronous Work-load split: 15X faster

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**XGC1 Performance: Weak scaling by number of planes using 1M vertex mesh (9.7K ions, 9.7K electrons per cell; 32 Summit nodes per plane)**

- Original version
- Kokkos version
- Lower is better
- 50M electrons/GPU
- 2.4T ions and electrons on 90%
- SUMMIT
  - 42 CPU cores per node
  - 4-way SMT per core
  - 6 GPUs per node
- using CUDA Fortran and OpenACC
- using CABANA and OpenACC

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**Compute Nodes**

**Avg. Sec. per Timestep**

- 500 to 4500

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**Number of Planes**

- 500 to 4500

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**50M electrons/GPU**

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**2.4T ions and electrons on 90%**

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**SUMMIT**

- 42 CPU cores per node
- 4-way SMT per core
- 6 GPUs per node

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**Using CUDA Fortran and OpenACC**

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**Using CABANA and OpenACC**
Example Scientific Discoveries last year enabled by SciDAC Institute collaborations
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]

Two big puzzles seen in the experimental RMP-driven edge transport:
1. Why is there the density pumpout?
2. How could an electron heat-barrier co-exist with density pumpout?

Puzzle 3: These two experimental observations are completely opposite to the existing “well-established” analytic model on stochastic transport [Rechester-Rosenbluth].

1. Convective density loss
2. Confinement in diffusion channel
3. Shallowing of $E_r$ well

All three need to be explained together.
For the first time, XGC succeeded in the total-f gyrokinetic simulation of RMP-neoclassical-turbulence-neutral interaction in diverted geometry

[R. Hager, 2019 APS-DPP Invited Talk]

- Finds enhanced 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 \( \sim 30\% \) by RMPs, as seen in experiments.
Answering the critical question on the (non)existence of pedestal in the target ITER plasma

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

  - We will continue the big runs (computing time could be an issue).
  - Next question: How will the pedestal be modified by electromagnetic turbulence?
Further investigation of the ITER divertor heat-flux width

<table>
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<th>Shot</th>
<th>R (cm)</th>
<th>a (cm)</th>
<th>I_P (MA)</th>
<th>B_{pol,OM} (T)</th>
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<td>1.4</td>
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<tr>
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<td>199</td>
<td>15</td>
<td>1.21</td>
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Further investigation of the ITER divertor heat-flux width

• The XGC-predicted divertor heat-flux width $\lambda_q$ has been well-validated

• Why $\lambda_q$(XGC, ITER) >6X wider than $\lambda_q$(Eich)?
  – To check if it is a pure size effect or $B_{pol}$ effect, a lower $B_{pol}$ ITER and a highest $B_{pol}$ C-Mod case simulated → No is the answer.

• Community question: How come such a strong difference at similar $B_{pol}$?

• The suspect “$\rho_i/a$ 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.

If we include the $a/\rho_i$ effect, there is a long distance between C-Mod and ITER
Evidence for different edge physics between higher and lower $\rho_i/a$ values.

In all the higher $\rho_i/a$ tokamaks, including low-current ITER, edge turbulence 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 across the separatrix.
Unlike the blobby turbulence, the full-current ITER contains a strong non-adiabatic electron response across the magnetic separatrix, as evidenced by a large phase difference between density and potential fluctuations ($\gtrsim \pi/2$) and a strong de-correlation between their amplitudes.
**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 gyro-orbits 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: Porting to GPUs and Testing of coupled codes on HPC
Collaboration with FASTMath
FASTMath(1): Meshing tool (M. Shephard)

- XGC uses unstructured triangular mesh due to separatrix and wall:
  - Mesh quality affects the simulation quality
  - Before the meshing by FASTMath, the meshing was performed manually.
    One case took a few days, but still overlooking details at many areas
  - M. Shephard developed an automated tool, by working with physicists

Last year, FASTMath enabled more accurate XGC solution by
- Improving mesh quality where flux curves interact with reactor wall
- Improving mesh gradation around the magnetic x-point
- Reordering mesh data for better memory access
PUMIpic: Parallel Unstructured Mesh PIC

- Mesh centric – no independent particle structure
- Particle migration and load balancing between pushes
- Focused on structures for execution on GPUs
  - Omega GPU-ready mesh-topology being integrated
- Since most of data structures are changed, XGC is rewritten in C++
- Test shows on-par performance using less memory

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<th>full sorting time (s)</th>
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</table>

Ion turbulence from XGC-PUMIpic in tokamak geometry on a highly coarse-grained mesh
FASTMath(3): New 3D solver (M. Adams)

Chacon’s fully implicit electromagnetic scheme implemented in XGC
• All the previous production runs were with electrostatic turbulence
• Summit is now powerful enough for electromagnetic simulation

- For electrostatic turbulence
  XGC used 2D solver + finite differencing in the third direction
- The EM scheme requires fully 3D solver
  • Implicit iteration requires efficient solver
  • PETSc/GMRES is used
- Significant effort invested in reducing iteration #
- Machine learning is being explored to optimize the preconditioner [J. Hittinger, R. Archbald]

*Iteration count is low enough for production on Summit [B. Studervant, L. Chacon]*
Other on-going collaborations with FASTMath

- Machine learning for preconditioner: *J. Hittinger and R. Archbald*
- Nonlinear Fokker-Planck collision operator that is more efficient and WDM-ready than the $N^2$ operation currently used in XGC: *Mark Adams*
- Method of Manufactured Solution for PIC solution to Vlasov-Poisson equation: *J. Hittinger, L. Ricketson, P.J. Tranquilli*
  - Expanded and corrected previous work by Riva et al. [Phys. Plasmas 2017]
  - Demonstrated implementation with 2D Vlasov-Poisson
Collaboration with RAPIDS
RAPIDS(1): Big data I/O (S. Klasky)
I/O was a big concern for XGC. ADIOS changed it to “No Concern.”

- ITER simulation produces ~20TB restart data per hour using ½ Summit.
  - Takes < 1 minute for writing on GPFS
  - Takes ~ 1 sec for writing on NVMe
- ADIOS is fast enough to write out 50PB a day for XGC, but way too big for GPFS → In situ, streaming data analysis is in progress.

XGC Checkpoint Writing on Summit
GPFS with I/O aggregation

Summit NVMe

Throughput (GB/sec)

Nodes

Throughput (GB/sec)

Number of Nodes
RAPIDS(2): Code coupling (S. Klasky)

- XGC is coupling with
  - the MHD code M3Dc1 for
    - magnetic equilibrium reconstruction as pedestal buildup
    - edge localized mode crash of the pedestal
  - the plasma-wall interaction code hPIC for
    - Plasma influx to the surface
    - Particle outflux from the surface
    - As described in the physics slides

- ADIOS enables code couplings
  - Coupling manager
  - In-situ staging
  - In-situ visualization
  - Coupling performance monitoring
  - Heterogeneous memory/process utilization
XGC asynchronously offloads the analysis computations to designated processors via ADIOS.

ADIOS enables:
- In-memory analysis
- Inter-network analysis
- WAN-coupled analysis

### Diagram:
- **XGC1 original**
  - XGC1
  - F Analysis
    - Calc1
    - Reduce1
    - Calc2,3
    - Reduce2
    - Calc4
    - Reduce3
    - Write

- **XGC1 modified**
  - XGC without F analysis
  - F Put
  - Adios Push
  - IMPI SST

- **F-analysis**
  - F Analysis
    - Calc1
    - Reduce1
    - Calc2,3
    - Reduce2
    - Calc4
    - Reduce3
    - Write

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**Maximize Data Locality**

**XGC1 on 1024 summit nodes with 9X analysis computations**

- XGC1- original
- XGC1- modified
- F-analysis

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Example Data Analysis Code of XGC1 Turbulence

I. Keramidas¹, J. Myra², S. Parker¹
Univ. of Colorado¹, Lodestar Corp.²

• One XGC1-run requires $10^{17}$ flop-hrs
• Enormous scientific interest in the data
• Powerful data science tools are widely available

Detailed analysis of neoclassical and turbulent particle fluxes

Turbulent particle flux at the last closed flux surface is shown


Other collaborations with RAPIDS

- Software process (Hoffman/Galbreath, Kitware)
  - Continuous Integration (CI) testing system
  - Incorporate a modern CMake build
  - Git workflow incorporated with CI
  - Integrate CDash into github

- EFFIS (Klasky, ORNL): End-to-end Framework for Fusion Integrated Simulation
  - Initial development in SciDAC-2 CPES (PI: Chang)
  - Integrated platform of services to compose, launch, monitor, analyze, and control coupled applications on all leadership HPCs
  - High Performant I/O for coupled codes
  - Process placement (inter or intra node)
  - Online dashboard functionality

Example EFFIS specification file

```bash
run:
  xgc:
    processes: 1024
    processes-per-node: 32
    path: xgc-build/xgc1-es

groups:
  diagnosis.1d:
    plot:
      psi-plot:
        x: psi
        y: i_gc_density_1d
```

CDash

EFFIS

Submit

Compose

Monitor

Communicate

Provenance

Toolkit

XGC1

XGCa

M3DC1

hPIC

Matlab

Visit

Paraview

Python

ADIOS

BPFile

SST

IMPI

SST-SP

HDFS

IMPI
Summary

• HBPS is making scientific discoveries that would not have been possible without the SciDAC framework and the US Leadership Class Computers
  Since last SciDAC Conference
  – Many Invited/Plenary Talks at major scientific conferences, including Smokey Mt 2018, IAEA-FEC 2018, APS-DPP 2019, International Data Driven Plasma Sciences 2019, KSTAR 2019, PACS 2019, + many more
  – 7 SciDAC-funded physics papers + many ASCR papers, (co-authored)
• Strong collaboration with FASTMath and RAPIDS in many subjects
• Other ASCR collaborations outside of SciDAC Institutes also strong
  o R. Moser (Texas): UQ, Multifidelity Monte Carlo (MFMC) methods
  o L. Chacon (LANL): math leadership
  o V. Carey (U. Colorado Denver): particle re-sampling
  o C. Hauck (ORNL): super time-stepping
• Preparation for WDM coupling with most Fusion SciDACs
• AI/ML is becoming an important part of the project
  • In-situ data analytics
  • Validation
  • Simulation acceleration
  • Anchored ML for prediction, by adding high-fidelity simulation data