**WDMApp: High-Fidelity Whole Device Model of Magnetically Confined Fusion Plasma**


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Grand Challenge: *Integration* of the knowledge provided by plasma models to understand, predict, and control the performance of fusion experiments

“I think the…21st century will be the century of complexity. We have already discovered the basic laws that govern matter and understand all the normal situations. We don’t know how the laws fit together, and what happens under extreme conditions….There is no limit to the complexity we can build using those basic laws.”----Stephen Hawking
A bit of history: Need for extreme-scale computing resources

Exascale Computing Project (ECP)

- Mission Need: July 2015: President established National Strategic Computing Initiative (NSCI) to maximize the benefits of HPC for US economic competitiveness and scientific discovery
- Accelerating delivery of capable exascale computing systems that integrates hardware and software capability to deliver approximately 100 times the performance of current 10 petaflop systems across a range of applications representing government needs
  • To be deployed in 2021 (Aurora at ANL, Frontier at ORNL)

• ECP was envisioned as a DOE 413.3b project with emphasis on software engineering that can be transformational for science

  ECP builds on the foundation of SciDAC Centers. Without SciDAC, with its blend of advanced computing and physics, strongly coupled with validation, ECP would not be possible.
FES Highest Priority (2015): Advancing Predictive Capability for Whole Device

"Developing an experimentally validated integrated predictive simulation capability that will reduce risk in the design and operation of next-step devices as well as enhance the knowledge gained from ITER."

2015 DOE Report to Congress

10-Year Problem Target of Fusion Exascale Computing Project (ECP) led by PPPL (Acknowledgements: S. Prager, M. Zarnstorff, and J. Mandrekas)

To carry out the simulation of non-inductively sustained burning plasma in a high-performance advanced regime, integrating the effects of energetic particles, extended MHD instabilities, and current drive.
Exascale Computing Program: Holistic Approach

Application Development
- Science and mission applications

Software Technology
- Scalable software stack
  - Correctness
  - Visualization
  - Data Analysis
  - Applications
  - Co-Design
  - Programming models, development environment, and runtimes
  - Math libraries and frameworks
  - Tools
  - System software, resource management, threading, scheduling, monitoring, and control
  - Memory and Burst Buffer
  - Data management in I/O and file system
  - Node OS, runtimes
  - Hardware interface

Hardware Technology
- Hardware technology elements

Exascale Systems
- Integrated exascale supercomputers
### Exascale Applications Cover 6 DOE Strategic Pillars

<table>
<thead>
<tr>
<th>National security</th>
<th>Energy security</th>
<th>Economic security</th>
<th>Scientific discovery</th>
<th>Earth system</th>
<th>Health care</th>
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<tbody>
<tr>
<td>Stockpile stewardship</td>
<td>Turbine wind plant efficiency</td>
<td>Additive manufacturing of qualifiable metal parts</td>
<td>Cosmological probe of the standard model of particle physics</td>
<td>Accurate regional impact assessments in Earth system models</td>
<td>Accelerate and translate cancer research</td>
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<td>Design and commercialization of SMRs</td>
<td>Urban planning</td>
<td>Validate fundamental laws of nature</td>
<td>Stress-resistant crop analysis and catalytic conversion of biomass-derived alcohols</td>
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<td>Nuclear fission and fusion reactor materials design</td>
<td>Reliable and efficient planning of the power grid</td>
<td>Plasma wakefield accelerator design</td>
<td>Metagenomics for analysis of biogeochemical cycles, climate change, environmental remediation</td>
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<td>Subsurface use for carbon capture, petro extraction, waste disposal</td>
<td>Seismic hazard risk assessment</td>
<td>Light source-enabled analysis of protein and molecular structure and design</td>
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<td>High-efficiency, low-emission combustion engine and gas turbine design</td>
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<td>Find, predict, and control materials and properties</td>
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<td>Carbon capture and sequestration scaleup</td>
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<td>Predict and control stable ITER operational performance</td>
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<td></td>
<td>Biofuel catalyst design</td>
<td></td>
<td>Demystify origin of chemical elements</td>
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WDMApp: $23.6M 2016-23
Vision: A High-Performant, First-Principles-Based Whole Device Model

2016-23
Integration
Full-f
delta-f

Applied Math + Computer Science
\[ F = F_0 + \delta F \]

Framework
Tight / Loose Coupling

2023-26
- Plasma-Material Interaction
- RF and Neutral Beam
- Extended MHD
- Energetic Particles

Multi-scale time advance
Key Recommendations:

First, the United States should remain an ITER partner as the most cost-effective way to gain experience with a burning plasma at the scale of a power plant.

Second, the United States should start a national program of accompanying research and technology leading to the construction of a compact pilot plant that produces electricity from fusion at the lowest possible capital cost.

The second recommendation motivated the 2021 NASEM Report on “Bringing Fusion to the Power Grid”
Sources

- **Accelerating Fusion Through Integrated Whole Device Modeling**
  
  A. Bhattacharjee, P. Bonoli, A. Boozer, J. Callen, J. Candy, C.-S. Chang, A. Friedman, L. LoDestro, G. Staebler, F. Waelbroeck (Chair, Theory Coordinating Committee)


  
  P. Bonoli, *Chair*, and L. Curfman-McInnes, *Co-Chair*

  
  C.-S. Chang, *Chair*, and M. Greenwald, *Co-Chair*
Questions from the NAS Panel (2018)

• What is the current status of U.S. research that supports advanced scientific computing and modeling for fusion energy?

• What are your views of strategic initiatives that would foster the international development of fusion energy, including participation in the ITER project?

• How advancements in both theoretical understanding and computing infrastructure might broadly strengthen fusion research in the U. S. and promote leadership in the field?
WDM hierarchy: High-fidelity to reduced models

• WDM requires a *fidelity hierarchy* of computational models.

• Pyramid structure

  1. Apex of the structure are high-fidelity kinetic models that require leadership-class computing resources, used to calibrate reduced models that form successive layers of the hierarchy.

  2. Fast, reduced models are used for large dataset validation of physics basis.

  3. Computing infrastructure needed depends on the level of the hierarchy----from exascale computing (and beyond) at the highest fidelity to capacity computing for reduced models.

  4. Necessary to develop a large database at all levels of hierarchy for prediction and uncertainty quantification. Machine learning can be very useful

  5. Strong effort in analytical theory needed at all levels.
Advancing Predictive Capability for Whole Device Model is a leading priority for FES community

From the “Final Report of the Committee on a Strategic Plan for US Burning Plasma Science Research (2019)” by the US National Academy of Sciences:

“The creation of the DOE Exascale Computing Project in fiscal year 2017 has provided the impetus for the realization of a high-fidelity whole device model of fusion plasma applicable to a high performance advanced tokamak regime, integrating the effects of turbulent transport, plasma collisions, and neutral particles, energetic particles, plasma-material interactions, as well as heating and current drive…Whole device modeling holds the promise of being a powerful predictive tool for current and future fusion devices that will access hitherto unrealized plasma regimes, and has the potential to produce scientific discoveries of new and emergent behavior of burning plasmas that have been so far studied piecemeal…. The project will be developed in a computational ecosystem that brings together plasma physicists with applied mathematicians, computer scientists, and other application scientists using a diverse range of software technologies and several co-design centers.”
Evolution of Kinetic Modeling Capability with Increasing Computing Power

**Gigaflops**
- 5-D electrostatic ion physics in simplified circular cylindrical geometry
- Core: 5D ion-scale electromagnetic physics in torus
- Edge: ion+neutral electrostatic physics in torus

**Teraflops**
- Core: 5D ion-scale electromagnetic physics in torus
- Edge: ion+neutral electrostatic physics in torus

**Petaflops**
- Core: 5D i+e scale electrostatic physics
- Edge: ions + electrons + neutrals, electrostatic physics

**Exaflops**
- Core-edge coupled 5D electromagnetic study of whole-device ITER, including turbulence, transport, large-scale instability, plasma-material interaction, rf heating, and energetic particles

**Beyond**
- 6D whole device modeling of all the relevant fusion reactor science with burn control
SciDAC Centers

A partnership between FES and ASCR divisions in the DOE Office of Science. PPPL/Princeton University leads three, and is a co-participant in four others:

• High-Fidelity Boundary Plasma Simulation (C.-S. Chang, PI)
• Center for Tokamak Transient Simulations (S. Jardin, PI)
• Simulation Center for Runaway Electrons Avoidance and Mitigation (D. Brennan (Princeton University, PI; A. Bhattacharjee, Co-PI)
• Tokamak Disruption Simulation (X. Tang (LANL), PI; W. Wang, Co-PI)
• Integrated Simulation of Energetic Particles (Z. Lin (UCI), PI; N. Gorelenkov, Co-PI)
• Advanced Tokamak Modeling Environment (J. Candy (GA), PI; J. Sachdev, Co-PI)
• Multi-Scale Gyrokinetics (D. Hatch (UT Austin), PI; G. Hammett, Co-PI)
Coupling the core and edge: first in fusion history

The core evolves more slowly than the edge

Core Turbulence from GENE

Edge Turbulence from XGC
Principal WDMApp Goals

- Demonstration and assessment of WDM **gyrokinetic physics** on experimental transport time-scale in a challenge problem for pedestal formation

- **Figure of Merit (FOM) of >50** for coupled code on exascale platforms, accomplished through algorithmic advancement, performance engineering and hardware improvement (*to be discussed in detail in answer to Q3*)

- Completion of **extensible integration framework** EFFIS 2.0 (End-to-End Framework for Fusion Integrated Simulations 2.0) and demonstration on exascale platform
WDMApp Challenge Problem

High-fidelity simulation of a whole-device burning plasma (specifically, ITER with full plasma current) operating in “high-mode” (H-mode), and prediction of the plasma pressure “pedestal” shape (height and width)

Pedestal determines the plasma pressure, hence fusion yield, in the burning core
Developing core-edge coupling of technology

1. We first use XGC-XGC coupling to develop the technology

2. Apply the technology to GENE/GEM and XGC coupling

XGC is the leading gyrokinetic code for simulating edge region, including a separatrix.

GENE and GEM are leading gyrokinetic codes for simulating core region.

First coupled simulation of turbulence in a Tokamak device.

J. Dominski et al., Physics of Plasmas 25, 072308 (2018)

Visualization: Dave Pugmire (ORNL)
Cross-verification between GENE and XGC: Non-linear ITG instability (J. Dominski, S. Ku, G. Merlo, C.S. Chang, F. Jenko, S. Parker)

Time-radius dynamics of the logarithmic gradient $R_0/L_T$:

Excellent agreement in the time-evolution of the global ion heat flux and temperature gradient. Radial average is taken over the widest region (0.3-0.7) after removing the simulation-boundary area.
Core-edge coupling

Coupling of XGC-core and XGC-edge


- True kinetic coupling between executables
- The coupled simulation is statistically equivalent to the reference simulation
- Study how to replace the XGC core simulation with a GENE simulation

Difficulty was in avoiding turbulence suppression from nonlinear de-phasing between two codes.

Failed example

Ion heat flux, $Q_i$
XGC – GEM coupling

\[ \phi, \text{XGC} \]

\[ \phi, \text{GEM-XGC coupling} \]

- \( R \) and \( Z \) scales are shown for both plots.
- The graphs compare \( \phi \) in XGC and GEM-XGC coupling scenarios.
**WDMApp coupling results**

- Linear results (n=24): frequency almost the same, growth rate differs ~1%, between coupled code and XGC reference.
- Nonlinear results (n=3,6,9,12…) show ~4% difference for the saturation level of heat flux, between coupled code and XGC reference.
- Coupled code adds little cost when using parallelized grid-quantity mapping (algorithm and performance enhancement). For example, 24.62s for XGC only, 25.23s for coupling with parallelized mapping.
What is EFFIS 2.0?

- EFFIS 2.0 is a workflow coordinator for the WDM App
  - A collection of services to compose, launch, monitor, and communicate between coupled applications
  - Automates “easy” deployment on DOE systems
  - Facilitates “easy” integration to analysis and visualization tools, components, frameworks, etc.
  - Unique features: in-situ memory-based data movement, placement options (e.g. same node), wide-area network, automated visualization
Tiered Science Challenge Goals

- **Basic challenge goal: for consistent measure of FOM**
  - Predict pedestal shape (height and width) in full-current ITER with electrostatic turbulence
  - Gyrokinetic ions and drift kinetic electrons
  - Execute simulation until pedestal reaches steady state
  - Pedestal shape largely determines energy-production efficiency of burning plasma in ITER

- **Advanced challenge goal: for more complete prediction with less uncertainty**
  - Include electromagnetic turbulence
  - Include tungsten impurity particles (ITER has tungsten wall)
  - Predict pedestal shape, and measure the divertor heat-load density

  - Expected bottleneck: performance of preconditioner for electromagnetic turbulence solver
  - Mitigation strategy: Use 3D PETSc solver and machine learning to speed up preconditioner
GENE-XGC Coupling
Optimization of GENE, XGC and GEM for large-scale Summit

Scope and objectives

- Port and optimize WDMAp codes on Summit computer in preparation for exascale systems
- Leverage the ECP Co-Design and Software Technologies projects for portability and performance
- Scale WDMAp codes GENE, XGC, and GEM to 20% of Summit

Impact

- Achieving high performance and scalability on a multi-GPU system is a critical requirement towards running WDMAp on Frontier and Aurora

Project accomplishments

- Successful porting to GPU of all three codes used in the WDM application: XGC, GENE, and GEM
- Use of CoPA-developed “Cabana” library in XGC, leading to high portability without loss of performance or scalability
- All 3 codes successfully ran on 1,024+ nodes on SUMMIT

ECP WBS

ADSE12-16 WDMAp

PI

Amitava Bhattacharjee, PPPL

Members

PPPL, ORNL, ANL, UNH, UT-Austin, U.Colorado-Boulder

 scope: Rectangular

impact: Rectangular

project accomplishments: Rectangular

deliverables: Rectangular

Deliverables Milestone Report

ADSE 12-16

Project: WDMAp
ST & CD Project Collaborations with WDMAApp

**ST**
- ADIOS-ECP: ADIOS Using ADIOS for I/O, code coupling, and in situ analysis/visualization
  - Indirect collaboration for analysis: VTK-M team, CODAR (FTK)
- ExaMPI: MPI is used in all codes (no support from ExaMPI)
- SOLLVE: OpenMP: OpenMP is being used in all codes (no support from SOLLVE)
- SPACK: Used for package management in EFFIS (no support from SPACK)
- PETSc: Used in WDMApp, for the field and collision solver: (M. Adams, not supported by WDMApp yet)

**CD**
- MGARD (CODAR): investigating the use for the unstructured XGC1 datasets (M. Ainsworth)
- Cabana (COPA): Used in XGC1 to provide platform portable performance for GPU optimization (S. Slattery)
- Savanna (CODAR): Used for the job submission and placement for EFFIS (K. Mehta)
- TAU (CODAR): Used to obtain performance information for the coupled runs (K. Huck)
Multiple-Time-Scale Coupling for advanced challenge problem

WDMApp turbulence capability ~1ms time-scale

Full Experiment ~1s time-scale

Multi-scale Coupling

Brute force requires resources far beyond exascale

Algorithmic innovation required
Challenge of Multiple-Time-Scale Coupling (continued)

Advanced challenge problem requires multiple approaches for risk mitigation

**Tango-GENE**
- GENE coupled to 1-D transport
- Recent innovation accelerates convergence near marginal stability

**Equation-free**
- Kinetic coupled to fluid moments
- Novel “lifting” operator preserves kinetic effects
- Currently implemented in XGCa
- 4.5x speedup in test cases

**Parallel-in-Time**
- Builds on MGRIT method
- New wrinkle: model reduction
- Synergistic with other approaches
- Additional parallelism improves scalability
- General framework compatible with wide variety of physics phenomena

Relative error vs. iteration

- *Original method*
- *Revised method*

Image courtesy of XBraid
Conclusions

• WDMApp is a leading priority of the fusion community, and will deliver a computational tool of unprecedented power and versatility.

• We have focused here on two primary goals: (1) Coupling of core gyrokinetic code (GENE and GEM) and edge gyrokinetic code (XGC), and performance of the coupled code with FOM > 50 (2) Development of a user-friendly extensible framework EFFIS 2.0 for code-coupling in WDMApp.

• The science is extremely interesting, and compute power will help realize Hawking’s vision for science in the 21st century.