Report of the Workshop on Integrated Simulations for Magnetic Fusion Energy Sciences

June 2 – 4, 2015

U.S. DEPARTMENT OF ENERGY | Office of Science

Sponsored by the Office of Fusion Energy Sciences and the Office of Advanced Scientific Computing Research

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Rockville, MD
June 2-4, 2015

Chair: Paul Bonoli, Massachusetts Institute of Technology
Co-Chair: Lois Curfman McInnes, Argonne National Laboratory

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Abstract

This report presents results from the DOE Workshop on *Integrated Simulations for Magnetic Fusion Energy Sciences*, `https://www.burningplasma.org/activities/IntegratedSimulations2015`. The workshop assessed recent progress and identified gaps and challenges in fusion theory and computation directly relevant to integrated simulations in the science applications of disruption physics and the plasma boundary, with whole device modeling as a long-term goal. Gaps in theory and simulation related to the integration of multiple processes and regions were assessed in terms of (1) how these gaps can be addressed in a ten-year timeframe; (2) new opportunities for integrated simulation with an emphasis on crosscutting fusion, applied mathematics, and computer science connections; and (3) identification of potential applications for extreme-scale computing. The report articulates priority research directions for seven synergistic panel topics, where DOE can achieve fundamental advances in integrated fusion simulations through sustained collaborations among fusion scientists, applied mathematicians, and computer and computational scientists.

Workshop Panels

Integrated Science Applications:

- **Disruption Physics**
    - **Panel Chair: Carl Sovinec** (University of Wisconsin-Madison)
    - **Panel Co-Chair: Dylan Brennan** (Princeton University)
    - **Panel Members:**
      Boris Breizman (University of Texas - Austin)
      Luis Chacón[1] (Los Alamos National Laboratory)
      Nathaniel Ferarro (General Atomics)
      Richard Fitzpatrick (University of Texas - Austin)
      Guo-Yong Fu (Princeton Plasma Physics Laboratory)
      Stefan Gerhardt (Princeton Plasma Physics Laboratory)
      Eric Hollman (University of California - San Diego)
      Valerie Izzo (University of California - San Diego)
      Steve Jardin (Princeton Plasma Physics Laboratory)
      Scott Kruger (Tech-X Corporation)
      Ravi Samtaney[1] (King Abdullah University of Science and Technology)
      Hank Strauss (HRS Fusion)
      Alan Turnbull (General Atomics)

- **Plasma Boundary Physics**
    - **Panel Chair: Tom Rognlien** (Lawrence Livermore National Laboratory)
    - **Panel Co-Chair: Phil Snyder** (General Atomics)
    - **Panel Members:**
      John Canik (Oak Ridge National Laboratory)
      Choong-Seock Chang (Princeton Plasma Physics Laboratory)
      Eduardo D'Azevedo[1] (Oak Ridge National Laboratory)
      Andris Dimits (Lawrence Livermore National Laboratory)
      Mikhail Dorf (Lawrence Livermore National Laboratory)
      Milo Dorr[1] (Lawrence Livermore National Laboratory)
      Richard Groebner (General Atomics)
      Greg Hammett (Princeton Plasma Physics Laboratory)
      Karl Hammond (University of Missouri)
      Sergei Krasheninnikov (University of California - San Diego)
      Tony Leonard (General Atomics)
      Zhihong Lin (University of California - Irvine)

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[1] Crosscutting expert from ASCR

Workshop Panels (continued)

- **Whole Device Modeling**
  - **Panel Chair: Jeff Candy** (General Atomics)
  - **Panel Co-Chair: Chuck Kessel** (Princeton Plasma Physics Laboratory)
  - **Panel Members:**
    Donald Batchelor (Oak Ridge National Laboratory)
    John Cary (Tech-X Corporation)
    David Green (Oak Ridge National Laboratory)
    Brian Grierson (Princeton Plasma Physics Laboratory)
    Jeff Hittinger[1] (Lawrence Livermore National Laboratory)
    Chris Holland (University of California - San Diego)
    Stan Kaye (Princeton Plasma Physics Laboratory)
    Alice Koniges[1] (Lawrence Berkeley National Laboratory)
    Arnold Kritz (Lehigh University)
    Lynda Lodestro (Lawrence Livermore National Laboratory)
    Orso Meneghini (General Atomics)
    Francesca Poli (Princeton Plasma Physics Laboratory)
    Tariq Rafiq (Lehigh University)

Mathematical and Computational Enabling Technologies:

- **Multiphysics and Multiscale Coupling**
  - **Panel Chair: Jeff Hittinger** (Lawrence Livermore National Laboratory)
  - **Panel Co-Chair: Luis Chacón** (Los Alamos National Laboratory)
  - **Panel Members:**
    Andrew Christlieb (Michigan State University)
    Guo-Yong Fu[2] (Princeton Plasma Physics Laboratory)
    Greg Hammett[2] (Princeton Plasma Physics Laboratory)
    Cory Hauck (Oak Ridge National Laboratory)
    Dan Reynolds (Southern Methodist University)
    Ravi Samtaney (King Abdullah University of Science and Technology)
    Mark Shephard (Rensselaer Polytechnic Institute)
    Mayya Tokman (University of California - Merced)
    Ray Tuminaro (Sandia National Laboratories)
    Carol Woodward (Lawrence Livermore National Laboratory)

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[2] Crosscutting expert from FES

Workshop Panels (continued)

- **Beyond Interpretive Simulations**
  - **Panel Chair: Donald Estep** (Colorado State University)
  - **Panel Co-Chair: Todd Munson** (Argonne National Laboratory)
  - **Panel Members:**
    Eduardo D'Azevedo (Oak Ridge National Laboratory)
    Omar Knio (Duke University)
    Scott Kruger[2] (Tech-X Corporation)
    Robert Moser (University of Texas - Austin)
    Eugenio Schuster (Lehigh University)
    Daniel Tartakovsky (University of California - San Diego)
    Bart van Bloemen Waanders (Sandia National Laboratories)
    Anne White[2] (Massachusetts Institute of Technology)

- **Data Management, Analysis, and Assimilation**
  - **Panel Chair: Wes Bethel** (Lawrence Berkeley National Laboratory)
  - **Panel Co-Chair: Martin Greenwald** (Massachusetts Institute of Technology)
  - **Panel Members:**
    Stan Kaye[2] (Princeton Plasma Physics Laboratory)
    Scott Klasky (Oak Ridge National Laboratory)
    Allen Sanderson (University of Utah)
    David Schissel[2] (General Atomics)
    John Wright[2] (Massachusetts Institute of Technology)
    John Wu (Lawrence Berkeley National Laboratory)

- **Software Integration and Performance**
  - **Panel Chair: David Bernholdt** (Oak Ridge National Laboratory)
  - **Panel Co-Chair: Bob Lucas** (University of Southern California / ISI)
  - **Panel Members:**
    John Cary[2] (Tech-X Corporation)
    Milo Dorr (Lawrence Livermore National Laboratory)
    Alice Koniges (Lawrence Berkeley National Laboratory)
    Orso Meneghini[2] (General Atomics)
    Boyana Norris (University of Oregon)
    Francesca Poli[2] (Princeton Plasma Physics Laboratory)
    Brian Van Straalen (Lawrence Berkeley National Laboratory)
    Patrick Worley (Oak Ridge National Laboratory)

Contents

Executive Summary

Fusion energy research has the goal of producing a safe and virtually limitless supply of energy for mankind. However, the great promise of fusion comes with the challenge of understanding the complex physics of both magnetic and inertial confinement fusion energy devices. The multiple physical processes in these devices interact nonlinearly over spatiotemporal scales spanning many orders of magnitude as they confine plasmas consisting of fusing deuterium and tritium gases at temperatures exceeding 150,000,000 degrees Celsius. The high cost of building future experiments and prototype fusion facilities such as the ITER device now under construction by a consortium of countries, combined with the complexity of these systems and the advances expected in extreme-scale computing over the coming decade, provides strong motivation for developing integrated simulation capabilities to predict key physical processes in these devices that can ultimately allow accurate simulation of an entire fusion device, thus minimizing risk to the device and guaranteeing its successful operation.

At the request of the Office of Fusion Energy Sciences (FES), U.S. Department of Energy, a series of four technical workshops were held in 2015 to seek community engagement and input for future program planning activities. The other three FES workshops focused on the topics of transients, plasma-materials interactions, and plasma science frontiers. This report describes the planning process and workshop that was held in collaboration with the Office of Advanced Scientific Computing Research (ASCR) on the role of integrated simulations for magnetic fusion energy sciences. The workshop assessed recent progress and identified gaps and challenges in fusion theory and computation directly relevant to integrated simulations in the science applications of disruption physics and the plasma boundary, with whole device modeling as a long-term goal. The study also broadened these science applications where appropriate. Gaps related to the integration of multiple processes and regions were assessed in terms of the following:

- Means for addressing these gaps in a ten-year timeframe.
- New opportunities for integrated simulation, with an emphasis on the crosscutting fusion, applied mathematics, and computer science connections.
- Identification of potential applications for extreme-scale computing.

As part of the workshop process, a call for whitepapers and a community teleconference were held to obtain community input, and a writing workshop was held for panel members and at-large invitees.

A key overarching finding is that opportunities abound for interdisciplinary FES-ASCR collaborations to pursue fundamental advances in integrated fusion simulations that fully leverage emerging extreme-scale architectures. These advances include high-fidelity models such as real-time plasma disruption forecasting from stability boundary maps and predictions of momentum, particle, and energy transport in burning plasmas obtained from gyrokinetic solvers or from caching vast databases. Opportunities were identified for developing predictive gyrokinetic simulations of the boundary pedestal and scrape-off layer where transitions to high-performance confinement modes occur that can ultimately determine overall plasma performance. Opportunities for integrated simulation were also identified that would make it possible to assess potentially damaging transient phenomena such as edge-localized modes, as well as lifetime predictions of divertor/wall plasma-facing components from erosion and tritium retention. Other opportunities were identified for whole device modeling, which would make it possible to integrate high-fidelity descriptions of multiple physics phenomena into a single simulation in order to assess risk and overall plasma performance in present-day experiments and ultimately in burning plasma devices.

Following an introduction in Secs. 1 and 2 to challenges and opportunities for high-performance integrated fusion simulations, Sec. 3 articulates workshop findings in terms of priority research directions determined by seven synergistic FES-ASCR panels, as well as several crosscutting recommendations; strategy and rationale are described in detail in Secs. 4 and 5.

Integrated Science Applications

Three panels were formed to address the fusion areas of (1) disruption prediction, avoidance, and mitigation; (2) plasma boundary physics, including the pedestal, scrape-off layer (SOL), and plasma-material-interactions; and (3) whole device modeling (WDM).

Disruption physics. The potential for catastrophic damage to a fusion reactor during a plasma disruption motivates the need to predict, avoid, and mitigate these transient events. A set of recommendations for accomplishing these goals consists of developing integrated simulation for all stages and forms of tokamak disruption, with and without mitigation, from instability through thermal and current quenches to the final deposition of energy on walls. This work will require improving multiscale, multiphysics algorithms, managing large amounts of computational data, and taking advantage of new extreme-scale computing opportunities. An automated plasma-state reconstruction and stability assessment system should also be developed in order to perform disruption forecasting, with the goal of facilitating disruption avoidance. Formulating and solving numerical optimization and inverse problems to inform stability forecasts are critical parts of this initiative, along with quantifying the uncertainty and reliability of stability predictions. Also, linear and nonlinear computational models must be validated, in order to establish confidence in the prediction and understanding of tokamak disruption physics with and without mitigation.

Plasma boundary physics. Boundary models require integration of multiple physical processes that cover a wide range of overlapping spatial and temporal scales, from the hot, confined pedestal zone with sharp gradients, to the cooler unconfined SOL and divertor plasma where heat fluxes reaching the walls must be within material limits, and finally the first few microns of the wall itself. The physics and simulation capabilities currently being developed in this area on petascale computing platforms have already benefited greatly from expertise in applied mathematics, computer science, and high-performance computing and will continue to do so as computing resources evolve toward exascale. These capabilities include kinetic turbulence simulations, related three-dimensional fluid simulations with gyro-Landau kinetic extensions, large-scale molecular dynamics simulations of materials, and couplings of lower-dimensional models (for fast analyses) to simulate interactions between zones and particle species. Prime candidates for substantial model development are as follows: the structure and dynamics of the coupled pedestal and SOL zones with turbulence, neoclassical collisions, and neutral gas fueling; dynamics of large transients such as edge-localized modes yielding high heat flux to walls, and methods for their mitigation and control; physics of the highly collisional, detached divertor plasma including advanced divertor designs; interaction of the boundary with radio frequency antennas; and coupling simulations of solid and liquid materials to those of the boundary plasma to assess surface erosion, recycling, and tritium retention.

Whole device modeling. Whole device models are required for assessments of reactor performance in order to minimize risk and qualify operating scenarios for next-step burning plasma experiments, as well as time-dependent or single-time-slice interpretive analysis of experimental discharges. Indeed, burning plasma experiments such as ITER will rely on whole device modeling for more accurate predictions of fusion performance, to control plasmas efficiently, to support the preparation for machine operation, and, in the longer term, to provide the modeling and control tools required for the physics exploitation phase. Significant improvements in WDM realism have occurred over the past decade (via more accurate core transport, pedestal stability, and wave heating models). Opportunities exist to take greater advantage of physics understanding obtained from high-fidelity whole device simulations, by directly utilizing high-fidelity kinetic simulations on extreme-scale platforms as part of a WDM and by developing model hierarchies suitable for inclusion into a fast, predictive WDM capability. Improvements in contemporary modeling efforts and advances in WDM capability depend on varying levels of theoretical, computational, and framework advances that will be greatly enabled by engagement with ASCR and the advent of extreme-scale resources. Recommendations for a credible path forward are (1) continued reliance on high-fidelity simulations for physics discovery and for the development of ever-improving model hierarchies and (2) continuation along the current path of WDM framework development that adds more flexible capabilities to incorporate models at all fidelity levels in order to explore both rigorous and ad hoc coupling schemes, enabling the study of trade-offs between accuracy and time to solution.

In addition to opportunities for WDM in disruption and boundary physics, workshop participants identified several new opportunities for WDM, including interaction of fast particles with thermal plasma waves and instabilities; steady-state plasma modeling with strong coupling of core transport to sources and MHD; inclusion of multiscale turbulence in WDM; development of a fast WDM capability for real-time simulation, numerical optimization, and uncertainty quantification; and the use of probabilistic WDM to assess the likelihood of key physical transitions or states occurring such as a plasma disruption, achieving a specific value of fusion energy gain Q, or exceeding the wall-damage threshold of divertor heat flux. Extreme-scale computing can help realize these goals.

Mathematical and Computational Enabling Technologies

Four panels were formed to address crosscutting ASCR areas of (1) multiphysics and multiscale coupling; (2) numerical optimization and uncertainty quantification; (3) data analysis, management, and assimilation; and (4) software integration and performance.

Multiphysics and multiscale coupling. Recent advances in multiscale, multiphysics coupling techniques—such as scale-bridging algorithms, time advancement, meshing, discretization, solvers, adaptivity, error analysis, and verification—have the potential to benefit fusion codes employing both multiple physics components and kinetic whole device models. Fully meeting these needs, however, is a significant applied mathematics and computer science challenge that will require novel algorithms and computing solutions. Advances in coupling algorithms for integrated simulation will require closer fusion and applied mathematics collaborations. The most effective algorithms for these problems will need to accommodate the specific characteristics of each driving physics application and will be intrusive, since they impact the foundation of simulation codes. To ensure that applied mathematics contributions have lasting impact, fusion scientists must be involved in the development and implementation of new algorithms so that they have ownership of and can support and maintain new capabilities.

Numerical optimization and uncertainty quantification. Scientific inference or prediction involves the synthesis of model simulations and experimental observations typically through the solution of inverse and numerical optimization problems combined with uncertainty quantification tools such as forward propagation of stochastic uncertainty. This area extends the predictive state of the art beyond interpretive simulations by improving confidence in fusion simulations and improving the efficiency of these simulations. These advances will provide increased confidence in the design of physical experiments and enable the design of robustly reliable fusion reactors, for example, by controlling and mitigating disruptions and by improving the edge pedestal quality and spread of the divertor heat-load. Collaborations should be formed that focus on developing and analyzing rigorous methodologies in these areas that can be applied to complex integrated models with complicated, evolving geometries. A concurrent effort should be devoted to designing and implementing efficient and reliable algorithms for the solution of inverse and numerical optimization problems as well as uncertainty quantification specialized to both kinetic whole device simulations and simulations involving coupled physics components.

Data analysis, management, and assimilation. Scientific discovery is driven by exploitation of data. However, extreme-scale computing, new computer architectures, the growing complexity of scientific processes, and the increasing importance of extended collaborations challenge traditional approaches to data assimilation, analysis, and visualization for integrated fusion simulations. This report emphasizes the needs for better systemization for data and metadata within individual projects and a community-wide approach overall, and between simulation codes and next-step experiments such as ITER; support for in situ methods of data analysis and visualization (especially for high-fidelity kinetic whole device simulations on extreme-scale platforms); automated capture and documentation of scientific workflows; fusion-specific analysis, visualization, and postprocessing capabilities; and an approach to improving the adoption and sustainability of new capabilities. Improvements and adoption of new tools and technologies for data management, analysis, visualization, and dissemination would increase the effectiveness of fusion simulation activities and foster stronger collaborations between theoretical and computational groups as well as with the experimental community.

Software integration and performance. Topics important to integrated simulation include general aspects of (large-scale, integrated) software systems, including workflow and coupling software, frameworks, and related topics; software engineering and software productivity; performance and portability; and community organization and governance. The ability of integrated simulation software to make effective use of current and future computer architectures is a significant concern that should be addressed through sustained, interdisciplinary partnerships among researchers in fusion, applied mathematics, and computer science. This report emphasizes the need for establishing and improving basic software engineering practices among the developers of integrated fusion software and for developing and disseminating software engineering best practices focused specifically on the characteristics of integrated or coupled software systems. Also, longer-term research is needed on the computer science of code composition to facilitate code coupling.

Crosscutting Themes

The recommendations outlined in this report are critical to meeting future challenges in integrated simulation for magnetic fusion energy sciences. Two crosscutting themes in particular have been identified that strongly couple the priority research directions set forth in the FES and ASCR recommendations:

- As the complexity of the models employed in magnetic fusion increases through integrated simulation, attention to model verification and validation will become front and center. In particular, development of reliable and validated model hierarchies is crucial for integrated simulation as a whole to succeed. These activities will naturally engage theoretical and computational plasma physicists, experimentalists in fusion energy sciences, applied mathematicians, and computer scientists. Thus, broad-based community support for model verification and validation is essential in order to realize the goals set forth in this report.
- FES and ASCR must expand opportunities for close collaboration among fusion scientists, applied mathematicians, and computer scientists in order to accomplish the goals in the recommended priority research directions. Such collaborative efforts would preferably engage physical scientists, applied mathematicians, and computer scientists from the outset of any new projects. Diversity in the size and scope of such projects is recommended: from smaller teams working on fundamental advancements, to larger teams focused more on development of new multiphysics codes and integration of new algorithms.

In summary, this workshop and report have assessed the role of integrated simulations in magnetic fusion energy sciences with a focus on identifying gaps, challenges, and new opportunities in fusion theory and computation in the science applications of disruption physics, the plasma boundary, and whole device modeling. The role of computational and enabling technologies was also considered in the crosscutting areas of multiphysics and multiscale coupling; numerical optimization and uncertainty quantification; data analysis, management, and assimilation; and software integration and performance. Strategies and a path forward in each of these areas have been articulated in terms of a set of priority research directions. Numerous opportunities for collaboration between FES and ASCR have been identified that will enable fusion energy scientists to take advantage of emerging extreme-scale architectures and ultimately develop the integrated simulation capabilities needed to predict key physical processes in burning plasmas and next-step devices.

1 Introduction: The Promise and Challenge of Fusion

The process of nuclear fusion has long held the promise of providing a limitless and safe supply of energy for humankind. Since the 1950s, scientists throughout the world have been engaged in controlled nuclear fusion research whereby the energy production that occurs naturally in the core of the sun is replicated in laboratory plasmas on Earth using isotopes of hydrogen (deuterium and tritium) at temperatures more than ten times higher than in the sun, as shown in Fig. 1. Deuterium can be distilled from all forms of water and is therefore a widely available, harmless, and virtually inexhaustible resource. Tritium is a fast-decaying radioisotope of hydrogen that, despite being relatively scarce, can be bred by using fast neutrons in a lithium blanket surrounding the core of a D–T fusion reactor. The isotope of lithium (Li^6) needed in the surrounding blanket is relatively abundant in nature. This report focuses on magnetic fusion energy research that today is being conducted on experimental devices such as tokamaks, spherical tori, reversed field pinches, and stellarators that confine very hot, dense plasma (ionized gas). These facilities are located both within the United States and around the world and with strong U.S. participation and interest. The next steps in the quest for a viable commercial fusion reactor concept will be the construction of the ITER device [1] and facilities to study nuclear science in order to test the key physics and technologies needed for a DEMO (DEMOnstration Power Plant).

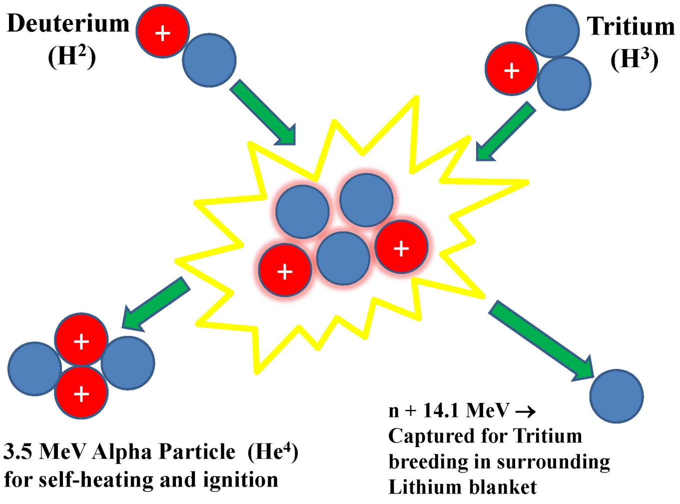


Figure 1: *Depiction of a D–T fusion reaction in a laboratory where deuterium (D) and tritium (T) nuclei fuse resulting in a helium atom, an energetic neutron, and heat [2].*

The scientific challenges we face in advancing to next-step devices are great. In order to minimize risk in such devices and ultimately ensure successful operation, it will be necessary to predict, avoid, and mitigate plasma disruptions, which are the premature termination of a tokamak discharge through the sudden loss of macroscopic stability and energy confinement. In ITER and future reactor-scale devices, disruptions will be capable of producing plasma heat fluxes and forces sufficient to damage in-vessel components, coils, and the vacuum vessel wall. In addition, the overall performance of a burning plasma is the result of a complicated interplay of physical processes that occur in a narrow layer at the plasma boundary known as the pedestal. The spatial profiles of density and temperature in the pedestal can form a "transport barrier," which then "lifts" the pressure profile to fusion-relevant conditions. However, the unregulated collapse of this pedestal or thermal barrier can result in the expulsion of enormous energy to plasma-facing components (PFCs) such as the divertor through quasi-periodic phenomena known as "edge-localized modes" (ELMs). Even without ELMs, the harsh environment of a burning plasma poses severe constraints on plasma-facing components because of damage from neutrons and high steady-state plasma heat fluxes. Better plasma–wall solutions will likely be needed for next-step devices, especially for nuclear science facilities and DEMO. Steady-state operating modes that are compatible with high fusion yields must also be developed in order for the tokamak to be a viable reactor concept. These will require development of external actuators that can be used to control the plasma current and pressure profiles as well as regulate or control disruptions and pedestal behavior. Achieving these scientific goals requires addressing the enormous challenge of integrating complex multiphysics, multiscale models to simulate dense, high-temperature plasmas confined by 3D magnetic fields that ultimately deposit their energy on material surfaces.

2 Integrated Fusion Simulations and Extreme-Scale Computing

Magnetic fusion energy (MFE) research is beginning to transition from the stage of scientific feasibility of main components, such as core energy confinement and large-scale stability, to questions associated with building an operating fusion power plant where all components must perform their critical functions in a predictable manner. Thus, in the next ten-year timeframe, research will focus on solidifying scientific understanding and fully exploiting experimental facilities. This will require integrating more multiphysics, multiscale phenomena and higher-fidelity physics models into simulations and expanding simulation capabilities toward prediction and design. The challenges and opportunities for moving forward range from near term, where important progress can be made with modest increases of effort, to much longer term, requiring new theoretical approaches, much more powerful computers, and mathematical methods applicable to the new physics models as well as to emerging extreme-scale computer architectures.

This section introduces workshop goals and outlines a number of challenges and opportunities at different levels of ambition. To set context, we provide an overview of recent work in MFE integrated simulations and highlight issues in emerging architectures for extreme-scale computing. Section 3 details priority research directions identified during the workshop.

2.1 Workshop Goals and Process

This workshop and report [3] address a charge that was communicated to the community in a letter from Dr. Edmund Synakowski, Associate Director of Science for Fusion Energy Sciences (FES), dated February 9, 2015 (see Appendix B, page 151). This workshop was conducted in collaboration with the Office of Advanced Scientific Computing Research (ASCR) in order to build on past successful partnerships between FES and ASCR that have made it possible to take advantage of advances in applied mathematics, computer science, and high-performance computing, in order to address grand-challenge-level problems in fusion energy sciences.

The goals of this workshop were to review recent progress and identify gaps and challenges in fusion theory and computation directly relevant to integrated simulations in the science applications of disruption physics and the plasma boundary, with whole device modeling as a long-term goal. In addition the workshop and this report have broadened these science applications taking into consideration recent progress and using the criteria of urgency, leadership-class computing benefit, readiness for progress within a ten-year timeframe, and world-leading potential. Recent progress in theory and simulation were considered since ReNeW [4] and the 2011 Fusion Simulation Program Execution Plan [5]. Gaps in theory and simulation related to the integration of physical processes and spatial regions were assessed in terms of the following:

- Means for addressing these gaps in a ten-year timeframe.
- New opportunities for integrated simulation, with an emphasis on the crosscutting fusion, applied mathematics, and computer science connections.
- Identification of potential applications for extreme-scale computing.

Workshop process. In order to achieve community consensus on these challenges and opportunities, a call for whitepapers was issued (see Appendix C, page 157), with a response period starting on March 16, 2015, and ending on April 24, 2015. A total of 121 whitepapers were received. A two-day community teleconference was held May 18-19, 2015, where oral presentations of 45 whitepapers were made to members of the workshop panels and the community at large. Members of the workshop panels were encouraged to submit whitepapers of their own; however, they did not give oral presentations during the community teleconference, in order to maximize time for members of the community not on the workshop panels to present their ideas. The list of whitepapers received can be found in the bibliography (starting on page 132). The whitepapers and corresponding oral presentations can be found on the public website for the workshop: `https://www.burningplasma.org/activities/IntegratedSimulations2015`.

To address these workshop goals and respond to the charge from DOE, panel members relied on the whitepapers, the community teleconference, additional materials such as existing reports, and interdisciplinary interactions supported through frequent teleconferencing. A workshop was held in Rockville, Maryland, June 2–4, 2015, in which preliminary results from each panel were presented and refined, with emphasis on crosscutting connections among topics in fusion, applied mathematics, and computer science. The workshop agenda can be found in Appendix D (page 161), and plenary workshop presentations can be found at the website above. An important goal of this workshop was to identify and further develop areas of common interest and benefit among the fusion, applied mathematics, and computer science communities as they relate to integrated simulation. In addition to the community teleconference in May and the workshop in June, the various panels conducted more than 40 teleconferences from February through July, 2015, with a teleconference held weekly among the panel chairs and co-chairs.

Workshop panel structure. The workshop was divided into three panels on topics in fusion energy sciences and four panels on topics in applied mathematics and computer science, as shown in Fig. 2. The fusion panels addressed Integrated Science Applications in the areas of *Disruption Physics* (Sec. 4.1), including prediction, avoidance, and mitigation; *Plasma Boundary Physics* (Sec. 4.2), including the pedestal, scrape-off layer, and plasma materials interactions; and *Whole Device Modeling* (Sec. 4.3). In addition to reviewing recent progress and identifying gaps and challenges in fusion theory and computation directly relevant to integrated simulations, each of the fusion panels considered the status of and prospects for validation against experiment, which are synergistic with activities of the DOE Workshop on Transients [6] and the DOE Workshop on Plasma–Materials Interactions [7]. Related issues are being addressed at the DOE Plasma Science Frontiers Workshop [8].

Panels on Mathematical and Computational Enabling Technologies (MCET, see Fig. 2) addressed crosscutting issues in fusion energy sciences directly related to integrated simulation. The panel on *Multiphysics and Multiscale Coupling* (Sec. 5.1) was tasked with identifying open challenges related to combining multiple complex physics models, including modeling and multiscale analysis, scale-bridging algorithms, time advancement, meshing, discretizations, solvers, and adaptivity. The focus of the panel on *Beyond Interpretive Simulations* (Sec. 5.2) was on the mathematical problems involved with predicting and controlling fusion processes, such as stochastic inverse problems for parameter estimation, sensitivity analysis, uncertainty quantification, numerical optimization, design, and control. The panel on *Data Management, Analysis, and Assimilation* (Sec. 5.3) studied aspects of fusion simulations related to integrated data analysis and assimilation that support end-to-end scientific workflows; knowledge discovery methods in multimodal, high-dimensional data; and integrating data management and knowledge discovery software architectures and systems. The panel on *Software Integration and Performance* (Sec. 5.4) focused on issues of workflows and code-coupling software, performance portability, software productivity, software engineering, and governance models for the fusion integrated modeling community.

Each panel consisted of a chair and co-chair with at least two fusion scientists on each of the MCET panels and at least two MCET researchers on each of the fusion panels. The detailed make-up of the panels with affiliations is given in Appendix E (page 163).

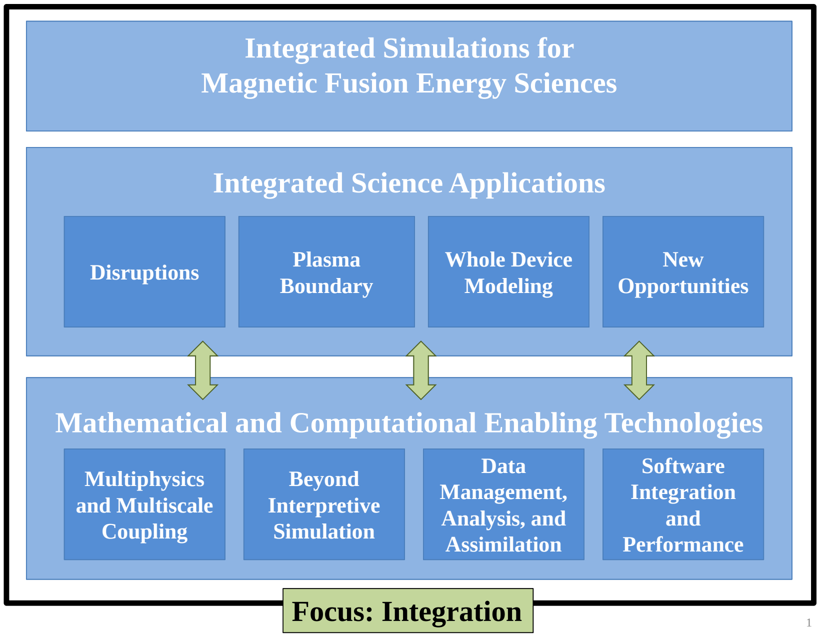


Figure 2: *Overview of the structure of the Workshop on Integrated Simulations for Magnetic Fusion Energy Sciences, showing the panel areas on Integrated Science Applications and panel areas on Mathematical and Computational Enabling Technologies.*

2.2 Challenges in Integrated Simulations for Magnetic Fusion Energy Sciences

The behavior of magnetically confined plasmas is described by the Maxwell-Boltzman system of equations, which can be written as

$$\frac{\partial f_\alpha(\mathbf{x},\mathbf{v},t)}{\partial t} + \mathbf{v}\cdot\frac{\partial f_\alpha}{\partial \mathbf{x}} + \frac{q_\alpha}{m_\alpha}(\mathbf{E}+\mathbf{v}\times\mathbf{B})\cdot\frac{\partial f_\alpha}{\partial \mathbf{v}} = \sum_\beta C(f_\alpha, f_\beta) + \sum_\alpha S(f_\alpha) \tag{1}$$

$$\nabla\times\mathbf{B} = \mu_0\mathbf{J} + \mu_0\epsilon_0\frac{\partial \mathbf{E}}{\partial t} \tag{2a}$$

$$\nabla\times\mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \tag{2b}$$

$$\nabla\cdot\mathbf{E} = \frac{\rho}{\epsilon_0} \tag{2c}$$

$$\nabla\cdot\mathbf{B} = 0. \tag{2d}$$

The field equations and Boltzmann equation are linked through the charge density ρ and the perturbed current density J, which can be expressed in terms of the particle distribution function as

$$\rho(\mathbf{x},t) = \sum_{\alpha} q_{\alpha} \int d^3\mathbf{v} f_{\alpha}(\mathbf{x},\mathbf{v},t) \tag{3a}$$

$$\mathbf{J}(\mathbf{x},t) = \sum_{\alpha} q_{\alpha} \int d^3\mathbf{v}\mathbf{v} f_{\alpha}(\mathbf{x},\mathbf{v},t). \tag{3b}$$

In Eq. (1) $f_{\alpha}(\mathbf{x},\mathbf{v},t)$ is the six-dimensional plus time distribution function for all charged plasma species, including electrons, ions, fusion-generated alpha particles, and impurity ions. The collision operator $C(f_{\alpha}, f_{\beta})$ (typically of the Fokker–Planck type), along with the source term $S(f_{\alpha})$, can represent additional rich physics (and associated computational challenges), such as radio frequency (RF) heating, neutral beam injection, pellet injection, interactions with neutrals, and atomic and molecular physics. The neutral gas particles can also be described by a similar kinetic equation where the electromagnetic interactions are absent (charge $q = 0$) and the collision operator differs. The primary challenge in integrated simulation of a tokamak plasma is the requirement to properly include the multiple physical processes represented in Eqs. (1–3), which span orders of magnitude in spatial and temporal scales. This fact is illustrated in Fig. 3, where one can see that spatial scales ranging from the electron gyroradius to the system size can span eight orders of magnitude (microns to tens of kilometers) and where temporal scales ranging from the electron gyroperiod to the pulse length can span fifteen orders of magnitude (nanoseconds to hours). The phenomena that must be modeled include plasma turbulence, large-scale magnetohydrodynamic (MHD) instabilities, wave–particle interactions for heating and current drive, energetic particle instabilities, radiation transport, atomic physics processes, and plasma–wall interactions. In addition to the multiphysics and multiscale aspects of Eq. (1), significant nonlinearities can exist; for example the third term on the left represents nonlinearities that are important in microturbulence and macroscopic dynamics. Also, many of the source terms can depend sensitively on $f_{\alpha}(\mathbf{x},\mathbf{v},t)$, and the transport can depend on the local gradient of plasma profiles. Indeed the ultimate goal of a whole device model is to simulate all of these physical processes at the relevant temporal and spatial scales [9].

The most prevalent approach to date for simulating the multiple physical processes in a tokamak plasma has been to take advantage of the separation of space and time, as shown in Fig. 4. The separation of timescales allows advanced models for heating and current drive sources, gyrokinetic codes for plasma turbulence, and extended MHD codes for macroscopic stability to be applied in relative isolation at given points in space and time. We note that each of these separate simulations may involve the integration of one or more physics subcomponents. Commonly, multiscale and multiphysics behavior in a tokamak plasma includes both weakly coupled systems with large separations of scales and strongly coupled systems with little scale separation (see Sec. 5.1.1). The challenges that arise for integrated simulation as a result of strongly coupled spatial and temporal scales when describing phenomena associated with plasma disruptions, the plasma pedestal and scrape-off layer, and the tokamak system as a whole are described in the following sections.

Disruption physics. The prediction, avoidance, characterization, and mitigation of disruptions are areas requiring integration of multiphysics and multiscale phenomena. For example, a principal pressure limit in tokamaks is set by the onset of neoclassical tearing modes (NTMs), which are destabilized and maintained by helical perturbations to the pressure-gradient-driven "bootstrap current." The resulting magnetic islands break up the magnetic surfaces that confine the plasma. Extended MHD simulations of the NTM onset and growth must resolve spatial scales from the microscale of the thermal ion gyroradius to the macroscale of the plasma minor radius. Stabilization of NTMs using RF waves in the electron cyclotron range of frequencies requires the inclusion of RF

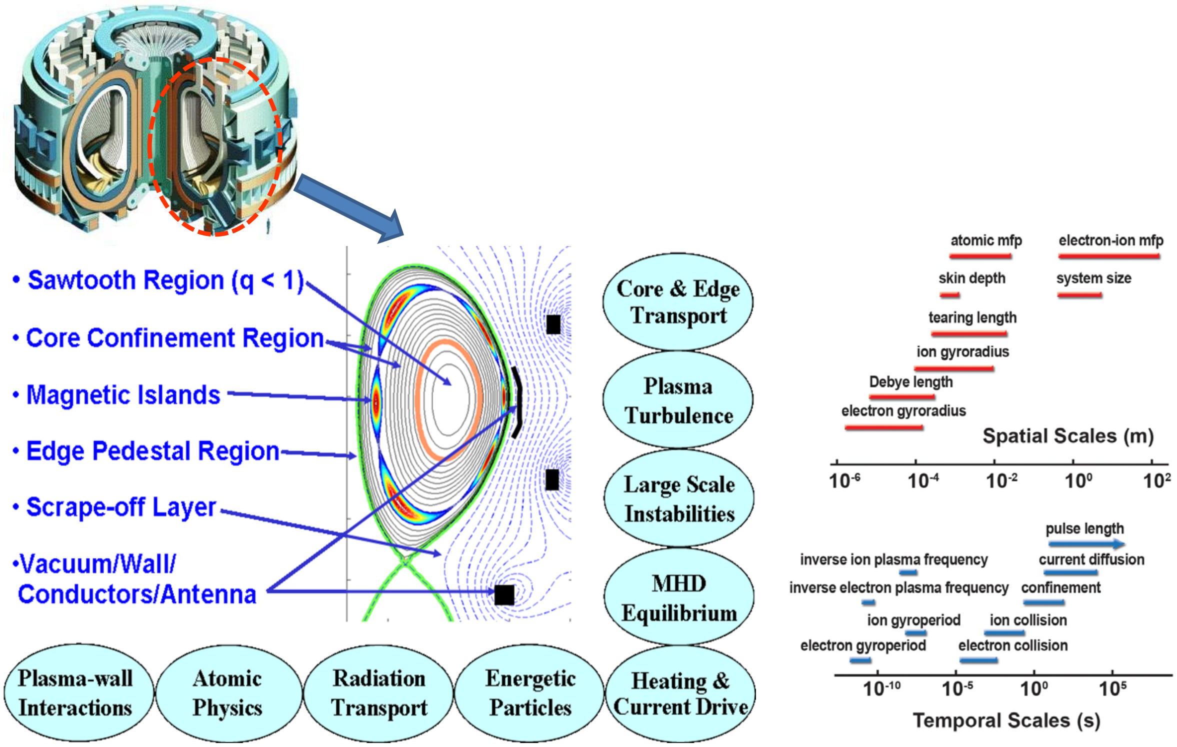
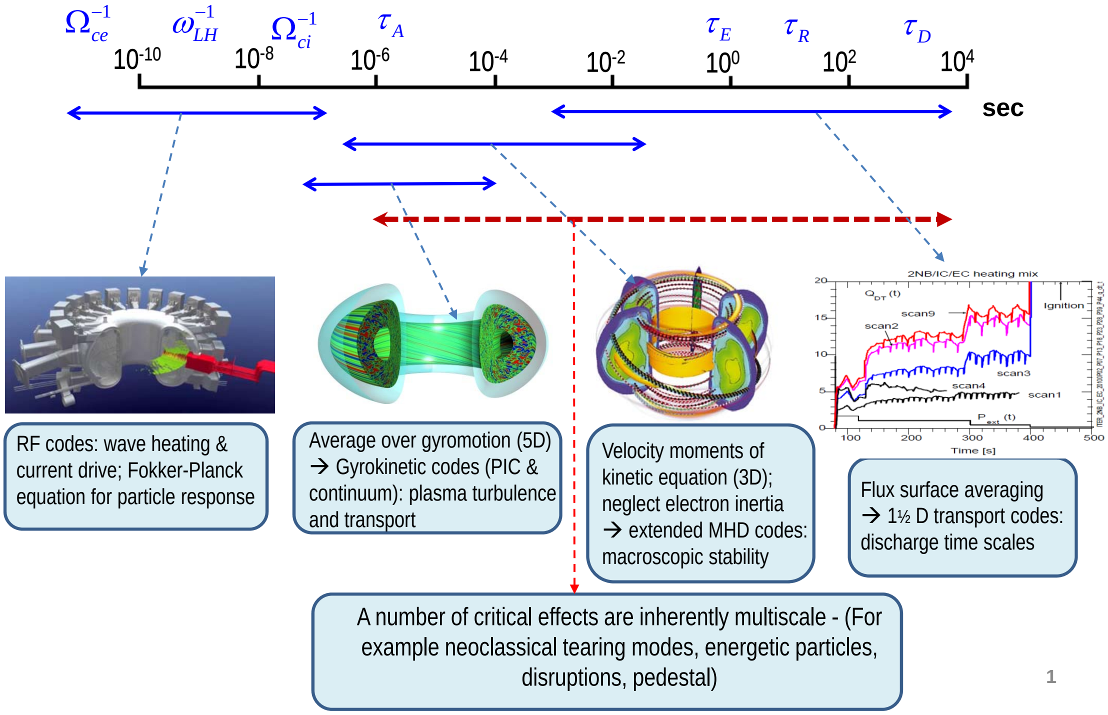


Figure 3: *Multiple physics processes, spatial scales, and temporal scales that must be accounted for in the whole device model of a tokamak [10].*

source effects effects in the MHD equations. To properly simulate island evolution associated with NTMs, one must include nonideal and asymmetric wall effects in toroidal geometry, which then must be coupled to physics models describing the plasma response. Modeling the eventual disruption after mode locking may require the inclusion of plasma–surface interactions, impurity dynamics, and radiation that depend on wall materials and conditioning. Disruption simulation must also include the effect of runaway electrons generated by the high electric field that is a consequence of the large resistivity of the colder plasma. Moreover, accurate modeling of disruption mitigation requires integrating models for impurity radiation, ionization/recombination, neutral dynamics and transport, and pellet ablation. Thus, modeling of disruption physics clearly requires integrated simulation that is both multiphysics and multiscale.

Plasma boundary physics. The plasma boundary, composed of the pedestal, scrape-off layer, and wall, is the narrower outer region of the tokamak where the range of spatial and temporal scales is especially large, resulting in an overlap of processes. The pedestal plasma typically transitions from being almost collisionless near the top of the pedestal to substantially collisional at the bottom, requiring methods appropriate for both regimes. The range of overlapping temporal scales often exceeds six orders of magnitude, with a similar overlap found in physically relevant spatial scales, where the gyroradius and ion drift wave scales can overlap the short gradient-scale lengths (see Fig. 4). The SOL has a number of especially challenging features, such as large amplitude turbulent structures even in the absence of ELMs, strong plasma and neutral variations along the magnetic



RF codes: wave heating & current drive; Fokker-Planck equation for particle response

Average over gyromotion (5D) → Gyrokinetic codes (PIC & continuum): plasma turbulence and transport

Velocity moments of kinetic equation (3D); neglect electron inertia → extended MHD codes: macroscopic stability

Flux surface averaging → 1½ D transport codes: discharge time scales

A number of critical effects are inherently multiscale - (For example neoclassical tearing modes, energetic particles, disruptions, pedestal)

Figure 4: *Application of simulation codes to take advantage of the separation of spatial and temporal scales that exist in a tokamak for certain physical processes; shown are examples of temporal-scale separations. Adapted from [11].*

field line resulting in orders-of-magnitude changes in collisional mean-free paths, strongly radiating impurity components, and long equilibrium timescales associated with particle fueling and pumping. The primary challenge in simulating plasma–materials interactions (PMIs) at the wall is the need to treat the smallest length and temporal scales in the system, that is, to directly simulate the interaction between individual atoms within the surface.

Whole device modeling. These discussions underscore the importance of integrated simulation in developing accurate models for disruption phenomena and the boundary plasma. However, these types of simulations really require the inclusion of many other physics phenomena, such as core turbulence or heating and current drive via the application of radio-frequency power or neutral beam injection power. Thus, whole device modeling can be viewed as integrated simulation carried to the "extreme." One of the great challenges of integrated simulation, especially as applied to the whole device, is the development of a validated set of models of varying fidelity that can be employed to optimize the use of computational resources to produce simulation outcomes with a required level of accuracy. Optimization of computational resources is necessary because a single high-fidelity simulation of a whole device will require a staggering amount of computational resources, while the demands of scientific inference, uncertainty quantification, and control and design generally require many simulations. Exploiting a set of models of varying fidelity in practice requires developing the capability of choosing from the set of models in some systematic fashion. This requires the systematic development of two types of model classes:

- Models using equations describing the physical processes to varying degrees of fidelity. The set of models is constructed in consideration of a "fidelity balance" that takes into account (1) the degree of physical fidelity that is possible given our understanding, (2) the degree of physical fidelity that is possible or desirable given computational resources, and (3) the fidelity needed to achieve a given level of accuracy in the simulation outcomes. Models in this class are sometimes referred to as "reduced" depending on the degree of physics fidelity.

- Empirical and phenomenological models that describe or process experimental data or express general physical processes in qualitative terms, for example, scaling laws that are generally derived from statistical fits of data.

These physics challenges also provide unique and interesting challenges in applied mathematics and computer science that embody the areas of multiphysics and multiscale coupling; verification, validation, uncertainty quantification, and optimization; integrated data management, analysis, and assimilation; and software integration and performance.

Multiphysics and multiscale coupling. Recent advances in multiscale, multiphysics coupling techniques have the potential to benefit fusion codes, but fully meeting these needs is a significant applied mathematics and computer science challenge that will require novel algorithmic and computing solutions. The requisite coupling techniques encompass applied mathematics topics such as modeling and multiscale analysis; scale-bridging algorithms; time advancement; meshing, geometry, and discretizations; solvers and preconditioners; adaptivity in space, order, and models; and coupling errors and verification. However, some of the most effective algorithms for fusion problems are likely to be intrusive and thus will require close collaboration between fusion scientists and applied mathematicians in order to develop and implement new algorithms.

Beyond interpretive simulations: Verification, validation, uncertainty quantification, optimization, and inverse problems. The fusion endeavor depends on the quality of scientific inference obtained from the combination of experimental, theoretical, and computational efforts. To what extent can we trust our models, data, and observations, and how does the assimilation of this information improve our understanding? The methods from statistics and applied mathematics that support more rigorous, quantitative, and potentially more valuable scientific inference have become known as uncertainty quantification (UQ), which includes a wide range of activities, such as forward propagation of stochastic uncertainty and variation; stochastic inverse problems; quantification of the effects of numerical, sampling, and model errors; and model validation.

Engineering design and control is a broad area encompassing parts of applied mathematics and numerical optimization. This activity applies mathematical techniques in conjunction with numerical simulations to, for example, determine design parameters to improve a quantity of interest, such as reducing the risk of a disruption in a fusion reactor, or determining when to apply a control to mitigate a disruption.

Applying systematic UQ and numerical optimization techniques to complex integrated simulations for fusion science will be challenging. Using more sophisticated analyses and numerical methods, however, can have significant impact. By increasing the quality of scientific inference, for example, questions can be answered with more confidence and rigor, leading to better understanding of the range of applicability of models and the reliability of predicted results.

Data management, analysis, and assimilation. The challenges in data management, analysis, and assimilation posed by integrated MFE simulations include most generally the need for a more systematic community-based approach to data and metadata. Further challenges imposed by I/O limitations on existing and future computing platforms also must be addressed. These challenges include (1) better systemization for data and metadata within individual projects and a community-wide approach overall; (2) support for in situ methods of data analysis and visualization; (3) automated capture and documentation of scientific workflows; (4) fusion-specific analysis, visualization, and postprocessing capabilities; and (5) an approach to improving the adoption and sustainability of the new capabilities. For example, the development of in situ workflows would be especially beneficial within large-scale computations where one must perform calculations with data that is not available as written output. Similarly, well-documented scientific workflows and metadata will aid validation and uncertainty quantification activities, where all the results can be traced back through all the processes and computations to the original input data, parameters, and assumptions.

Software integration and performance. One important challenge in the area of software performance of MFE simulation codes is the readiness of these codes for new architectures, including current leading-edge environments such as hybrid or accelerated systems and emerging extreme-scale machines. In particular, it is not known how the solvers and mathematical algorithms currently employed in these codes will fare on new architectures. Different algorithms and even different formulations may be better suited to new architectures, and application developers may need to rethink how best to solve specific physics problems rather than how best to port current algorithms to coming machines. A second challenging area for software engineering concerns the fact that the fusion community has much less experience, from a software engineering standpoint, in working with integrated systems in computational science and engineering. For example, researchers must work across multiple disparate code bases as they develop their integrated applications. A significant amount of the code coupling that currently takes place is based on adaptation of existing component codes rather than codes that are built specifically for the coupling. A third challenge for software performance in fusion energy sciences is the need for more universal application of basic software engineering best practices. This need is especially acute in the context of integrated simulation, where by definition the codes are more likely than in many other domains to be used and modified outside of their core development team.

2.3 Integrated Fusion Simulations and High-Performance Computing

Although integrated simulation has been part of fusion energy research for some time, the ability to carry out such simulations with increasing physical fidelity and a broader coupling to models of various processes has been enabled by rapid growth in computational capabilities, as well as DOE initiatives that have encouraged partnerships among researchers in fusion, applied mathematics, and computer science to begin addressing the challenges listed above. Some of the achievements that are a consequence of these initiatives are briefly discussed in this section.

FES/ASCR partnerships and achievements. Starting in 2001, DOE began funding the Scientific Discovery through Advanced Computing (SciDAC) [12] initiatives in ASCR and various application areas in the Office of Science, including FES. From the perspective of the fusion community, the purpose of these initiatives has been to advance scientific understanding in fusion energy sciences by taking advantage of advances in high-performance computing through partnerships with applied mathematicians and computer scientists in the corresponding ASCR SciDAC institutes, as well as in the applied mathematics and computer science community at-large. Eight fusion centers are currently funded under this initiative:

- Center for Simulation of Plasma Microturbulence (CSPM) [13]
- Gyrokinetic Simulation of Energetic Particle Turbulence and Transport (GSEP) [14]
- Center for Simulation of Wave-Plasma Interactions (CSWPI) [15]
- Center for Extended Magnetohydrodynamic Modeling (CEMM) [16]
- Center for Simulation of Energetic Particles in Burning Plasmas (CSEP)
- Center for Edge Physics Simulation (EPSI) [17]
- Plasma Surface Interactions: Bridging from the Surface to the Micron Frontier through Leadership Class Computing (PSI-SciDAC) [18]
- Advanced Tokamak Modeling Project (AToM) [19]

In addition to the FES SciDAC centers, ASCR currently funds four SciDAC institutes. The goals and objectives for the SciDAC institutes are to develop (1) tools and resources for lowering the barriers to effectively use state-of-the-art computational systems, (2) mechanisms for taking on computational grand challenges across different science application areas, (3) mechanisms for incorporating and demonstrating the value of basic research results from applied mathematics and computer science, and (4) plans for building up and engaging the nation's computational science research communities. The four SciDAC institutes are as follows:

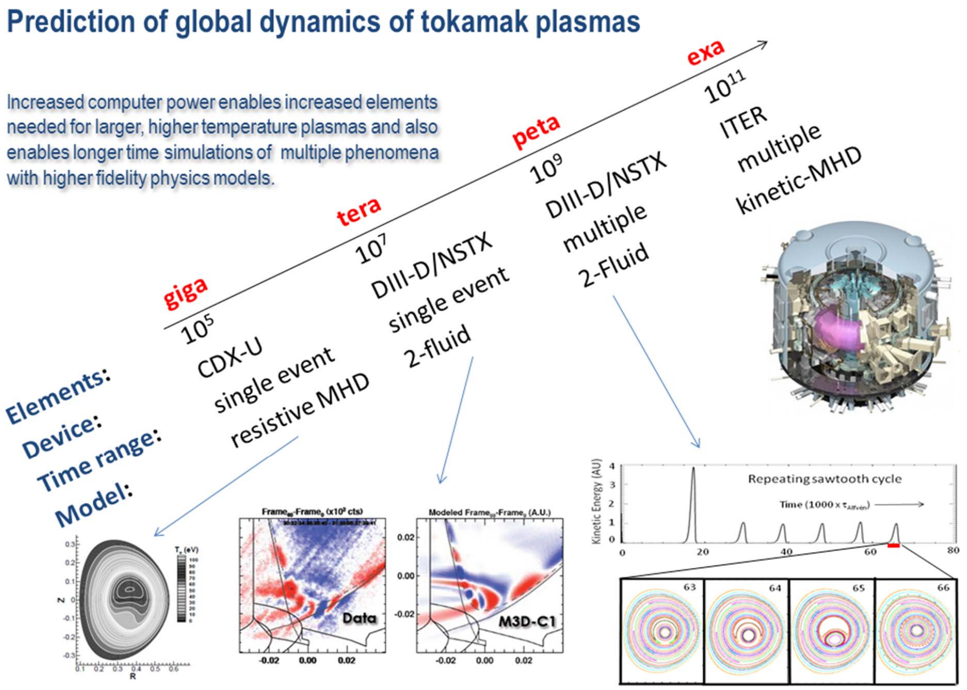
- FASTMath: Frameworks, Algorithms, and Scalable Technologies for Mathematics [20]
- QUEST: Quantification of Uncertainty in Extreme Scale Computations [21]
- SUPER: Institute for Sustained Performance, Energy and Resilience [22]
- SDAV: Scalable Data Management, Analysis and Visualization [23]

Starting in 2005 and continuing until 2011, DOE launched one of the first focused efforts in integrated simulation with three "prototype fusion simulation projects," or proto-FSPs, as part of the SciDAC program:

- Center for Simulation of Wave Interactions with MHD (SWIM) [24]
- Center for Plasma Edge Simulation (CPES) [25]
- Framework Application for Core-Edge Transport Simulation (FACETS) [26]

In addition to these SciDAC centers, another major effort with extensive collaboration among fusion scientists and applied mathematicians is the Edge Simulation Laboratory (ESL) [27]. Notably, these proto-FSPs carried out the framework development needed to perform the integrated simulations required by their physics missions, resulting in the FACETS, IPS (Integrated Plasma Simulator), and EFFIS (End-to-end Framework for Fusion Integrated Simulation) frameworks. The framework developed in the SWIM prototype FSP is based on a "loose coupling" of physics components with file-based transfers of information between the components, while the FACETS framework is based on a "tightly coupled" approach resulting in a single executable code with MPI for distributed-memory computing but otherwise one memory space. The EFFIS framework utilizes the general-purpose Kepler workflow system at its core.

Theory and computation in magnetic fusion energy research have long taken advantage of the latest developments in numerical algorithms and high-performance computing, dating back to the 1970s. These have greatly enriched the complexity of the physical descriptions incorporated into the models employed over the years. Two examples of this increasing model complexity are shown in this section for the areas of extended MHD and plasma turbulence. Figure 5 demonstrates how the progression from gigaflop to petaflop computing facilitated the transition from resistive MHD to two-fluid model descriptions and from simulation and comparison with experiment for single to multiple events (in time). This progression also enabled comparisons in experimental devices ranging from small-scale experiments to the major fusion user facilities, requiring an increase in computational unknowns (or elements) from 10^5 to 10^9. Note that exascale computing capabilities would enable the use of kinetic-MHD models to simulate multiple events in time in an ITER-sized device using 10^{11} elements. What is not so obvious in Fig. 5 but should be emphasized is the critical role of applied mathematics and computer science in the development and improvement of algorithms needed to take advantage of emerging computing architectures, as further discussed for various panel topics in Secs. 4 and 5 (see especially crosscutting discussion in Secs. 4.1.3, 4.2.3, 4.3.3, 5.1.2, 5.2.2, 5.3.2, and 5.4.2).


Prediction of global dynamics of tokamak plasmas

Increased computer power enables increased elements needed for larger, higher temperature plasmas and also enables longer time simulations of multiple phenomena with higher fidelity physics models.

Figure 5: *Increasing enrichment of physical description that has been achieved in the simulation of extended or global MHD phenomena with increasing high-performance computing capability. Adapted from S. C. Jardin [28].*

2.4 Emerging Extreme-Scale Computing Architectures

History. During the ten years since the start of the proto-FSP projects in 2005, the performance of the #1 system on the Top500 worldwide ranking of supercomputers [29] has increased by 120×, and the aggregate of the top 10 systems has increased by 166×,[3] enabling a tremendous expansion of the use of coupled multiphysics simulation as well as an increasing emphasis on computationally intensive validation, verification, and uncertainty quantification across many scientific domains. With these greater computational capabilities has come a similar rise in the number and volume of data sets produced by these simulations.

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[3] Comparing the November 2005 and November 2014 lists.

Coincidentally, the 2005–2007 timeframe is also generally agreed to mark the breakdown of Dennard scaling [30]. This was an important turning point impacting the architecture of high-performance computers, at which the primary performance gains in computers shifted from increasing the CPU clock frequency to increasing the number of cores in the CPU. Consequently, parallelism, both at the node level and at the system level, became the primary factor in increasing the capability of high-performance computing systems. Extending the Top500 comparison above, the aggregate core count of the top 10 systems has increased by 31× since November 2005.

Exascale concerns and architectural trends. Looking to computers with exascale performance levels, one sees a number of basic issues affecting the evolution of the hardware and, consequently, the environment in which large-scale fusion simulations will have to execute:

- Increasing computational capabilities now come from increasing concurrency. The trend toward massive levels of concurrency is a significant departure from the environment to which researchers have been accustomed for roughly the past twenty years or more.
- Power consumption has become an important constraint for the design of future systems, in order to control operational costs. These constraints are significantly below industry projections of power consumption based on current technology roadmaps. Thus, energy (power) has become a major driver of design throughout the system.
- One consequence of the focus on energy is the differentiation between more complex and power-hungry "latency-optimized" core designs and "throughput-optimized" cores that consume less power, typically through simplification and increased use of instruction-level parallelism, for example in SIMD or vector units, or simultaneous multithreading within CPU or GPU cores. This introduces yet more concurrency into the architecture.
- The cost per bit of memory chips, their power consumption per bit, and their bandwidth are improving slowly. These factors motivate increased use of nonvolatile memory, which consumes less power and is expected to be cheaper but has much lower bandwidth and higher latency. Memory bandwidth can be increased by packaging memory close to the processor chip, rather than in standard DIMMS; but such packages have limited capacity and higher cost.
- More and smaller transistors result in higher failure rates per system. While *undetected* hardware errors will, one hopes, continue to be rare, *detected but uncorrected* hardware errors are likely to become much more frequent.

As the HPC community attempts to respond and adapt to these changes, architectural trends for extreme-scale computers have largely coalesced around two basic "swim lanes." The many-core lane involves processors with a rapidly increasing number of relatively lightweight cores, while the hybrid lane involves multiple processor types, which are sometimes characterized as latency optimized and throughput optimized.

Current and next-generation leadership-class systems. The 2012 deployment of the Cray XK7 "Titan" system [31] at the Oak Ridge Leadership Computing Facility (OLCF) marked the clear bifurcation between the two swim lanes in DOE's major computational facilities. Titan is a current exemplar of the hybrid swim lane, with a 16-core server-class AMD Opteron CPU and an NVIDIA Kepler GPU accelerator. The many-core swim lane is represented by the IBM Blue Gene/Q "Mira" system [32] at the Argonne Leadership Computing Facility (ALCF). Mira nodes

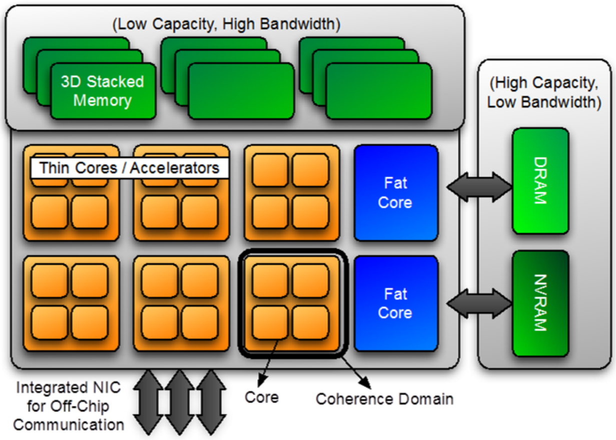


Figure 6: *Proposed abstract machine model for the node-level architecture of a future exascale system, developed by the joint Berkeley-Sandia Computer Architecture Lab [41,42]*

comprise a low-power PowerPC processor containing 16 cores, each with four hardware threads. On a per-node basis, the Cray system is roughly five times more powerful than the IBM.

The differences between the two swim lanes will become even more noticeable in the next generation of leadership-class systems [33], scheduled to be deployed in the 2017–2018 timeframe as part of the CORAL (Collaboration of Oak Ridge, Argonne, and Livermore) joint procurement. These systems are expected to deliver $\sim 6\times$ to $10\times$ the application performance of current systems, in excess of 100 petaflops. The Summit system [34], to be deployed at the OLCF, will comprise a small number (~3,400) of powerful nodes, with multiple IBM POWER CPUs and multiple NVIDIA GPUs, with most of the performance coming from very high degrees of parallelism in the GPUs. The Aurora system [35], destined for the ALCF, will have ~50,000 Intel Xeon Phi nodes, each with a large number cores (>60 per node) of a single type. Along with 2016 systems being delivered to Los Alamos National Laboratory and the National Energy Research Supercomputing Center (NERSC), they will also be among the first large-scale systems in the DOE complex to incorporate significant nonvolatile memory into the system architecture.

Extrapolating to exascale. The National Strategic Computing Initiative [36] aims at deploying early in the next decade systems with exascale performance (capable of executing $O(10^{18})$ operations per second), with price, power consumption, and footprint similar to those of current (2015) high-performance systems.

The exascale systems may have architectures similar to the CORAL systems, suitably extended: higher transistor density, more nodes, more cores per node, and more heterogeneity in the core architectures (see Fig. 6). However, it becomes increasingly hard and expensive to shrink device sizes at the rate prescribed by Moore's law. Consequently, the exascale generation of systems may have to take a more "adventurous" approach to increasing performance, which is even harder to anticipate.

But regardless of the architectural details, these systems will provide unprecedented resources for scientific discovery and are critical for meeting DOE computational mission needs over the next decade [37–40], including addressing the challenges in integrated simulations for magnetic fusion energy sciences introduced in Sec. 2.2.

Programming future systems. Adapting applications to the next generations of systems will require significant efforts: first and foremost, in finding and exposing the required levels of parallelism, at all three levels (instruction level, thread level, node level). Applications will need to manage the multiple levels of memory/storage and core heterogeneity (CPU/GPU). Resilience is an area of increasing concern; and it may become useful, or even necessary, for applications to take a larger role in dealing with resilience issues. Similar uncertainties exist concerning the extent to which applications will need to explicitly consider power consumption and power management (such as dynamic frequency scaling).

Overall, however, applications are expected to see more heterogeneity (even on systems with homogeneous processor architectures) because of variations in performance and capability across large-scale systems. These variations may arise from any number of reasons and require the use of asynchronous algorithms and the avoidance of global synchronizations.

The programming models used for high-performance scientific computing have not changed significantly in the past twenty years. MPI and OpenMP will continue to be available in the next decade and will evolve, both in design and implementation efficiency; ongoing research in programming models and runtimes may provide improved mechanisms for mapping applications to the new platforms, such as support for a global name space, support for dataflow programming paradigms, and support for parallel iterators that can leverage both CPUs and GPUs. Even within the confines of MPI and OpenMP, it will be worthwhile to adopt programming paradigms that are likely to scale better, such as the use of one-sided communication, sparse collectives, and nonblocking collectives in MPI and the use of task models. More significant changes in programming environments may provide more compact and expressive ways of programming future systems; however, the practical barriers to adoption of so-called revolutionary changes in programming models are high.

The uncertainty about the details of the future evolution of extreme-scale computing and the existence already of two architectural swim lanes will pose significant challenges to application developers. The need to prepare applications for coming generations of computer architectures is not a mere "porting" exercise but an opportunity to revisit implementation details, algorithms, and even the fundamental modeling and solution methods in order to identify approaches that may be better matched not only for immediate target systems but also for longer-range architectural trends [43]. And it will certainly be useful to pay more attention to software architecture and software engineering in order to produce software that is more easily modified and adapted as the details emerge (and change) [44].

Implications for integrated simulations for magnetic FES. While we emphasize changes at the largest scales, the key characteristics of these systems flow downward in both time and space. While leadership-class systems are national-scale resources, institutional and departmental clusters will be made of the same building blocks. The capabilities of server-class processors used in high-end systems make their way over time into desktop and laptop systems. Consequently, scalable solution strategies will affect the full spectrum of fidelity and scale of integrated fusion simulation, not just the most computationally intensive physics models.

2.5 Opportunities for Integrated Simulations: New Fusion Science Frontiers

The unprecedented computing resources expected to become available over the next ten years, coupled with partnerships among fusion scientists, applied mathematicians, and computer scientists, will create opportunities for dramatically improving the fidelity of integrated fusion simulations and for developing the capability to predict and control fusion processes. Below, we briefly summarize these opportunities and concomitant challenges in the areas of disruption physics, boundary physics, and whole device modeling. In addition, opportunities in several new areas are identified.

Disruption physics. An exciting opportunity for integrated simulation in disruption physics studies is the possibility of *characterizing* disruptions. Accomplishing this requires accounting for multiple physical processes, including the kinetic effects of thermal and energetic particles, radiation, neutral dynamics, plasma–surface interaction, detailed external electromagnetics, turbulent transport, and appropriate sources, all carefully coordinated in three-dimensional, time-dependent macroscopic simulations. Another opportunity for high-performance computation in this area is to inform control algorithms of the likelihood of a disruptive event through probabilistic forecasting that is analogous to weather prediction.

Plasma boundary physics. The strong coupling of the pedestal, SOL, and wall leads to several critical problems that provide unique opportunities that can be be addressed only by integration at the extreme scale. These include simulating the structure and dynamics of the coupled pedestal and SOL including the dynamics of transients such as ELMs and methods for their mitigation and control to prevent excessive wall heating; simulating the highly collisional detached divertor and its interaction with the upstream plasma; simulating the interaction of the boundary with RF antennas; and coupling materials simulations to the boundary plasma, including study of advanced divertor and materials concepts.

Whole device modeling. One of the overarching opportunities for high-performance computing in the context of WDM is the vision of a WDM framework that adds a more flexible capability to incorporate models at all fidelity levels, thus enabling researchers to explore both rigorous and ad hoc coupling schemes and address trade-offs between accuracy and time to solution. This is illustrated in Fig. 7, where a possible hierarchy of increasing model fidelity for core transport in the WDM is shown. The development and validation of gyro-Landau fluid turbulence codes provide core transport models that can be used in WDM where fast turnaround is crucial. Embedded gyrokinetic calculations in transport solvers represent increasing fidelity and computational requirements where core transport simulations with two species (electrons and a single ion) in present-day devices are possible using a few tens of thousands of cores but will require hundreds of thousands of cores in a reactor scale device with multiple species, including electrons, deuterium, tritium, energetic alpha-particles, helium ash, at least one beam species, tungsten, and beryllium. Also shown in Fig. 7 is the opportunity to include multiscale (ion and electron gyroradii) effects in WDM through a focused validation and database development effort. Exascale systems provide a natural opportunity for carrying out the parameter scans necessary to study and characterize multiscale turbulence and to inform the construction of tractable model hierarchies of enhanced electron transport.

In addition to WDM initiatives aimed specifically at disruption physics and the boundary, several challenging new areas were identified as opportunities for future research.

- Interaction of fast particles with thermal plasma waves and instabilities including the development of more detailed formalisms for the coupling of the thermal and energetic components
- Steady-state plasma modeling with strong coupling of core transport to sources and MHD
- Development of model hierarchies for multiscale turbulence that are tractable for WDM
- Fast WDM capability for real-time simulation, numerical optimization, and UQ
- Probabilistic WDM to assess the likelihood of key physical transitions or states occurring, such as a plasma disruption, achieving a specific value of fusion gain Q, or exceeding a threshold value of divertor heat flux

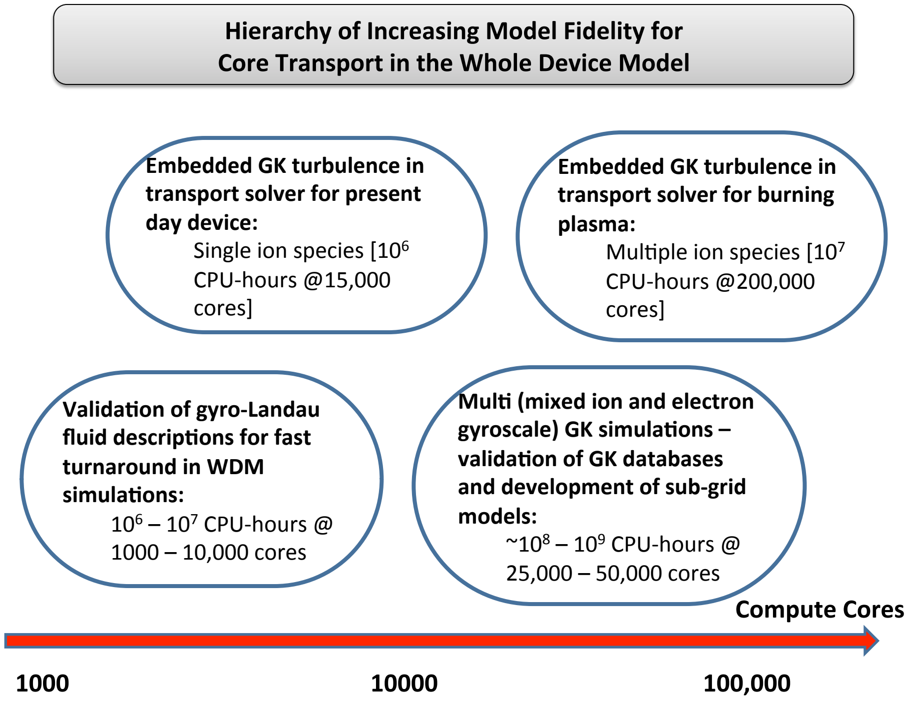


Figure 7: *Hierarchy of increasing model fidelity for core transport in whole device models.*

These new opportunities significantly broaden the scope for WDM beyond what was originally contemplated (i.e., disruption and boundary physics).

The opportunities for integrated simulation described thus far are primarily component based, where efficient, accurate, and interchangeable physics models are coupled to a simulation in order to integrate multiple physical processes. We note that approaches based on the use of the particle-in-cell (PIC) technique are also under development that allow multiple physical processes to be included in a single simulation. This is especially useful where separation of spatial and/or temporal scales is difficult. Also, PIC-based algorithms are highly amenable to extreme-scale architectures. The first verified and validated realization of this approach is being developed for the boundary where, for example, kinetic PIC simulations of three-dimensional electrostatic turbulence including both the pedestal and SOL regions have been performed (see Fig. 20). The next step will be to assess the fidelity of this method for the boundary and ultimately to include the entire device. Extending these simulations, which currently include transport from collisions (neoclassical) and electrostatic turbulence with central heating, to properly account for electron-scale turbulence will require extreme-scale resources because this might require a gyrokinetic electron treatment. Also, physics processes such as radio-frequency wave-particle interactions are still best incorporated in these types of simulations as coupled components. Thus, PIC-based algorithms can be considered as components themselves of a larger integrated simulation or whole device model. It is expected that use of PIC methods to describe multiple physical processes in a single simulation will be synergistic with coupled component-based approaches, resulting in the acceleration of the highest-fidelity physics models into WDM frameworks.

Verification, validation, and UQ. To date, the fusion community has applied some level of code verification (ensuring that the code implements the model correctly) and model validation (determining the extent to which a model accurately predicts one or more physical phenomena). However, new partnerships among fusion scientists, applied mathematicians, and computer scientists will provide an opportunity to do much more in this area. Common practice for model validation in many fields has been to compare experimental data (with some characterization of uncertainty, such as error bars) qualitatively with the results computed from a deterministic model without a characterization of the errors or uncertainty in the computed results. Numerical errors introduce biases, however; initial conditions, boundary conditions, and model parameters all introduce uncertainty. Thus, the results computed from models should be characterized by probability distributions, as is the case for experimental results. In fusion, this perspective is gaining ground; however, the full power of quantitative model validation through direct comparison of the distributions has yet to be realized. Moving to more sophisticated analyses of UQ applied to magnetic fusion science can have significant impact. By increasing the quality of scientific inference, questions can be answered with more confidence and rigor, leading to better understanding of the range of applicability of models and the reliability of predicted results, as well as indicating fruitful areas of scientific investigation when significant model errors are identified.

Extreme-scale integrated fusion simulations. The exascale requirements of the new science opportunities discussed in this section are summarized in Fig. 8. Shown are examples of the highest-fidelity physics models in four important areas where integration is needed: disruption prediction, avoidance, and mitigation; the pedestal and SOL; the plasma–wall interface; and core transport. An example is given for each area of a high-fidelity physics model simulation that would be enabled by exascale resources, combined with the requisite expertise from applied mathematics and computer science for multiphysics and multiscale coupling (Sec. 5.1); numerical optimization, inverse problems, verification, validation, and UQ (Sec. 5.2); data management, analysis, and assimilation (Sec. 5.3); and software integration and performance (Sec. 5.4). These include the possibility of extended MHD analysis of NTM island growth, locking, and disruption; core gyrokinetic simulations of transport in burning plasmas obtained from embedded gyrokinetic solvers or from caching vast databases constructed from the gyrokinetic solvers; gyrokinetic simulations of the pedestal, including the transition to high-performance confinement modes; and lifetime predictions of plasma-facing components such as the divertor as well as the tritium retention of the first wall.

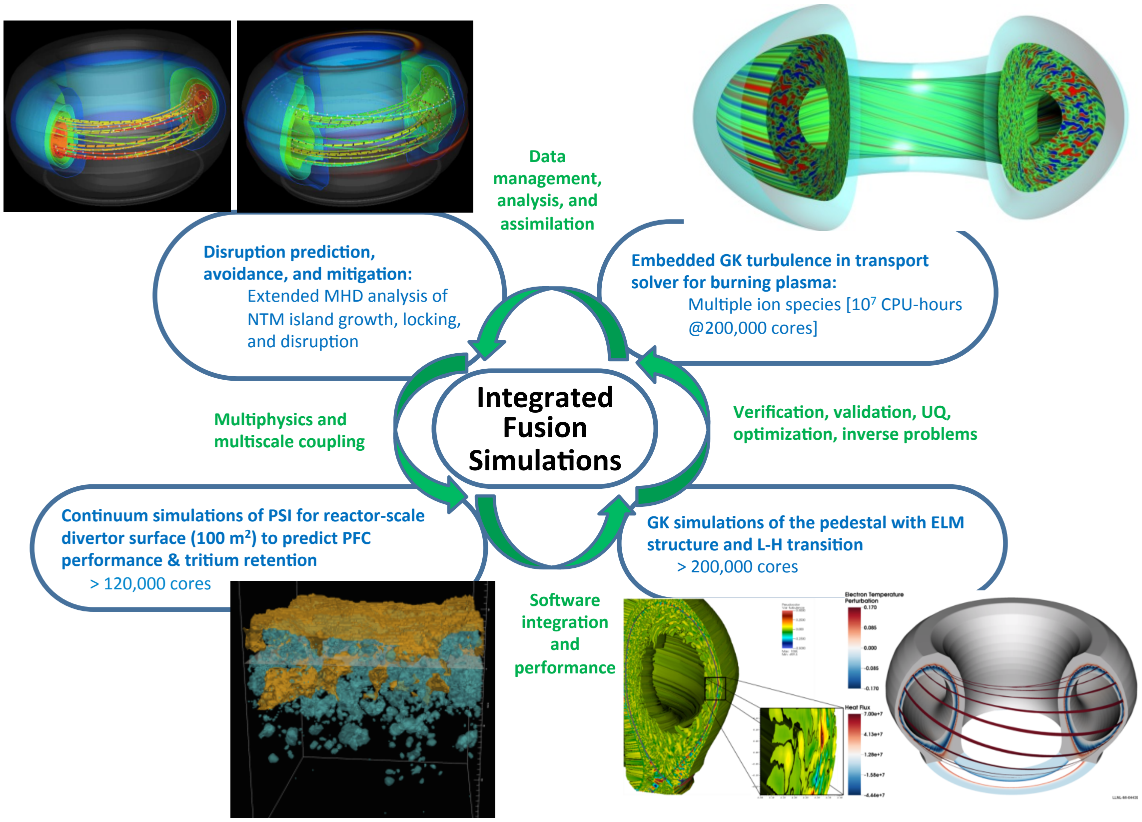


Figure 8: *Exascale requirements for the whole device model of a tokamak when using the highest-fidelity physics models available for core transport, the pedestal and scrape-off layer, plasma–materials interactions at the wall, and global MHD stability. Integrated fusion simulation is achieved by applying techniques from multiphysics and multiscale coupling; verification, validation, UQ, numerical optimization, and inverse problems; and data management, analysis, and assimilation. All require careful attention to software integration and performance on emerging architectures. Image at upper left is nonlinear MHD simulation of global instability leading to thermal quench and localized heat deposition on the surrounding wall (courtesy of S. Kruger, Tech-X Corp). Image at upper right is gyrokinetic simulation of core plasma turbulence (courtesy of J. Candy, General Atomics). Images at lower right are gyrokinetic simulation of edge-core coupling of plasma turbulence (courtesy of C. S. Chang, PPPL) and BOUT++ simulation of nonlinear ELM structure showing* T_e *perturbation (courtesy of X. Xu, LLNL). Figure at lower left is a molecular dynamics simulation of a tungsten surface exposed to 100 eV helium plasma for 285 ns (courtesy of K. Hammond, Univ. of Missouri).*

3 Priority Research Directions

In this section we describe a set of priority research directions developed by each panel in order to meet the challenges and take advantage of the opportunities discussed for each of the integrated science application areas and the mathematical and computational enabling technology areas. The strategy and rationale behind these priority research directions are described in detail in Secs. 4 and 5. The section concludes with several overarching issues that have been identified for all priority research recommendation areas.

3.1 Disruption Prevention, Avoidance, and Mitigation

Stability with respect to disruptive transients and protection against material damage when such disruptions occur are top priorities of research on magnetic confinement for fusion. Numerical simulation contributes to research on disruptions; but new initiatives are needed in order to realize the full potential of integrated modeling, recent advances in mathematics and computation, and forthcoming changes in computer architectures. The evolution of disruptions involves many physical effects occurring at wide ranges of temporal and spatial scales. Characterizing the different forms of disruption and designing systems that reliably mitigate their harmful effects will require an unprecedented level of model integration. Maintaining stable operation of reactor-grade discharges will also benefit from new efforts in integrated modeling. The reconstruction of plasma and magnetic-field states is a central component of stability assessment, and present approaches are not compatible with the scale of computing that is needed for mapping and forecasting stability. The stability and response calculations also need more complete modeling to achieve predictability over the relevant range of parameters. Based on these findings, the following priority research directions are recommended for the area of disruption physics.

- **[PRD-Disruptions-1]** Develop integrated simulation for all stages and forms of tokamak disruption from instability through thermal and current quenches to the final deposition of energy with and without mitigation. Because disruptive transients couple many different physical effects, characterizing them and engineering mitigation systems will benefit from a tailored form of whole device modeling. Complete numerical descriptions will include three-dimensional macroscopic dynamics, kinetics for runaway electrons and majority species, neutral and impurity transport, radiation, external electromagnetics, and plasma-surface interactions. Applications include magnetic-island locking, density-limit disruptions, runaway-electron generation, and mixing of impurities injected for mitigation.

- **[PRD-Disruptions-2]** Develop an automated plasma state reconstruction and stability assessment system with the goal of facilitating disruption avoidance. Linear stability and response analyses have potential for contributing to plasma control. Many computations will be needed to validate the models and to map stability over operational space. Automated processing of profiles and linear computations with essential flow, two-fluid, and kinetic effects need to be developed and coordinated to work at database scales.

- **[PRD-Disruptions-3]** Verify and validate linear and nonlinear computational models in order to establish confidence in the prediction and understanding of tokamak disruption physics with and without mitigation. Validating the predictive capability of linear computation for guiding operations can use existing disruptivity and active probing data in the near term. Uncertainty analysis is essential for validation and will be used to optimize the stability assessment system. Validating nonlinear simulations of transients will be challenged by the scale of individual computations, and hence practical limits on testing sensitivity to parameters.

Integrated simulation of disruptive transients requires improved theoretical models, effective multiscale and multiphysics algorithms, large-scale computing for each simulation, and management of large datasets. Analyzing plasma states for stability forecasting entails the formulation and solution of inverse and numerical optimization problems, along with quantifying the uncertainties in data and computation. Advances in capacity computing are also needed in order to analyze plasma states over the multidimensional parameter space and to support the demands of model validation. Details are provided in Sec. 4.1.4.

3.2 Plasma Boundary

Much of the challenge of the practical realization of fusion energy involves the boundary region, where the confined plasma, hotter than the core of the sun, must cool dramatically as it moves outward and eventually contacts the surrounding material wall. The physical processes in this region thus exhibit an even greater range of length scales and timescales than in the core. In addition, plasma interactions with neutral gas and the wall become important. The varying physical parameters can be identified with the three zones of the boundary: (1) the hot, confined edge pedestal plasma, a region with sharp gradients that has a profound influence on global fusion performance; (2) the cooler scrape-off layer plasma, which is located on open magnetic field lines that intersect material divertor plates and which must maintain the distribution of heat flux to these surfaces to be within material limits, while also shielding the core from sputtered impurities; and (3) the wall itself, which must withstand intense plasma bombardment that also results in neutral particle injection back into the plasma. Because of the complexity within and across these zones, extreme-scale computational models can play an important role in the development of a comprehensive predictive capability. We recommend the following priority research directions.

- [**PRD-Boundary-1**] Develop a high-fidelity simulation capability and predictive understanding of the coupled pedestal/SOL system and its structure and evolution in the presence of microturbulence and collisional transport. This capability will enable predictions of the temperature and density at the core interface, which strongly influence fusion performance, and also of particle and energy fluxes into and through the SOL, which determine wall heat loads and material erosion. Fuel and impurity neutral particles emitted from the wall/SOL in turn provide sources to the pedestal and core. Efforts should include simulating kinetic effects across and along the magnetic field as well as stochastic electron motion in 3D magnetic fields. Models include 5D electromagnetic gyrokinetic codes, 3D and 2D fluid codes, and 6D neutral Monte Carlo codes. Needed advances include methods to account for coupling of scales between the equilibrium and turbulence, implicit time integration, code optimization for high resolution, coupling schemes, and data management and validation procedures.

- [**PRD-Boundary-2**] Incorporate the dynamics of transients, particularly intermittent edge-localized mode events that eject bursts of particles and energy into the SOL, leading to large transient heat loads on the walls. This effort will require including the temporal wall response of impurity sputtering, and particle pumping or outgassing, and the impact of applied 3D magnetic fields. A key output of the work is to assess the maximum tolerable ELM size compatible with sufficient material lifetimes. Models include 3D MHD and two-fluid codes for ELM growth and ejection, coupling to 5D EM-GK, wall codes, and plasma/neutral transport codes. Needed advances are similar to those in [**PRD-Boundary-1**], with the addition of efficient, possibly adaptive, gridding techniques capable of treating rapid evolution of the local magnetic field.

- [**PRD-Boundary-3**] Develop a simulation capability that integrates the moderately collisional midplane SOL plasma with the highly collisional divertor plasma in order to model the detached divertor plasma regime, which is planned for ITER and other devices because of its effective power-handling features. The modeling challenge arises because ion and electron mean-free paths for the two SOL regions can vary by as much as 5 orders of magnitude based on recent measurements, and important divertor region interactions such as impurity radiation and coupled neutral particle transport must be incorporated. Models include 5D EM-GK codes, 3D and 2D fluid codes, 6D neutral Monte Carlo codes, and wall codes. Needed advances include coupling schemes between a 5D EM-GK midplane code and 2D fluid with neutrals divertor codes, or extension of 5D EM-GK to include the highly collisional divertor region. Other advances needed are similar to those in [**PRD-Boundary-1**].

- [**PRD-Boundary-4**] Integrate RF antenna/plasma-absorption simulations with SOL/pedestal plasma transport simulations, filling a notable gap in present capability. The SOL plasma strongly affects the wave coupling to the core, and the RF fields are expected to modify the SOL; this interaction must be studied with high fidelity to enable quantitative predictions for present-day devices and ITER. Existing 2D codes for the RF antenna and boundary plasma provide a starting point for the development, which eventually should couple 3D RF and transport models. Advances are required in coupling algorithms, especially using different meshes, as well as other algorithm improvements mentioned for [**PRD-Boundary-1,2,3**].

- [**PRD-Boundary-5**] Develop an enhanced capability to couple wall response models to plasma models. A related activity is to examine advanced divertor concepts, including alternate magnetic-geometry divertors and liquid walls. Models include molecular dynamics and kinetic Monte Carlo codes, 2D and 3D plasma transport codes, and 4-5D EM-GK codes. Especially important for coupling are efficient wall models for erosion/redeposition of surfaces, impurity release, and tritium trapping within the wall. Needed advances include coupling algorithms, especially utilizing implicit techniques to manage the large timescale separation between plasma and material processes.

As discussed in Sec. 4.2.4, these priority research directions emphasize the goal of developing high-fidelity models for key operational issues that were identified through the whitepaper and workshop process, with an emphasis on integrating models across the three boundary zones. The capabilities achieved will thus provide important integrated boundary components for whole device simulations. As briefly indicated in each item and detailed in Sec. 4.2.3, a number of algorithmic advances are needed to reach these goals.

3.3 Whole Device Modeling

Whole device models are required for reactor performance prediction as well as interpretive analysis of experimental discharges. Although significant improvements in WDM realism have occurred over the past decade, clear opportunities exist to take greater advantage of physics understanding obtained by high-fidelity simulations. These can be accomplished by directly utilizing these simulations as part of a WDM or by distillation into reduced models suitable for inclusion into a fast, predictive WDM capability. One of the great long-term challenges in integrated simulation is to address multiscale and multiphysics phenomena, such as the complex interaction between low-n MHD (sawtooth/kink, tearing) modes and short-wavelength drift-wave fluctuations. Based on these needs and challenges, the following priority research directions are recommended for whole device modeling of tokamak systems:

- **[PRD-WDM-1]** Increase development of and support for modular WDM frameworks. A sustainable path forward for whole device modeling will require both support for mission-critical legacy tools and development and expansion of newer components and workflows that can more effectively utilize leadership-class computing resources. This effort should be supported by steady programmatic commitment, should leverage contemporary efforts rather than starting from scratch, and should converge toward a reduced set of community tools compatible with the ITER Integrated Modeling and Analysis Suite (IMAS) and other standards.

- **[PRD-WDM-2]** Continue and expand efforts to understand and distill physics of gap areas. Addressing gaps in fusion physics understanding and achieving predictive simulation of these processes require a multipronged approach that includes (1) exploration of gap areas using both theoretical exploration and large-scale simulation of current and emerging fundamental model equations; (2) synthesis of physics insights obtained, in order to improve or develop new reduced models and modeling techniques; and (3) facilitating a pipeline of components at all fidelity levels into whole device modeling via a flexible framework structure.

- **[PRD-WDM-3]** Increase connection to experiment through validation. Mathematical formulations and corresponding software infrastructure are needed in order to enable robust validation of individual and coupled physics models at all fidelity levels and verification of corresponding numerical simulations. This effort combines the formulation and implementation of rigorous UQ methodologies appropriate for coupled systems identified in Sec. 3.5 with the data management capabilities identified in Sec. 3.6.

Over the next decade, a range of opportunities for improving WDM capability will depend on varying levels of theoretical, computational, and framework advances. Recommendations for a credible path forward are broadly consistent with the following theme: continuation along the current path of framework development that will grow to incorporate models at all fidelity levels and explore both rigorous and ad hoc coupling schemes. This path forward contains numerous opportunities for engagement with ASCR that will speed physics discovery and module development. Details are discussed in Sec. 4.3.4.

3.4 Multiphysics and Multiscale Coupling

Multiscale, multiphysics model coupling involves a breadth of applied mathematics topics, including modeling and multiscale analysis; scale-bridging algorithms; time advancement; meshing, geometry, and discretizations; solvers and preconditioners; adaptivity in space, order, and models; and coupling errors and verification. As such, this area is on the critical path to meet the goals of integrated simulation of magnetic fusion devices, especially where these goals require extreme-scale computing. Recent advances in multiscale, multiphysics coupling techniques have the potential to benefit some fusion codes, but fully meeting these needs is a significant applied mathematics and computer science challenge that will also require novel algorithmic and computing solutions. These solutions will emerge only if allowed by a broad, highly collaborative research environment. Specifically, we identify the following priority research directions, discussed further in Sec. 5.1.4.

- **[PRD-MultiXCoupling-1]** Invest in model development and analysis. Suitable multiscale algorithmic treatments begin with appropriate models and analysis of these models. A high priority is to foster near-term collaborations on this topic for problems where such analysis is needed.

- **[PRD-MultiXCoupling-2]** Develop efficient scale-bridging algorithms that address the particular challenges of fusion science. Systematic scale-bridging schemes that ensure consistency and accuracy are fundamental to the integrated simulations of burning plasmas, and the development of new scale-bridging algorithms not only is on the critical path for progress but also may benefit from new extreme-scale architectures.

- **[PRD-MultiXCoupling-3]** Develop time integration algorithms better suited to specific problems in fusion energy science. Time advancement techniques are essential to successful scale-bridging and coupled-physics simulations, and many advances recently have been made. Still, much work needs to be done to tailor these algorithms to MFE applications.

- **[PRD-MultiXCoupling-4]** Develop new techniques to address the geometrical complexities of fusion devices. Large anisotropies, complex device boundaries, and evolving magnetic field structures all pose severe challenges for integrated simulations that must be considered early during problem formulation, even though improvements can mature on a longer timescale.

- **[PRD-MultiXCoupling-5]** Develop new solvers and preconditioners congruent both with specific fusion science applications and with extreme-scale architectures. Physical processes, problem formulation, and discretization all directly impact the nature of the problems for which solvers and preconditions must be designed. In the medium to long term, solver algorithms will also need to make effective use of evolving HPC architectures.

- **[PRD-MultiXCoupling-6]** Develop new techniques that enable adaptivity of space, order, and models. Focusing resources only on those regions where additional resolution, accuracy, and/or physical fidelity are needed will be essential in the long term as a broad scale-bridging strategy for certain problems.

- **[PRD-MultiXCoupling-7]** Develop improved techniques to understand and control coupling errors. This effort requires a long-term commitment, since significant advances need to be made in verification methodologies before they can be applied routinely to complex multiscale, multiphysics simulation codes.

Addressing each of these research directions will be critical to meet the current and future challenges of integrated simulation for magnetic fusion energy sciences. Substantial work remains to be done, and advances will require more tightly coupled collaborations between fusion scientists and applied mathematicians.

3.5 Beyond Interpretive Simulations

This panel focused on issues related to using physics-based models (1) to investigate aspects of fusion processes that are currently intractable, expensive, or dangerous to observe and, ultimately, (2) to design experiments and reactors. Scientific inference or prediction involves a combination of model simulation and experimental observation typically achieved through the solution of numerical optimization and inverse problems combined with uncertainty quantification tools such as forward propagation of stochastic uncertainty. Important goals include improving confidence in simulation predictions, designing physical experiments, forming the basis for improved efficiency in high-performance fusion simulations, and designing robustly reliable reactors, for example, by controlling and mitigating disruptions. Details are found in Sec. 5.2.4. The specific recommendations of this panel follow.

- **[PRD-BeyondInterpretive-1]** Utilize applied mathematics to develop and rigorously analyze numerical optimization algorithms and UQ methodologies capable of addressing complex, coupled numerical fusion simulations with complicated, evolving geometries.

- **[PRD-BeyondInterpretive-2]** Develop joint fusion energy science and applied mathematics activities in numerical optimization and UQ to formulate relevant and impactful applications, leverage existing methodologies, develop new capabilities, and identify gaps that need to be addressed.

- **[PRD-BeyondInterpretive-3]** Support the extreme-scale computing needs for numerical optimization and UQ by devising new algorithms and providing appropriate computational resources.

Uncertainty quantification, numerical optimization, and inverse problems are drivers for extreme-scale computing. The physics-based models relevant to fusion energy science will challenge the frontiers of these mathematical disciplines and push researchers to develop novel algorithms and implementations targeting such complex models. Progress can occur only through collaborations between fusion energy scientists and applied mathematicians in order to ensure that the methods and tools developed are applicable to targeted science drivers in the short, medium, and long terms. In particular, the physics-based models should be instrumented for uncertainty quantification and numerical optimization as they are being developed.

3.6 Data Management, Analysis, and Assimilation

The computational work carried out by fusion researchers is among the most sophisticated and demanding in science. In general, however, the state of “data science” for fusion simulations would benefit from significantly increased attention. Improvements in and adoption of new tools and technologies for data management, analysis, visualization, and dissemination would increase the effectiveness of fusion simulation activities and foster stronger collaborations between groups and with the experimental community. New discoveries may be overlooked because of the difficulty of navigating and fully exploiting the potential of the huge, complex data sets already produced. The needs will only be greater as computing platforms move toward the exascale.

The need for a more systematic, community-based approach to data and metadata was widely recognized in submitted whitepapers, as were the challenges imposed by I/O limitations on existing and future computing platforms. This need is not particular to fusion applications and has spawned an active program of research and development across the DOE Office of Science. Concerted efforts, however, will be required to apply the infrastructure to fusion-specific problems. Overall, a sustained and coordinated effort will be required in order to develop shared solutions in the data management space. Specifically we identify the following promising research directions; details are provided in Sec. 5.3.4.

- **[PRD-Data-1]** Develop community data and metadata standards based on broad input from users and developers: These standards should explicitly represent the relationships between data objects and descriptions of data quality and validity. Implementation should build on strong abstractions that can support the inevitable evolution of software and hardware technologies.

- **[PRD-Data-2]** Develop and deploy infrastructure and algorithms that support in situ analysis for fusion simulation codes: Work is actively under way to develop underlying in situ infrastructure, however nascent; in order to be useful to the fusion community, projects must be initiated to help fusion code teams adopt this infrastructure, as well as to develop and deploy fusion-specific analysis, data management, and visualization methods in this in situ infrastructure.

- **[PRD-Data-3]** Improve support for MFE-centric workflows including capture of data provenance: Tools are needed that support end-to-end workflows, including experimental and simulation processes and dissemination of research products (e.g., databases, publications).
- **[PRD-Data-4]** Build federated, curated data repositories: Utilizing community data and metadata standards, fusion data should migrate to these repositories supporting remote access under flexible access control to meet investigator requirements. This effort will require a transition towards common abstractions, common ontologies, common schemas, common APIs, and common formats. Data creation, access, searching, and browsing through a shared, easily adopted toolset are needed.
- **[PRD-Data-5]** Engage in R&D and deployment of visualization and analysis methods targeted to the needs of the fusion community. These include methods for robust comparison of data from diverse sources, for visual data exploration of high-dimensional simulation output, for effective visualization of uncertainty and variability, for working with ensemble collections of data, and for accommodating the integration of metadata and provenance into the visual data exploration and analysis processes.
- **[PRD-Data-6]** Develop a strategy for promoting adoption and sustainment of shared tools that support data management, analysis, and visualization for fusion applications: Addressing this recommendation will require concerted engagement from all stakeholders, including developers, users, and DOE.

A roadmap for addressing these issues is urgently needed. The steps outlined above are critical to meeting future challenges in computation and more specifically for fusion sciences. Addressing these challenges will not be quick or easy, but progress can be incremental if guided by a broadly based and widely accepted plan. The fusion community should be open to ideas or solutions developed in other communities but should not hesitate to lead where appropriate.

3.7 Software Integration and Performance

The area of Software Integration and Performance spans a range of topics important to integrated simulation: general aspects of (large-scale, integrated) software systems, including workflow and coupling software, frameworks, and related topics; software engineering and software productivity; performance and performance portability; and community organization and governance as they pertain to the development and maintenance of software. These topics cut across those of all the other panels of this workshop. Given this breadth and these interconnections, the panel identified wide range of challenges and opportunities. We then determined the following six recommendations for future action; details are provided in Sec. 5.4.4.

- **[PRD-Software-1]** Implement software engineering best practices, consistently, throughout the fusion integrated simulation community. A core set of recommended practices should be identified and documented. They should be brought to the community through an outreach program staffed with experienced practitioners, with a mandate to provide assistance and follow-up to promote understanding and adoption.

- [**PRD-Software-2**] Bring together fusion researchers, applied mathematicians, and performance experts to focus on the performance and portability of fusion codes on current and future hardware platforms. This effort may involve taking a step back and considering different algorithms or even different formulations from those typically used today.

- [**PRD-Software-3**] Develop community standards and conventions for interoperability. This effort might include agreement on common data structures and data file formats, metadata and provenance, and names and units of measure for input and output data, as well as calling conventions and APIs. This recommendation builds on and extends [**PRD-Data-1**] to deeper levels of interoperability within integrated simulation software.

- [**PRD-Software-4**] Develop best-practice guidelines and recommendations to address the particular software engineering challenges of integrated simulation. Needs in this area include techniques for structuring and writing code with integration in mind, common directory structures, compatible build systems, and means to ensure the correctness of code in both standalone and integrated contexts.

- [**PRD-Software-5**] Perform research on the computer science of code composition. Extend ongoing work to systematize the physics and mathematics of code coupling, identifying the patterns and developing the abstractions that will facilitate the creation of composite software systems in a systematic fashion. This work also should build on and extend experience with computational frameworks and workflow environments in fusion and other research communities to address the additional computational patterns identified elsewhere in this report, including large ensembles, in situ data analysis, and tight connections between simulation code and data management and provenance capture systems.

- [**PRD-Software-6**] Determine a strategy to ensure the sustainability of key fusion integrated simulation infrastructure for long enough to establish a sustainable community of developers and users around it, as well as a strategy to encourage fusion code developers to take an active role in the integrated simulation community, as opposed to staying focused on standalone simulations.

While these recommendations may not all be considered to have as strong a “research” component as one might expect, we believe that the recommendations will have the most significant impact on the fusion integrated simulation community in the five- to ten-year timeframe in the area of software integration and performance and will greatly facilitate and accelerate the ability to make progress on integrated fusion simulations.

3.8 Overarching Themes

The priority research directions outlined above are critical to meeting future challenges in integrated simulations for magnetic fusion energy sciences. Several overarching themes have been identified that are important to recognize in order to achieve the goals articulated in the priority research directions.

- [**Overarching-1**] A key overarching finding is that opportunities abound for interdisciplinary FES/ASCR collaborations to fully leverage emerging extreme-scale computing resources for fundamental advances in integrated fusion simulations. These advances include high-fidelity simulations such as real-time disruption forecasting from stability boundary maps, predictions of core transport in burning plasmas obtained from embedded gyrokinetic solvers or from caching vast databases, gyrokinetic simulations of the pedestal including the transition to high-performance confinement modes, and lifetime predictions of plasma-facing components such as the divertor as well as the tritium retention of the first wall. All these fusion simulation topics require sustained and deep collaborations in applied mathematics and computer science for modeling and algorithmic advances as well as robust, high-performance, sustainable software. Such collaborative efforts need to engage application scientists, applied mathematicians, and computer scientists, preferably with involvement occurring from the outset of any new projects. Diversity in the size and scope of such projects is recommended: from smaller teams working on fundamental algorithmic advancements through larger teams focused more on development of new multiphysics codes and integration of new algorithms into existing production fusion codes.

- **[Overarching-2]** As the complexity of models employed in magnetic fusion increases through integrated simulation, attention to model verification and validation will become front and center. In fact, the need for careful model validation in all aspects of the priority research directions cannot be overstated, since it will be the final arbiter of the accuracy of the simulation (and measurement) capabilities that are being developed. Model verification and validation in this context will apply not only to individual physics components but also to integrated simulations that combine multiple physics effects. These activities will naturally engage theoretical and computational plasma physicists, experimentalists in fusion energy sciences, applied mathematicians, and computer scientists. Thus, broad-based support for model verification and validation is essential in order to realize the goals set forth in the priority research directions.

- **[Overarching-3]** A crucial element for realization of the goals of this workshop will be stable and predictable access to high-performance computing resources. These resources must address both capability and capacity computing needs, including short, moderate, and long time simulations on the largest-scale available machines, as well as at the 5,000–200,000 core level. In addition to multiphysics, multiscale fusion simulations that will require all resources of an exascale machine in order to meet the challenges described in this report, there is a significant need for research on innovative workflows, data structures, and algorithms to support efficient concurrent execution of many related moderate-concurrency simulations running for long periods of time. For example, studies to carry out uncertainty quantification, investigate model sensitivities, and perform numerical optimization require scans consisting of hundreds of related jobs running at, say, the 50,000 core concurrency level. Research is needed on issues such as memory locality and workflows to move beyond simplistic ensemble approaches by exploiting commonalities among closely related runs to fully leverage extreme-scale architectures. In addition, in order to reduce the time that is needed for the development of model hierarchies that can be used in WDM, algorithms that exploit the concurrency of extreme-scale platforms must be developed for these outer loop simulations.

4 Integrated Science Applications

This section provides background and details about priority research directions, introduced in Sec. 3, for three integrated science applications: disruption prevention, avoidance, and mitigation (Sec. 4.1); plasma boundary (Sec. 4.2); and whole device modeling (Sec. 4.3). Following a summary for each integrated science application, we explain background and recent progress, challenges and opportunities, and crosscutting issues in mathematics and computer science. We then discuss strategy and path forward, including more details about priority research directions. Crosscutting issues in mathematics and computer science are discussed in Sec. 5.

4.1 Disruption Prevention, Avoidance, and Mitigation

Stability with respect to disruptive transients will be paramount in ITER and in future large tokamaks. Significant progress has been made in understanding both the initiation and the evolution of disruptive transients, but many opportunities for integrated simulation remain in efforts to avoid, characterize, and mitigate disruptions. Automating the reconstruction of plasma states and quantifying uncertainties will facilitate assessing the value of stability computations for operations planning and for future uses of computation in control systems. Understanding the evolution of transients when disruption occurs is important for designing systems that protect experimental hardware. The transients are multiphysics processes that couple wide ranges of temporal and spatial scales. Expanding the scope of nonlinear integrated simulation will contribute to answering fundamental questions involving the onset and evolution of disruption and to designing effective mitigation systems.

4.1.1 Background and Recent Progress

Disruption, the premature termination of tokamak plasma discharges through sudden loss of macroscopic stability and energy confinement, poses one of the most serious challenges to the tokamak concept for fusion energy. In ITER and future reactor-scale devices, disruptions will be capable of producing heat fluxes, relativistic beams of electrons, and forces sufficient to damage physical structures. The root causes of disruptions include inadequate operations planning, failure of feedback control or other systems, and natural fluctuations that exceed the nonlinear metastability of a confinement state (see Fig. 9). Fundamental scientific questions remain about the onset and evolution of disruptions and how best to predict, avoid, and mitigate them. Many of these questions involve the interaction of diverse physical processes on multiple scales, which must be addressed through an integrated approach to modeling.

Solving the challenges of tokamak disruption in the burning plasma era will require concerted experimental and theoretical research. Integrated simulation that is rigorously validated against experiment can play a major role. As illustrated in Fig. 10, two distinct categories of numerical computation are needed to assess macroscopic stability and understand and characterize disruptive transients. Stability assessment informs operations planning and underlies *avoidance* of disruptions. Here, "avoidance" means both the routine maintenance of the discharge trajectory and last-minute redirection of the discharge if disruption becomes likely. If stability can be assessed and forecast computationally in real time, numerical results can be incorporated into experimental control systems. Stability is most often judged through mathematical perturbation of dynamical models about axisymmetric equilibrium profiles. The profiles are found by solving the nonlinear force-balance (Grad-Shafranov) equation with input from laboratory data and from transport modeling. An unstable condition is indicated by a growing mode of the linear system. In stable

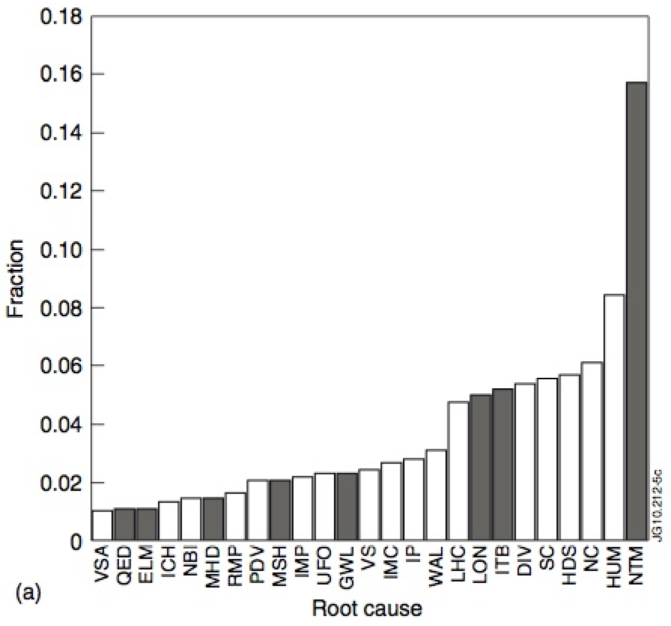


Figure 9: *Ranking of disruption chain root element causes of 1654 unintentional JET disruptions, years 2000 to 2010, distinguishing physical and technical/procedural causes from Ref. [45]. Physics and technical root causes are shown by grey and white colored boxes, respectively. The most frequent cause of disruptions was found to be the neoclassical tearing mode (NTM), which is physics-related. The second most common cause of disruptions was human error (HUM).*

conditions, proximity to a threshold can be inferred from the response to applied perturbations. Researchers are not certain, however, that most disruptions can be predicted by analyzing the linear stability of axisymmetric systems, and not all linear instabilities lead to disruption. The challenges for stability assessment, described in Sec. 4.1.2, include reconstructing equilibria with sufficient accuracy, modeling all the physical effects that influence stability, and quantifying the robustness of the stability properties of computed equilibria with respect to uncertainty and error.

When disruption cannot be avoided, ITER and future large tokamaks require *mitigation* to minimize damage from extreme localized heating on surfaces, from electromagnetic forces on structures, and from the impact of relativistic "runaway" electrons (RE) that can be created during disruption. Injecting heavy impurities when disruption is imminent, for example, radiates thermal energy

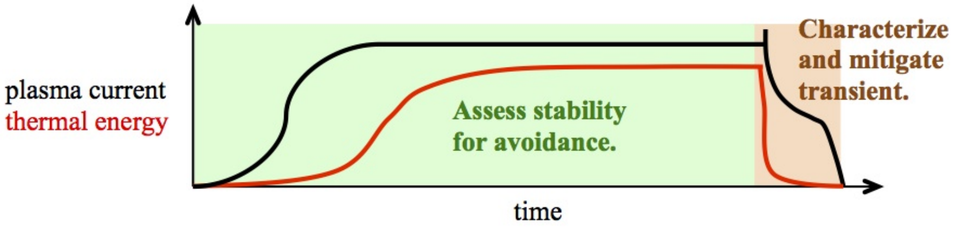


Figure 10: *Schematic time evolution of a disrupting discharge showing the steady, thermal-quench, and current-quench phases and the applicability of computations for stability assessment and for nonlinear transient characterization.*

broadly. This reduces localized heating, but it may increase the risk of RE generation. Therefore, development of effective mitigation strategies requires accurate *characterization* of disruptive transients. Disruptive evolution involves many effects, including nonlinear macroscopic dynamics, relativistic and nonrelativistic particle kinetics, electromagnetic responses of external structures, radiation, neutral dynamics, and plasma–surface interaction. Numerical models of some of these processes exist, but predictive simulation requires integrating the physical elements and quantifying the effects of uncertainties. Achieving this integration in a way that is accurate and makes use of future computational resources will require state-of-the-art and emerging developments in applied mathematics and computer science.

The 2009 ReNeW report [4] calls out the importance of controlling disruptions in its Thrust 2. Among the key issues are characterization of disruptions, capability to predict disruptions, capability to avoid disruptions, and means to minimize the impact of disruptions. In order to better predict the onset of a disruption, kinetic effects for both the majority species and energetic ions have been added to linear MHD codes so that they can more accurately predict instability boundaries [wp2,wp113]. Work has also begun on extending the kinetic MHD description to nonlinear simulations with the goal of creating a self-consistent drift-kinetic (5D) model suitable for long timescale simulations. Theoretical work has contributed to our understanding of the response to intrinsic and applied non-axisymmetric magnetic-field perturbations, using both linear and nonlinear response models. Progress with two-fluid capabilities of the extended MHD codes includes numerical algorithms, verification of two-fluid finite-Larmor radius effects on the drift-tearing mode, and efforts to validate the modeling through comparison with experiments [wp70].

Applying electron cyclotron current drive to stabilize magnetic islands before they have a chance to lock or otherwise grow has been demonstrated experimentally. Formulations to include the effect of electron cyclotron current drive in the MHD equations have been developed and used in a nonlinear 3D simulation to qualitatively reproduce this experimentally observed effect.

The current quench phase of the disruption results as a consequence of an instability leaving behind a low temperature plasma, a vertical displacement event (VDE) causing the plasma to impact the wall, or an intentional injection of gas (mitigation). Recent progress in 2D modeling of VDEs includes important benchmarks of the TSC and DINA codes. The tokamak MHD (TMHD) reduced model has been implemented in new codes that speed the analysis of currents conducted from the plasma surface through the complex external structures of experiments [wp32,wp121]. The TMHD computations contribute to validation of the wall-touching kink mode as the driver for asymmetric conductive currents and mechanical forcing. Three-dimensional simulations of current quench events have been performed with the M3D code to clarify the mechanism for the asymmetrical wall currents and forces, and projections have been made for the resulting forces on the ITER wall. New "resistive wall" capabilities have been added to the NIMROD and M3D-C1 codes to enable these 3D implicit MHD codes to study disruption physics with a more realistic separation of timescales than that used in earlier studies.

The RE electric-field threshold observed in recent experiments [wp34] is larger than expectations from the standard Connor-Hastie model, motivating recent theoretical investigations. The roles of radiation and scattering have been clarified. Significant progress has also been made in the kinetic theory of runaway generation, including effects of enhanced radiation because of electron elastic scattering with high-Z impurities. Microinstabilities are receiving renewed attention for enhancing scattering. In early tokamaks, the "fan" instability was observed in the presence of runaway electrons and interpreted qualitatively on the basis of local stability theory.

A recently developed ray-tracing code COIN (COnvective INstability) [wp8] is designed to address finite system size, plasma nonuniformity, and magnetized waves in order to examine kinetic instabilities of a runaway beam for any given equilibrium configuration of the plasma and

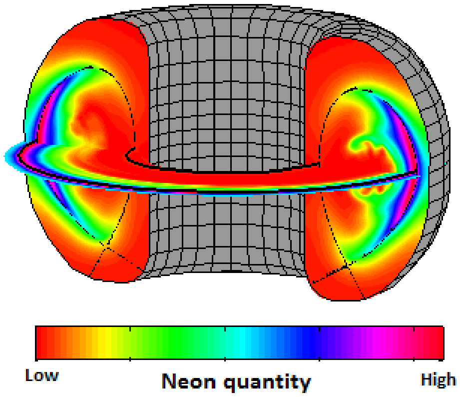


Figure 11: *Concentration of edge-injected Ne impurity after dynamic mixing, as predicted by integrated nonlinear simulation, combining 3D MHD and radiation modeling. Image courtesy of V. Izzo (UCSD).*

any distribution function of the RE. Other studies model the development and mitigation of an axisymmetric runaway avalanche that consumes the full equilibrium current. Initial simulations apply a self-consistent nonlinear fluid RE model to the evolution of the internal resistive kink mode in order to study the effects on MHD evolution.

Nonlinear 3D MHD simulations of mitigation by massive gas injection have been performed to support experiments on DIII-D (shown in Fig. 11) and project these to ITER [wp54]. They also include analysis of runaway electron confinement and variability for rapid shutdown scenarios.

4.1.2 Challenges and Opportunities

The multitude of effects that influence the macroscopic stability of tokamak discharges and their evolution during disruptive transients leads to theoretical challenges in identifying and modeling all of the important contributions. We first discuss challenges and opportunities in forecasting disruption and predicting its onset, followed by challenges involved in simulations of disruption dynamics and mitigation: the process of mode locking, thermal and current quench phases, relativistic runaway electrons, and the unique challenges for mitigation. The focus here is on theoretical topics and their importance for tokamak experiments, while only briefly describing the associated mathematical and computational challenges that are considered in more detail in Sec. 4.1.3.

Avoidance and onset prediction. Extensive pre-shot planning and real-time active control systems are used to guide modern tokamak discharges through all phases of operation. Improving the stability assessments used in planning and incorporating computational results into active controls seek to reduce the rate of disruption from the current best of 4% in JET to less than 1% in ITER [wp2][4]. However, significant advances in physical understanding and computing are required. For example, discrepancies exist between plasma responses measured experimentally by using MHD spectroscopy and the most complete linear model of resistive wall modes (RWMs), including drift and kinetic effects in conditions of low rotation, which are most representative of ITER [wp112]. The observed stability is less robust than that of the best numerical predictions. Other situations defy a simple connection between linear stability and disruptive instability. Short-wavelength ideal modes saturate benignly without causing disruption. In contrast, the onset of nonlinearly unstable NTMs includes the creation of a magnetic island of finite width, typically from some other event such as a sawtooth crash or ELM. By itself, the island-triggering instability is not a sufficient predictor of disruption, but it must be considered.

In addition to the variety of possible physical effects, sensitivity to the plasma state makes macroscopic stability assessment challenging. For both classical resistive tearing instabilities and ideal-MHD instabilities, the linear onset conditions are understood but are often sensitive to the details of plasma profiles, including the magnetic winding (safety factor), plasma pressure, flow, fast-ion distribution, and shaping [wp113]. Application of stability computation for avoidance and for post-shot analysis must consider the limited number of measurements used for mathematical reconstruction, errors in those measurements, numerical errors in solving the force-balance and stability computations, and physical limitations of the modeling. Precise stability assessment is, therefore, unlikely. However, probabilistic forecasting that is analogous to weather prediction is a realistic goal [wp66]. By using active probing of experiments and frequently updated measurements, together with empirical knowledge of precursor signatures, computation can inform control algorithms of the likelihood of a disruptive event.

Both planning and control are important for disruption avoidance, but incorporating computation into active control has not been demonstrated and presents a unique opportunity [wp53]. Two strategies for informing active control are envisioned: (1) reconstructing equilibrium and assessing stability in real time [wp33,wp60] and (2) real-time referencing of precomputed stability maps over relevant regions of the multidimensional parameter space [wp9]. In addition to the physical uncertainties and sensitivities noted above, each strategy presents a number of challenges. Fast real-time reconstruction performed with present-day experiments uses data only from external magnetic and internal motional Stark effect (MSE) diagnostics, and numerical resolution of the equilibrium computations is coarse. Current post-shot reconstruction of sufficient quality for stability computation includes pressure and flow measurements from multichannel Thomson scattering and other measurements. In practice, this relies on detailed prior knowledge of various offsets and uncertainties within different data channels, in addition to physics knowledge of the limitations of the equilibrium model response to the constraints of the data, and is currently done by hand with human judgment. The equilibrium computations also need to be well resolved numerically for accurate stability assessment. The stability-mapping strategy must identify the physical parameters that have the greatest influence on stability and conduct enough stability and plasma-response computations to resolve the multidimensional parameter space. It also needs to map laboratory measurements reliably into the parameter-space coordinates and rapidly evaluate the likelihood of disruptive instability from the stored computational results.

Clear physical, mathematical, computational, and technological gaps remain for control strategy and for improvements to operations planning through computation. First, our models for assessing stability are not validated for forecasting disruption over a sufficiently large space of parameters. All expectations for using linear computation to improve disruption avoidance hinge on model validation and improvement. Second, accurate reconstruction of tokamak plasma and magnetic-field states needs to be automated. This is a necessary step for real-time analysis, but it is also required for systematic validation with existing data. In addition, it will facilitate interaction with developments for the whole device modeling described in Sec. 4.3. Third, assessing stability over multidimensional parameter space requires equilibrium and stability computation at scales far beyond present efforts. Fourth, incorporating and analyzing equilibrium reconstructions for real-time control must integrate laboratory data management with fast and accurate numerical computation.

Magnetic islands, plasma rotation and locking. Mode locking is the process in which non-axisymmetric magnetic field exerts torque on the plasma through interaction with external conducting structures or through an increase in viscous transport, ultimately stopping plasma rotation. Locking events generally exhibit a bifurcation in which the plasma rapidly transitions from a rotating state with a small, static non-axisymmetric field to a stationary state with a large non-axisymmetric field. The transition is qualitatively described by the nonlinear theory of island penetration, which involves the balance of electromagnetic torque with viscous momentum diffusion and external sources of torque. However, a quantitative model for the onset of this bifurcation does not yet exist. The nonrotating state is highly prone to disruption for reasons that are not entirely understood. Because of the low rotation frequency expected in ITER and next-step devices, mode locking is expected to be one of the dominant causes of disruptions in these devices, as it has been in JET. ("NTM" events in Fig. 9 imply locking.) The transport of angular momentum in the presence of magnetic asymmetry, how the plasma state evolves to a locked condition, and why this state leads to disruption are active research topics and represent gaps in current understanding.

Non-axisymmetric modes may be present in the plasma as a result of linear or nonlinear instability of the axisymmetric equilibrium. In particular, classical tearing modes and RWMs are common linear instabilities that lead to significant torque on the plasma. NTMs are stable linearly but are unstable nonlinearly because of nonlocal particle kinetics. As noted above, calculating the onset criterion for tearing modes, RWMs, and NTMs is challenging. When calculating the transport associated with these modes, the mode amplitude, which is unconstrained by linear theory, must be calculated with nonlinear or quasilinear models. Non-axisymmetric modes may also be driven by externally applied magnetic fields. The fields may be applied intentionally for ELM suppression, or they may be a consequence of non-axisymmetries in the device (error fields). The non-axisymmetric field in the plasma is the combination of the externally applied field and the field generated by the plasma response. Understanding of plasma response, while incomplete, has improved considerably since ReNeW, and models of this response have been successfully validated for a limited set of experimental conditions.

The multiphysics aspects of island evolution and external-field penetration present challenges for integrated modeling. Nonideal and asymmetric wall effects in toroidal geometry are minimal requirements, which must be coupled to physics models describing the plasma response. Quantitatively accurate simulation of mode locking will require a detailed model of external electrically conducting structures and device-specific characterization of error fields. The onset condition for NTM depends on perpendicular thermal transport and thermal ion polarization drift. Multiple nonideal processes also affect the evolution of islands. The plasma microturbulence that transports thermal energy across magnetic field is influenced by the presence of magnetic islands. Energetic particles and magnetic tearing also have synergistic interaction; the particles affect tearing and other macroscopic modes, while their transport is influenced by magnetic fluctuations. Energetic particle transport can also be driven by instabilities such as Alfvén eigenmodes and energetic particle modes. Extended MHD modeling of these processes needs to resolve spatial scales from the microscale of thermal ion gyroradius to the macroscale of plasma radius. The timescales include the microsecond particle orbit time, the millisecond turbulence time, and the tens of milliseconds island evolution time. Modeling the eventual disruption after locking may require plasma-surface interaction, impurity dynamics, and radiation that depend on wall materials and conditioning.

Thermal quench. Apart from hot VDEs, disruptive transients typically start with the thermal quench (TQ), a rapid decrease of the plasma temperature from its pre-quench value down to several 10s of eV. The timescale for this varies, but it can occur in as little as 1 ms in a large tokamak,

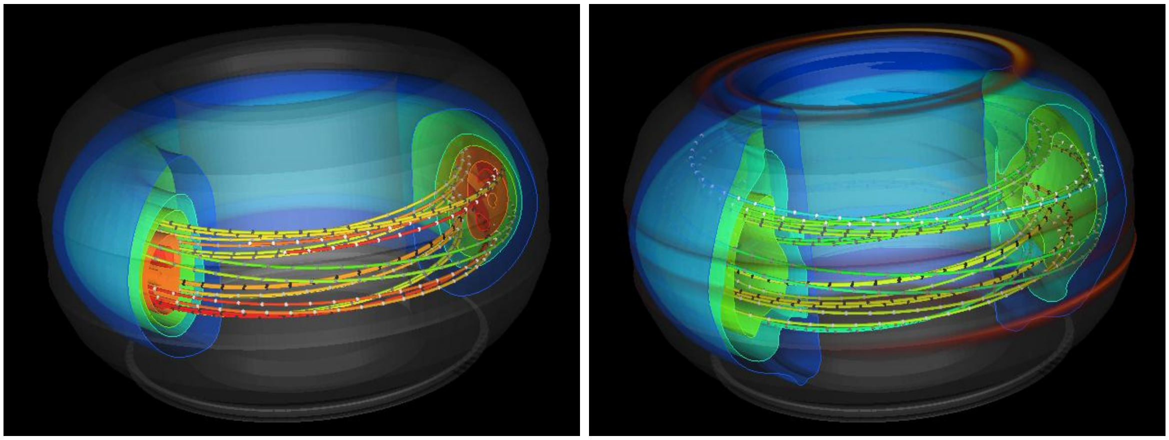


Figure 12: *Nonlinear MHD simulation of global instability leading to thermal quench and localized heat deposition on the surrounding wall. Images courtesy of S. Kruger (Tech-X Corp.).*

hundreds or thousands of times faster than the pre-quench energy confinement time. The TQ may be caused by one or more 3D global instabilities that destroy magnetic surfaces and hence the confinement properties of the device, as shown in Fig. 12. TQ also results when an accumulation of high-Z impurities causes radiative collapse. The rapid heat loss during the TQ produces damaging thermal loads on surrounding material surfaces. The sudden decrease in plasma temperature causes a sudden increase in resistivity that leads to the subsequent current quench (CQ) and associated large electric field that drives energetic electrons to relativistic speed during the CQ.

High plasma density also causes TQ in tokamaks. Beyond an empirically determined limit, which is proportional to the plasma current divided by system size, disruption becomes extremely likely. The empirical scaling of the density limit is robust, and yet the physical mechanism triggering the disruption has remained elusive. The phenomenon involves impurity density, radiation, energy transport, turbulence, and MHD instability. How the physical mechanisms are coupled and what primary mechanism is responsible for the observed scaling are open questions that can be addressed by integrated simulation. Two leading theories are based on radiative cooling of the plasma by impurities; one considers turbulence, transport, and thermal loss that propagate inward from the edge, while the other is based on radiative cooling within magnetic islands that causes explosive island growth. Integrated simulation will be able to distinguish the effects underlying this apparently universal phenomenon.

At present the detailed mechanism of how heat is lost during the TQ is poorly understood. Large, free-streaming parallel heat transport along chaotic temporally evolving magnetic lines certainly plays a role, as does a concomitant impurity influx from the surrounding structures. However, these phenomena have been modeled only approximately. Gaps exist in our understanding and modeling abilities for both areas. It is not clear whether a fluid (extended MHD) model with realistic anisotropic thermal conduction and with evolving impurity species (including radiation) can quantitatively model a TQ in a large tokamak or whether a more fundamental (kinetic) description is required.

The TQ phase of the disruption is likely the most challenging aspect of disruption modeling for the following reason. At the start of the TQ, the tokamak temperature can be at its maximum value, which will be over 10 keV in ITER. The corresponding Lundquist number will be in the range of $S \sim 10^9$ or more. This value is considerably larger than that used in published nonlinear extended-MHD calculations, because it implies long timescales (compared with the Alfvén transit time) and fine-scale structures that develop as a result of the breaking and reconnecting of magnetic field lines. After the TQ, when the temperature has decreased dramatically, the post-TQ plasma will likely have S $\sim 10^5$, which does not require as much spatial and temporal resolution, although the actual time period for the CQ is considerably longer than that for the TQ.

Plasma–surface interaction during the TQ leads to the generation of impurities and must be included as a boundary source term in the MHD modeling. Effects from neutral dynamics are also likely and should be evaluated [wp96]. Since this topic relates to the edge modeling area (Sec. 4.2), opportunities exist for incorporating the plasma–wall interaction models developed there. However, the extremely large heat flux and radiation impacting the wall during disruptions are well outside the range occurring during normal tokamak operation, and the plasma–wall interaction models may have to be extended to include extreme heat-flux phenomena such as melting and sublimation.

Current quench. The magnetic energy associated with electrical current carried by plasma is released during the CQ phase of a disruption. Low temperature following the TQ implies relatively fast resistive decay, but the timescale is still much longer than Alfvénic times. The TQ transient also upsets positioning control, and the plasma configuration drifts both radially and vertically (cold VDE). The motion induces surface currents in the plasma and eddy currents in external conducting structures. It also conducts current along open magnetic field-lines into the external structures. This current has both symmetric and asymmetric components. Without mitigation, the magnetic forces associated with these currents may be sufficient to cause structural damage in ITER [wp7,wp108], especially with asymmetry driven by external-kink instability induced by contact with the wall [wp120]. Disruptions also produce toroidal rotation, and possible resonance between oscillating wall forces and low-frequency harmonics of conducting structures would exacerbate damage. Modeling that reliably predicts current paths and forces can help protect expensive experimental hardware by providing guidance for control, mitigation, and design.

For this disruption scenario, integrating multiple important effects poses a significant challenge for modeling. Coupling to detailed external electromagnetics is required for computing current paths accurately [wp121]. To date, 3D MHD computations have considered only simplified axisymmetric wall models. The intense plasma–surface interaction initiated during the TQ also influences conducting currents through sheath effects, secondary emission, and impurity transport. In addition, runaway electrons can acquire the current that remains during the quench, and they impose kinetic effects on the evolution. Yet another disruption scenario is loss of vertical stability through control error. This leads to hot VDE disruption, where a well-confined region of high-temperature plasma rests against the chamber wall. The disruption evolution is then particularly slow, as governed by the resistive wall penetration time. This scenario challenges the ability of nonlinear integrated simulation to cover all temporal and spatial scales to a greater extent than other disruptive transients.

Runaway electron generation and confinement. The TQ enhances the electric field significantly because of the large resistivity of the cooled plasma, and the enhanced field can generate an avalanche of relativistic runaway electrons. The electric field then decreases to a level near the avalanche threshold on a timescale that is comparable to the avalanche growth time. Understanding the processes of the formation and loss of REs requires continued theoretical study and improved numerical modeling to achieve the quantitative predictability needed for confidence in mitigation techniques [wp10]. Areas of particular importance include relativistic kinetic effects on the avalanche growth mechanism, pitch-angle scattering and synchrotron losses of the runaways, and the stability and evolution of the runaway distribution function [wp8]. Studying this topic has broad scientific value, since it has applicability in other contexts including atmospheric events (lightning) and astrophysical and solar phenomena.

Most theoretical analyses of runaway avalanche assume a beamlike distribution of the current-carrying electrons. Beamlike distributions have been observed in experiments, but other measurements (TEXTOR, DIII-D, JET) show a large population of lower energy electrons with a roughly isotropic angular distribution. The origin of this population and its contribution to the total current still need better understanding. It is plausible that large-angle collisions of the beamlike runaways with bulk plasma electrons create an accompanying population of lower energy particles. An accurate near-threshold modeling of the runaway avalanche in realistic geometry will enable quantification of this mechanism to see whether it can explain the low-energy component of the electron distribution and its role in larger machines. Experimental observations of runaway beams also exhibit crescent and ring shaped spatial distributions, which rapidly alternate by means of some unknown mechanism. Effort has been made to understand the inward curved structure, but more study is needed.

As an aspect of current quench, all modeling needs described previously for CQ also apply to integrated simulation with RE effects. Test-particle RE modeling has been applied in nonlinear 3D CQ computation to investigate their confinement during disruption, and RE effects on the resistive internal kink have been investigated with a fluid approximation of the RE minority. Like other energetic particle effects, integrating RE kinetics into nonlinear simulation presents significant challenges, particularly given the timescale of the CQ. Ongoing theoretical developments on pitch-angle scattering and synchrotron losses have implications for integrated simulation. An unabridged description of Møller (electron-electron) scattering is essential for the near-threshold regime, and drift-orbit losses are significant in smaller devices. The work on microinstabilities mentioned in Sec. 4.1.1 will address whistler-wave scattering, which can enhance RE losses during the decay phase of runaway beams. Incorporating these effects in CQ simulations may require the development of reduced models as well as new numerical algorithms for full-scale kinetic modeling.

Disruption mitigation. Disruption mitigation strategies involve the injection of large quantities of impurities so that the thermal quench is dominated by radiative rather than conducted heat loss, although MHD activity has a significant role in the TQ evolution. Mitigation modeling therefore requires impurity radiation, ionization/recombination, neutral dynamics and transport, and pellet ablation. In some cases, opacity and radiation transport may be important. Like present-day experimental studies of mitigation, existing simulation results start with healthy-plasma conditions. Simulating mitigation of disrupting conditions represents a gap in predictive capability and will require integrating the physical effects described in Sec. 4.1.2 with those that influence the injected impurity radiation.

The two impurity injection concepts selected for the ITER disruption mitigation system are massive gas injection (MGI) and shattered pellet injection (SPI). In both cases, accurate models for the deposition of neutrals do not exist. For MGI, the penetration of a high-density directed neutral gas jet into the plasma edge differs from that of a single neutral particle because of the shielding of the jet interior from the surrounding hot plasma. SPI injects a cloud of gas, liquid, and solid fragments of various sizes; and a model for penetration and ablation is even more challenging. Integrated simulations including the ablation of the tiny pellet fragments must contend with much smaller spatial scales in the vicinity of the fragments (see Fig. 13). They must be coupled to the macroscopic MHD evolution, because of the global response of the plasma as the pellet cools the edge region with a back-reaction on the ablation process as the fragments continue their inward trajectory. This has been accomplished for whole-pellet fueling by using adaptive meshing (Fig. 14) but not for SPI.

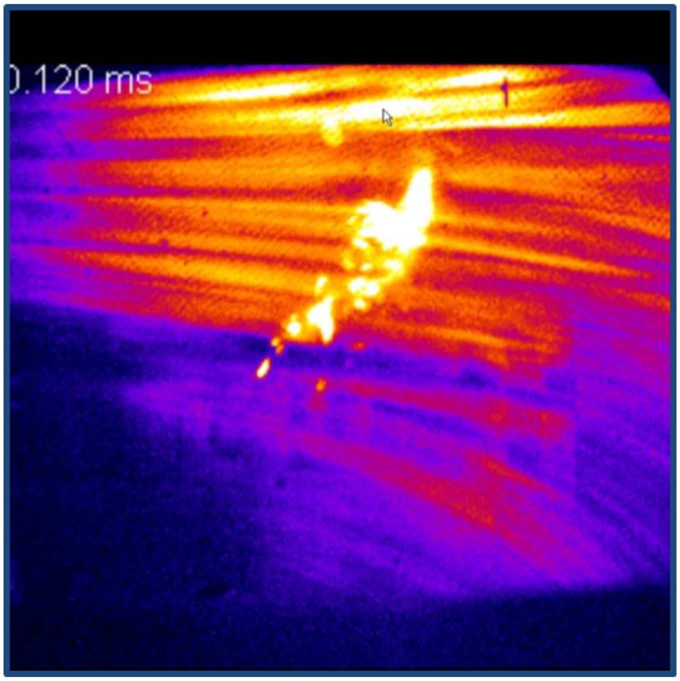


Figure 13: *Fast camera image of shattered-pellet injection in DIII-D, showing the radiation pattern from a collection of small shards penetrating the plasma edge. Image courtesy of R. Moyer (UCSD).*

4.1.3 Crosscutting Issues in Applied Mathematics and Computer Science

Numerical computations that describe plasma evolution during disruptions in tokamaks are characteristically multiscale. They solve extensions or reductions of resistive MHD for the particle density, flow velocity, temperature, and magnetic field as functions of space over the evolution of a disruption. The same equations also describe Alfvén and ion-acoustic waves that propagate over device scales in orders of magnitude less time than do the disruptive transients. The spatial distortions have features ranging from the ion gyro-orbit radius, or smaller, to the device scale. Thus, the problems are multiscale temporally and spatially. The magnetic field imposes extreme anisotropy in transport properties and leads to distinct polarizations in normal modes of the system. Moreover, the orientation and topology of magnetic field evolve during disruptive transients. Modeling macroscopic dynamics in magnetic confinement systems has benefitted from, and has motivated topics in, computational mathematics. Continuing progress relies on furthering and strengthening the scientific partnerships with the applied mathematics and computer science communities.

Implicit methods for multiphysics and multiscale systems. [Crosscutting Sec. 5.1]. Multiscale computations for macroscopic dynamics have been accomplished through semi-implicit and fully implicit methods with full and reduced modeling. The semi-implicit methods fall into the general category of partitioned time integrators, where numerical mathematics has advanced in recent years [wp24,wp94]. Application of these developments to disruption modeling may improve performance with relatively little coding. Research on applying exponential integrators to macroscopic modeling is another promising avenue [wp91]. Two-fluid and kinetic descriptions include

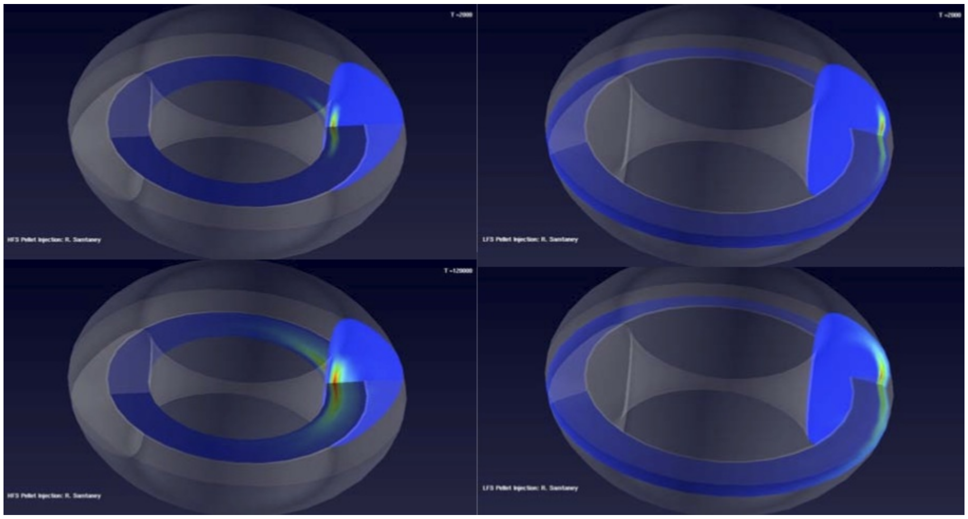


Figure 14: *Particle-density response in MHD modeling of pellet fueling on high- and low-field sides using adaptive mesh refinement. Image courtesy of R. Samtaney (KAUST).*

plasma drift-wave effects that have significant influence on the stability of macroscopic modes, and exponential integrators may be able to capture these effects more efficiently than can currently used methods. Development of implicit methods for multiphysics systems is also needed in order to reliably address all the envisioned integrated-simulation capability [wp94]. Parallel-in-time methods may lead to better use of parallel computation for evolution over long timescales. Other recent advances that address stiff systems include asymptotic-preserving methods.

Scalable algebraic solvers. [Crosscutting Secs. 5.1]. At present the solution of large, sparse algebraic systems is the most computationally demanding part of simulating macroscopic dynamics with implicit and semi-implicit fluid-based plasma models. Computational developments for parallel direct methods for sparse systems and for multigrid methods have enabled simulation capabilities. However, novel preconditioning strategies for iterative methods are needed in order to make further progress and to address increasing stiffness with increasing spatial resolution.

Integration of multiple physical effects, moving beyond interpretive simulations. [Crosscutting Secs. 5.1, 5.2, 5.3, and 5.4]. Strategies need to be formulated for integrating multiple physical effects in disruption modeling. The evolution of transients involves the various effects described in Sec. 4.1.2. Planning computation from the abstract sense of operators mapping from a domain space to a range space will help organize the complex physics and facilitate developments from applied mathematics and computer science [wp86]. The challenges include coupling the distinct domains of plasma dynamics and external electromagnetics for detailed structural geometry, coupling domains of different dimensionality for surface physics (lower dimensionality) and kinetic dynamics (higher dimensionality), and managing increased stiffness from fast radiative processes. Integrating software is another important aspect of the multiphysics simulations. Plasma simulation codes are typically implemented for standalone computation and are not amenable to integrated simulation without modification. Strategies for the long-term objectives should avoid inefficient one-off couplings that require multiple revisions over the life of the initiative. Another challenge is formulating and solving the numerical optimization and inverse problems for the multiphysics systems that describe disruptive transients. The simulations bridge vast scales and raise new mathematics-theoretical issues not apparent in traditional "single physics" problems, and the sheer size of the parameter and data space creates extraordinary computational challenges through the "curse of dimensionality."

Emerging architectures and data issues. [Crosscutting Sec. 5.1, 5.3, and 5.4]. The availability of increased computational resources may enable the application of kinetic-based computation to large-scale phenomena. Physically local processes, such as radiation, may be well suited to new accelerator technologies, effectively expanding the modeling without slowing computations. However, the reliance of implicit disruption computations on parallel algebraic software libraries, such as PETSc and Trilinos, requires their adaptation to changing hardware. Computational advances also lead to more demands for data management. Deciding what is worth the relatively high computational cost of I/O is not trivial, and analysis and data reduction conducted while computations are running will be important. Data that is saved during extreme-scale computation will likely be voluminous and require data mining and pattern recognition.

Linear stability assessment. [Crosscutting Secs. 5.2, 5.3, and 5.4]. Assessing the linear stability of axisymmetric tokamak profiles fitted to experimental measurements or produced from whole device modeling offers other opportunities for applied mathematics and computer science. Automating plasma-state reconstruction for stability computations needs to propagate errors in measurement and uncertainties from fitting to yield estimates of the uncertainties in the computed equilibria and their influence on stability. This involves the solution of stochastic inverse problems. Data management needs to consider input from a variety of experimental channels. Envisioned output includes maps of stability over parameter spaces of high dimensionality with user-useful descriptions of the results. Generating these maps requires the construction and stability assessment of many plasma states and will require high-capacity computing. Effective management of the output and highly reduced models of the findings can inform experimental controls in the near term. The long-term vision of real-time profile analysis and stability computation will have unique data-management requirements and unique needs with respect to uncertainty from data limitations.

Experimental design and data issues in disruption avoidance. [Crosscutting Secs. 5.2 and 5.3]. A fundamental objective of the profile analysis described in Sec. 4.1.4 is to determine the predictive capability of linear stability analysis for disruption avoidance. Scientific inference is central to this objective, and methods for solving numerical optimization and inverse problems along with uncertainty quantification are needed. Optimal experimental design can inform experimental campaigns of which measurements discriminate among computed results. Data that is typically ignored because of large uncertainty can be included in ways that improve the analysis. Also available are techniques for weighting input based on the specific objectives of the computations. For example, the needs for macroscopic stability computation differ from those of transport analysis, and the optimal profile fit for each may differ. The development of reduced models for experimental control will benefit from techniques for optimizing under uncertainty. In addition, new developments for profile analysis can take advantage of existing software for numerical optimization and uncertainty quantification, if it is written to provide information such as adjoints and Hessian computations.

4.1.4 Strategy and Path Forward

Solving the problem of disruption in modern tokamaks requires model development, computational infrastructure, and rigorous validation campaigns. The priority research directions proposed here encompass a range of simulation-based activities that will have spin-off benefits for all macroscopic stability studies of magnetic confinement. Contributions from applied mathematics and computer science are integral to these initiatives.

- **[PRD-Disruptions-1]** Develop integrated simulation for all stages and forms of tokamak disruption from instability through thermal and current quenches to the final deposition of energy with and without mitigation.

Considering the challenges discussed in Sec. 4.1.2, one can see that many aspects of tokamak disruption are understood at just a rudimentary level. Integrated simulation can be instrumental in addressing disruption physics, but modeling all the important aspects of disrupting discharges requires considerable extension and improvement to present capabilities. Characterizing disruptions and modeling mitigation techniques ultimately require important kinetic effects of thermal and energetic particles, radiation, neutral dynamics, plasma–surface interaction, detailed external electromagnetics, turbulent transport, and appropriate sources—orchestrated in three-dimensional time-dependent macroscopic simulations. At present, most disruption simulations use resistive-MHD modeling coupled with simplified external electromagnetics or with radiation modeling for mitigation. The proposed priority research direction is ambitious. Its aim is a form of whole device modeling with emphases that differ from those of predicting confinement. Here, the pivotal disruption-related questions involving magnetic islands, runaway electrons, open field-line currents, and mitigation define "use cases" that prioritize research activities. Critically needed will be theoretical guidance on reduced models for important effects, as well as algorithms and solvers from recent scientific computing research.

Magnetic island evolution in modern tokamaks is a multiscale, multiphysics process, and integrated simulation is required for a full description. Nonetheless, studies for this use case can start by applying scientific inference methodology to address how well standard resistive-MHD models with realistic flows, realistic geometry, and external electromagnetics describe islands in experiments. Predicting conditions that can be determined experimentally, such as the torque threshold for locking and the onset of island growth, is a high-level goal for scientific inference. Beyond the resistive-MHD basis, two-fluid computation, energetic-particle effects, and drift kinetics are either already available or emerging in macroscopic simulation codes. Smaller experiments can contribute to model validation over a range of conditions [wp70]. However, solving integrated 3D models with these effects over the timescale of island evolution in large tokamaks needs algorithmic advances to be practical. Contributions from applied mathematics and computer science will play a crucial role in achieving this. The development of improved preconditioners for the large sparse matrices that are motivated by the disparate physical processes being modeled would lead to immediate benefit. Developing suitable models of electron transport, neutral dynamics, and radiation are important for understanding thermal quench and could proceed in parallel with the efforts for island onset and locking.

Characterizing the current quench defines use cases of the physics of open field-line currents and runaway electrons. Quantifying the electromagnetic forces on conducting structures requires detailed external electromagnetics, driven by the MHD free energy of the disrupting plasma. Comprehensive prediction of the plasma response will require nonideal effects, modeling of plasma–surface interaction, neutrals, and radiation. At present the most advanced macroscopic simulation tools have been coupled only to simplified models for external electromagnetics. The TMHD model of the plasma core has received more extensive development in this regard and can potentially be applied for rapid-turnaround computations after further development and benchmarking deems this to be warranted. Coupling of macroscopic core-plasma modeling to detailed external electromagnetics can proceed in parallel. Practical models of edge plasma dynamics and plasma–surface interaction need to be developed in collaboration with theory and the edge simulation activities.

Self-consistent investigation of runaway electrons requires kinetic modeling of the fast electron population and a focus on thermal quench physics, including bulk electron thermal transport and impurity radiation. Numerical models that have been applied for fast-ion kinetics provide a starting point for modeling runaway electrons, but long-timescale nonlinear simulation will benefit from improvements in the algorithms and implementations. Theoretical developments in scattering and synchrotron radiation are needed to guide the computational modeling. Emerging capabilities for electron drift kinetics and neutral dynamics can contribute to thermal transport modeling if supported by computational advances. The developments for radiation and neutral modeling will also enable a use case on density-limit disruptions.

Engineering a reliable mitigation system is an important use case for integrated simulation. Modeling based on resistive-MHD coupled to impurity radiation is making contributions to understanding the mixing processes. Validation is far from complete, however, and is identifying limitations of the simulations. Ideally, integrated mitigation simulation includes all impurity dynamics, and the effects of mitigation strategies can be tested in the various disruption scenarios. It can also be used to judge the benefits or harm of different mitigation strategies on thermal quench, current quench, and runaway electron generation. Like the other use cases, mitigation studies will proceed with increasingly detailed models, but ultimately they require the greatest extent of integration.

- **[PRD-Disruptions-2]** Develop an automated plasma state reconstruction and stability assessment system with the goal of facilitating disruption avoidance.

A priority research direction focusing on 2D equilibrium reconstruction and linear macroscopic stability will benefit all aspects of disruption modeling, including avoidance, prediction, characterization, and mitigation. Practical approaches for avoidance test the linear stability of 2D equilibria, and the reliability of a prediction depends sensitively on the fidelity of the equilibrium. At present, including kinetic information (thermal and flow) and weighting data according to its quality are painstaking processes that are often accomplished by hand. In some cases, critical information is supplied through transport analysis. Developing software that reliably automates these aspects of reconstruction and assesses uncertainties will boost macroscopic stability computation in general. It will facilitate assessing the value of linear macroscopic stability for predicting disruption, which would be too time-consuming by current means. Some efforts in this direction are already under way; coordinating and extending the efforts will provide a basis for this PRD. More reliable initial conditions for nonlinear time-dependent computation will be another benefit. Automated reconstruction will also provide a necessary step toward real-time processing. Enhancing and modernizing linear stability computations are a complementary part of this initiative. The importance of including flow, kinetic, and two-fluid effects in macroscopic linear stability computations is gaining increasing appreciation. Computational performance improvement, including parallel computation of legacy applications, will be necessary for validation and for possible real-time applications.

Disruption prediction and avoidance are the primary goal of a profile stability analysis system. A validated macroscopic stability capability could potentially be used during the operational planning of tokamak discharges for all configurations, from startup through shutdown. Coupling to transport computations will inform whole device modeling about macroscopic stability limitations. One strategy for avoiding instability is to generate stability and response maps for discharges. This will need profiles and stability computations over a sufficiently large part of the multidimensional parameter space near planned trajectories to inform feedback systems of which corrective steps are safe. A crucial element of this strategy is the provision of sufficient capacity computing.

Control through real-time reconstruction and stability analysis is another possible use case that can drive development. Parallel implementation of fast asymptotic stability methods is tractable. However, the feasibility of real-time analysis depends on many physical, computational, and technical factors and on their reliability when assembled into a control system.

- **[PRD-Disruptions-3]** Verify and validate linear and nonlinear computational models in order to establish confidence in the prediction and understanding of tokamak disruption physics with and without mitigation.

Magnetically confined plasma is a physically complex system that is sensitive to coil currents, sources of heat and current, and the conditioning of surfaces. The integrated macroscopic simulation described in the first priority research direction necessarily involves reduced models, and the knowledge of conditions in experiments is not precise. The methodology of validation provides a standard by which our models, and hence our understanding of macroscopic dynamics, can be judged. It will also help avoid pitfalls from uncertainties in input and laboratory data. Although validation activities for macroscopic dynamics are under way, the benefits of bringing validation methodology to disruption modeling justifies a separate initiative. Topics for validation include all areas of disruption modeling; but application to linear and nonlinear stability, magnetic penetration and island locking, RE dynamics, and mitigation have particular significance.

Many disruptions are attributed to loss of macroscopic stability, but the reliability of using the linear stability of 2D equilibria as a basis for predicting disruption has not been validated. A concerted effort is needed to assess how well linear stability computations account for disruptive instabilities over a broad range of conditions. For nonlinearly unstable NTMs, quantifying uncertainties in conditions at onset can help identify which seeding effects are most important for nonlinearly unstable islands. These studies can proceed with existing experimental data and in collaboration with new experiments. The sensitivity of the models to uncertainties in experimental measurements needs to be quantified. Implications for the feasibility of avoidance through operational planning would be an important outcome of this study. The concept of probability-based disruption forecasting is also testable through linear stability validation.

The prevalence of locking and magnetic-island effects in disruptions deserves focused effort. The ability to compute quantitative estimates of torque and rotation thresholds for both the penetration of static error fields and the birth of rotating islands should be demonstrated computationally and validated against experimental data. When asymmetry results from instability, validation studies must consider nonlinear modeling to quantify effects on transport. Linear modeling of the plasma response may be appropriate, however, when the external field drives asymmetry; validation will quantify its limitations. In either case, neoclassical and turbulent transport should be calculated in the perturbed non-axisymmetric magnetic geometry, as well as the electromagnetic torque due to the interaction of the non-axisymmetric fields with external conducting structures.

Mitigation systems in ITER and future tokamak experiments must be reliable in order to prevent catastrophic losses in instances when disruption is not avoided. Here, the value of a rigorous engineering-level validation of mitigation simulation is most apparent. Present work focuses on the extent and underlying influences of radiation symmetry with massive-gas injection. Modeling that represents the shattered-pellet approach will need validation in order to understand its penetration and radiation symmetry under a variety of conditions.

The path forward for integrated disruption simulations should include all three priority research directions. While activities associated with each exist today, the initiatives will call attention to them, launch new development and validation campaigns, and provide clear aims for macroscopic modeling research over the coming decade.

4.2 Plasma Boundary

Much of the challenge of the practical realization of fusion energy plays out in the boundary region, where the confined plasma, hotter than the core of the sun, must cool dramatically as it moves outward and eventually contacts the surrounding material wall. The boundary encompasses three zones: (1) the hot, confined edge pedestal plasma, a region with sharp gradients that has a profound influence on global fusion performance; (2) the cooler scrape-off layer (including the remote divertor) plasma, where magnetic field lines begin to intersect the wall, which must maintain the distribution of heat flux to these surfaces to be within material limits, while also shielding the core from sputtered impurities; and (3) the wall itself, which must withstand intense plasma bombardment. Each zone covers a broad range of length and temporal scales and complex, interlinked physics processes. For example, microturbulence and larger-scale transient events drive energy losses through this strongly inhomogeneous plasma region, ultimately leading to ejection of 3D plasma filaments to the walls. In addition, plasma and neutron fluxes to the walls can create trapping sites within the material that hinder recovery of tritium and can also change the surface structure, resulting in modified sputtering rates and heat conductivity.

4.2.1 Background and Recent Progress

Realizing the promise of controlled fusion requires attainment of conditions that are in some respects more extreme even than those in the core of the sun. The challenge of achieving these conditions is felt most acutely in the boundary region, where a transition occurs between the fusion plasma, far hotter than the core of the sun, and the material surfaces, which must be kept from melting and protected from excessive erosion. This boundary region begins with the outermost region of the confined plasma, which in high-performance ("H-mode") plasmas is referred to as the "pedestal" because the very sharp plasma pressure gradients in this region appear to be "lifting" up the core pressure profiles as if they were sitting on a pedestal as shown in Fig. 15. Moving outward, the pedestal plasma connects to the SOL plasma, which is an unconfined plasma layer where the magnetic field lines are open and intersect material surfaces. The equilibrium magnetic field is often structured such that the near-pedestal SOL plasma enters into a region more remote, known as the divertor, where the plasma cools and density increases before contacting material surfaces. These surfaces are termed the divertor plates and walls [Fig. 15(a)], which are collectively known as plasma facing components. Peak plasma heat fluxes at the divertor plates can exceed 10 $\mathrm{MW/m^2}$, comparable to that in arc welding and higher than that on the space shuttle during reentry, illustrating one of the materials science challenges presented by fusion devices.

While the boundary region provides a number of critical functions for a fusion device, the development of predictive simulation models is challenged by its rich combination of multiscale and multicomponent physics interactions. In order to enable both high fusion performance and long material lifetimes, the temperature must transition from $\sim 10^3$ ℃ in the material surfaces (to avoid melting) to $\sim 10^4$ ℃ in the plasma near the wall (to avoid excessive erosion), up to $\sim 10^6$ ℃ at the pedestal-SOL interface, and finally to $\sim 3 \times 10^7$ ℃ at the top of the pedestal (to provide conditions required by the core region to produce high fusion power density). In addition to the dramatic temperature variation, the boundary is characterized by steep gradients in other plasma and neutral atom equilibrium quantities such as density, pressure, and current density. These variations lead to various complications for model development beyond that used for core simulations, including (1) rapidly changing particle collisionalities that range from the long mean-free-path kinetic regime at the inner pedestal, moderately collisional at the magnetic separatrix, and in the strongly collisional fluid regime in the SOL-divertor region, and (2) short equilibrium

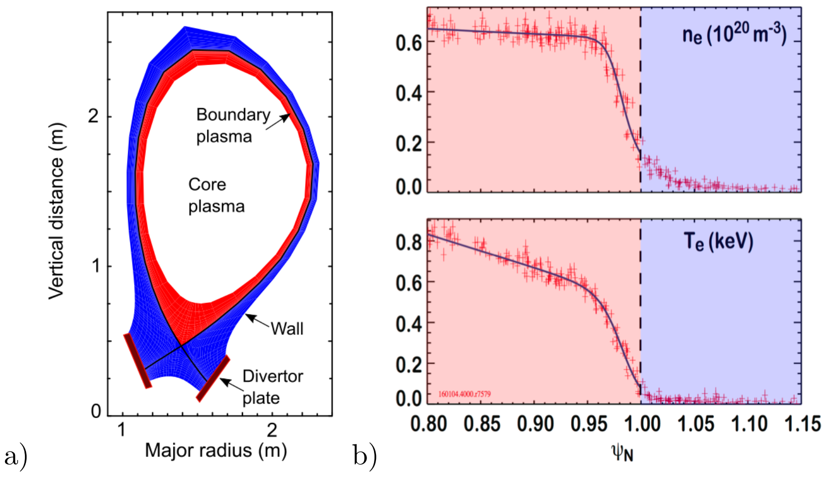


Figure 15: *(a) Poloidal cross-section of a tokamak illustrating the 3 zones of the boundary region: the pedestal plasma (red), the scrape-off layer plasma (blue), and the surrounding material wall and divertor plates. The transition between these zones is determined by the magnetic separatrix (black line). (b) Midplane profiles of electron density and temperature from a DIII-D discharge versus normalized poloidal flux with unity being the separatrix between the pedestal and SOL zones.*

profile scale lengths that can overlap with the length scales characteristic of plasma turbulence and particle drift orbits. Indeed the range of spatiotemporal scales in the boundary is so broad, as shown in Fig. 16, that comprehensive boundary simulations present a formidable challenge to theory and computational techniques. Furthermore, the particle and energy fluxes to the wall are large enough to substantially alter the material structure, bringing in even smaller temporal and spatial material scales to be modeled. Enhanced simulation of this range of processes leads to computational requirements that would greatly benefit from exascale computation. Furthermore, while numerous issues can be identified locally within the pedestal, SOL, or PFCs, the compact radial extent of the boundary region results in strongly coupled interactions. Simulation progress for each of the three zones is discussed in turn, followed by progress in integration.

Pedestal. High-performance operation in tokamaks is achieved by the spontaneous formation of the pedestal in the outer few percent of the confined plasma. This edge transport barrier strongly improves global energy confinement and generally improves global stability, resulting in dramatically enhanced fusion performance and the potential for more cost-effective fusion reactors. However, the large pressure gradient and the resulting bootstrap current (a toroidal current driven by the steep gradient) in the pedestal can drive instabilities called ELMs, which periodically eject impulsive heat and particle loads into the SOL that then impact the PFCs in localized regions that may reduce component lifetimes in reactor-scale devices. A predictive understanding of pedestal formation and structure, as well as the physics of ELMs and their mitigation, is essential for prediction and numerical optimization of the fusion performance of ITER and future reactors. A key goal is to achieve a robust and very high-pressure pedestal in order to enable high fusion reactivity in the core (fusion energy is predicted to scale roughly as the square of the plasma pedestal pressure), while minimizing the impact of transients such as ELMs on the PFCs.

Two principal challenges in understanding the physics of the pedestal (and SOL) region are the wide range of overlapping spatiotemporal scales, shown in Fig. 16, and the breadth of physical processes involved. Despite these challenges, substantial progress has been made in the past few

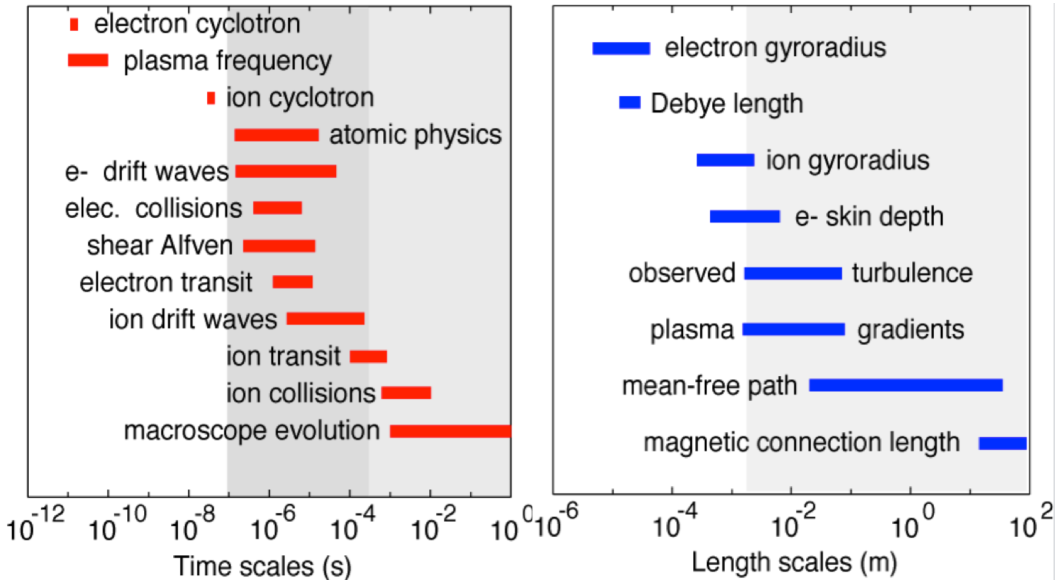


Figure 16: *Length scales and timescales for the pedestal region. The ranges shown are for a typical plasma on the DIII-D tokamak during a given discharge, indicating the wide range of overlapping physical scales. In the SOL divertor region, the collision times become much shorter than shown because of an increase in density and reduction in temperature (see Fig. 19).*

years. Much of this progress is summarized in a 2013 review paper, describing a U.S. DOE joint research target on understanding pedestal physics [46,47], as well as in more recent publications and several community white papers noted in the remainder of this paragraph. Because of the importance of the bootstrap current as well as neoclassical (i.e., collisional, in the presence of drift orbits) ion heat transport, very high-accuracy neoclassical codes have been developed, including the full collision operator, accounting for the effects of impurities. These include both closed-field line solvers such as NEO, which are highly efficient and have been used extensively in integrated workflows, and XGC0/XGCa [wp40,wp82] and COGENT [wp28], which cross the separatrix and can study the effects of ion orbit loss to divertor plates. Gyrokinetic (GK) codes originally developed for core studies (e.g., GS2, GYRO, GENE, GEM, GTC) have been applied to study microinstabilities in the closed field-line pedestal region with increasing physics capabilities [wp41,wp42,wp46,wp58,wp 82]. In addition, a new electromagnetic GK code, CGYRO, has been developed to enable precise calculation of collisional effects that become important in the pedestal region; and electrostatic turbulence has been studied with the XGC1 code [wp40,wp82], which includes both pedestal and SOL.

Magnetohydrodynamic (MHD) stability codes such as ELITE and MISHKA, are routinely used to evaluate the stability of the pedestal to peeling-ballooning modes, which are intermediate wavelength instabilities driven by current and pressure gradients that constrain the pedestal pressure and drive both ELMs and the edge harmonic oscillation (EHO) found in quiescent H-mode discharges. Extended MHD codes such as BOUT++, NIMROD, M3D-C1, and JOREK have been used to study nonideal effects on peeling-ballooning modes and to study ELM dynamics [wp6,wp118]; and kinetic effects have been added in some cases by using gyrofluid methods [wp118]. An example of an ELM simulation from BOUT++ is shown in Fig. 17. MHD codes have also revealed the importance of accounting for the overlap of mode and equilibrium scales, which causes effects such as the kink term (associated with the current gradient) to be important even for very high toroidal mode

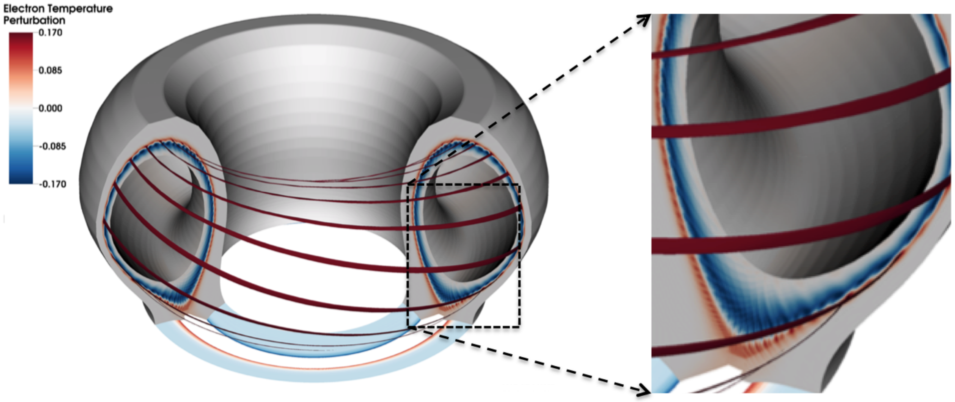


Figure 17: *BOUT++ simulation of 3D nonlinear ELM structure showing the perturbation to the electron temperature. Expanded view shows structure on both sides of the separatrix and in the divertor region with heat flux on the divertor plate.*

numbers, revealing the need for computational tools that can account for both kinetic effects and strong variation of the equilibrium. Nonaxisymmetric variations in the equilibrium magnetic field, sometimes referred to as resonant magnetic perturbations (RMPs), are also seen to have important effects on transport and stability.

A predictive model for the pedestal structure, EPED, has been developed by combining insight from both MHD and GK calculations. The model posits that the pedestal is finally constrained by a combination of transport from kinetic ballooning modes and longer wavelength ELMs or harmonic oscillations caused by peeling-ballooning modes. Combining these two constraints enables prediction of the pedestal height (pressure, or temperature at given density) and width, which can be compared with measurements, as has been done in more than 700 cases on five tokamaks, typically finding agreement to standard deviation ∼0.2-0.25 (Fig. 18). In recent work, EPED has been coupled to core transport models via the OMFIT/IPS framework to enable study of core-pedestal coupling [wp73,wp100,wp102]. However, EPED has not yet been coupled to SOL physics; and both pedestal density and impurity content are taken as inputs, rather than computed self-consistently via pedestal-SOL-PFC integration.

SOL. The SOL region plays two major roles: (1) it determines the distribution of escaping core plasma particles, momentum, and heat to PFCs where the peak heat flux, sputtering rate, fueling, and helium ash removal are major issues; and (2) it shields the pedestal/core plasma from the wall impurities generated by sputtering and dust mobilization and controls the penetration of wall-recycled neutral particles that help fuel the core. For this discussion, the SOL includes the divertor region, which is more remote from the pedestal than the midplane SOL. The neutral gas in the SOL arises primarily from recycling of the fuel particles stored in the walls. While the plasma heat striking the walls is removed to heat sinks via conduction, the DT (deuterium/tritium fuel) plasma particles build up within the material as a neutral gas until a steady state is reached with neutral DT gas being released (recycled) into the SOL at the same rate as DT ions strike the wall. The escaping gas is then reionized in the SOL or pedestal. In order to maintain the proper DT mixture, separate fuel of D and T is required, as well as the pumping of some of the DT along with the helium produced by the DT fusion reaction. The D/T/He exhaust plasma fluxes are generally guided along the open magnetic fields to a specially designed section of the wall known as the divertor through

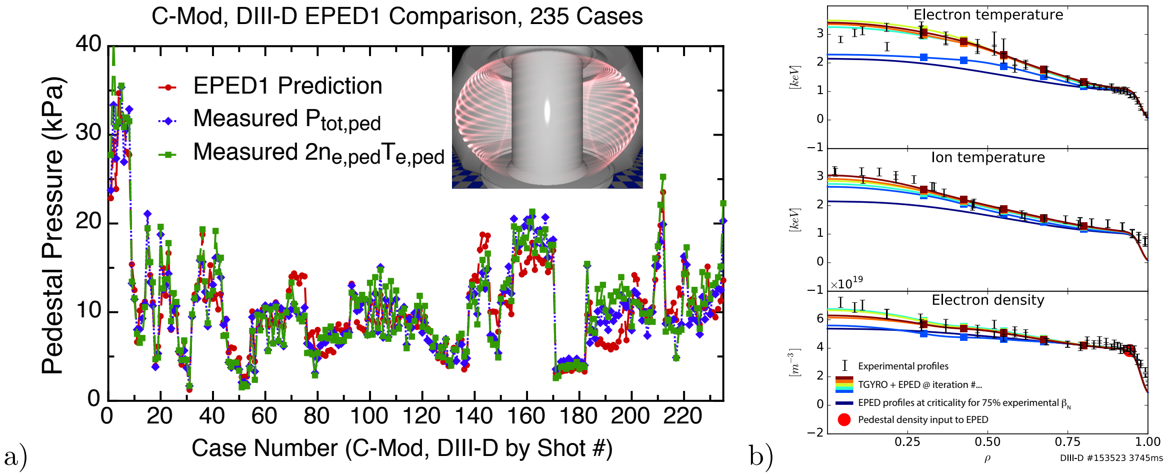


Figure 18: *(a) EPED model predictions of the pedestal pressure are compared with measurements from the Alcator C-Mod and DIII-D tokamaks in 235 cases. More than 150,000 peeling-ballooning calculations were required for these predictions, and a sample mode structure is inset. (b) Combining EPED pedestal predictions with predictions of core turbulent and neoclassical transport has enabled initial predictions of profiles across the core and pedestal and studies of core-pedestal interaction. The example shown is from an ITER-like plasma in the DIII-D tokamak.*

adjustments to magnetic coil currents. In contrast, energy loss by neutron and line-radiation fluxes is broadly distributed to surrounding walls. A central issue for magnetic fusion devices is to operate them such that the steady-state peak heat flux to the divertor material surface does not exceed $\sim$10 MWm^{-2}. This requirement is expected to be challenging for ITER and a major concern for future higher-power devices. Possible methods for managing the heat load include detached plasma divertors and alternative magnetic configurations (see Sec. 4.2.4). Transient heat loads from ELMs are also an issue; in order to avoid surface melting or vaporization, the energy flux striking the wall must be less than $S_E \sim 40\tau_L^{1/2}$ (MJ m^{-2} s$^{1/2}$), where τ_L is the time for the energy to travel through the SOL to the material surface.

Since the ReNeW report in 2009, numerous advances have been made in simulations of the SOL region. Focusing first on plasma transport, the experimentally observed 3D filamentary "blob" transport can now be simulated with a reduced 2D macro-blob model and is combined with the 2D UEDGE plasma/neutral transport code to form UEDGE-MB. This model has been applied to present-day devices, showing significant differences from the previous simple convection-only 2D blob filament model. The OEDGE model is used in an interpretive mode where it utilizes as much experimental data as possible to constrain the simulation and then predicts processes such as neutral penetration to the core and impurity radiation. A coupled fluid plasma and Monte Carlo neutrals model available in the SOLPS code has been used to model divertor experiments and the proposed innovative divertor configuration Super-X. Similarly, UEDGE, with a coupled fluid-neutral model, has also been used to model present-day divertor experiments as shown in Fig. 19, where the large increase in DIII-D divertor density shown arises from strong plate recycling and is accompanied by a reduction in the electron temperature to $\sim$1 eV. UEDGE has now been upgraded to include the multiple nearby magnetic X-points in the divertor region known as a Snowflake configuration. The Snowflake and Super-X divertors are examples of ongoing innovation to spread the peak heat flux on divertor surfaces to an acceptable level.

In further model development, a parallel 2D plasma/neutral version of UEDGE has been de-

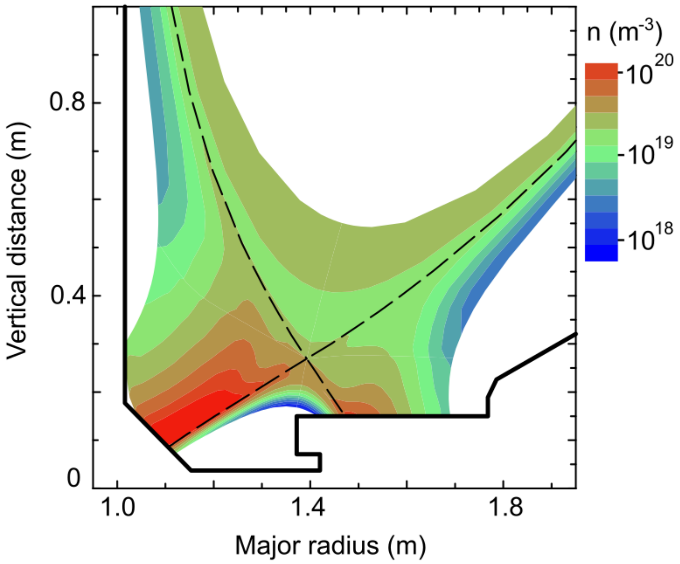


Figure 19: *Ion density in the divertor region from UEDGE fluid simulation showing a ten-fold increase in plate density compared with midplane density. The separatrix (dashed line) strikes the raised baffle to facilitate comparison with divertor Thomson scattering data giving $T_e \sim 1$ eV near the plate. Image courtesy of G. D. Porter, LLNL.*

veloped through collaborative research within the FACETS SciDAC project. A new Landau-fluid closure has been formulated and implemented in UEDGE for kinetic parallel electron transport. The 3D Monte Carlo transport model EMC3-Eirene for the main fuel plasma and neutrals has begun to be applied in order to understand the impact of applied 3D magnetic perturbations (for ELM stabilization) on the SOL plasma [wp59,wp68]. Drift-kinetic and gyrokinetic plasma models have been developed that can now span the separatrix and have been applied to explain the non-Maxwellian character of the midplane ions via XGC PIC codes developed under the EPSI/CPES SciDAC project and via a counterpart continuum code COGENT developed through the collaborative ESL project. Kinetic code simulations that include both the pedestal and SOL are illustrated in Fig. 20. The inclusion of electrostatic turbulence in XGC1 is discussed in the next paragraph. PIC simulations of the plasma sheath with VPIC have resulted in improved energy transmission coefficients as part of the PSI SciDAC project.

Advances in turbulence modeling capability (including the magnetic separatrix region) include the 2D SOLT code [wp77] applied to several U.S. tokamaks and the 3D electromagnetic fluid code BOUT++ applied to DIII-D discharges with approximate experimental features reproduced for a specific discharge. BOUT++ has also been used to analyze the breakup of ejected plasma filaments owing to secondary instabilities and to begin direct comparison with experimental diagnostics of near-separatrix turbulence. BOUT++ has recently been generalized to include kinetic effects of finite ion Larmor radius and Landau damping along the magnetic field [wp118]. Also, 3D electrostatic turbulence has been included in kinetic XGC1 PIC simulations (see Fig. 20b) to begin to analyze the divertor heat-flux width problem as discussed in more detail in the Integration subsection (page 51). Continuum codes have not had as much development effort but should also be able to do this problem, probably within 3–5 years at the current development rate with similar levels of physics (or with more complete physics sooner with additional resources)[wp28,wp41]. The fluid code shows good scaling to ~50,000 processors, and GK PIC and continuum/Eulerian codes

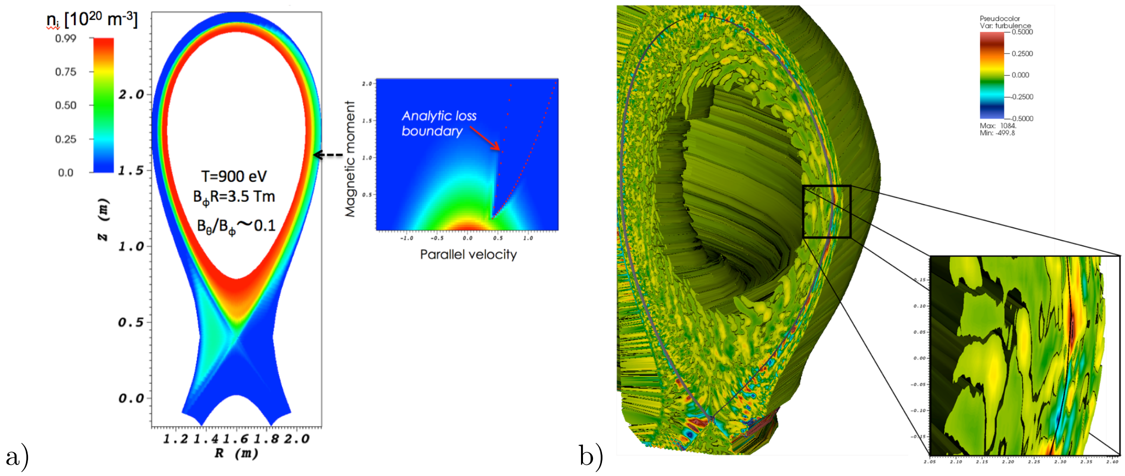


Figure 20: *(a) COGENT 4D (2r,2v) kinetic simulation showing ion density and velocity-space loss cone for an initial uniform Maxwellian distribution function after 1.2 ms; magnetic mirror-trapped ions in SOL and loss cone are substantially reduced when the full collision model is turned on (not shown). (b) Contours of turbulent electrostatic potential from an XGC1 5D (3r,2v) gyrokinetic simulation that spans the pedestal and SOL in DIII-D magnetic geometry. A black line indicates the magnetic separatrix. The enlarged outer-midplane box-view shows large amplitude fluctuations near the separatrix and in the SOL, together with ExB-flow shearing of turbulence in the pedestal.*

are most likely to be scalable to exascale.

PMI. The wall material must be able to withstand high heat flux and ion flux while avoiding excessive wall inventory of tritium. For efficient heat removal to a cooled substrate, the PFC should be thin so as to increase the conductive heat flow. The plasma, however, also causes erosion of this thin material by sputtering. In order to ensure adequate PFC lifetime, plasma conditions must be achieved that ensure that the majority of the sputtered material is ionized close to the surface and redeposited nearby. In a steady-state reactor, this process will result in surfaces that are dominated by the redeposited layers, which have currently unknown properties (e.g., thermal conductivity). The self-consistent generation of this continually eroding and depositing surface layer and the properties of the redeposited material must be understood and characterized, including that of mixed materials as in ITER where the divertor will be tungsten and the main chamber wall beryllium. The wide variety of processes that can occur within the near-surface material is illustrated in Fig. 21.

The material can retain deuterium and tritium fuel, and the tritium inventory in particular needs to be kept low for regulatory/safety and cost reasons. Periodic removal of tritium may be possible, but many layers of the PFC can become damaged by redeposition and internally by high-energy ions/neutrals and neutrons. Similarly, helium entering the PFC (e.g., tungsten) can cause blistering of the surface and/or the growth of "fuzz" structures (microsized tendrils of tungsten) in certain surface temperature ranges that may degrade the conductivity of the material and/or lead to enhanced generation of impurities that could penetrate through the SOL to the pedestal and core. The timescales and length scales of the processes governing material evolution in response to plasma/radiation damage span several orders of magnitude and can, in some cases, overlap with the scales of the near-surface plasma, presenting a challenge for the coupling of wall evolution to plasma models [wp107].

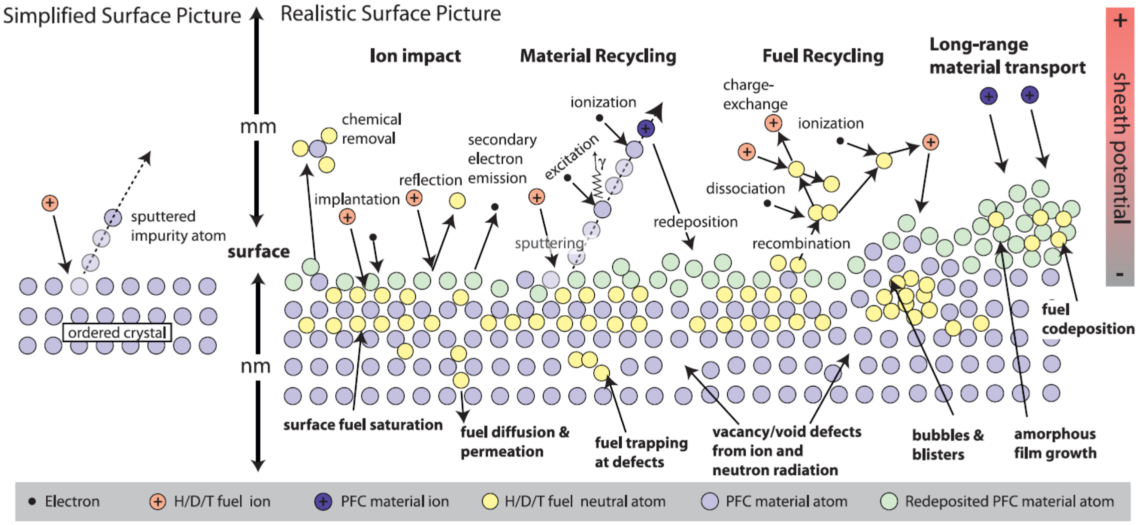


Figure 21: *Comparison of a simplified plasma/surface model where only sputtering occurs (left) with a realistic model (right) where many types of interactions occur within the material during bombardment by a fusion plasma. From B. Wirth et al. [48].*

Over the past three years, the PSI SciDAC project has performed many simulations of molecular dynamics (MD) and accelerated molecular dynamics (which utilizes methods for enhancing sampling rates of particle-lattice interactions simulations). Both methods study materials processes at the atomic scale, with the aim of exploring the behavior of helium and hydrogen in tungsten, as input to and benchmarks for larger-scale simulations and as investigations of mechanisms of material deformation relevant on the appropriate spatial and temporal scales. An example of such an MD simulation is shown in Fig. 22. Of particular interest is the development of helium bubbles of different sizes. These results are used to parameterize the much faster continuum model Xolotl, which can then follow the bubble evolution over longer timescales. Other base-program work has advanced the simulation application and capabilities. The WBC/REDEP Monte Carlo ion code has successfully modeled experiments of tungsten erosion/redeposition on the DiMES probe in the DIII-D tokamak. More recently, the similar ERO code has been used for such studies. Simulations of the surface melting processes, including vapor shielding for large transient heat fluxes, have been studied with the integrated plasma/neutral/material HEIGHTS code [wp97].

Integration. Because of the close connection between the various zones of the boundary, a number of simulations have included two or more of these domains simultaneously. Many of these codes are mentioned briefly in the SOL subsection but are highlighted again here for their integration features. Edge plasma transport codes (2D [SOLPS and UEDGE] and 3D [EMC3-Eirene] provide integrated models of the pedestal and SOL, while coupling to the wall is generally through boundary conditions to describe particle recycling and sputtering of impurities [wp68]. These simulations generally target steady-state solutions in which the balance of particle fueling and pumping results in long timescales (∼0.1 s). The 4D (2r,2v) PIC drift kinetic code XGC0 (EPSI/CPES SciDAC project), coupled to the DEGAS 2 Monte Carlo neutral code, has also been used to compute plasma profiles including the pedestal and SOL, although for a considerably shorter time than the fueling/pumping equilibrium. Generally, these transport-only simulations use ad hoc turbulent cross-field transport coefficients, thus presenting a clear opportunity for future advancements.

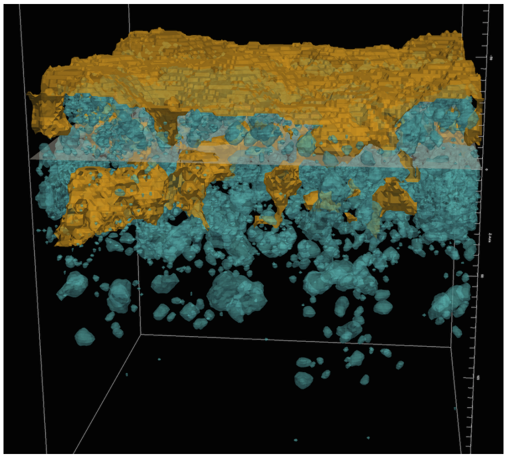


Figure 22: *Visualization of a molecular dynamics simulation of a tungsten* ($100\ m^2$) *surface exposed to 100 eV helium plasma for* ~ 285 *ns, corresponding to a fluence of* $\Phi = 4.7 \times 10^{21}\ m^{-2}$*, at a normal-incidence helium flux* $\Gamma = 1.6 \times 10^{28}\ m^{-2} s^{-1}$*. Bluish surfaces are helium bubbles; yellow surfaces are empty spaces and/or represent the external surface at this point in time. The white plane corresponds to the original surface. Image courtesy of K. Hammond (Univ. of Missouri).*

Turbulence simulations that encompass the pedestal and SOL have been performed by 3D fluid plasma codes such as BOUT++ with electromagnetic fields and show the characteristic strong, intermittent plasma filaments (or "blobs") being born near the separatrix and then moving into the SOL. Such models, even with kinetic corrections, need to be compared with gyrokinetic simulations deep in the pedestal where kinetic effects are likely stronger. Recently, GK simulations of the pedestal/SOL electrostatic turbulence including neutrals have been performed by XGC1 (see Fig. 20) [wp82] solving for electrostatic turbulence; these simulations need to be extended to electromagnetic fields. The results report a scaling of the heat-flux width on the divertor plate with the poloidal magnetic field similar to experimental data for attached plasmas. Improved mesh resolution and extended simulations times are needed.

Other advances in coupling include the time-dependent 2D fluid UEDGE code (pedestal + SOL plasma and neutrals) with a version of the continuum WallPSI code that describes the uptake and release of neutral gas during an ELM pulse; the results show how such time-varying gas inventory impacts the rebuilding of the pedestal plasma after the pulse. Also, coupled simulations of tungsten dust-particle trajectories through the plasma have been computed with DUSTT to UEDGE transport, where the plasma electrons ablate the dust, thus generating an additional impurity source in the SOL beyond wall sputtering [wp98].

4.2.2 Challenges and Opportunities

As in the previous section, each of the three boundary zones is discussed in turn, followed by major integration issues.

Pedestal. The pedestal presents a set of challenges to traditional theoretical and computational methods. Because the plasma pressure varies by 1–2 orders of magnitude across the pedestal and because the density, temperature, flow velocity, radial electric field and current also vary substantially, a wide range of key dimensionless parameters is encompassed in this narrow region. The pedestal plasma typically transitions from being almost collisionless near the top of the pedestal to being strongly collisional at the bottom, requiring methods appropriate for both regimes. More fundamentally, the broad range and overlap of spatiotemporal scales across the pedestal challenge the assumed separation of equilibrium ("macro") and turbulence ("micro") scales upon which much existing theory and computation rely, and thus extensions of basic theory and substantial computational resources are expected to be needed. For example, across a single pedestal, the timescales associated with electron drift waves span a wide range (because of the wide variation of equilibrium quantities), which overlaps with the wide range of temporal scales associated with Alfvén waves, which in turn overlaps with ion drift wave and ion transit temporal scales, which in turn can overlap with the fast timescales on which the equilibrium itself is observed to evolve, for example during an ELM. The range of overlapping temporal scales often exceeds six orders of magnitude. A similar overlap is found in physically relevant spatial scales, where the gyroradius and ion drift wave scales can overlap the short gradient-scale lengths. Simple estimates indicate that treating this full range of scales could utilize exascale computing resources, provided that efficient, scalable algorithms can be developed and tuned for next-generation machines.

Despite these challenges, substantial recent progress in development of numerical tools and physics understanding has laid a strong foundation to build on. Critical problems that can be addressed include the following.

(a) Electron-scale turbulent transport: Turbulence driven by electron-drift-scale instabilities such as the electron temperature gradient mode is expected to drive significant transport in the pedestal region. Because electron drift scales are in many cases well separated from equilibrium scales, significant progress should be possible by employing existing electromagnetic gyrokinetic codes with realistic collision operators and geometry to characterize such turbulence, verify nonlinear code results, and validate results against measurements from turbulence diagnostics. To simulate the entire pedestal region as a series of local simulations would require substantial HPC resources.

(b) Improved pedestal structure models: Existing pedestal structure models calculate constraints on the pressure and pressure gradient and use the pedestal density and impurity concentration as inputs. Natural extensions of such models could take advantage of results from (a), and eventually (c) below, either directly calculating, or using a reduced model including collisional neoclassical transport to predict density and temperature profiles across the pedestal region where separatrix values are used as boundary conditions. Including the physics of neutral particle sources from recycled particles and/or gas puffs that reach into the pedestal also is important. This would enable coupling to the SOL, as described below, and eventually coupling to the PFCs as well, which will be needed for determining impurity sources.

(c) Ion/Alfvén-scale turbulence: Because ion-drift scales can strongly overlap with equilibrium scales in the pedestal, treating ion-scale turbulence, driven by modes such as the kinetic ballooning mode and the ion-temperature gradient mode, fully quantitatively presents significant challenges. MHD studies indicate that equilibrium-scale terms, such as the kink term, contribute significantly to mode stability, even at the very high toroidal mode numbers expected for the peak of the turbulent spectrum. Significant code development, verification, and validation effort are needed to assess and improve the capabilities of existing and new gyrokinetic and gyrofluid codes in order to accurately capture the full range of relevant physics. Additional work on developing and implementing new gyrokinetic formulations may be needed. Developing this capability will further enable quantitative assessment of ion and Alfvén-scale turbulent transport across the pedestal.

(d) Interaction of electron and ion scales: Once the capabilities of (a) and (c) are developed, additional computational resources can be engaged to study the interaction of electron and ion scales; a wide range of such interactions involving zonal flow dynamics and turbulent cascades is seen in electron- and ion-scale core simulations. Because of the wide variation of the electron and ion scales across the pedestal, treating the full range of these scales across the full radial domain of the pedestal will require enormous computational resources, likely exascale.

(e) Dynamic evolution of pedestal profiles: Extending turbulence simulations to longer timescales and coupling them to transport codes having particle and energy sources should enable studies of the full dynamic evolution of the pedestal profiles between transient events.

(f) ELM and EHO dynamics: Further study is needed of the nonlinear dynamics of peeling-ballooning modes, including the impact of rotation, and kinetic effects, with a focus on understanding the physics determining whether the mode saturates (e.g., forms an EHO) or bursts as an ELM. Detailed dynamics and ELM transport will require coupling to the SOL and PFC as discussed below.

(g) 3D effects: Resonant magnetic perturbations induced by external 3D coils can suppress or mitigate ELMs. Existing codes calculate the plasma response to imposed RMPs and aspects of 3D neoclassical transport. Incorporating 3D effects in electromagnetic gyrokinetic simulations may be needed in order to develop a predictive understanding of ELM suppression and density modification by RMPs. This work is expected to further increase computational resource requirements.

(h) Pedestal formation: Studying formation of the pedestal (also known as the L-H transition) and its dependence on source power, rotation, ion orbit loss, and other key physics is likely to require cross-separatrix kinetic codes able to reproduce first L-mode turbulence and then its suppression via electric field shear or other effects. Also of interest are studies of partial transitions, such as the I-mode state, where a temperature pedestal forms without a density pedestal.

A common thread across many of these key problems is the need for comprehensive electromagnetic gyrokinetic (or, if need be, 6D kinetic) simulations, which incorporate electron, Alfvén, and ion scales, and strong coupling to equilibrium scales. Significant physics extensions of existing codes, or development of new codes that incorporate all these features, as well as improvements in numerical algorithms and scaling, should enable comprehensive, high-fidelity studies of the pedestal.

SOL. The SOL has a number of characteristics that are especially challenging for both theory and simulation. Among these features are large-amplitude turbulent structures even in the absence of ELMs, strong plasma and neutral variations along the magnetic field line and sometimes toroidally (adding one or two transport dimensions compared with core modeling), changes from moderate collisionality to strong collisionality, strongly radiating impurity components, and long equilibrium timescales associated with particle fueling and pumping. All these complexities will benefit greatly from enhanced computational resources that extend to exascale. Critical problems to be addressed for the SOL include the following.

(a) Plasma scale-lengths across the separatrix: What determines the plasma scale-lengths across the separatrix is a key question directly impacting the width of the divertor heat-flux profile. Observations of plasma turbulence indicates that near the separatrix, fluctuation amplitudes become especially large and form filamentary, outward propagating structures, loosely referred to as “blobs.” A central issue to be addressed by nonlinear electromagnetic simulations is the mechanism and scaling of microturbulent filament production and how this process contributes to the determination of the radial density and temperature scale lengths near the separatrix. Fluid codes have shown good scaling to ~50,000 processors, and gyrokinetic PIC and continuum/Eulerian codes can essentially use the full capacity of Titan at ORNL and thus are most likely to be scalable to exascale. As in all extensions to exascale, possible changes in programming models will need to be considered. Such studies should also include the effect of ionization of recycled neutral gas as a source of plasma.

(b) Propagation of plasma filaments: Plasma transport in the SOL is dominated by 3D filaments, both large-amplitude, long-toroidal-wavelength ELMs and smaller, more numerous filaments that contribute substantially to the energy loss between or in the absence of ELMs. How these structures propagate through the SOL and get deposited on PFCs determines the local steady-state heat-flux load. Such transport is inherently 3D and is believed to dominantly follow the static magnetic field lines, but small changes to the magnetic field and spreading across fields lines both may be important.

(c) Long-timescale transport simulations: The 2D and 3D transport models used for long-timescale (~1 s) SOL simulations [wp68] combine plasma, neutral, and impurity species, and most have some description of the pedestal. Kinetic transport models are beginning to address a similar range of physical processes but currently on a much shorter timescale (1–10 ms). Owing to their dimensionality, most implementations are not expected to directly utilize extreme computing, but they should be important components for whole device models. The opportunity here is to upgrade the radial turbulence transport models, which could be done by coupling to turbulence simulations or distilling reduced models of such transport by parameterizing a large number of turbulence simulations.

(d) Impurity transport through the SOL: The SOL serves as a filter to reduce the influx of sputtered wall impurities that can reach the pedestal region and beyond into the core. Traditional transport models simply use convective/diffusive operators to describe how impurity ions might reach the pedestal. Because the turbulent fields in the SOL are highly localized filaments propagating to the wall, a more fundamental model of the resulting inward impurity transport in such fields is needed. Some preliminary turbulence simulations have included impurity species, and such work should be extended to develop better SOL impurity transport models.

(e) Efficient coupling of neutrals and plasma: A useful advance well within reach is to improve the coupling of neutrals and plasma components. Present coupling with the highest-fidelity neutral Monte Carlo codes results in long convergence times, especially when steady-state scenarios are desired where the long-timescale particle fueling/pumping aspects are included. Other methods for accurate and efficient modeling of neutral dynamics for high densities where nonlinear collision processes occur should be explored. This problem should lend itself well to collaborative exploration of multiscale/projective integration techniques by fusion scientists and applied mathematicians.

(f) Transport by cross-field drifts: Classical cross-field particle drifts (i.e., ExB and curvature/gradient-B particle drifts) have been implemented in 2D transport codes for a number of years both in the United States and in Europe; but routine simulations using these terms has proven difficult, especially for H-mode plasmas with reduced turbulent transport. Simulations that are successful (converge to a steady state) show that such effects are important for a detailed evaluation of the peak divertor heat flux. Here collaboration with applied mathematicians on higher-order spatial discretization with modern methods to avoid artificial oscillations, or refined meshes that utilize efficient parallelization on many-processor nodes, could be effective.

(g) Detached divertor modeling: The modeling of detached divertor plasmas, where the electron temperature drops to ~1 eV such that volume plasma recombination becomes important, is both challenging and relevant because ITER and some reactor designs envisage utilizing such conditions by radiating most of the plasma heat flux before it strikes the divertor plate. From present-day simulations and recent detailed Thomson scattering measurements on the DIII-D tokamak, such plasmas are collisional, with ions having mean-free paths of less than a millimeter, while on the same magnetic field line near the midplane the mean-free path is on the order of 1 m such that kinetic effects can be important. A divertor model must include Coulomb and charge-exchange collisions as well as neutral-neutral collisions and should also include the kinetic midplane effects.

PMI. The primary challenge in PMI simulations is the trade-off between speed and accuracy, with speed typically being sacrificed in order to accurately treat the physics that occurs at the smallest length and timescales in the system. PMI simulations often use molecular dynamics, which simulates the Newtonian dynamics of individual atoms within the material in the presence of an interatomic electrostatic potential obtained from consideration of the electron structure of material atoms by using density functional theory. The extremely short timestep required, typically on the order of 10^{-15} s or less, limits the simulated particle flux and fluence to values that are far from experimentally relevant (by many orders of magnitude). Even with exascale computing, the extension of existing molecular dynamics algorithms to macroscopic length and timescales will be difficult because of challenges in time parallelization. Critical problems to be addressed for PMI include the following.

(a) Coarse-grained materials modeling: In the 5–10 year timeframe, the development of a continuum reaction–diffusion simulation capability is planned, which will be capable of simulating the surface evolution and composition over large length scales and timescales than are conceivable even with atomistic simulations. This development is the focus of a collaboration among fusion, applied mathematics, and computer science researchers within the PSI-SciDAC project [18]. If this capability is successfully scaled to exascale, it could provide the ability to simulate large-area surfaces ($\sim$m^2) at experimentally accessible fluxes and fluences.

(b) Coupling of the surface to the plasma sheath: A coupling of PMI and plasma transport simulations is necessary to account for the strong redeposition of eroded material, which involves transport processes occurring over a wide range of length scales and timescales. For the main SOL plasma, the timescales are much longer than for PMI processes, so that a one-way coupling is sufficient to define the flux of redeposited material needed by the surface evolution simulation. However, the same is not true of the plasma sheath near the surface, where the scales of the plasma and material can overlap at conditions anticipated in a reactor [wp107]. In order to self-consistently treat the plasma–material interface region, a coupling of a fully kinetic (6D) sheath simulation to a coarse-grained materials model is anticipated, with both the individual components and the coupling method presenting opportunities for collaboration among fusion, applied mathematics, and computer science researchers.

(c) Coupling the sheath to the SOL and pedestal: A further, direct coupling of a surface/sheath simulation to a pedestal/SOL plasma transport simulation would enable studies of the simultaneous, long-time evolution of the plasma and surface. In the nearer term, this coupling will be achieved by a parameterization of the surface/sheath results that includes effects such as surface roughness, which can be incorporated into plasma codes through databases in much the same way that surface data such as sputtering yields are incorporated at present.

Integration. The zones of the boundary region are strongly coupled owing to their close proximity to one another. Here, a number of the key boundary processes needing integration are itemized.

- Electromagnetic turbulence spanning the separatrix
- ELM dynamics, including propagation from the pedestal to SOL to the wall
- Impurity transport from the wall across the SOL to the pedestal and core
- Prediction of density profiles and fueling requirements for the pedestal/SOL
- Formation of the pedestal (“L–H transition”) including cross-separatrix dynamics
- Coupling to the core to enable global prediction of confinement and fusion power
- Evolving wall conditions and their impact on the SOL and pedestal

The detailed plan to move forward with the integration of boundary processes is given as priority research directions in Sec. 4.2.4. These PRDs will then form modules that can be used in coupling to the core as addressed in Sec. 4.3 on whole device modeling.

4.2.3 Crosscutting Issues in Applied Mathematics and Computer Science

As a prelude to the discussion of how the ASCR crosscutting panels can provide key expertise to address the physics problems presented, a summary is given of recent advances in simulation capability already made possible by existing collaborations on mathematical and computational enabling technologies (the full project names are explained in Sec. 2.3).

AToM: Combines OMFIT and IPS for coupled core-pedestal modeling using EPED/TGLF/NEO, as shown in Fig. 18. The IPS framework has enabled parallelization of the EPED model, including the capability to use 150,000 cores in order to complete all 245 cases shown in the figure in a few minutes, which facilitates validation, uncertainty quantification, and integrated modeling

EPSI/CPES: PETSc solvers and code verification; heterogeneous programing in MPI, OpenMP, and Cuda; load balancing; heterogeneous load sharing between CPUs and GPUs; multilevel threading; Adios I/O and workflow; in-memory on-the-fly data management using DataSpaces; parallel particle sorting; unstructured triangular meshing; extreme-scale parallelization; efficient time advance, large-scale visualization (XGC family)

ESL: High-order, mapped-multiblock, finite-volume discretization algorithms; Chombo support for (MPI-based) parallel, distributed locally rectangular data structures in multiple dimensions; linear solvers from hypre and PETSc; visualization tools provided by VisIt, including interrogation of 4D/5D distribution functions and postprocessing of moment data (COGENT/NEO/CGYRO)

FACETS: PETSc solvers, parallelization of UEDGE; enhancements to BOUT++; coupling algorithms for core/edge and edge/wall

PSI: Visualization of material structural changes utilizing molecular dynamics simulations

SWIM: Development of an integrated plasma simulator, enabling efficient use of HPC resources

As we move forward, many applied mathematics and computational science issues continue for edge models given the wide range of spatial and temporal scales that must be addressed and the number of interacting components that must be included. Here we describe these issues in the context of the boundary priority research directions; and we identify the panel(s) on mathematical and computational enabling technologies where such methods are described in more depth.

Efficient spatial discretization algorithms. [Crosscutting Sec. 5.1]. The plasma boundary has several challenging features that require particularly accurate mesh representation and discretization. The first is related to the shear in the magnetic field as the separatrix is approached. For divertor tokamaks, the separatrix is associated with a null (X-point) in the poloidal magnetic field that divides the closed magnetic field region from the open SOL region. In the vicinity of the X-point, the total magnetic field is strongly sheared; that is, the field-line length and local direction change rapidly. This shearing complicates the motion of particles and the self-consistent electromagnetic field associated with plasma turbulence and transport. Systematic application of a mapped-block technology to help address this problem would be useful, as would higher-order discretizations.

Another issue is the scale length of the toroidally averaged plasma and neutral particle poloidal variations followed in transport simulations, which can be small (<1 cm) near the divertor target plates compared with the midplane variation. This strongly nonuniform mesh spacing is advantageous for efficiently capturing this change in scale size. Further, localized ionization fronts arise for detached plasma conditions in the divertor region, a freestanding interface where the recycling gas is abruptly ionized. Here, a dynamic mesh adaptation algorithm would greatly improve the ability to resolve these sharp interfaces between the plasma and gas components.

Efficient timestepping algorithms. [Crosscutting Secs. 5.1 and 5.4]. Plasmas naturally have a wide range of timescales owing in part to the large difference in the electron and ion masses (see Fig. 3). For low-frequency plasma turbulence and transport in fusion devices (below the ion cyclotron frequency), the drift of ions and electrons across the magnetic field have comparable timescales, but the streaming motion along the magnetic field differs by the square root of the mass ratio for equal temperatures, yielding a factor of 60 difference in timescales for a deuterium plasma (and a factor of 360 when tungsten impurity ions are included). For the first steps in [**PRD-Boundary-1,2**] of simulating linear instabilities and their saturated turbulence, the fluctuating magnetic field needs to be included self-consistently. Including these fluctuating magnetic fields has been challenging because of the so-called Ampere-cancellation problem, wherein two large terms in Ampere's equation nearly cancel. Several approaches have been tried, with some algorithms apparently having more success than others [wp41] for some applications, but the optimal solution is not clear. A detailed investigation of this problem by applied mathematicians could help. Moreover, the Alfvén-wave timescale, which becomes very fast in low-density regions of the plasma, could benefit from a robust implicit treatment. Handling the wide range of collisionality is also challenging, where the timescales associated with the collision operator near the detached region could become $\sim 10^4$ faster than dynamics of interest and will require an efficient implicit treatment; again, collaborations with applied mathematicians could help. As in any use of implicit methods, one must confirm that no essential physical timescales are averaged over; preconditioners can often be used to improve efficiency [**PRD-Boundary-1,2,3,4**].

The edge plasma profiles evolve on a slower timescale than does the saturation of turbulence, markedly so when plasma–wall interactions of hydrogen particle recycling as neutral gas, the gas pumping and reionization, and impurity sputtering are included [**PRD-Boundary-1,2,3,4**]. These longer timescales can again benefit from implicit timestepping in a transport module that has a reduced description of the turbulent cross-field transport or uses multiscale or projective integration methods. As the range of timescales included expands, however, preconditioners can become more difficult to utilize owing to the large condition-number of the related matrices that must be inverted (iterative methods can also be more challenging for hyperbolic-type problems, though some applied mathematics research has been successful here.) Also, as architectures evolve, inversion techniques may require more development to become efficient. Thus, a blend of implicit and explicit methods is attractive, which treat only the fastest processes implicitly, with slower processes being treated explicitly. Such algorithms would be of great benefit for the transport portion of [**PRD-Boundary-1,2,3,4**].

Coupling algorithms and model hierarchies. [Crosscutting Secs. 5.1 and 5.4]. Because of the distinct physical regions of the boundary, coupling algorithms can be useful. Some of the large models provide such coupling by a common description of species (e.g., all particles or all continuum components) and a continuous spatial domain (e.g., pedestal + SOL). Such models are an important aspect of understanding and ultimately predicting the properties of the boundary plasma, and they are expected to utilize very large-scale computing resources, including exascale. Codes also exist that provide high-fidelity models of various physics aspects, such as turbulence in the pedestal and in the near-separatrix regions; highly collisional regions of the SOL divertor region, erosion and redeposition at the wall; and particle migration within walls. Coupling of these models can provide an efficient method for investigating extensive parameter variations with high resolution. Most of the examples for the latter group of codes involve coupling at a surface between regions, where robust methods need to be developed [**PRD-Boundary-1,2,5**]. Also needed is a systematic set of reduced models as understanding emerges that can be used in whole device models.

Other issues involve volumetric coupling between dissimilar model elements, such as a particle plasma with a continuum plasma model and particle neutrals with a continuum plasma model [**PRD-Boundary-1,2,3**]. The integration of boundary models with RF antenna models involves coupling codes from two independently developed areas. Since the antenna is embedded in the plasma, volumetric coupling between the RF fields and the plasma and neutral gas is required [**PRD-Boundary-4**].

Data storage, diagnostics, and verification and validation. [Crosscutting Secs. 5.1, 5.2, 5.3, and 5.4]. An enormous amount of data will be generated from 5D boundary turbulence simulations, as well as from lower-dimension transport simulations. A systematic procedure is needed to determine which data should be stored, the format for storage (including metadata and provenance), and a procedure for easy retrieval. In situ diagnostics should continue to be developed to provide key physics insights and to mimic experimental diagnostics such as phase-contrast imaging of turbulence, beam-emission spectroscopy, density reflectometry, Thomson scattering density and temperature profiles, and charge-exchange recombination spectroscopy. These activities should involve especially close collaborations among fusion, applied mathematics, and computer science researchers. In order to facilitate model validation procedures, simulation data should be in a format compatible with experimental data, and ideally in the same format where possible [**PRD-Boundary-1,2,3,4**].

A standard data storage format for simulations will also facilitate the critical verification procedures to ensure that the numerical models faithfully represent the equations on which they are based. Often in nonlinear regimes and in complex geometries of the boundary, no analytical results are available, and code-code comparisons become essential, a procedure that has been used effectively for core turbulence models. The method of manufactured solutions is another powerful tool that should be used to verify codes in the boundary's complex regimes [**PRD-Boundary-1,2,3,4**].

Visualization of the data should also be advanced because unexpected physics insight can often arise from data visualization [**PRD-Boundary-1,2,3,4**]. For example, visualization has been an important tool for the EPSI and PSI SciDAC projects in understanding the dynamics of plasma filaments, divertor heat load, and material evolution. Visualization efforts should be emphasized in all aspects of boundary modeling.

Uncertainty quantification and predictability. [Crosscutting Secs. 5.1 and 5.2]. A critical need exists to identify the source of errors and uncertainties for boundary models and to quantify the effects on simulation results. Because a number of the basic boundary processes are not yet fully understood, for example, the full range of relevant microinstabilities and related plasma transport in the different regions or the time-history of hydrogen storage in and release from walls, UQ has to pay particular attention to model uncertainty and error. The solution of stochastic inverse problems coupled with sensitivity analysis may be useful for identifying aspects of model uncertainty that has significant impact on simulation results. Thus, an important opportunity exists to greatly advance this area of the science in the next 5–10 years. At present, the SciDAC project EPSI (XGC1 code) and the SciDAC Institute QUEST are working together to develop improved methods of UQ for extreme-scale edge plasma simulations [**PRD-Boundary-1,2,3,4**].

Utilization of new architectures. [Crosscutting Secs. 5.1 and 5.4]. As in all simulation areas, the advent of new architectures (see Sec. 2.4) raises the question of scalability of existing codes. This area will require substantial investment of effort in which expertise in mathematical and computational enabling technologies will be invaluable. For example, nonlinear system solvers and implicit time integration packages such as PETSc and SUNDIALS, used by several boundary codes, might need to be rewritten to scale well on alternative architectures. As these architectures become clearer, reduced-scale, testbed computers will be helpful in testing new codes [**PRD-Boundary-1,2,3,4**].

4.2.4 Strategy and Path Forward

The boundary region of a tokamak fusion reactor is of critical importance because the fusion plant yield and component lifetimes are largely set by its properties. A key long-term goal is to develop the capability to accurately predict and optimize this coupled pedestal/SOL/material system. While recent advances in understanding have laid a strong foundation, the development of high fidelity models of its complex interacting processes is still in a comparatively early stage. Development and application of significant new capabilities are needed. Here we present a strategy to accelerate scientific progress, taking advantage of expected advances in high-performance computing.

Present work on transport, extended MHD, and gyrokinetic codes, employing both continuum and PIC algorithms, should be continued, while also engaging the theory and applied mathematics communities to develop analytic formalisms and numerical methods that enable accurate, efficient treatment of kinetic and short equilibrium-scale effects self-consistently. Particularly valuable would be a strong initiative on developing gyrokinetic codes that are able to accurately account for collisional, electromagnetic, and short-equilibrium-scale effects in the edge region. Also useful would be a more modest effort to develop codes to efficiently solve the full 6D plasma equations, providing a tool for assessing the accuracy of 5D gyrokinetics, sheath models and extended fluid simulations. Likewise, various integration approaches should be compared, ranging from a number of distinct coupled modules [wp15,wp16,wp35,wp42,wp100,wp102] to more tightly coupled approaches [wp40,wp82]. Extensive code verification, as well as detailed validation of simulation results, is essential at all stages of development.

Many important applications of boundary simulation codes arise as their capabilities expand. Here we identify five integrated priority research directions critical to the goal of prediction and numerical optimization of the coupled pedestal/SOL/material system that can enable the promise of fusion power.

[**PRD-Boundary-1**] Develop a high-fidelity simulation capability and predictive understanding of the coupled pedestal/SOL system and its structure and evolution in the presence of microturbulence and collisional transport. This capability will enable predictions of the temperature and density at the core interface, which strongly influence fusion performance, and also of particle and energy fluxes into and through the SOL, which determine wall heat loads and material erosion. Fuel and impurity neutral particles emitted from the wall/SOL in turn provide sources to the pedestal and core. Efforts should include simulating kinetic effects across and along the magnetic field as well as stochastic electron motion in 3D magnetic fields. Models include 5D electromagnetic gyrokinetic codes, 3D and 2D fluid codes, and 6D neutral Monte Carlo codes. Related whitepapers:

[wp28,wp41,wp42,wp46,wp50,wp58,wp68,wp71,wp72,wp77,wp80,wp82,wp102,wp105,wp118].

- Further characterize linear plasma microinstabilities in the pedestal and SOL, including kinetic effects, detailed collision models, impurity effects, electromagnetic fluctuations and realistic magnetic geometry. Progressively include coupling to the strongly varying equilibrium profiles.

- Move to nonlinear simulations of turbulent transport, first on electron scales, and then on ion scales where coupling to strong equilibrium variations is essential; include impurity transport. Carry out extensive code verification, including careful code-code comparisons for parameters representative first of present-day devices and then of ITER-size devices, which are computationally more demanding.

- Validate nonlinear turbulence simulations with experimental data. Utilize well-documented data set with a variety of diagnostics for spatial and temporal character of plasma fluctuations; (e.g., beam emission spectroscopy, phase-contrast imaging, and probes for fluctuations; maintain strong collaboration with experimentalists.

- Utilize turbulent transport models and results to predict slow equilibrium plasma profile evolution of the pedestal/SOL/wall system. Develop reduced models for use in efficient boundary transport simulation and whole device modeling efforts. Also extend high-fidelity simulation codes to longer timescales while including profile evolution, collisional neoclassical transport, plasma sources, and impurities. Validate with experimental data: Thomson scattering, reflectometry, charge-exchange recombination spectroscopy, and probes for equilibrium plasma profiles; spectroscopy and bolometric tools for radiative loss profiles.

In all these steps, applied mathematicians and computer scientists aid with the following: IMEX methods, adaptive mesh methods, MHD+gyrokinetic coupling, the Ampere cancellation problem, numerical code optimization on evolving computer architectures, coupling methods including between continuum and particle representations, methods for data storage and retrieval and systematic validation procedures and metrics. Priorities: robust implicit algorithms, IMEX and multirate methods, and Ampere cancellation problem.

[PRD-Boundary-2] Incorporate the dynamics of transients, particularly intermittent edge-localized mode events that eject bursts of particles and energy into the SOL, leading to large transient heat loads on the walls. This effort will require including the temporal wall response of impurity sputtering, particle pumping or outgassing, and the impact of applied 3D magnetic fields. A key output of the work is to assess the maximum tolerable ELM size compatible with sufficient material lifetimes. Models include 3D MHD and two-fluid codes for ELM growth and ejection, coupling to 5D EM-GK, wall codes, and plasma/neutral transport codes. Related whitepapers: [wp6,wp50,wp62,wp97,wp102,wp118].

- Determine the effect of applied 3D RMP fields on ELM stability, and compare one-fluid MHD models with two-fluid (separate ion and electron fluids) models. Include the effect of finite plasma pressure at the separatrix region.

- Verify nonlinear ELM ejection models by comparisons of simulation codes, identifying the key physics requirements. Include potential of filamentation of the ELM pulse by the time it reaches the wall.

- Validate simulations with experimental data, using an initial standardized set with a variety of diagnostics. Include wall effects of surface temperature rise and vapor shielding. Develop reduced models for inclusion in whole device model.

- Include SOL/pedestal recovery phase following the ELM pulse. Include microinstability models as in [**PRD-Boundary-1**] as well as coupling to wall model for gas release or absorption and sputtering/redeposition and a neutral transport model to understand particle refueling.

Contributions in applied mathematics and computer science are as in [**PRD-Boundary-1**], with an emphasis on the Ampere cancellation problem and electron motion in locally stochastic 3D magnetic fields.

[**PRD-Boundary-3**] Develop a simulation capability that integrates the moderately collisional midplane SOL plasma with the highly collisional divertor plasma in order to model the detached divertor plasma regime, which is planned for ITER and other devices because of its effective power-handling features. The modeling challenge arises because ion and electron mean-free paths for the two SOL regions can vary by as much as 5 orders of magnitude based on recent measurements, and important divertor region interactions such as impurity radiation and coupled neutral particle transport must be incorporated. Models include 5D EM-GK codes, 3D and 2D fluid codes, 6D neutral Monte Carlo codes, and wall codes. Include coupling schemes between a 5D EM-GK midplane code and 2D fluid with neutrals divertor codes, or extend 5D EM-GK to include the highly collisional divertor region. Related whitepapers: [wp28,wp68,wp82,wp96].

- Demonstrate neutral/plasma/radiation coupling in highly collisional, detached divertor plasma regime for long particle-pumping timescales, efforts likely requiring implicit time advance. As available, verify solutions between codes: fluid-fluid or kinetic-fluid.

- Validate detached plasma models with experimental data, especially divertor Thomson scattering measurements of electron density and temperature and impurity line-radiation spectroscopy.

- Provide coupling between kinetic midplane models and fluid divertor models, or extend kinetic model to full domain. Develop highly implicit algorithms needed to deal with very high collision rate. Develop reduced models for whole device modeling.

Mathematical and computational enabling technologies aid with implicit models for the strong collisional regime and for coupling kinetic/fluid models, as well as providing data extraction and comparison algorithms and helping improve code performance.

[**PRD-Boundary-4**] Integrate RF antenna/plasma-absorption simulations with SOL/pedestal plasma transport simulations, filling a notable gap in present capability. The SOL plasma strongly affects the wave coupling to the core, and the RF fields are expected to modify the SOL; this interaction must be studied with high fidelity to enable quantitative predictions for present-day devices and ITER. Existing 2D codes for the RF antenna and boundary plasma provide a starting point for the development, which eventually should couple 3D RF and transport models. Related whitepapers: [wp3,wp29,wp101,wp117].

- Couple 2D RF antenna to 2D SOL/wall model that includes RF sheath effects. Include computing on a common mesh or developing/utilizing interpolation routines and adaptive mesh algorithms. Assess requirements for different types of heating, for example, ion cyclotron or lower hybrid. Include energy source terms from RF fields for the plasma transport model.

- Compare with experimental data, focusing on trends of coupled power with SOL density and SOL response to RF power level.

- Couple 3D RF code to edge plasma/neutral model. Develop spectral solver in plasma interior: high-order FE/FD + Fourier, and adaptive mesh methods. Conduct solution matching (overlap method), which requires 3D reconstruction of signal and expensive computation. Compare 2D and 3D couplings.

- Validate with experimental data and assess development of reduced models. Provide capability in whole device modeling.

Researchers in applied mathematics and computer science aid with higher-order differencing; coupling finite-element, finite-difference, and Fourier methods; adaptive meshing; and data extraction and comparison algorithms.

[PRD-Boundary-5] Develop an enhanced capability to couple wall response models to plasma models. A related activity is to examine advanced divertor concepts, including alternate magnetic-geometry divertors and liquid walls. Utilize molecular dynamics and kinetic Monte Carlo codes, 2D and 3D plasma transport codes, and 4–5D EM-GK codes. Especially important for coupling are efficient wall models for erosion/redeposition of surfaces, impurity release, and tritium trapping within the wall. Related whitepapers: [wp25,wp80,wp97,wp98,wp107,wp111,wp115].

- Couple Monte Carlo erosion/redeposition code to fluid/kinetic plasma/neutral code, first with loose coupling, then strong coupling. Investigate implicit coupling algorithms. Compare with experimental data provided by sample probes removed for laboratory examination or by developing in situ diagnostic techniques.

- Develop and implement model of tritium and helium build-up in walls via continuum and coarse-grained simulations, calibrated by extension of molecular dynamics simulations. Couple continuum simulation to SOL transport codes.

- Add models for liquid walls, including motion of the conducting liquid in strong magnetic fields. Further develop models to assess effectiveness of liquids to remove plasma exhaust heat and to evaluate plasma contamination.

- Extend geometrical plasma/neutral modeling capabilities to include geometrical complexities of divertor concepts with alternative magnetic configurations. Provide assessments through systematic simulations and comparisons.

Mathematical and computational enabling technologies aid with coupling algorithms, implicit methods, and interfacing particle and fluid models, as well as data extraction and comparison algorithms.

4.3 Whole Device Modeling

Whole device models are required for assessments of reactor performance as well as time-dependent or single-time-slice interpretive analysis of experimental discharges. Because WDMs calculate temperature and density profiles based on heating and fueling sources, the fusion power produced by a reactor—proportional to the volume-averaged product of the deuterium and tritium pressures—is a key predictive capability. Significant improvements in WDM realism have occurred over the past decade (through more accurate core transport, pedestal stability, and wave heating models). Still, important opportunities exist to take greater advantage of physics understanding obtained from high-fidelity simulations, by directly utilizing these simulations as part of a WDM or by distillation into reduced models suitable for inclusion into a fast, predictive WDM capability. One of the great long-term challenges in integrated simulation is to address multiscale and multiphysics phenomena, such as the complex interaction between low-n MHD (sawtooth/kink, tearing) modes and short-wavelength drift-wave fluctuations. The vision for a WDM described in the following sections was distilled from the numerous whitepapers submitted to this panel as well as to crosscutting panels (see `https://www.burningplasma.org/activities/?article=IS_Whitepapers`).

4.3.1 Background and Recent Progress

A whole device model is generally described as an assembly of physics models that provides an integrated simulation of the plasma. The most basic components are the plasma equilibrium (geometry) and the transported profiles (density, temperature, flows, current). Existing WDM components have been developed based on an ordering in the small parameter $\delta \doteq \rho_i/a$, where ρ_i is the ion gyroradius and a is the "machine" (plasma minor radius) size. This ordering (the *drift-ordering*) identifies three timescales (equilibrium force-balance, fluctuation, and transport) and two space scales (profile and fluctuation). The profiles evolve on the transport timescale when an imbalance exists between the second-order outward flux driven by transport processes (collisional and turbulent) and the nominally second-order sources (particles, energy, and momentum). In addition to these basic processes one must consider plasma radiation losses, current drive sources, bootstrap current, pedestal dynamics, and so forth. Although a WDM is often a time-dependent simulation of a plasma, it can also be a time-slice analysis for which sources are fixed in time and the profiles iterated to steady state ($\partial n/\partial t = \partial T/\partial t = 0$). Two important aspects of the WDM are its *physics scope* (how many phenomena are included) and its *fidelity hierarchy* (how accurate is each model). A schematic illustration of the physics scope is shown in Fig. 23. The implicit goal in WDM development is to enhance both the scope and the fidelity. These enhancements typically lead to higher computational requirements. Maintaining a range of physics fidelity in models is desirable to allow a flexible WDM that can emphasize some physics effects relative to others and to enable a trade-off between accuracy and time to solution. The physics fidelity hierarchy can be illustrated by the bootstrap current (see Fig. 23), where a basic model may be the Hirshman model for the low collisionality limit, which is improved by the Sauter model to cover some collisionality regimes, further improved by NCLASS allowing multiple ion species, and even further improved by a direct solution of the neoclassical kinetic equations. Moving beyond standard neoclassical theory, however, will require nontrivial coupling between turbulent and collisional dynamics. Maintaining accurate WDM simulation capability with modest turnaround time is vital, since these simulations are utilized extensively in experimental interpretation, experimental planning, scenario physics studies, and fusion plasma facility design. That said, it is not uncommon to perform a simulation that will take significantly longer utilizing a sophisticated physics model, possibly simulating a smaller time window appropriate for the physics of interest.

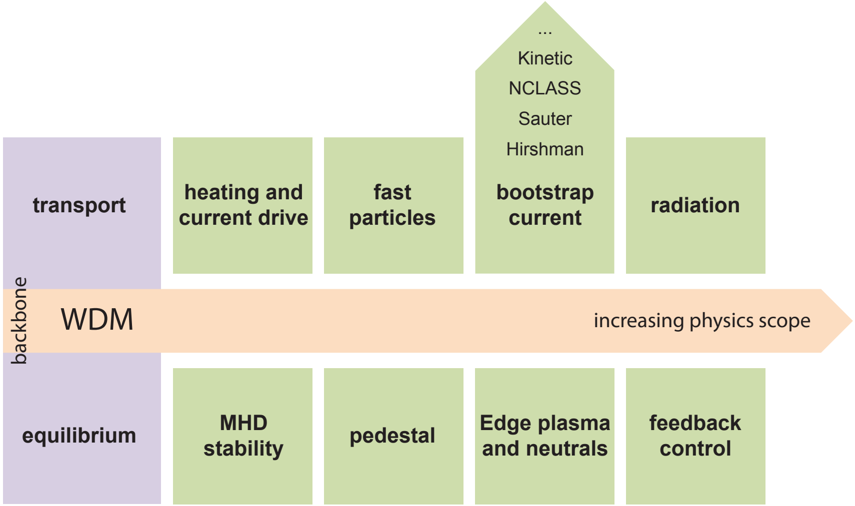


Figure 23: *Schematic diagram of the whole device model showing its most basic components (equilibrium and transport) plus additional components that illustrate increasing physics scope. Also, using the bootstrap current as an example (not exhaustive), a series of progressively more accurate components illustrates the fidelity hierarchy for this process.*

Although historically much of the WDM effort has concentrated on the core plasma evolution, including edge plasma and plasma wall interactions, as well as associated physics (e.g., antenna coupling, sputtering and erosion), is required in order to represent the core plasma realistically. A tool that simulates the spatial domain from the plasma center to the confining plasma chamber is the ultimate plasma physics goal of the whole device model. Researchers have also proposed going beyond this and including the engineering systems that surround and support the plasma, for example, thermomechanics, neutronics, and electromagnetics. Here electromagnetics refers to including complex 3D structures, ferromagnetic materials, and coupling to mechanical analysis. In fact, poloidal field coils, axisymmetric conducting structures, flux and field measurements, and feedback control systems have been incorporated in WDM simulations already and integrated as part of free-boundary plasma equilibrium evolution. The next steps for this area could include more complex conducting structures and their interaction with plasma MHD and disruption dynamics.

WDM codes for the study of tokamak plasmas with varying degrees of physics fidelity have been in use for roughly 40 years. Those most often used in the United States include TRANSP, ONETWO, Baldur, WHIST, Corsica, and TSC, with a substantial fraction of the codebase dating back to the 1970s and 1980s. Typically, they contain multiple physics models, along with their own equilibrium and transport solvers, for performing transport timescale plasma evolution to simulate experiments and future devices. A National Transport Code Collaboration (1999–2003) was funded to promote sharing and community ownership of transport physics modules and ultimately to develop a modern framework for these integrated simulations. The module library exists at `w3.pppl.gov/ntcc` and is still in use. Following this, efforts within the SciDAC SWIM (Simulation of Wave Interactions with MHD) project created a loosely coupled framework for assembling, data sharing, and executing a series of core physics models producing a WDM, based on TSC equilibrium and transport models (and other internal physics models). Another SciDAC project, called FACETS (Framework Application for Core-Edge Transport Simulation), pursued a tightly coupled edge-to-core plasma WDM approach, initially coupling a new core solver (using various transport modules) and the edge (represented with UEDGE).

The importance of these activities was to (1) explore more efficient ways to integrate multiple physics models that can improve over time, (2) support models with varying levels of physics fidelity for given physics phenomena, (3) accommodate physics codes developed by a range of scientists, (4) provide a means for physics model couplings, and (5) support a flexible approach to physics simulations. More recently (2011–2012) the Fusion Simulation Project planning activity identified an ambitious plan to develop a new national WDM capability based on the best of the existing WDM codes, as well as significant expansions of that capability. This project was not pursued, and most institutions returned to sustaining and expanding their local modeling codes. The WDM framework developed in the SWIM project turned into the Integrated Plasma Simulator (IPS), and received further attention to demonstrate progressively more capability and more applications. Most recently, the IPS framework (that includes TSC) and OMFIT workflow manager are being pursued and expanded within the AToM SciDAC project. Meanwhile, supported institutional efforts on WDMs in the United States include TRANSP at PPPL, ONETWO/TGYRO at GA, and Corsica at LLNL. WDM activities also exist in Europe, Japan, and Korea and in the ITER Integrated Modeling and Analysis Suite (IMAS).

The application of and activities associated with WDM include (1) experimental discharge interpretation and predictive planning, (2) experimental discharge/simulation data comparison, validation, (3) predictive simulation and design of future facilities, (4) discharge physics scenario exploration, (5) plasma control algorithm simulations, (6) physics subroutine or other software development, (7) data management and handling, and (8) supplying of plasma descriptions to other analyses that are not included in the WDM. Components used to provide WDM functionality are as follows.

- Equilibrium (free and fixed boundary): TSC, TEQ, VMEC, TOQ, EFIT, ISOLVER
- Energy, particle, rotation, anomalous transport: RLW, Coppi-Tang, Bohm-gyroBohm, CDBM, MMM, GLF23, TGLF
- Pedestal (pedestal pressure enforced): PEDESTAL (analytic ballooning), EPED
- Neoclassical physics (bootstrap current): Hirshman, Sauter, NCLASS, NEO
- Cyclotron radiation: Trubnikov, CYTRAN
- Bremsstrahlung radiation: plasma formulary
- Line radiation and charge exchange: Post/Jensen coronal equilibrium, P/J noncoronal equilibrium, ADAS
- Sawtooth instability: prescribed crash times or Porcelli trigger, Kadomtsev or hyper-resistivity and thermal diffusivity for crash prescription
- Ideal MHD stability: DCON, GATO, PEST, BALMSC, Peeling-ballooning (pedestal)
- Fast-ion confinement: enhanced diffusion models, critical gradient models, NOVA-K
- Neoclassical tearing modes: 2D equilibrium ISLAND, 2D equilibrium modified Rutherford equation (MRE), 2D equilibrium MRE and frequency
- Heating and current drive (ion cyclotron, electron cyclotron, lower hybrid, neutral beam): GENRAY, GENRAY/CQL3D, TORIC, TORIC/FP, TORAY, TORBEAM, LSC, NFREYA, NUBEAM, AORSA
- Fokker-Planck: FPPRF, CQL3D
- Boundary plasma: B2-Eirene correlations, 2-point model, UEDGE, fluid neutrals, DEGAS2, SOLPS

All these categories can be pushed further to higher physics fidelity (the list reflects this in some cases), and for other categories the models are rarely used because of their heavy computational load (e.g., ideal MHD, boundary plasma, embedded gyrokinetics) and are used mainly on time-slices or very short durations. The ordering reflects simpler to more sophisticated models. In some cases the transition to higher fidelity would involve a large leap in computational demand (e.g., moving beyond Porcelli trigger model); in other cases no high-fidelity models exist (NTMs, for example), and simple/empirical models are used. However, replacing all the physics models in a WDM with a small number of comprehensive, first-principles physics models is far beyond current or even near-term capabilities. While even modest improvements in fidelity can come at a cost too great for acceptable turnaround time, in other cases the question of the best theory from which to build a higher-fidelity simulation capability is a topic of current research, as in the case of NTMs. These considerations make the need for continuing and enhancing lower-fidelity (reduced) models critical and fundamental for achieving progress. Approaches to include higher-fidelity models are being explored and can form the basis for longer-term WDM development, and strategies to utilize these high-fidelity models more efficiently on HPC platforms are being developed. Figure 24 provides a schematic view of the interaction envisioned among major physics areas with varying fidelity for whole device modeling. The evolution of WDMs is clearly defined as growing the physics included in the simulations and pushing the included physics to higher fidelity. This evolution is also deeply connected to faster computing platforms and the software developed to take advantage of them, improved numerical algorithms, and advanced parallelization schemes that function on hybrid and GPU systems.

Particularly challenging and urgent plasma physics problems can provide focus to the directions for WDM development regardless of the physics fidelity level. The plasma behavior of ITER, a large and powerful reactor-scale device now under construction by a consortium of countries of which the United States is a partner, can produce significant damage to hardware or limit the access to the burning plasma operating conditions it was designed to test. Ultimately these same issues will arise in next-step fusion facilities such as a fusion nuclear science facility or the demonstration power plant (DEMO), which are envisioned as steps in the fusion development pathway. Similarly, present experiments provide challenges to WDM that are appropriate analogs to virtually all the ITER plasma issues listed below. These physics challenges, discussed in detail in the next section, can be summarized briefly as follows:

1. Coupling of plasma edge and material interactions to the core plasma
2. Interaction of fast particles with thermal plasma waves and instabilities
3. Dynamics of NTM, sawtooth, and other low-n instabilities
4. Modeling of plasma disruption behavior
5. Steady-state plasma modeling with strong coupling of core transport to sources and MHD
6. Multiscale turbulence
7. Fast WDM capability for real-time simulation, numerical optimization, UQ
8. Probabilistic WDM

4.3.2 Challenges and Opportunities

A fundamental attribute of a whole device modeling capability is the collection of physics models that compose it. The continuous expansion of the physics scope described by the collection of models is needed for WDM progress. These physics models can have a range of physics fidelity. Indeed, the concept of fidelity hierarchy is critical to enable the WDM to run efficiently with reasonable turnaround yet allow simulations with a broad range of goals.

If a high-fidelity physics simulation exists (typically with high computational demands), then

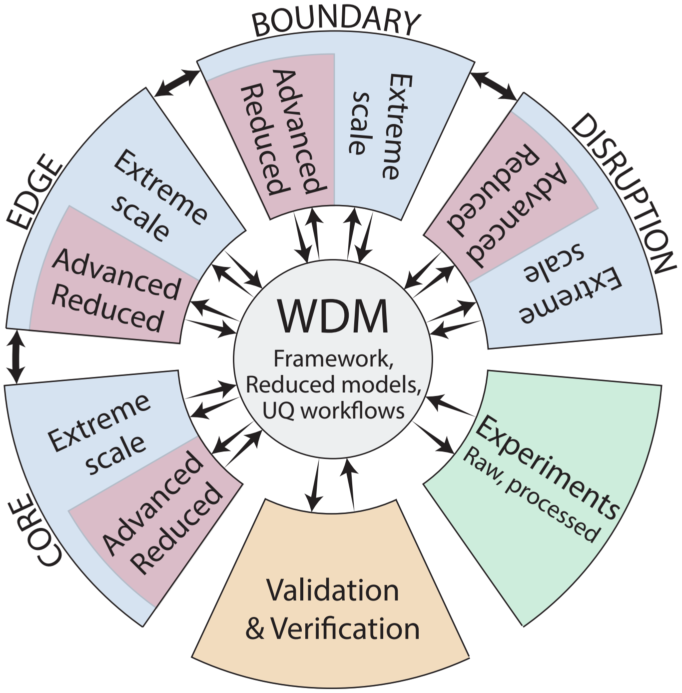


Figure 24: *Schematic overview of envisioned interaction between topical areas, V&V technology, and experimental data, along with the essential connectivity provided by WDM frameworks. Note that, in this illustration, experimental data encompasses not just raw measurements but also the processed results (such as smoothly varying kinetic profiles obtained from fits to point measurements), which are commonly used as inputs to and compared with WDM calculations. In this vision, the WDM framework provides a robust mechanism for managing data flow between experiment and validation tools through a variety of UQ-aware workflows.*

including it as a component within a WDM is most often considered impractical, particularly for a time-dependent simulation spanning seconds of real time (i.e., an entire plasma discharge). Instead, the WDM relies on lower-fidelity models to provide reasonable turnaround time for simulations, say 1 hour to 1 week. These lower-fidelity models are often called reduced models, although the terminology is not precise. They can be derived directly from primitive kinetic equations (e.g., GYRO to TGLF) theoretically or computationally or constructed separately (full wave versus ray tracing, orbit following Monte Carlo NB versus orbit averaged Fokker-Planck NB). The lower-fidelity models are often available in a sort of hierarchy with progressively increasing physics fidelity. In order to provide improved integrated simulation capability in the form of whole device modeling, these reduced models must be continuously developed and improved.

The pursuit of highest-fidelity (often described as first-principles) simulations is critical to exploring more detailed and inclusive physics behavior. These simulations are moving in the direction of multiphysics to unify the more traditional topical physics areas (MHD, kinetics, transport, RF, fast particles, boundary), since a number of actual physics processes may show strong couplings that make the separation inaccurate. Whether this separation leads to important physics impacts should be motivated by experiments and/or theory. In a sense these simulations are evolving toward a WDM since they are coupling multiple physics (e.g., RF and MHD, pedestal and SOL, transport and MHD). They rely on new theoretical formulations and computational development to produce a simulation tool. However, experience shows that very high-fidelity simulations are not routinely benefiting production WDM enough, and an opportunity exists for the fusion program to significantly enhance this interaction. On a five- to ten-year timescale, it seems prudent to more aggressively develop and experimentally validate reduced models from the highest-fidelity models, provide HPC computational access to the very high-fidelity models, and perform short-duration production WDM simulations that utilize high-fidelity models directly. Examples of high-fidelity options are COGENT, CGYRO, and XGC in the pedestal/boundary area; TGYRO-GYRO and TRINITY-GS2 as embedded turbulence modules in the core; and NIMROD and M3D-C1 for extended MHD. Over time the WDM will absorb very high-fidelity (computationally intensive) physics models (based on computer speed enhancements and computational platforms), but in some instances the highest-fidelity models may simply not be practical for production whole device modeling.

Coupling plasma edge and material interactions with the core plasma. Efforts in this area have in the past sought to identify and implement a range of differing fidelity representations for the scrape-off layer physics, divertor physics, plasma material interaction physics, neutrals physics, ELM crash/recover and pedestal physics, and RF transmission physics (see, for example, Sec. 4.2). Currently 2D SOL plasma and kinetic or fluid neutrals edge modeling are used in conjunction with a 1D core transport solver, providing greater self-consistency for particle transport prediction. These are not in common use, however, because of their high computational requirements; and they still depend on simplified assumptions and ad hoc inputs (for example, perpendicular plasma transport). Broadly speaking, the theory and simulation needs in this area include improved understanding and predictive capability for an array of complex phenomena. These are the (1) source of high Z impurities and their impact on plasma burn performance, (2) establishment of highly radiating divertor regimes to manage extreme power flows, (3) impact of ELMs on the plasma edge and plasma facing components (divertor, first wall, launching structures), (4) particle transport of fusion fuel, helium ash, and impurities in the core, pedestal, scrape-off layer, and divertor, (5) plasma–material interactions and the coupling of these to the core plasma, and (6) interaction of RF (ICRF and LH) waves with the SOL plasma, toward coupling to the core plasma, and the parasitic mechanisms that reduce the power to the core or result in plasma–material interactions.

Future opportunities include development of higher-fidelity physics components through more sophisticated individual models with core-edge coupling strategies and more inclusive cross-separatrix multiphysics, multiscale models, improving the connection from wall to SOL to plasma pedestal and core.

Interaction of fast particles with thermal plasma waves and instabilities. The historical challenges in this area include a more detailed understanding and predictive capability for the self-consistent interaction between energetic ions (alpha particles, beam, and ICRH ions) and thermal plasma waves, as is expected to occur in burning plasmas such as ITER and DEMO. Because energetic ions can transfer energy to thermal plasma waves (for example, Alfven waves), these waves can grow to an amplitude that may cause fast-ion loss or redistribution. Similarly, a more detailed understanding is sought for the interaction between waves generated by ICRH heating and energetic ions.

The electron distribution function is important in order to properly model the damping, heating, and current driven by electron cyclotron and lower hybrid waves. 1D Fokker-Planck (FP) treatments have been incorporated through adjoint formulations and are routinely available. However, researchers now recognize that 2D FP effects are significant, leading to 15–30% higher driven current compared with that of 1D FP. Although 2D FP is available, it is much less routine and is time-consuming for time-dependent simulations. However, since EC current drive is envisioned to be used in feedback control of neoclassical tearing modes and sawteeth instabilities and LH current drive is anticipated for off-axis current-profile control, access to the more accurate high-fidelity 2D FP treatments in the WDM is essential.

Work continues on development of more self-consistent descriptions of the coupling between energetic ions and the thermal plasma, whether via perturbative inclusion of fast-ion dissipation in the MHD pressure tensor or by nonperturbative inclusion of fast ions in gyrokinetic solvers.

Future opportunities include development of more detailed formalisms for coupling the thermal and energetic components and near-term projects such as faster or more elegant FP solvers to compute energetic particle distributions (in the absence of plasma waves) or multiple simultaneous fast-particle populations. 3D FP solutions, with explicit radial dependence, would be a new area to explore.

Dynamics of NTM, sawtooth, and other low-n instabilities. These are challenging problems for which inclusion into a WDM remains almost entirely absent or severely lacking in realism but are critical because of the impact they can have on ITER burning-plasma operation. Here the classic challenge is to predict the trigger for onset and subsequent growth and saturation of NTMs and thereby assess their impact on core plasma performance. Related to this is deducing the mechanisms for detection and suppression. An approach for NTMs or TMs could start with linear resistive stability but must include island dynamics and transport in order to properly address the physics of these modes. Similarly, more realistic models of the kink/sawtooth instability are needed, including thermal kinetic effects as well as resonant-layer interaction with small 3D fields and energetic particles (from heating as well as alpha particles). In addition, the community is seeking improved theoretical understanding of ELM instability (its post-trigger crash and recovery, and capability to trigger NTMs) and resistive wall mode behavior in the vicinity of the no-wall beta limit (below, at, and above) and its stabilization by feedback and rotation.

More aggressive, longer-term challenges include derivation and numerical solution of unified extended-MHD/drift-wave equations that describe island formation, currents, and drift-wave cross-field transport, with the ultimate capability of self-consistently simulating island evolution, saturation, and stabilization via feedback.

Modeling of plasma disruption behavior. The general aims here are to understand and predict the impacts of plasma motion, wall interaction, SOL currents, and structural currents in both present and future (ITER and DEMO) devices. Also needed is simulation of the plasma responses to disruption (and mitigation) or unintentional disruption triggers (large island, large impurity influx, H-to-L transitions) and thermal quench. Predicting the current quench phase, as well as onset of runaway electrons and schemes for their mitigation is also a goal. 2D plasma equilibrium device modeling continues to be used for design analysis of disruptions for future facilities such as ITER, including plasma wall contact, wall heating, electromagnetic currents and forces, halo/hiro currents, and runaway electron modeling. Techniques to improve the treatment of these phenomena should be pursued, subject to comparisons with higher-fidelity simulations.

Two levels of research thrusts are envisioned for disruption modeling. First, computations for disruption avoidance will likely be linear, checking for unstable modes and for the plasma response in stable conditions. This is detailed in part 1 of Sec. 4.1.2. For operations planning, these would be run from WDM predictions of the equilibrium profile at a sufficiently large number of time slices over the WDM simulation. UQ/margin assessment is needed to address the profile ensemble created through simulations. Linear computations may contribute to control, either through stability maps or possibly through real-time reconstruction and analysis. Computations for characterizing disruption transients and for improving mitigation will mainly be multiphysics 3D nonlinear simulations that start from WDM profiles or reconstructions. Extended MHD codes provide a more enhanced equilibrium treatment including 3D force balance with islands and stochasticity. These high-fidelity nonlinear simulations are not likely to be used when rapid turnaround is required, however. Adding more plasma effects may slow things to the point where it is not faster than nonlinear extended MHD. Improved reduced models of predisruption NTMs are desirable but will require advances in underlying physical understanding to go beyond approaches based on the modified Rutherford equation.

Steady-state plasma modeling with strong coupling of core transport to sources and MHD. The traditional research challenges in this area include understanding improved confinement regimes (the formation of ion transport barriers) as influenced by safety factors (and rational surfaces) and plasma rotation. While significant progress has been made along these lines, some experimental plasmas with very high non-inductive or bootstrap currents have shown MHD activity strongly correlated to the presence of fast particles, transport barriers, and edge or global modes that are observed at high safety factors. The challenge here is to predict the stable burning plasma regime accessible in steady state and its controllability through actuators for heating and current drive. In reactors the effect of actuators becomes progressively weaker because of the large fraction of self-heating and self-driven bootstrap current. For example, in ITER, we expect 40–50% of total plasma current or heating power to be externally driven, while in a power plant this could shrink to 10–25%, thus providing minimal latitude for plasma control. This implies a greater sensitivity to the transport modeling, since it determines the current profile, pressure gradients, and MHD and provides a complex control problem.

Also lacking are tractable physics models that predict the onset of internal transport barriers (or other events) that are driven by processes outside the drift ordering (such as external current drive sources and MHD). A better, more unified theory encapsulating both gyrokinetic and extended-MHD theory is needed in order to explore and understand the sensitivities of such transport phenomena and, ultimately, the strong coupling between plasma transport, current, external sources, plasma rotation, small 3D fields, and MHD. Lower-fidelity, empirical model generation and model coupling are directions for this area, in addition to high-fidelity model development. This strong coupling problem could be initially addressed in a time-slice simulation using multiple medium- to high-fidelity models.

Multiscale turbulence. Nonlinear microturbulence simulation capability has evolved to a relatively sophisticated state, and time-slice turbulence and fluctuation analysis for experimental discharges has become a routine exercise. What characterizes all but a handful of these simulations, however, is a restriction to relatively long wavelengths in the range $k_\perp \rho_i < 1$. While this can perhaps be justified empirically based on comparisons with experiment, and theoretically based on mixing-length arguments, we nevertheless have reason to expect that electron transport is systematically underpredicted in this limit. Particularly in cases where ion-scale turbulence is partially or fully suppressed (inside transport barriers or the pedestal), proper simulation of turbulent transport requires resolution of electron scales ($k_\perp \rho_e \sim 1$). For realistic mass ratios, full multiscale turbulence simulations are a factor of 10^3 more expensive than are ion-scale ones. Thus, exascale systems provide a natural opportunity for carrying out the parameter scans necessary for studying and characterizing multiscale turbulence and for informing the construction of improved reduced models of the enhanced electron transport.

We also note some connection here with spherical tokamaks, for which the challenges are doubly complicated. Not only are multiscale simulations required in order to properly estimate electron transport, but the larger value of gyroradius to system size makes the drift ordering less reliable than in tokamaks and significantly less reliable than in reactors. However, precisely because the gyroradius to system-size scale separation is weaker than in tokamaks, spherical tokamaks serve as a more numerically tractable benchmark for unified magnetohydrodynamic-gyrokinetic (MHD-GK) approaches.

Fast WDM capability for real-time simulation, numerical optimization, UQ. The primary objective here is to make WDM execution as fast as possible while maintaining an acceptable level of experimental fidelity. In this way we can explore development of control algorithms through linear and nonlinear model-based feedback algorithms and can carry out during-discharge, real-time WDM simulation to attempt to track the discharge, allowing appropriate safe termination, identifying imminent limits, and deriving proper control actions that minimize consequences. These low-fidelity WDMs can be used for achieving dynamic phase optimizations (adjusting gains for phase of the discharge), minimizing power requirements for plasma current ramp-up to desired relaxed configuration, or maximizing fusion gain through power management of multiple heating and current drive sources. The challenge is to retain critical physics while moving to very high efficiency, thereby presenting a possible engagement opportunity for experts in mathematical and computational enabling technologies.

Probabilistic WDM. Stochastic or probabilistic influences enter a WDM in multiple ways. Obviously, parameters and model inputs determined from experimental data (for example, beam-source voltage fluctuations or dust particles in the plasma scrape-off layer) are subject to stochastic variation both from natural randomness and as a model of experimental error. Additional inputs are affected by numerical stochastic effects (for example, time averages of nonlinear initial-value turbulence simulations and finite-sample Monte Carlo computations of a neutral beam model). Probability is also used as a model for phenomena that cannot be resolved because of computational or other limitations. For example, a defining feature of many of the individual and coupled-physics phenomena central to a predictive WDM capability is extreme sensitivity to controlling physics parameters and/or extremely rapid transition in values. This is observed, for instance, in the scaling of turbulent transport with driving temperature gradients and the triggering of L-H transitions and tearing modes. On the scale of feasible resolution, such phenomena can lead to behavior that is effectively nondeterministic.

As discussed in Sec. 5.2 and Sec. 5.3, mathematical science tools are clearly needed in order to describe the effects of stochastic variations affecting WDM on the output results. In addition to approximating probability distributions of important quantities of interest, capabilities must be developed to assess the probabilities of key physical transitions or states occurring. Example uses cases for these tools are the determination of probabilities that in a given scenario the plasma disrupts, achieves a specific value of fusion gain Q, that the divertor heat fluxes will exceed a threshold value, or even that the plasma will enter H-mode.

4.3.3 Crosscutting Issues in Applied Mathematics and Computer Science

Addressing the challenges of whole device modeling requires strong collaboration among fusion scientists and experts in mathematical and computational enabling technologies. This interaction is shown schematically in Fig. 24. Here we summarize the key areas of engagement that derive from WDM operation and capabilities.

Maintain/modernize key legacy components and frameworks. [Crosscutting Secs. 5.1 and 5.4]. Complex and mission-critical legacy components dominate the current WDM landscape. These components should continue functioning on both current and emerging HPC platforms. Currently, the computational platforms primarily used for integrated modeling are institutional clusters (128–512 cores) and capacity systems such as those at NERSC. WDM components can include large-scale solvers (core gyrokinetic turbulence, heating and current drive, nonlinear MHD), although the workhorse components detailed in Sec. 4.3.1 are less computationally expensive. As frameworks evolve, an opportunity exists to implement more sophisticated coupling algorithms for light- and middle-weight components with strongly varying spatiotemporal scales. For the large-scale codes, ongoing performance optimizations will be required for new platforms with hybrid architectures and accelerators, extreme core counts, and so forth. Methods must also be developed for migrating computational applications to different data layouts, as needed for good performance on GPUs and Phis. Moreover, tools must be developed for nonintrusive performance assessment. The sometimes opposing challenges of portability and performance represent significant software engineering opportunities.

Early inclusion of advanced solver/iteration algorithms. [Crosscutting Sec. 5.1]. Often, involvement of applied mathematicians and computer scientists in the improvement of fusion codes occurs late in the development lifecycle. For high-fidelity multiscale research issues (and potential upcoming initiatives) outlined in Sec. 4.3.2, opportunities exist for applied mathematicians to review the basic equations and work with physicists to develop innovative new numerical methods. For example, some methods trade computational work for improved scaling at larger problem sizes or dimensionality. Therefore, we can explore methods not typically thought about when formulating a computational approach to a problem by physicists alone. We remark that advanced solvers are still needed for existing efforts—particularly iteration and acceleration methods for embedded gyrokinetic transport solvers with noisy fluxes or generalization of parallelized grid tools for nonlinear MHD and other fluid solvers.

Large-scale data management and integration. [Crosscutting Secs. 5.3 and 5.4]. Various tools and protocols for data management could be integrated into WDM frameworks, thereby enhancing and broadening some WDM workflows while simultaneously providing a flexible tool for data management tasks. In particular, with regard to large-scale datasets generated by the biggest fusion codes, better management schemes could be developed to improve workflows for analysis, verification, and validation. Intriguing ideas are to develop searchable databases describing simulation data and to create a data-caching system to reuse results of large-scale simulation for V&V or reduced-model development. This line of research seeks to broaden the connection of WDM frameworks to the historically separate problem of data management.

Incorporation of numerical optimization and UQ approaches into workflows. [Crosscutting Secs. 5.2 and 5.4]. The goal of this effort is to transition to a capability that allows researchers to efficiently utilize current and next-generation HPC systems for uncertainty quantification (UQ), solution of inverse and numerical optimization (NO) problems, control, and risk and margin quantification with existing, validated, community-accepted components. In order to support existing WDM (or more broadly Integrated Modeling, IM) workflows, initial work should focus on developing and implementing new framework capabilities that enable the ensemble calculations needed for UQ and NO without requiring changes to the underlying core physics model code bases. A variety of different approaches and workflows will be needed, reflecting the wide range of use cases encompassed within WDM. For instance, the UQ and NO needs and resource requirements for a high-fidelity prediction of a steady-state reactor scenario will be different from those used for real-time control and feedback simulation. In the longer term, as existing models are updated and new models developed, researchers in fusion and applied mathematics should collaborate to implement capabilities for more advanced approaches such as adjoint calculations in new components as appropriate and necessary.

Improved access to HPC codes and resources. [Crosscutting Sec. 5.4]. The application in WDM of high-fidelity physics components or multiphysics components requires stable and predictable access to the HPC platforms where they can be executed efficiently. Thus users of integrated and whole device modeling tools and frameworks must have access to significantly more capacity computing resources in order to ensure enhanced productivity. This may require changes to the usual protocols for usage on these types of platforms. Also, if the role of high-fidelity components (developed via SciDAC or elsewhere) is to grow, WDM frameworks must be able to effectively manage their complex execution and I/O requirements.

4.3.4 Strategy and Path Forward

In this section we provide priority research directions, as well as the physics basis and justification, for the crosscutting issues presented in the previous section.

[PRD-WDM-1] Increase development of and support for modular WDM frameworks.

The magnetic fusion program today widely relies on large, complex legacy tools (TRANSP, TSC, ONETWO, Corsica) and emerging usage of newer efforts (IPS, OMFIT, IMAS). A sustainable path forward will require support both for the most mission-critical legacy tools and for development and expansion of the newer efforts that can more effectively utilize leadership-class computing resources and execute next-generation workflows. This research includes new methods to facilitate problem setup, execution, and analysis (via command line, shell scripts, graphical user interfaces, etc.). More detailed suggestions include the following; see Sec. 5.4 for discussion of related issues in software integration.

- Define a fixed target for integrated modeling and particularly for WDM. By fixed we mean permanence with a long-term programmatic commitment and support for community efforts. A moving target (i.e., short-term projects with varying goals and mandates) is not likely to get any buy-in. The suggestion is to merge useful capabilities from proto-FSP and other efforts; that is, do not start from scratch again.
- Build community buy-in to common integration targets by transitioning disparate legacy integration components to a reduced set of community integration frameworks. Demonstrate this capability for existing workflows and current and near-term (5-year) modeling capabilities.
- Work to ensure compatibility with the Integrated Modeling and Analysis Suite developed for the ITER project.
- Continue integration of HPC codes within WDM frameworks.
- Recover the NTCC Modules Library component “qualification” process including revision control in a centralized repository.
- Encourage software engineering best practices, for example regression testing, modern interface design, and documentation.

[PRD-WDM-2] Continue/expand efforts to understand and distill physics of gap areas.

Many gaps in theory and associated simulation capability have been identified by the community. Addressing the theoretical challenges associated with these gaps must take place in parallel to building a next-generation WDM capability. The strategy is not to define the next-generation WDM capability in terms of these gaps but to incorporate new capabilities as they are developed and to facilitate cross-code verification and experimental validation through the framework itself. We envision continuation and expansion of efforts aimed at using large-scale, high-fidelity codes to advance understanding in physics gap areas. Significant and fundamental gap areas that emerge from the physics challenges in Sec. 4.3.2, and the related requirements, are as follows:

1. Improved gyrokinetic models of the plasma edge, including electron dynamics and the associated electric field across the separatrix, and more generally a unified gyrokinetic theory spanning core to edge.

2. Improved formulations of MHD to rigorously include kinetic dissipation mechanisms. These will facilitate more accurate exploration of key effects of low-n 3D fields on space-time evolution of tokamak magnetic topology (dissipative reconnection, magnetic island growth, stochastic fields) and associated transport and better understanding and modeling of NTMs and externally imposed RMPs.

3. Improved kinetic-fluid formulations that include both drift-wave and turbulence physics, as well as low-n extended MHD physics. These could be either kinetic-type or many-moment fluid-type formulations.

4. Comprehensive framework for modeling boundary plasmas whose collisionality ranges from collision-dominated (Braginskii equations) to collisionless regimes and includes many physical processes—SOL instabilities, complex divertor geometries, neutral recycling, plasma–material interactions, and so forth.

The goals of these efforts are twofold: (1) deeper understanding of the underlying physics processes through traditional non-integrated HPC simulations whereby the ability to control and facilitate high-fidelity simulations via a WDM framework should accelerate this approach; and (2) synthesis of these insights to develop and improve reduced models that embody our understanding of the physics processes. This approach provides the opportunity to tackle the multiphysics aspects of the gap areas above with a coherent and sound theoretical foundation. With regard to reduced model development, this will likely require ensembles of computations rather than a single "hero run." Data management, analysis, and visualization at this scale (needed to understand the simulations in order to develop reduced models) is another opportunity for engagement of computer scientists and applied mathematicians.

[PRD-WDM-3] Increase connection to experiment through validation.

Each of the challenges and opportunities identified in Sec. 4.3.2 will require either extensive validation against current experiments or new development efforts for the probabilistic WDM capability case. The specific opportunity here is to increase the role of validation in the model development process through the use of tools that fulfill validation hierarchies and compute associated metrics. Such an approach will require expertise in large-scale data management and analysis for both HPC code output and the experimental observations they will be tested against (which will come from a hierarchy of experiments) and in the development and implementation of advanced UQ techniques to be incorporated into validation metrics. By using these tools to track model performance more systematically and prioritize development needs (including new experiments and diagnostic capabilities), the community can accelerate development of a validated predictive capability that addresses the key research issues and shortcomings in the present modeling capability identified in Sec. 4.3.2.

The significant experimental data analysis and management challenges will also create new opportunities to leverage expertise in mathematical and computational enabling technologies. As an example, the community might investigate whether HPC resources combined together with advanced data-mining algorithms can enable development of next-generation empirical reduced models, particularly for those areas where high-fidelity tools are unavailable, such as the presence of magnetic islands. These efforts might include neural network or other multidimensional fitting schemes formulated in terms of dimensionless plasma parameters. Another opportunity for collaboration with computer scientists is the implementation of data-caching tools to enable online "on-time" (immediate) access to massively parallel nonlinear simulation results, which would support the validation effort and open the opportunity for simulation data-mining. The standard being developed by ITER for experimental and model-based data is IMAS. Enabling support for the IMAS data structure will be essential in any WDM data management efforts, and this requirement presents yet another opportunity for collaboration with ITER researchers. Also needed is improved, standardized, and simplified connection to raw and processed experimental tokamak data. For this reason, the community might seek to develop an API for unified access to experimental data across U.S. experimental devices, perhaps utilizing IMAS capabilities, as well as common HPC formats such as NetCDF/HDF, and the fusion MDS+ archiving system. This system would also incorporate improved standardized equilibrium reconstruction, profile fitting, and associated numerical optimization and UQ tools identified as a key need for improved disruption and transients modeling.

Another area of potential collaboration with applied mathematicians and computer scientists is improved code robustness for large-scale HPC simulations. For any WDM effort that relies on such codes as key components (e.g., one that uses nonlinear initial-value gyrokinetic simulations to predict core transport), both the HPC-scale modules and the WDM framework must be sufficiently robust.

5 Mathematical and Computational Enabling Technologies

This section provides background and details about priority research directions, introduced in Sec. 3, for mathematical and computational enabling technologies in four key areas: multiphysics and multiscale coupling (Sec. 5.1); beyond interpretive simulations, featuring numerical optimization and uncertainty quantification (Sec. 5.2); data management, analysis, and assimilation (Sec. 5.3); and software integration and performance (Sec. 5.4). Figure 25 illustrates how these topics are important aspects of integrated fusion simulations. For each panel topic, we explain background and recent progress, crosscutting fusion motivation, and challenges and opportunities, followed by a discussion of strategy and path forward, including more details about priority research directions. Motivating issues in integrated science applications are discussed in Sec. 4.

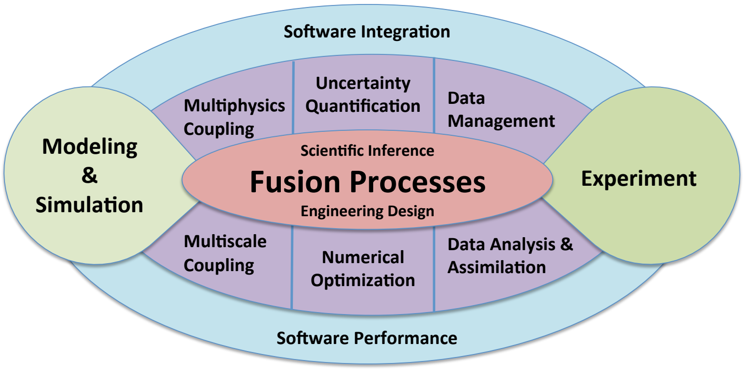


Figure 25: *Computational and enabling technologies are important aspects of integrated simulations in magnetic fusion energy sciences. This diagram illustrates the relationships among ASCR panel topics. Details about fusion processes are discussed in Sec. 4; for example, see Fig. 24.*

5.1 Multiphysics and Multiscale Coupling

The Multiscale and Multiphysics Coupling panel was organized to identify open challenges and problems in the formulation, discretization, and numerical solution of multiscale, multiphysics models for integrated simulation in MFE sciences. We define *multiphysics* problems as those that involve two or more physical processes that interact (couple) in some way. *Multiscale* problems are those that exhibit significant behavior over a wide range of scales—usually several orders of magnitude. The primary goal of this panel was to make specific recommendations for multiscale, multiphysics coupling research (1) that identify the applied mathematics needs and gaps in the ten-year plan for integrated simulation in MFE sciences based on the scientific goals identified in the physics panels and (2) that allow for strategic thinking about how integrated simulation should be done with more rigorous mathematical underpinnings.

The MFE community has had a long tradition of dealing with difficult, stiff multiphysics systems, both theoretically and computationally. The progress made by this community in understanding magnetized fusion plasmas has been exceptional, and many fusion scientists have successfully made use of (or directly participated in) advancements in computational mathematics. However, the modeling and simulation challenges ahead are orders of magnitude more complex and will best be addressed by a close interaction among MFE application scientists, applied mathematicians, and computer scientists. A secondary goal of this panel was therefore to identify processes that could facilitate more fruitful interdisciplinary collaborations.

Underpinning the recommendations of this panel is the disruptive transition in computer architectures, particularly in the drive toward exascale computing (which we broadly term here *extreme-scale* computing). These changes will provide unprecedented levels of computational resources and opportunities to enable new science but likely will require significant effort to use these resources effectively. Thus, new simulation capabilities will come not only through evolution of existing algorithms, but also by embracing and exploiting heterogeneity to develop entirely new algorithmic solutions for stiff multiple timescale and length-scale multiphysics applications. Applied mathematics will play a central role in enabling next-generation science via extreme-scale computing, both in general and in the MFE context.

Multiscale, multiphysics model coupling involves a broad range of applied mathematics topics, including modeling and multiscale analysis; scale-bridging algorithms; time advancement; meshing, geometry, and discretizations; solvers and preconditioners; adaptivity in space, order, and models; and coupling errors and verification. As such, this area is on the critical path toward integrated simulation of magnetic fusion devices, especially where these goals require extreme-scale computing. Recent advances in multiscale, multiphysics coupling techniques have the potential to benefit some fusion codes, but fully meeting these needs raises a significant applied mathematics and computer science challenge that will also require novel algorithmic and computing solutions. These solutions will emerge only if allowed by a broad research environment.

5.1.1 Background and Recent Progress

For clarity, we first distinguish between the couplings between physics and/or scales and the coupling of codes or models. The former are intrinsic relationships in the complete mathematical expression of the problem. The latter is the result of trying to recover some aspect of the former by using components that partially describe some of the physics and/or scales. From the mathematical perspective, considerations for multiscale, multiphysics coupling should be guided by the principle that it is better to consider the complete collection of physics or scales at the outset and make informed choices (e.g., asymptotics, strength of coupling, overlap of timescales) about how to split or partition it than to start with a collection of models and try to determine how to glue them together.

We adopt the terminology of [49] in describing the strength of physical and algorithmic coupling. Specifically, in the continuous mathematical model, the coupling of physics or scales is strong or weak. When the finest scales are resolved, coupling is usually weak; when one attempts to step over scales (e.g., use an asymptotic model) the coupling between scales and/or physics becomes strong (and often nonlinear). In contrast, the algorithm or strategy to solve the discrete approximation of a model is either tightly or loosely coupled. Using loose coupling strategies, such as traditional operator splitting, for weakly coupled problems is usually robust. However, loose coupling strategies for strongly coupled systems often fail because the discrete problem is ill posed or numerically ill behaved. In contrast, tight coupling strategies, such as nonlinearly converged fully implicit treatments, work well for weakly coupled systems, although the computational cost may not justify the approach. Tight coupling is really the only systematic approach for strongly coupled systems, but care still must be taken to ensure that the correct asymptotic limits are obtained discretely. Tight-coupling solution strategies typically demand significant effort to develop efficient and scalable solutions methods.

The mathematical concerns for multiscale, multiphysics couplings are mostly the standard concerns of numerical analysis: consistency of the discrete model with the problem being approximated, stability of the algorithm, convergence of the discrete solution to physical solutions of the problem being approximated, and performance (in terms of operations, memory, scalability, energy, etc.) of the algorithm. To these standard issues we add asymptotic well-posedness: Does the discrete algorithm converge asymptotically (in small parameter(s) of the original system) with uniform accuracy to the correct asymptotic limit(s) of the problem being approximated?

Within this context, we highlight seven computational mathematics topics that touch on multiscale, multiphysics coupling: models and multiscale analysis; scale-bridging algorithms; time advancement algorithms; meshing, geometry, and discretization; solvers and preconditioners; adaptivity in space, order, and models; and coupling errors and verification. Admittedly, these topics are neither entirely disjoint nor exhaustive, but they provide a convenient framework in which to discuss potential areas for collaboration between physicists and applied mathematicians. We provide a description and brief overview of each area here and will relate these topics to more specific integrated simulation challenges in Sec. 5.1.3. Related issues in numerical optimization and uncertainty quantification are discussed in Section 5.2.

Models and multiscale analysis. The basis for models of magnetized plasmas is a kinetic description in which the state of each particle species is given by a non-negative distribution function defined over a six-dimensional position-momentum phase space. Although the kinetic equation (see Eq. 1) is itself derived from the more fundamental Liouville equation, kinetic descriptions are sufficient for modeling magnetically confined plasmas. Assuming statistical independence, one can reduce the N-particle Liouville equation to a single-particle Vlasov equation that features particle advection and acceleration due to electromagnetic fields that satisfy Maxwell's equations. Corrections to incorporate correlations are added by using collision operators that are defined locally in space and time but are integral and/or differential operators with respect to momentum.

Kinetic equations are currently too expensive for end-to-end simulations, because of the dimension of the phase space and the large variation of scales that the equations can support. Reduced descriptions can address this challenge in several ways: as stand-alone models, as preconditioners for more complicated systems, as members of a hierarchy, or as components of hybrid descriptions.

Any strategy to control simulation error must balance model reduction errors with discretization and model coupling errors. In multiscale settings, numerical algorithms should naturally be designed to preserve, at the discrete level, important continuum properties of the kinetic equation. For plasma simulations, these properties include conservation, stability, and asymptotic limits. In multiphysics settings, the coupling between different processes must take into consideration the information to be communicated among the chosen set of reduced models, for example between components of a whole device model or between the plasma edge and the tokamak wall.

One common approach for generating reduced models is by asymptotic approximations based on collisional, field-induced, and large system limits. These approximations may dramatically reduce the number of unknowns required for simulations by dimensional reductions and/or by the removal of fine-scale dynamics that do not need to be resolved. The fusion community has a strong tradition of deriving models of reduced complexity by using suitable asymptotic approximations. For example, collisional limits lead to fluid equations for ions and electrons; the quasi-neutral limit leads further to extended MHD, resistive MHD, and finally to ideal MHD equations in the very large system-scale limit. In strong magnetic fields, gyrokinetic approximations remove one dimension of the phase space, and drift-kinetic approximations eliminate the gyromotion completely. The major drawback to asymptotic approximations is that they may be highly inaccurate outside the asymptotic regime for which they are designed.

Reduced models could also be derived by coarse discretization in the momentum variables, allowing the design of adaptive, multilevel hierarchies. In the fusion community, moment methods have been used extensively, although other approximation schemes are possible. The major challenge is to find transition-regime models that connect fluid approximations of kinetic equations with full phase-space discretizations, while remaining well posed. Indeed, linear hierarchies typically lack important structural features, while the complexity of nonlinear hierarchies can make the development of suitable algorithms extremely challenging.

Even reduced models of plasmas may exhibit dynamics over a large range of spatial and temporal scales. In many dissipative systems, however, the balance of forces at underresolved scales leads to features at operational scales. Meanwhile, dispersive systems often exhibit high-frequency modes that can be effectively averaged out. In such cases, current research in numerical methods focuses on accuracy and stability properties that are independent of these underlying scales. Two well-known and related approaches that have received recent attention are *asymptotic preserving* methods [50,51] and *well-balanced* methods [52]. Asymptotic preserving methods are used when small-scale balances lead asymptotically to a further reduced model. They are important both for single-model simulations and for coupling models together by domain decomposition or with scale-bridging algorithms. Well-balanced models are designed to capture special solutions of particular interest, such as steady states.

Scale-bridging algorithms. Efficient numerical integration of multiscale systems require targeted algorithms able to bridge the scale disparity (see Fig. 3). Families of scale-bridging algorithms of relevance to magnetic fusion energy include those based on heterogeneous multiscale modeling [53] and projective integration methods, methods arising directly from the asymptotically preserving and micro-macro decompositions (described in the previous section), and methods that employ a concurrent hierarchy of models.

Heterogeneous multiscale methods and projective integration methods exploit the separation of scales between microscale and macroscale processes. In such frameworks, a coarse-level model is missing a key piece of information, either in a distinct region (e.g., complex boundary condition) or throughout the entire domain (e.g., equation of state). This missing information is then provided by running locally an ensemble of small-scale, but higher-fidelity, microscale simulations. While such algorithms may be used to introduce high-quality microscale information into coarser macroscale simulations (or, for projective integration, to construct the coarse model itself), their primary challenges include initialization of each microscale simulation and formulation of consistent macro/micro models.

Hybrid algorithms combine models at various levels of description, using high-resolution models only as needed for solution accuracy. These algorithms include standard domain decomposition approaches, locally adaptive hierarchies, and multilevel representations. A well-known two-level approach is the so-called macro-micro decomposition (related to delta-f methods in plasma physics), in which the solution is written as the sum of a low-dimensional approximation (often an equilibrium component) and a correction. These two pieces form a coupled set of equations that, in many cases, can be solved more efficiently than the original equation by employing error-balancing techniques.

Various scale-bridging algorithms utilize a hierarchy of models at various scales in order to accelerate convergence of the highest-fidelity model. The most well-known of these are multigrid methods, which use the same model at different resolutions to generate scalable linear or nonlinear solvers. Recently the idea of using model hierarchies in a multigrid framework has gained attention, with the key idea of using different levels of models at different levels of the V-cycle to provide only required model fidelity at each level of the V-cycle. Here, hybrid models could even be employed, for example, using a fluid model to accelerate convergence of a higher-cost kinetic simulation.

Almost all scale-bridging algorithms require discretizations that are asymptotically preserving in order to ensure that a given model and its asymptotic approximations are consistent in relevant asymptotic regimes. This property is important for coupling between models in a hybrid approach and for convergence and effective preconditioning in multigrid approaches. The lack of the asymptotic preserving property results in the numerical representation producing intolerable errors when the scale in question is not resolved. Because of the coupled nature of the multiscale hierarchy, this error will propagate throughout the hierarchy. Given the disparity of scales in MFE, the development and specialization of scale-bridging algorithms will be challenging and will require targeted research beyond existing approaches.

As an example, Figure 26 demonstrates the benefits of careful asymptotic treatment in a multiscale problem. It depicts the radiation temperature for a 2D crooked pipe problem using an implicit Monte Carlo algorithm (left) and a modern multiscale (high-order/low-order, or HOLO) asymptotic preserving algorithm. Both these algorithms attempt to bridge the scales, but only the multiscale algorithm exploits a hierarchical asymptotic formulation. As a result, it provides a significantly sharper solution at the boundary between optically thin regions (inside the pipe) and optically thick ones (outside the pipe) [Figure 26(a)]. In addition to being more accurate, the multiscale HOLO algorithm delivers a much more efficient algorithm [Figure 26(b)].

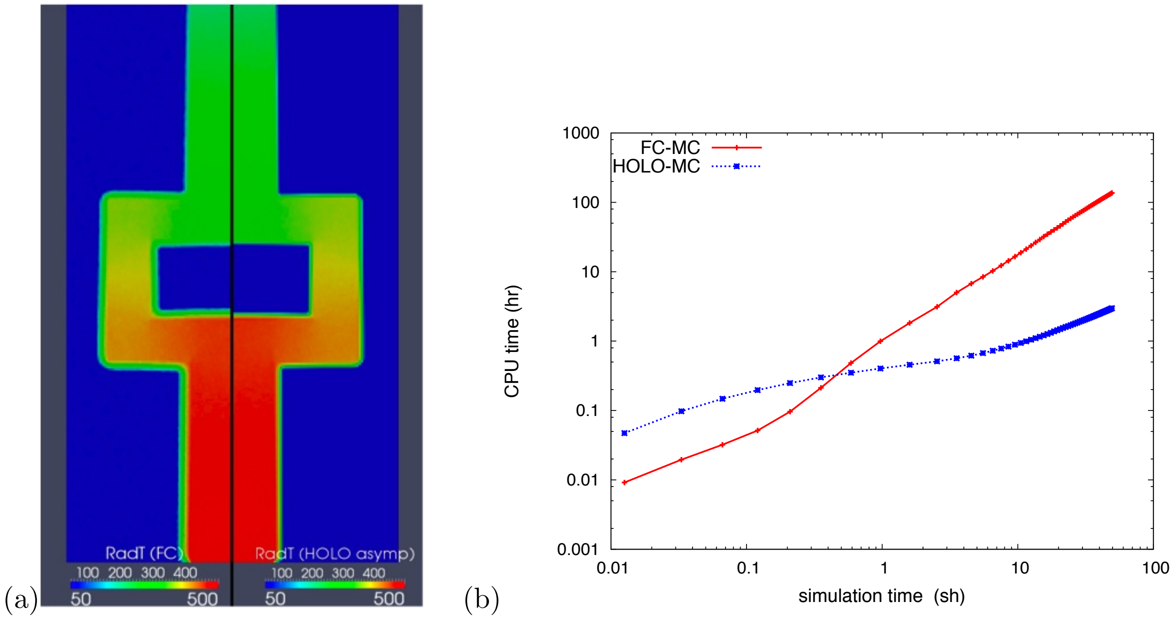


Figure 26: *Comparison of radiation temperature for a 2D crooked pipe problem between implicit Monte Carlo (left) and an asymptotic preserving scheme, HOLO Monte Carlo for radiation transport that (a) demonstrates a significantly sharper solution at the interface between optically thin and thick regions and (b) demonstrates substantial improvement in time to solution for long-time simulations. From [54].*

Time advancement. Numerous applications in fusion energy sciences involve modeling a physical system with evolution equations. Computing temporal dynamics of such systems accurately and efficiently is one of the key topics in integrated modeling of fusion devices. Since a majority of systems encountered in fusion modeling involve a wide range of temporal scales (see Fig. 3), efficient temporal solvers for stiff systems are necessary. For this reason, MFE scientists have been at the forefront of research in semi-implicit methods for stiff hyperbolic systems. Still, the growing complexity of the physical models in fusion simulations demands corresponding increases in the efficiency and sophistication of temporal schemes, which by necessity must be adapted for the specific problems at hand. Adaptation of the latest advances in time integration to development of efficient methods for fusion simulations presents numerous opportunities to improve code performance and to extend computations to currently intractable parameter regimes.

Among the wide variety of production fusion plasma codes, two important types are (1) macroscopic fluid codes, based on different flavors of MHD models, and (2) microturbulence transport codes, based on gyrokinetic models. The time integration schemes used in MHD codes are generally linearly implicit or semi-implicit. The choice of implicit terms is typically motivated by problem-specific, physics-based decompositions, with a goal of generating subsystems that are more amenable to scalable algebraic solvers. Progress has been made in developing theory for the convergence and stability of such partitioned approaches, as well as in developing a posteriori estimates of temporal error for adaptive timestep control, but much work remains to be done in these areas toward the goal of robust, accurate, and computationally efficient splitting techniques. Transport and microturbulence codes introduce a range of additional temporal discretization issues, such as expensive evaluations of particle orbits in particle-in-cell models and nontrivial Jacobian operator spectrums in gyrokinetic models that are difficult to account for in a straightforward time integrator.

Significant advances have been made in the field of time integration in the past few decades (see [wp91] and the references therein). New implicit integrators have been constructed with a range of desirable properties, for example, implicit schemes with optimized error constants for a given problem or those specifically designed to reduce the computational time of the linear solves embedded within an implicit integrator. A new class of exponential integrators has been introduced that offers computational advantages, particularly for problems where constructing a preconditioner is difficult. A number of innovations have been made in the coupling of implicit or exponential integrators with Krylov solvers and other algorithms to derive efficient time integration techniques (e.g., Rosenbrock-Krylov and exponential-Krylov methods). More traditional approaches, such as the fully implicit Newton-Krylov methods with "physics-based" preconditioners, the FAS (full approximation scheme) multigrid methods, and exponential integrators, have also shown promise for MHD. Additional important advances include the development of methodologies to construct (1) multimethods, that is, globally accurate and stable time integrators that include several different discretizations such as explicit, implicit, or exponential applied to different terms in an equation (e.g., IMEX); (2) splitting schemes with embedded error estimators to ensure the global accuracy and stability of the split terms; (3) asynchronous multirate time stepping that advances different terms with different timesteps while achieving a global target accuracy; (4) integral [55] and spectral [56] deferred correction methods, effective for simulating hyperbolic systems, which offer a compact stencil in time at the cost of more local computation (important in the new computing paradigm) and provide a pathway for breaking the well-known explicit order barrier for strong stability preserving methods; (5) methods that form a consistent nonlinear residual, enabling the development of higher-order temporal methods, strongly coupled nonlinear solvers (e.g., Newton-Krylov), and adjoint-based beyond forward simulation computational analysis; and (6) parallel-in-time integrators [wp24,wp91,wp94] beyond the early parareal algorithm.

The complexity of these new powerful techniques in time integration requires that physicists and mathematicians work closely to identify the most relevant tools in temporal discretization and use them to construct a method optimized to the specific problem for efficiency and accuracy. Physical intuition is an important guiding tool in the development of powerful algorithmic solutions, but sound mathematics is needed to provide a solid theoretical foundation. Preliminary results of adapting some of these techniques to problems in fusion (e.g., [57–63]) indicate that the effort required to fashion a time integrator well suited for a given plasma model can be more than justified by significant gains in performance, reliability, and resiliency.

Meshing, geometry, and discretizations. Mesh-based methods are extensively applied to study the behavior of plasmas in tokamak geometries in two and three dimensions, and MFE numerical modelers have needed to deal with complex geometries from the beginning. Both the physical components defining the reactor (e.g., inner wall, outer wall, vacuum vessel) and the magnetic fields in magnetically confined fusion plasmas introduce challenges for accurate spatial discretization and meshes, including interior convex corners, extremely narrow features, and highly curved boundaries; even for the linear stability analyses, the characterization of toroidal effects permeates the physics at the microscopic and macroscopic levels. Many of these issues can leverage advances from other fields. Strong anisotropies encourage alignment with magnetic field lines to reduce the number of degrees of freedom. Mapped multiblock and fully unstructured grids, extensively developed for aerospace problems, allow alignment with the magnetic field, as shown in Figure 27(a); the latter can handle the outer wall geometry, while the former could take advantage of embedded boundary representations. For both structured and unstructured mapped meshes, ongoing work is developing robust high-order treatments (e.g., high-order curvilinear elements) that better address large deformations in the mesh without catastrophic loss of accuracy. However, open questions remain on how to deal accurately with the challenges of evolving geometry, such as the formation or loss of magnetic islands, and extreme geometric variations, such as the severe shear between any two radially separated field lines in the toroidal direction due to incongruent (and typically irrational) winding numbers. Within the fusion simulation community, there is also ongoing work on initial mesh generation of high-quality unstructured meshes and of high-quality mappings from measured data and from computed equilibria.

Recent advances in spatial discretization have been primarily in the area of high-order methods, whether finite-difference, finite-volume, finite-element, spectral-element, or even low-noise PIC schemes. One driver is the push to exascale, where the trade-off between operations and data motion now favors methods with more flops per byte transferred. Active areas of research include high-order finite volume methods, discontinuous Galerkin methods, mimetic methods (which discretely preserve properties of the continuous operators, such as positivity, divergence, and curl), and sparse grid representations. High-order methods require high-order curvilinear meshes, and this is another area that has seen recent advances.

In addition, an often-overlooked discretization issue occurs at boundaries and, in particular, interfaces between coupled regions. Stable high-order boundary conditions can be particularly challenging for finite-difference and finite-volume formulations. Time-dependent boundary conditions also require care to ensure that the proper compatibility conditions on the boundary are satisfied to produce the desired temporal accuracy. For problems where the domain is partitioned into different physical regions coupled through an interface (as opposed to a monolithic approach where all regions are discretized implicitly and advanced simultaneously), stability (and even consistency) has long been a problem; but recent work that enforces the correct interface compatibility relations provides a path for robust interface treatment.

Increasingly the ability to address the multiple scales of physical behavior of fusion plasmas requires the coupled combination of particle methods with mesh-based solvers for partial differential equations. Similarly, coupling is desired between different physical processes either separated by domain boundaries or collocated but on different meshes, such as neutral particle transport and gyrokinetics in the edge region. Care must be taken during exchanges between scales, domains, and meshes to map fields accurately between representations. The considerations that must be addressed include the following:

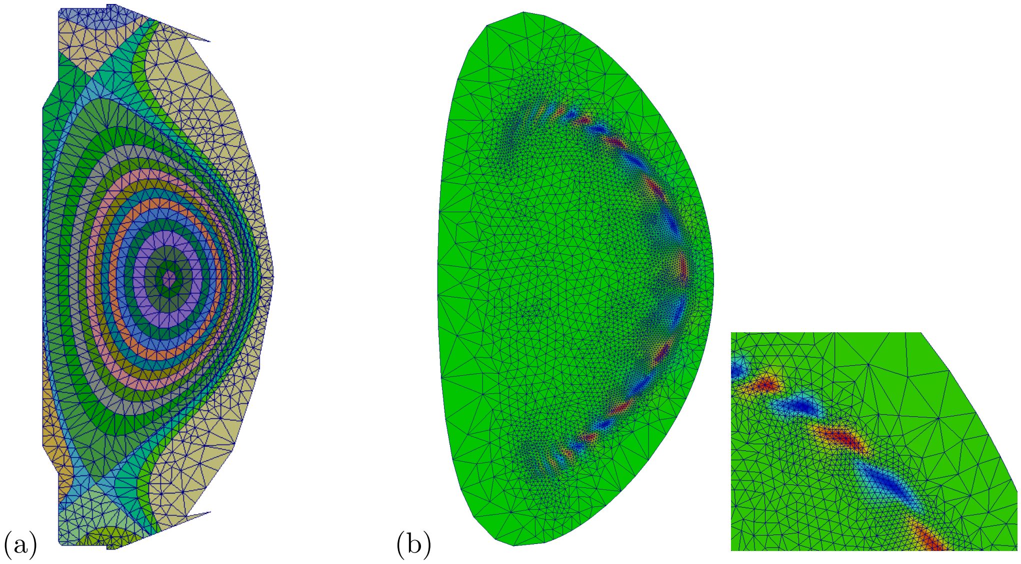


Figure 27: *(a) Example of a coarse mesh appropriate for PIC simulations; actual meshes would be much finer overall but would maintain the characteristics of the example shown here; (b) 2D adapted mesh from an extended MHD simulation.*

- Defining appropriate, compatible relationships between interacting parameters and/or variables between representations
- Preserving invariants across scales, interfaces, and meshes
- Accounting for the appropriate distributions of fields and/or discrete values, including geometry mismatch assumptions on the different scales

A reasonably straightforward implementation of combined particle and mesh methods employs a distributed representation of the particles while assuming that the mesh size is small so that the mesh can be copied on all processes. As higher-fidelity simulations are developed for high-performance computing systems, this assumption is no longer valid, and effective methods to deal with both the particles and mesh being distributed are needed. A similar decomposition challenge exists in continuum kinetic simulation, where the phase space and configuration space problems need to communicate efficiently while occupying vastly different distributed resources.

Solvers and preconditioners. Efficient solution techniques, both linear and nonlinear, underpin and enable a number of important capabilities that will be essential for the integrated simulation of magnetic fusion energy systems. Such solvers are required for implicit time advancement schemes (needed to bridge temporal disparate scales) and are heavily leveraged for stability analysis (e.g., eigenvalue computation) and for numerical optimization and UQ tasks, such as control and sensitivity analysis. Implicit time integration [64] and Newton-Krylov approaches [65] have made inroads in fusion simulation, but many opportunities still exist for further application to more complex fusion problems.

Preconditioned Newton-Krylov solvers have been successfully applied to highly nonlinear systems of MFE relevance such as gyrokinetics and MHD. Efficient preconditioners must effectively approximate (at least crudely) the inverse of the linear system across a wide range of scales represented within the problem that one is interested in solving. Designing effective preconditioners for fusion applications is particularly challenging because of the intricate coupling and disparate scales associated with the underlying phenomena of interest. This complexity is particularly pronounced when modeling the boundary region of a tokamak system. As the complexity of interactions increases (e.g., coupled models that include gyrokinetics and MHD formulations), preconditioning capabilities must address the increasingly challenging linear systems originating in these sophisticated numerical models.

Advances continue to be made in solver technologies. Significant improvements have been made in the convergence and robustness for both nonlinear solvers (e.g., exploring the use of Anderson acceleration and nonlinear multigrid, implicit-explicit methods, and careful use of operator splitting) and linear solvers. Current research trends that merit exploration in the plasma simulation context include problem-specific adaptable algorithms such as K-cycle-based multigrid, compatible relaxation, and bootstrap and energy minimization algebraic multigrid, as well as the use of eigenanalysis to augment coarse operators within domain decomposition. There is also ongoing research to improve scalability on hundreds of thousands of compute cores, including communication-avoiding methods, new multilevel methods with either increased parallelism (e.g., processing hierarchy levels concurrently) or less communication/increased data locality (e.g., sparsified non-Galerkin coarse grid operators), and methods better adapted to hierarchical architectures (e.g., recursive domain decomposition). Significant progress also has been made in the development of advanced solver principles, including domain decomposition [66], multigrid [67,68], physics-based solvers [57,58,62,69,70], and auxiliary preconditioners [71]. However, the effectiveness of many black-box solvers is often limited when applied naively to highly complex systems such as magnetically confined fusion plasmas, because assumptions made in the solver development are often violated. Therefore, research is needed either to adapt principles to complex scenarios (e.g., subspace projections to approximate nonlocal behavior) or to craft the linear systems addressed by the solvers carefully. The key is that promising solver avenues are often driven by a combination of domain-specific knowledge (e.g., used to create reduced models) and preconditioner expertise as to how such information can be employed to build effective solvers for high-fidelity calculations.

Adaptivity in space, order, and models. Adaptivity generally refers to changing the mesh (r-adaptivity), adding or removing mesh cells/nodes/elements (h-adaptivity), or changing the order of the underlying numerical representation (p-adaptivity) dynamically in response to the solution. Adaptivity is a key component of a scale-bridging algorithm. Mathematically, the motivation is to attain a more uniform truncation error in the discrete solution of the underlying partial differential equations. Physically, the motivation may be to resolve high-gradient phenomena, wherein the refinement criteria are usually determined heuristically or determined based on the "physics."

For multiscale simulations, dynamic adaptation in space can help resolve internal current layers, localized high-gradient regions changing dynamically in space, and small-scale features. As an example, Figure 27(b) shows an isotropically adapted mesh developed for investigating edge-localized modes in an extended MHD code. Typically, adaptive mesh refinement (AMR) methods are explicit in time. A research frontier is to efficiently and scalably combine fully implicit methods with dynamic adaptation (see, for example, [72]). In general, the development of efficient and effective inversion algorithms for linear systems arising from implicit or semi-implicit temporal discretizations in an AMR context remains an open area of research.

For multiphysics simulations, a research frontier is to dynamically change the mathematical model of the physics as the resolution changes (i.e., adaptive mesh and algorithm refinement). An example in the context of global magnetic reconnection is to invoke kinetic models inside the thin reconnection layer while still operating with a fluid MHD model in the outer region. Achieving good weak and strong parallel scaling of adaptive mesh codes on petascale and future exascale architectures remains a challenge.

Coupling errors and verification. Current methods for solving multiphysics systems usually invoke an approach that splits the solution of the full system into solutions of component systems in some way, giving rise to errors related to the coupling that is, at best, approximated by this splitting. In cases where the coupling is weak, the splitting error is usually small. However, splitting tightly coupled processes can lead to significant splitting errors. Unfortunately, splitting errors are seldom quantified [49].

Current research in time integration methodologies focuses on systems with varying timescales with the goals of reducing splitting error while maintaining efficiency of split schemes. New methods allow for consistent integration of multiple timescales within a single system through advanced partitioning, ensuring robustness and stability while providing more accurate coupling [wp24,wp91]. Of course, these approaches are more expensive than traditional low-order splitting schemes, so an active area of research is to address efficiency through both adaptation of step sizes to control temporal error and the use of multiple methods within a single integrator.

Recent work in a posteriori error estimation methodologies attempts to quantify coupling errors. Error transport methods evolve a set of equations for the solution error along with the state solution itself. Adjoint methods not only can give the a posteriori error in a quantity of interest but also can attribute how much of the solution error is due to the splitting. These methods can help scientists understand accuracy loss due to splitting the models within these coupled multiphysics simulations, but their application to problems as complex as those in MFE applications will require significant advances.

For any given simulation, one must understand the accuracy of the computed solution; verification is crucial to this process. As discussed in Sec. 5.2.1, code verification is the process of determining whether a code solves correctly the mathematical model it implements, usually through systematic convergence studies on problems with known solutions. For multiphysics problems, formal code verification is usually conducted on the component systems, which fails to test coupling errors. For differential equation-based models, testing single components is a well-known process, but formal code verification should be applied more to particle-based methods [wp23]. A lack of test cases for multiscale, multiphysics problems is an issue across many disciplines; in MFE science, a weaker form of verification, code-to-code comparison or benchmarking, is therefore frequently used [wp2,wp5,wp31,wp33,wp36,wp39,wp41,wp58,wp84,wp105]. Benchmarking also has its limitations; for example, it can be nontrivial to ensure that different codes are solving the same problem, and discrepancies are difficult to attribute (which code is wrong?).

The method of manufactured solutions (MMS) alleviates some of these difficulties by allowing the definition of suitable test cases that stress more (though not all) aspects of the code beyond simple linearized, single-physics, analytic (asymptotic) solutions. Manufactured solutions can be designed to include multiple physical models, multiscale model hierarchies, and nonlinearities. Error estimation techniques can then be used to determine the sizes and dominant sources of errors. Current research in verification methods includes the generation of MMS problems for multiphysics that can test a code within its regime of validity. However, applying this approach to MFE problems will be challenging and will require additional research.

As indicated throughout, all seven of these computational mathematics topics are active areas of research, and new techniques have made inroads—to varying degrees—into fusion community codes. One successful path has been through the Frameworks, Algorithms, and Scalable Technologies for Mathematics (FASTMath) SciDAC institute [20], which develops and deploys scalable mathematical algorithms and software for distributed and adaptive unstructured and structured meshes for finite-element, finite-difference, and finite-volume discretizations; dynamic load balancing and mesh-quality improvement tools; time integrators; preconditioners; and linear, eigen-, and nonlinear solvers. Members of the FASTMath team actively collaborate with the fusion community, for example, providing solvers for the Center for Plasma Surface Interactions [18]; developing extreme-scale particle data management, parallel mesh generation, and fast multigrid algorithms and solvers for the Center for Edge Physics Simulation [17]; providing meshing software and solvers for the Center for Extended Magnetohydrodynamic Modeling [16]; and developing the distributed high-order, mapped multi-block finite volume framework and solvers that support the Edge Simulation Laboratory [27] and Advanced Tokamak Modeling Project [19].

5.1.2 Crosscutting Fusion Motivation

From the whitepapers solicited from the MFE community many common themes emerged that relate to the applied mathematics topics involved in multiscale, multiphysics coupling. We briefly review these, corresponding to issues introduced in Secs. 4.1.3, 4.2.3, and 4.3.3, as the science-driven motivation for the challenges and opportunities identified in Sec. 5.1.3.

Need to couple two or more physical processes. Integrated simulation is about coupling physical processes, and many whitepapers identified gaps where particular types of coupled simulation are needed. Several papers identified the need for better models to express kinetic effects in MHD codes, especially for nonthermal particles, such as runaway electrons [wp10,wp31,wp32,wp54,wp62,wp102,wp113], energetic particles [wp9], and neutrals [wp96]. Another frequently identified gap was the need for better coupling of impurity generation, propagation, and interaction with kinetic and MHD descriptions of the plasma, especially in the edge region [wp25,wp28,wp40,wp45,wp54,wp56,wp68,wp80,wp82,wp87,wp97,wp98,wp102,wp107]. The coupling of RF to core turbulence, MHD instabilities, SOL plasma, and PMI was the subject of a number of whitepapers [wp3,wp5,wp29,wp40,wp82,wp101,wp117]. The coupling of models from the core, across the pedestal, and out to the edge came up several times [wp65,wp68,wp87,wp102]. The need for kinetic electron treatments with self-consistent electromagnetic models was discussed in [wp41,wp52]. One whitepaper identified the broader need for consideration of the couplings beyond the reactor vessel to include thermomechanical effects, neutron and photon transport, and so forth [wp26].

Need to accommodate a wide range of scales. Many whitepapers reiterated the challenges of the wide range of scales present in the physics of magnetically confined fusion. From a broad perspective, a fundamental challenge in magnetic fusion is that important physical effects can occur from kinetic scales all the way up to transport scales [wp28,wp42,wp65]. For disruptions, already a wide range of scales is present in simple resistive and extended MHD models, even before incorporating additional physical processes such as radiation, neutral dynamics, or runaway kinetic electrons [wp31,wp67,wp103]. The wide range of temporal and spatial scales in the boundary region was discussed in [wp80,wp82], and, in particular, the challenges of handling additional timescales introduced by plasma-material interactions and impurities [wp25,wp107,wp115]. Several papers emphasized that some physical processes, particularly in the edge and in plasma–wall interactions, do not exhibit a separation of scales [wp36,wp40,wp82], while others, such as RF coupling to the equilibrium evolution, are separated by five orders of magnitude in time [wp101]. The use of heterogeneous multiscale and projective integration techniques for scale-bridging was either highlighted by, or could be relevant to, specific whitepapers from the community [wp13,wp15,wp41,wp42,wp67,wp69,wp90,wp102,wp103,wp107]. Several whitepapers also promoted or presented approaches that could benefit from the use of hierarchies of models as scale-bridging techniques [wp1,wp52,wp59,wp94].

Need for more fidelity. Fidelity in this context can mean increased resolution of scales or increased physical fidelity (better models). Few whitepapers explicitly expressed the need for the former; increased accuracy was called for in stability calculations [wp9], and the use of mesh adaptivity was discussed in the context of fluid [wp97] and kinetic [wp58,wp90] edge codes. More common were calls for increased physical fidelity. For disruptions, this included improved models of MHD resistive inner regions [wp33], shatter pellet injection [wp54,wp56], and kinetic effects in extended MHD [wp109,wp112]. Needed are numerous improved physics models in the boundary, including sheath models [wp29,wp77], improved fluid [wp68] and kinetic models [wp77] for turbulent transport, and better models for impurities and PMI [wp77,wp82,wp96,wp105,wp111]. In WDM, examples of increased physical fidelity included calls for treatment of open flux surfaces [wp39,wp65] and the addition of more kinetic effects [wp41,wp47,wp57], particularly for the edge.

Need for hierarchies of models. Each physical process in MFE simulation can be described by a range of models of varying physical fidelity. Several whitepapers called for the development and use of hierarchies of models, particularly in boundary physics [wp77,wp80,wp111] and WDM [wp5,wp14,wp35,wp36]. From the mathematical perspective, the concept of a hierarchy of models is usually restricted to a set of nested models where the transformation between each level of model is well defined and systematic. Hierarchies of models are preferred in multiscale modeling because they help ensure self-consistency; such is the case in the systematic closures discussed in [wp14,wp111]. The use of hierarchies of models as a scale-bridging technique was already mentioned in the discussion of the wide range of scales.

Need for further reduced model development. A strong theme throughout the whitepapers was the need for more reduced model development [wp3,wp4,wp15,wp25,wp36,wp39,wp49,wp 57,wp71,wp77,wp87,wp93,wp97,wp111], particularly for use in practical WDM. While this has not traditionally been an area where fusion and applied mathematics researchers have collaborated, applied mathematicians could bring different perspectives to activities involving development of systematic, self-consistent multiscale models.

Need for verification of integrated simulation models. Throughout the whitepapers was a consistent call for increased verification and validation of integrated simulation. While validation and calculation verification for the purposes of quantitative error estimation are outside the scope of this panel, code verification, particularly for multiscale and multiphysics coupling, is of great concern. Across all physics areas, the majority of whitepapers discussed verification in the form of benchmarking, that is, code-to-code comparison [wp28,wp36,wp40,wp47,wp71,wp80]. In particular, one role for high-fidelity "first-principles" codes is the verification of reduced models. Some whitepapers called for more rigorous order verification [wp23,wp31,wp57,wp58] and in situ error estimation techniques [wp91,wp94], especially to determine the necessary resolution requirements [wp23,wp57]; in fact, difficulties were stated in utilizing more rigorous techniques, such as the method of manufactured solutions [wp41].

Need for scalable parallel algorithms. Especially for the disruption and boundary physics areas, the need for scalable solution strategies was emphasized, particularly as HPC architectures continue to evolve toward extreme scales. Of course, the architectures across all scales of computing are changing, with an increased emphasis on concurrency and reduced power over clock speed, so scalable solution strategies may have an impact on more than just the most computationally intensive physics models. One repeated need was dealing with heterogeneous architectures, such as support for GPUs for extended MHD [wp56] and PMI codes [wp25]. More general expressions of the need for scalable algorithms were made for both fluid edge and gyrokinetic core and edge codes [wp41,wp57,wp58,wp68] as well as for WDM [wp47]. Distributed particle data management algorithms for particle-in-cell algorithms were discussed in [wp1]. One whitepaper raised the issue of parallel-in-time algorithms for PMI simulations [wp107].

Need for computationally efficient algorithms. Improving the performance of numerical solution techniques also appeared as a theme across all physics areas. In several cases, the concern was for improved preconditioners for implicit discretizations [wp42,wp56,wp59,wp94]. The use of mesh adaptivity for improved efficiency was also identified [wp58,wp59,wp83]. The remaining examples were general statements about the need for faster time to solution [wp9,wp87], particularly for controls [wp93].

Need for robust integrated algorithms. The topic of robustness appeared in several whitepapers, but in particular in the context of WDM [wp4,wp16,wp35]. What is unclear is whether this robustness is an issue of code robustness, algorithmic stability, or reliability of solvers to converge; the latter two topics are relevant to multiscale, multiphysics coupling. Other examples included robustness to topological changes of the solution (for example, magnetic island formation) and to device geometry [wp82] and the robustness of RF codes when coupled to additional physics [wp5]. Resilience, which is expected to be a challenge for exascale computing, was identified by one author [wp58].

Need to handle complex geometry. Multiple whitepapers touched on the challenges of modeling multiscale, multiphysics processes on complex geometric domains. Realistic geometry in runaway electron avalanche [wp8] and in understanding MHD instabilities [wp44,wp53] was identified as a need. The complex geometry of antennas [wp3,wp29,wp117] and plasma-facing components [wp3,wp29,wp40,wp82], where thin Debye-length-scale sheaths form, is important to disruption and boundary region physics. A particular challenge in the edge is dealing with the complex magnetic separatrix geometry [wp28,wp40,wp77,wp82].

Need for modularity in the composition of integrated models. Among the whitepapers was a recurrent theme that integrated simulation, and WDM in particular, will benefit from easily composed modular components [wp4,wp14,wp35,wp42,wp65]. Certainly, this has historically been the approach of many WDM efforts. Notably absent was discussion of how to allow such flexibility while ensuring self-consistency and robustness (i.e., stability and reliable solver convergence). The mathematical perspective of modular software design as a composition of operators [wp86] provides an interesting perspective that may help to bridge this gap.

5.1.3 Challenges and Opportunities

Table 1 shows a crosscutting characterization of the physics use cases (as identified in the workshop) according to the set of applied mathematics topics identified in Sec. 5.1.2. The characterization has been done in terms of both relevance and priority (short-term in red, mid-term in blue, long-term in green). Priority has been assigned according to (perceived) urgency (i.e., whether a task is on

Table 1: Prioritization of multiscale, multiphysics coupling topic research in physics area use cases: near-term (🔴), mid-term (🔵), long-term (🟢).

			Multi-X Topics						
			Models & multiscale analysis	Scale-bridging algorithms	Time advancement	Meshing, geometry, & discretization	Solvers & Preconditioners	Adaptivity	Coupling errors & verification
			D1	D2	D3	D4	D5	D6	D7
Disruptions	A.1.1	Integrated models: Two-fluid solver + discretization			🟥	🟥	🟥		
	A.1.2	Integrated models: Fluid-kinetic coupling (runaway *e*, energetic particles)	🟥	🟥	🟦		🟦	🟩	🟩
	A.1.3	Integrated models: Coupling with wall dynamics (melting, ionization, multiphase, radiation)	🟥	🟥	🟦	🟦	🟦	🟩	🟩
	A.2	Parameterized assessment: Model hierarchy to quantify errors in sampling of parameter space	🟦	🟦					
Boundary	B.1	Pedestal characterization	🟥	🟥	🟥	🟦	🟥	🟩	🟩
	B.2.1	Detached divertor plasmas: Fast collisional algorithms (neutrals, plasma)	🟥	🟥	🟦	🟦		🟩	🟩
	B.2.2	Detached divertor plasmas: Plasma + neutrals + radiation coupling strategies	🟥	🟥	🟦	🟦	🟦	🟩	🟩
	B.2.3	Detached divertor plasmas: Kinetic + fluid coupling	🟥	🟥	🟦	🟦	🟦	🟩	🟩
WDM	C.1.1	Time-dependent baseline: Coupling 1D + fast dynamics components	🟥	🟥	🟥	🟥	🟦		🟩
	C.1.2	Time-dependent baseline: Coupling MHD + kinetics for NTM trigger	🟥	🟥	🟥	🟦	🟦	🟩	🟩
	C.2.1	ELMs, sputtering, impurity transport: Effective impurity source at edge	🟥						🟦
	C.2.2	ELMs, sputtering, impurity transport: Kinetic high-Z impurity transport	🟦	🟦	🟩	🟩	🟩		🟩
	C.3.1	ITER core transport and ITBs: Coupling core models + RF	🟥	🟥	🟥	🟦	🟦		🟩
	C.3.2	ITER core transport and ITBs: Coupling with edge (HMM, projective integration)	🟦	🟦	🟦		🟦		🟩
	C.3.3	ITER core transport and ITBs: Reduced models for ITB triggers	🟦						
	C.3.4	ITER core transport and ITBs: Accelerate GK core simulations			🟦	🟦	🟦	🟩	
	C.3.5	ITER core transport and ITBs: Sensitivity studies in high-D (> 20) space							🟦
	C.4	Q=10 ITER scenario: Coupling MHD + EP + transport	🟥	🟥	🟥	🟦	🟦	🟩	🟩
	C.5.1	Steady-state ST: Global GK simulations	🟥	🟥	🟥	🟦	🟦		🟩
	C.5.2	Steady-state ST: Coupled ions-electrons, realistic mass ratios	🟦	🟦	🟦		🟩		🟩
	C.5.3	Steady-state ST: EM effects (high-β)	🟦	🟦	🟦		🟩		🟩

a critical path), tractability, and maturity of the area. Based on this characterization, we can begin to assess the various challenges and opportunities presented by the physics use cases from an applied mathematics standpoint.

D1. Models and multiscale analysis. The need for model development and multiscale analysis is pervasive throughout the physics use cases in all panels. Since a suitable multiscale algorithmic treatment first requires appropriate model development and analysis, this step is a high priority in most use cases. Therefore, it offers much opportunity for short-term collaborations between applied mathematicians and plasma physicists.

Clear opportunities exist in the coupling between fluid descriptions and kinetic species (energetic particles, runaway electrons, neutrals; A.1.2, B.1, B.2.1, B.2.2, B.2.3, C.1.1, C.1.2, C.4, C.5.2, C.5.3) and/or the coupling of distinct multiphysics components (wall physics, RF, core-edge; A.1.3, B.2.2, C.3.1, C.3.2). In disruptions studies, specific applications include the characterization of disruption onset (which requires coupling of extended MHD (XMHD) with majority and minority kinetic species); disruption evolution (which requires coupling of XMHD, kinetic species ions and runaway electrons and the structure, as a resistive wall, as a boundary condition for the plasma, and as a source of material); and mitigation, both with pellets and with gas injection (which requires XMHD + gas or pellet modeling). Boundary studies will require coupling of plasma and kinetic species for pedestal characterization and of neutrals and wall physics for detached divertor studies. WDM will require coupling XMHD and kinetic models for NTM trigger studies; coupling of core, edge, and RF models for studies of ITER core transport and internal transport barrier (ITB) formation; and coupling of plasma and kinetic models for high-Z impurity transport and ELMs studies.

In all these applications, the challenge with model coupling will be to ensure the underlying asymptotic well-posedness, stability, and consistency of the formulations targeted, in the presence of disparate timescales (which require some level of implicitness in the time integrator) and length scales (which require adaptivity).

D2. Scale-bridging algorithms. The ultimate goal of model development and multiscale analysis is to express these models in well-performing algorithms. Hence, in the table, this topic goes hand in hand with topic D1. By well-performing, we mean that the algorithms are stable, consistent, and able to bridge the scales efficiently.

The need for scale-bridging algorithms is pervasive throughout the physics use cases and is on the critical path for progress in the integrated simulation of burning plasmas in the next 5 to 10 years. Whether many of the physics goals are met will ultimately depend on whether these problems can be solved with available computers. Brute-force algorithms will fail to deliver the answers sought.

Scale-bridging algorithms are particularly relevant for simulations that must couple macroscopic models (typically fluid) with microscale models (typically kinetic) or for simulations in which costly high-fidelity simulations may be accelerated by using lower-cost simplified models. Such algorithms are relevant to all three primary physical topic areas of this workshop. For example, these methods could be used to couple extended MHD fluid models with kinetic models for energetic particles in modeling disruptions. Similarly, they could be used to couple edge physics models with atomistic models of the tokamak divertor or wall, or even to develop the underlying formulations for coupling between models for whole device modeling. Some of the couplings required are interfacial (e.g., plasma–wall interactions), whereas others are volumetric (coupling of XMHD+kinetic or RF). These will present different mathematical challenges and will demand different solution strategies.

Specific opportunities lie in the development of efficient algorithms for extended MHD models (which underpin many physics hierarchies in MFE plasmas; A.1.1), coupling algorithms for informing fluid models with minority kinetic species (energetic particles, runaway electrons, neutrals; A.1.2, B.1, B.2.1, B.2.2, B.2.3, C.1.1, C.1.2, C.4, C.5.2, C.5.3), and heterogeneous physics modules (wall physics, RF, core-edge; A.1.3, B.2.2, C.3.1, C.3.2). We expect this topic to lead to rich interactions between the applied mathematics and plasma physics communities, with significant research opportunities for cross-fertilization and capability development.

D3. Time advancement. Time advancement is in many instances a critical component of a scale-bridging algorithm, since the numerical stiffness often originates in temporal-scale disparity supported by the underlying models.

Careful development of time advancement schemes is essential. The naive use of well-known schemes, uninformed by topics D1 and D2, will likely fail for physical systems of the complexity envisioned in many of the physical use cases. As indicated in Sec. 5.1.1, modern timestepping solutions will need to be targeted to the application and, as such, will be intrusive and will require some level of code refactorization. The challenge, then, will be to muster the required commitment and level of collaboration between applied mathematicians and plasma physicists to provide the manpower required for fruitful results.

Significant opportunity exists for impact of topic D3 throughout the physics use cases, as identified in Table 1. Of particular relevance will be the development of suitable temporal schemes for extended MHD (A.1.1), fluid-kinetic couplings (A.1.2, B.1, B.2.1, B.2.2, B.2.3, C.1.1, C.1.2, C.4, C.5.2, C.5.3), core-edge couplings (C.3.1, C.3.2), wall-plasma couplings (A.1.3, B.2.2), and gyrokinetic models (flux-tube and global; C.3.4, C.5.1). Progress in these applications will require targeted time-advancement approaches, of the sort described in Sec. 5.1.1. Parallel-in-time integrators may help to enable full space optimization methods (see Sec. 5.2) and to leverage extreme-scale computing resources for all these applications to bridge timescale disparities.

This topic also offers significant opportunity for fruitful interaction between applied mathematicians and application scientists. Indeed, deep knowledge of the mathematical properties and options of various timestepping schemes will mean the difference between failure and success.

D4. Meshing, geometry, and discretizations. Fusion devices are geometrically complex, and the physical fidelity demanded in the next 5 to 10 years will require the modeler to respect the geometrical complexity of the problem, which in turn will put a premium on meshing. This will generally be true for any physics use case that needs to deal with the fusion reactor boundary (e.g., A.1.3, all of B, and C.2.1, C.2.2). In general, we consider dealing with such geometrical complexity a mid-term priority, since one needs to define the mathematical description first before discretization. That said, it is important to make early formulation and implementation choices taking into account that meshing complex geometry will eventually enter the picture.

Spatial discretization choices (e.g., finite differences vs. finite elements in various flavors or Eulerian vs. Lagrangian) will generally be problem dependent and should be driven by the underlying mathematical requirements (stability, consistency, efficiency) as well as physical ones (geometry complexity, adaptivity, etc). Careful discretization choices are expected to play a critical role in the development of effective two-fluid solvers (A.1.1) and fluid-kinetic couplings (A.1.2, A.1.3, B.1, B.2.1, B.2.2, B.2.3, C.1.1, C.1.2, C.4, C.5.2, C.5.3), particularly when one considers spatial adaptivity as an option (see D6). One important aspect to consider is the need to transfer simulation information between different representations (particle-mesh or different meshes) or through interfaces, where the different representations or partitions are chosen to better suit particular physical processes. For instance, neutral models (which do not require field-aligned meshes) will have to interact with plasma ones, which may benefit significantly from such meshes.

This area is ripe for fruitful interactions between mathematicians and application scientists, and a great deal of intellectual capital can be leveraged for work.

D5. Solvers and preconditioners. This topic is considered of mid- to long-term priority for most physics use cases. It is a critical aspect of most scale-bridging algorithms (of timestepping in particular) but can be properly addressed only after formulation and discretization stages have matured. In practice, there will be an iteration loop between topic D5 and topics D1, D2, and D3.

Off-the-shelf nonlinear (e.g., Newton or Anderson) and linear (e.g., Krylov or multigrid) solvers will likely be a good starting point for most applications. In multiscale contexts, tight nonlinear coupling will be necessary, and the challenge will be the development of effective accelerators (e.g., preconditioning). These will represent a fertile ground for collaboration between applied mathematicians and plasma physicists, since success will draw as much from physics insight as from the availability of modern, optimal solvers. Applied mathematicians and fusion scientists must be encouraged to work together to devise suitable preconditioners for multiphysics/multiscale systems associated with sophisticated gyrokinetics, MHD, and kinetic-MHD formulations, including formulations and meshes appropriate for regions near the edge of a tokamak.

Short-term impact opportunities for solver and preconditioner development are in extended MHD modeling (A.1.1). Longer-term opportunities will be found in the development of efficient solvers for fluid+kinetic models (A.1.2, A.1.3, B.1, B.2.3, C.1.1, C.1.2, C.4, C.5.2, C.5.3), plasma+multiphysics models (A.1.3, B.2.1, B.2.2, C.1.1), and standalone kinetic models (C.2.2, C.3.4, C.5.1, C.5.2).

D6. Adaptivity in space, time, order, and models. Adaptivity is also considered a mid-term priority, in general, but essential in the long term as a broad scale-bridging strategy. Spatiotemporal adaptivity can be considered only after a suitable discretization strategy has been defined and suitable error estimators are available. Similarly, model adaptivity (the natural step beyond spatial refinement) can be considered only after a careful model and multiscale analysis has been performed. Both can result in significant performance gains if used appropriately.

We emphasize that the transition to exascale will provide “only” a 10^3 boost in computing power beyond petascale capabilities. In 3D, this will at best afford an order of magnitude increase in resolution per physical dimension, likely less if solution algorithms scale unfavorably with mesh refinement. This, on its own, is unlikely to deliver new science. New science will likely emerge from the judicious use of the exascale-computing leap, for instance, by enabling new multiphysics couplings via the development of robust scale-bridging algorithms. Adaptivity (in its various forms) will be a key component of the latter and therefore offers significant opportunity for impact. However, it also presents significant challenges, since adaptivity in most of its variants is hard to retrofit into existing codes and will likely require new codes.

Specific areas ripe for the broad use of adaptivity are extended MHD modeling (A.1.1), pedestal region and ELM modeling (B.1), and various kinetic or fluid+kinetic models (either by Lagrangian particles, or by adaptive mesh refinement in Eulerian formulations).

In the disruption context, adaptivity will help follow XMHD island formation and saturation by addressing the spatial-scale disparity dominating reconnection dynamics at rational surfaces and during sawteeth evolution, originating from high plasma conductivity and/or two-fluid effects. Also instrumental will be modeling of disruption mitigation strategies such as pellet injection and gas jet injection. The use of locally refined meshes will, however, result in stiffer numerical formulations and will make the use of implicit techniques a necessity, again stressing the need for suitable solvers.

The combination of XMHD+spatial adaptivity+implicit solvers is currently a research frontier.

In boundary physics, the plasma boundary pedestal region is generally thin compared with the size of the core and is another case where adaptive mesh refinement may mitigate spatial resolution requirements. Furthermore, AMR may be useful for resolving ELMs at the plasma edge for accurate and converged simulations of such phenomenon.

In the context of WDM, microturbulence gyrokinetic simulations using an Eulerian approach currently employ fairly coarse velocity space resolution. Adaptivity in velocity space will improve the resolution of trapped particles and phase-space filamentation physics, presenting another interesting research opportunity.

This topic offers significant opportunities for interaction between mathematicians and application scientists, since adaptivity needs to be informed by careful error estimation, including model coupling error, and will likely be most successful in well-defined asymptotic hierarchies.

D7. Coupling errors and verification. While in Table 1 this topic has been relegated to the long term, it is in fact critical for all physics use cases and in practice will require continuous monitoring during the development path of multiphysics, multiscale algorithms.

Coupling itself can be a dominant source of numerical error, and two convergent numerical descriptions may lose convergence when coupled without sufficient care. Often, asymptotic well-posedness comes at the cost of low temporal and/or spatial order of accuracy. This is true in stiff single-physics systems and will be even more the case in a multiphysics, multiscale context. In such contexts, the challenge will be to increase the order of accuracy (using, for instance, spectral deferred correction strategies), characterize the coupling error between stiff subsystems, and ensure a convergent algorithm. The use of in situ quantitative a posteriori error estimators should be encouraged as a means to monitor coupling errors over a wider range of problems.

Code verification will also require constant attention to ensure correctness throughout the implementation process. Code verification will have to be performed both at the individual component level and for coupled formulations. Code-to-code comparison is fraught with perils, but it can be useful. Well-defined mathematical techniques such as the method of manufactured solutions will be expected to play an important role, as will community-agreed test cases that allow the direct assessment of algorithms.

5.1.4 Strategy and Path Forward

Multiscale, multiphysics model coupling has been identified by all three integrated science applications as being on the critical path to meet the goals of extreme-scale integrated simulation of magnetic fusion devices in the next decade. Meeting these needs, however, will involve significant applied mathematics and computer science challenges that will not be addressed solely by incremental progress from current strategies: it will also require novel algorithmic and computing solutions. These solutions will emerge only if allowed by a broad research environment.

Specifically, in relation to the seven topical areas within multiscale, multiphysics coupling, we recommend the following priority research directions.

- [**PRD-MultiXCoupling-1**] Invest in model development and analysis. Suitable multiscale algorithmic treatments begin with appropriate models and analysis of these models. A high priority is to foster near-term collaborations on this topic for problems where such analysis is needed.

- [**PRD-MultiXCoupling-2**] Develop efficient scale-bridging algorithms that address the particular challenges of fusion science. Systematic scale-bridging schemes that ensure consistency and accuracy are fundamental to the integrated simulations of burning plasmas, and the development of new scale-bridging algorithms not only is on the critical path for progress but may also benefit from new extreme-scale architectures.

- **[PRD-MultiXCoupling-3]** Develop time integration algorithms better suited to specific problems in fusion energy science. Time advancement techniques are essential to successful scale-bridging and coupled-physics simulations. Many recent advances have occurred, but much works needs to be done to tailor these algorithms to MFE applications.

- **[PRD-MultiXCoupling-4]** Develop new techniques to address the geometrical complexities of fusion devices. Large anisotropies, complex device boundaries, and evolving magnetic field structures all pose severe challenges for integrated simulations that must be considered early during problem formulation, even though improvements can mature on a longer timescale.

- **[PRD-MultiXCoupling-5]** Develop new solvers and preconditioners congruent both with specific fusion science applications and with extreme-scale architectures. Physical processes, problem formulation, and discretization all directly impact the nature of the problems for which solvers and preconditions must be designed. In the mid to long term, solver algorithms will also need to make effective use of evolving HPC architectures.

- **[PRD-MultiXCoupling-6]** Develop new techniques that enable adaptivity of space, order, and models. Focusing resources only on those regions where additional resolution, accuracy, and/or physical fidelity are needed will be essential in the long term as a broad scale-bridging strategy for certain problems.

- **[PRD-MultiXCoupling-7]** Develop improved techniques to understand and control coupling errors. This effort requires a long-term investment and commitment, since significant advances need to be made in verification methodologies before they can be applied routinely to complex multiscale, multiphysics simulation codes.

Detailed connections of these initiatives to the three integrated science applications are provided in Sec. 5.1.3.

Advances in multiscale, multiphysics algorithms for integrated simulation for magnetic fusion energy sciences will require more tightly coupled collaborations. The most effective algorithms for these problems will need to accommodate the specific characteristics of each driving physics application. In addition, such algorithms will be intrusive, since they impact the core of simulation codes; it will be insufficient to rely solely on modularized libraries. To ensure that applied mathematics contributions have lasting impact, fusion scientists must be involved in the development and implementation of new algorithms so that they have ownership of and can continue to support and to maintain any new capabilities.

Close collaboration between fusion scientists and applied mathematicians is essential to advance the development of multiscale, multiphysics algorithms. Such collaborative efforts need to support *both* domain scientists and applied mathematicians. Increased diversity in the types of such opportunities is needed. For instance, smaller multidisciplinary teams, not driven by physics deliverables, may be more appropriate for fundamental work on multiscale, multiphysics algorithms. To explore the complex technical landscape of approaches to whole-device MFE simulation, moderate-sized teams could be formed; these teams could explore trade-offs of various integrated approaches, such as the cost/benefit of implicitness in a rigorous asymptotically preserving hybrid kinetic/fluid approach or the boundaries of applying strongly coupled implicit/IMEX multifluid approaches. Large multidisciplinary teams are needed for science-result-driven projects that require integration of new technologies into more complete-physics production codes.

To attract, inform, and retain interest from the applied mathematics community in problems of interest to magnetic fusion energy sciences, we recommend that new mechanisms be explored. In order to create a larger pool of potential collaborators, formal training opportunities help; examples include tutorials, webinars, workshops, summer schools, and limited visiting researcher programs at fusion facilities. Exploratory research initiatives could also foster new collaborations between applied mathematicians and MFE scientists. The development and availability of stripped-down applications that capture key features of MFE coupling challenges would facilitate exploration and the development of new algorithms by applied mathematicians—not only within DOE research projects but potentially within the broader applied mathematics community; the challenge will be ensuring that these new advances are incorporated into full MFE applications.

5.2 Beyond Interpretive Simulations

This section focuses on issues related to utilizing physics-based models to investigate aspects of fusion processes that are currently intractable, expensive, or dangerous to observe and, ultimately, to design experiments and reactors. Scientific inference or prediction involves the synthesis of model simulations and experimental observations typically through the solution of inverse and numerical optimization problems together with uncertainty quantification tools such as forward propagation of stochastic uncertainty. Potential benefits to fusion science include improving confidence in simulation predictions, designing physical experiments, forming the basis for improved efficiency in high-performance fusion simulations, and designing robust and reliable reactors (e.g., by controlling and mitigating disruptions). By their nature, uncertainty quantification, numerical optimization, and inverse problems are drivers for extreme-scale computing.

5.2.1 Background and Recent Progress

The goal of the next phase of fusion research, to test the key physics and technologies of a burning plasma device, spans inquiry-focused science and design-focused engineering. This is paralleled by a range of problems in mathematical sciences that must be addressed, which in the context of the complexity of fusion processes provide significant challenges to both theory and application.

A simple definition of scientific inference is predicting unobserved behavior of fusion processes based on limited model and experimental observations. The need arises because experimental observations of fusion processes are both expensive to obtain and limited in terms of observation quantities. Similarly, high-fidelity fusion simulations are computationally expensive and limited in terms of physical description. Nevertheless, scientific inference is important to many fusion research goals. Scientific inference for fusion processes depends on an amalgamation of experimental data and complex physical models and hence does not fall entirely into either statistics or mathematics.

Engineering design and control of fusion reactors require the use of mathematical techniques in conjunction with numerical simulations to determine parameters to improve a quantity of interest, such as reducing the risk of a disruption, or to determine when to apply a control to mitigate a disruption. Such problems can be posed in either deterministic or stochastic settings, which impact the numerical methods applied and the time required. The goal is to improve on current practice, while performing the equivalent of only a limited number of numerical simulations. Engineering design and control thus encompass parts of applied mathematics and numerical optimization.

The mathematical and statistical tools involved in scientific inference and engineering design and control include the following:

- Mathematical and numerical analysis of coupled, complex multiphysics, multiscale models, in which the components are themselves complex problems.
- Sensitivity analysis of solution behavior with respect to data and parameters and computation of derivative information with respect to model inputs.
- Propagation of probability distributions describing stochastic variation and uncertainty for input quantities and parameters through complex models.
- Quantitative error estimation for all sources of stochastic and deterministic error and uncertainty and development of strategies for efficient distribution of computational resources in order to obtain simulation results of desired accuracy. This includes development of methodologies for selection between physics models of different fidelity and computational costs while maintaining a desired level of accuracy in output quantities.

- Formulation and solution of inverse problems for determination of information about model parameters and data input into a model based on observations of output quantities computed from model solutions. Two particularly important examples are data assimilation and calibration and computing unobservable quantities from experimental observables.

- Formulation and solution of numerical optimization problems such as simulation-constrained optimization problems and stochastic optimization problems with probabilistic constraints. These problems arise at various levels, from coupling of models for different fusion processes (e.g., solution transfer) to designing systems with desirable behavior.

We can organize these tools, along with the problems to which they apply, into two broad categories.

Numerical Optimization (NO). This category covers a range of problems encountered in fusion science, including reactor design, avoidance and mitigation of instabilities, and plasma control. The mathematical foundation includes large-scale optimization with simulation constraints and discrete variables, optimal control problems with state and control constraints, constrained parameter and state estimation, stochastic optimization with probabilistic constraints, and robust optimization.

Uncertainty Quantification (UQ). This category includes code and calculation verification, validation of models, treatment of experimental data and error, sensitivity analysis, propagation of uncertainty and stochastic variation, stochastic inverse problems and inference, model selection, design of experiments, and detection of critical events.

In Fig. 28 we illustrate the role of UQ and NO as the bridge that enables moving from simulation and experiment to scientific inference and engineering design.

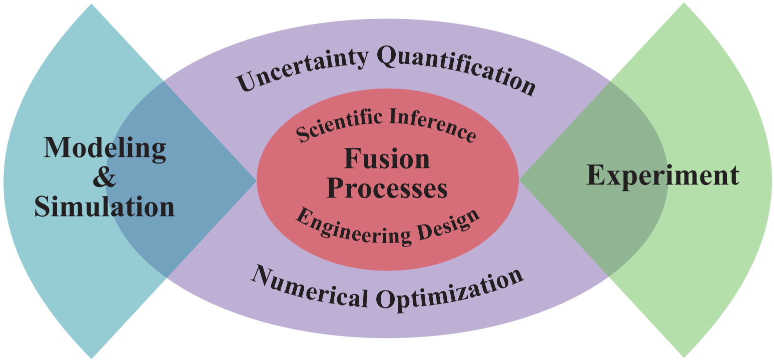


Figure 28: *Uncertainty quantification and numerical optimization provide the tools that enable the combined use of modeling and simulation with experimental observation in order to make scientific inferences about fusion processes leading to the stage of engineering design and control of fusion reactions.*

NO and UQ have a long tradition in many engineering disciplines; but the techniques and mathematical foundations have not been strongly established for the complex multiphysics, multiscale systems encountered in fusion energy science. As discussed in Sec. 5.2.4, these two topics share many common needs, from scientific description to handling of bifurcations and mathematical difficulties related to complex geometries that evolve over time to treatment of experimental data and error. A primary focus of NO is development of convergent algorithms for fusion-related problems. UQ techniques can be applied to both numerical simulations and NO applications and algorithms, including code and calculation verification, validation of models, and stochastic inverse problems. Both activities lend themselves to extreme-scale computing.

Research in UQ and NO for fusion systems begins on a strong foundation advanced by communities both in DOE (e.g., the SciDAC QUEST Institute [21]) and outside DOE. Recent progress in UQ includes a steadily improved mathematical foundation, advances in computational methods, and applications to large-scale simulations. NO has seen developments in a range of methods, both derivative-free and derivative-based approaches, that are applicable to large-scale simulation-constrained optimization problems, increasing treatment of stochasticity and probabilistic constraints in these problems, and the inclusion of discrete and categorical variables.

NO is computationally expensive and requires the equivalent of several forward numerical simulations. By their nature, UQ and numerical optimization under uncertainty, the intersection of UQ and NO, are even more expensive because of the mathematical barrier of the "curse of dimensionality," in which the computational overhead scales exponentially with the effective dimension of the probability space induced by the model's inputs and parameters. Consequently, these problems can always scale to available resources. On the other hand, increasing the computational resources increases the range of problems that can be tackled, leading to a demonstrated increase in impact on science and engineering. Such resources also allow increased robustness, efficiency, and reliability of computational results.

Sophisticated algorithms can further increase the range of problems that can be tackled. Naive algorithms (e.g., employing brute-force computation) can easily overwhelm machines of any size. More advanced algorithms require fewer simulations but involve computing more information from simulations, such as derivatives, and in this way broaden the range of problems that can be solved. Adding UQ and NO capabilities such as derivative and adjoint computations to an existing simulation code can be difficult, however, and numerical simulation developers should consider integration of these tools natively into future simulation codes.

Verification and validation. This report emphasizes the importance of validating the fidelity of fusion models and quantifying the regimes of conditions for which the models are valid. Model validation is a crucial ingredient of scientific inference. Model validation for fusion is a complex undertaking that involves all aspects of uncertainty quantification, although for a more narrowly defined goal. For example, comparing experimental data affected by stochastic experimental error with stochastic model outputs involves the technical problem of comparing nonparametric probability distributions. This comparison is complicated by the fact that the physical processes affecting or included in experiments and models are typically different. In this context, "validation" of computations using comparisons of single realizations of experimental data and simulation results is not very meaningful.

In "classic" verification and validation practice, verification is divided into two aspects: code verification and calculation verification. Code verification is concerned with code correctness: testing to ensure that the approximate numerical solutions converge to solutions of the given model using problem formulations with known solutions. Calculation verification is concerned with estimation of the error in the approximate solution (or quantities of interest computed from approximate solutions) for a problem where the exact solution is unknown; hence it depends on quantitative a posteriori error estimation. Both aspects are necessary for systematic model validation. In practice, however, code verification tends to be a continuous background activity (perhaps even part of regression testing) whereas calculation verification is more closely linked to model validation.

Connection to data management. For many UQ and NO tasks, data management is extremely important, from the management and treatment of experimental data to the storage of intermediate information from forward simulations and the processing of the forward simulation data to efficiently compute sensitivities. The relevant issues are explored in Sec. 5.3.

5.2.2 Crosscutting Fusion Motivation

Fusion problems related to plasma control and operation of the boundary plasma lead to many interesting mathematical challenges and opportunities. A successful reactor design and operating process must address complexities such as microturbulence, instabilities such as Alfvén and MHD modes, dynamical interactions between different behaviors at different spatial scales, and deleterious operating modes causing erosion (disruptions, sawteeth, and edge-localized modes) [wp64]. Addressing these complexities typically involves formulating and solving inverse and numerical optimization problems in the presence of uncertainty. An example of a typical numerical optimization problem is controlling the steady-state plasma shape under an electromagnetic field in tokamaks with a fixed gap of a few centimeters, while simultaneously controlling the plasma instability arising in plasma poloidal cross-sections and keeping the maximum tolerable currents as low as possible. The solution of such numerical optimization problems must be risk-adverse in terms of maintaining safety margins [wp85]. Additional complexities come from the fact that fusion involves coupling of processes across at least three distinct subregions where the geometries for each region can be complex and may evolve over time [73].

The goal is to predict the behavior of fusion processes and to perform engineering design and control of fusion processes. Potential impacts of mathematical progress include the following:

- Building community confidence and credibility in models
- Designing better fusion reactors and demo reactors
- Enabling better design and operation of experiments
- Improving plasma control system performance and safety design
- Determining the dominant uncertainties
- Avoiding disruptions requires high-quality equilibrium reconstruction in real time
- Designing the operation of the boundary plasma

In a number of ways, we can point to the history of the design and operation of nuclear fission reactors to see the strong potential for positive benefits of UQ and NO for the study and engineering of fusion processes.

The problems and techniques associated with UQ and NO are common activities for modern fusion science. These activities have been pursued primarily by application scientists, leading to a set of challenges particular to fusion science. However, UQ and NO are *mathematical* problems, and rigorous mathematical foundations and solution methodologies are necessary for resolving the scientific challenges. Moreover, resolution of some of the mathematical issues promises to lead to increased computational efficiency and broaden the applications that can be tackled. Thus, support of interdisciplinary research between fusion and mathematical scientists is strongly needed.

5.2.3 Challenges and Opportunities

The mathematical challenges arising in fusion science include the following.

- Fusion processes are coupled, complex multiphysics systems, whose models combine descriptions of physical processes of varying deterministic and stochastic nature acting through a wide range of scales. Three coupled systems are (1) core and pedestal, which is important for optimizing core performance consistent with a radiative boundary; (2) transport, MHD, and sources, which is important for addressing the long-pulse steady-state; and (3) scrape-off layer, divertor, and PMI, which is important for addressing plasma and material properties during high heat flux [wp102]. As discussed in Sec. 5.1, significant technical challenges remain for the mathematical and numerical analysis of coupled multiphysics, multiscale systems such as those that arise in fusion.

- Modeling the fusion system and its constituent processes is an active area of research. Some of the processes are not well understood [wp47,wp58], while others can be resolved by a range of models that vary in both the fidelity of the results and the cost to compute [wp110]. The highest-fidelity computational models are extremely expensive to run. The analysis becomes particularly difficult in the context of fusion process characteristics such as bifurcations and other sources of nonsmoothness and geometrically distorted domains that evolve as a function of the state.

- Significant amounts of experimental data for fusion processes are available from both physical and computational experiments, yet only specific kinds of behavior can be observed, while other key behaviors cannot be observed in a quantitative fashion [wp58,wp99]. As discussed in Sec. 5.3, describing and processing the experimental data into forms useful for modeling present numerous challenges. Moreover, testing the physical processes independently is hard or impossible, the physics are profile dependent, and the coupling is tight and nonlinear.

- The results of the numerical simulations are affected significantly by multiple sources of error and uncertainty. Sources or errors include measurement, numerical, and modeling errors. The stochastic elements involve high-dimensional probability spaces with complex structure, and quantifying the stochastic properties of parameters and data can be difficult. The computation of approximate probability distributions using finite sampling of computationally expensive models with high-dimensional input spaces presents serious challenges because of the "curse of dimensionality."

- Understanding and controlling complex fusion processes are difficult. Moreover, the numerical optimization problems have state and control constraints that may not be well understood or modeled, such as the distance to an instability. Operating near an instability, however, may be desirable for peak performance of the device. The design and control problems can include a mixture of continuous (e.g., power, phase, and duration) and discrete (e.g., turn on/off and frequency) decisions. Integer or categorical variables may be involved (e.g., the number of actuators and the types of sensors). In addition, stochastic formulations need to treat physical events of low probability. The probability of such rare events presents a well-known challenge for accurate approximation by finite sampling.

- Determining desirable properties of the models for various activities (from designing feedback controllers to performing uncertainty quantification) can be difficult.

In addition to fundamental mathematics research, interdisciplinary efforts, and specific fusion simulation research, we emphasize that overcoming these challenges involves extreme demands on computational resources. Developing efficient HPC simulations must be a priority.

5.2.4 Strategy and Path Forward

We identify three priority research directions.

[**PRD-BeyondInterpretive-1**] Utilize applied mathematics to develop and rigorously analyze numerical optimization algorithms and UQ methodologies capable of addressing complex, coupled numerical fusion simulations with complicated, evolving geometries.

[**PRD-BeyondInterpretive-2**] Develop joint fusion energy science and applied mathematics activities in numerical optimization and UQ to formulate relevant and impactful applications, leverage existing methodologies, develop new capabilities, and identify gaps that need to be addressed.

[**PRD-BeyondInterpretive-3**] Support the extreme-scale computing needs for numerical optimization and UQ by devising new algorithms and providing appropriate computational resources.

Achieving these goals requires a parallel effort in mathematical sciences research.

Scientific description. A strong need exists to establish interdisciplinary collaborations among experimentalists, modelers, computational physicists, and mathematical scientists in order to define and continuously refine the UQ and NO activities [74]. The definition and goals of the UQ and NO efforts must evolve in scope and rigor as the understanding of physics, mathematics, and computation advances. A key ingredient to the successful application of mathematical techniques to scientific fusion questions will be the clear definition of those questions by the fusion community. Working together, fusion and mathematical scientists must prescribe details such as the following [73,74]:

- Sequences of models for different phenomena, for example, what the models can represent about the processes and the scale of validity
- Identification of important inputs, parameters, and variables input into models, including definitions of variable ranges and domains and information concerning uncertainty and variation in the values
- Widely accepted set of quantities of interest characterizing crucial properties of fusion processes
- Scientific and engineering questions to be addressed, and acceptable ranges of uncertainty in answers

Treatment of experimental results. As discussed in Sec. 5.3, a significant amount of experimental data about fusion processes is available, but many research challenges are involved with processing experimental data into forms useful for mathematical models. These are complicated by incomplete understanding of fusion processes and by a number of puzzling experimental observations.

One of the chief mathematical challenges is the fact that processing observable data into desirable quantities useful for modeling often requires formulating and solving an inverse problem for physics-based mathematical models, which themselves have a complicated nature. Another challenge is that the data has to be accompanied with mathematical descriptions of the uncertainty and range of error for the data values. In many cases, systematic statistical tools are needed for filtering experimental results in order to remove "bad" or misleading values from data sets. Another challenge is developing feasible validation techniques for coupled multiphysics models, where experimental results are available only for components of the system process [wp30,wp50,wp53,wp58,wp76,wp78,wp99,wp102][74,75].

The needs of verification and validation of simulation results place extra demands on data processing, including complete documentation of assumptions, conditions, and range of validity of both simulation and experimental results. These issues are explored fully in Sec. 5.3.

Treatment of mathematical complexities arising in fusion processes. Fusion presents unique challenges to mathematical analysis of models, UQ, and NO. For example, the domains for different spatial regions of fusion reactors have complex shapes with characteristics that are difficult to treat, including extreme narrowness, interior convex corners, lack of convexity, and highly curved boundaries. Moreover, in high-fidelity simulations the regions evolve in time as a function of the state. Thus, the geometry of the spatial regions both affects the accuracy of computed solutions and is affected by numerical errors in computed states.

Fusion models consist of a mixture of elliptic, parabolic, and hyperbolic systems that typically exhibit bifurcations in relevant parameter domains. For example, dominant bifurcations include transport confinement bifurcations (L-H mode transition, internal transport barriers) and macroscopic instability bifurcations. The presence of bifurcations can result in strong local changes in model behavior and/or loss of regularity in solutions, which in turn may have a strong effect on the accuracy of both numerical simulations and approximation of stochastic structure.

Another example of mathematical complexity is the need to evaluate threshold conditions for fusion processes in the presence of numerical error and stochastic uncertainty [73].

Development of UQ and NO methods for fusion models. Fusion models present significant mathematical challenges arising both from the complex nature of the partial differential equations representing component processes in fusion and from the coupled multiphysics formulations of system-level models. In particular, the development of UQ and NO techniques for coupled models is far less developed than for "single physics" models, and there is a strong need for development of theory and efficient computational UQ and NO algorithms and error estimation for complex multiphysics fusion models.

On the level of modeling, there is a strong need to develop and mathematically analyze physically grounded approaches for coupling models of different physical processes, especially in the situation of different kinds of descriptions (e.g., stochastic and deterministic). The coupling between components introduces significant errors into simulation; this problem needs to be analyzed mathematically.

On a mathematical level, there is a need to understand how to define and compute first- and second-order derivative information for model outputs for coupled physics models, including the development of efficient high-performance algorithms. One aspect of this problem is the proper definition of adjoint operators associated with coupled physics models, along with algorithms for the approximation of adjoints [wp53,wp78,wp92,wp95,wp102][73,74].

Propagation of stochastic variation/uncertainty. Probability distributions are commonly used to model experimental error, natural stochastic variation, and uncertainty in model input parameters and data. The consequence is that output quantities computed from the models have a stochastic nature that is described completely by probability distributions and partially by statistics such as the mean and variance. The "forward propagation" problem is to approximate the output probability distribution, or some statistics, for the targeted output quantities.

Since fusion models are complex, approximations of output probability distributions and statistics are affected by issues such as numerical simulation error and model error, both of which are significant. In addition, available physical models for various component processes often vary in terms of both fidelity to the physics and computational cost of evaluation. On the stochastic side, the dimension of the space of inputs for a fusion model is large, which has a strong negative impact on the accuracy of sampling techniques such as Monte Carlo methods because of the "curse of dimensionality." All these factors place a high premium on development of efficient high-performance algorithms for the forward propagation problem.

Also needed are quantitative a posteriori error estimates for computed statistical information from fusion models that quantifies both deterministic (e.g., numerical error) and stochastic (e.g., finite sampling) sources of error. Additionally, algorithms are needed for selecting discretizations, models, and samples in order to achieve a desired accuracy in output quantities as efficiently as possible. A key aspect of achieving such efficiency is devising algorithms for reducing the dimension of the input space for fusion models by determining which parameters and data have the most effect on targeted output quantities.

Reduced-order methods and surrogate models also need to be explored in order to decrease the cost of computing sample solutions and the use of multifidelity statistical models. Many statistical techniques have not yet been extended to treat coupled physics models.

Fusion also presents special challenges for forward propagation. One challenge is the use of stochastic models for complex physical processes, such as the use of averaging and finite sampling to model chaotic stochastic systems and turbulent dynamics. Another is the need to estimate the probability of extreme values of functionals of model solutions that are forced stochastically where the extreme values occur with low probability [wp11,wp17,wp30,wp38,wp53,wp76,wp78,wp83,wp 92,wp95,wp110] [73].

Formulation and solution of inverse problems. The inverse problem lies at the heart of the challenge of combining experimental data with complex fusion models in order to predict and control the behavior of fusion processes, calibrate models, and design physical and computational experiments. For example, parameter and state estimation is concerned with inferring unknown model inputs characterizing a physical process, such as parameters, source terms, initial or boundary conditions, and/or model structure, from experimental observations of model output. Also, processing experimental data to obtain quantities useful for modeling often involves solution of an inverse problem for a physics model. The formulation and solution of inverse problems for coupled multiphysics models are relatively underdeveloped in mathematical terms at present.

The inverse problem for fusion has several characteristics that offer challenges for mathematical sciences and computation. In general, the inverse value for a single model output consists of a manifold of possible corresponding values, a generalization of a contour curve in higher dimensions. Special formulations of inverse problems are particularly important for fusion science. For example, data assimilation is concerned with the serial incorporation of data into models in order to refine model and improve model predictions. Another example is optimal experimental design to help guide experimentation, data acquisition, and sensor placements in order to maximize the information obtained from experiments while minimizing costs.

Moreover, inverse problems for fusion research will generally be stochastic. For example, when the observations on the output are subject to experimental error that is modeled stochastically, then the inverse problem requires computing a probability distribution for the inverse solution. This stochastic inverse problem also suffers from the "curse of dimensionality" that complicates the accurate approximation of the solution [wp11,wp17,wp85,wp92] [73,76].

Numerical optimization problems with constraints and uncertainty. Constrained numerical optimization problems for coupled systems of partial differential equations arise naturally in the study of fusion processes and the design and control of fusion reactors. Fusion processes complicate the formulation and solution of numerical optimization problems. The number of control and design variables can be extremely large, while design variables span a number of components in a system model. Extending methodologies to handle complex geometries that evolve over time in response to the state is a challenge. Moreover, the constraints and objectives generally have a stochastic nature, thus requiring the formulation of a stochastic optimization problem. A number of simulation issues such as numerical error and model fidelity affect the computation of an optimal solution. In addition, the computation of derivative information is a complex issue in the context of coupled multiphysics models. We also note that application to fusion involves treatment of discrete and categorical variables.

Thus, algorithms must be formulated, developed, and analyzed for various numerical constrained optimization problems with characteristics ranging from simulation constraints to state and control constraints and probabilistic constraints. In general, robust methodologies and solutions are needed that minimize the risk of failure arising from various sources of error and stochastic variation. These are particularly important in the context of numerical optimization problems determining failure events [wp64,wp85,wp110] [76].

High-performance UQ and NO algorithms for fusion processes. Many standard approaches for UQ and NO for physics models treat the models as "black boxes" requiring only model evaluation for specified input data and parameter values. While this approach minimizes the need to alter model simulation codes, it raises significant barriers to devising algorithms for UQ and NO that obtain true efficiency on high-performance computers. Because a single high-fidelity fusion simulation is already prohibitively expensive in terms of computational cost, and the "curse of dimensionality" means that solving any UQ or NO problem requires significant numbers of simulations, a strong need exists to develop and implement efficient algorithms for UQ and NO computations in coupled multiphysics fusion models.

An example is the native implementation of methods for computing derivative information, for example, automatic differentiation, finite difference, and analytic techniques. In the context of coupled multiphysics models, research is needed on how to obtain system-level derivative information from derivative information for component models. Such component derivative information may be computed by using different techniques with different error terms, and coupling further complicates the analysis. Some components may not provide derivative information, but other available derivative information still must be used to obtain partial system-level derivative information. Furthermore, higher-order derivatives, such as Hessians, can be beneficial for numerical methods; methodologies for obtaining such high-order system-level derivatives need to be developed. Architecture-dependent checkpointing algorithms for extreme-scale machines that consider, for example, the memory/disk hierarchy would improve the efficiency of adjoint calculations. In general, the embedding of tools to enable efficient solution of UQ and NO problems requires a paradigm shift in developing codes for fusion simulations, given the past emphasis on producing model solutions [wp85][73,74,76].

5.3 Data Management, Analysis, and Assimilation

Scientific discovery is driven by exploitation of data. However, extreme-scale computing, new computer architectures, the growing complexity of scientific processes, and the increasing importance of extended collaborations challenge traditional approaches to data assimilation, analysis, and visualization for integrated fusion simulations. Scattered efforts have begun to address these gaps; but a more concerted, coordinated effort is required. The need for a more systematic, community-based approach to data and metadata was widely recognized in the whitepapers. Also widely recognized were the challenges imposed by I/O limitations on existing and future computing platforms. This report tries to capture the challenges through a set of use cases that illustrate the real-world applications for new capabilities.

5.3.1 Background and Recent Progress

Careful management of data and associated metadata is a critical part of any scientific enterprise. Unfortunately, most current fusion simulation efforts lack systematic, projectwide organization of their data. At the same time, extreme-scale computing, new computer architectures, the growing complexity of scientific processes, and the increasing importance of extended collaborations challenge traditional approaches to data assimilation, analysis, and visualization. Already, I/O considerations in high-performance computing have imposed restrictions that limit the range of postprocessing tasks available to users. In addition, for data to be fully useful, to share its meaning among a collaboration, and to retain its meaning over time, it must be enhanced with sufficient metadata to explain its origins and use and to place it into the context of the scientific enterprise that created it. Currently no widely adopted and systematic approach to these issues exists within the fusion community [wp37].

However, some efforts have begun to address these challenges. For experimental data, the MDSplus system [77] has emerged as a de facto standard. In MDSplus, data is stored in a set of self-descriptive trees, which also contain information to drive a workflow engine—the dispatcher—which executes data acquisition and analysis tasks. This guarantees the recording of a minimum level of metadata and provenance information for automated acquisition, processing, and analysis. In practice, however, a good deal of analysis is also carried out under manual control, leaving the provision of the more complete level of metadata to individual users. In order to address this issue and the analogous set of issues for simulation data, a project was initiated in 2012 [78–81], called the MPO (Metadata, Provenance and Ontology). MPO researchers have developed a web service, based on a RESTful API [82] that allows users to instrument any analysis script with callouts that automatically populate a database, documenting their scientific workflows to their preferred level of detail [83]. Data and all processes that create or modify that data are represented mathematically as a directed acyclic graph, providing explicit information about the relationships between elements. A web interface allows workflows to be navigated, searched, or browsed. Another noteworthy activity, ElVis, allows running computations to export live updates in the form of data visualizations [84]. These can serve a real-time monitoring function for long-running jobs [wp89].

Fusion data comprising millions to billions of individual particles has been a visualization challenge that has required specialized rendering platforms, such as the Manta ray-tracing system [85], to display all the data in an interactive setting (see Fig. 29). Alternatively, tools such as FastBit [86] allow fast index range-based queries, thereby limiting analysis and visualization processing to the subset of data that is of interest (a process known as "query-driven visualization" [87]). These tools, deployed in systems such as VisIt [88], have allowed fusion scientists to explore their data in a semi-interactive setting. Fusion-specific analysis tools that allow scientists to follow the

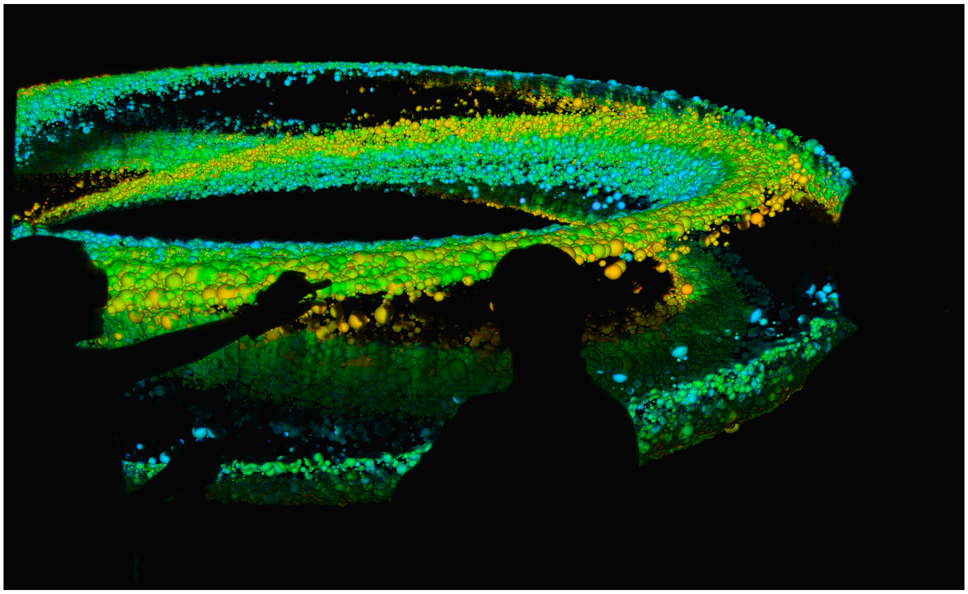


Figure 29: *Visualization of gyrokinetic particles from a magnetic fusion simulation using the GTC simulation code. This visualization is displayed by using the Manta ray-tracing system on the large display at the SCI Institute's Evans Visualization Center. Data courtesy of S. Ethier (PPPL). Image courtesy of A. Sanderson (Univ. of Utah).*

time-dependent topology of the magnetic field have also been developed [89]. Such tools have been extremely important because they are code independent and can be deployed in either in situ or post hoc fashion.

The SciDAC Scientific Data Management, Analysis, and Visualization (SDAV) Institute [23] focuses on developing and deploying methods that enable scientific knowledge discovery on DOE HPC platforms. SDAV has been engaged with the fusion community in several different ways in recent years. For example, one project involving SDAV personnel and members of the XGC code team has focused on enabling study of high-resolution edge effects using a combination of in situ infrastructure coupled to XGC and modern visual data exploration and analysis infrastructure (see Fig. 30). Another fusion-facing project in SDAV has focused on analysis methods for finding features known as blobs [90]. Figure 31 shows the output from two consecutive timesteps from XGC1 simulation of plasma in an ITER model. The output is from synthetic diagnosis that mimics what might be observed through gass puff imaging (GPI). The parallel implementation of this blob detection algorithm has been demonstrated to have sufficient response time that it could possibly keep pace with GPI devices on fusion tokamaks. Furthermore, with a suitable distributed workflow engine [91], this feature detection work can be conducted in near-real time [92].

The SDAV mission also includes maintaining production-quality visualization and analysis software infrastructure and extending it in ways that are useful for science communities. One good example is visual data exploration of high-dimensional data from fusion simulations (see Figs. 36 and 37), in which a specific need of the fusion community was met by adding a new method to a production-quality visualization application (VisIt), which is freely available for download and is installed and supported at all DOE facilities.

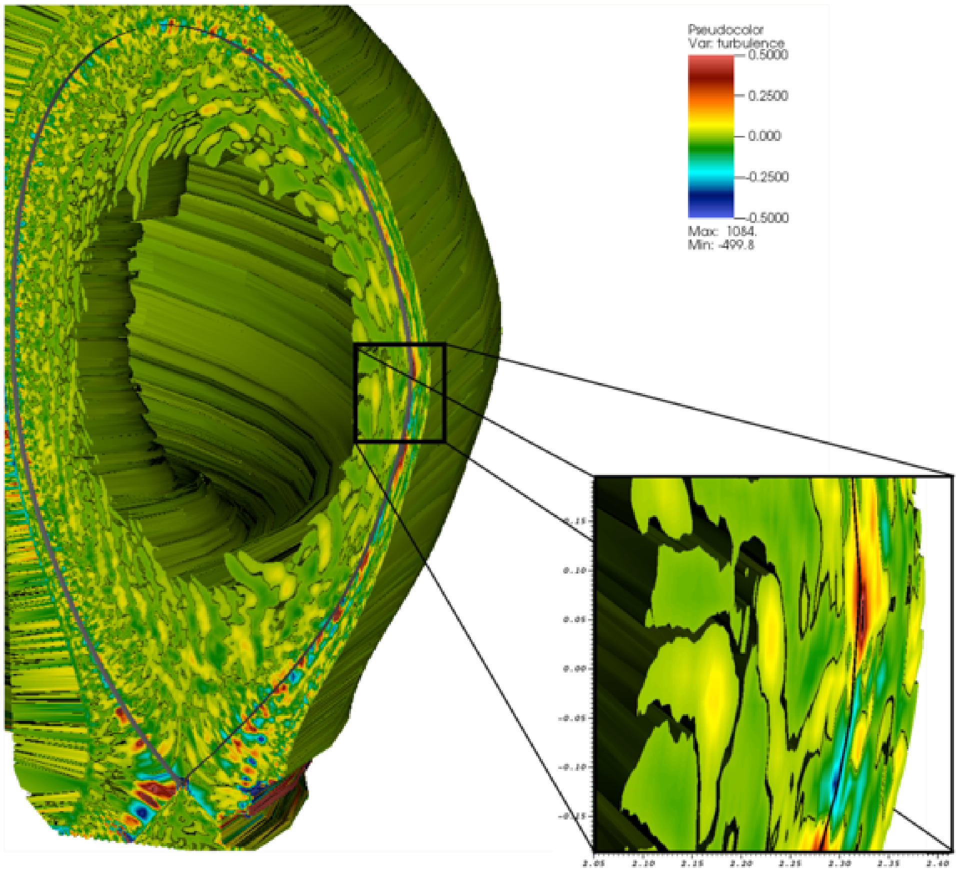
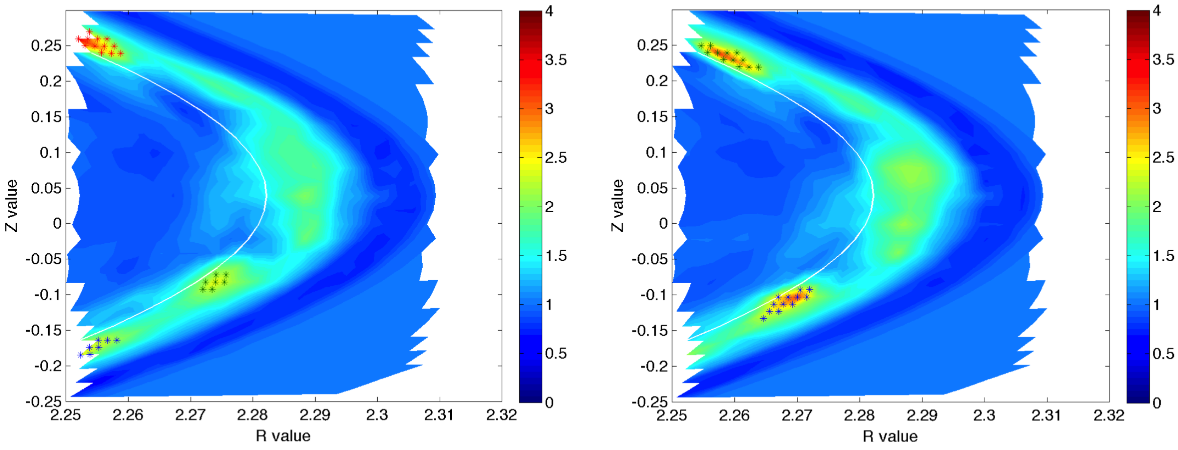


Figure 30: *Visualization showing the turbulence front from the plasma edge being spread inward in multiscale interaction with the evolving background profile under the central heat source. Eventually, the whole volume becomes turbulent, with the spatial turbulence amplitude distribution being just enough to produce the outward heat transport to expel the centrally deposited heat to the edge. The edge turbulence source is continuously fed by the heat flux from the core. This is how the plasma profile, the heat source, and the turbulence self-organize. Image courtesy of D. Pugmire (ORNL).*

5.3.2 Crosscutting Fusion Motivation

The motivation for data needs in integrated fusion simulations is perhaps best understood by referring to four use cases, which are "composites" of the material submitted in the whitepapers and augmented by discussions in several fusion panels.

Use Case 1: In situ calculations within large-scale computations. A researcher is running the transport component as part of a multiphysics integrated simulation on the latest HPC platform. The user needs to perform calculations with data that is not available as written output, specifically (1) to compute turbulence-driven energy flow between scales; (2) to compute impurity transport via modeling the impurity as a passive scalar advected by the turbulent flows; (3) to implement a synthetic diagnostic that requires the full time and space resolution over the full spatial domain (see Fig. 32); (4) to exchange information between physics components; or (5) to record provenance information describing the in situ workflow, including the calculations described in several whitepapers [wp12,wp20,wp22,wp51,wp52,wp61,wp83,wp116].



Blobs from timestep 63 Blobs from timestep 64

Figure 31: *Detection of elongated filament structures in the plasma edge ("blobs") on the synthetic diagnosis output from an XGC1 simulation of the NSTX device. Image source: Wu et al. 2014 [92].*

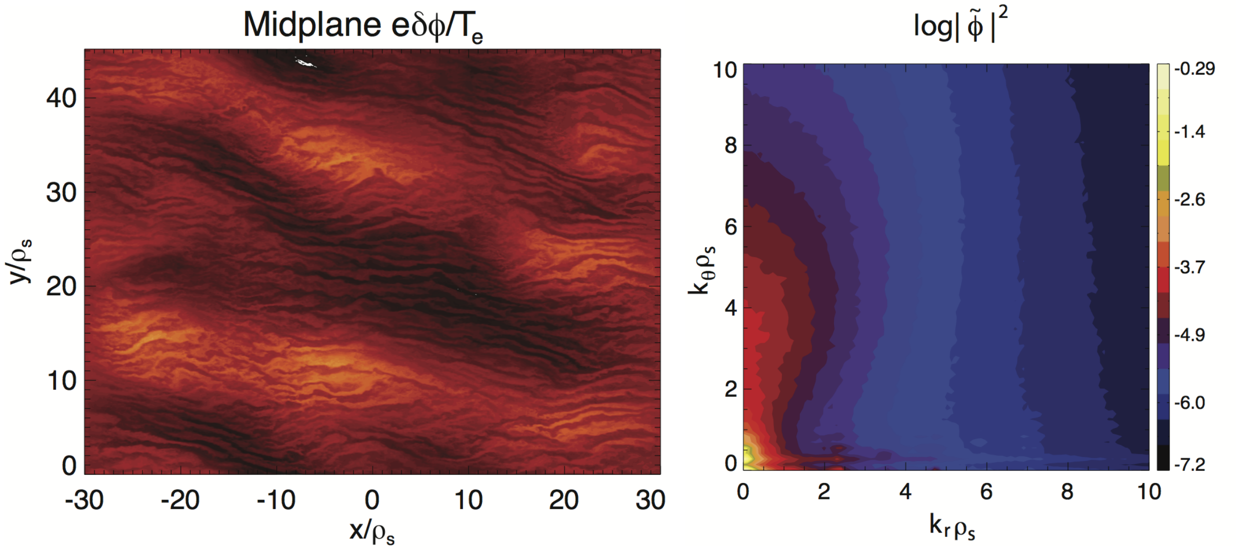


Figure 32: *Normalized electrostatic potential fluctuations in real (left) and wavenumber (right) space from a large multiscale plasma turbulence simulation using the GYRO code [93]. This calculation included both ion and electron-scale dynamics requiring 15 million core-hours to complete [94]. The simulation shows the coexistence of radially extended ETG streamers and the larger ion temperature gradient features explaining the experimental levels of electron heat transport and profile stiffness. Sufficient I/O is not available to do all the desired analysis and visualization, as discussed in Use Case 1. Image source: Howard et al., 2014 [94].*

Use Case 2: Well-documented validation and uncertainty quantification activities. A set of experiments is performed as part of a large collaboration to test the predictions of a computational model. A rich set of metadata, including data provenance, definitions, and access information, is available from the experiment. Some of this data is used as input for the simulation. The entire simulation workflow is documented and annotated. The simulations are catalogued to provide more transparent access for the collaboration. Comparisons are carried out between the experiment and simulation outputs. The results of the comparisons are also catalogued with a rich set of metadata. When the results are published, the publication is linked to all the data used. All of the results can be traced through all of the processes and computations back to the original input data, parameters, and assumptions. The metadata allows the data to retain its meaning over an extended period of time [wp12,wp22,wp37,wp48,wp61,wp73,wp74].

Use Case 3: A crisis in data provenance. After several years, a problem with the original data is found—a calibration error is uncovered in a critical measurement over a period of time that includes the studies described in Use Case 2. The new calibration is applied, and the raw data is now correct; but researchers need to determine whether any of the miscalibrated data was used in the simulations or for the subsequent validation comparisons. If the measurements were used, did they have a significant impact on the published results? The researchers use the metadata and provenance information and establish that indeed some of the incorrect data was used. (They also find numerous other cases where this data was used, presented, and published.) The simulations are rerun, using the stored metadata to guarantee that the same calculations are done. The effects of miscalibration turn out to be small but measurable. An erratum is published in the original journal [wp37,wp50].

Use Case 4: Near-real-time data analysis in support of decision making. For fusion experiments, control room decisions based on analysis, visualization, and assimilation of data in near-real time are essential for activities such as preventing disruptions (see Sec. 4.1.1). A research group would like to expand this operational model by extending the analysis into the realm of HPC. This activity requires the solution of several problems. First, data preparation must be automated. To this end, the team has applied machine learning techniques, such as Gaussian process regression, to their data, providing automated profile fits and uncertainty estimation. The second set of issues concerns streaming the processed data to HPC systems, marshaling the required resources, and returning results in a timely manner. The "feedback loop," originating at the experiment and going over the network to the HPC center and back again to the experiment, could include a set of researchers who are conducting the experiment remotely, with the assistance of personnel on site. Given the cost of operating large experiments, all these activities must be conducted in a reliable, time-constrained fashion [wp21].

5.3.3 Challenges and Opportunities

We summarize our findings as follows.

Need for data and metadata systemization within each project and for community data and metadata standards. A well-defined data "standard," or "data model," including appropriate metadata definitions and infrastructure, is a central activity for ensuring the robust success of any scientific community and endeavor [wp48]. Currently, however, data resulting from both experiments and simulations lacks a widely used systemization for data, metadata, and provenance throughout the workflow, inhibiting the natural collaborative nature of data production, analysis, and dissemination. Because of their larger scale, experimental teams have made more progress toward these goals than have simulation teams. Nevertheless, exchange and comparison of data between experiments tend to be as labor intensive as between different simulation models. Data provenance and metadata are also crucial for protecting the investment in data. Incentives do not always align with the desired outcome. Foundational software is expensive to develop, but projects may be transient. Overall, the data created may have a much longer useful lifespan than do the simulation codes used to create them. Several of the workshop participants noted that the fusion community would be well served to take a long-term view of investments in data technology, to think of data lifespan in terms of decades (if not longer), and to design and implement solutions that will facilitate longevity of data [wp74].

In addition to the improvements each project can make to advance its systemization of data and metadata, a concerted effort to develop community-wide standards, even if incomplete, could bring significant value. Community-centric data standards have taken hold in many domains and enable collaboration on larger projects by larger communities than has otherwise been possible in the past [wp48]. Examples abound, including the Climate and Forecast convention used by the worldwide climate community [95], which defines metadata that provide a definitive description of what the data in each variable represents and the spatial and temporal properties of the data. This enables users of data from different sources to decide which quantities are comparable, and it facilitates building applications with powerful extraction, regridding, and display capabilities. Another example is the HDF-EOS format, which has been used in production by NASA since 1999 as the format for storing and archiving a wealth of data from satellites [96].

Community-centric data standards for the fusion community offer a number of potential benefits [wp48]. A community-centric data standard opens the potential to eliminate many of the challenges that arise when exchanging data with colleagues or the community. It enables the community to reach a critical mass that entices commercial and open source tools that support the standard, reducing the effort spent within the community creating one-off tools for specialty data formats. It offers the potential path to partly address the software sustainability problem, where the lifespan of project-centric software efforts is vulnerable to lapses in individual project funding.

In fusion, de facto standards have emerged, but no concerted effort has been undertaken in this direction. MDSplus [77], IMAS [97], and EFIT eqdsk files [98] are examples of data standards that facilitate data exchange and collaboration, demonstrating that the advantages from sharing can drive behaviors in productive directions even in the absence of broader coordination. While promising, however, these efforts are not sufficiently broad enough in scope to accommodate the requirements of the fusion community, which include the need to collect and manage provenance [wp12,wp37,wp74] from simulation and experimental data repositories of enormous size [wp21,wp51] and with all their associated metadata. The name spaces for fusion-related data are huge: for existing experiments they can run to 10^5 named items (ITER is planning for 10^6) and on the order of 10^5 instances of each.

A community-centric data model requires up-front investment, including, nontrivially, community agreement; but it has a payoff in the form of reducing, if not eliminating, the redundant effort resulting when each individual researcher “rolls their own” data format. With a community-centric data model, researchers can quickly share both data and software tools for working with such data—essentially reducing an $N \times M$ problem to order N. The degree of standardization need not be absolute to be useful. At a minimum, however, shared data models, abstractions, and vocabulary supporting the full diversity of data types and metadata are essential.

Data standards would dramatically enhance the ability to search for, access, browse, and work with a diversity of data. One may wish to find calculations that meet specific criteria or to find and reuse workflows. These types of needs highlight the important interplay among metadata, provenance, data models, and formats; the potentially long lifespan of data; and the software infrastructure that implements these capabilities. The ability to search for data relies on the ability to have something to search for (the source of which is metadata), as well as somewhere to look for such data. Thus the metadata must be shared or federated in a way that is convenient to data consumers. The metadata must also provide sufficient information on data location and format to retrieve the underlying data, assuming the user has permission. This requires the existence of federated or centralized data repositories and an archive that is widely accessible, long-lived, searchable, and browsable.

Need to support in situ methods. The growing scale of data from fusion simulations presents challenges that cannot be met by conventional approaches. Simulations such as EPSI routinely generate checkpoint files that are on the order of petabytes per day, and these are expected to similarly grow in size by an order of magnitude in the next five years [wp20]. XGC1 generates about 4 TB of data every 30 seconds on Titan, a data rate that exceeds the 50 GB/s capacity of Titan's filesystem [wp22]. And even if writing such datasets to persistent storage were possible, working with such datasets is difficult and time consuming; and systems with sufficient memory and I/O capacity to postprocess such data are not always readily available [wp51]. The transition to exascale computing will only aggravate this situation.

Currently ORNL's Titan machine has a peak computational rate of about 27 petaflops, a memory footprint of about 710 terabytes, and an I/O capacity of about 1.4 TB/s [31]. NERSC's Edison has a peak computational rate of about 2.5 petaflops, a memory footprint of about 357 TB, and an I/O capacity of about 168 GB/s [99]. In a 2009 report, projections for exascale class machines have computational capacity growing by 3 orders of magnitude, while I/O capacity is projected to grow only by about 1 order of magnitude [100]. More recent information in presentations suggests that while the computational capacity is still projected to grow by 3 orders of magnitude, the I/O capacity will grow more modestly, perhaps by as little as a factor of 2× to 4× over present (2015) levels. The implication for computational science projects is clear: it is going to be increasingly, perhaps prohibitively, expensive to save data to persistent storage for subsequent analysis and visualization.

One approach that has the potential to address these challenges is in situ processing, where analysis, visualization, and other data-centric operations are conducted while simulation data is still resident in memory (see, e.g., Fig. 33). The term *in situ* is generally used to refer to a family of different approaches, ranging from purely in situ (i.e., in place), where data does not move at all, to *in transit*, where data is moved from cores or nodes performing the computation to other nearby nodes or cores for visualization and analysis processing. These approaches avoid the increasingly prohibitive cost of I/O while providing the ability to perform key analysis operations. An additional benefit is the potential to perform analysis operations on data at full spatiotemporal resolution: for example, from the calculation that created Fig. 32 [wp51]. These codes often do postprocessing for "synthetic diagnostics," a method essential for code validation. The required frequencies or spatial coverage may not be available at the coarser sampling rate and resolution of the save files but would be available with in situ analysis. These problems are arising well below the exascale. In the future autonomous selection of key features in data will be needed in order to trigger data writing, analysis, or visualization [wp75].

Three primary fusion community needs can be identified in the in situ space. The first is for production-quality, petascale- and exascale-capable in situ software infrastructure. The second is for algorithmic implementations that will run in these infrastructures, algorithms that meet specific fusion science needs. The third is for effort to actually assist in modifying codes to use in situ infrastructure as well as to develop and deploy fusion-centric in situ analysis methods.

While some in situ implementations support some notion of "zero-copy operation," where the in situ methods operate on data in the same address space as the simulation, many other types of in situ operations, as well as coupled-code models, require movement of data from one set of cores or nodes to another. As with the broader in situ topic, this set of challenges involves two dimensions. The first is the need for robust, reusable infrastructure for moving data between coupled code components, regardless of whether the application is a coupled-code integrated sim-

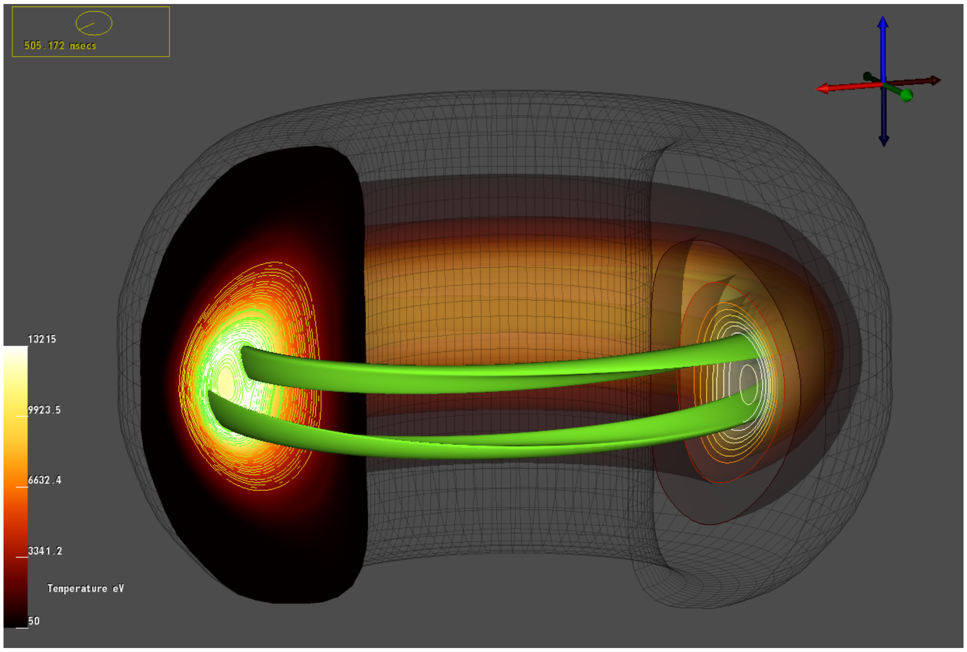


Figure 33: *Visualization of the magnetic field topology and the breakup of magnetic flux surfaces into a series of island chains with a 2:1 island chain that dominates the inner core of the simulation [89,101]. Such visualization and topological analysis can be performed by using in situ or post hoc approaches. Image courtesy of A. Sanderson (Univ. of Utah).*

ulation [wp26,wp42], or between processing stages of an analysis workflow coupled with a running code [wp20]. The second need arises when the data exchanged between processing stages, or different modules of a coupled code, needs to undergo some sort of transformation. This situation arises, for example, when the cooperating codes have different mesh types or different units of measure for data. Whereas infrastructure for moving data is arguably general purpose, operations such as data transformation are highly domain-specific.

Fortunately, the need for production-quality in situ infrastructure is not unique to the fusion science community. ASCR recognizes that this need cuts across essentially all areas of computational science and is making investments in this type of software infrastructure. The kinds of algorithms and methods that would run in situ are potentially diverse, but the main point here is that the fusion community has some specific needs for analysis and visualization and that algorithm design and code implementation are a fusion-focused activity.

While in situ methods hold much promise for bridging the widening gap between compute and I/O capacity, codes will still need to write data to persistent storage. Hence, the role of I/O infrastructure is still on the critical path for the fusion community going forward. Some of the specific needs are for stable, production-quality I/O infrastructure that performs well on large HPC platforms, is easy to use, has sufficient flexibility to support a variety of different use modes (e.g., "pulsed" vs. "streamed"), supports inclusion of arbitrary metadata, provides a growth path to future storage systems (e.g., those that are object- or record- rather than file-based), and can be counted on to be around for a long time [wp48].

Need to capture and document scientific workflows. Workflows (see, e.g., Fig. 34), which may be thought of as a chain or sequence of processing steps executing on a single machine or multiple machines, come in several varieties. Here, "processing steps" refers to any number of potential operations, including analysis, visualization, data reorganization, data compression, data reduction/subsetting, data indexing, data movement, and data storage. An in situ workflow executes a sequence of processing operations performed on the same machine as a simulation, while data is still resident in memory on the simulation platform. Ex situ workflows execute a sequence of operations on machines external to the simulation platform, but they may be executed concurrently with the simulation. Post hoc workflows use as input data written to persistent storage, either by a simulation or from an experiment. All cases share a number of common themes, challenges, and needs; and all play a key role in a diversity of MFE science projects.

As discussed in Sec. 5.2, verification and validation with uncertainty quantification present perhaps the most demanding and complex set of workflow requirements, entailing a combination of in situ analysis for uncertainty analysis and movement of data from an experiment to simulation for validation studies. Without integration of metadata, workflows, and data provenance from in situ and ex situ processes, the chain of provenance is broken; and what could be a coherent body of data becomes fragmented. The community needs tools that facilitate recording of provenance in a wide range of contexts and workflows and tools that enable the creation and usage of standard data dictionary in the service of collaboration, search, data discovery, and browsing.

The concept that workflows are central to many different science domains has the attention of the computer science research community. ASCR hosted a workshop in April 2015 titled "Automating Computational Workflows for DOE Scientists" [102]. The central findings of that workshop, which also reflect ideas from the 2013 ASCAC Data Subcommittee report [103]), are that although workflow concepts hold much promise for streamlining and accelerating computational and data-centric activities across a broad range of sciences, numerous research and practical challenges still remain.

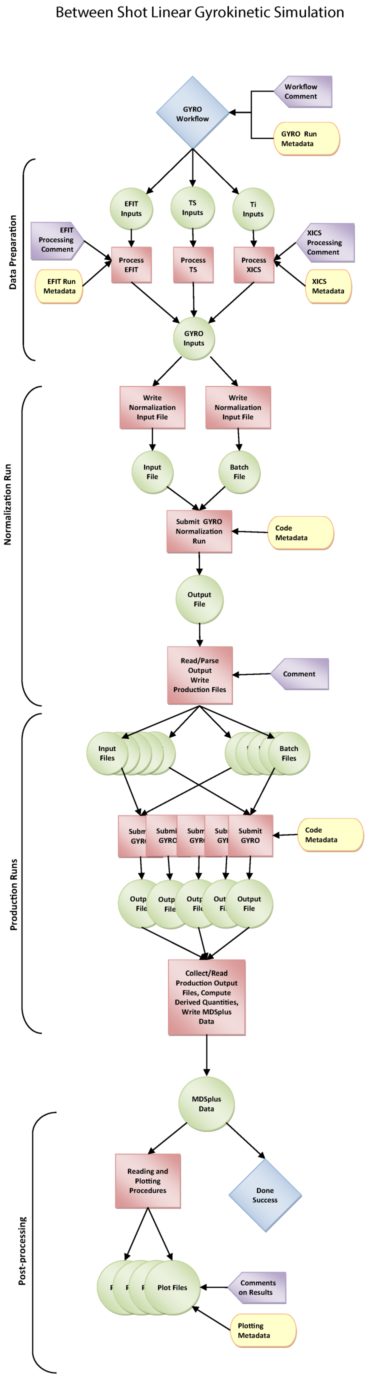


Figure 34: *Workflow for preparing inputs and running a gyrokinetic simulation similar to the one shown in Fig. 32. Image courtesy of M. Greenwald (MIT).*

The traditional laboratory notebook is the paradigm for workflow capture. If properly used, it records the purpose and intent of the scientist, the methods of investigations, a description of any apparatus or measuring schemes, the data recorded, the analysis methods including any assumptions, the results of analysis, and the final results of the experiment and conclusions. Essentially it tells the complete story of the research with nothing important omitted. Modern technology has made each of these steps more powerful and more complex but has fragmented the information into a bewildering collection of disconnected files and records. Thus our challenge is to rebuild the former capability in the modern environment.

Efforts in this direction have begun. In the United States, the Metadata, Provenance, and Ontology Project stores provenance and descriptive metadata and allows users to search and browse information about the workflows they or their collaborators have performed [wp37]. Rather than requiring users to adopt a particular workflow engine, this project allows users to "instrument" any workflow tool with callouts using a RESTful API. A web server provides a live display of the workflow as it is executes—providing a monitoring function and a lab notebook style interface with modern searching and browsing capabilities. Work with a similar set of goals has begun in Europe [104], where the approach is to create wrappers for each existing code or procedure. Discussions between the two groups about possible collaborations has begun. The ability to capture and store metadata about workflow processing steps, along with information about data—from experiment or simulation—is acutely needed, along with implementations that have a low barrier to entry and that are sustainable over a long period of time. Taking a broad view, this type of capability would span a broad set of activities, beginning with data collection and generation, and including all intermediate processing steps, through data curation and publication of results.

Projects such as the IPython Notebook offer the ability to compose workflows, which include simulation and data manipulation, analysis, and visualization operations and are an integrated environment for workflow development and execution. Centers such as NERSC are beginning to deploy this kind of capability in support of science projects. [wp61].

Additional fusion-specific visualization and analysis challenges and opportunities. One of the current visualization exploration challenges is the higher-dimensional aspects. Fusion simulation data may be 4- to 6-dimensional: two or three spatial dimensions, a temporal dimension, and two or more dimension in some other space, like velocity or energy. Figure 35 is an example showing a time-evolving field with energetic particles colorized by their energy. While one can abstract such higher dimensions with methods such as parallel coordinates [105], visual data exploration and analysis can be difficult. More often the fusion scientist reduces the dimensionality of the data by fixing one or more spatial dimensions while exploring the velocity space, or vice versa.

Recent work in the area of high-dimensional visualization includes extending commonly used data subsetting techniques to account for the underlying multidimensional nature of the data. For example, a "slice" in a spatial dimension of one variable, which is a familiar data subset selection metaphor, produces a data subset that is the extraction of a high-dimensional dataset in the same spatial dimension (see Fig. 36), revealing specific phenomena of interest. Then, with this subset, additional analysis can be performed on that high-dimensional subset over time to track the evolution of the phenomena of interest (see Fig. 37). This capability was developed as part of the SDAV portfolio through interactions with the fusion community and is now included in the freely downloadable production version of the VisIt visualization software application [107].

Another form of high-dimensional visualization and analysis arises when considering uncertainty and variability. The fusion community has identified uncertainty as something that needs to be included as part of the end-to-end process, from data collection to analysis, visualization, publication, and data curation. Ensemble analysis methods have been called out as needs for better understanding model sensitivities in multiscale gyrokinetic model development [wp52]. Some prior work exists in the area of visualizing uncertainty [108], as well as in visual data exploration and

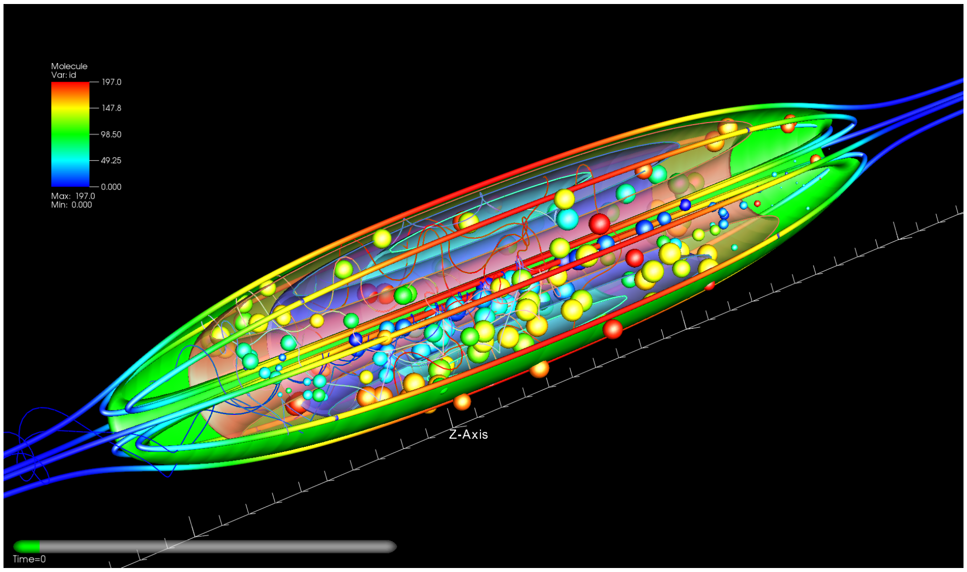


Figure 35: *Visualization of a hybrid kinetic-MHD simulation; dynamic field plus 5+D particles [106]. Analyzing such large amounts of multivariate data was facilitated by interactive query-based tools deployed in the VisIt visualization and analysis toolkit. Such tools provide fusion scientists with an interactive integrated environment to visually correlate and analyze volumetric data, which is leading to a better understanding of the role of energetic particles in the excitation and stabilization of plasma instabilities and disruptions. Simulation, analysis, and visualization performed by C. Kim (General Fusion Inc.).*

analysis of the variability across ensemble member calculations with an eye toward predictive uncertainty [109]. Despite these examples of progress, however, the use of such methods requires a high degree of interaction among fusion scientists, computer scientists, and mathematicians to tune and adapt to a particular problem.

One of the basic challenges with some fusion codes is their usage of complicated nonstandard coordinate systems. For instance, GS2 simulations are performed in field-line-following coordinates using toroidal flux tubes [110]. While such coordinate systems make the nonlinear gyrokinetic equation computationally easier, the resulting data (in five dimensions) is hard to visualize in the flux-tube domain. Other methods specific to fusion energy are required.

Many workshop participants expressed a desire for robust methods for model and data intercomparison. This activity highlights the need for improved approaches to data infrastructure for data sharing and analysis. Particular needs include synthetic diagnostic comparison [wp51], as part of the basis for validation methodology [wp50], and implementation of metrics for assessing validation [wp52,wp107]. One promising approach lies in the area of structural, geometric, or topological analysis of simulation and experimental data. Such methods provide a basis for quantitative analysis that is robust and that works across data of different scales and different sources [wp52], and would be helpful in meeting validation needs (see [PRD-Disruptions-3], [PRD-WDM-3]).

Challenges of adoption and sustainability. Even where the needs outlined above are addressed, the science does not benefit if users do not adopt the solutions. Application scientists need to perceive value in adopting principles and tools with minimal effort on their part [wp74]. For example, metadata and provenance capture should be as automatic as possible—perhaps as simple as inserting a header file into each file in the code base along with some simple addition to the build system. Similarly, data standards should be as easy to use—even if not as familiar—as

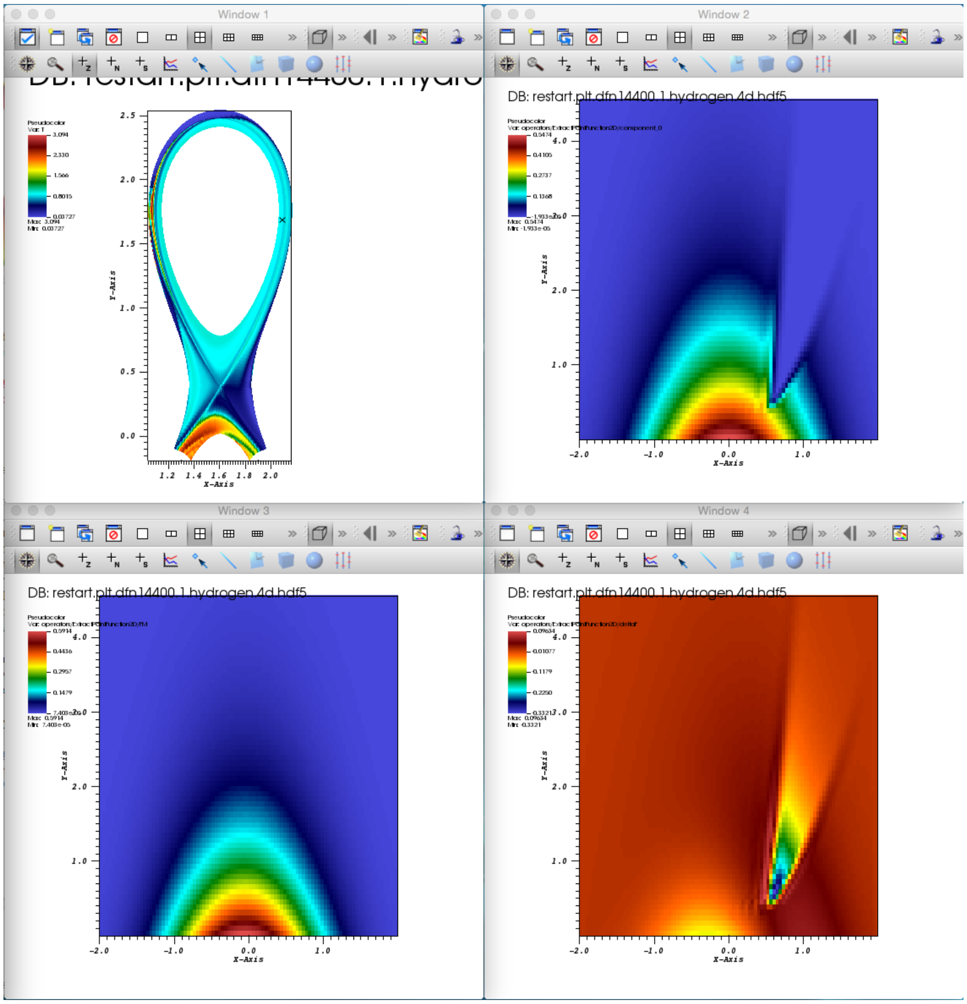


Figure 36: *Distribution function at a given location in 2D space. (Top left) Projection of simulation results to 2D by computing temperature. The query location is marked with an "x." (Top right) 2D velocity distribution at the marked point. (Bottom left) Ideal Maxwellian distribution for the temperature at the queried location. (Bottom right) Difference between actual distribution function and ideal Maxwellian distribution. In this figure, the distributions show a "loss cone" in a fusion simulation. This "loss cone" is due to particles leaving the system, resulting in a cone-shaped region in the distribution where velocity density is significantly lower than in a Maxwell distribution. Image courtesy of G. Weber (LBNL).*

whatever particular format a scientist has devised. To achieve this objective, software engineers, computational scientists, and applied mathematicians will need to encapsulate the complexity of the underlying technologies.

New capabilities will not benefit science if they are not supported and sustained over useful periods of time. Often, institutional or sponsor support is lacking after the initial research and development phase. This situation negatively impacts user adoption in a vicious circle: users must be convinced that new tools and technologies will be sustained before they undertake the work required to adopt them. At the same time, if adoption rates are low, the economies of scale do not appear, and the cost of support and sustainment cannot be justified. All stakeholders must play a part in breaking the circle.

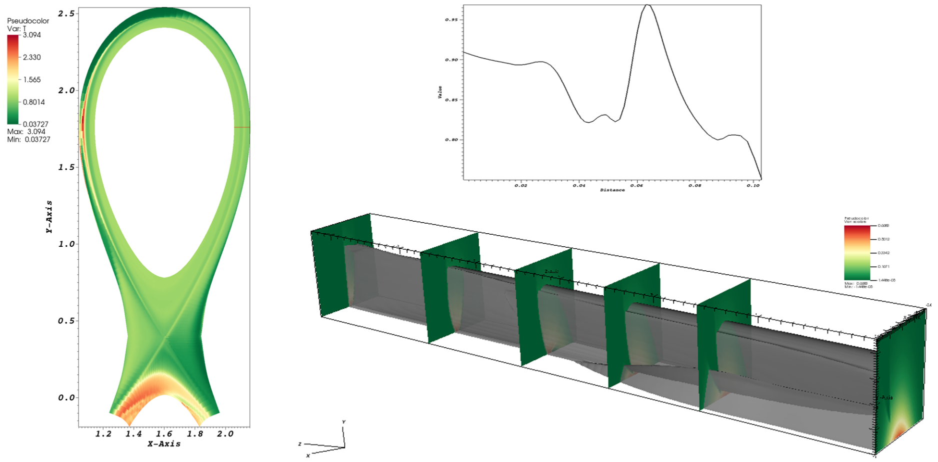


Figure 37: *Generalization of a VisIt "line out" plot to distribution functions. (Left) Plot of temperature in the spatial dimensions. (Right, top) "Regular" lineout plot showing the temperature variation along this line. (Right, bottom) New lineout plot showing the variation of the distribution functions along the same line. Since each distribution function comprises two velocity dimensions, the lineout plot results in a 3D "stack of 2D slices" along the line. Isosurface extraction as well as slicing show the evolution of the distribution along the lineout. In this figure, the lineout plot shows the evolution of a "loss cone" in a fusion simulation. This "loss cone" arises because of particles leaving the system, resulting in a cone-shaped region in the distribution where velocity density is significantly lower than in a Maxwell distribution. Image courtesy of G. Weber (LBNL).*

5.3.4 Strategy and Path Forward

Improvements and adoption of new tools and technologies for data management, analysis, visualization, and dissemination would increase the effectiveness of fusion simulation activities and foster stronger collaborations among groups and with the experimental community. The computational work carried out by fusion researchers is among the most sophisticated and demanding in science. But while exceptions exist, in general the state of "data science" for fusion simulations is not particularly mature and would benefit from significantly increased attention. New discoveries are undoubtedly overlooked because of the difficulty in navigating and fully exploiting the potential of the huge, complex datasets already produced. The needs will only be greater as computing platforms move toward the exascale.

- **[PRD-Data-1]** Develop community data and metadata standards based on broad input from users and developers. These standards should explicitly represent the relationships between data objects and descriptions of data quality and validity. Implementation should build on strong abstractions that can support the inevitable evolution of software and hardware technologies.

- **[PRD-Data-2]** Develop and deploy infrastructure and algorithms that support in situ analysis for fusion simulation codes. It is not enough that in situ infrastructure exists, however nascent; to be useful to the fusion community, projects must be initiated to help fusion code teams adopt this infrastructure, as well as develop and deploy fusion-specific analysis, data management, and visualization methods in this in situ infrastructure.

- **[PRD-Data-3]** Improve support for MFE-centric workflows including capture of metadata and data provenance. Tools are needed that support end-to-end workflows including experimental and simulation processes and dissemination of research products (e.g., databases, publications). Workflows may be small, such as running a simulation code and writing data to disk, or may be large and complex, such as those in our use cases that involve distributed resources, multiple processing stages, and multiple potential data sources and sinks.

- **[PRD-Data-4]** Build federated, curated data repositories. Utilizing community data and metadata standards, fusion data should migrate to these repositories supporting remote access under flexible access control to meet investigator requirements. This effort will require a transition (perhaps in decreasing order of importance) to common abstractions, common ontologies, common schemas, common API, and common formats. Data creation, access, searching, and browsing would be supported through a shared, easily adopted toolset. The repositories would support various approaches for federation or data sharing by storing all information required for data access as easily obtained metadata. "Beyond grep" searching relies on robust and rich metadata, which could include data origin, processing methods, analysis results (structural, feature detection, data quality, etc.), and owner. This type of searching would require an evolution in the lexicon of search terms: while searching for data containing given words is straightforward, new terms (and associated standards) useful for the fusion community would need to be defined and accessible/searchable as metadata. Such data infrastructure and data products would be widely used throughout the MFE community for years to come for comparison, verification, validation, UQ, archival, publication, and compliance with federal regulations that mandate public access of data produced by federally funded research.

- **[PRD-Data-5]** Engage in R&D and deployment of visualization and analysis methods targeted to the needs of the fusion community. These include methods for robust comparison of data from diverse sources, for visual data exploration of high-dimensional simulation output, for effective visualization of uncertainty and variability, for working with ensemble collections of data, and for accommodating the integration of metadata and provenance into the visual data exploration and analysis processes.

- **[PRD-Data-6]** Develop a strategy for promoting adoption and sustainment of shared tools that support data management, analysis, and visualization for fusion applications. Addressing this recommendation will require concerted engagement from all stakeholders, including developers, users, and DOE.

A roadmap for addressing these issues is urgently needed. The steps outlined above are critical to meeting future challenges in computation and more generally for fusion sciences. Addressing these challenges will not be quick or easy, but progress can be incremental if guided by a broadly based and widely accepted plan. The fusion community should be open to ideas or solutions developed in other communities but should not hesitate to lead where it is appropriate.

5.4 Software Integration and Performance

The panel on Software Integration and Performance covers a range of topics important to integrated simulation: general aspects of (large-scale, integrated) software systems, including workflow and coupling software, frameworks, and related topics; software engineering and software productivity; performance and performance portability, and community organization and governance pertaining to the development and maintenance of software. As illustrated in Fig. 25, these topics cut across all the other panels of this workshop.

5.4.1 Background and Recent Progress

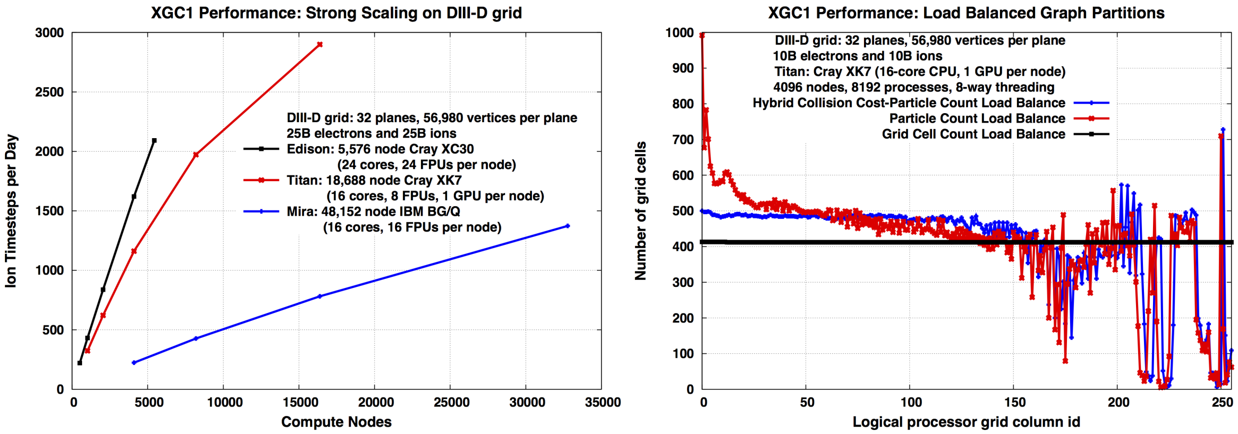
Integrated simulation has a long history in the fusion energy field. In many respects, however, the "modern era" of fusion integrated simulation might be said to have begun with the launch of the so-called prototype fusion simulation projects (proto-FSPs), funded through the SciDAC program during 2005–2011: the Center for Plasma Edge Simulation (CPES) [25,111,112], the Center for Simulation of Wave Interactions with Magnetohydrodynamics (SWIM) [24,113], and the Framework Application for Core-Edge Transport Simulations (FACETS) [26,114] project.

The three proto-FSP projects investigated different physical, mathematical, and computational aspects of fusion integrated simulation. Following the SciDAC model, these projects were among the first in the fusion community to involve tightly integrated cross-disciplinary teams, including physicists, applied mathematicians, and computer scientists. All three projects used explicit workflow system or framework concepts, as distinct from the physics codes being coupled, as a central element of their software architectures, another first in this domain. The CPES project developed an end-to-end framework for fusion integrated simulation (EFFIS) [115] with the general-purpose Kepler workflow system [116,117] at its core. The SWIM project developed the general-purpose IPS framework [118], based on a simplified version of the Common Component Architecture [119]. The FACETS project developed a new framework that utilized a purpose-designed component architecture [120].

The current round of the SciDAC program, which began in 2010 (SciDAC-3), includes one project that is officially identified as being focused on integrated modeling, the Advanced Tokamak Modeling (AToM) [19] project, which is in many respects a follow-on to the SWIM project. However, the other two SciDAC-3 projects also include integrated simulation in their current or future plans: the Center for Edge Physics Simulation (EPSI) [17] is a follow-on to the CPES project, and the Plasma-Surface Interactions project aims to integrate the plasma boundary with materials models for the wall. (This panel included representatives of all six of these SciDAC projects.)

As part of the SciDAC program, these integrated simulation projects have been expected to connect to various institutes that provide computer science and applied mathematics expertise to the program. Of particular relevance to this panel, the SciDAC-2 Performance Engineering Research Institute (PERI), and SciDAC-3 Institute for Sustained Performance, Energy, and Resilience (SUPER) [22] have focused on tools and techniques for performance engineering in general as well as the performance needs of applications (Fig. 38). These institutes and other more fundamental performance-related R&D projects track the evolution of the computer architectures described in Sec. 2.4 and work to understand the performance implications for applications and how to design applications to maximize performance and performance portability for a broad range of application domains.

Workflow tools, which are one approach for integrating software, have been developed primarily in the context of distributed (or grid) computing environments. The Kepler system used by the CPES and EPSI projects, as well as the ITER IMAS, is but one example of tools in this space.



(a) (b)

Figure 38: *Two aspects of the performance of the XGC1 plasma microturbulence edge code [121]. Panel (a) shows that the code is able to scale effectively to full system size on current DOE high-performance computing systems for fixed-size (strong-scaling) production simulations. The data for the same problem across systems demonstrates scaling to significant fractions of these systems. Panel (b) illustrates multiple sources of load imbalance when running XGC1 in parallel. Some degree of load imbalance is present in nearly all parallel applications. Treating it effectively is critical to performance and to parallel scalability. This example examines the impact of treating both particle and grid-based load imbalances simultaneously on the decomposition of the computational grid. Courtesy of P. H. Worley (ORNL).*

The level of research activity and the pace of development in this area have slowed in recent years; however, a number of tools remain in active use by various projects across many application domains.

Component frameworks, with a formally defined component architecture, are another way of integrating software and were used by the FACETS and SWIM projects. These projects were informed to a significant extent by the SciDAC-1 Center for Component Technology for Terascale Simulation Software (CCTTSS) and SciDAC-2 Center for Technology for Advanced Scientific Component Software (TASCS) projects and their work on the CCA, but component-based software development is not currently an actively funded research topic in ASCR. Nevertheless, the concept of modularity, one of the key underpinnings of component-based software engineering (CBSE), is widely accepted as a best practice in the design of software and is, therefore, a design principle of many scientific applications. Some of the other more detailed or subtle aspects of CBSE appear to varying degrees in modern scientific applications.

Software engineering emerged from the workshop discussions as an area of significant concern. Historically, this has not been a research area for ASCR, although the recently launched Interoperable Design of Extreme-Scale Application Software (IDEAS) project [122] may indicate a change. IDEAS is focused on software productivity issues, including interoperability of the major DOE-supported solver libraries, and general software engineering practices for high-end scientific computing. While the project is supported primarily by ASCR, the Office of Science Biological and Environment Research (BER) program supports work with several of the terrestrial ecosystem projects as a “laboratory” to motivate and validate software productivity research.

5.4.2 Crosscutting Fusion Motivation

This panel identified motivating challenges that cut across both the Integrated Science Applications and the Mathematical and Computational Enabling Technologies areas.

Disruption physics. Understanding the formation, evolution, avoidance, and mitigation of disruptions in plasmas is mathematically challenging and computationally intensive on current architectures [wp103]. In the modeling of actual disruption events, many symmetries, which are used in other contexts to reduce the computational effort, are broken, thus multiplying both the cost and the challenge [wp90]. It is not clear to what extent current solution approaches can be mapped effectively to current and coming high-end hardware architectures, and a deeper exploration of both current and alternative approaches is needed.

At the other end of the spectrum in this area is profile analysis, which attempts to map the stability characteristics of large parameter spaces in the plasma through the duration of the discharge. This entails massive numbers of simulations that are, individually, modest in scale. A great deal of existing experimental data can be used to validate computational models, and researchers want to predict stability maps for ITER and other future experimental devices. The computational challenge in this case involves orchestrating and tracking the execution of massive ensembles of simulation tasks, each of which ingests and produces data that also has to be marshaled, staged, and tracked, thus also connecting directly to the Data Management, Analysis, and Assimilation area (Sec. 5.3).

Plasma boundary. As described in Sec. 4.2.1, the plasma boundary encompasses the pedestal, scrape-off, and wall regions of a tokamak reactor. Although the simulation of the plasma boundary provides only part of what is needed for a whole device model, it comprises a substantial integrated simulation challenge in and of itself. Codes that focus on a specific part of the boundary problem (e.g., the pedestal and near-separatrix region) make certain choices with respect to coordinate systems, gridding, centering of variables with respect to the grid, and the like, which exploit known characteristics of that particular region. The reconciliation of these choices in an integrated simulation has mathematical, algorithmic, data distribution, and format issues that need to be addressed. Some of these issues are considered elsewhere in this report. Clearly at least part of the software integration challenge in the boundary area (as in the others) can be addressed through the promotion and adoption of software engineering best practices. The issue of performance is of particular importance in the boundary plasma area, because several components are especially computationally intensive. These include high-dimensional kinetic models of plasma turbulence and molecular dynamics models of plasma–materials interactions. A number of the existing boundary plasma codes already rely on ASCR-developed numerical libraries for some well-defined mathematical operations, such as the solution of linear and nonlinear systems, which have been identified as requiring continued development for advanced architectures. Given the new challenges presented by exascale architectures, additional software tool support will be needed to achieve high performance and portability. A major concern in the boundary area is how to minimize the impact of performance-required modifications, as well as those required to achieve integration goals, on a significant existing code base.

Whole device modeling. Because of the breadth and diversity of integration involved in whole device modeling, some of the more fundamental aspects of software development emerge as primary needs in this area.

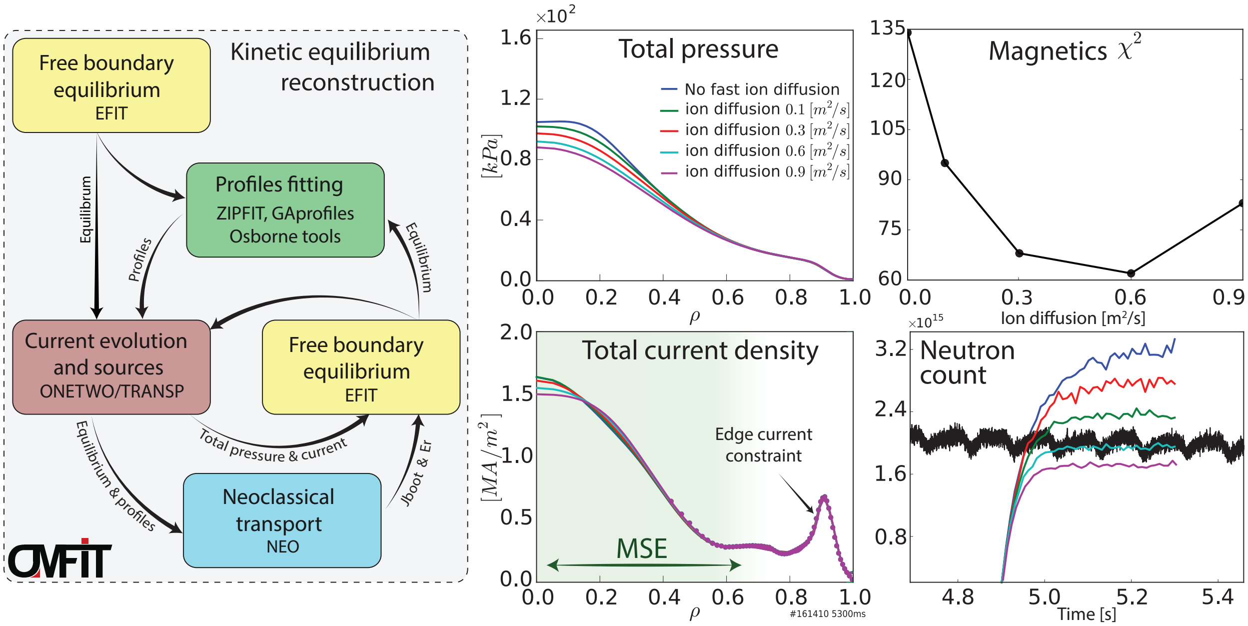


Figure 39: *Schematic of a kinetic equilibrium reconstruction workflow, implemented in the OMFIT framework, and illustrative results [123].*

At the heart of this area is software architecture, particularly including workflow or framework environments capable of supporting a wide range of integrated simulations in a common environment [wp47] (Fig. 39). Such environments also need to provide both the abstractions and the basic computational support for modern multiphysics, multiscale coupling strategies (see Sec. 5.1), as well as the ability to orchestrate large-scale parameter studies, sensitivity analysis, and other numerical optimization and uncertainty quantification [wp49,wp50] approaches (see Sec. 5.2), and novel time-stepping and time-parallel algorithms. Frameworks also need to support and interface with data management systems for both experimental and simulation data, minimizing to the extent possible the need for the physics components themselves to take responsibility for such interfaces (see Sec. 5.3).

Of course the physics components are the heart of WDM [wp26]. Existing components for WDM, as well as other types of integrated simulation, span a wide range of computational cost, performance, and scalability. Many opportunities exist for code modernization, performance optimization, and even algorithmic overhauls to improve this situation on a code-by-code basis. But WDM and other integrated simulation frameworks will always need to be able to deal with such disparities in order to take maximum advantage of the available computational resources. Because many WDM components are, or are based closely on, standalone single-physics fusion codes, promoting interoperability and standards for interfaces and/or data exchange can facilitate their integration.

Multiphysics and multiscale coupling. The discussion of multiphysics and multiscale coupling focuses primarily on the physical and mathematical issues. Drawing on experience and insights from similar work in other domains, the applied mathematics community is in a position to suggest solutions to multiphysics, multiscale coupling problems in fusion integrated simulation and to define and address the research questions that distinguish fusion problems from prior experience. The next step is to understand from the software perspective how the implementation of coupling solutions in fusion integrated simulation can be generalized and abstracted so that every new coupling does not require a new one-off software design.

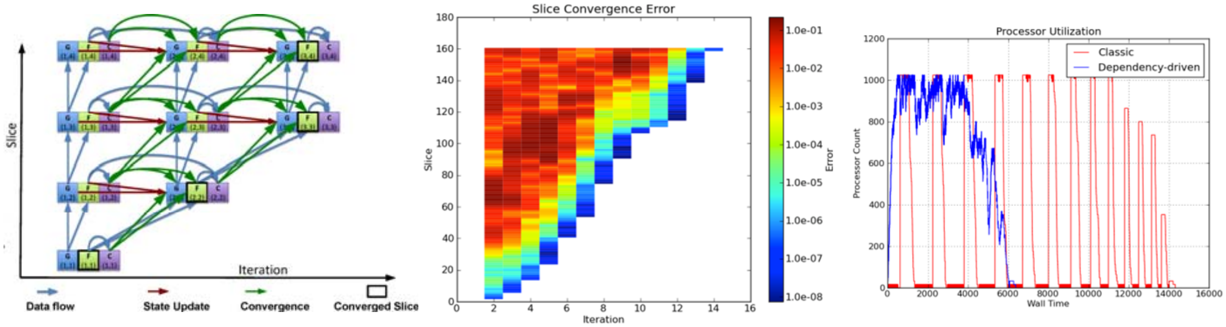
Beyond interpretive simulations. Numerical optimization and uncertainty quantification place fusion integrated simulation into a new context, with a significant multiplier on both the cost and complexity compared with individual simulations [wp83]. Solving inverse and numerical optimization problems and performing uncertainty quantification inherently depend on carrying out multiple simulations. They also involve coordination with the treatment of data (see Data Management, Analysis, and Assimilation, Sec. 5.3). Performance issues in this new context extend beyond the individual simulation to include the startup and teardown of simulation tasks. New software architectures that allow collections of simulations to be evaluated concurrently in a single invocation of a single executable may be worth exploring for some applications.

Data management, analysis, and assimilation. While a number of specific connections between data management and software issues have already been cited, the general message is that the software needs to help make the data management and analysis capabilities as easy to use as possible for the developers of physics components and integrated simulation users [wp37,wp73]. This effort includes integrating frameworks rather than individual physics components with the data management infrastructure to the extent possible, as well as generalization of interfaces for in situ analysis capabilities wherever possible. The development of community standards for data and metadata is, in part, a community governance issue to which we can contribute.

5.4.3 Challenges and Opportunities

Performance issues. Workshop participants expressed a broad range of performance-related concerns for integrated simulation. On the one hand, we have the challenges of current and future computer architectures (described in Sec. 2.4 and 5.4.1) and ensuring that simulation codes can use them effectively. On the other hand, we have the complexities introduced by the coupling of codes, as well as the impact of numerical optimization and uncertainty quantification techniques, visualization and analysis processes, and other aspects of integrated simulation that can have a significant impact on both performance and cost.

Today's fusion simulation codes vary widely in their readiness for new architectures, including current leading-edge environments such as hybrid or accelerated systems; emerging architectures pose even greater challenges. Researchers recognize that they risk being overtaken by new architectures and being unable to compete effectively for access to HPC resources, with concomitant risks to their scientific productivity. A particular concern of many application developers is how the solvers and mathematical algorithms they are currently using will fare on new architectures. A point that emerged from the discussion is that different algorithms and even different formulations may be better suited to new architectures and that application developers need to prepare to take a step back and focus on how best to solve their physics problem rather than how best to port their current algorithms to coming machines (Fig. 40). In this context, close engagement with the applied mathematics community would be invaluable to help fusion code developers identify and implement mathematical solutions that are better suited for future hardware. Workshop participants noted the impact SciDAC partnerships have had on some applications, by bringing together fusion, applied mathematics, and performance researchers; and they felt that it would be extremely productive if partnerships of this kind could be expanded to reach larger numbers of fusion applications [wp88].



(a) (b) (c)

Figure 40: *Implementation of the parareal [124,125] parallel-in-time algorithm within the IPS framework employs a novel implementation using task-based parallelism to avoid the sequential bottleneck present in the "classic" implementation of parareal. Panel (a) illustrates the data dependencies that form the basis of the algorithm. Panel (b) shows a convergence heat map for all 160 time slices of the simulation (y-axis) as the algorithm iterates (x-axis). Panel (c) shows the total time required (x-axis) and the utilization of available compute resources (y-axis) for the dependency-driven parareal implementation (blue curve) compared with the classic implementation (red curve). From [126].*

On their own, however, these kinds of "porting" activities are not sufficient to ensure that fusion codes will be ready for the architectures that follow the next-generation systems. The workshop participants recognized the need for a longer-range view of the performance problem that would yield a sustainable approach that would facilitate not just the first port but each and every successive port. One of the challenges here is in understanding the performance of individual components in a coupled simulation context, how that differs from the performance in a standalone context, and how codes can be engineered to perform well in both situations. A starting point for such an undertaking might be to develop a concept of "performance-aware software." This would provide an "always-on" performance-monitoring capability as a way of obtaining the quantitative information needed to achieve understanding. How to effectively provide such performance information is an open research question—both built-in instrumentation infrastructure and nonintrusive external measurement techniques could be envisioned as possible approaches. How to analyze the information and most usefully characterize the performance, including performance variability, is another open research question, particularly in the integrated simulation context.

An additional performance challenge for integrated simulation stems from the increasing use of advanced computational techniques, such as numerical optimization and uncertainty quantification, parallel-in-time algorithms, and even testing. These techniques typically have a multiplicative effect on the cost of the simulation run and may benefit from novel formulations of the problems. Similarly, approaches such as in situ analytics and visualization also change the performance considerations of simulation jobs.

The opportunities in the performance area lead us to recommend a fusion-math-performance partnership to address both the near- and longer-term needs (see [**PRD-Software-2**], Sec. 5.4.4). We believe this is a high-priority issue in order to ensure that the integrated simulation community can keep pace with changing hardware.

Software engineering issues. Two software engineering concerns arose in workshop discussions. The first is the fact that basic software engineering best practices are not as universally used as they should be in this domain. Here we include the use of version control repositories, bug trackers, tests, and systematic ways to communicate among developers and with and among users. While this situation is fairly common across all of computational science, we believe that it is particularly important in *integrated* simulation, where the codes are more likely than in many other domains to be used and modified outside their core development team. At this level, the software engineering issues are well understood. What is needed is to identify a “minimal” set of best practices [wp100], as well as teams of knowledgeable and experienced practitioners to help disseminate the practices throughout the community, ensure that they are understood, and assist in their implementation (typically in the form of a consultant). In some cases, the availability (or simply awareness) of the infrastructure to support these basic software engineering practices (e.g., a version control repository that is accessible to all members of the development team, and a bug tracker available to the team and perhaps also to users). Such infrastructure can be costly and onerous to set up and maintain at the project level, especially given security requirements on anything that is exposed on the Internet. While third-party code hosting platforms can provide these services, we believe that there is value in making these tools available at the institutional or community level.

The second level of software engineering concerns is more focused on the *integrated* aspect of integrated simulation and on the fact that we have much less experience, from a software engineering standpoint, in working with integrated systems in computational science and engineering. The issues here are fundamental. For example, how can we make it easier for researchers to work across multiple disparate code bases as they develop their integrated applications? A significant amount of the code coupling that currently takes place in integrated fusion simulation is based on adaptation of existing component codes rather than codes that are purpose-built for the coupling. This means that the developer of an N-component integrated application is working across at least N different code bases. If these codes are all structured differently, with different directory layouts and different build systems, the cognitive burden can be tremendous. While we do not believe that imposing strict standards across the whole domain is either necessary or realistic, encouraging more commonality certainly would be useful. This has the incidental benefit of simplifying some of the practical, and important, decisions that the developers of new codes have to make. This challenge is not only about the build system or the layout of the files in the code tree. It is also about how the codes themselves can be architected and designed to facilitate integration rather than making it harder. These are research questions, at various levels of complexity, that need to be investigated in order to develop recommendations that can be disseminated to the community.

More complex issues in the software engineering of *integrated* applications have to do with ensuring confidence in the component codes and the results they produce (Fig. 41). Note that this is in the sense of code *verification*; we consider *validation* to be a science issue rather than a computing issue, although obviously proper verification is a prerequisite. Testing is a typical strategy for gaining confidence in code, and regular and extensive testing is a hallmark software engineering best practice. Testing is, however, primarily an “offline” strategy, in that it is separate from science runs and that the correct answers must already be known in order to define a test. Contracts are another approach for gaining confidence in code. Unlike tests, contracts are implemented *within* the code base, expressing requirements on inputs, invariants, and outputs of routines, all of which can be checked during execution (for example, a routine may require that an input matrix be unitary and produce a sorted array of eigenvalues) to ensure that the routine is being invoked with appropriate inputs and is delivering outputs that conform to its specifications. Contracts can be enforced during production science runs. Both offline and online strategies are important in a comprehensive effort to ensure code quality. But, even assuming a component is well covered with tests (or contracts) for standalone use, those tests do not necessarily guarantee correctness when it is used in an integrated context because the *way* in which the code is used and the expected inputs and outputs are in some way different from the standalone case (or else it would not be worth doing

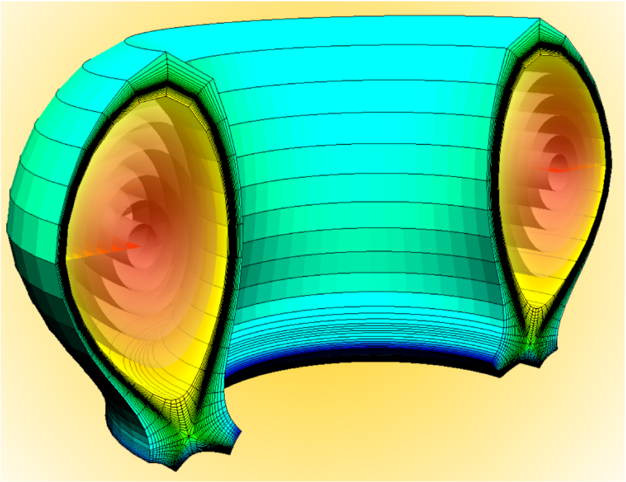


Figure 41: *Visualization of a coupled core-edge simulation using FACETS. The visualization shows that C^1 continuity was achieved across the boundary [127,128].*

the integration). The key question in this context is how to design the tests to provide as complete a coverage as possible. As practiced today, test design is largely ad hoc, even for standalone cases. It would be extremely useful to develop and disseminate test design strategies with a particular emphasis on the integrated context (but also standalone) to help developers to be more systematic and thorough in their testing practices.

Because of the different levels of complexity in the development and dissemination of guidelines for basic software engineering practices versus those targeting software integration issues, we divide this area into two distinct recommendations. [**PRD-Software-1**] relates to the basic software engineering practices and constitutes "low-hanging fruit" for this community, meaning that, with relatively little effort, significant improvements should be possible in the level of software engineering being practiced. [**PRD-Software-4**] focuses on the particular issues of *integrated* software systems. It is no less important but will require more time and effort to implement. Overall, the scientific computing community has significant experience with various kinds of integrated simulation, but it has not yet been thoughtfully examined as a body, and simplified and generalized.

Community and governance issues. Major opportunities were identified in the development of community-based standards to promote interoperability [wp114]. In this context, the notion of "interoperability" covers a broad range, from the ability to easily exchange data, to the ability to make calls between components, or even to the ability to transparently replace one component with an equivalent one. The time and effort typically required to agree upon and implement interoperability standards can also vary over a similarly broad range. The community will need to consider the costs and benefits in order to determine a detailed prioritization of standardization activities and how far it is worth going. But the workshop discussions included some observations based on prior experience (often in other domains). Agreement on basic information can be both simple and quick to achieve and relatively easy to implement. One example might be the names and units of measure associated with common data fields (especially those likely to be exchanged between components in a coupled simulation context), as the climate modeling community has done with the Climate and Forecast Conventions [95]. Similarly, agreement on metadata and provenance elements to be captured in conjunction with integrated simulation workflows would facilitate work spanning different workflow and data management environments. A step up from these in cost might be specific formats for data files. On the other hand, this is a more powerful level of interoperability because it implies that files produced by one component can be consumed directly by another. Self-describing data formats, such as HDF5 [129], combined with conventions for data fields and units of measure, can greatly simplify implementation of standards at this level. These kinds of activities are consistent with those recommended in [**PRD-Data-1**], and for similar reasons.

Stepping up another level in cost and complexity, data structures and object or subroutine interfaces (APIs) can facilitate direct data exchange and other interaction between two separate code bases. However they are often much more challenging to agree upon because they tend to directly impact code structure and performance. There is an art to finding the right level at which to define APIs for interoperability while minimizing the constraints imposed on the structure and implementation of codes conforming to that API. A common failure mode for API design activities is to work at too low a level to allow sufficient flexibility among the stakeholders. Many researchers in the DOE computer science and applied mathematics communities have experience in designing APIs that should be tapped to inform such activities in the fusion community. Perhaps the highest level of interoperability is achieved when an entire component can be swapped out and replaced with another component, transparently to the rest of the simulation. This is a useful concept in integrated simulation because it allows for the interchange of different implementations of the same physics. For example, one RF solver can be replaced with another conforming to the same interface; or one transport solver can be replaced with another.

Other integrated simulation activities are under way around the world, with the EU Integrated Tokamak Modeling (ITM) activity (and its successors) and ITER's Integrated Modeling and Analysis Suite (IMAS) being among those more visible to the U.S. fusion community. From perspectives of both program management and research, the U.S. fusion community should explicitly consider how best to work with and interoperate with other integrated simulation activities such as these [wp88]. Doing so will generally entail some effort to explore and evaluate the package or approach and to understand the technical and strategic directions. Note that choosing to interoperate at some level with another integrated simulation activity does not necessarily mean *agreeing with* or adopting either the technical or strategic directions of the other project. Rather, the degree of alignment on directions may influence considerations as to the viability and likelihood of achieving and maintaining the desired level of interoperability. In many cases, different elements of the integrated simulation environment need to be considered separately. For example, during the workshop Simon Pinches, head of Integrated Modeling for ITER, stated that they have different degrees of commitment to the data model, workflow environment, and individual physics components they are using in IMAS. More specifically, they are most strongly committed to the data model but less so to any particular physics component or workflow engine.

From a governance perspective, the primary concern we heard had to do with the level of sustainability and level of support available for some of the tools and libraries that fusion researchers might want to use as fundamental building blocks of their applications. DOE-funded research products in the computer science and applied mathematics (CS/AM) areas may become attractive on which to base fusion simulation codes. Because they are the result of novel research, however, in many cases there is no easy alternative should the CS/AM project cease to be supported—a problem that more than one fusion project has experienced. While we recognize that long-term support cannot be guaranteed to every CS/AM project that might be considered useful to a researcher in another domain, some concept of "productization" or at least long-term support and maintenance for certain key packages clearly would be mutually beneficial [wp100].

A secondary governance concern is that many of the developers of physics components that might be useful in an integrated simulation context remain strongly focused on the standalone use cases in which they were originally developed, and take little or no interest in their integrated uses. Since successful integration often requires significant understanding of the structure and function of the component codes, and in many cases modifications to them, having the developers engaged in integration activities is extremely helpful.

These considerations lead us to two recommendations in the community and governance area. [**PRD-Software-3**] focuses on community standards for interoperability, where the details of the specific topics and levels of interoperability desired must constitute the initial part of the initiative. We believe that the integrated simulation community can benefit significantly from these activities, and many useful standards can be agreed with modest levels of effort. [**PRD-Software-6**], on the other hand, draws attention to the community's infrastructure challenge, which we expect to be significantly more complex to address.

Software issues. Of all the topics covered by this panel, the software itself presents some of the most significant and longest-term challenges. Integrated simulation, particularly in fusion energy sciences, is a relatively young topic, and experience is limited. The majority of couplings are still done in a "one-off" fashion, and we do not have a good "recipe" to guide developers through the process, much less provide guidance as to how to design and structure their software to facilitate and simplify the process or to make it sustainable over the long term [wp61,wp86]. Newer considerations, such as the large "ensemble" jobs required by numerical optimization and uncertainty quantification, the integration with data management systems, and the increase use of in situ visualization and analysis also have important impacts on the design and implementation of integrated simulation environments.

In general, however, the workshop participants felt that there are strong prospects to improve the situation. Over the years, across many domains, a significant amount of experience has been gained with the *physics* and *applied mathematics* of coupled simulation, and at this level the computational science and engineering community as a whole is beginning to see the important patterns and abstractions in these areas that can be generalized and reused to make new coupling problems easier to solve at these levels. While the *computer science of coupling* lags behind the physics and applied mathematics, there are many point-solutions in this area as well, including the proto-FSP projects and other past and current integrated simulation activities in the fusion community, which can be used to begin the process of developing abstractions and patterns for the computational aspects of integrated simulation [wp100] to complement those for the physics and mathematical aspects. In order to be successful, such an initiative will have to build on ongoing work in the physics and mathematics of coupling, which will provide more extensive groundwork, particularly within the fusion domain. It will also need to consider how to incorporate new and emerging "computational patterns" (e.g., large ensembles and in situ analysis) to ensure both efficient and reliable execution.

In order to be useful to the fusion community, however, such an initiative cannot be a free-for-all of code development to explore new ideas. Coupled simulation involves significant software infrastructure, which is expensive to create and maintain. Researchers should be encouraged to carry out their work, insofar as possible, in the context of established infrastructure in order to avoid unnecessarily diluting the R&D resources with creation and support of many tools with significant duplication of effort [wp100,wp114]. A modest level of diversity and competition is useful and desirable, but these need to have sufficient levels of both capability and support in order to serve as productive infrastructure for the fusion researchers, while simultaneously providing a testbed for innovative computer science ideas.

This topic is perhaps the most substantial R&D need identified in the general area of software integration and performance. It is both broad and long-term, with a great many detailed questions that need to be addressed. However, we feel that such an initiative in the context of integrated fusion simulation would produce significant benefits for other domains where code composition and integrated simulation are important. [**PRD-Software-5**] therefore recommends a major initiative in this area.

5.4.4 Strategy and Path Forward

Based on the preceding, we have developed a set of recommendations for initiatives we believe would be valuable to advancing the fusion community's capabilities in integrated simulation over the next five to ten years.

- [**PRD-Software-1**] Implement software engineering best practices, consistently, throughout the fusion integrated simulation community. A core set of recommended practices should be identified and documented. They should be brought to the community through an outreach program staffed with experienced practitioners, with a mandate to provide assistance and follow-up to promote understanding and adoption.

- [**PRD-Software-2**] Bring together fusion researchers, applied mathematicians, and performance experts to focus on the performance and portability of fusion codes on current and future hardware platforms. This effort may involve taking a step back and considering different algorithms or even different formulations from those typically used today.

- [**PRD-Software-3**] Develop community standards and conventions for interoperability. This effort might include agreement on common data structures and data file formats, metadata and provenance, and names and units of measure for input and output data, as well as calling conventions and APIs. This recommendation builds on and extends [**PRD-Data-1**] to deeper levels of interoperability within integrated simulation software.

- [**PRD-Software-4**] Develop best-practice guidelines and recommendations to address the particular software engineering challenges of integrated simulation. Needs in this area include techniques for structuring and writing code with integration in mind, common directory structures, compatible build systems, and means to ensure the correctness of code in both standalone and integrated contexts.

- [**PRD-Software-5**] Perform research on the computer science of code composition. Extend ongoing work to systematize the physics and mathematics of code coupling, identifying the patterns and developing the abstractions that will facilitate the creation of composite software systems in a systematic fashion. This work also should build on and extend experience with computational frameworks and workflow environments in fusion and other research communities to address the additional computational patterns identified elsewhere in this report, including large ensembles, in situ data analysis, and tight connections between simulation code and data management and provenance capture systems.

- [**PRD-Software-6**] Determine a strategy to ensure the sustainability of key fusion integrated simulation infrastructure for long enough to establish a sustainable community of developers and users around it, as well as a strategy to encourage fusion code developers to take an active role in the integrated simulation community, as opposed to staying focused on standalone simulations.

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Bibliography

Electronic versions of whitepapers are available for download from the workshop website via: `https://www.burningplasma.org/activities/?article=IS_Whitepapers`

The call for whitepapers requested that each whitepaper submitter identify a primary panel affiliation and optionally secondary panel affiliations. The list below indicates these panel affiliations:

- **Panel A:** Disruption Physics (Sec. 4.1)
- **Panel B:** Plasma Boundary Physics (Sec. 4.2)
- **Panel C:** Whole Device Modeling (Sec. 4.3)
- **Panel D:** Multiphysics and Multiscale Coupling (Sec. 5.1)
- **Panel E:** Beyond Interpretive Simulations (Sec. 5.2)
- **Panel F:** Data Management, Analysis, and Assimilation (Sec. 5.3)
- **Panel G:** Software Integration and Performance (Sec. 5.4)

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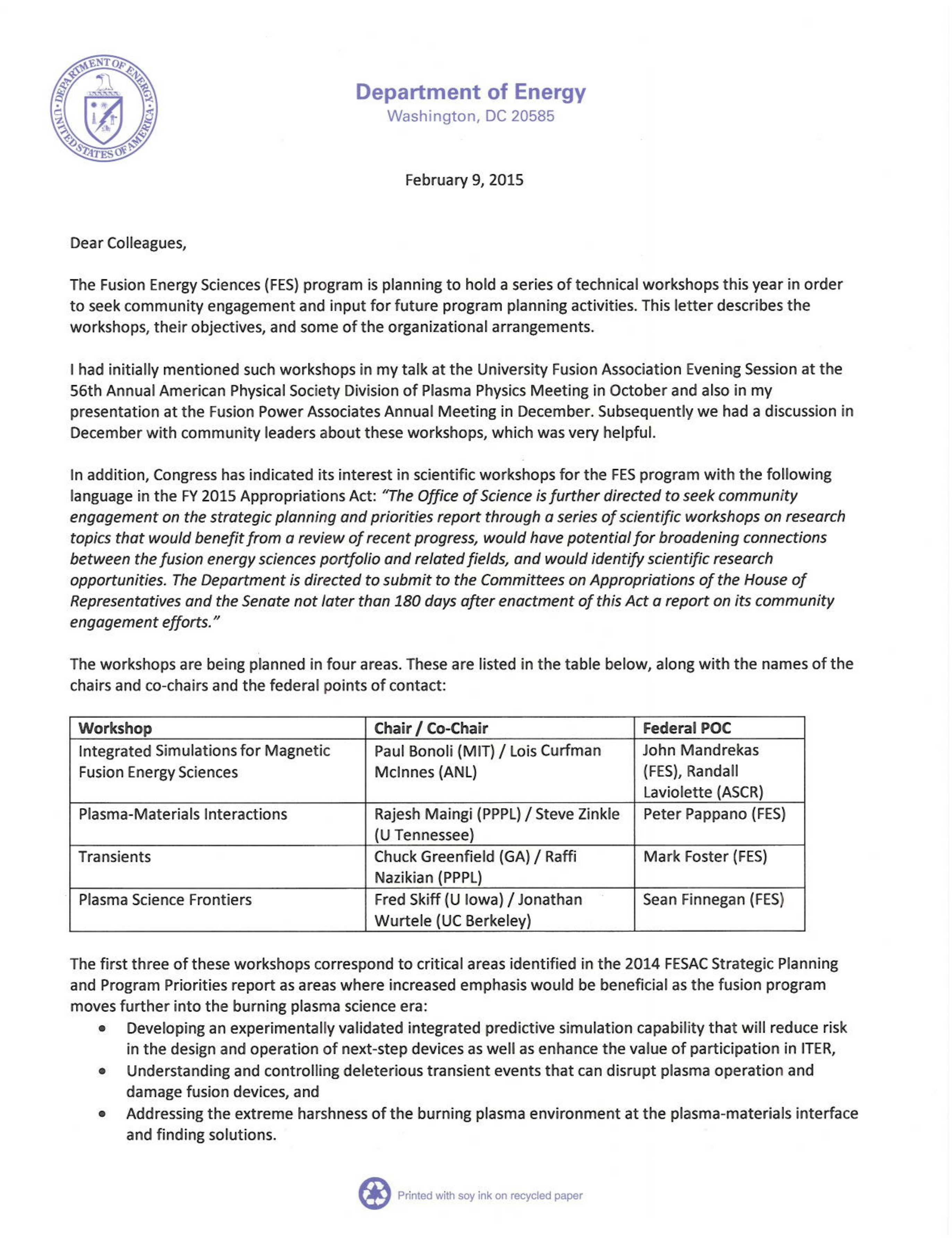
A. Acronyms and Abbreviations

AMR	adaptive mesh refinement
API	application program interface
ASCR	Advanced Scientific Computing Research
DOE	Department of Energy
ELM	edge-localized mode
EHO	edge harmonic oscillation
EM	electromagnetic
EP	energetic particle
FAS	full approximation scheme
FES	Fusion Energy Sciences
GK	gyrokinetic
GPI	gas puff imaging
HMM	heterogeneous multiscale modeling
H-mode	high-performance mode
HOLO	high-order/low-order
HPC	high-performance computing
IM	integrated modeling
IMEX	implicit-explicit
ITB	internal transport barrier
ITER IMAS	ITER Integrated Modeling and Analysis Suite
MCET	Mathematical and Computational Enabling Technologies
MD	molecular dynamics
MFE	magnetic fusion energy
MGI	massive gas injection
MHD	magnetohydrodynamics
MHD-GK	magnetohydrodynamic plus gyrokinetic
MMS	method of manufactured solutions
NO	numerical optimization
NTM	neoclassical tearing mode
PFC	plasma-facing component
PIC	particle-in-cell
PMI	plasma–materials interactions
PRD	priority research direction
RE	“runaway” electrons
RF	radio frequency
RMP	resonant magnetic perturbation
RWM	resistive wall mode
SciDAC	Scientific Discovery through Advanced Computing
SOL	scrape-off layer
SPI	shattered pellet injection
ST	spherical tokamak
UQ	uncertainty quantification
VDE	vertical displacement event
WDM	whole device modeling
XMHD	extended magnetohydrodynamics



Department of Energy
Washington, DC 20585

February 9, 2015

Dear Colleagues,

The Fusion Energy Sciences (FES) program is planning to hold a series of technical workshops this year in order to seek community engagement and input for future program planning activities. This letter describes the workshops, their objectives, and some of the organizational arrangements.

I had initially mentioned such workshops in my talk at the University Fusion Association Evening Session at the 56th Annual American Physical Society Division of Plasma Physics Meeting in October and also in my presentation at the Fusion Power Associates Annual Meeting in December. Subsequently we had a discussion in December with community leaders about these workshops, which was very helpful.

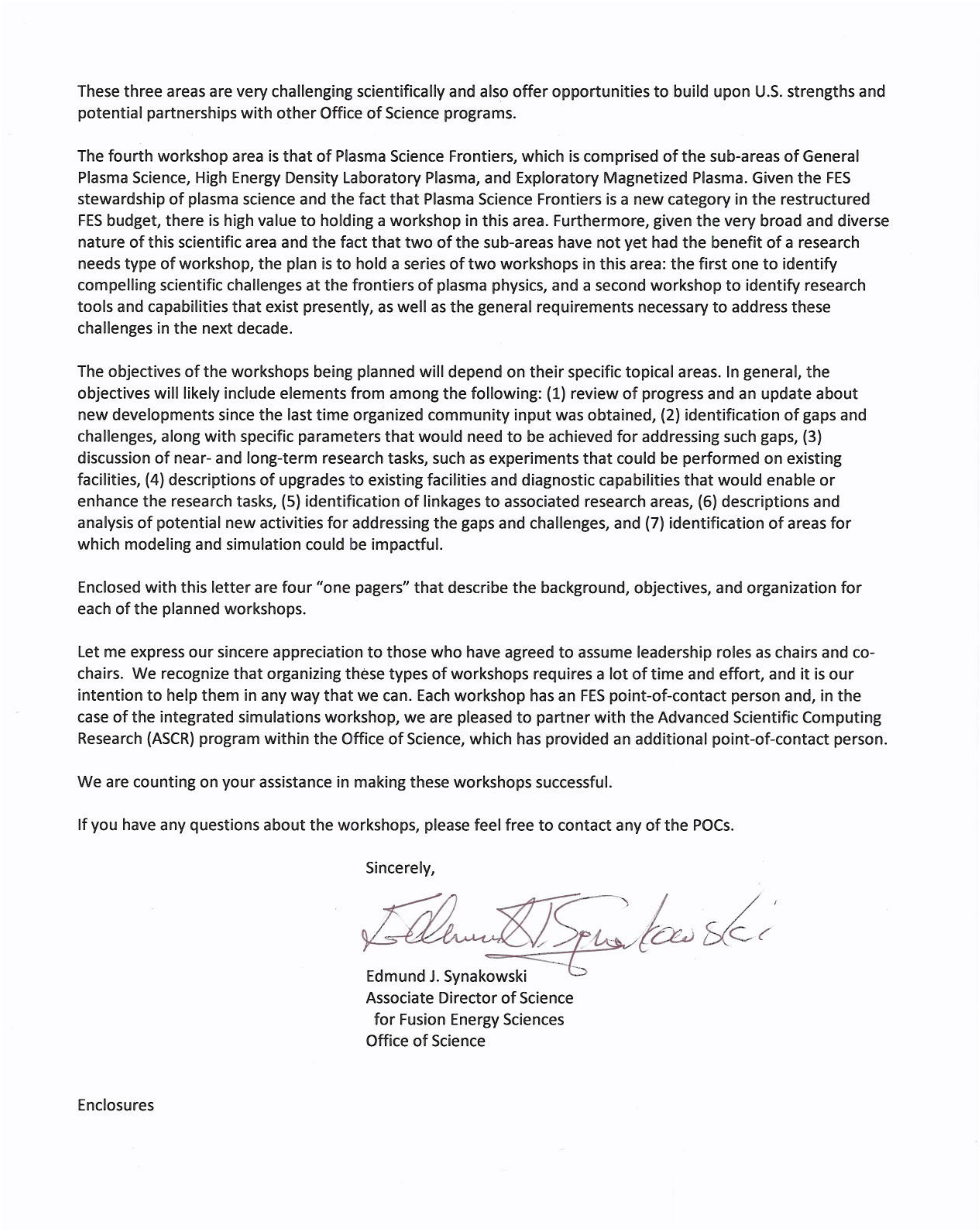
In addition, Congress has indicated its interest in scientific workshops for the FES program with the following language in the FY 2015 Appropriations Act: *"The Office of Science is further directed to seek community engagement on the strategic planning and priorities report through a series of scientific workshops on research topics that would benefit from a review of recent progress, would have potential for broadening connections between the fusion energy sciences portfolio and related fields, and would identify scientific research opportunities. The Department is directed to submit to the Committees on Appropriations of the House of Representatives and the Senate not later than 180 days after enactment of this Act a report on its community engagement efforts."*

The workshops are being planned in four areas. These are listed in the table below, along with the names of the chairs and co-chairs and the federal points of contact:

Workshop	**Chair / Co-Chair**	**Federal POC**
Integrated Simulations for Magnetic Fusion Energy Sciences	Paul Bonoli (MIT) / Lois Curfman McInnes (ANL)	John Mandrekas (FES), Randall Laviolette (ASCR)
Plasma-Materials Interactions	Rajesh Maingi (PPPL) / Steve Zinkle (U Tennessee)	Peter Pappano (FES)
Transients	Chuck Greenfield (GA) / Raffi Nazikian (PPPL)	Mark Foster (FES)
Plasma Science Frontiers	Fred Skiff (U Iowa) / Jonathan Wurtele (UC Berkeley)	Sean Finnegan (FES)

The first three of these workshops correspond to critical areas identified in the 2014 FESAC Strategic Planning and Program Priorities report as areas where increased emphasis would be beneficial as the fusion program moves further into the burning plasma science era:

- 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 value of participation in ITER,
- Understanding and controlling deleterious transient events that can disrupt plasma operation and damage fusion devices, and
- Addressing the extreme harshness of the burning plasma environment at the plasma-materials interface and finding solutions.



These three areas are very challenging scientifically and also offer opportunities to build upon U.S. strengths and potential partnerships with other Office of Science programs.

The fourth workshop area is that of Plasma Science Frontiers, which is comprised of the sub-areas of General Plasma Science, High Energy Density Laboratory Plasma, and Exploratory Magnetized Plasma. Given the FES stewardship of plasma science and the fact that Plasma Science Frontiers is a new category in the restructured FES budget, there is high value to holding a workshop in this area. Furthermore, given the very broad and diverse nature of this scientific area and the fact that two of the sub-areas have not yet had the benefit of a research needs type of workshop, the plan is to hold a series of two workshops in this area: the first one to identify compelling scientific challenges at the frontiers of plasma physics, and a second workshop to identify research tools and capabilities that exist presently, as well as the general requirements necessary to address these challenges in the next decade.

The objectives of the workshops being planned will depend on their specific topical areas. In general, the objectives will likely include elements from among the following: (1) review of progress and an update about new developments since the last time organized community input was obtained, (2) identification of gaps and challenges, along with specific parameters that would need to be achieved for addressing such gaps, (3) discussion of near- and long-term research tasks, such as experiments that could be performed on existing facilities, (4) descriptions of upgrades to existing facilities and diagnostic capabilities that would enable or enhance the research tasks, (5) identification of linkages to associated research areas, (6) descriptions and analysis of potential new activities for addressing the gaps and challenges, and (7) identification of areas for which modeling and simulation could be impactful.

Enclosed with this letter are four “one pagers” that describe the background, objectives, and organization for each of the planned workshops.

Let me express our sincere appreciation to those who have agreed to assume leadership roles as chairs and co-chairs. We recognize that organizing these types of workshops requires a lot of time and effort, and it is our intention to help them in any way that we can. Each workshop has an FES point-of-contact person and, in the case of the integrated simulations workshop, we are pleased to partner with the Advanced Scientific Computing Research (ASCR) program within the Office of Science, which has provided an additional point-of-contact person.

We are counting on your assistance in making these workshops successful.

If you have any questions about the workshops, please feel free to contact any of the POCs.

Sincerely,

Edmund J. Synakowski

Edmund J. Synakowski
Associate Director of Science
for Fusion Energy Sciences
Office of Science

Enclosures

Workshop on Integrated Simulations for Magnetic Fusion Energy Sciences

Chair: Paul Bonoli (MIT), Co-Chair: Lois Curfman McInnes (ANL)

Background

Motivated by the opportunities afforded by the extraordinary advances in high-performance computing, the Fusion Energy Sciences (FES) program, in partnership with the Advanced Scientific Computing Research (ASCR) program, has supported a number of world-leading multi-institutional and interdisciplinary efforts in the last decade under the Scientific Discovery through Advanced Computing (SciDAC) program, addressing grand challenge problems in fusion energy sciences. While most of these efforts treat phenomena in relative isolation by taking advantage of scale separation, FES and ASCR have also supported efforts that have taken the first steps toward integration, recognized as the next necessary undertaking for developing credible predictive capability. FES and ASCR solicited community input several times during the last decade, including the 2007 Fusion Simulation Project workshop, a two-year fusion simulation planning study, the 2009 ASCR-led workshop on Scientific Grand Challenges and the Role of Computing at the Extreme Scale, and others. In addition, experimentally validated integrated simulation has been among the top recommendations of several Fusion Energy Sciences Advisory Committee (FESAC) and other community studies, including the Greenwald report, the ReNeW report, and the recent FESAC report on strategic planning.

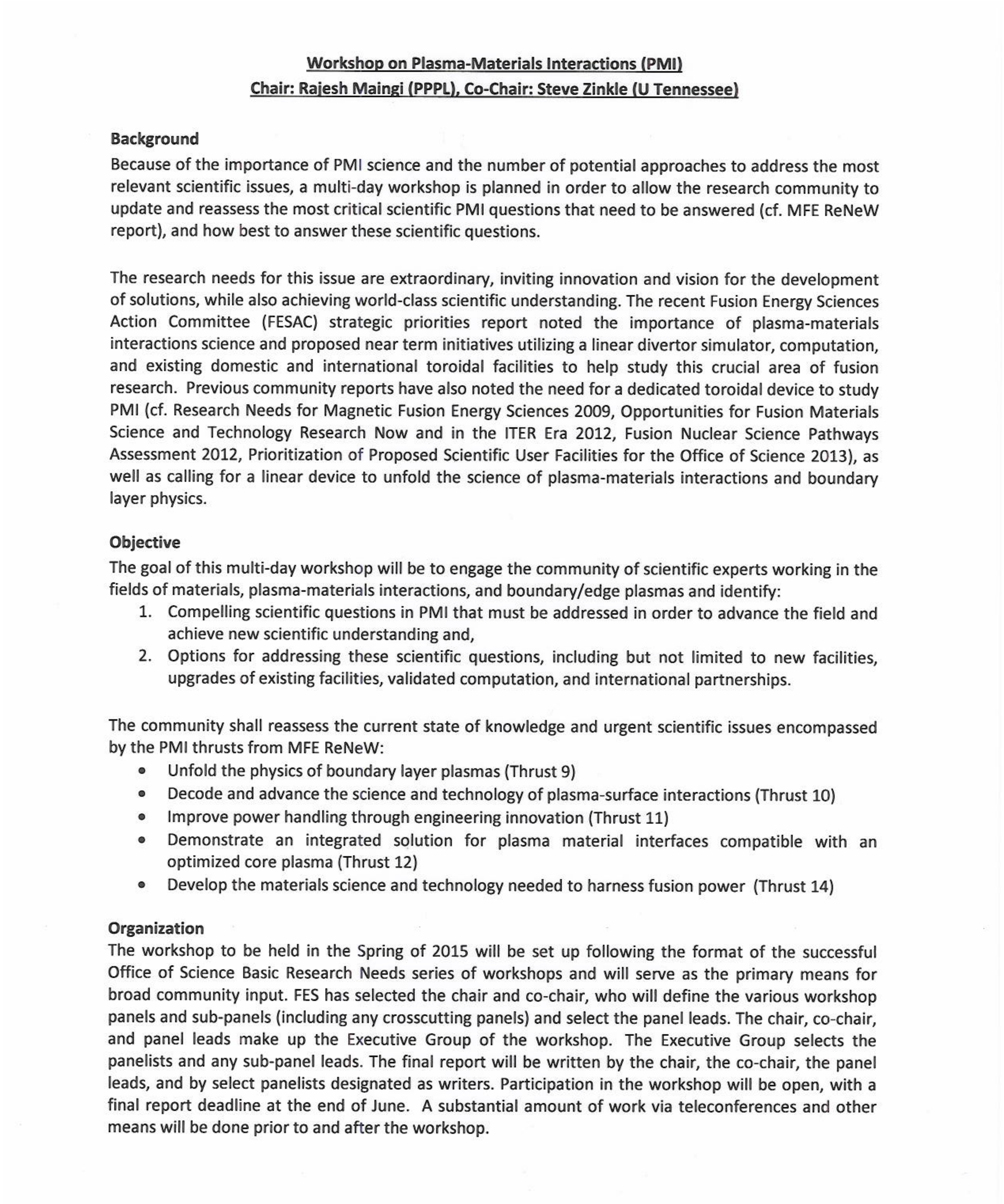
Objective

The main goal of this workshop will be to review recent progress and identify gaps and challenges in fusion theory and computation directly relevant to the leading scientific opportunities for integrated simulations identified by previous community studies. In addition, the workshop should reassess these opportunities and adjust or broaden them appropriately, taking into consideration recent progress and using the criteria of urgency, leadership computing benefit, readiness for progress within a ten-year time frame, and world-leading potential.

The leading scientific opportunities identified by previous studies have been remarkably robust and consistent: the prediction, avoidance, and mitigation of major disruptions and the physics of the plasma boundary, with Whole Device Modeling as the long-term goal. These scientific priorities are also consistent with the findings of the recent FESAC report on strategic planning. The workshop will achieve its objectives by considering recent advances, including research tools and capabilities developed by the eight FES SciDAC Centers and computational expertise at the ASCR SciDAC Institutes; advances and associated challenges in emerging extreme-scale computing hardware; recent progress in verification and validation and uncertainty quantification; "big data" issues; and the emerging needs of ITER. Crosscutting issues such as the status of measurement capabilities that are relevant to the experimental validation mission will also be addressed through coordination with the other workshops in this series.

Organization

The workshop will follow the format of the successful Office of Science Basic Research Needs series of workshops. FES and ASCR will select the chair and co-chair(s), who will define the various workshop panels and sub-panels (including any crosscutting panels), and select the panel leads. The chair, co-chair(s), and panel leads will make up the Executive Group of the workshop. The panel leads will select the panelists and any sub-panel leads. The workshop report will be written by the chair, the co-chair(s), the panel leads, and by select panelists designated as writers. Input from the entire community will be solicited during the preparation for the workshop, and participation will be open, but the total number of attendees will be limited to preserve the "working meeting" character of the workshop. A substantial amount of work via teleconferences and other means will be done prior to the workshop to allow the preparation of a draft report during the last day of the workshop.



Workshop on Plasma-Materials Interactions (PMI)

Chair: Rajesh Maingi (PPPL), Co-Chair: Steve Zinkle (U Tennessee)

Background

Because of the importance of PMI science and the number of potential approaches to address the most relevant scientific issues, a multi-day workshop is planned in order to allow the research community to update and reassess the most critical scientific PMI questions that need to be answered (cf. MFE ReNeW report), and how best to answer these scientific questions.

The research needs for this issue are extraordinary, inviting innovation and vision for the development of solutions, while also achieving world-class scientific understanding. The recent Fusion Energy Sciences Action Committee (FESAC) strategic priorities report noted the importance of plasma-materials interactions science and proposed near term initiatives utilizing a linear divertor simulator, computation, and existing domestic and international toroidal facilities to help study this crucial area of fusion research. Previous community reports have also noted the need for a dedicated toroidal device to study PMI (cf. Research Needs for Magnetic Fusion Energy Sciences 2009, Opportunities for Fusion Materials Science and Technology Research Now and in the ITER Era 2012, Fusion Nuclear Science Pathways Assessment 2012, Prioritization of Proposed Scientific User Facilities for the Office of Science 2013), as well as calling for a linear device to unfold the science of plasma-materials interactions and boundary layer physics.

Objective

The goal of this multi-day workshop will be to engage the community of scientific experts working in the fields of materials, plasma-materials interactions, and boundary/edge plasmas and identify:

1. Compelling scientific questions in PMI that must be addressed in order to advance the field and achieve new scientific understanding and,
2. Options for addressing these scientific questions, including but not limited to new facilities, upgrades of existing facilities, validated computation, and international partnerships.

The community shall reassess the current state of knowledge and urgent scientific issues encompassed by the PMI thrusts from MFE ReNeW:

- Unfold the physics of boundary layer plasmas (Thrust 9)
- Decode and advance the science and technology of plasma-surface interactions (Thrust 10)
- Improve power handling through engineering innovation (Thrust 11)
- Demonstrate an integrated solution for plasma material interfaces compatible with an optimized core plasma (Thrust 12)
- Develop the materials science and technology needed to harness fusion power (Thrust 14)

Organization

The workshop to be held in the Spring of 2015 will be set up following the format of the successful Office of Science Basic Research Needs series of workshops and will serve as the primary means for broad community input. FES has selected the chair and co-chair, who will define the various workshop panels and sub-panels (including any crosscutting panels) and select the panel leads. The chair, co-chair, and panel leads make up the Executive Group of the workshop. The Executive Group selects the panelists and any sub-panel leads. The final report will be written by the chair, the co-chair, the panel leads, and by select panelists designated as writers. Participation in the workshop will be open, with a final report deadline at the end of June. A substantial amount of work via teleconferences and other means will be done prior to and after the workshop.

Workshop on Transients

Chair: Charles Greenfield (GA), Co-Chair: Raffi Nazikian (PPPL)

Background

It is well known that transient events such as disruptions and Edge Localized Modes can have deleterious effects on tokamak plasmas, with the potential to cause damage to plasma facing components and first wall structures, as well as degrading plasma performance. Although these events are generally tolerated in present tokamaks, they are predicted to have more severe impacts on ITER and future burning plasma devices. If not prevented or mitigated, these events will have unacceptable impacts on the operational availability of these devices and shorten the lifetime of the in-vessel components. It is critical to develop the means to minimize these events and their consequences when they do occur.

The fusion community, through the comprehensive ReNeW process (*Research Needs for Magnetic Fusion Energy Sciences,* 2009), developed a proposed research thrust in this area – "Control transient events in burning plasmas". Subsequent Fusion Energy Sciences Advisory Committee (FESAC) reports (*Report of the FESAC Subcommittee on the Priorities of the Magnetic Fusion Energy Science Program,* 2013 and the *Report on Strategic Planning: Priorities Assessment and Budget Scenarios*, 2014) have endorsed this as one of the highest priority magnetic fusion research topics. Several workshops have already been held to examine in more detail the underlying physics issues and specific aspects of the ITER disruption mitigation system, and the U.S. Burning Plasma Organization (USBPO) currently has an active task force coordinating research on this topic.

Objective

Building on the ReNeW effort, other workshop results, and the ongoing USBPO disruptions task force plans, this workshop will review recent progress and identify the remaining science and technology challenges that must be addressed to demonstrate that magnetically confined tokamak plasmas with the characteristics desired for a fusion power plant can be robustly produced, sustained, and controlled without deleterious effects on the device's materials and structure. Based on thorough understanding of the remaining science and technology challenges, the workshop will identify specific research opportunities that can address these challenges in the next decade. These may include both domestic research and international partnerships and will be informed by the requirements of ITER and future burning plasma devices.

Organization

The workshop will be set up following the format of the successful Office of Science Basic Research Needs series of workshops. Fusion Energy Sciences will select the chair and co-chair(s) who will define the various workshop panels and sub-panels (including any crosscutting panels) and select the panel leads. The chair, co-chair(s), and panel leads make up the Executive Group of the workshop. The panel leads select the panelists and (if necessary) any sub-panel leads. The workshop report will be written by the chair, the co-chair(s), the panel leads, and any panelists designated as writers. A multi-day workshop will be held that will allow for a vigorous discussion of the scientific and technical issues and opportunities in this area. A substantial amount of work via teleconferences and other means will be done prior to the workshop to allow the preparation of a draft report during the last day of the workshop. Input from the entire community will be solicited during the preparation for the workshop, and participation will be open, but the total number of attendees will be limited to preserve the "working meeting" character of the workshop.

Since transient events will also be a subject of interest to the integrated simulations' effort, the activities of this workshop should be coordinated as appropriate with related activities of the integrated simulations workshop, including sharing participants and possibly establishing cross-cutting panels.

Workshop on Plasma Science Frontiers

Chair: Fred Skiff (U Iowa), Co-Chair: Jonathan Wurtele (UC Berkeley)

Background

The reorganization of the Fusion Energy Sciences (FES) budget structure in FY 2015 brings together three program elements at the frontiers of plasma science–viz., general plasma science, high energy density laboratory plasmas, and exploratory magnetized plasma. These three activities support a rich and diverse portfolio of plasma science, sharing many common intellectual threads with the potential for broadening connections between the fusion energy sciences portfolio and related fields.

Objective

The Plasma Science Frontiers (PSF) activities in FES seek to engage the community of scientific experts working in the fields of general plasma science, high energy density laboratory plasmas, and exploratory magnetized plasma in a series of two community-led workshops to identify:

1. Compelling scientific challenges at the frontiers of plasma physics, and
2. Research tools and capabilities that exist presently, as well as the general requirements necessary to address these challenges in the next decade.

The report(s) generated from these workshops will inform FES in planning and executing its strategic vision for the FES stewardship of the PSF activities, taking into consideration the recommendations from the Fusion Energy Sciences Advisory Committee [1] and the National Research Council [2].

Organization

The first workshop, "Scientific Frontiers," will focus on identifying the grand scientific challenges in plasma science. The starting point will be the six critical plasma processes that were identified in the 2007 National Research Council plasma science report [2] as being not well understood: explosive instabilities, magnetic self-organization, turbulence and transport, correlations in plasmas, multiphase plasma dynamics, and particle acceleration and energetic particles. The goal of the workshop will be to bring together input received from across the community (via one-page white papers) on updates to the state of the art and where the frontiers are since the 2007 report.

The second workshop, "Research Needs," will focus on identifying the research needs required to address scientific challenges at the forefront of plasma physics. It will specifically address existing experimental tools and capabilities, as well as future performance requirements at the intermediate scale and computational hardware and software needs.

Both workshops will follow the format of the successful Office of Science Basic Research Needs series of workshops. FES will select the chair and co-chair(s), who will define the various workshop panels and sub-panels (including any crosscutting panels) and select the panel leads. The chair, co-chair(s), and panel leads will make up the Executive Group of the workshop. The panel leads will select the panelists and any sub-panel leads. The workshop report will be written by the chair, the co-chair(s), the panel leads, and any panelists designated as writers. Input from the entire community will be solicited during the preparation for the workshop, and participation will be open, but the total number of attendees will be limited to preserve the "working meeting" character of the workshop. A substantial amount of work via teleconferences and other means will be done prior to the workshop to allow the preparation of a draft report during the last day of the workshop.

[1] "Report on Strategic Planning: Priorities Assessment and budget scenarios" (2014)
[2] "Plasma Science: Advancing Knowledge in the National Interest" (2007)

DOE Workshop on Integrated Simulations for Magnetic Fusion Energy Sciences
Call for Whitepapers - Due by April 24, 2015

https://www.burningplasma.org/activities/IntegratedSimulations2015

In preparation for the upcoming DOE Workshop on Integrated Simulations for Magnetic Fusion Energy Sciences, jointly sponsored by the offices of Fusion Energy Sciences (FES) and Advanced Scientific Computing Research (ASCR), the workshop chair Paul Bonoli and co-chair Lois Curfman McInnes invite all members of the FES and ASCR communities to submit whitepapers. The objectives of the whitepapers are to prepare topics for discussion at the workshop and to identify content to include in the workshop report.

The workshop goals are to review recent progress and identify gaps and challenges in fusion theory and computation directly relevant to the topic of disruption prevention, avoidance, and mitigation and that of plasma boundary physics, with whole device modeling as the long-term goal. In addition, the workshop will reassess these challenges and their concomitant opportunities and will adjust or broaden them appropriately by taking into consideration recent progress and using the criteria of urgency, extreme-scale computing benefit, readiness for progress within a ten-year time frame, and world-leading potential.

The workshop is organized into panels that broadly cover three fusion topics (A,B,C) and crosscutting issues in computational mathematics and computer science (D,E,F,G) in the context of integrated simulations for magnetic fusion energy sciences. The scope of each of these panels will build on prior workshop findings (as indicated in the resources listed at the end of this document) and will include recent advances in FES SciDAC Centers and ASCR SciDAC Institutes. Whitepapers should address one or more of the following specific panel topics:

A. **Disruption prevention, avoidance, and mitigation**: gaps and challenges in theory, guidance from experiment, status of simulation capabilities, status of validation and measurement capabilities.
B. **Plasma boundary, including the pedestal, scrape off layer, and plasma-materials interactions**: gaps and challenges in theory, guidance from experiment, status of simulation capabilities, status of validation and measurement capabilities.
C. **Whole device modeling**: software, status of integrated modeling, validation and measurement capabilities, the roles of first-principles models (e.g., requiring extreme-scale computing platforms) and reduced models.

D. **Multiphysics and multiscale coupling**: mathematical formulations (e.g., models, meshing, discretization), algorithms (e.g., solvers and time advancement, coupling between scales and domains), quantitative a posteriori error analysis, verification.
E. **Beyond interpretive simulations**: stochastic inverse problems for parameter determination, sensitivity analysis, uncertainty quantification, optimization, design, control (so-called 'outer loop' issues).
F. **Data management, analysis, and assimilation**: integrated data analysis and assimilation that support end-to-end scientific workflows; knowledge discovery methods in multi-modal, high-dimensional data (qualitative and quantitative); integrating data management and knowledge discovery software architectures and systems.

    White papers for this topic should include use cases that define the technology needs. It will be valuable to have use cases that describe an end-to-end problem scenario, complete with as much specific information as possible about science needs and resource utilization (e.g., amount of data moved/processed, over what period of time, lifetime/lifespan of data and data products, types of facilities used like centrally located SC centers or computing collocated with experimental facilities). Also valuable would be clear statements of desired/required analysis and "data mining" objectives with a brief description of the application area.

G. **Software integration and performance**: workflows and code coupling software, performance portability, software productivity and software engineering, governance models for the fusion integrated modeling community.

Instructions: Each whitepaper should indicate if an oral presentation is desired or not, specify a primary panel topic from the list A-G above and optionally secondary and/or crosscutting topics. The subtopics listed for panels A-G are intended for guidance and are not meant to be limiting. In formulating a whitepaper, please consider the following: (a) *motivation:* What specific challenge or opportunity facing the fusion community does the whitepaper address? (b) *approach:* What are the potential approaches to meeting that challenge or opportunity (optional)? and (c) *impact:* What would be the impact on the fusion community by meeting this challenge or opportunity (a positive impact) or not (a negative impact)?

Format and Submission Guidance for Whitepapers:

1. Whitepapers must be submitted in PDF format, maximum of 2 pages, inclusive of all text, tables, and figures. References are not included in the 2-page limit. Use no smaller than 11-point font and at least 1-inch margins. Each file's size should not exceed 5 MB. There is no limit to the number of whitepapers that an individual or group of co-authors may

submit. Each whitepaper should provide contact information (name, institution, email address) for a single corresponding author.

2. Submit each whitepaper to the email address ISwhitepapers@burningplasma.org. In the subject header of the email, please specify the primary panel topic of the whitepaper (A-G listed above). Please send a separate email for each whitepaper submission rather than bundling multiple whitepapers in one email.
3. Whitepapers will be accepted through April 16, 2015.
4. Oral presentations will be given via teleconference on May 18-19, 2015 for those whitepaper submissions requesting orals. We will try to accommodate all requests for oral presentations but may have to limit speakers depending on final numbers.

All whitepapers received will be posted or linked, for public viewing, on the workshop website. This website is hosted by the US Burning Plasma Organization, a national organization of scientists involved in burning plasma research that is often used by the fusion community to collect and archive relevant material. Whitepapers will feed into the draft workshop report and will be used to help organize workshop discussions.

Resource Documents: This workshop will build on prior workshop findings as indicated in the following resource documents:

2014 FESAC Strategic Planning Panel: report, whitepapers, references:
https://www.burningplasma.org/activities/?article=2014%20FESAC%20Strategic%20Planning%20Panel

2011 FSP Planning Study:
Report: http://w3.pppl.gov/fsp/FSP_Summary_FILES/FSP_Program_Execution_Plan.pdf
General information: http://w3.pppl.gov/fsp/Overview.html
FSP Validation wiki: http://www.psfc.mit.edu/FSP-Validation/index.php/Main_Page
2011 FSP Project Definition Workshop: https://ice.txcorp.com/trac/2011_FspDefinitionWorkshop
FSP Science Drivers wiki:
http://fspscidri.sites.lehigh.edu/index.php?title=Main_Page#Integrated_Science_Application_Plans

2010 Report on the Workshop on Scientific Grand Challenges: Crosscutting Technologies for Computing at the Exascale:
http://science.energy.gov/%7E/media/ascr/pdf/program-documents/docs/Crosscutting_grand_challenges.pdf

2009 Report on Fusion Energy Sciences and the Role of Computing at the Extreme Scale (part of an ASCR-led workshop series):

http://science.energy.gov/~/media/fes/pdf/workshop-reports/FES_Grand_Challenges_Report_final.pdf

2009 FES Research Needs Workshop (while simulations were just a part of this workshop, the report provides a good overview of magnetic fusion challenges): report, whitepapers, references:
https://www.burningplasma.org/web/renew.html

2007 FSP Workshop Report:
http://science.energy.gov/~/media/fes/pdf/workshop-reports/Fsp_workshop_report_may_2007.pdf

2014 Workshop on Software Productivity for Extreme-scale Science: report, whitepapers, references:
http://www.orau.gov/swproductivity2014/

2013 Workshop on Applied Mathematics Research for Exascale Computing: report, whitepapers, references:
https://collab.mcs.anl.gov/display/examath/Exascale+Mathematics+Home

2013 ASCAC Data Subcommittee Report on Synergistic Challenges in Data-Intensive Science and Computing:
http://science.energy.gov/~/media/ascr/ascac/pdf/reports/2013/ASCAC_Data_Intensive_Computing_report_final.pdf

2012 Report on the Workshop on Extreme-Scale Solvers: Transitions to Future Architectures:
http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/reportExtremeScaleSolvers2012.pdf

DOE FES/ASCR Workshop on
Integrated Simulations for Magnetic Fusion Energy Sciences

Hilton Hotel, Rockville, MD
June 2-4, 2015
https://www.burningplasma.org/activities/IntegratedSimulations2015

Final Agenda

Day 1: Tuesday, June 2 (8:30 am - 6:15 pm)

8:30 am	**Welcome and Logistics**
	John Mandrekas and Randall Laviolette, DOE
8:45 am	**Fusion Energy Sciences (FES) Introduction**
	Ed Synakowski and James Van Dam, DOE
9:00 am	**Advanced Scientific Computing Research (ASCR) Introduction**
	Steve Binkley, DOE
9:15 am	**Review of Workshop Agenda, Goals, and Preliminary Input**
	Paul Bonoli (MIT) and Lois Curfman McInnes (ANL)
9:45 am	Break
10:15 am	**Emerging Extreme-Scale Architectures and Programming Models**
	Marc Snir, ANL
11:00 am	Full-group Discussion
11:15 am	**The ITER Integrated Modelling Programme**
	Simon Pinches, ITER
12:00 pm	Full-group Discussion
12:15 pm	Lunch Break (attendees on your own)
1:30 pm	**Panel A: Disruptions: Preliminary Report**
2:00 pm	**Panel B: Plasma Boundary: Preliminary Report**
2:30 pm	**Panel C: Whole Device Modeling: Preliminary Report**
3:00 pm	Breakout Instructions, Q&A
3:15 pm	Break
3:45 pm	**Concurrent Breakout Sessions #1: Challenges and Opportunities in Integrated Simulations for Magnetic Fusion Energy Sciences: Physics Perspectives**
	Panels A,B,C (with crosscutting math/CS participants)
6:15 pm	Adjourn for the day (dinner on your own)

Day 2: Wednesday, June 3 (8:30 am - 6:15 pm)

8:30 am	Summary of Day 1, Review Agenda for Day 2
8:45 am	**Panel A: Disruptions: Outbrief #1**
9:05 am	**Panel B: Plasma Boundary: Outbrief #1**
9:25 am	**Panel C: Whole Device Modeling: Outbrief #1**
9:45 am	Full-group Discussion
10:15 am	Break
10:45 am	**Perspectives on Collaborative Computational Science from an ASC Code Team** Mike Glass, SNL
11:30 am	**Perspectives on Multi-institutional Collaborative Computational Chemistry & Materials** Theresa Windus, Iowa State University
12:15 pm	Full-group Discussion
12:30 pm	Lunch Break (attendees on your own)
1:45 pm	**Panel D: Multiphysics and Multiscale Coupling: Preliminary Report**
2:05 pm	**Panel E: Beyond Interpretive Simulations: Preliminary Report**
2:25 pm	**Panel F: Data Management, Analysis, and Assimilation: Preliminary Report**
2:45 pm	**Panel G: Software Integration and Performance: Preliminary Report**
3:05 pm	Breakout Instructions, Q&A
3:15 pm	Break
3:45 pm	**Concurrent Breakout Sessions #2: Challenges and Opportunities in Integrated Simulations for Magnetic Fusion Energy Sciences: Math/CS Perspectives** Panels D,E,F,G (with crosscutting fusion participants)
6:15 pm	Adjourn for the day (dinner on your own)

Day 3: Thursday, June 4 (8:00 am - 12:00 pm)

8:00 am	Summary of Day 2, Review Agenda for Day 3
8:05 am	**Panel D: Multiphysics and Multiscale Coupling: Outbrief #2**
8:25 am	**Panel E: Beyond Interpretive Simulations: Outbrief #2**
8:45 am	**Panel F: Data Management, Analysis, and Assimilation: Outbrief #2**
9:05 am	**Panel G: Software Integration and Performance: Outbrief #2**
9:25 am	Full-group Discussion
9:45 am	Break
10:00 am	**Concurrent Breakout Sessions #3: Challenges and Opportunities in Integrated Simulations for Magnetic FES: Revisiting Crosscutting Issues** Panels A,B,C (with crosscutting math/CS participants)
11:15 am	**Outbriefs from Panels A, B, C** (15 minutes each)
12:00 pm	Workshop wrap-up, review timeline, process and assignments for report
12:05 pm	Workshop adjourns for most participants (lunch on your own)
1:30-3:30 pm	Working session for writing leads

E. Workshop Participants

Chair: Paul Bonoli (Massachusetts Institute of Technology)
Co-Chair: Lois Curfman McInnes (Argonne National Laboratory)
DOE/FES Point of Contact: John Mandrekas
DOE/ASCR Point of Contact: Randall Laviolette

The workshop was organized into panels that broadly cover three fusion integrated science applications (A,B,C) and crosscutting issues in mathematical and computational enabling technologies (D,E,F,G) in the context of integrated simulations for magnetic fusion energy sciences.

Integrated Science Applications:

- **Panel A: Disruption Physics**
  - **Panel Chair:** Carl Sovinec (University of Wisconsin-Madison)
  - **Panel Co-Chair:** Dylan Brennan (Princeton University)
  - **Focus:** Gaps and challenges in theory, guidance from experiment, status of simulation capabilities, status of validation and measurement capabilities.
  - **Panel Members:**
    Boris Breizman (University of Texas - Austin)
    Luis Chacón[4] (Los Alamos National Laboratory)
    Nathaniel Ferarro (General Atomics)
    Richard Fitzpatrick (University of Texas - Austin)
    Guo-Yong Fu (Princeton Plasma Physics Laboratory)
    Stefan Gerhardt (Princeton Plasma Physics Laboratory)
    Eric Hollman (University of California - San Diego)
    Valerie Izzo (University of California - San Diego)
    Steve Jardin (Princeton Plasma Physics Laboratory)
    Scott Kruger (Tech-X Corporation)
    Ravi Samtaney[4] (King Abdullah University of Science and Technology)
    Hank Strauss (HRS Fusion)
    Alan Turnbull (General Atomics)

- **Panel B: Plasma Boundary Physics**
  - **Panel Chair:** Tom Rognlien (Lawrence Livermore National Laboratory)
  - **Panel Co-Chair:** Phil Snyder (General Atomics)
  - **Focus:** Gaps and challenges in theory, guidance from experiment, status of simulation capabilities, status of validation and measurement capabilities.
  - **Panel Members:**
    John Canik (Oak Ridge National Laboratory)
    Choong-Seock Chang (Princeton Plasma Physics Laboratory)
    Eduardo D'Azevedo[4] (Oak Ridge National Laboratory)

---

[4] Crosscutting expert from ASCR

Andris Dimits (Lawrence Livermore National Laboratory)
Mikhail Dorf (Lawrence Livermore National Laboratory)
Milo Dorr[4] (Lawrence Livermore National Laboratory)
Richard Groebner (General Atomics)
Greg Hammett (Princeton Plasma Physics Laboratory)
Karl Hammond (University of Missouri)
Sergei Krasheninnikov (University of California - San Diego)
Tony Leonard (General Atomics)
Zhihong Lin (University of California - Irvine)

- **Panel C: Whole Device Modeling**
  - **Panel Chair:** Jeff Candy (General Atomics)
  - **Panel Co-Chair:** Chuck Kessel (Princeton Plasma Physics Laboratory)
  - **Focus: Software, status of integrated modeling, validation and measurement capabilities, the roles of first-principles models (e.g., requiring extreme-scale computing platforms) and reduced models.**
  - **Panel Members:**
    Donald Batchelor (Oak Ridge National Laboratory)
    John Cary (Tech-X Corporation)
    David Green (Oak Ridge National Laboratory)
    Brian Grierson (Princeton Plasma Physics Laboratory)
    Jeff Hittinger[4] (Lawrence Livermore National Laboratory)
    Chris Holland (University of California - San Diego)
    Stan Kaye (Princeton Plasma Physics Laboratory)
    Alice Koniges[4] (Lawrence Berkeley National Laboratory)
    Arnold Kritz (Lehigh University)
    Lynda Lodestro (Lawrence Livermore National Laboratory)
    Orso Meneghini (General Atomics)
    Francesca Poli (Princeton Plasma Physics Laboratory)
    Tariq Rafiq (Lehigh University)

Mathematical and Computational Enabling Technologies:

- **Panel D: Multiphysics and Multiscale Coupling**
  - **Panel Chair:** Jeff Hittinger (Lawrence Livermore National Laboratory)
  - **Panel Co-Chair:** Luis Chacón (Los Alamos National Laboratory)
  - **Focus:** Mathematical formulations (e.g., models, meshing, discretization), algorithms (e.g., solvers and time advancement, coupling between scales and domains), quantitative a posteriori error analysis, verification.
  - **Panel Members:**
    Andrew Christlieb (Michigan State University)
    Guo-Yong Fu[5] (Princeton Plasma Physics Laboratory)

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[5] Crosscutting expert from FES

Greg Hammett[5] (Princeton Plasma Physics Laboratory)
Cory Hauck (Oak Ridge National Laboratory)
Dan Reynolds (Southern Methodist University)
Ravi Samtaney (King Abdullah University of Science and Technology)
Mark Shephard (Rensselaer Polytechnic Institute)
Mayya Tokman (University of California - Merced)
Ray Tuminaro (Sandia National Laboratories)
Carol Woodward (Lawrence Livermore National Laboratory)

- **Panel E: Beyond Interpretive Simulations**
  - **Panel Chair:** Donald Estep (Colorado State University)
  - **Panel Co-Chair:** Todd Munson (Argonne National Laboratory)
  - **Focus:** Inverse problems for parameter estimation, sensitivity analysis, uncertainty quantification, numerical optimization, and design and control.
  - **Panel Members:**
    Eduardo D'Azevedo (Oak Ridge National Laboratory)
    Omar Knio (Duke University)
    Scott Kruger[5] (Tech-X Corporation)
    Robert Moser (University of Texas - Austin)
    Eugenio Schuster (Lehigh University)
    Daniel Tartakovsky (University of California - San Diego)
    Bart van Bloemen Waanders (Sandia National Laboratories)
    Anne White[5] (Massachusetts Institute of Technology)

- **Panel F: Data Management, Analysis, and Assimilation**
  - **Panel Chair:** Wes Bethel (Lawrence Berkeley National Laboratory)
  - **Panel Co-Chair:** Martin Greenwald[5] (Massachusetts Institute of Technology)
  - **Focus:** Integrated data analysis and assimilation that support end-to-end scientific workflows; knowledge discovery methods in multi-modal, high-dimensional data (qualitative and quantitative); integrating data management and knowledge discovery software architectures and systems.
  - **Panel Members:**
    Stan Kaye[5] (Princeton Plasma Physics Laboratory)
    Scott Klasky (Oak Ridge National Laboratory)
    Allen Sanderson (University of Utah)
    David Schissel[5] (General Atomics)
    John Wright[5] (Massachusetts Institute of Technology)
    John Wu (Lawrence Berkeley National Laboratory)

- **Panel G: Software Integration and Performance**
  - **Panel Chair:** David Bernholdt (Oak Ridge National Laboratory)

- **Panel Co-Chair:** Bob Lucas (University of Southern California / Information Sciences Institute)
- **Focus:** Workflows and code coupling software, performance portability, software productivity and software engineering, governance models for the fusion integrated modeling community.
- **Panel Members:**
  John Cary[5] (Tech-X Corporation)
  Milo Dorr (Lawrence Livermore National Laboratory)
  Alice Koniges (Lawrence Berkeley National Laboratory)
  Orso Meneghini[5] (General Atomics)
  Boyana Norris (University of Oregon)
  Francesca Poli[5] (Princeton Plasma Physics Laboratory)
  Brian Van Straalen (Lawrence Berkeley National Laboratory)
  Patrick Worley (Oak Ridge National Laboratory)

General:

- **Participants at Large:**
  - **Focus:** Participants at Large were asked to attend the workshop in order to observe and provide feedback to the panels.
  - **Participants at Large:**
    Amitava Bhattacharjee (Princeton Plasma Physics Laboratory)
    William Dorland (University of Maryland)
    Mike Glass[6] (Sandia National Laboratories)
    Frank Jenko (University of California - Los Angeles)
    Esmond Ng (Lawrence Berkeley National Laboratory)
    Simon Pinches[6] (ITER)
    Marc Snir[6] (Argonne National Laboratory)
    William Tang (Princeton Plasma Physics Laboratory)
    Xianzhu Tang (Los Alamos National Laboratory)
    François Waelbroeck (University of Texas - Austin)
    Theresa Windus[6] (University of Iowa and Ames Laboratory)
    Michael Zarnstorff (Princeton Plasma Physics Laboratory)

- **Observers:**
  Steve Binkley (ASCR, DOE)
  Rich Carlson (ASCR, DOE)
  William Harrod (ASCR, DOE)
  Thuc Hoang (NNSA, DOE)
  Thomas Ndousse-Fetter (ASCR, DOE)
  Lucy Nowell (ASCR, DOE)
  Karen Pao (ASCR, DOE)
  Ceren Susut (ASCR, DOE)
  Ed Synakowski (FES, DOE)
  James Van Dam (FES, DOE)

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[6] Plenary speaker