Importance of Advanced Computers and Computation to Fusion Development

Paul Bonoli

(On behalf of the authors of the Report on Integrated Simulations for Magnetic Fusion Energy Sciences)

Plasma Science and Fusion Center

Massachusetts Institute of Technology

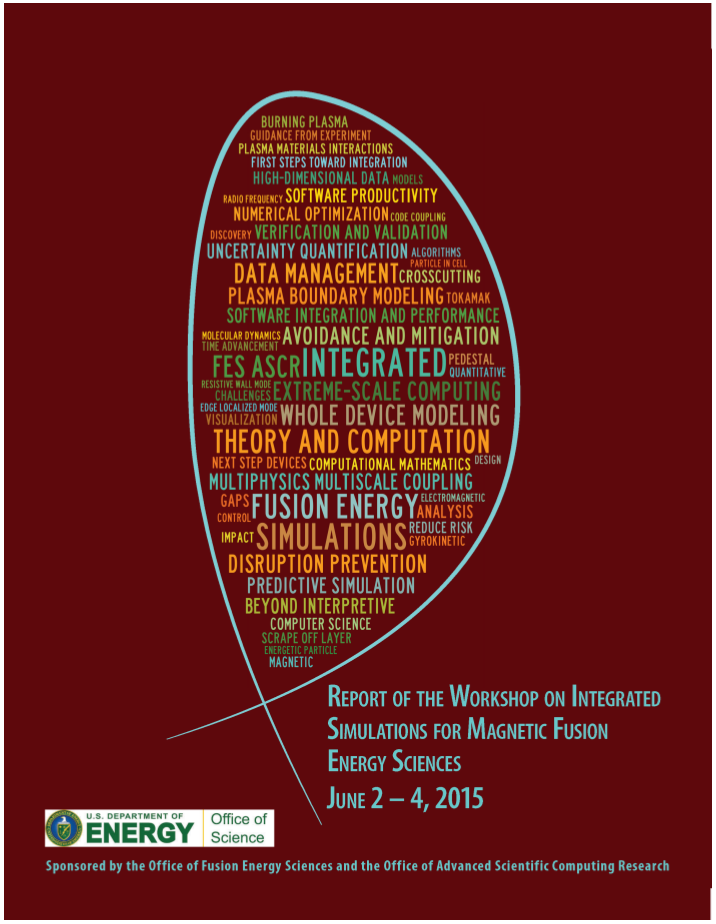
Cambridge, MA 02139

Fusion Power Associates
36th Annual Meeting and Symposium
"Strategies to Fusion Power"

December 16-17, 2015

Topic of this talk is timely in view of the recent DOE planning activity on integrated simulations for magnetic fusion energy sciences

- Report identified gaps in theory and simulation, especially as related to integration of multiple processes and regions:
  - **Examined how these gaps could be addressed in the ten year time frame.**
  - **Identified new opportunities for integrated simulation including the roles of physics, applied mathematics, and computer science**
  - **Emphasis on crosscutting fusion / applied math / computer science connections**
  - **Identified potential applications for extreme-scale computing**



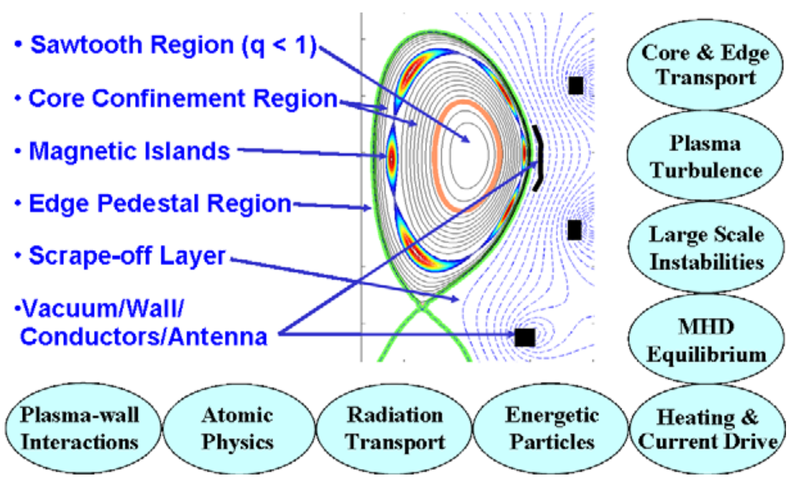
https://www.burningplasma.org/activities/IntegratedSimulations2015

Essential Role of advanced computers and computation in fusion development

- **Provide the predictive capability needed to develop the physics and engineering basis for a commercially viable fusion reactor.**
- **Why high performance computation is needed:**
  - **System complexity – multiple physical processes, multiple and overlapping spatial and temporal scales.**
  - **Requires integration at all levels ranging from "binary" process up to the "whole device".**
  - **High cost of experiments.**
  - **Catastrophic consequences of failure (e.g. disruptions).**

The tokamak offers unique opportunities and challenges for advanced computation and integrated simulations

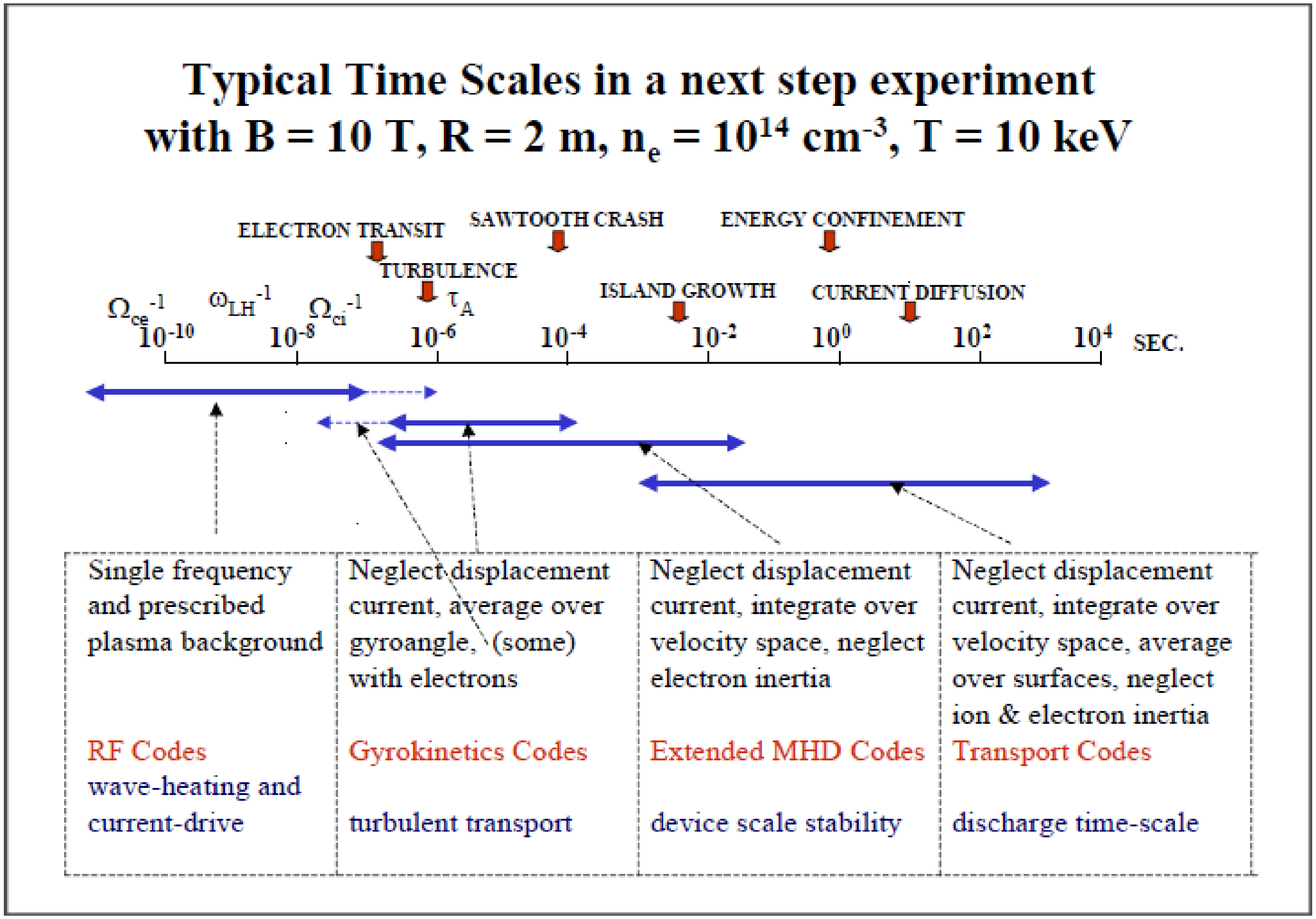
- **The modeling, system simulation, and validation areas critically require advanced computation tools to enable the high confidence design and verification planned for ITER operation.**



2007 FSP Workshop Report

- System-scale simulations integrate multiphysics & multiscale processes focused on understanding whole-system behavior:
  - Goes beyond traditional approach which focuses on detailed understanding of components
- Includes interdisciplinary simulations incorporating expertise from physics, applied math, and computer science
- Work flows require managing, visualizing, and analyzing ultra-large datasets

Physical processes in a tokamak discharge span multiple time and spatial scales



2002 FESAC ISOFS Report

Advanced Computation will necessarily involve interdisciplinary opportunities between physicists, applied mathematicians and computer scientists

Integrated Science Applications

- Disruption Prevention, Avoidance, and Mitigation
- Plasma Boundary including the Pedestal, SOL, and PMI
- Whole Device Modeling
- New Opportunities

Mathematical and Computational Enabling Technologies

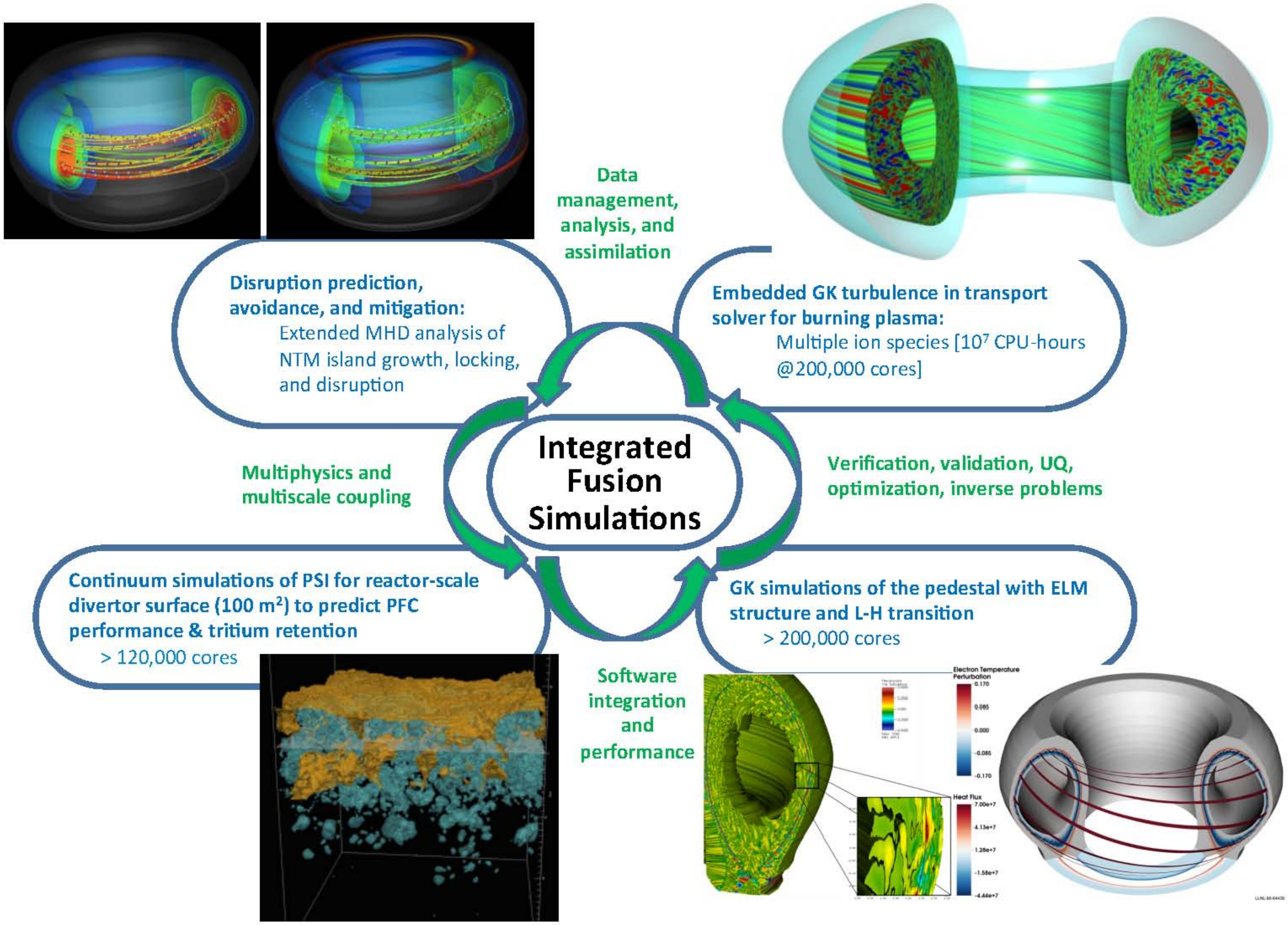
- Multiphysics and Multiscale Coupling
- Beyond Interpretive Simulation
- Data Management, Analysis, and Assimilation
- Software Integration and Performance

Focus: Integration

Mathematical and Computational Enabling Technologies

Multiphysics and Multiscale Coupling	Data Management, Analysis, and Assimilation
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	**Focus:** integrated data analysis & assimilation that support end –to-end scientific workflows; knowledge discovery methods in multimodal, high-dimensional data; integrating data management and knowledge discovery software architectures and systems
E: Beyond Interpretive Simulations	**Software Integration and Performance**
Focus: stochastic inverse problems for parameter determination, sensitivity analysis, uncertainty quantification, optimization, design, control (so-called ‘outer loop’ issues)	**Focus:** workflows and code coupling software, performance portability, software productivity and software engineering, governance models for the fusion integrated modeling community

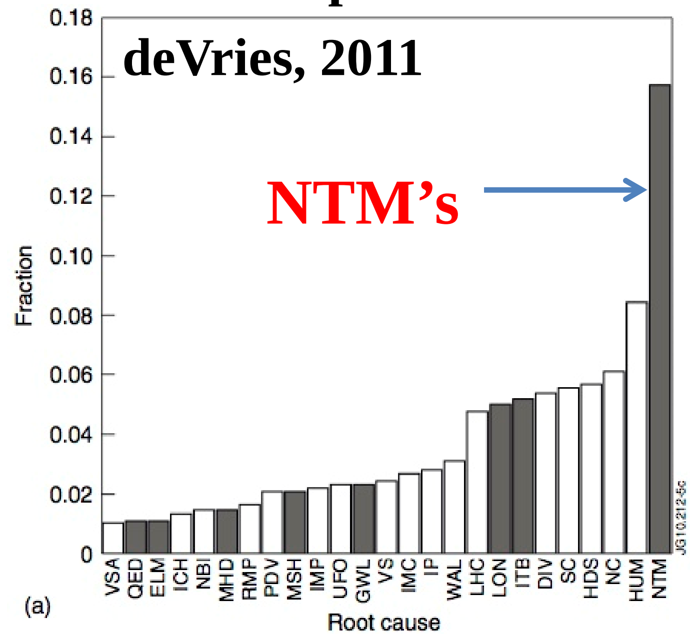
Physics vision for integrated simulations pushes computation to the extreme-scale



Disruption prevention, avoidance, and mitigation

- **The tokamak configuration is susceptible to macroscopic instability when operated in fusion-relevant conditions:**
  - Plasma is far from thermodynamic equilibrium with surroundings.
  - Discharge-terminating events are triggered by:
    - Natural fluctuations,
    - Equipment failure, and
    - Error in operations planning.
- **Unmitigated disruption in ITER and future tokamaks will have unacceptable consequences:**
  - Extreme localized heating can damage surfaces and other components.
  - Deposition of relativistic electrons also damages components.
  - Electromechanical forcing can distort coils and structures.

JET Disruption Database

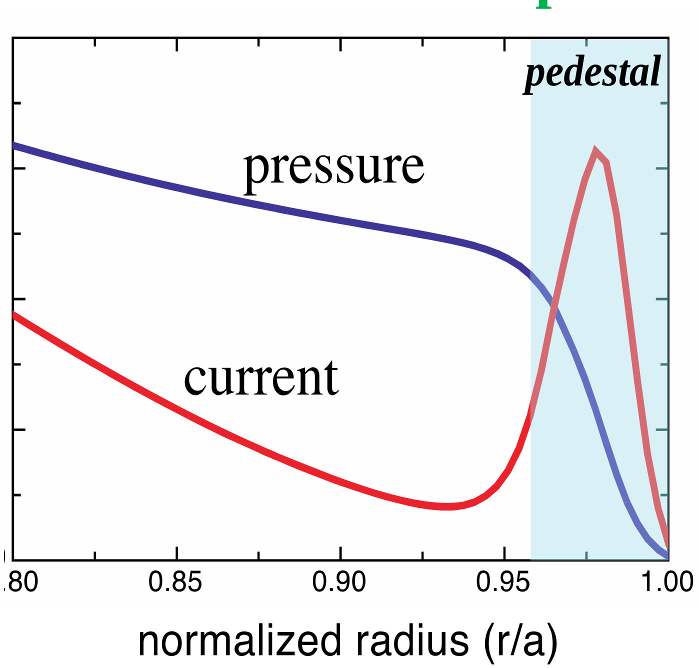


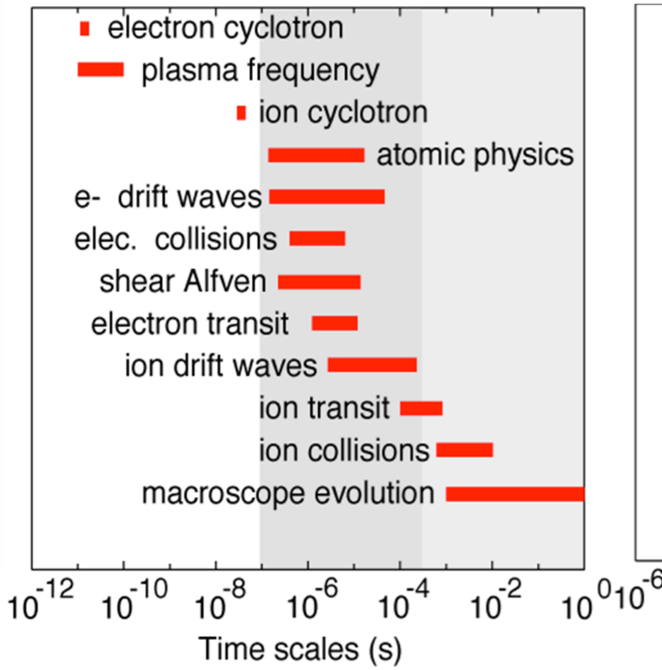
- **Integrated simulation can help avoid disruptive conditions and inform the engineering of effective mitigation systems.**
  - Improved characterization of disruptions is necessary.

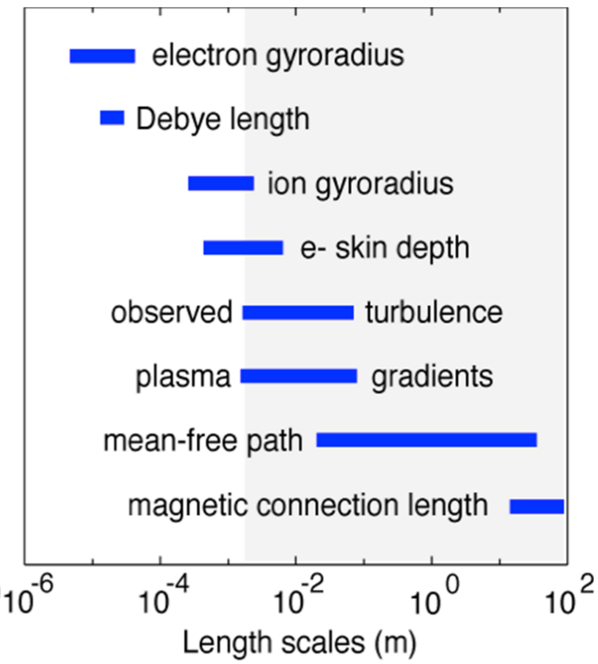
Disruption Physics: Priority Research Directions

- **Develop integrated simulation that models all forms of tokamak disruption from instability through thermal and current quenches to the final deposition of energy with and without mitigation.**
  - Modeling capable of addressing fundamental questions on mode locking, runaway-electron generation and evolution, and open-field currents.
  - Integrated modeling will facilitate the engineering of effective mitigation systems.
- **Develop a profile-analysis system that automates reconstruction and coordinates transport modeling and stability assessment for disruption studies.**
  - Automated profile analysis will benefit all forms of disruption modeling.
  - Automation is a necessary step for real-time analysis.
- **Verify and validate linear and nonlinear computational models to establish confidence in the prediction and understanding of tokamak disruption physics with and without mitigation.**
  - Validation methodology will help judge what effects are most important.
  - Prospect for predictability need to be addressed.

Challenge of the Plasma Boundary: Temperature must go from hundreds of degrees at the wall up to tens of millions at top of pedestal, while preserving long material lifetimes

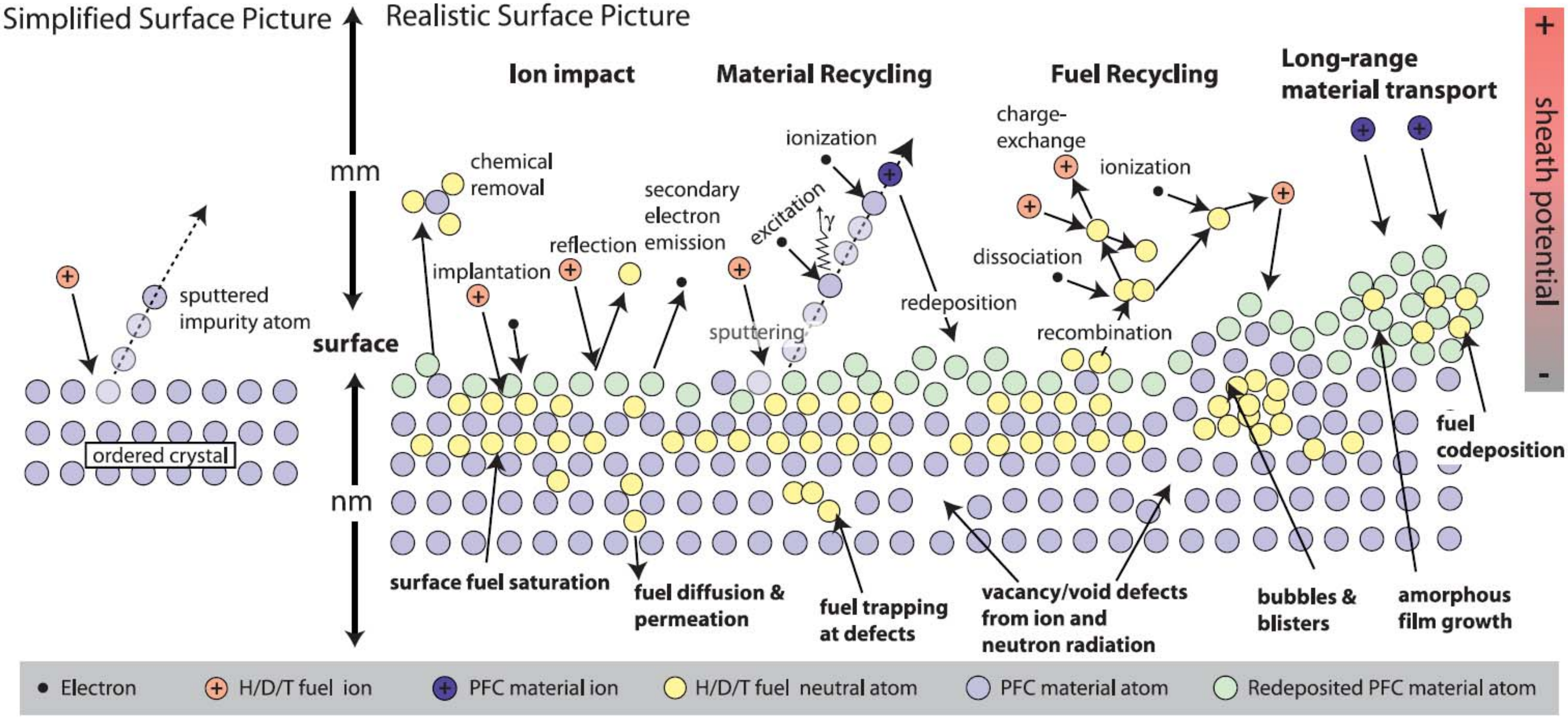






- **Problem is profoundly multiscale**
- **Essential role for verification and validation and uncertainty quantification**
  - Uncertainties in inputs, propagation of errors in high dimensions
  - Benefit from multiple algorithms for code-code comparisons, sophisticated UQ techniques (opportunity to develop validated model hierarchies)
  - Geometric complexity, evolving geometry, bifurcating solutions

Accurate simulation of the plasma-materials-interface must account for the wide variety of processes that can occur within the near-surface material interface



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.

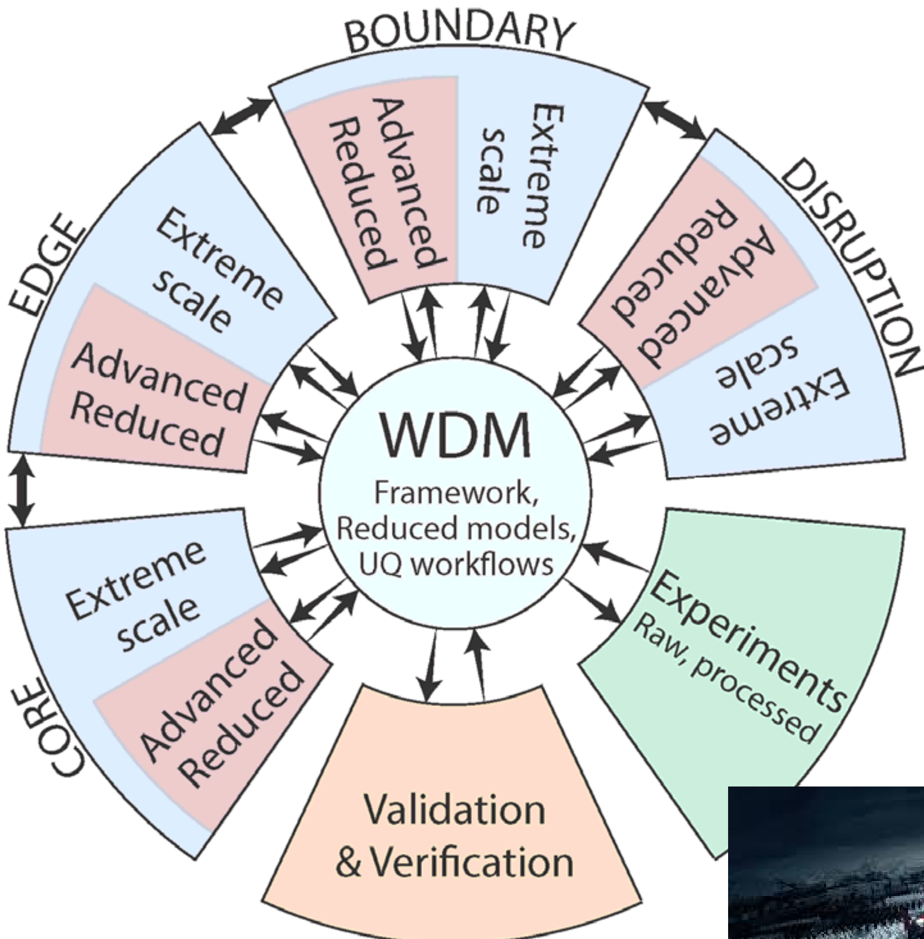
Boundary Physics: Priority Research Directions

- **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.**
- **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.**
- **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.**
- **Integrate RF antenna/plasma-absorption simulations with SOL/pedestal plasma transport simulations, filling a notable gap in present capability.**
- **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.**

Challenges for the Whole Device Model

- **The Whole Device Model is multiphyiscs and multiscale.**
- **There is an urgent need to minimize the time required for physics knowledge gained from highest fidelity physics simulations to be employed in Whole Device Models:**
  - **Model hierarchies are a useful concept for accomplishing this goal.**
- **Model hierarchies are characterized by a range of physics fidelity:**
  - **Development of reliable model hierarchies will require extensive validation against experiment to define regimes of applicability.**
  - **Ultimately must balance accuracy and simulation goals against time to solution.**
- **WDM framework and workflows must therefore be flexible.**

"Death star" vision for the WDM showing the interaction between topical areas



- **Flexibility envisioned for the WDM is embodied in the use of both Advanced Reduced models and Extreme Scale Simulations.**

- **WDM framework provides verification and validation technology (UQ workflows) plus connection to experimental data (both raw and processed).**

Key opportunities identified for WDM

- **Coupling of plasma edge and material interactions to the core plasma**
- **Modeling of plasma disruption behavior**
- **New opportunities:**
  - **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**
  - **Simulating the multiscale dynamics of NTM, sawtooth, and other low-n instabilities**
  - **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**

Whole Device Modeling:
Priority Research Directions

- **Increase development of and support for modular WDM frameworks.**
  - Support for mission-critical legacy tools and development and expansion of newer components and work flows that can more effectively utilize leadership-class computing resources.
  - Converge toward a reduced set of community tools compatible with the ITER Integrated Modeling and Analysis Suite (IMAS) and other standards.
- **Continue and expand efforts to understand and distill physics of gap areas using a multipronged approach that includes:**
  - Exploration of gap areas using both theoretical exploration and large-scale simulation of current and emerging fundamental model equations.
  - Synthesis of physics insights obtained, in order to improve or develop new reduced models and modeling techniques.
  - Facilitating a pipeline of components at all fidelity levels into whole device modeling via a flexible framework structure.
- **Increase connection to experiment through validation.**
  - Effort combines the formulation and implementation of rigorous UQ methodologies appropriate for coupled systems with data management capabilities.

Summary and Conclusions

- **Advanced computers and computation have the potential to greatly impact the state of integrated simulations in the areas of:**
  - Disruption physics, including prevention, avoidance, and mitigation
  - Plasma boundary, including the pedestal, scrape off layer, and plasma-materials-interactions
  - Whole device modeling
- **New opportunities anticipated beyond the disruption and boundary areas are:**
  - 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
  - Use of probabilistic WDM to assess the likelihood of key physical transitions or states occurring
- **Realizing these opportunities will require broad based support for a programs of model verification and validation**
- **Interdisciplinary collaborations will play an essential role in the areas of:**
  - Multiphysics and multiscale coupling
  - Beyond interpretive simulations: numerical optimization and uncertainty quantification
  - Data analysis, management, and assimilation
  - Software integration and performance