Challenges and opportunities for integrated modeling

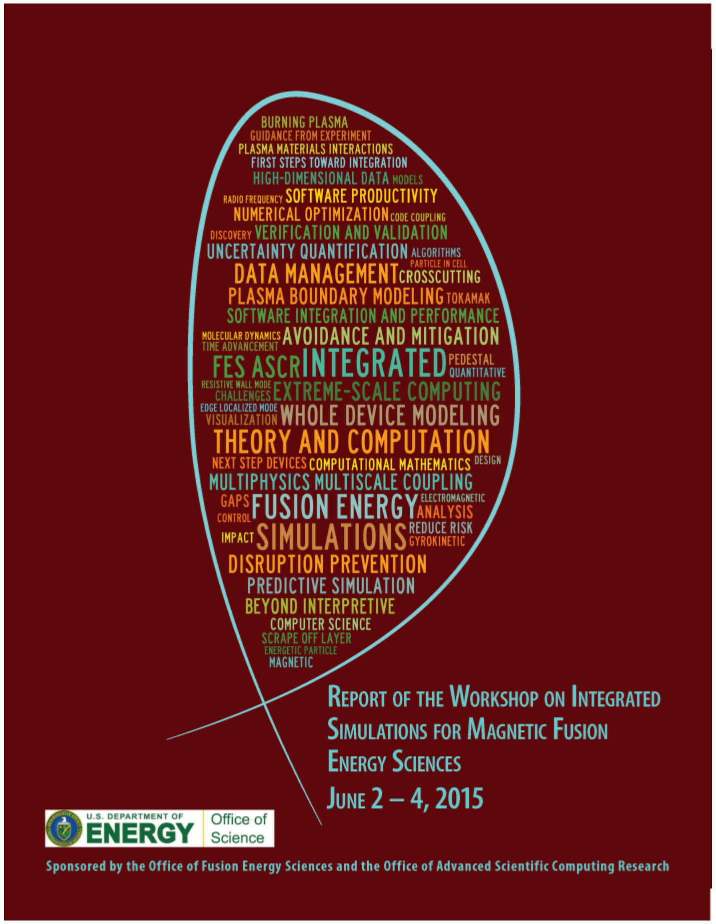
Presented by Francesca Poli

These slides are extracted from the summary of the IS Workshop given by

Paul Bonoli (MIT) and

Lois Curfman McInnes (ANL)

to DOE, on *November 12, 2015*

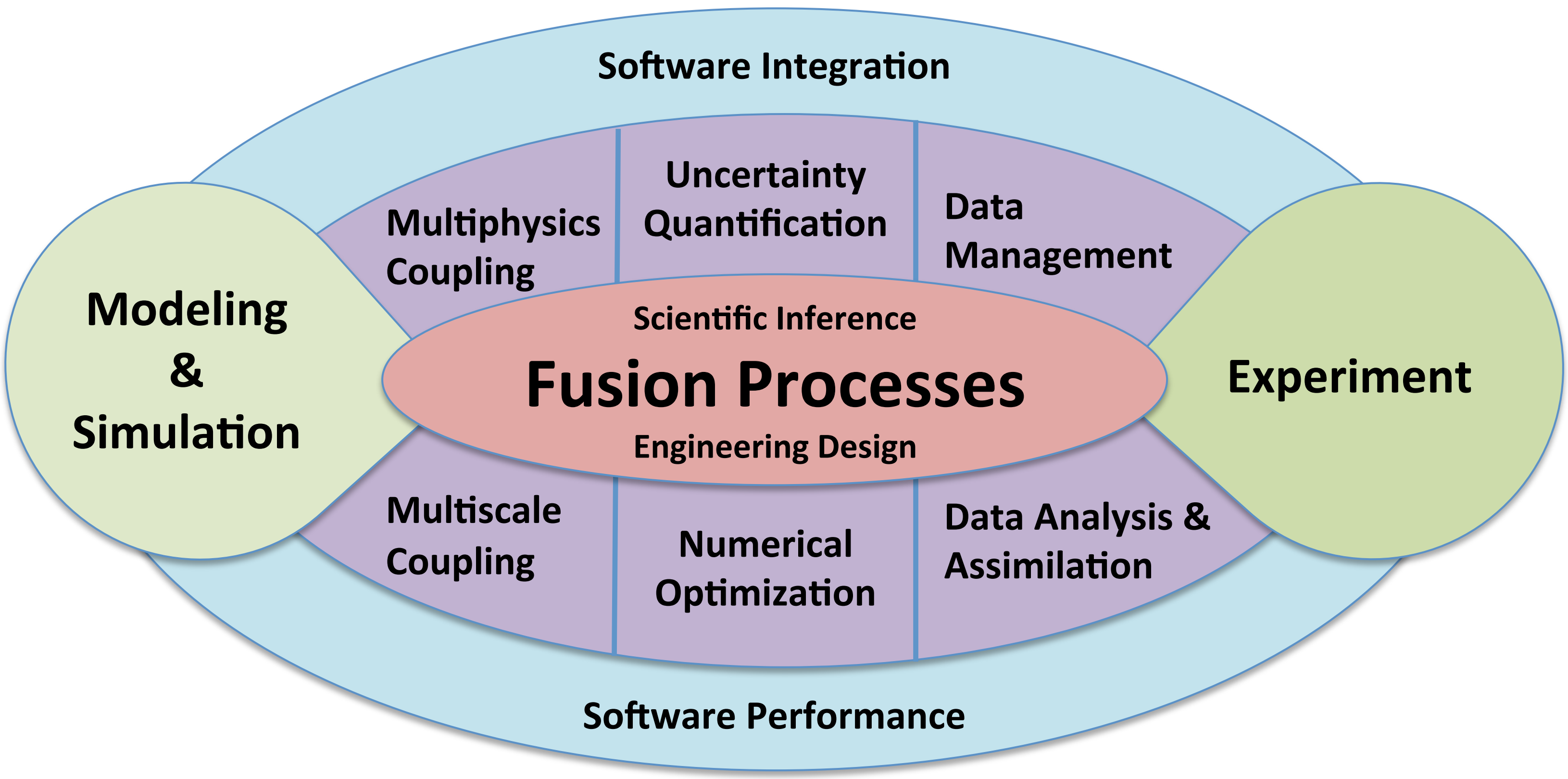


https://www.burningplasma.org/activities/IntegratedSimulations2015

Charge from DOE

- **"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."**
- **"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."**

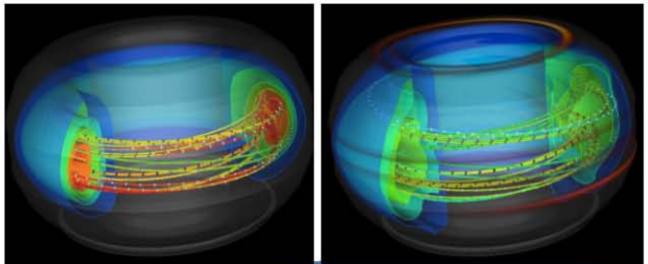
Computational and enabling technologies in integrated fusion simulations

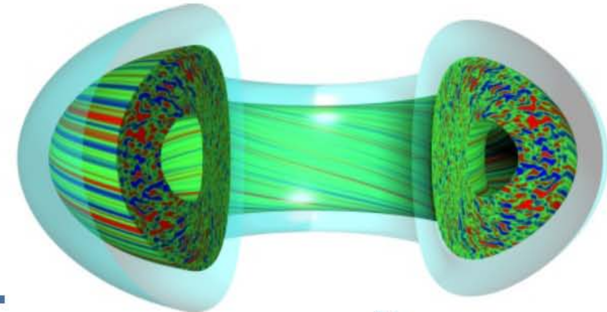


Summary and Conclusions

- **The role of integrated simulations in magnetic fusion energy sciences has been assessed with a focus on identifying gaps, challenges 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:**
  - 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
- **Role of computational and enabling technologies was considered in the crosscutting areas:**
  - Multiphysics and multiscale coupling
  - Beyond interpretive simulations: numerical optimization and uncertainty quantification
  - Data analysis, management, and assimilation
  - Software integration and performance
- **Strategies and a path forward were articulated for each of these areas**

Vision for integrated extreme-scale simulations





Data management, analysis, and assimilation

Disruption prediction, avoidance, and mitigation:
Extended MHD analysis of NTM island growth, locking, and disruption

Embedded GK turbulence in transport solver for burning plasma:
Multiple ion species [10^7 CPU-hours @200,000 cores]

Integrated Fusion Simulations

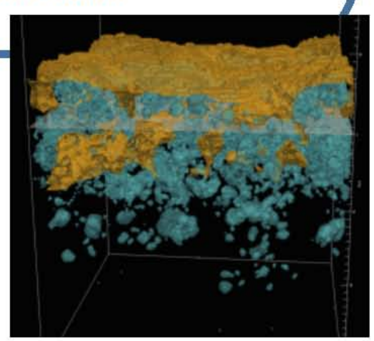
Multiphysics and multiscale coupling

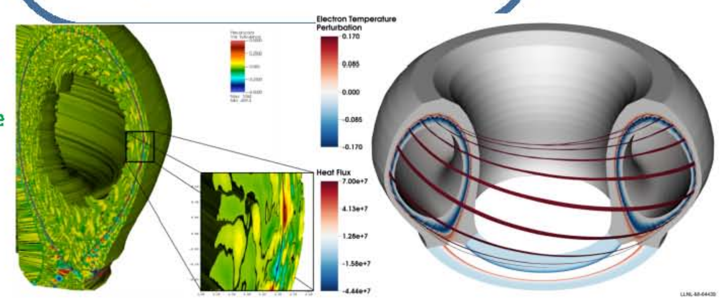
Verification, validation, UQ, optimization, inverse problems

Continuum simulations of PSI for reactor-scale divertor surface (100 m^2) to predict PFC performance & tritium retention
> 120,000 cores

GK simulations of the pedestal with ELM structure and L-H transition
> 200,000 cores

Software integration and performance





Key findings of this workshop and report - 1

- **Opportunities abound for interdisciplinary FES/ASCR collaborations to fully leverage emerging extreme-scale computing resources for fundamental advances in integrated fusion simulations including:**
  - Simulating all stages of plasma disruption behavior
  - 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
  - Coupling plasma heat/particle loads with material interactions and the core plasma
  - Lifetime predictions of plasma-facing components such as the divertor as well as the tritium retention of the first wall
  - **Algorithm and code development should be adapted at an early stage through sustainable partnerships between FES and ASCR.**

Key findings of this workshop and report - 2

- **New opportunities identified for integrated simulations in magnetic fusion energy sciences**
  - 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

Key findings of this workshop and report - 3

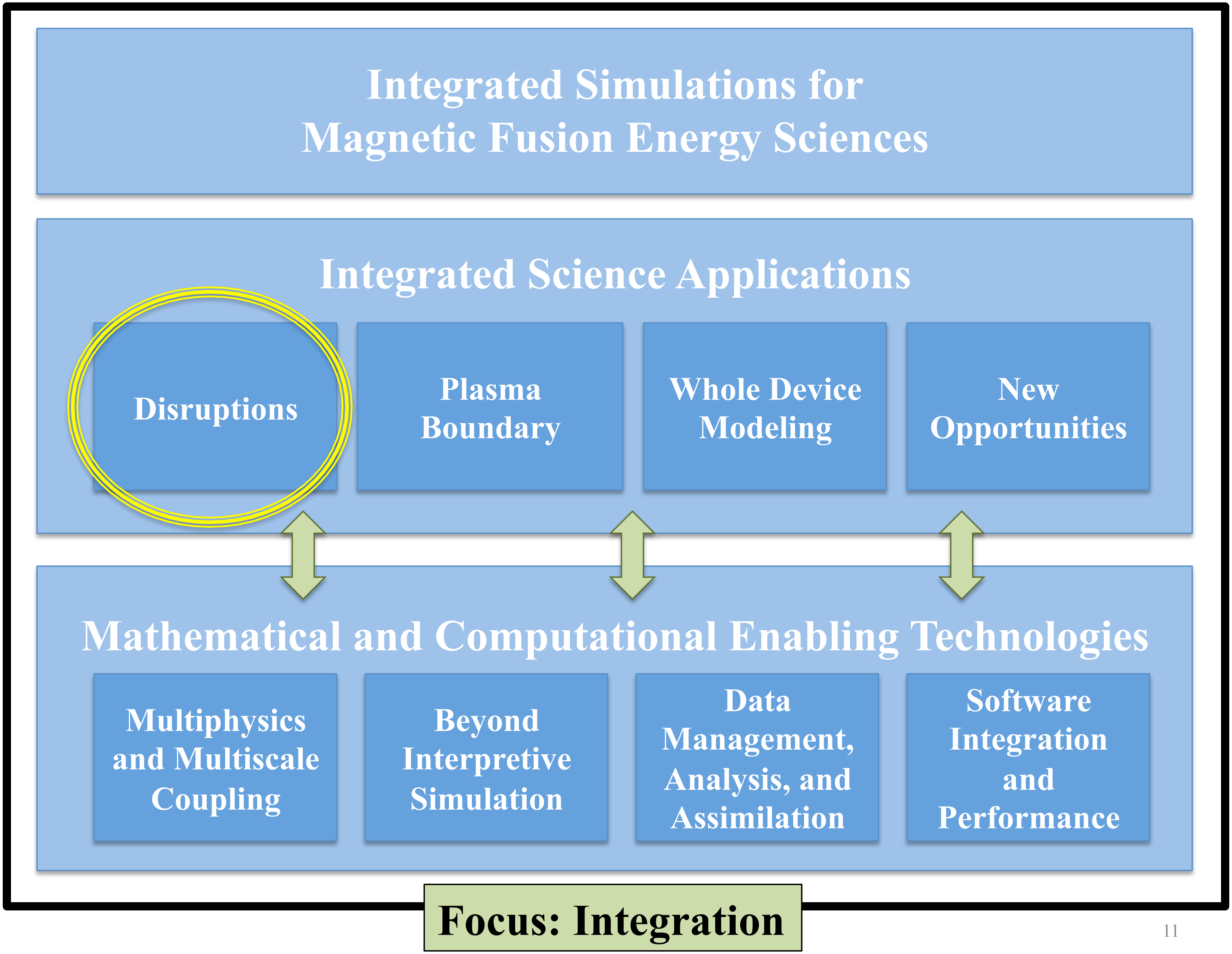
- **Need strong and broad-based support for model verification and validation:**
  - **Essential for the development of reliable model hierarchies:**
    - Models should range from highest physics fidelity to “reduced” descriptions that have been validated in their regimes of applicability.
    - Hierarchies must balance physics fidelity (accuracy) against time to solution for whole device modeling applications.
  - V&V will apply not only to individual physics components but also to integrated simulations that combine multiple physics effects.
  - Will naturally engage theoretical and computational plasma physicists, experimentalists in fusion energy sciences, applied mathematicians, and computer scientists.

Key findings of this workshop and report - 4

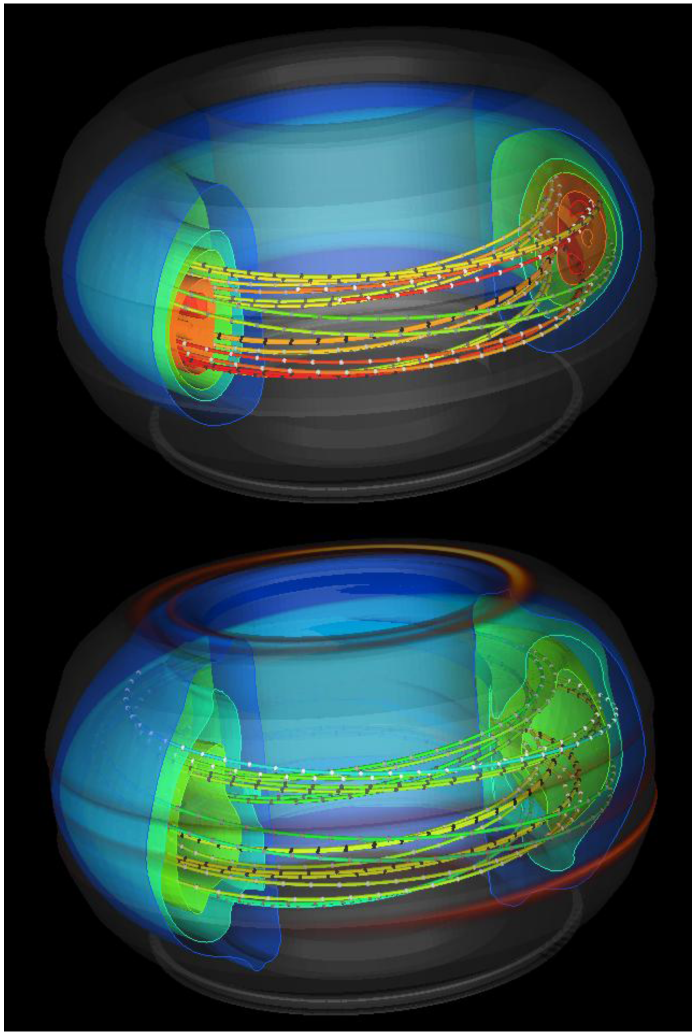
- **Need research on innovative workflows, data structures, and algorithms to support efficient concurrent execution of many related moderate-concurrency simulations running for long periods of time:**
  - Supports studies to carry out uncertainty quantification, investigate model sensitivities, and perform numerical optimization:
    - Scans consisting of hundreds of related jobs running at ~ 50,000 core concurrency level.
  - Research needed on issues such as memory locality and workflows to move beyond simplistic ensemble approaches:
    - Exploit commonalities among closely related runs to fully leverage extreme-scale architectures.
  - Reduce the time that is needed for the development of model hierarchies that can be used in WDM:
    - Develop algorithms that exploit the concurrency of extreme-scale platforms.

Key findings of this workshop and report - 5

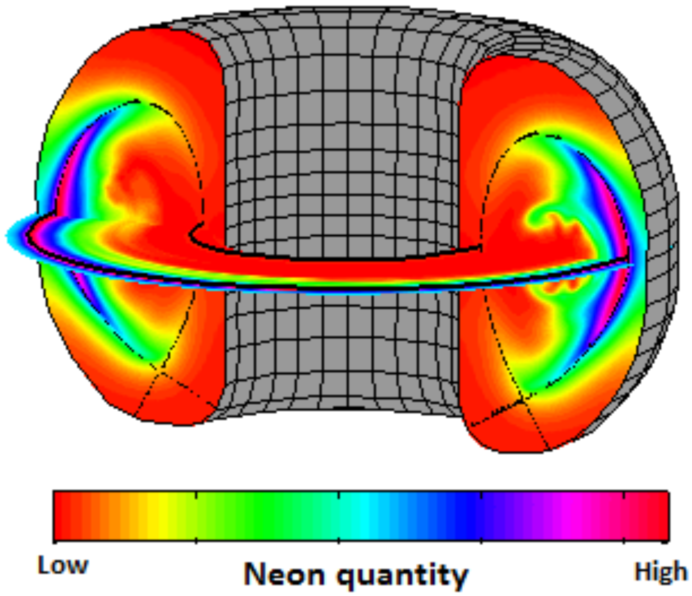
- **Crucial element for realization of the goals of this workshop will be stable and predictable access to high-performance computing resources and workflows:**
  - HPC resources must accommodate a range of applications and needs.
  - **Both capability & capacity computing needs exist:**
    - Largest-scale available machines: Short, moderate, and long time simulations
    - Moderate time (~ few day) simulations at > 100,000 – 150,000 core level
    - Long time (~30 day) simulations at the 25,000 – 50,000 core level
    - Short turnaround ("low latency') simulations at the 5,000-15,000 core level


Integrated Simulations for
Magnetic Fusion Energy Sciences
Integrated Science Applications
Disruptions
Plasma Boundary
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

Nonlinear MHD simulations are helping to elucidate the physics of disruptions and mitigation

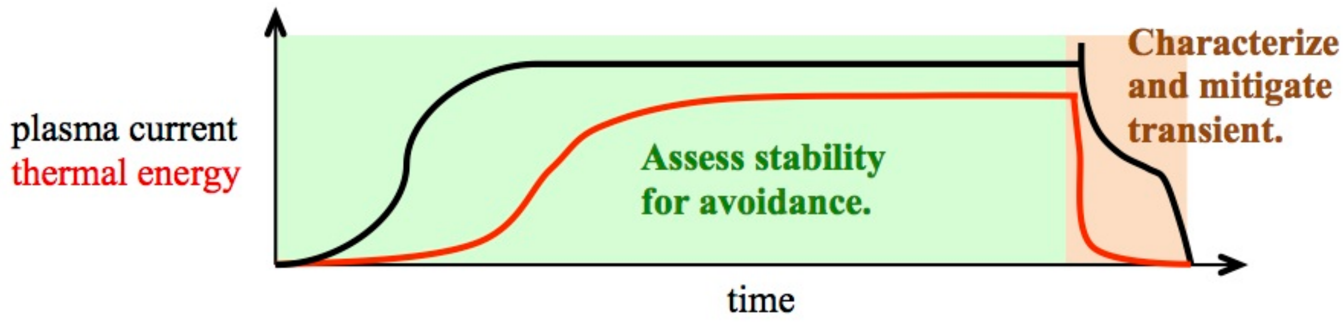


Nonlinear MHD simulation of global instability leading to thermal quench and localized heat. Image courtesy S. Kruger, Tech-X Corporation.



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).

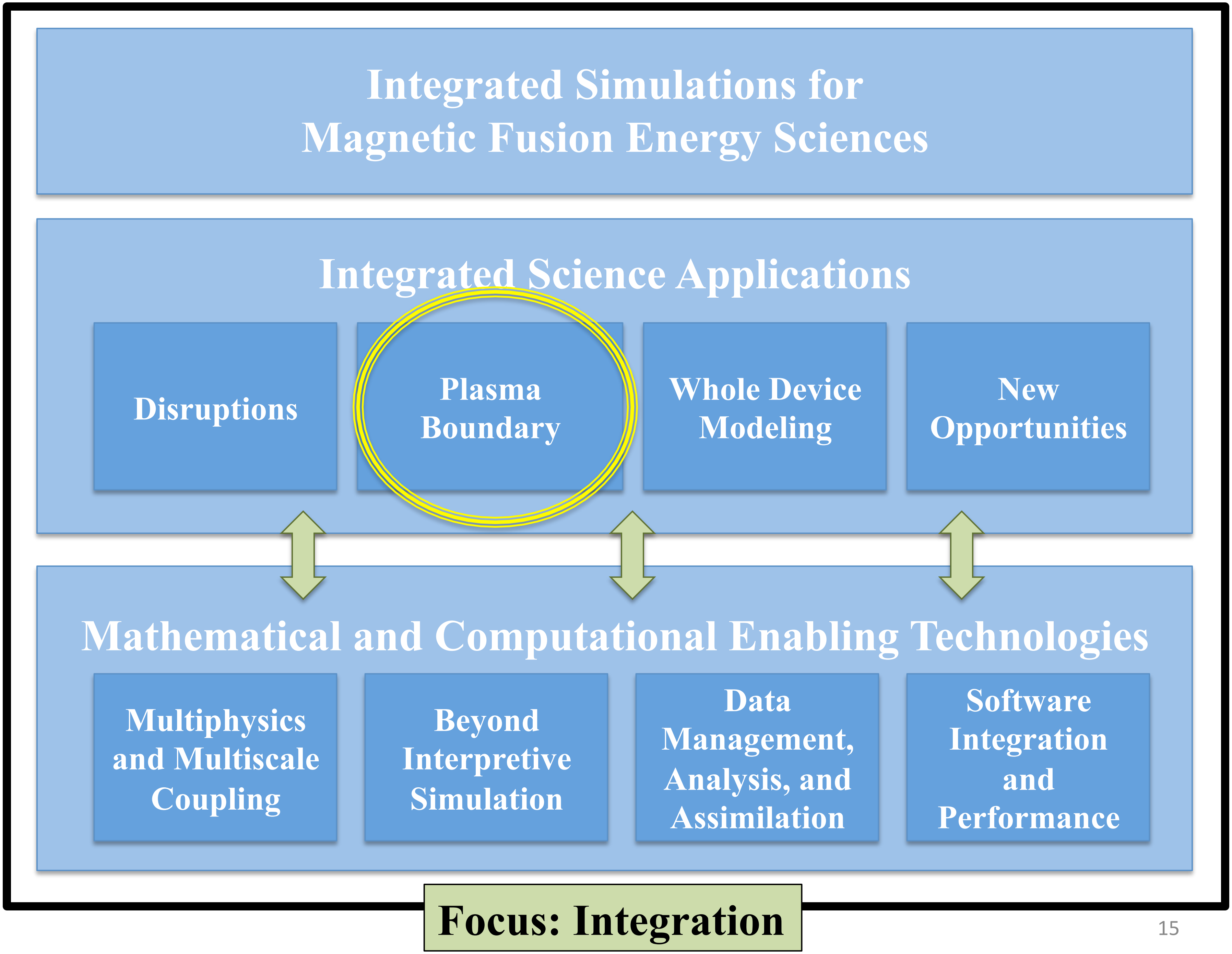
Disruption physics - challenges and opportunities



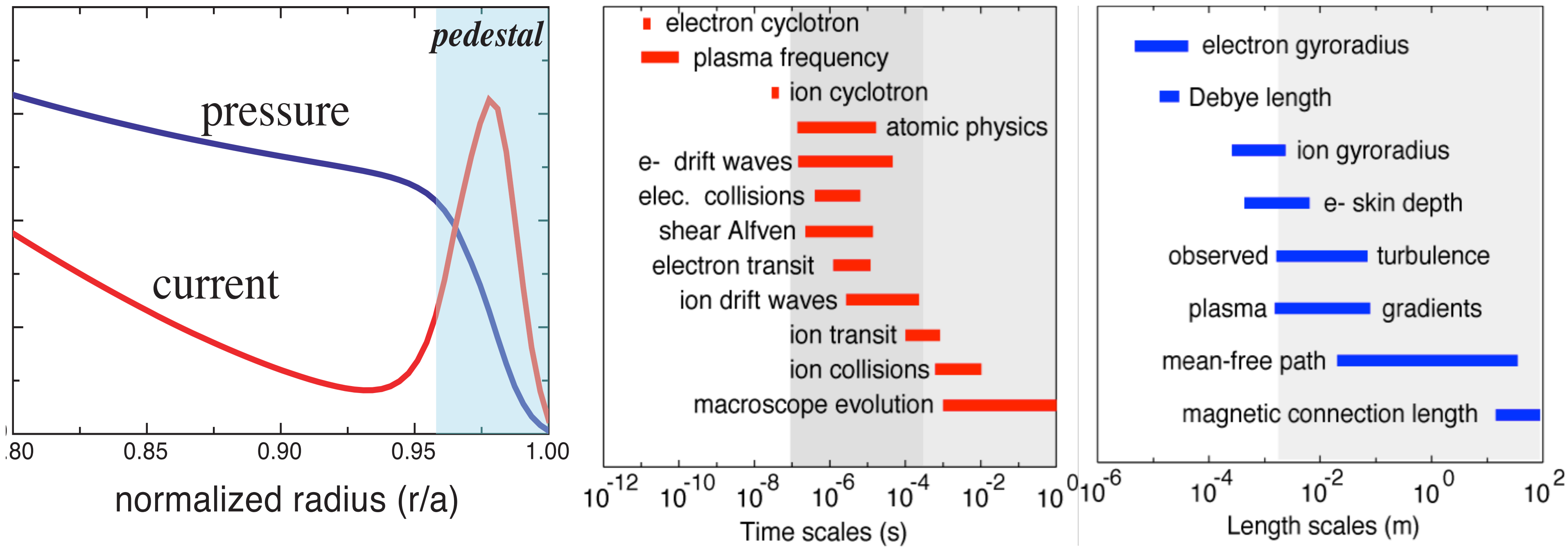
- **Avoidance and onset**
  - The predictive capability of linear stability computation needs validation.
  - Locking of resonant magnetic perturbations is a common, yet poorly understood, precursor to disruption.
  - Stability at low rotation is less robust than the best numerical predictions.
- **Thermal quench**
  - The primary channel of electron energy transport is not known.
  - Plasma-surface interaction likely affects the dynamics of disrupting discharges.
- **Current quench**
  - Electrical current paths depend on the geometric details of external conductors.
  - The experimentally observed electric field for runaway electron generation has not been explained.
- **Mitigation**
  - The penetration capability of shattered-pellets is not known.
  - The significance of rotation and neutral dynamics needs to be studied.

Disruption Physics: Priority Research Directions

- **[PRD-Disruption-1] 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.
- **[PRD-Disruption-2] 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.
- **[PRD-Disruption-3] 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.

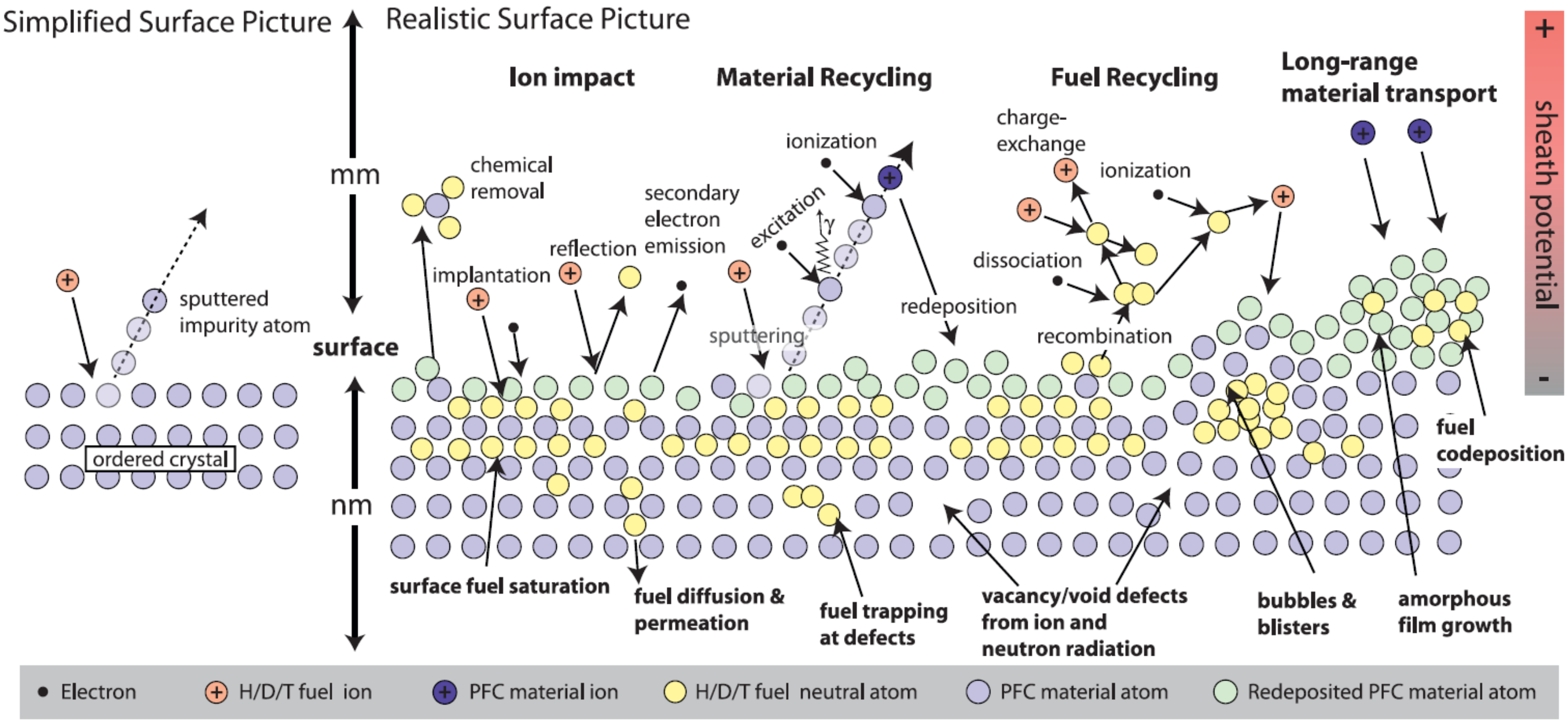

Integrated Simulations for
Magnetic Fusion Energy Sciences
Integrated Science Applications
Disruptions
Plasma Boundary
Whole Device Modeling
New Opportunities
Mathematical and Computational Enabling Technologies
Multiphysics and Multiscale Coupling
Beyond Interpretive Simulation
Data Management, Analysis, and Assimilation
Software Integration and Performance
Focus: Integration

Wide range of scales, strong multiphysics coupling: Need HPC, multiple algorithms, strong fusion-math-CS collaboration



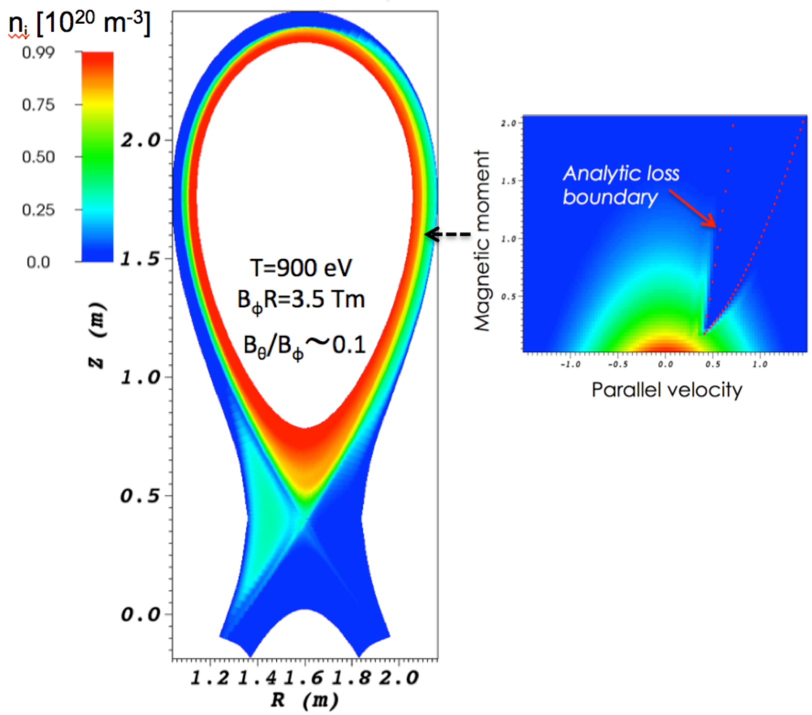
- **Problem is profoundly multiscale**
  - Potential to benefit substantially from exascale and beyond, challenge in efficient algorithms for comprehensive physics
- **Essential role for verification and validation and uncertainty quantification**
  - Uncertainties in inputs, propagation of errors in high dimensions, challenges of V&V at scale
  - Benefit from multiple algorithms for code-code comparisons, sophisticated UQ techniques
  - Geometric complexity, evolving geometry, bifurcating solutions
- **Large, complex simulation and experimental data sets**
  - Provenance/reproducibility, metadata, complex workflows, synthetic diagnostics, needs for V&V
- **Solvers and couplers for chaotic systems, interface between different dimensionality models**

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

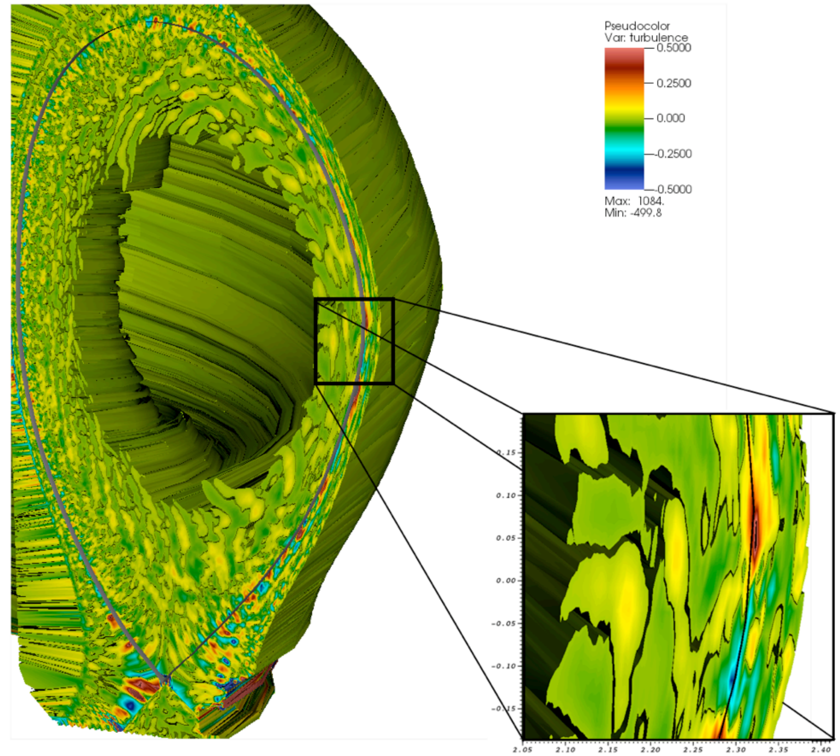


Comparison of a simplified plasma/surface model where only sputtering occurs (left) with a realistic model (right) where many types of interactions occur within the material during bombardment by a fusion plasma. From B. Wirth.

Kinetic simulations are rapidly advancing our understanding of edge and scrape off layer physics



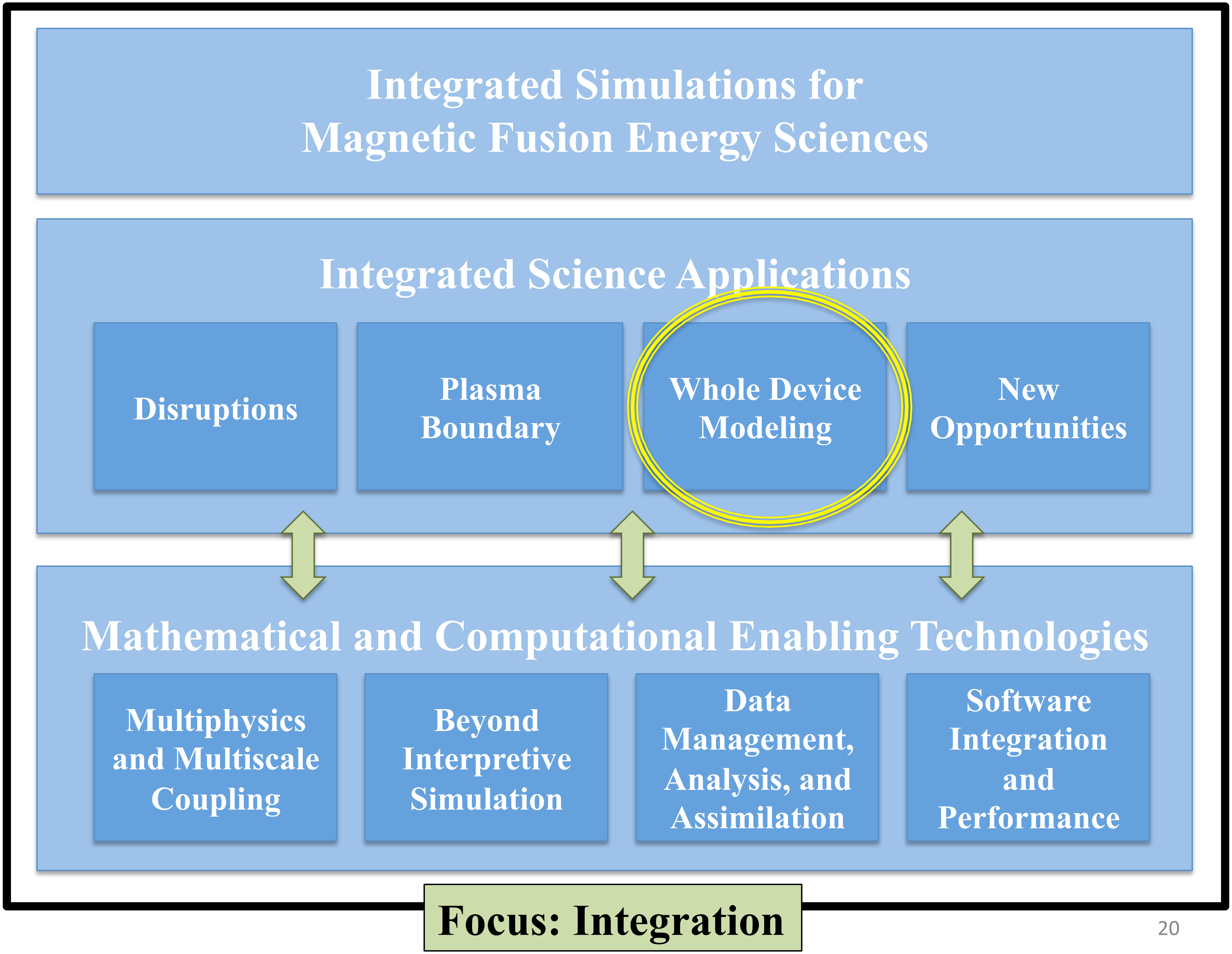
COGENT 4D (2r,2v) kinetic simulation showing ion density and velocity-space loss cone for an initial uniform Maxwellian distribution function after 1.2 ms



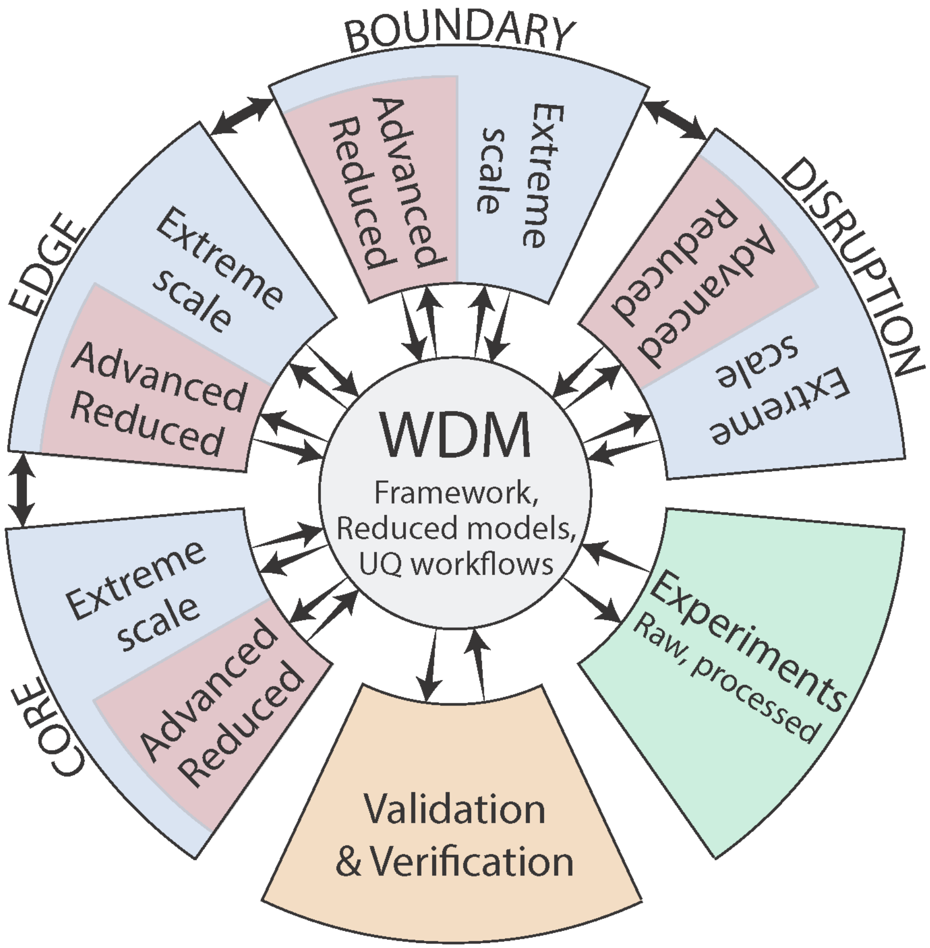
Contours of turbulent electrostatic potential from an XGC1 5D (3r,2v) gyrokinetic simulation that spans the pedestal and SOL in DIII-D magnetic geometry.

Boundary Physics:
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.**
- [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.**
- [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.**
- [PRD-Boundary-4] **Integrate RF antenna/plasma-absorption simulations with SOL/pedestal plasma transport simulations, filling a notable gap in present capability.**
- [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.**


Integrated Simulations for
Magnetic Fusion Energy Sciences
Integrated Science Applications
Disruptions
Plasma Boundary
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

Schematic overview envisioned 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).**

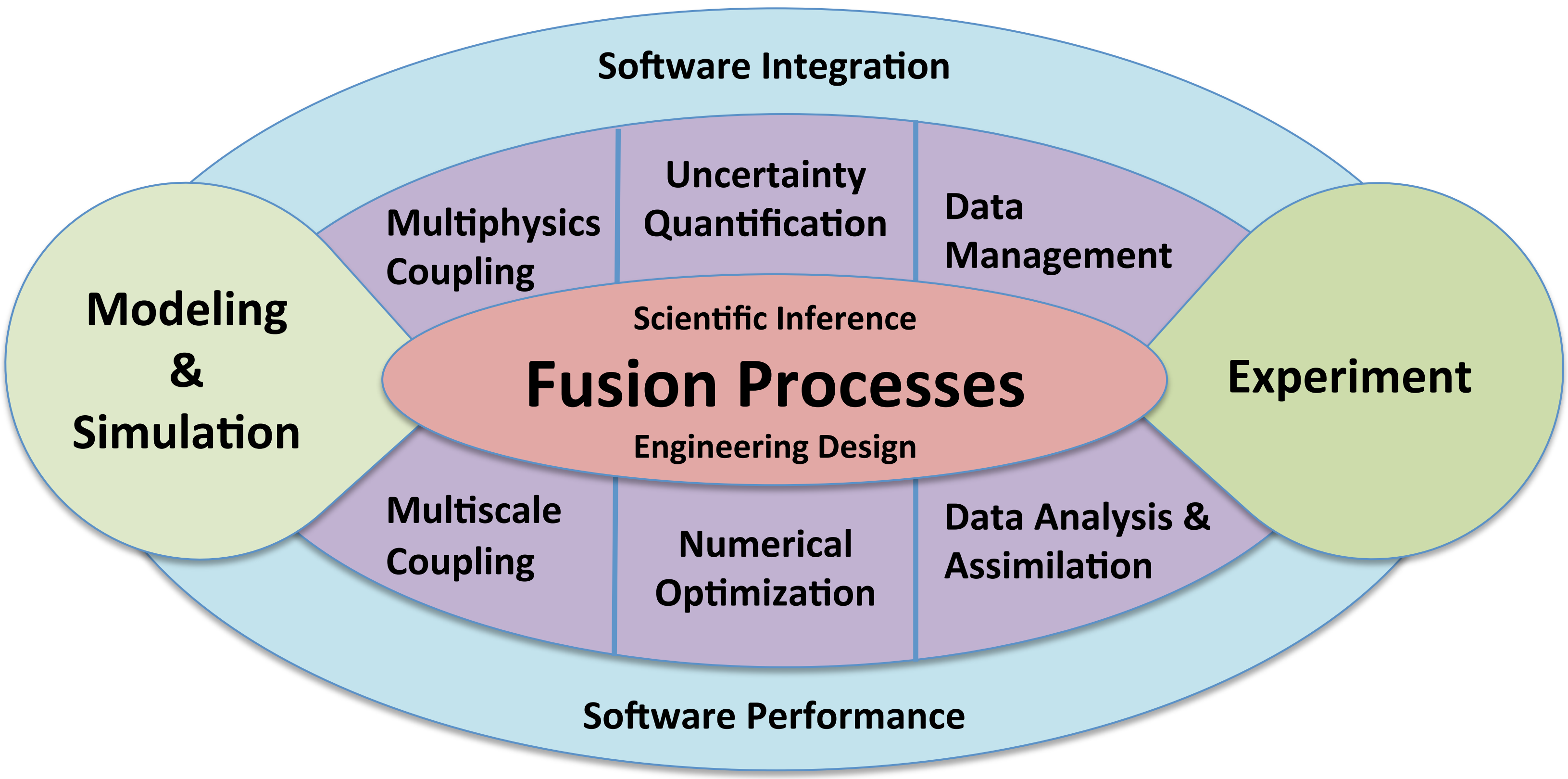
Key physics challenges identified for WDM

- **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

- **[PRD-WDM-1] Increase development of and support for modular WDM frameworks.**
  - A sustainable path forward includes both 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.
  - Should leverage contemporary efforts and 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 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.
- **[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.
  - Effort combines the formulation and implementation of rigorous UQ methodologies appropriate for coupled systems with data management capabilities.

Computational and enabling technologies in integrated fusion simulations



Multiphysics & multiscale coupling focus

- **Open challenges and problems in the *formulation*, *discretization*, and *numerical solution* of multiscale, multiphysics models for integrated simulation for magnetic fusion energy sciences**
  - ***Multiphysics***: involve two or more physical processes that interact (couple) in some way
  - ***Multiscale***: significant behavior over wide range of scales
    - Usually several orders of magnitude
    - Typically in the independent variables like space and time
- **Numerical mathematics concerns:**

Consistency

Stability

Convergence

Asymptotic well-posedness

Performance

- **Recent advances throughout community, including SciDAC FASTMath collaborations with fusion projects**

Multiphysics and Multiscale Coupling:
Priority Research Directions

- **[PRD-MultiXCoupling-1] Invest in model development and analysis.**
- **[PRD-MultiXCoupling-2] Develop efficient scale-bridging algorithms that address the particular challenges of fusion science.**
- **[PRD-MultiXCoupling-3] Develop time integration algorithms better suited to specific problems in fusion energy science.**
- **[PRD-MultiXCoupling-4] Develop new techniques to address the geometrical complexities of fusion devices.**
- **[PRD-MultiXCoupling-5] Develop new solvers and preconditioners congruent both with specific fusion science applications and with extreme-scale architectures.**
- **[PRD-MultiXCoupling-6] Develop new techniques that enable adaptivity of space, order, and models.**
- **[PRD-MultiXCoupling-7] Develop improved techniques to understand and control coupling errors.**