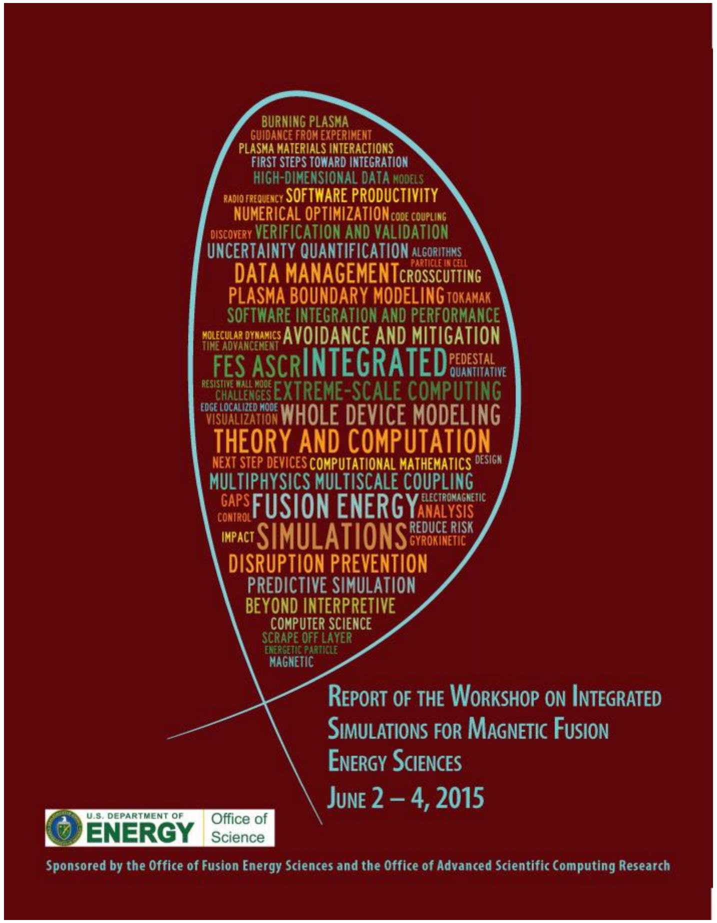
# Report of the Workshop on Integrated Simulations for Magnetic Fusion Energy Sciences


**Paul Bonoli**
**Massachusetts Institute of Technology**
**and**
**Lois Curfman McInnes**
**Argonne National Laboratory**


**DOE Points of Contact:**
**FES: John Mandrekas**
**ASCR: Randall Laviolette**

*FESAC Meeting*
*North Bethesda, MD*
*January 13-14, 2016*




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

# Charge from DOE

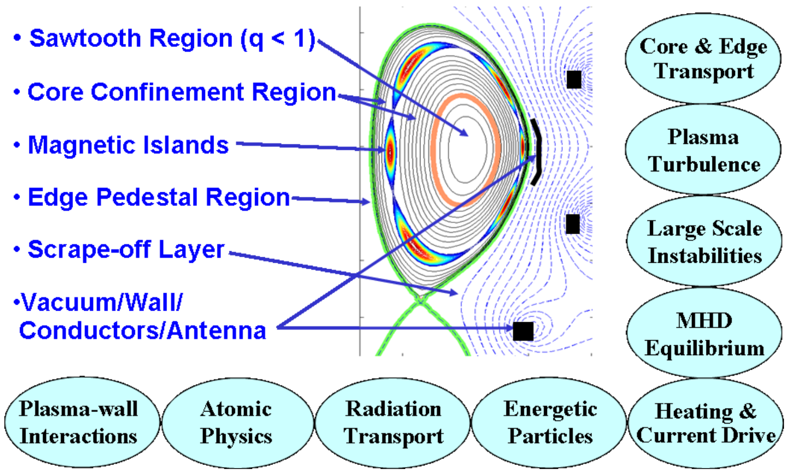
- **“Review recent progress and identify gaps and challenges in fusion theory and computation** directly relevant to the topic of disruption prevention, avoidance, and mitigation and that of plasma boundary physics, **with whole device modeling as the long-term goal.”**
- **“Reassess these opportunities 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.”**

# Approach for workshop and report

- **Community-wide call for whitepapers, ending on April 24, 2015 (delineated by panel topics shown on next slide):**
  - Panels received 121 whitepapers
- **Community Teleconference, May 18–19, 2015**
  - Oral presentations from 45 whitepaper submissions
  - Discussions of whitepapers by panels
- **Teleconferences conducted among panel chairs / co-chairs and individual panels**
  - 70 panel members including chairs and co-chairs
  - About 40 teleconferences from March – July 2015
- **“Writing” workshop held June 2-4, 2015**
  - Attended by panel members, “participants at large”-(12), and “observers”-(10)
- **Workshop report finalized (July – September, 2015)**

# The tokamak offers unique opportunities and challenges for integrated simulations

- **The modeling, system simulation, and validation areas critically require Whole Device Modeling (WDM) tools to enable the high confidence design and verification planned for ITER operation.**




- **Whole device modeling integrates multiphysics and 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, computer science, and observational data
- Validated simulations: require managing, visualizing, and analyzing ultra-large datasets

# Integrated Simulations for Magnetic Fusion Energy Sciences

## Integrated Science Applications

- Disruptions
- Plasma Boundary
- Whole Device Modeling
- New Opportunities

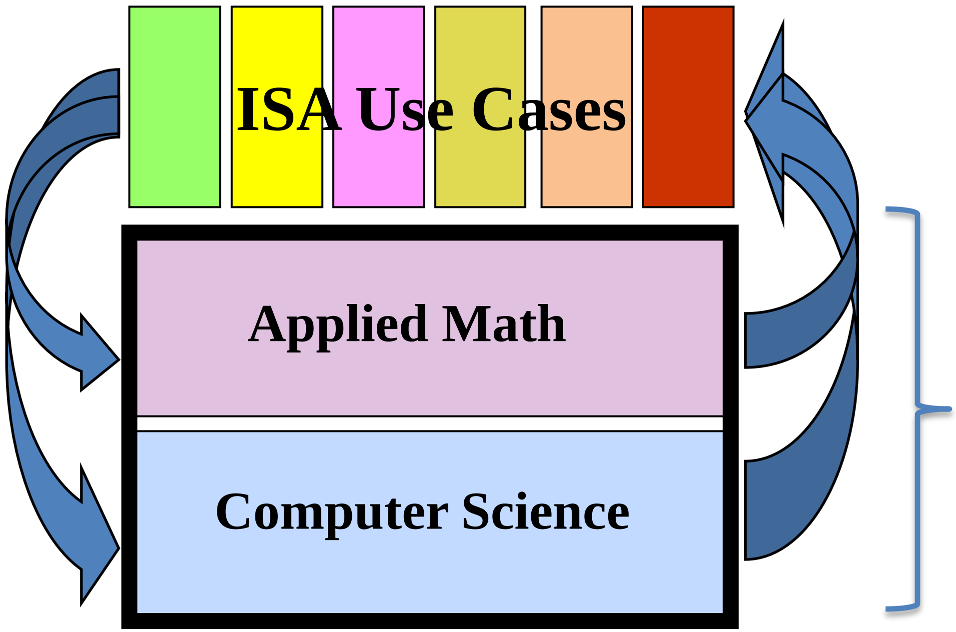
## Mathematical and Computational Enabling Technologies

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

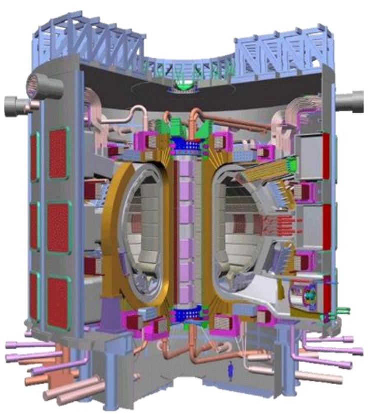
**Focus: Integration**

# ‘Philosophy’ of mathematical and computational enabling technologies

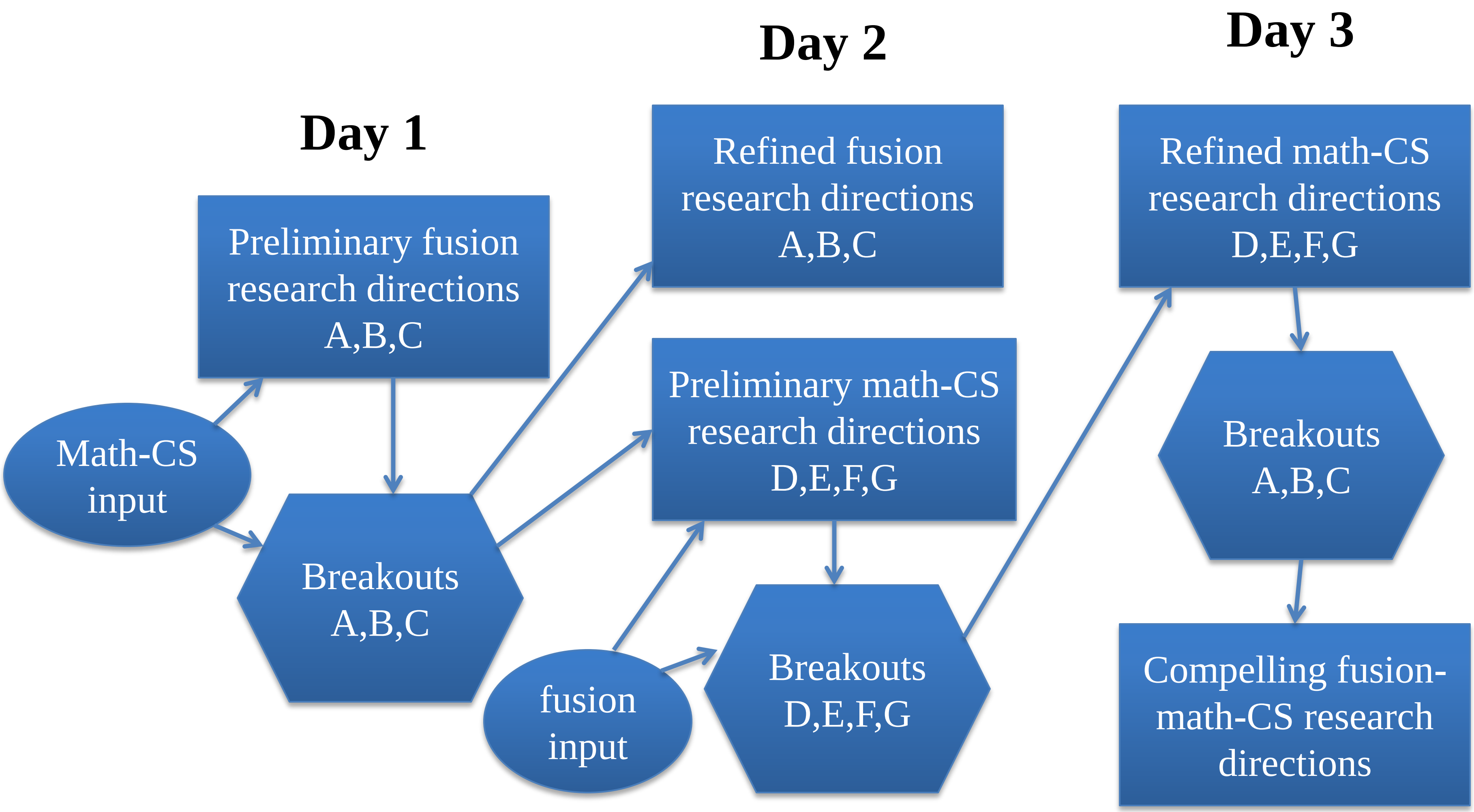
**Magnetic fusion energy**
**Integrated Science Applications (ISAs) drive**




**Enabling technologies respond to all**



# Workshop process involved extensive iterations between fusion and math / CS panels




**Emphasis:**

- **Role of integrated simulations**
- **Potential for extreme-scale computing**

- **Fusion panels: A,B,C**
- **Math-CS panels: D,E,F,G**

# Emerging extreme-scale computing resources

- **Exascale Computing**
  - Accelerating delivery of a capable exascale computing system that integrates hardware and software capability to deliver approximately 100 times the performance of current 10 petaflop systems across a range of applications representing government needs
    - Within a similar size, cost, and power footprint as today's systems
    - Fosters new generation of scientific, engineering, and large-data applications
    - Deployed in 2023
  - Mission Need: July 2015: President established **National Strategic Computing Initiative (NSCI)** to maximize the benefits of HPC for US economic competitiveness and scientific discovery
- **DOE computing facility upgrade plans: 2016-2018**
  - Peak performance in 100-200 petaflop range
  - Powerful nodes
    - Manycore processors or multiple GPUs
  - New memory devices, deeper hierarchies
  - http://science.energy.gov/~/media/ascr/pdf/facilities/ASCR_Computiing_Facility_Upgrades.pdf

**NERSC: Cori**
Intel Xeon Phi, 2016
**CORAL collaboration**
ORNL Summit, LLNL Sierra:
IBM POWER CPU +
NVIDIA Volta GPU, 2017-18
ANL Aurora: Intel Xeon Phi, 2018-19

# Extreme-scale: Computational power for next-generation integrated simulations

## Sustainable collaborations: fusion + math + computer science

- **"Third paradigm": computation and simulation**
  - **Better models**
    - Better resolve model's full, natural range of length or time scales
    - Accommodate physical effects with greater fidelity
    - Allow the model degrees of freedom in all relevant dimensions
  - **Multiphysics and multiscale coupling**
    - Combine multiple complex models
  - **Beyond interpretive simulation**
    - Solve inverse problems
    - Perform optimization or control
    - Quantify uncertainty
    - Verification and validation
- **"Fourth paradigm": Integrating simulations and data**
  - **Data management, analysis, and assimilation**
    - Validated simulations capitalizing on the ability to manage, visualize, and analyze ultra-large datasets

**Software integration and performance**

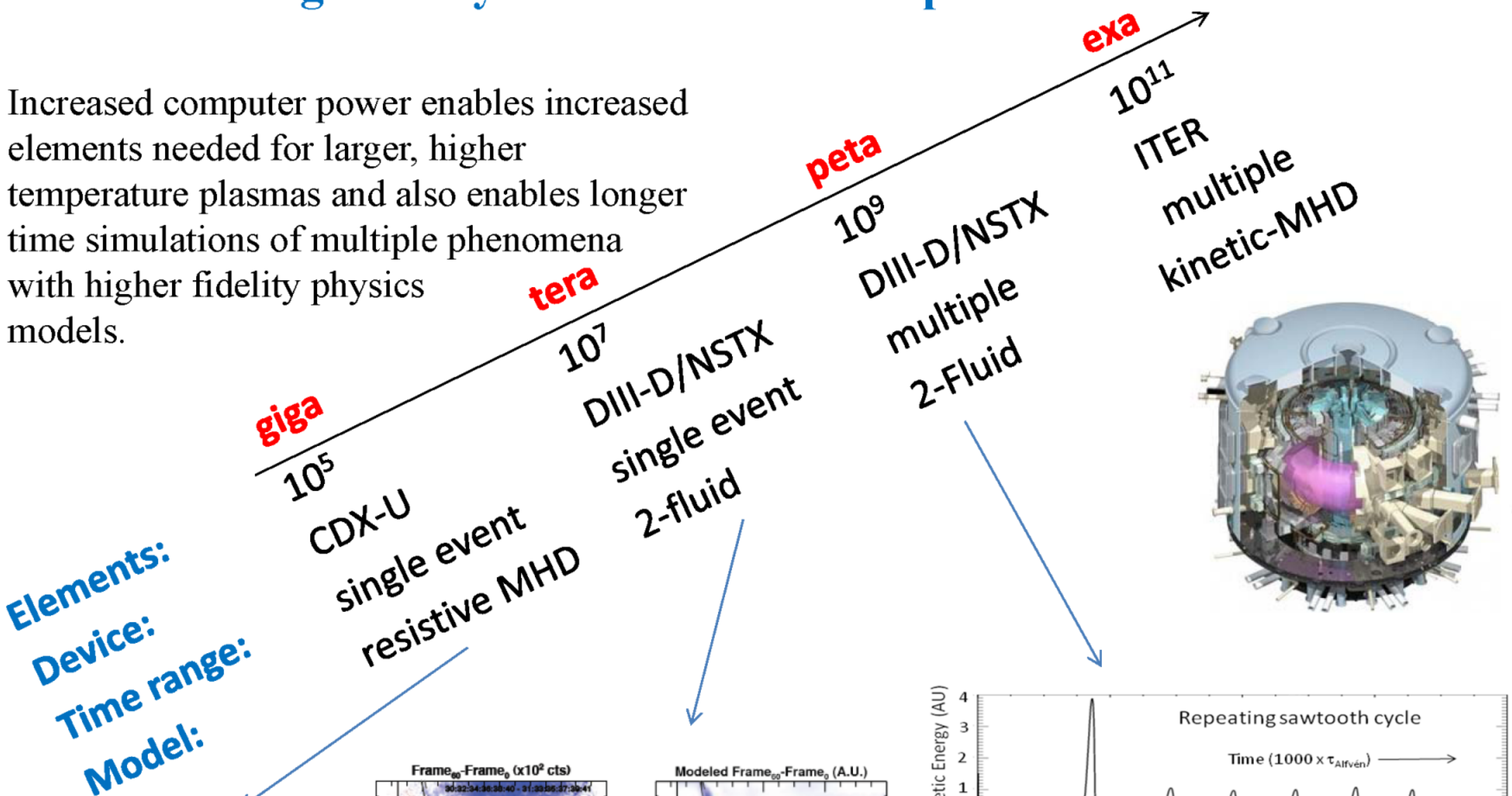
# Integrated simulation in fusion energy sciences has benefited historically from ASCR partnerships

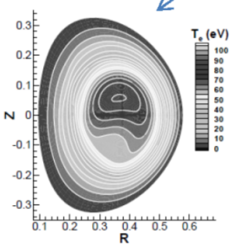
- **("Base") Fusion SciDAC Centers**
  - Center for Simulation of Plasma Microturbulence (CSPM)
  - Gyrokinetic Simulation of Energetic Particle Turbulence and Transport (GSEP)
  - Center for Simulation of Wave-Plasma Interactions (CSWPI)
  - Center for Extended Magnetohydrodynamic Modeling (CEMM)
  - Center for Simulation of Energetic Particles in Burning Plasmas (CSEP)
- **SciDAC-3 Centers: Fusion-Math-CS Partnerships**
  - Center for Edge Physics Simulation (EPSI)
  - Plasma Surface Interactions: Bridging from the Surface to the Micron Frontier through Leadership Class Computing (PSI-SciDAC)
  - Advanced Tokamak Modeling Project (AToM)
- **SciDAC-3 Institutes**
  - FASTMath: Frameworks, Algorithms, and Scalable Technologies for Mathematics
  - QUEST: Quantification of Uncertainty in Extreme Scale Computations
  - SDAV: Scalable Data Management, Analysis and Visualization
  - SUPER: Institute for Sustained Performance, Energy and Resilience
- **Proto-type Fusion Simulation Projects (2005-2011)**
  - Center for Simulation of Wave Interactions with MHD (SWIM)
  - Center for Plasma Edge Simulation (CPES)
  - Framework Application for Core-Edge Transport Simulation (FACETS)
- **Base-program funded**
  - Edge Simulation Laboratory (ESL)

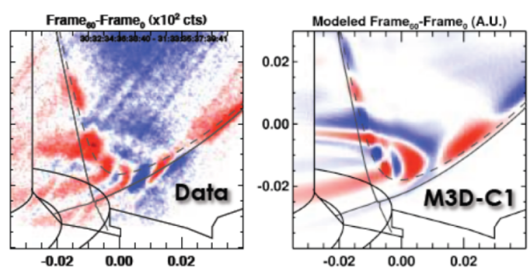
# HPC advances have enabled simulations of global MHD phenomena to be extended to higher temperatures, longer times, larger device sizes, and multiple events

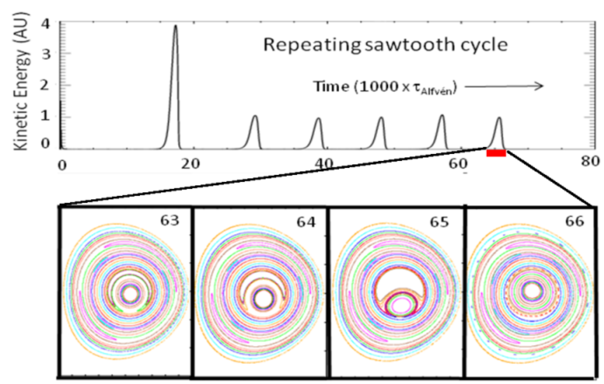
## Prediction of global dynamics of tokamak plasmas

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.

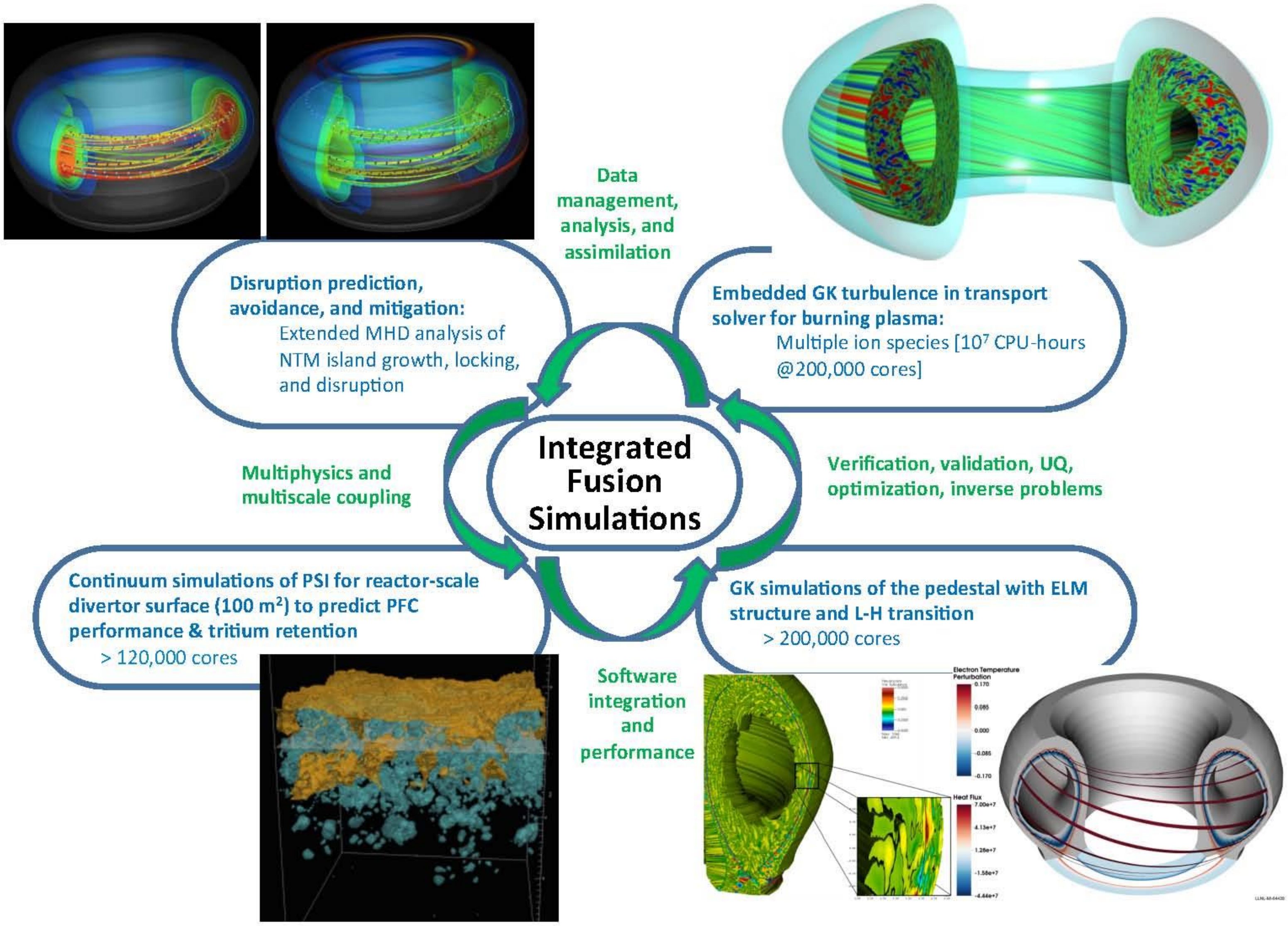


# Vision for integrated extreme-scale simulations



# Integrated Science Applications

## A. Disruption Physics (avoidance, characterization, and mitigation)

**Chair**: Carl Sovinec (UW)

**Co-chair**: Dylan Brennan (Princeton)

**Focus**: gaps and challenges in theory, guidance from experiment, status of simulation capabilities, status of validation and measurement capabilities

## B. Boundary Physics (pedestal, scrape off layer, and PMI)

**Chair:** Tom Rognlien (LLNL)

**Co-chair**: Phil Snyder (GA)

**Focus:** gaps and challenges in theory, guidance from experiment, status of simulation capabilities, status of validation and measurement capabilities

## C. Whole Device Modeling

**Chair:** Jeff Candy (GA)

**Co-chair:** Chuck Kessel (PPPL)

**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

***Common focus for all panels: Looking for new opportunities for integrated simulation.***

# Disruption Physics (prevention, avoidance, and mitigation)

**Panel Chair:** Carl Sovinec (University of Wisconsin-Madison)

**Panel Co-Chair:** Dylan Brennan (Princeton University)

**Panel Members**:

Boris Breizman (University of Texas - Austin)

Luis Chacon[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)

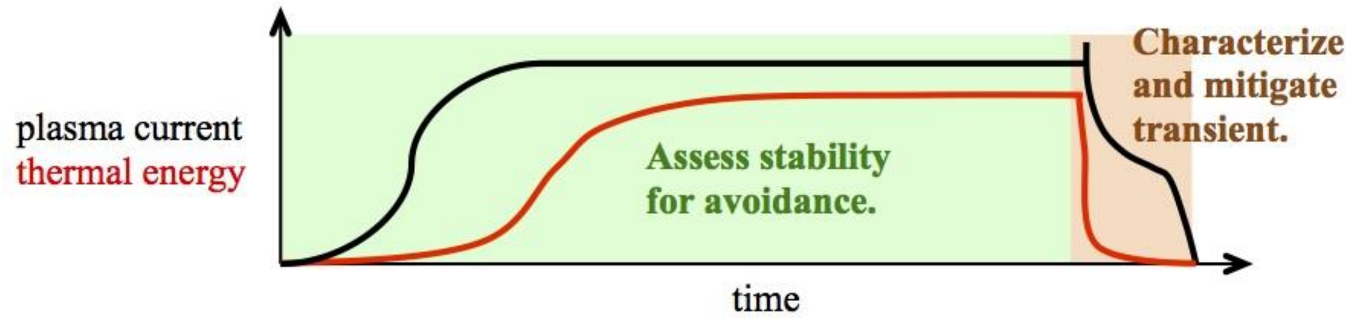
Ravi Samtaney[1] (King Abdullah University of Science and Technology)

Hank Strauss (HRS Fusion)

Alan Turnbull (General Atomics)

[1]Crosscutting expert from ASCR

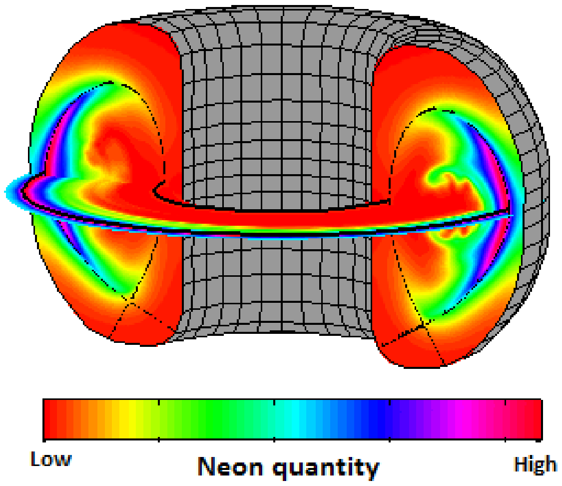
# Disruption physics - challenges and opportunities




- **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.
- **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.**
  - Complete numerical descriptions will include 3D macroscopic dynamics, kinetics for runaway electrons and majority species, neutral and impurity transport, radiation, external electromagnetics, and plasma - surface interactions
  - Models must address fundamental questions on mode locking, runaway-electron generation and evolution, and open-field currents
  - Applications include magnetic-island locking, density-limit disruptions, runaway-electron generation, and mixing of impurities injected for mitigation



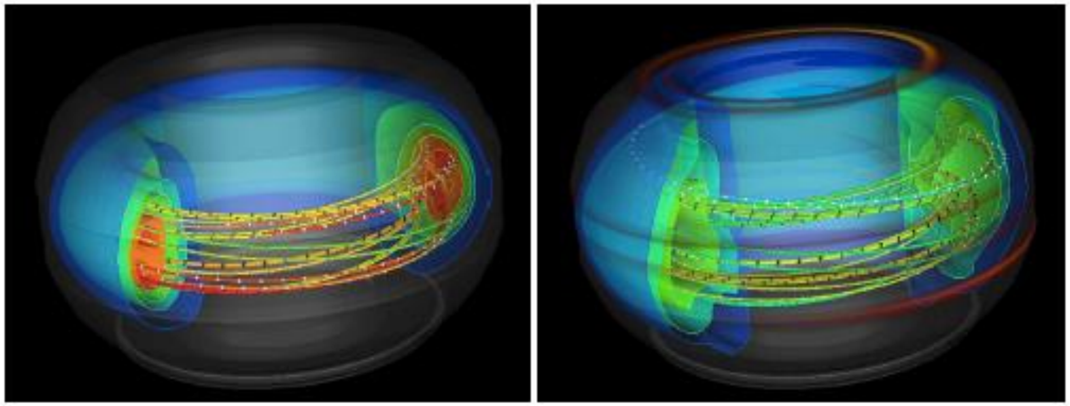

**Integrated nonlinear simulation of edge-injected Ne impurity concentration after dynamic mixing, predicted by combining 3D MHD and radiation modeling. Image courtesy of V. Izzo (UCSD).**

# Disruption Physics: Priority Research Directions

- **[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 and is a necessary step for real-time analysis
  - 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
  - Many computations will be needed to validate the models and to map stability over operational space

# Disruption Physics: Priority Research Directions

- **[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**:
  - 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



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

# Crosscutting math / CS issues for disruption physics

- **Integrated simulation of disruptive transients requires:**
  - Effective multiscale and multiphysics algorithms - advances in time-integration can facilitate studies of characterization and mitigation
  - Large-scale computing for each simulation
  - Management of large datasets
- **Analyzing plasma states for stability forecasting entails:**
  - 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.
- **Implicit computation on new architectures**
  - Implicit computation provides as much as 4 orders of magnitude performance improvement over explicit computation.
  - Wave-propagation physics leads to mathematical stiffness and ill-conditioned algebraic systems.
- **Software integration**
  - New combinations for multiphysics computation are expected.
  - Plasma-surface interaction, neutral dynamics, and more detailed external electromagnetics are needed.

# Boundary Physics (pedestal, scrape off layer, and plasma-materials-interactions)

**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)

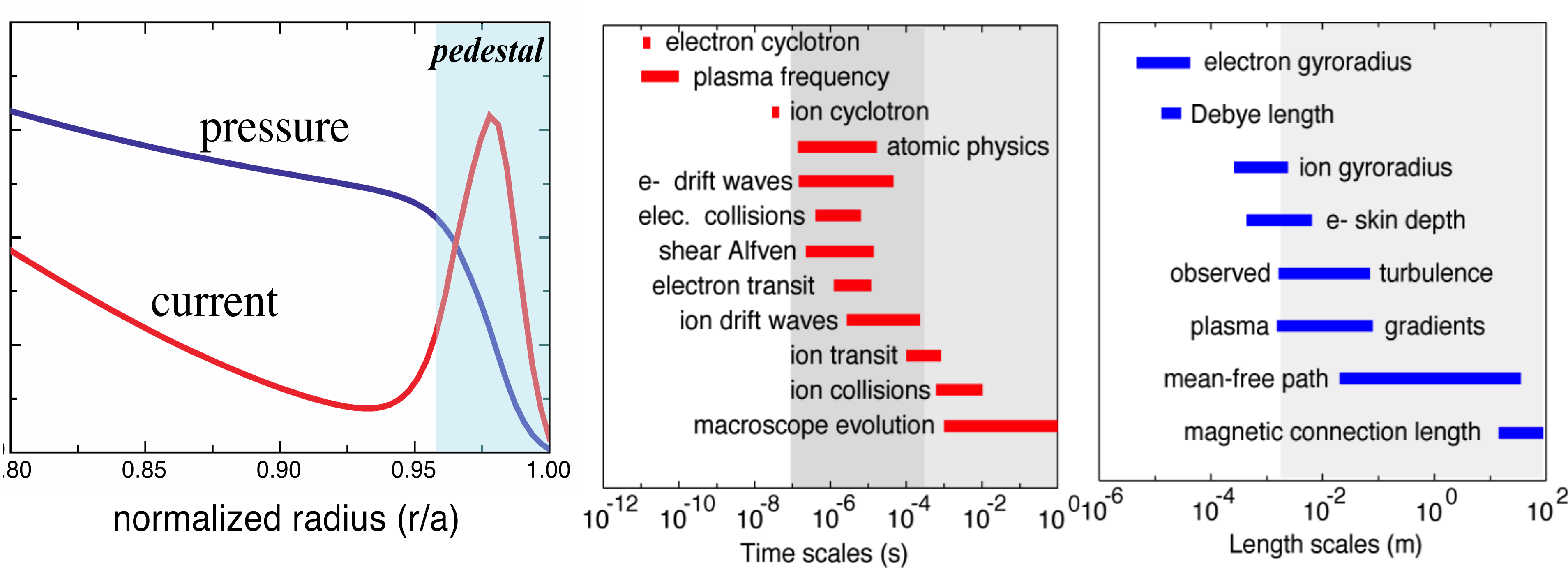
Sergei Krasheninnikov (University of California - San Diego)

Tony Leonard (General Atomics)

Zhihong Lin (University of California - Irvine)

[1]Crosscutting expert from ASCR

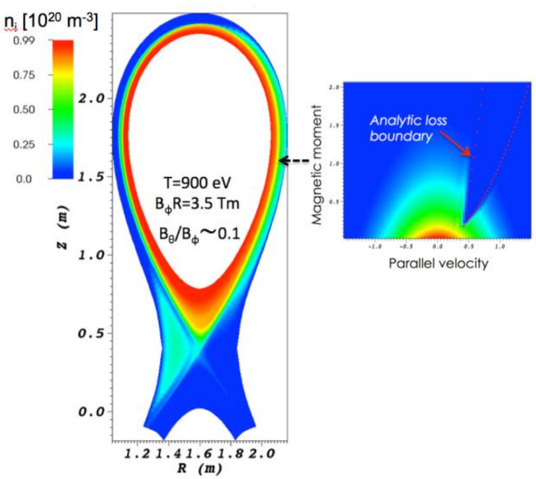
# Challenge of the Plasma Boundary: Temperature must go from hundreds of degrees at the wall up to millions of degrees at top of pedestal, while preserving long material lifetimes



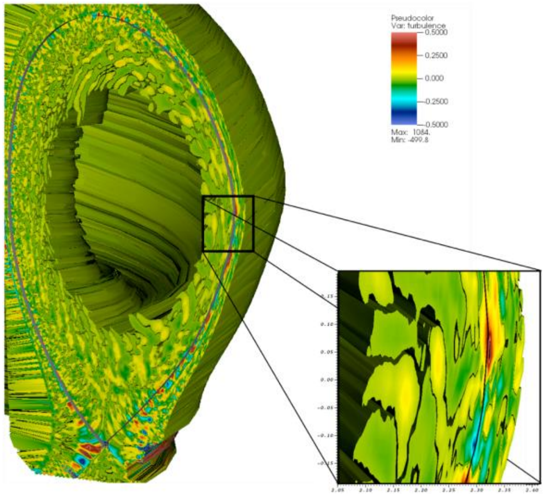

- **Problem is profoundly multiscale**
- **Temperature and density at the core interface strongly influence fusion performance, as well as particle and energy fluxes into and through the SOL, which determine wall heat loads and material erosion.**
- **Fuel and impurity neutral particles emitted from the wall/SOL in turn provide sources to the pedestal and core.**

# 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:**
  - Involves simulating kinetic effects across and along the magnetic field as well as stochastic electron motion in 3D magnetic fields
  - Models include 5D electromagnetic (EM) gyrokinetic codes, 3D and 2D fluid codes, and 6D neutral Monte Carlo codes



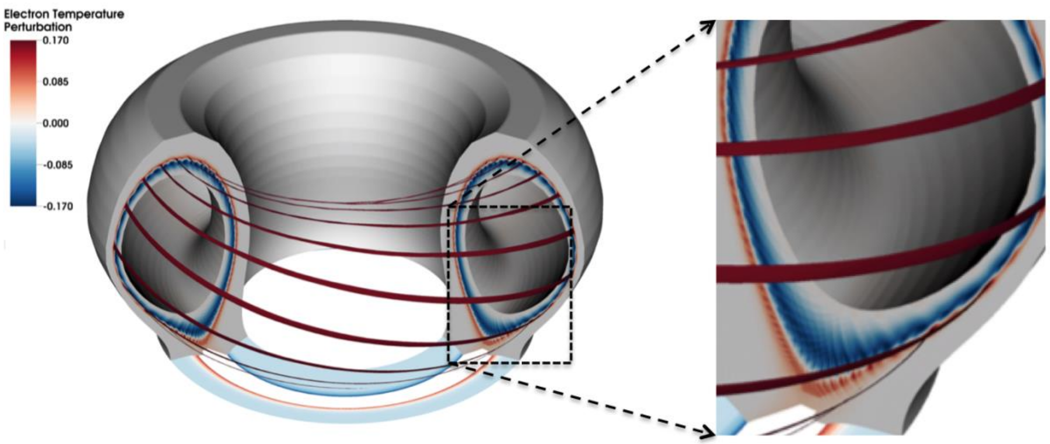

**COGENT 4D (2r,2v) kinetic simulation showing ion density and velocity-space loss cone for an initial uniform Maxwellian distribution function after 1.2 ms**



**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

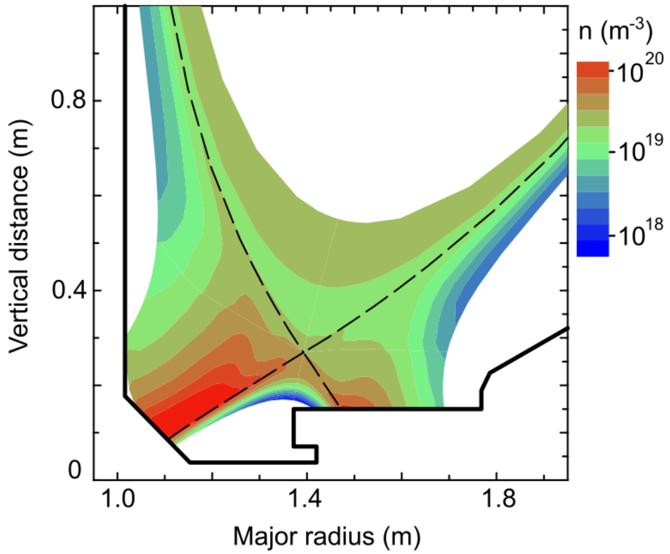
- **[PRD-Boundary-2] Incorporate the dynamics of transients, particularly intermittent edge-localized mode events that eject bursts of particles and energy into the SOL, leading to large transient heat loads on the walls:**
  - Include the temporal wall response of impurity sputtering, and particle pumping or outgassing, and the impact of applied 3D magnetic fields
  - 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 codes, wall codes, and plasma/neutral transport codes




**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.**

# Boundary Physics: Priority Research Directions

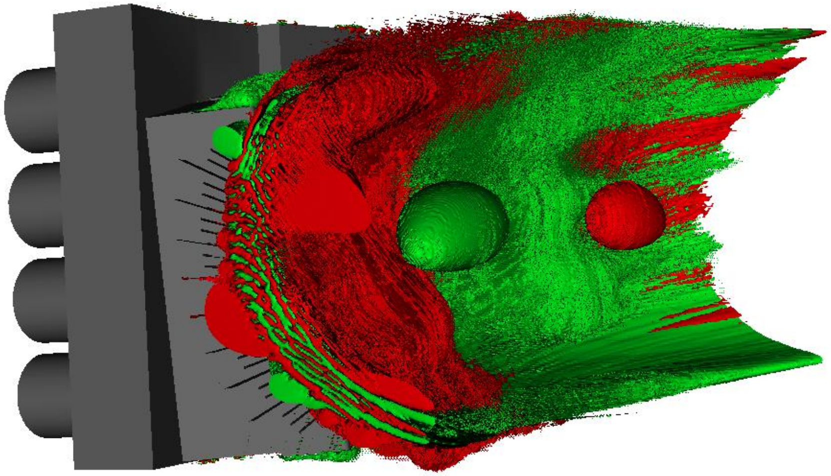
- **[PRD-Boundary-3] Develop a simulation capability that integrates the moderately collisional midplane SOL plasma with the highly collisional divertor plasma:**
  - Needed to model the detached divertor plasma regime, which is planned for ITER and other devices because of its effective power-handling features
  - Ion and electron mean-free paths for the two SOL regions can vary by as much as 5 orders of magnitude
  - 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




**Ion density in the divertor region from UEDGE fluid simulation showing a ten-fold increase in plate density compared with midplane density. Image courtesy of G. D. Porter, LLNL.**

# Boundary Physics: Priority Research Directions

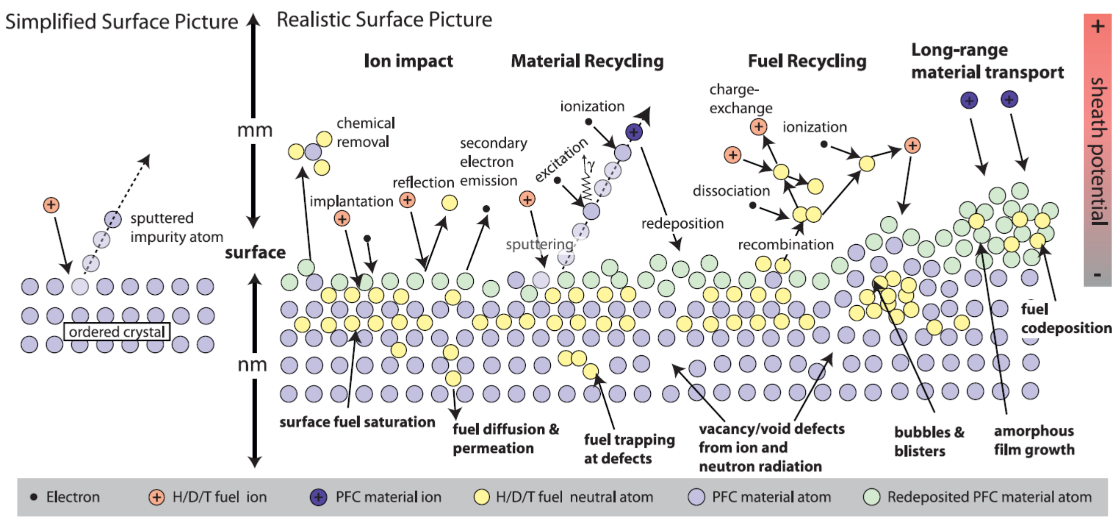
- **[PRD-Boundary-4] Integrate RF antenna/plasma-absorption simulations with SOL/pedestal plasma transport simulations, filling a notable gap in present capability:**
  - The SOL plasma strongly affects the wave coupling to the core, and the RF fields are expected to modify the SOL
  - Interaction must 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



**Contours of the vertical electric field induced by the field-aligned ICRF antenna in the Alcator C-Mod device. Both fast waves (large blobs near reactor core) and slow waves (short-wavelength behavior near plasma-facing antenna surfaces) are present. Image courtesy of T. Jenkins (Tech-X).**

# Boundary Physics: Priority Research Directions

- **[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




**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. Image courtesy of B. Wirth.**

# Crosscutting math / CS issues for boundary physics

- **IMEX (implicit/explicit) time advance**
  - Bridging turbulence-to-transport timescales; electron-scale modes
- **High order spatial/temporal algorithms**
  - Steep gradients, large range of timescales
- **Adaptive meshes**
  - Velocity space & divertor configuration space
- **Coupling algorithms that work**
  - Need to couple Monte Carlo to fluid and kinetic plasma models
  - Neutrals and wall models combined with whole-device modeling
  - Interface 3D antenna model to 2D SOL/wall
- **Verification, validation with UQ**
  - Verification procedure / hierarchy for components
- **Synthetic diagnostics and data management**

# 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)

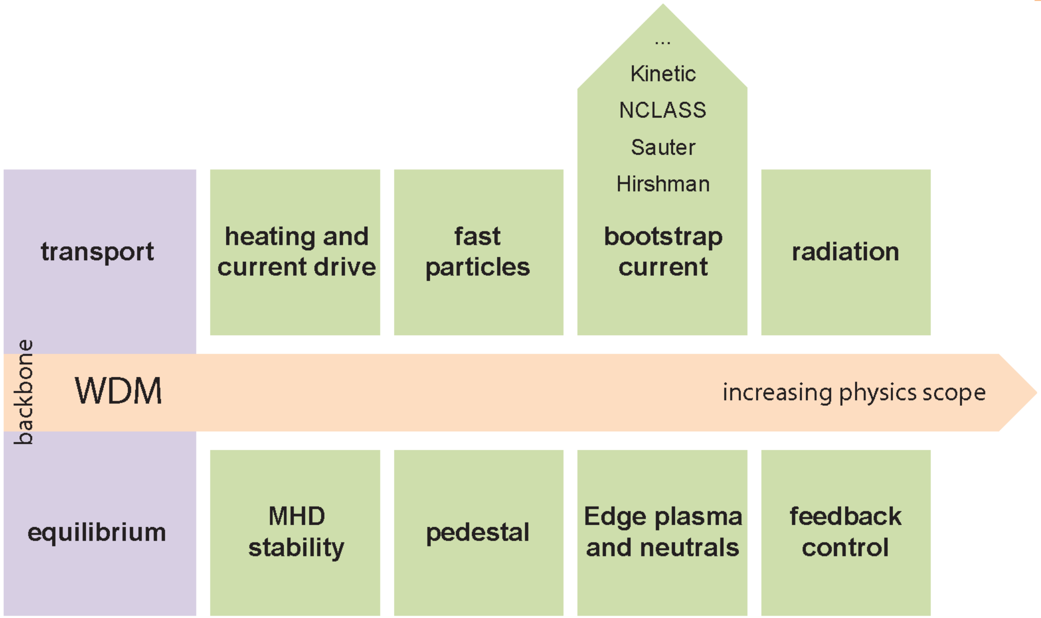
[1]Crosscutting expert from ASCR

# 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:**
  - **A useful concept for accomplishing this goal is the development of model hierarchies which 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.**

# Whole Device Modeling: Priority Research Directions

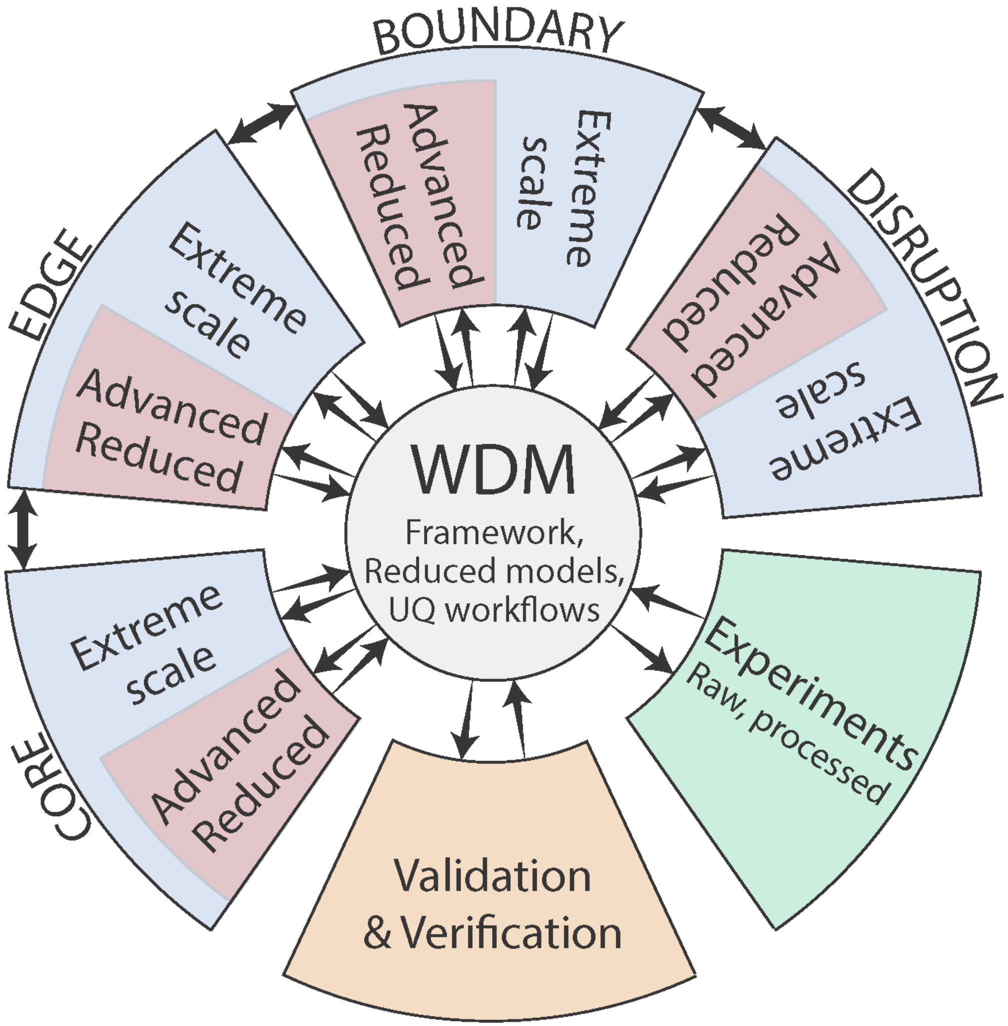
- **[PRD-WDM-1] Increase development of and support for modular WDM frameworks:**
  - Support for both mission-critical legacy tools and development and expansion of newer components and work flows that can more effectively utilize leadership-class computing resources.
  - Leverage contemporary efforts and converge toward a reduced set of community tools compatible with the ITER Integrated Modeling and Analysis Suite (IMAS) and other standards.




**Whole device model showing its most basic components (equilibrium and transport) plus additional components that illustrate increasing physics scope.**

**Using the bootstrap current as an example, a series of progressively more accurate components illustrates the fidelity hierarchy for this process.**

# Whole Device Modeling: Priority Research Directions




- **[PRD-WDM-2] Continue and expand efforts to understand and distill physics of gap areas using a multipronged approach that includes:**
  - **Improve or develop new reduced models and modeling techniques**
  - **Facilitate 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 to validate individual and coupled physics models at all fidelity levels and verify corresponding numerical simulations**
  - **Effort combines the formulation and implementation of rigorous UQ methodologies appropriate for coupled systems with data management capabilities.**

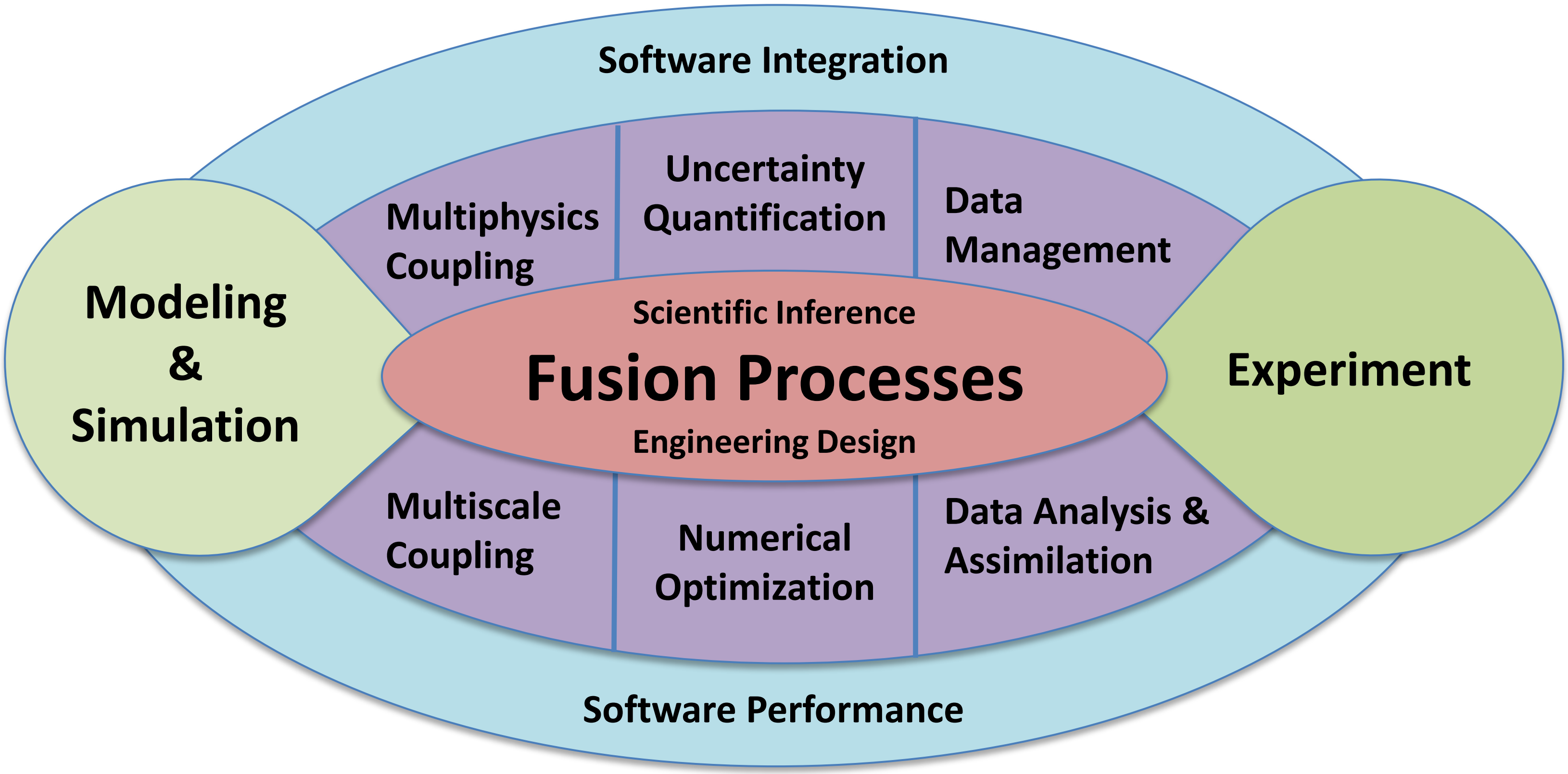
# New opportunities identified for WDM

- **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**

# Crosscutting math / CS issues for Whole Device Modeling

- **Maintain/modernize key legacy components and frameworks**
  - Complex and mission-critical legacy components must function on both current and emerging HPC platforms.
  - Opportunities will emerge to implement more sophisticated coupling algorithms for higher fidelity components with strongly varying spatiotemporal scales.
- **Early inclusion of advanced solver/iteration algorithms**
  - High-fidelity multiscale research issues present opportunities for applied mathematicians to review the basic equations and work with physicists to develop innovative new numerical methods.
  - Advanced solvers are needed now 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**
  - Need searchable databases describing simulation data; need a data-caching system to reuse results of large-scale simulation for V&V or reduced-model development
- **Incorporation of numerical optimization and UQ approaches into workflows**
- **Improved access to HPC codes and platforms**
  - WDM of high-fidelity multiphysics components requires access to the HPC platforms where they can be executed efficiently.

# Computational and enabling technologies in integrated fusion simulations



# Mathematical and Computational Enabling Technologies

## D: Multiphysics and Multiscale Coupling

**Chair:** Jeff Hittinger (LLNL)

**Co-chair:** Luis Chacon (LANL)

**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

## F: Data Management, Analysis, and Assimilation

**Chair:** Wes Bethel (LBNL)

**Co-chair:** Martin Greenwald (MIT)

**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

**Chair:** Donald Estep (Colorado State Univ)

**Co-chair:** Todd Munson (ANL)

**Focus:** stochastic inverse problems for parameter determination, sensitivity analysis, uncertainty quantification, optimization, design, control (so-called ‘outer loop’ issues)

## G: Software Integration and Performance

**Chair:** David Bernholdt (ORNL)

**Co-chair:** Bob Lucas (USC/ISI)

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

# Multiphysics and Multiscale Coupling

**Panel Chair: Jeff Hittinger (LLNL)**

**Panel Co-Chair: Luis Chacon (LANL)**

**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)

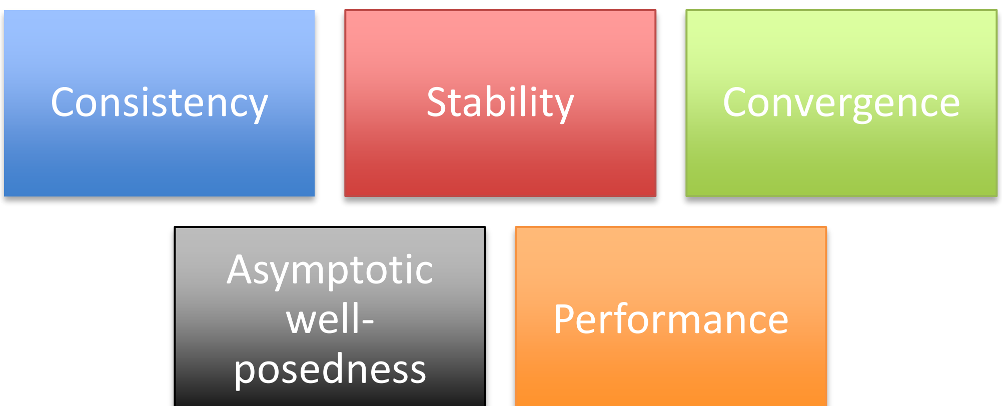
Ray Tuminaro (Sandia National Laboratories)

Carol Woodward (Lawrence Livermore National Laboratory)

[2] Crosscutting expert from FES

# 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:**




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

# How we think about coupling

**Couplings between physics and/or scales**

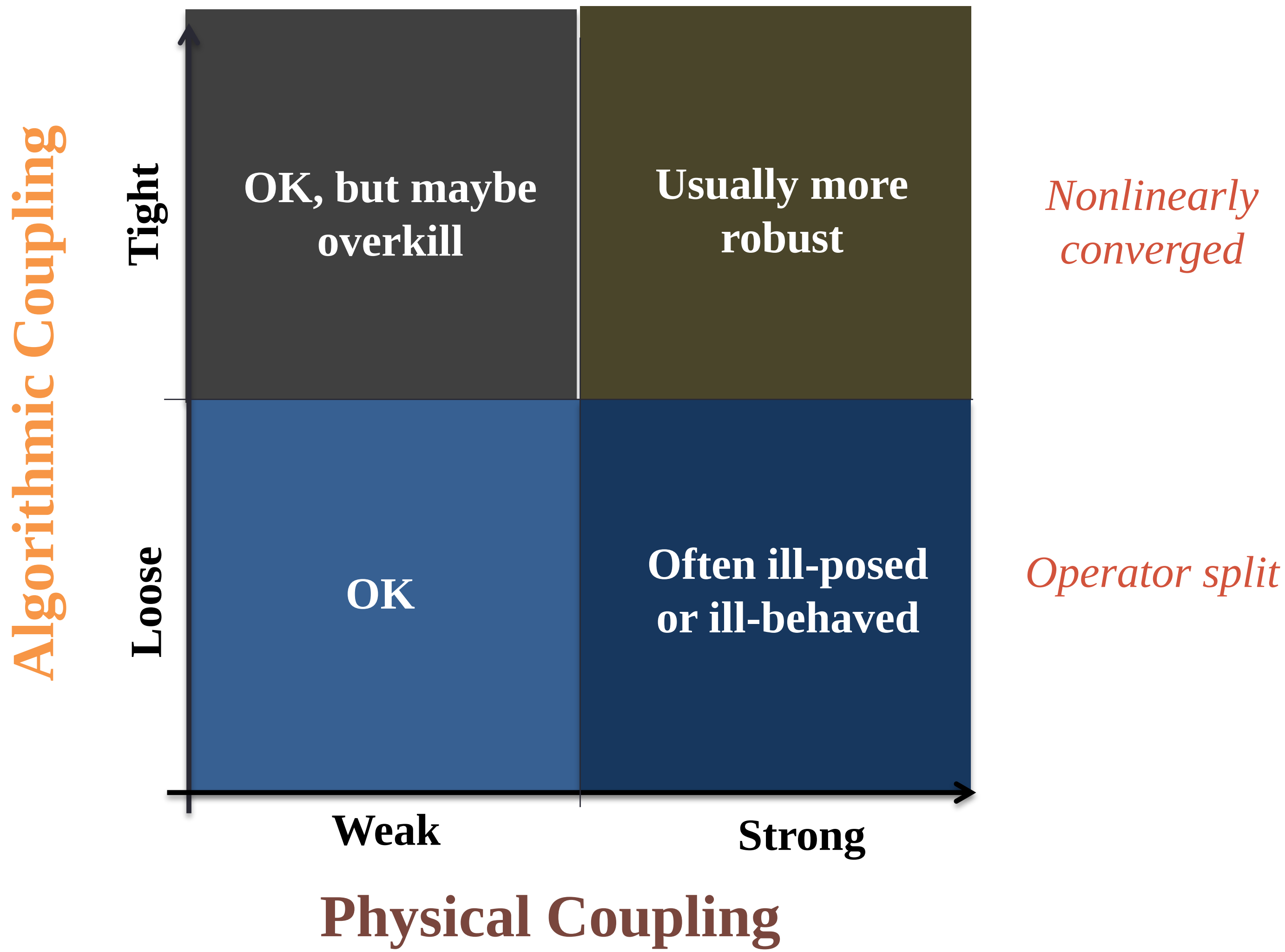
- Intrinsic relationships in complete mathematical expression of problem

**Coupling of codes or models**

- Attempt to recover physical couplings using components that partially describe some physics and/or scales

It is better to consider the complete collection of physics or scales at the outset and make informed choices about how to split or partition it than to start with a collection of models and try to determine how to glue them together.

# On the strength of coupling



# 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.**

# Prioritization of multi-x topics in physics areas

- Near-term
- Mid-term
- Long-term

| | | | Multi-X Topics | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | Models & multiscale analysis D1 | Scale-bridging algorithms D2 | Time advancement D3 | Meshing, geometry, & discretization D4 | Solvers & Preconditioners D5 | Adaptivity D6 | Coupling errors & verification D7 |
| Disruptions | A.1.1 | Integrated models: Two-fluid solver + discretization | | | Near-term | Near-term | Near-term | | |
| Disruptions | A.1.2 | Integrated models: Fluid-kinetic coupling (runaway *e*, energetic particles) | Near-term | Near-term | Mid-term | | Mid-term | Long-term | Long-term |
| Disruptions | A.1.3 | Integrated models: Coupling with wall dynamics (melting, ionization, multiphase, radiation) | Near-term | Near-term | Mid-term | Mid-term | Mid-term | Long-term | Long-term |
| Disruptions | A.2 | Parameterized assessment: Model hierarchy to quantify errors in sampling of parameter space | Mid-term | Mid-term | | | | | |
| Boundary | B.1 | Pedestal characterization | Near-term | Near-term | Near-term | Mid-term | Near-term | Long-term | Long-term |
| Boundary | B.2.1 | Detached divertor plasmas: Fast collisional algorithms (neutrals, plasma) | Near-term | Near-term | Mid-term | Mid-term | | Long-term | Long-term |
| Boundary | B.2.2 | Detached divertor plasmas: Plasma + neutrals + radiation coupling strategies | Near-term | Near-term | Mid-term | Mid-term | Mid-term | Long-term | Long-term |
| Boundary | B.2.3 | Detached divertor plasmas: Kinetic + fluid coupling | Near-term | Near-term | Mid-term | Mid-term | Mid-term | Long-term | Long-term |

# Prioritization of multi-x topics in physics areas

Near-term | Mid-term | Long-term

| | | | Multi-X Topics | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | D1 | D2 | D3 | D4 | D5 | D6 | D7 |
| WDM | C.1.1 | Time-dependent baseline: Coupling 1D + fast dynamics components | Near-term | Near-term | Near-term | Near-term | Mid-term | | Long-term |
| WDM | C.1.2 | Time-dependent baseline: Coupling MHD + kinetics for NTM trigger | Near-term | Near-term | Near-term | Mid-term | Mid-term | Long-term | Long-term |
| WDM | C.2.1 | ELMs, sputtering, impurity transport: Effective impurity source at edge | Near-term | | | | | | Mid-term |
| WDM | C.2.2 | ELMs, sputtering, impurity transport: Kinetic high-Z impurity transport | Mid-term | Mid-term | Long-term | Long-term | Long-term | | Long-term |
| WDM | C.3.1 | ITER core transport and ITBs: Coupling core models + RF | Near-term | Near-term | Near-term | Mid-term | Mid-term | | Long-term |
| WDM | C.3.2 | ITER core transport and ITBs: Coupling with edge (HMM, projective integration) | Mid-term | Mid-term | Mid-term | | Mid-term | | Long-term |
| WDM | C.3.3 | ITER core transport and ITBs: Reduced models for ITB triggers | Mid-term | | | | | | |
| WDM | C.3.4 | ITER core transport and ITBs: Accelerate GK core simulations | | | Mid-term | Mid-term | Mid-term | Long-term | |
| WDM | C.3.5 | ITER core transport and ITBs: Sensitivity studies in high-D (> 20) space | | | | | | | Mid-term |
| WDM | C.4 | Q=10 ITER scenario: Coupling MHD + EP + transport | Near-term | Near-term | Near-term | Mid-term | Mid-term | Long-term | Long-term |
| WDM | C.5.1 | Steady-state ST: Global GK simulations | Near-term | Near-term | Near-term | Mid-term | Mid-term | | Long-term |
| WDM | C.5.2 | Steady-state ST: Coupled ions-electrons, realistic mass ratios | Mid-term | Mid-term | Mid-term | | Long-term | | Long-term |
| WDM | C.5.3 | Steady-state ST: EM effects (high-$\beta$) | Mid-term | Mid-term | Mid-term | | Long-term | | Long-term |

# Beyond Interpretive Simulations:
## Numerical Optimization and Uncertainty Quantification

**Panel Chair:** Don 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 at 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)

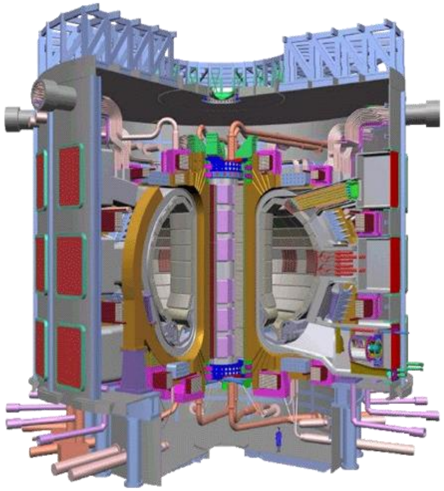
[2] Crosscutting expert from FES

# Advancing fusion energy science requires more than isolated simulation campaigns.

- **Successful reactor design & operating process must address**
  - Complexities such as microturbulence
  - Instabilities such as Alfven and MHD modes
  - Dynamical interactions between different behaviors at different spatial scales
  - Deleterious operating modes causing erosion

**Requires formulating and solving inverse and numerical optimization problems in the presence of uncertainty**

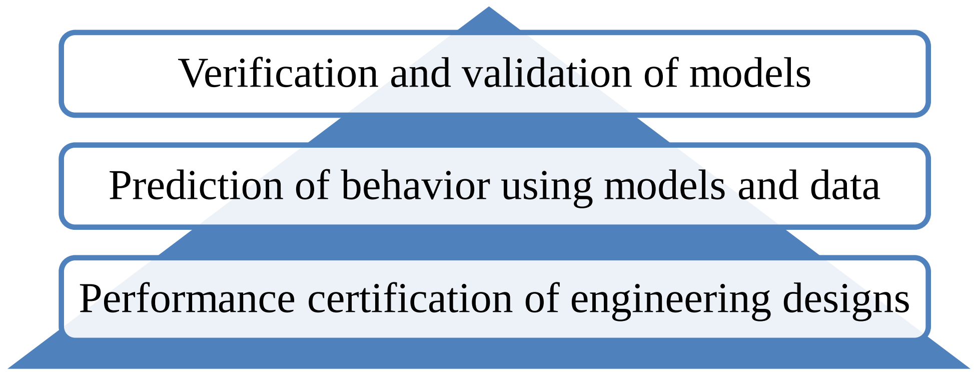
- **Example: Controlling steady-state plasma shape under an electromagnetic field in a tokamak**
  - with a fixed gap of a few centimeters,
  - while simultaneously controlling plasma instability arising in plasma poloidal cross-sections
  - and keeping the maximum tolerable currents as low as possible



# Beyond interpretive simulations

**Scientific inference:** Involves synthesis of model simulations and experimental observations typically through solution of **inverse and numerical optimization problems** together with **uncertainty quantification**

**Benefits:**
- Improving confidence in simulations
- Designing physical experiments
- Forming the basis for improved simulation efficiency
- Designing robust and reliable reactors

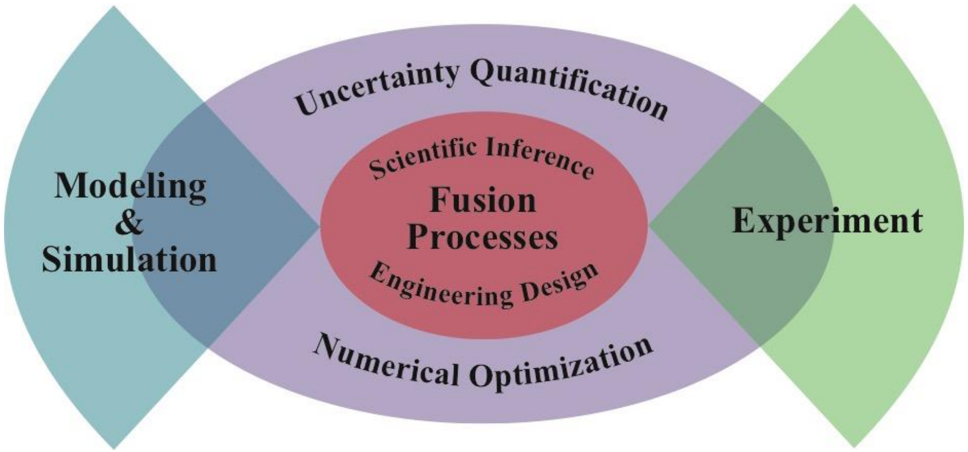



**Numerical Optimization (NO) with simulation constraints**
- Avoidance and mitigation of events (control)
- Parameter & state estimation (inverse problems)
- Robust optimization for design and control
- Constraints including chance constraints
- Discrete and categorical variables

**Uncertainty Quantification (UQ)**
- Sensitivity analysis
- Propagation of uncertainty and variation
- Stochastic inverse problems and inference
- Model selection and design of experiments
- Detection of critical events

**Recent advances throughout communities both in DOE (e.g., SciDAC QUEST) and outside DOE**

# Beyond Interpretive Simulations:
## 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.**

# Need interdisciplinary collaborations to define and continuously refine UQ and NO activities

- **Definition and goals must evolve in scope and rigor as understanding of physics, mathematics, and computation advances. Needs include:**
  - Sequences of models for different phenomena (what models can represent, scale of validity)
  - Identification of important inputs, parameters, variables, including definitions of variable ranges and information concerning uncertainty in values
  - Widely accepted quantities of interest characterizing crucial properties of fusion processes
  - Scientific and engineering questions to be addressed, and acceptable ranges of uncertainty in answers
- **Challenges**
  - Treatment of experimental results and data
  - Treatment of mathematical complexities arising in fusion processes
  - Propagation of stochastic variation/uncertainty
  - Formulation and solution of inverse problems (often experimental error is modeled stochastically)
  - Numerical optimization problems with constraints and uncertainty
  - High-performance NO and UQ for complex, multiphysics, coupled fusion processes (beyond 'black-box')

# Data Management, Analysis & 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)

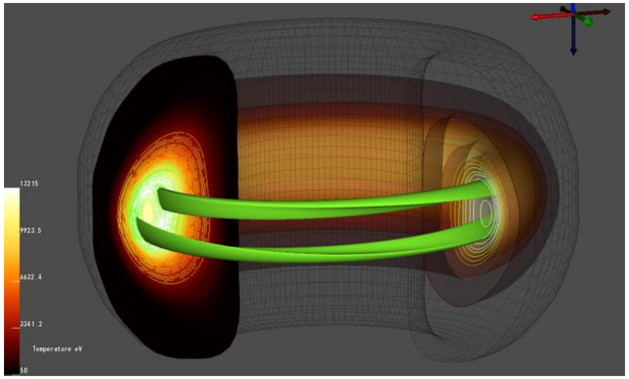
John Wright[2] (Massachusetts Institute of Technology)

John Wu (Lawrence Berkeley National Laboratory)

[2] Crosscutting expert from FES

# Scientific discovery is driven by exploitation of data

- **Careful management of data, its creation and transformation (analysis) and all of the associated metadata: critical aspect of scientific enterprise**
- **New set of challenging data problems**
  - I/O challenged computer architectures
  - Fragmented processes for storing and describing data
  - Complex and collaborative workflows (in-situ and ex-situ)
- **Integrated simulation for MFE exemplifies these challenges and also provides a testbed for solutions**
- **Recent advances throughout community, including SciDAC SDAV**




**Magnetic field topology and magnetic flux surfaces in a series of island chains. Image courtesy of A. Sanderson (Univ of Utah).**

# Data use cases

**“Composites” of material submitted in whitepapers and discussed in fusion panels:**

- **In situ calculations within large-scale computations**
  - MFE-specific computations, coupled models, synthetic diagnostics, data exchange, recording provenance
- **Well documented validation and UQ activities**
  - Experimental data collected for use in testing predictions of computational model, detailed documentation of processing chains
- **Crisis with data provenance**
  - Calibration (or other) error introduced into multi-generational analysis/computation, error discovered later, want to understand impacts of that error on subsequent uses.
- **Near-real-time data analysis in support of decision making**
  - Control-room decisions based on analysis, visualization, and assimilation of data to prevent disruptions

# Data Management, Analysis & Assimilation: Priority Research Directions

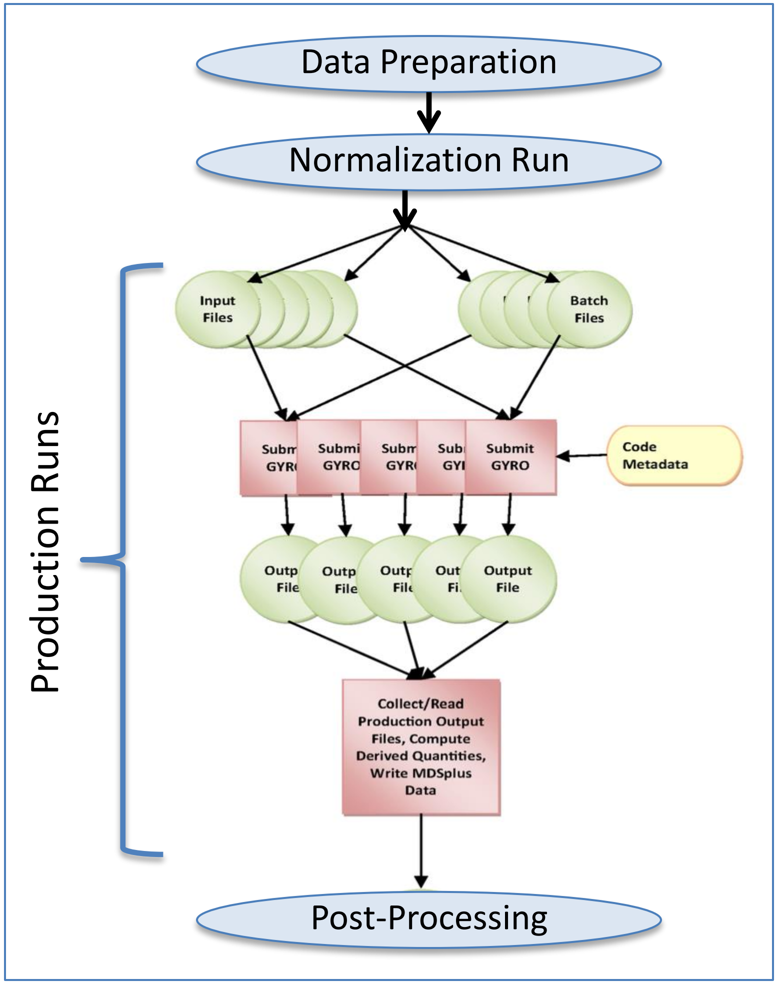
- **[PRD-Data-1] Develop community data and metadata standards based on broad input from users and developers.**
- **[PRD-Data-2] Develop and deploy infrastructure and algorithms that support in situ analysis for fusion simulation codes.**
- **[PRD-Data-3] Improve support for MFE-centric workflows including capture of data provenance.**
- **[PRD-Data-4] Build federated, curated data repositories.**
- **[PRD-Data-5] Engage in R&D and deployment of visualization and analysis methods targeted to the needs of the fusion community.**
- **[PRD-Data-6] Develop a strategy for promoting adoption and sustainment of shared tools that support data management, analysis, and visualization for fusion applications.**

# Improve support for MFE-centric workflows

**Workflow: Chain or sequence of processing steps executing on a single machine or multiple machines, come in several varieties.**

**Workflows (in situ, ex situ, post hoc) to support fusion-centric science activities.**

- Provenance capture
- Metadata management
- Data movement
- Data "processing", data analysis & visualization
- Use in diverse, distributed computing environments
- Support real-time analysis and coordination between experiments and HPC centers
- Capable of dealing with very large volumes of data
- Literate programming in "lab notebook" like interface for (ex situ) workflow management, end-to-end documentation of workflow




Workflow for preparing inputs and running a gyrokinetic simulation (M. Greenwald)

# Software Integration and Performance

**Panel Chair:** David Bernholdt (Oak Ridge National Laboratory)

**Panel Co-Chair:** Robert Lucas (University of 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)

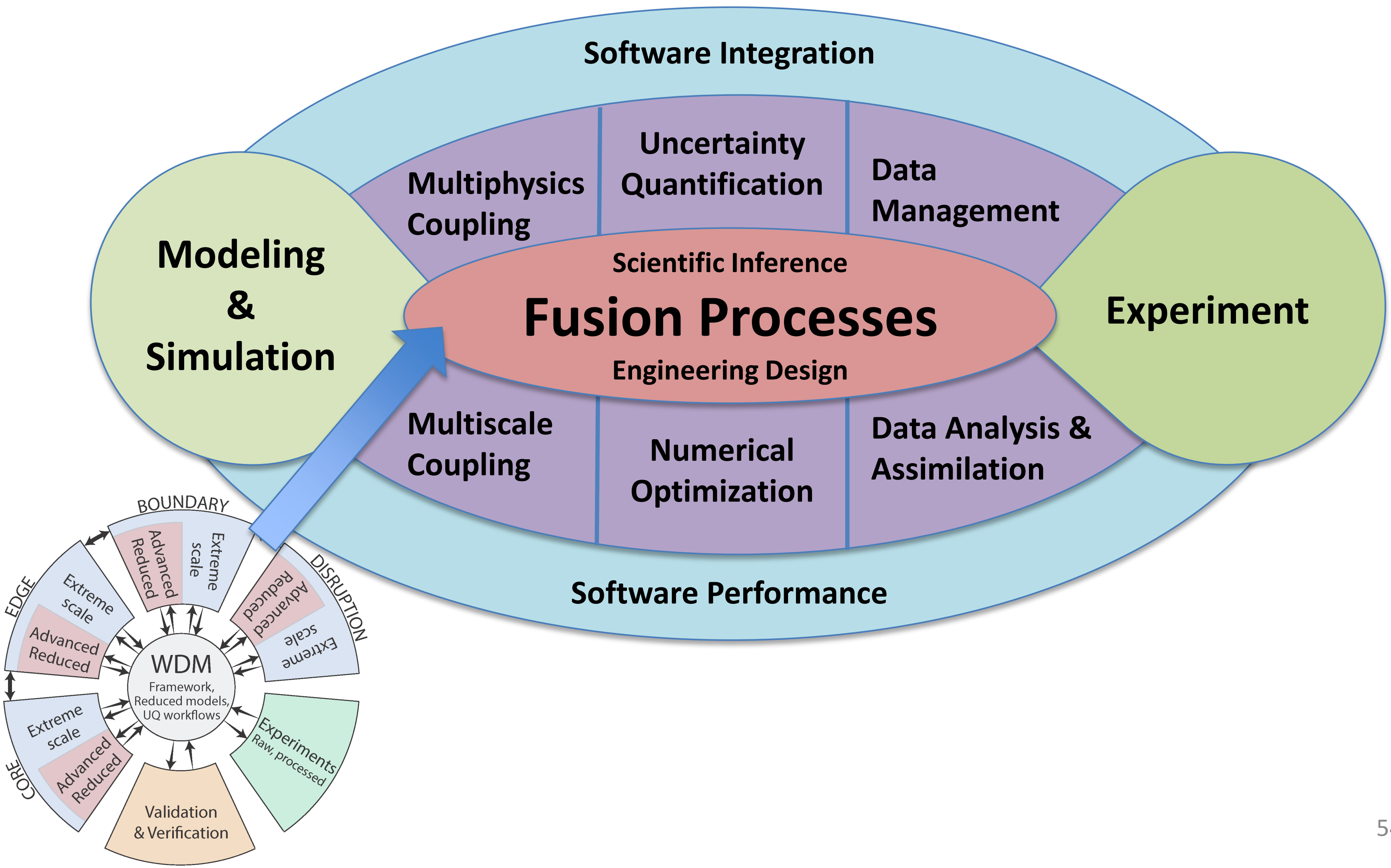
Francesca Poli[2] (Princeton Plasma Physics Laboratory)

Brian Van Straalen (Lawrence Berkeley National Laboratory)

Patrick Worley (Oak Ridge National Laboratory)

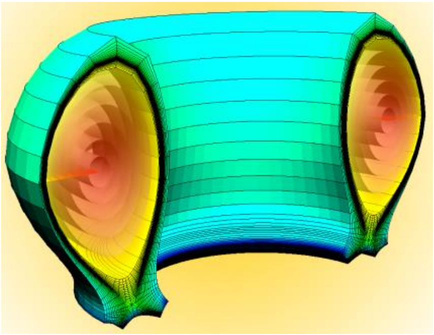
[2] Crosscutting expert from FES

# Software integration and performance: Permeate all aspects of work



# Software integration & performance

- **Code design, maturity, and integration**
  - Different codes for different purposes; need to (re)structure codes to make them more readily composable
  - Common for single-physics codes to be in both standalone and integrated contexts
  - Useful design pattern: 'Component' approach, with interchangeability of conceptually similar codes
- **Performance and portability**
  - Must plan for emerging extreme-scale architectures: performance-aware software
  - Understanding performance in coupled contexts
  - Need to expose performance models and performance variation
- **Culture, community, and governance issues**
  - Sharing code; institutional investments in own codes; tension between 'research' and 'production' software
- **Software productivity and software engineering for integrated fusion applications**
  - Methodologies for revision control, build systems, bug tracking, documentation, refactoring, interoperability, performance portability, etc.
  - Testing (unit, integration, system level, performance, etc.)
- **Recent progress**
  - Fusion proto-FSPs (FACETS, SWIM, CPES); SciDAC projects: AToM, EPSI
  - SUPER SciDAC Institute, IDEAS software productivity project
- **Related work**
  - EU Integrated Tokamak Modeling, ITER's Integrated Modeling and Analysis Suite (IMAS): compatibility useful and desirable



Coupled core-edge simulation using FACETS

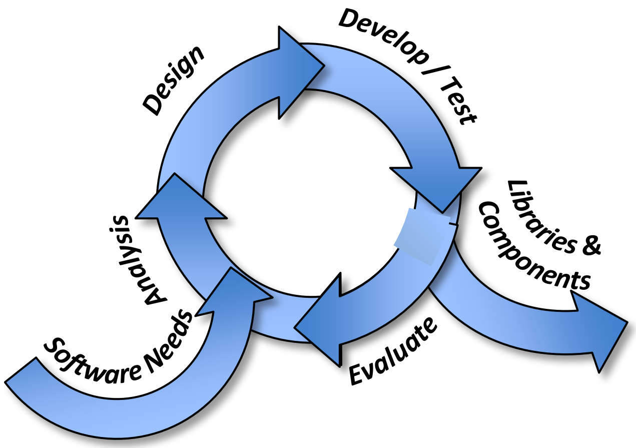
# Software Integration and Performance:
## Priority Research Directions

- **[PRD-Software-1]** **Implement software engineering best practices, consistently, throughout the fusion integrated simulation community.**
- **[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.**
- **[PRD-Software-3]** **Develop community standards and conventions for interoperability.**
- **[PRD-Software-4]** **Develop best-practice guidelines and recommendations to address the particular software engineering challenges of integrated simulation.**
- **[PRD-Software-5]** **Perform research on the computer science of code composition.**
- **[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.**

# Addressing portable performance at scale

**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.**

- May need to take a step back and consider different algorithms or even different formulations from those typically used today




**For pre-exascale fusion applications, software productivity questions include:**

**(1) Will application X scale on platform Y?**

**→ <u>Need:</u> Software performance engineering methodology for platform Y**

**(2) Will component A scale on platforms Y and Z?**

**→ <u>Need</u>: Software engineering processes to enable porting to new platforms**

**(3) Can component A work with application X?**

**→ <u>Need</u>: Software engineering to develop interoperable interfaces**

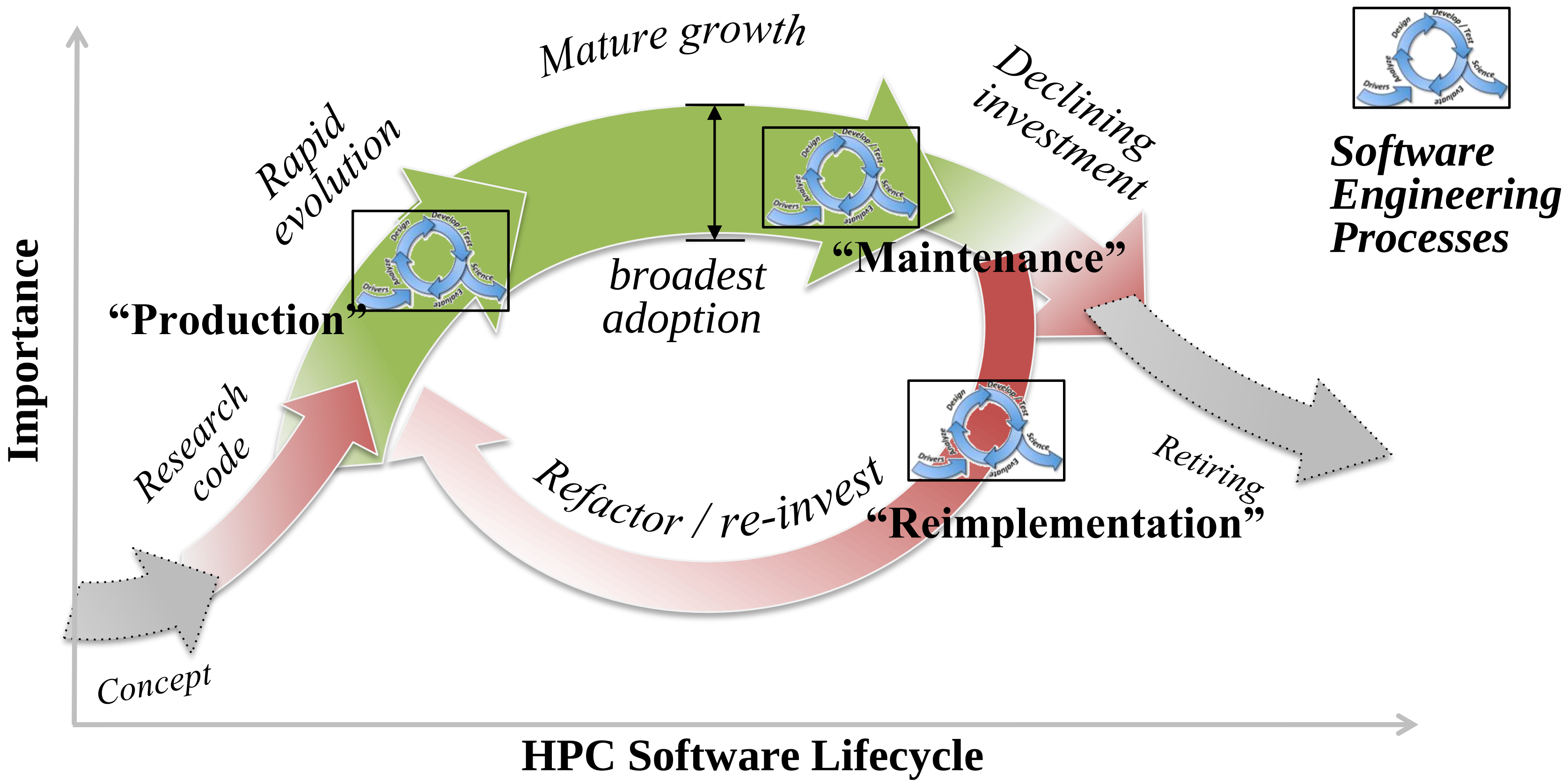
**(4) How hard is it to integrate component B?**

**→ <u>Need</u>: Develop a methodology and processes to refactor to use libraries and components**

**(5) How could we have made that easier?**

**→ <u>Need</u>: Develop a repeatable, deployable approach to improve software productivity for fusion applications at scale**

# Addressing software engineering & productivity challenges for integrated fusion simulations




**Need:** Put steps in place to encourage adoption and reuse of research components and libraries, and improve longevity of FES and ASCR software investments through refactoring and interoperability.

# 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**

# Summary and Conclusions

- **Opportunities abound for interdisciplinary FES/ASCR collaborations to fully leverage emerging extreme-scale computing resources for fundamental advances in integrated fusion simulations:**
  - Collaborations at both the smaller and larger scales are envisioned.
- **All strategies call for a strong and broad-based support for model verification and validation that leverage expertise from applied math and computer science in uncertainty quantification and numerical optimization:**
  - Application of verification and validation technologies to integrated simulations will be a particular challenge.
- **Research will be needed on innovative workflows, data structures, and algorithms to support efficient concurrent execution of many related moderate concurrency simulations running for long periods of time:**
  - Will ultimately allow exploitation of extreme scale platforms.
- **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.

# Back-up Slides

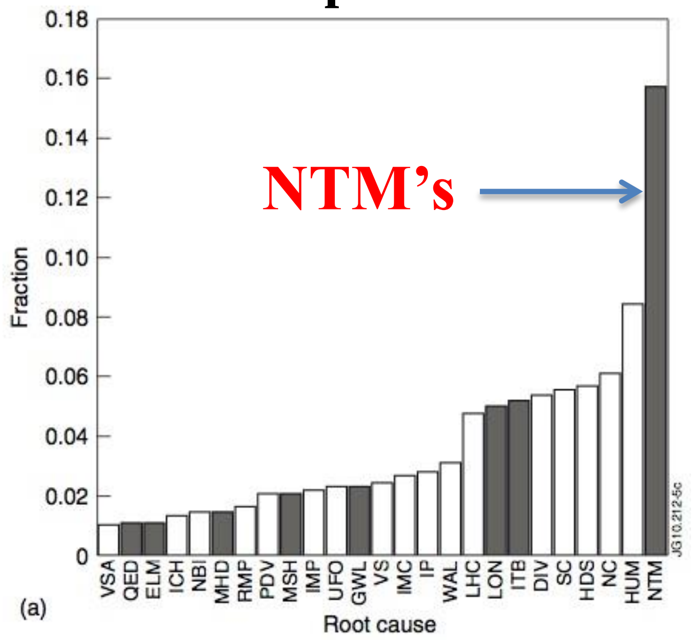
# Workshop goals

- Identify theory/simulation advances since RENEW (2009) and more recently the 2011 FSP Execution Plan.
- Identify gaps in theory/simulation, especially related to integration of multiple processes and regions:
  - How could these gaps be addressed in the shorter (5 year) and longer (10 year) timeframes?
  - Identify new opportunities for integrated simulation including the roles of physics, applied mathematics, and computer science
  - Emphasize crosscutting fusion / applied math / computer science connections
  - Identify potential applications for extreme-scale computing

# Disruption physics - background

- **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.

**JET Disruption Database**




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

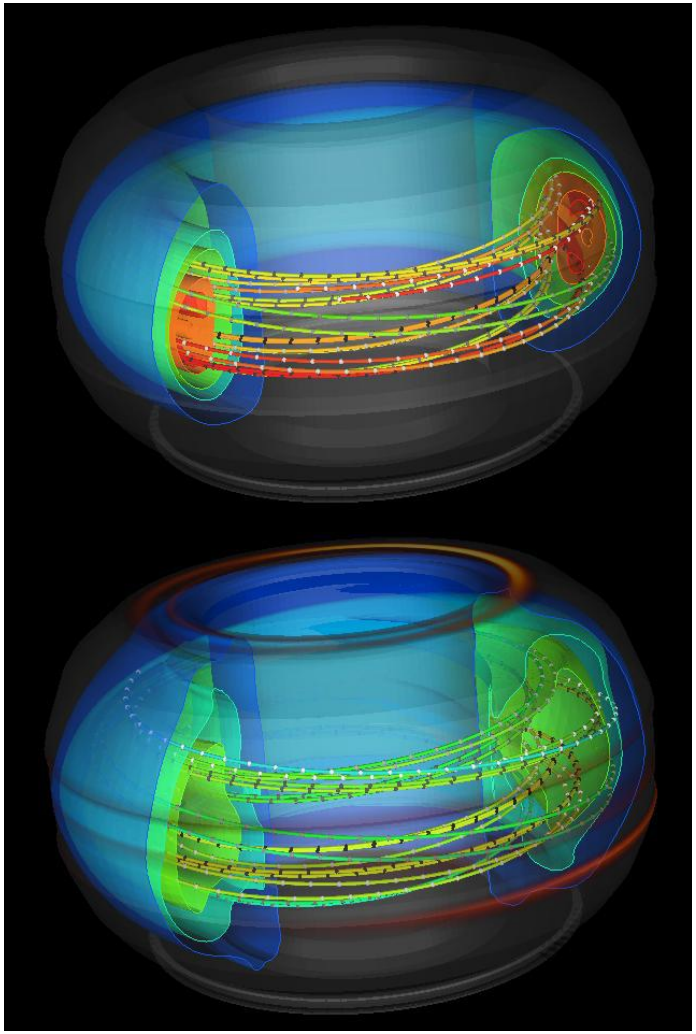
# Recent progress in disruption modeling

- The understanding of externally imposed non-axisymmetric perturbations has improved through validation and benchmarking campaigns.
- Synchrotron radiation and scattering effects on the runaway-electron threshold voltage have been analyzed theoretically.
- Drift and energetic-ion effects are now considered in linear stability computations and in nonlinear simulation.
- Progress on modeling vertical displacement events includes:
  - 2D simulation benchmarking,
  - asymmetric wall-force predictions for ITER,
  - development of reduced modeling and detailed external electromagnetics.
- Majority-species drift kinetics for macroscopic dynamics have progressed analytically and computationally.
- Modeling and validation of mitigation through massive gas injection (MGI) reveal causes of toroidal localization.

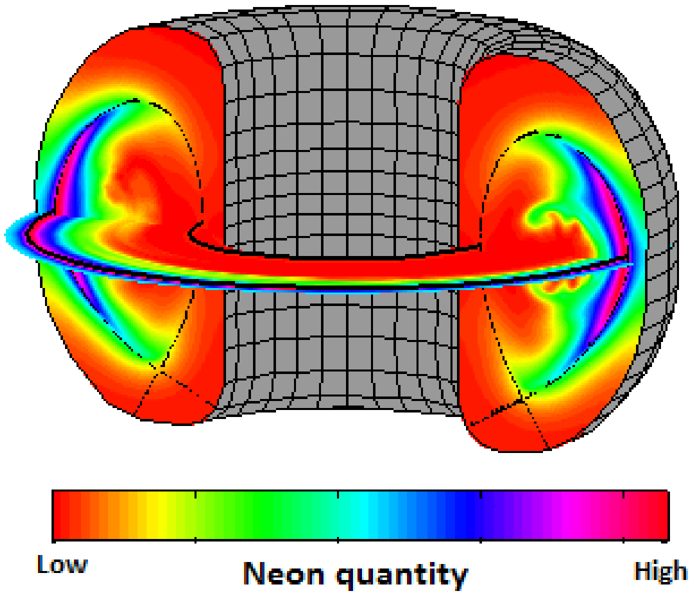
# Disruption Physics:
# Priority Research Directions

- **[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.

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

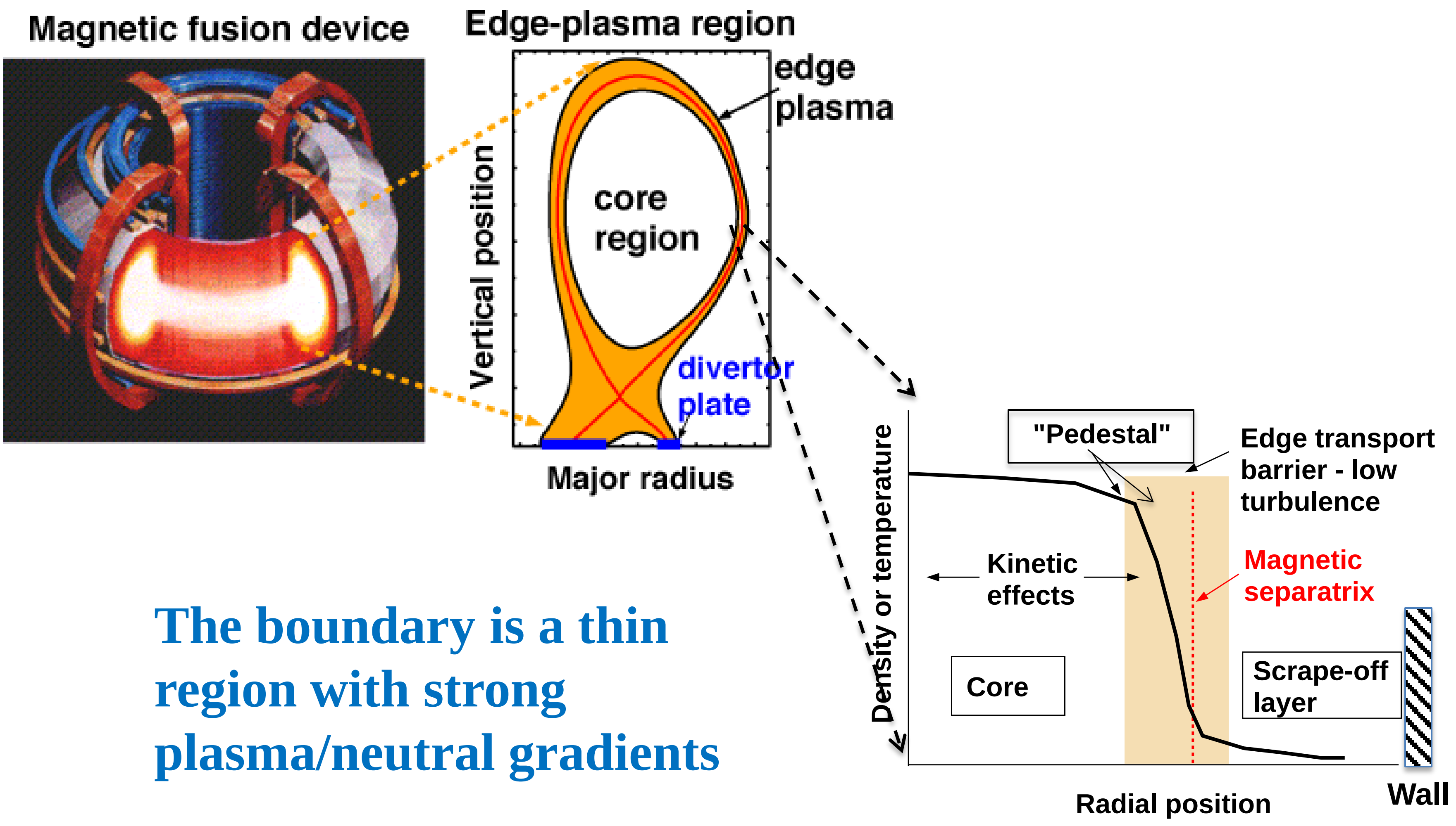


Nonlinear MHD simulation of global instability leading to thermal quench and localized heat. Image courtesy S. Kruger, Tech-X Corporation.



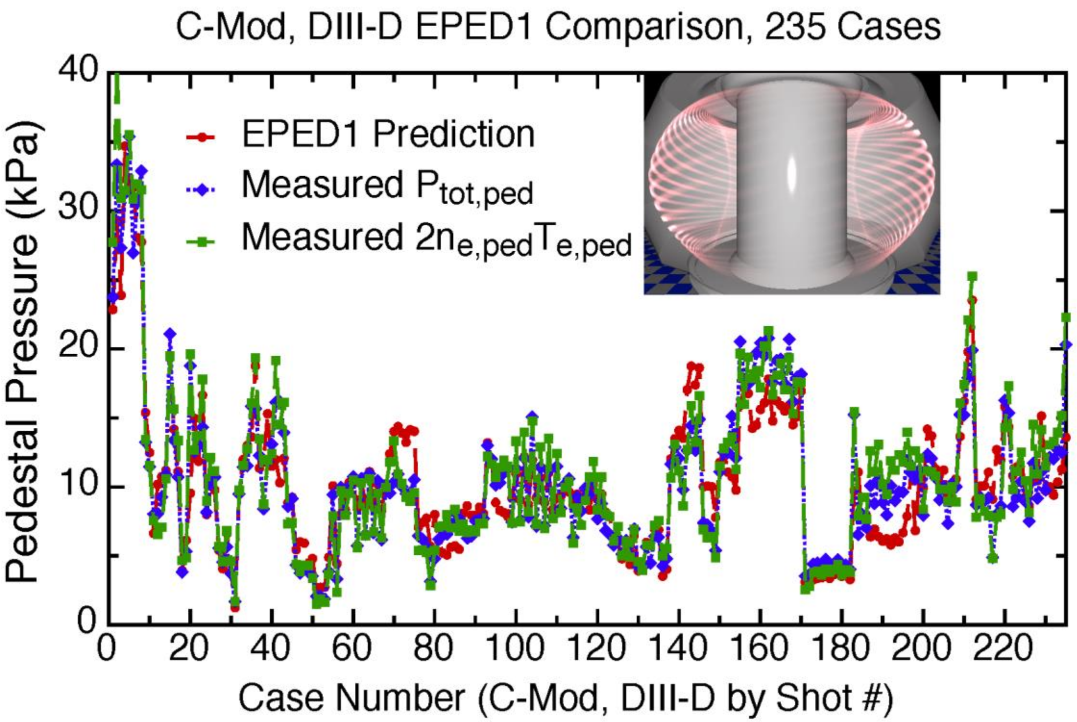

Concentration of edge-injected Ne impurity after dynamic mixing, as predicted by integrated nonlinear simulation, combining 3D MHD and radiation modeling. Image courtesy of V. Izzo (UCSD).

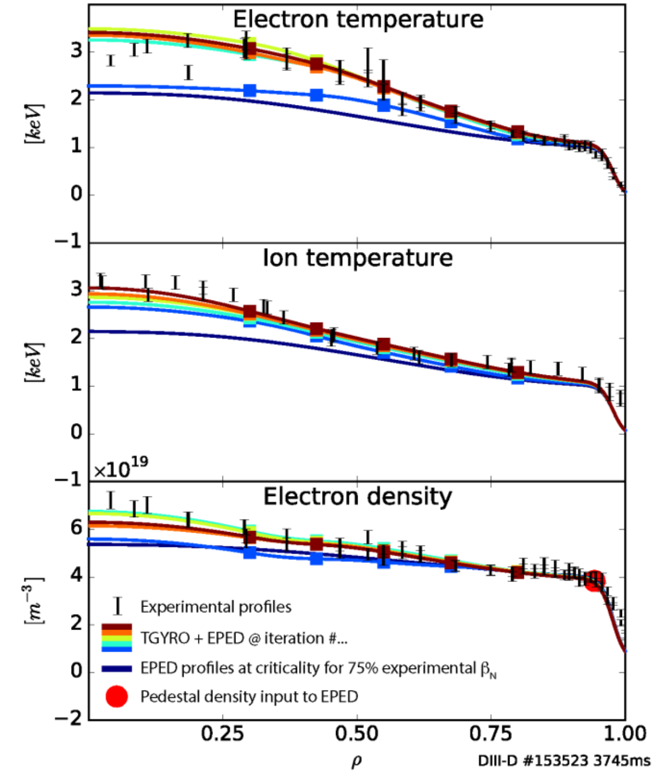
# Challenge: Temperature must go from hundreds of degrees at the wall up to tens of millions at top of pedestal, while preserving long material lifetimes




The boundary is a thin region with strong plasma/neutral gradients

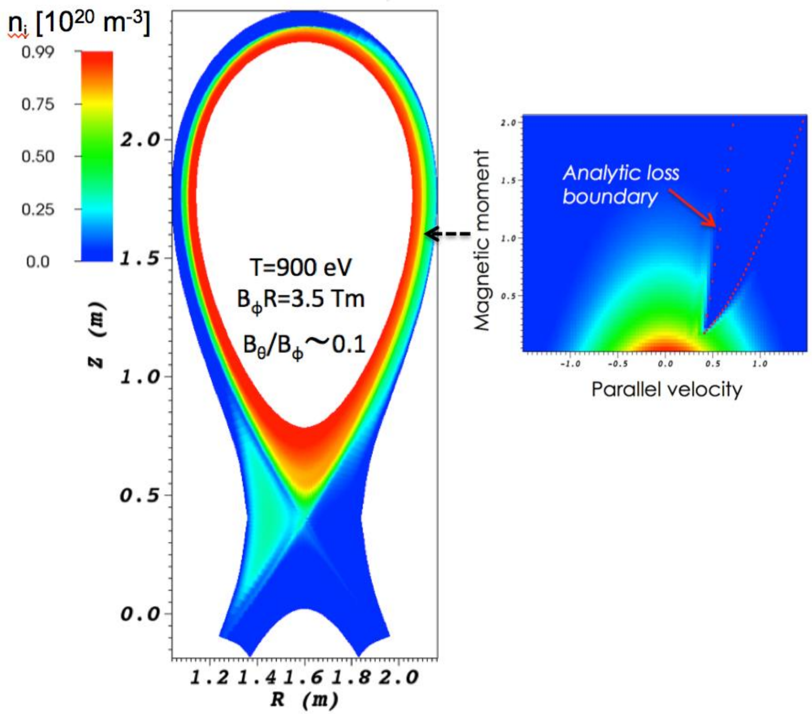
# Pedestal properties have been successfully predicted using constraints that combine transport from kinetic ballooning and peeling-ballooning modes.



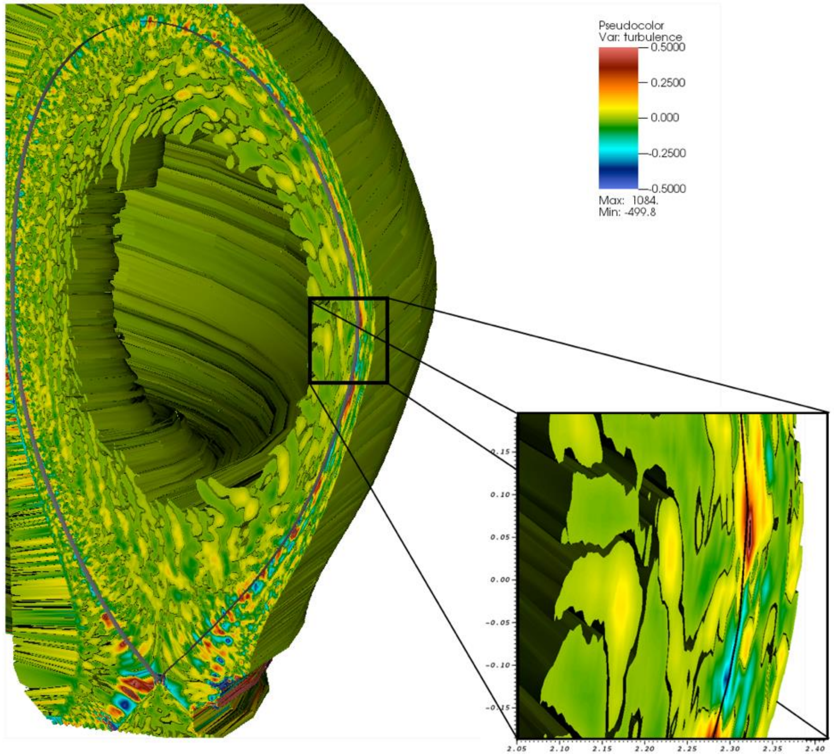




**EPED model predictions of the pedestal pressure compared with measurements from the Alcator C-Mod and DIII-D tokamaks in 235 cases. More than 150,000 peeling-ballooning calculations were required for these predictions, and a sample mode structure is inset. Example shown is from an ITER-like plasma in the DIII-D tokamak.**

# 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

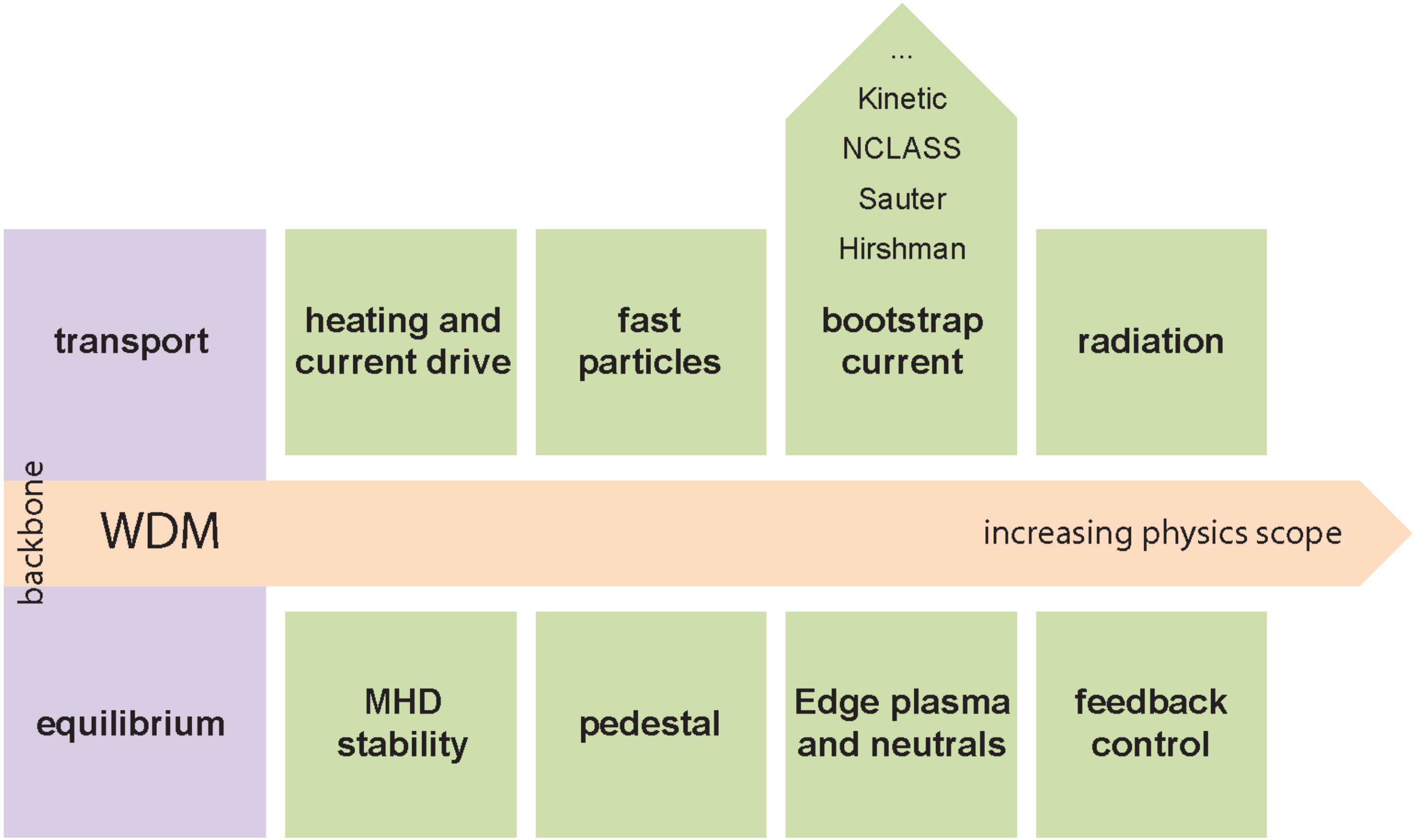



Contours of turbulent electrostatic potential from an XGC1 5D (3r,2v) gyrokinetic simulation that spans the pedestal and SOL in DIII-D magnetic geometry.

# Boundary Physics: Priority Research Directions

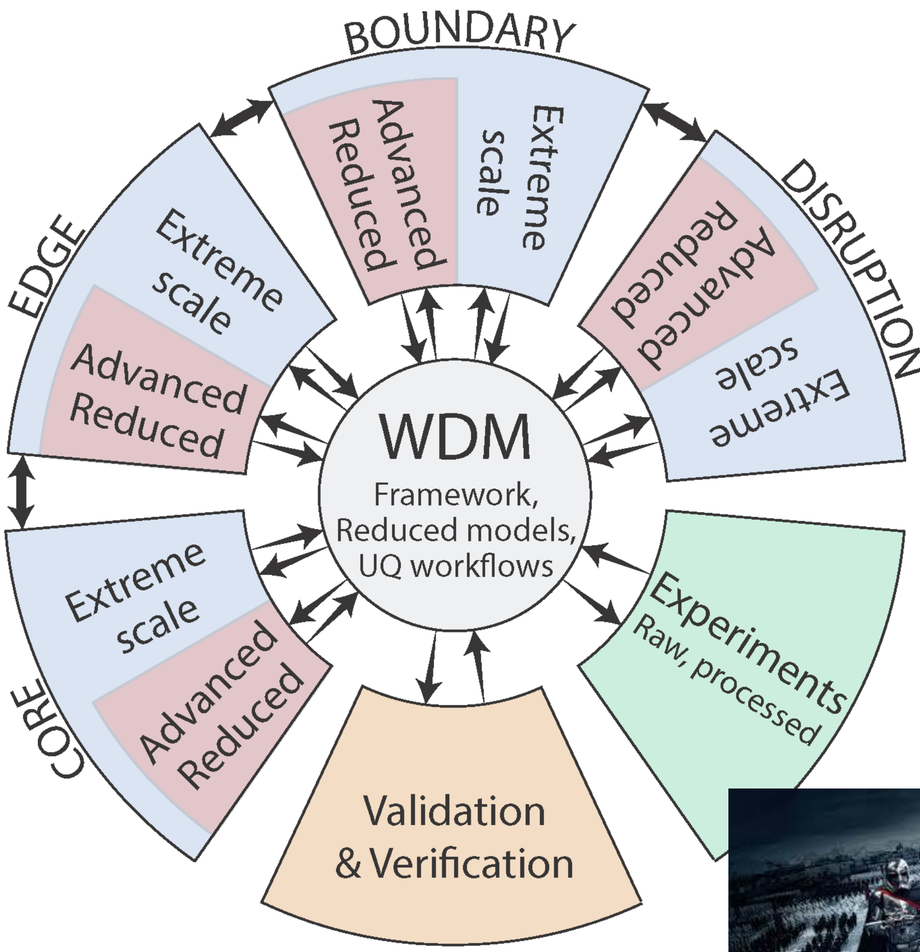
- **[PRD-Boundary-1] Develop a high-fidelity simulation capability and predictive understanding of the coupled pedestal/SOL system and its structure and evolution in the presence of microturbulence and collisional transport.**
- **[PRD-Boundary-2] Incorporate the dynamics of transients, particularly 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.**

# The "Whole Device Model" is really just another form of Integrated Simulation




- Whole device model showing its most basic components (equilibrium and transport) plus additional components that illustrate increasing physics scope.
- Using the bootstrap current as an example, a series of progressively more accurate components illustrates the fidelity hierarchy for this process.

# 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).**

# 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.