Role of Integrated Simulations in Disruption Physics Research

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Outline

- This is actually a summary of the DOE Workshop and Report on Integrated Simulations in Magnetic Fusion Energy Sciences as it pertains to disruptions.
- Review Background and Process
  - DoE charge letter, panel structure
  - Call for whitepapers, community teleconference, writing workshop
  - Goals of the workshop
- Review of Recent Progress
- Gaps and Opportunities
  - Physics / Applied mathematics / Computer Science
- Strategy and Path Forward:
  - Priority Research Directions

Background

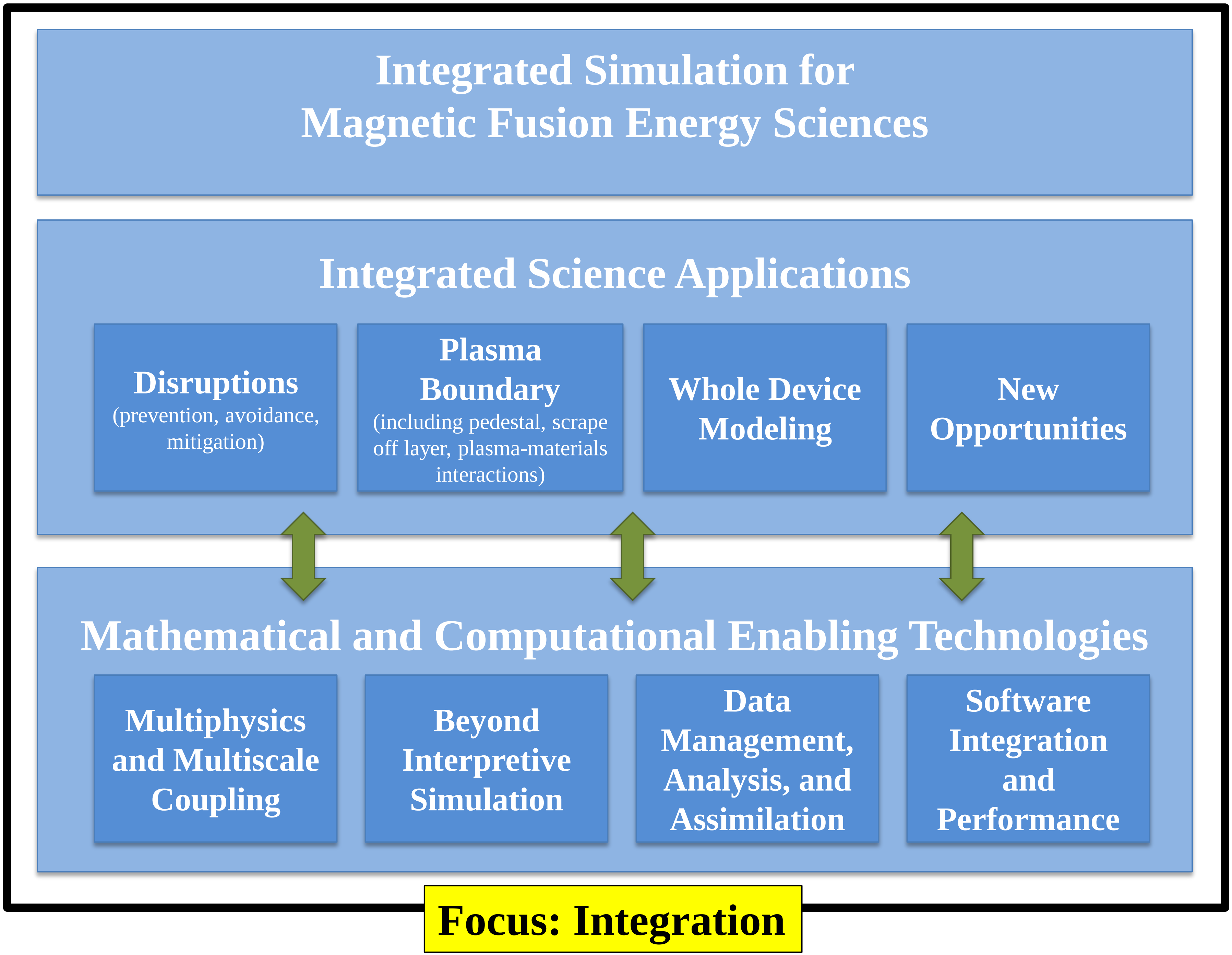
- Integrated Simulation Workshop is one of the four FES Community Planning Workshops conducted in 2015:
  - https://www.burningplasma.org/activities/?article=Integrated%20Simulations
  - DOE Points of Contact:
    - John Mandrekas (FES)
    - Randall Laviolette (ASCR)
- Workshops were held on Transients and Plasma-Material-Interactions, with Plasma Science Frontiers Workshops to be held in (August & October, 2015):
  - https://www.burningplasma.org/activities/?article=FES%20Community%20Planning%20Workshops%202015

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**
  - **World-leading potential**

Goals of this Workshop

- 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**


Integrated Simulation for
Magnetic Fusion Energy Sciences
Integrated Science Applications
Disruptions
(prevention, avoidance, mitigation)
Plasma Boundary
(including pedestal, scrape off layer, plasma-materials interactions)
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

Integrated Science Applications

A. Disruption Physics (prevention, 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

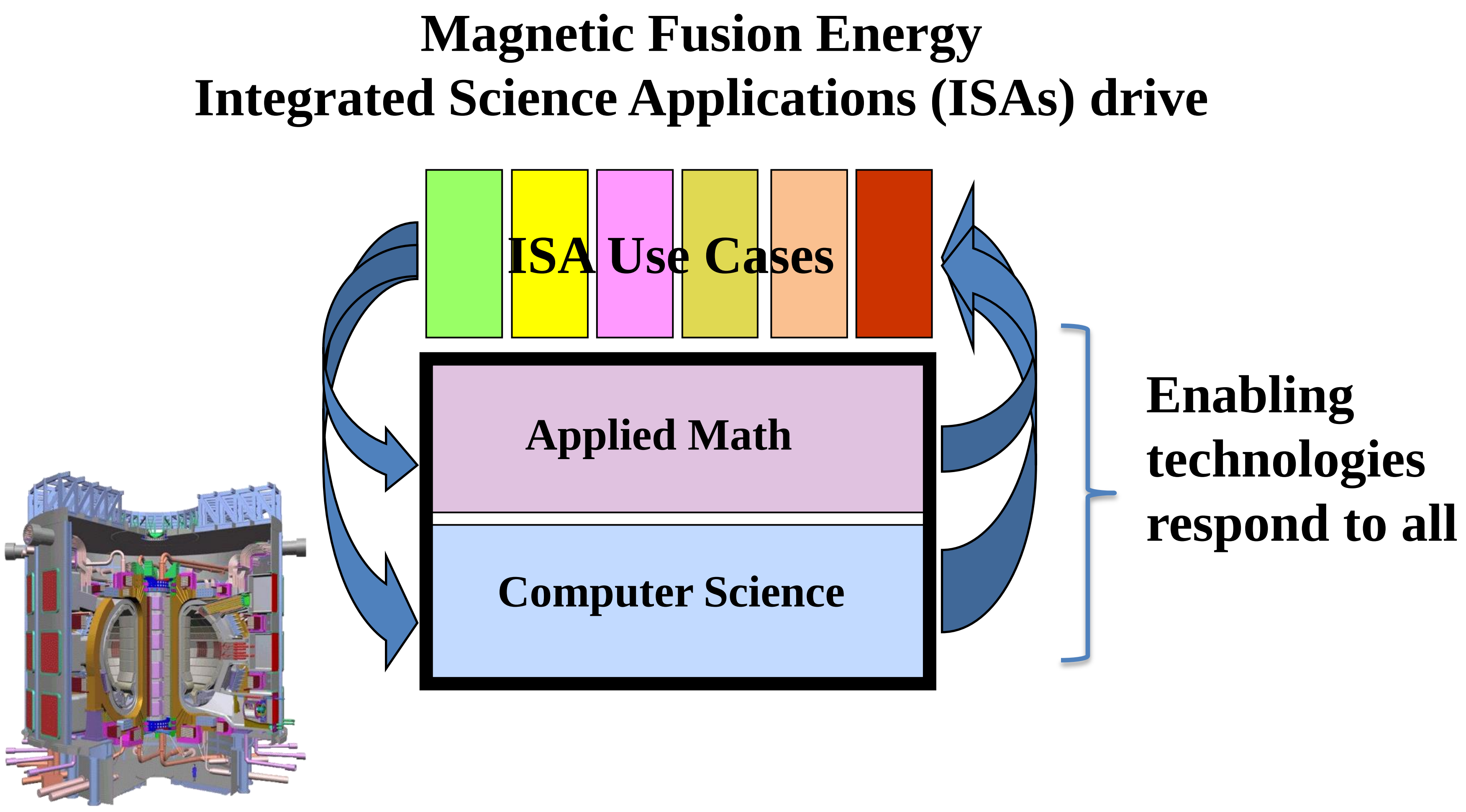
Chair: Jeff Candy (GA)

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.

Interaction with Mathematical and Computational Enabling Technologies



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.

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

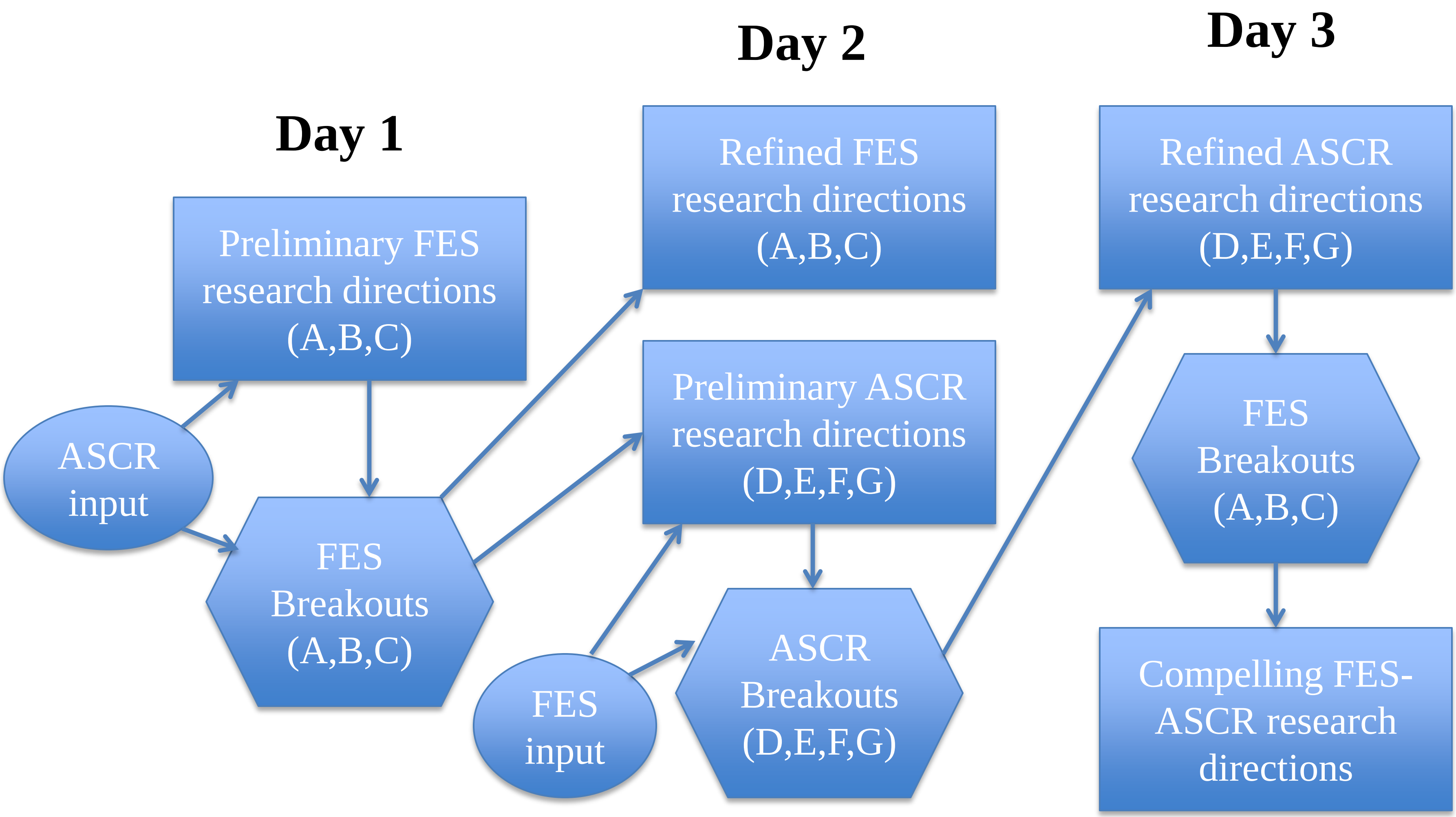
Process Thus Far

- Community wide call for whitepapers ending on April 24, 2015:
  - Panels received 121 whitepapers
- Community Teleconference, May 18–19, 2015:
  - Oral presentations from 45 whitepaper submissions.
  - Discussions of whitepapers by panels.
- Teleconferences among panel chairs / co-chairs and individual panels:
  - About 35 teleconferences thus far (March, 2015 – present).
- “Writing” workshop held June 2-4, 2015:
  - Attended by panel members and “participants at large”.
- Workshop report is now being finalized.

Disruption Panel (A): Process

- Panel members were selected to balance experimental, theoretical, computational, and applied mathematics perspectives.
- The panel held conference calls and exchanged information through e-mail, web postings, and the video conference.
- 11 whitepapers were invited to ensure coverage of critical topics.
- The community submitted a total of 28 whitepapers that listed disruption simulation as primary or secondary area.
  - **Topics include avoidance, characterization, mitigation, kinetic stability, runaway electron physics, halo currents, external structures, fast linear computation, reduced models, multi-scale modeling, data analytics, and validation.**

Workshop Process for Identifying Compelling FES-ASCR Research Directions



Emphasis:

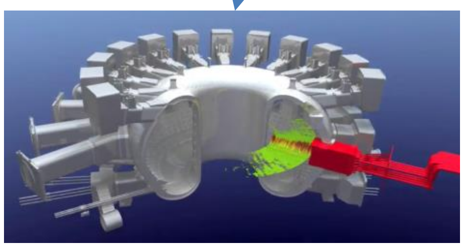
- **Role of integrated simulations**
- **Potential for extreme-scale computing**

Fusion physics panels: A,B,C
ASCR math/CS panels: D,E,F,G

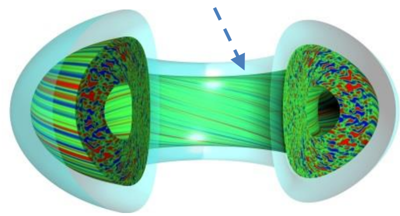
Today's Approach: Scale Separation

Ω_{ce}^{-1} ω_{LH}^{-1} Ω_{ci}^{-1} τ_A τ_E τ_R τ_D

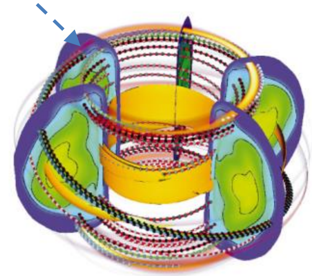
10^{-10} 10^{-8} 10^{-6} 10^{-4} 10^{-2} 10^{0} 10^{2} 10^{4} sec



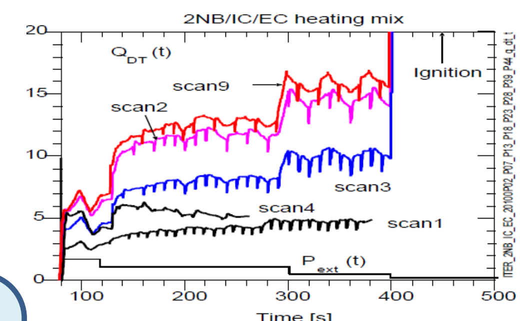
RF codes: wave heating & current drive; Fokker-Planck equation for particle response



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



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

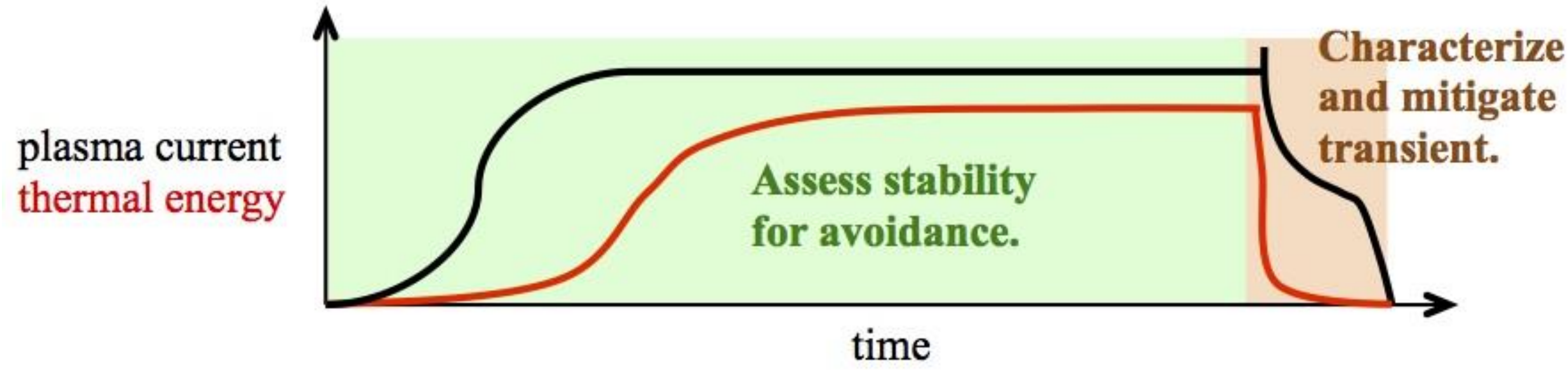


Flux surface averaging → 1½ D transport codes: discharge time scales

A number of critical effects (*Neoclassical Tearing Modes, Energetic Particles, Disruptions, etc.*) are inherently multiscale

Adapted from: D.E. Post, J. Fusion Energy, 2005

Approach

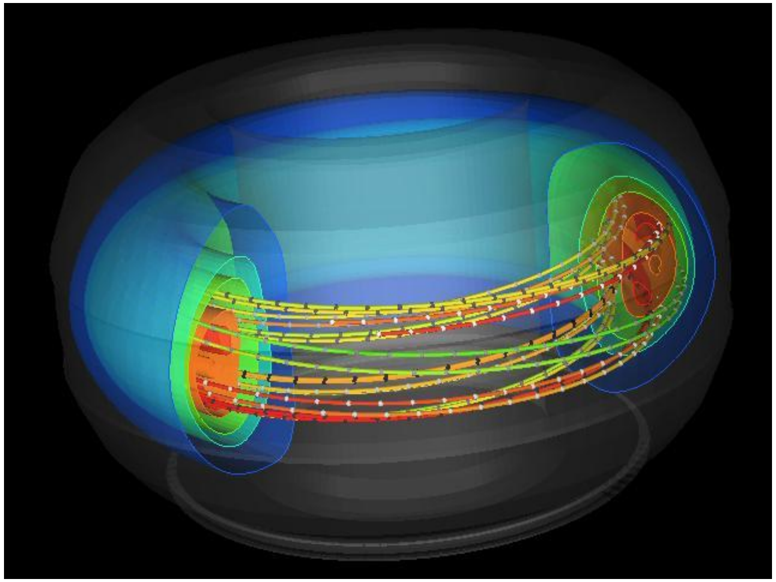


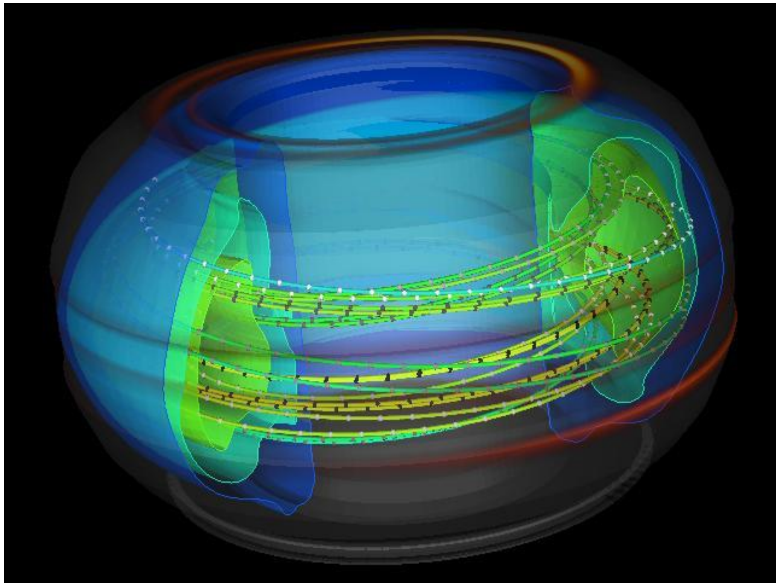
- **Two distinct categories of numerical computation are needed:**
  - **Assess macroscopic stability for avoidance.**
  - **Understand and characterize disruptive transients.**
- **"Avoidance" is used to mean both the routine maintenance of the discharge trajectory and last-minute redirection of the discharge if disruption becomes likely.**
- **Disruptive evolution involves nonlinear macroscopic dynamics, relativistic and non-relativistic particle kinetics, electromagnetic responses of external structures, radiation, neutral dynamics, and plasma-surface interaction.**

Recent Progress in Disruption Modeling - Highlights

- 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 including:
  - 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.

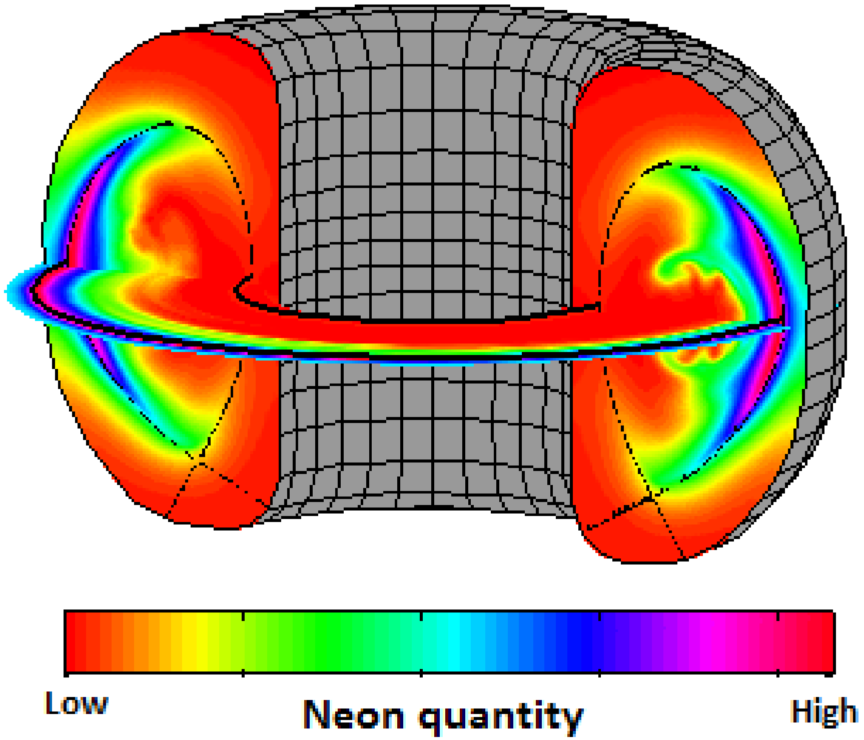
Recent progress in simulating disruptive transients





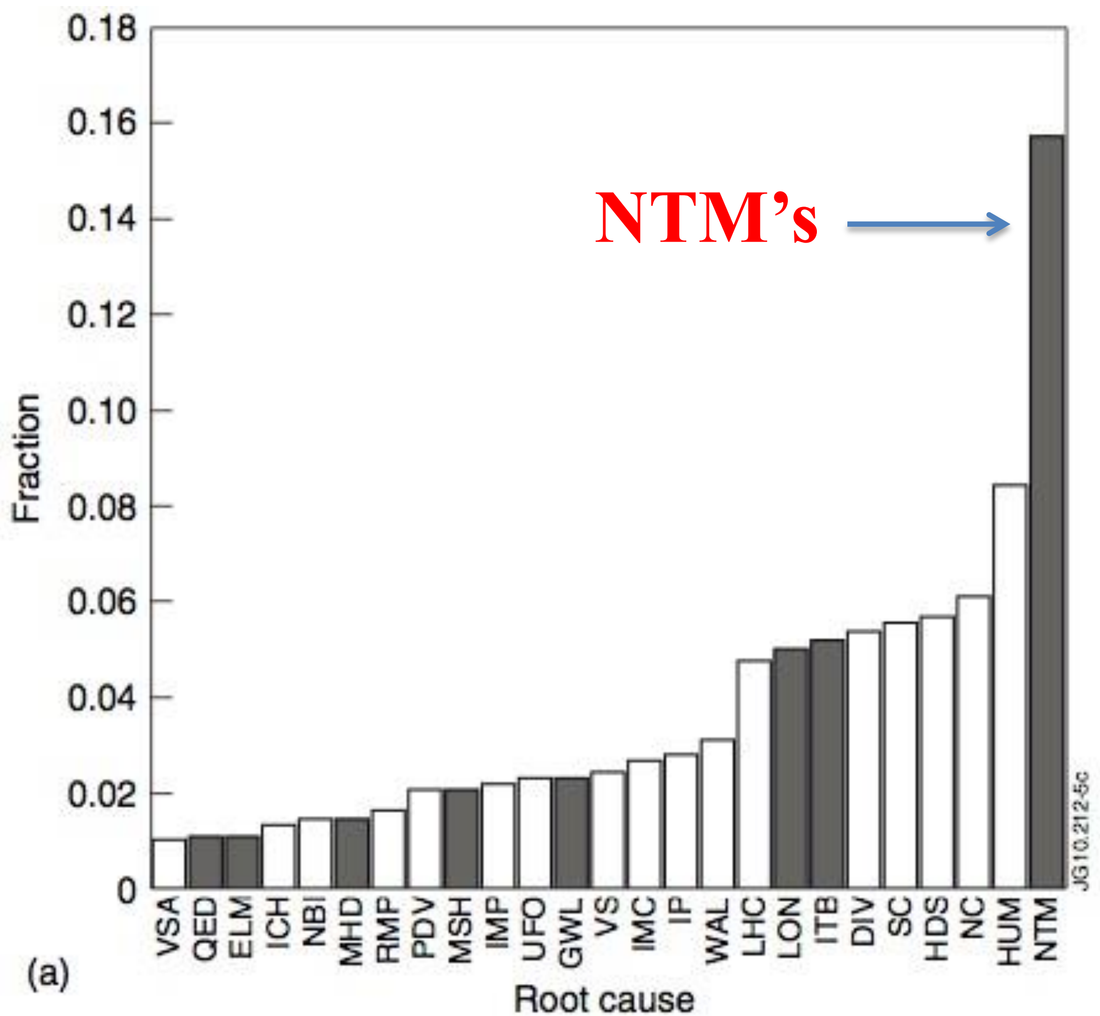
- Nonlinear MHD simulation of global instability leading to thermal quench and localized heat deposition on the surrounding wall (S. Kruger).

Recent progress in simulating disruption mitigation



- Nonlinear 3D MHD simulation combined with radiation modeling of mitigation via massive gas injection (MGI) in DIII-D (V. Izzo).
- Simulation shows concentration of edge-injected Ne impurity after dynamic mixing

The challenge: JET data base indicates a number of root causes of disruptions in JET



- **Root causes of disruptions include:**

  Inadequate operations planning.

  Failure of feedback control or other systems.

  Natural fluctuations that exceed the nonlinear meta-stability of a confinement state.

P. C. deVries, M. F. Johnson, B. Alper, et al., Nucl. Fusion 51, 053018 (2011).

Challenges and Opportunities - Physics

- **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.
  - The interaction of relativistic particles with matter is of broad scientific interest.
- **Mitigation**
  - The penetration capability of shattered-pellets is not known.
  - The significance of rotation and neutral dynamics needs to be studied.

Challenges and Opportunities - Computation

- **Multiple scales**
  - Distortions are device-scale; resonant layer thickness is 100 – 1000 times smaller.
  - Equilibration is fast relative to island development, wall time, and quench times.
  - Modeling kinetic effects increases the dimensionality of the system.
- **Multi-physics effects**
  - Present-day 3D simulations use implicit single- and two-fluid modeling with limited external electromagnetics, radiation, and fast-ion kinetics.
  - Comprehensive characterization needs plasma-surface interaction, neutral dynamics, majority-species and runaway-electron kinetics.
- **Data analysis**
  - Linear stability analysis and initial conditions for nonlinear simulations are based on profiles fitted to experimental discharges.
  - Incorporating "kinetic" data and adjusting for quality need to be automated.
  - Stability is sensitive to profiles, and uncertainties have not been quantified.

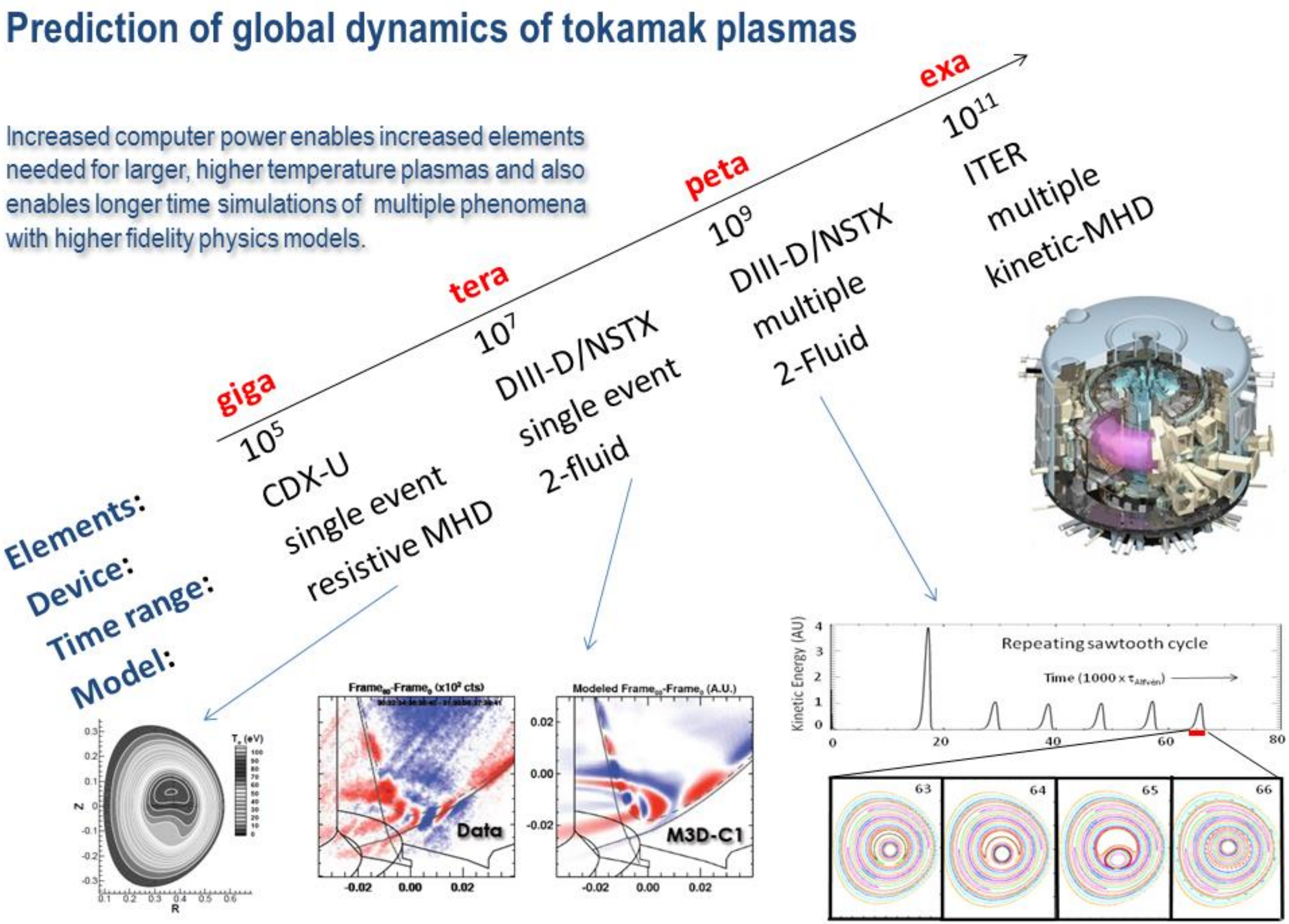
Challenges – Computation (continued)

- **Code integration**
  - Radiation and external electromagnetics software have been coupled for mitigation and wall-force studies.
  - Coupling RF propagation and deposition has been demonstrated and required significant development.
  - Plasma-surface interaction, neutral dynamics, and more detailed external electromagnetics are needed.
- **Plasma control**
  - Fast linear stability computation for real-time control may be feasible.
  - Accurate and fast profile fitting would be the most challenging aspect.

Crosscutting Issues Identified for ASCR

- **Validation**
  - Databases have not been systematically analyzed for linear stability.
  - Nonlinear modeling without reduced modeling is computationally expensive.
- **Multi-scale computation**
  - Advances in time-integration can facilitate studies of characterization and mitigation.
  - Computational performance depends on algebraic solvers.
- **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.
- **Data analysis**
  - Profile reconstruction uses a number of input channels.
- **Software integration**
  - New combinations for multi-physics computation are expected.

HPC has enabled significant advances in Extended MHD



CEMM (S. Jardin, PPPL)

Recommendations and Path Forward
"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.