Computational Challenges of Integrated Simulations for Disruption Studies

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Magnetically confined plasma is necessarily far from thermodynamic equilibrium with surrounding surfaces and structures. With sufficiently large perturbation, the metastability of the system is violated, and confinement is lost on a rapid time-scale. Disruptive evolution of the plasma/magnetic-field system in tokamaks always exhibits macroscopic dynamics, regardless of the root cause [1]. Integrated simulations are needed for avoidance, prediction, characterization, and mitigation. Here, we introduce the classes of numerical simulations that are needed and outline the associated computational challenges.

Characterizing disruptive behavior and exploring means to *mitigate* the physical damage from disruptions require spatially 3D simulations that describe the plasma and magnetic field over time. At a first-principles level, the equations that describe the dynamics are known: Maxwell's equations, plasma kinetic equations, models for line radiation, etc. However, comprehensive modeling of disruptions will not be feasible over the next decade, even with efficient use of exa-scale computation. All tractable models reduce the system and/or the dynamics to varying degrees. The most commonly used model for present-day characterization and mitigation is visco-resistive MHD [2,3], with non-ideal wall effects in characterization studies and impurity radiation in simulations of mitigation experiments.

Even the relatively simple visco-resistive MHD model encompasses multiple spatial and temporal scales. When applied to parameters relevant to the ITER experiment [4], $B \sim 5\ \mathrm{T}$, particle density $n \sim 10^{20}\ \mathrm{m}^{-3}$, and temperature $T \sim 15\ \mathrm{keV}$ with major and minor radii of 6 m and 2 m, respectively, Alfvén waves circle the chamber in microseconds (τ_A), whereas global resistive diffusion would occur over hours (τ_r) if the device could operate that long. During the early phase of many disruptions, the thermal quench, energy is transported to the vessel walls in concentrated regions with enormous heat-flux density. Temperature drops rapidly (~1 ms expected for ITER [1]), shortening $\tau_r \sim T^{3/2}$ by orders of magnitude, although it remains much larger than τ_A. The sudden increase in resistivity before the current density has time to change creates a large electric field. This process accelerates electrons to relativistic energies (runaway electrons), increasing risks to the device if not controlled. Global-scale ideal MHD instabilities have growth times of tens or hundreds of τ_A, but they seldom cause disruptions in large modern tokamaks [5]. More frequently, slow variants of ideal instabilities arise, where the time-scale is set by diffusion of magnetic flux through conducting surfaces. Symmetric and asymmetric vertical displacement events (VDEs) are particularly harmful examples. The confined plasma can remain intact for a prolonged time while resting against the first wall, then becomes unstable to 3D MHD.

Besides non-ideal wall effects, non-ideal plasma effects lead to evolution that is slow relative to ideal instability. The visco-resistive model predicts linear growth on a hybrid time that is between τ_r and τ_A [6]; $\sqrt{\tau_A \tau_r}$ can be used for estimation. However, plasma drifts, electron responses, kinetic effects of both thermal and energetic ions [7-9], and plasma micro-turbulence, which are outside the scope of the visco-resistive MHD model, are important for these slower dynamics. The range of spatial scales is also more challenging, as internal boundary layers form along surfaces of resonance between the magnetic winding and the helical structure of the modes. With the MHD model, the width of these layers in the linear phase is analogous to a resistive skin depth, but more detailed models exhibit multiple scales. The ion skin depth is the largest of the possible scales, and it is 100 times smaller than the minor radius. Over time these localized layers broaden into helical magnetic islands, and growth slows nonlinearly [10] if confinement is not lost. Macroscopic evolution through such non-ideal plasma responses is important for several different aspects of disruptions. While plasma flow can saturate island development at acceptable levels, the interaction of magnetic islands with external conducting structures imposes drag [11]. Loss of mode rotation, "locking," affects the overall mode of operation, and frequently leads to disruption [5].

Overlap of magnetic islands, as either a primary cause or a secondary effect, initiates thermal quenches due to the concomitant magnetic field stochastization. Efforts to mitigate concentrated energy deposition during a thermal quench inject impurities to radiate energy broadly, and non-ideal plasma evolution plays a central role in impurity penetration [12].

The computational challenges associated with characterizing disruption and exploring mitigation are those of modeling macroscopic dynamics in magnetically confined plasma, plus the challenges of incorporating radiation modeling, neutral dynamics, external magnetostatics, and runaway electron kinetics. The multi-scale nature of these applications requires implicit methods to address the mathematical stiffness, as reviewed in [13], and the large sparse matrices for linearly implicit and nonlinearly implicit methods are ill conditioned. Hot magnetized plasma is also anisotropic. The anisotropy leads to distinct polarizations of propagating waves, including the Alfvénic class of waves that equilibrates forces over large scales. Transport properties, such as viscosity and thermal conductivity, along and across magnetic field-lines differ greatly. Numerical methods need to represent anisotropy accurately in conditions of changing magnetic topology, and high-order and spectral elements [14-16] or special treatments of fluxes [17] are used. When included, kinetic effects add information on particle distributions over velocity-space coordinates. Particle-based methods track drift orbits that cover global spatial scales [18]. Individual particle computations are independent, but the field information is not localized, and parallel load balancing is not trivial. Continuum methods discretize at least two velocity coordinates [19,20]. They avoid statistical sampling, and implicit computation is more straightforward, but they are memory- and communication-intensive. Incorporating external magnetostatics requires coupling to codes that are suited to modeling the detailed 3D geometry of conducting surfaces and magnetic coils. Radiative cooling from atomic physics has been integrated with MHD successfully [3], but independent flow and energy dynamics of different charge states and neutrals need to be addressed.

Avoiding and *predicting* disruptions require a class of models and computations that are distinct from characterization and mitigation. Avoidance and prediction entails modeling of equilibrium evolution, along with stability analysis, to plan the operation of discharges. In addition, real-time analysis for control systems and for triggering mitigation is envisioned. Linear stability analysis of axisymmetric equilibria yields the most essential stability information, because violent ideal instabilities in tokamaks do not saturate nonlinearly and tokamak plasma is largely symmetric over the toroidal angle during normal operation. The fastest stability analysis tool (DCON [21]) solves Euler-Lagrange equations as a system of coupled ODEs. This approach is expected to be sufficiently fast for use in real-time analysis. Other methods solve eigenvalue problems for ideal and non-ideal models using 2D discretization over the poloidal plane for each toroidal Fourier component. More comprehensive prediction requires modeling the nonlinear triggering processes that lead to disruption. An example is integrated multi-scale simulation of multiple interacting islands with neoclassical kinetic effects, plasma micro-turbulence, and momentum transport, which is beyond present-day capabilities for multi-scale modeling.

MHD linear stability computation is sensitive to the accuracy of the equilibrium data and to the details of its pressure and current profiles. When used for post-shot analysis of laboratory discharges, profiles are structured to fit internal and external magnetic measurements, spectroscopic analysis, and measureable shape information [22]. While solving the nonlinear elliptic force-balance equation is straightforward for 2D equilibria, incorporating sufficiently discriminating laboratory data is not. Whether sufficient data can be collected and processed for real-time analysis is an open technical question. Pre-shot planning differs from real-time analysis in that it needs equilibria from predictive whole-device computation. Accurate equilibrium information is also used as the initial condition for nonlinear characterization and mitigation studies, so equilibrium processing affects all disruption simulation areas.

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