Tokamak Disruption Simulation (TDS) Center: Toward Robust and Efficient Simulation using Scalable Formulations, Solvers, and UQ

Abstract / Motivation
Disruption modeling for characterization, prediction, and mitigation is essential for realizing tokamak fusion in TDS. Advanced plasma models (multifluid, kinetic, & hybrid) are being explored for modeling electron dynamics, fast reconnection, transport in 3D fields, and strong neutral jet - plasma interactions. To enable these advanced TDS studies, our partnership is applying and extending advanced ASCR-developed scalable algorithms and software for:

- Implicit/IMEX extended MHD and multifluid electromagnetic (EM) plasma formulations as continuum models and moment based accelerators for hybrid continuum/kinetic models.
- Iterative nonlinear/slinear, and physics-based block preconditioners, to enable optimal multigrid solvers for physics-compatible spatial discretizations.
- Uncertainty quantification for high-dim. spaces using reduced sampling, surrogate models, and multifidelity approach.

Highlight: Implicit / IMEX Plasma Fluid Formulations and Scalable Solvers
Extended MHD and multifluid plasma models are being evaluated/extended for simulation of moderately-dense to dense collisional systems. Significant progress has been made towards capabilities for tokamak magnetic-field evolution.

- Extended MHD [1,2] (Generalized Ohm’s law formulation). Progress is being made towards MFS relevant simulation capabilities. E.g., use EFIT interface for experimental equilibrium, study on magnetic field evolution during a sawtooth oscillation for a doubly-diverted D shaped tokamak [3].
- We have implemented EFIT interface for experimental device configuration evaluations. Currently PIXIE3D fits tokamak cross section into elliptical boundary and defines poloidal and toroidal magnetic field. Equilibria sustained in absence, of dissipation and forcing. Mesh and computed ITER poloidal flux shown.
- Pursuing MHS3 macro-scale dynamics.
- Resistive and vacuum wall capabilities in development for VDE modeling.
- Evaluating scalable MHD [1,4,5], extended MHD [2], and multifluid plasma [6,7] block preconditioners for critical TDS apps. E.g. for multifluid model these allow overstepping of EM waves, plasma & cyclotron frequency, and collisional time-scales, by $10^4$ [6,7]. For MHD weak scaling results up to 1M cores have been obtained [5].
- Drekar MHD & multifluid electromagnetic plasma models are progressing towards capabilities for discontinuous solutions relevant for massive gas injection for disruption mitigation. Drekar has demonstrated initial scalable implicit / IMEX solutions of multifluid plasma, and accurate solution of multifluid in asymptotic MHD limits [7].

Drekar Multifluid EM Plasma (collisions/ionization/recombination)

- Goal: Help guide / moderate tokamak disruption thermal quench, and runaway electron avalanche, with radiative cooling and low-energy electrons from high Z impurities.
- Preliminary proof-of-principle 1D study of a core of 0.1 eV, n = 10^{20} Ne, A=7 neutral gases expanding in a 100 eV, n = 10^{20} Deuterium plasma. Profiles at t = 1 microsecond.

Highlight: High Z gas transport, ionization, and recombination with multifluid model
- In a disruption, plasma temperature will drop from 10 keV to a few eV in a few ms.
- This energy can be mostly channelled through runaway electrons.
- Complete avoidance is impractical.
- Optimal scenario is to avoid runaway avalanche.

Drekar Multifluid EM Plasma (collisions/ionization/recombination)

Highlight: Uncertainty Quantification
Development of robust and efficient uncertainty quantification (UQ) using efficient sampling, surrogate / reduced order modeling (ROM), neural nets (NN), and multifidelity / multifidelity approaches, for sensitivities, forward UQ, and inverse UQ for data-informed model improvement.

- Exploring multi-level and multi-fidelity methods to reduce the burden on high-fidelity models. (1) Highest-fidelity simulations can be prohibitive for use in UQ and only (O(10) - O(100)) might be possible. (2) Low fidelity “design” models often predictive of basic trends, (3) Plasma physics has a natural model hierarchy (resistive MHD, extended MHD, multifluid EM plasma, kinetic e.g. PIC). (4) Can we leverage low-fidelity models in mathematically / statistically rigorous manner?

E.g. MLMC Methods for Efficient UQ

Demo of multilevel Monte-Carlo (MLMC) UQ for a 2D Resistive MHD Tearing Mode on coarse, medium, and fine meshes. Estimates of accuracy and cost of simulations are obtained with exploratory studies, then MLMC algorithm defines efficient sequence of computations to either minimize cost for a given accuracy, or maximize accuracy at a fixed cost, for statistically estimated QoI. (with FASTMATH UQ Scadac team)

Highlight: High Z gas transport, ionization, and recombination with multifluid model

Exploring the Utilization of Machine Learning (Deep NN) as Surrogate Models / ROM
- Deep Neural Networks (DNN) seek to detect and exploit low dimensional feature spaces, (2) Nonlinear ROM for evolution and QoI
- Current research: how to enforce physics constraints?

Initial Studies using NN as Surrogate for OX-Merger Model
Convergence of the loss function for a NN with 2 hidden layers (left) and with 4 hidden layers (right) for the OX-margi semi-analytic electron avalanche avoidance model. These NN surrogates are to be used for estimating statistical quantities for UQ of the OX-Merger model.

Exploring Multi-Fidelity Deep NN in TDS Model
- Deep Neural Networks (DNN) seek to detect and exploit low dimensional feature spaces, (2) Nonlinear ROM for evolution and QoI
- Current research: how to enforce physics constraints?

Simple Demo: using NN as ROM for 2D Resistive Tearing Mode

This very preliminary LSTM-ROM NN method uses a 2 stage learning process, (1) 0D simple temporal snapshots are used compute orthogonal POD basis, the coefficients at each time step are computed using a projection of the snapshots onto these bases, (2) the LSTM NN is then trained on these snapshots at each time step. $3^2$ POD modes are used. Run time PDES: 250 sec on 72 cores; LSTM-ROM PDES: 5 sec, NN training: 50 sec., NN ROM computation: 1 sec. (with RAPIDS Scadac inst.)

Major Next Steps
- Carry out significant retrained and extended MHD stability computations using EFIT experimental equilibria, study instabilities, breakdown of magnetic structure.
- Carry out initial INCITE-scale fast-reconnection and massive gas injection (MGJ) type prototype problems
- Demonstrate high-order reduced MHD in MFEM, and HDG MHD, on MCF relevant resistive MHD problems
- Perform comprehensive UQ studies (forward, inverse) on 0D OX merger RE, begin studies on 1D, 2D neutral MGI models with transport effects for neutrals/ions/electrons.
- Explore efficient reduced sampling and multifidelity UQ approaches with Goll surrogates, and ROM, and NN-ROM for dynamics of parameterized MHD / plasma codes

Incomplete List of References
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2019 DOE Scidac Principal Investigators’ (Pi) Meeting, Rockville, MD; July 16-18, 2019