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

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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/linear solvers, 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.

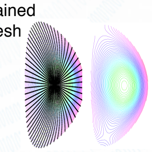
Highlight: Implicit / IMEX Plasma Fluid Formulations and Scalable Solvers

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 MCF relevant simulation capabilities. E.g. PIXIE3D has been used for studying magnetic field evolution during a sawtooth oscillation for a doubly-diverted D shaped tokamak [3].

$$\mathbf{E} = -\underbrace{\mathbf{u}\times\mathbf{B}}_{\text{Ideal}} + \underbrace{\eta\mathbf{J}}_{\text{Resistive}} + \underbrace{\frac{d_i}{n}(\mathbf{J}\times\mathbf{B} - \nabla p_e - \nabla\cdot\overline{\overline{\Pi}}_e)}_{\text{Hall}} + \underbrace{\frac{d_e^2}{n}\frac{d\mathbf{J}}{dt}}_{\text{e inertia}}$$

- We have implemented EFIT interface for experimental device configuration equilibriums. Currently PIXIE3D fits tokamak cross section into elliptical boundary and defines poloidal and toroidal magnetic field. Equilibriums sustained in absence, of dissipation and forcing. Mesh and computed ITER poloidal flux shown.
- Pursuing MHD 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 methods 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 for accurate evolution of multifluid plasmas, and accurate solution of multifluid in asymptotic MHD limits [7].

Drekar Multifluid EM Plasma (collisions/ionization/recombination)

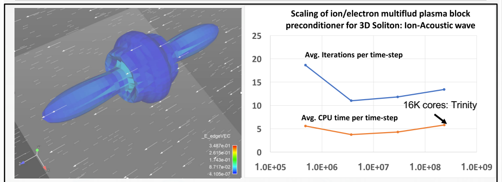
$$\partial_t\rho_s + \nabla\cdot(\rho_s\mathbf{u}_s) = -\rho_s n_e(I_s+R_s) + m_s n_e(n_{s-1}I_{s-1} + n_{s+1}R_{s+1})$$

$$\partial_t(\rho_s\mathbf{u}_s) + \nabla\cdot(\rho_s\mathbf{u}_s\otimes\mathbf{u}_s + p_s\underline{\mathbf{I}} + \underline{\boldsymbol{\Pi}}_s) = q_s n_s(\mathbf{E}+\mathbf{u}_s\times\mathbf{B}) + \sum_{t\neq s}\alpha_{s;t}\rho_s\rho_t(\mathbf{u}_t-\mathbf{u}_s)$$
$$-\rho_s\mathbf{u}_s n_e(I_s+R_s) + \frac{m_s}{m_{s-1}}n_e\rho_{s-1}\mathbf{u}_{s-1}I_{s-1} + (n_e\rho_{s+1}\mathbf{u}_{s+1} + n_{s+1}\rho_e\mathbf{u}_e)R_{s+1}$$

$$\partial_t\mathcal{E}_s + \nabla\cdot[(\mathcal{E}_s+p_s)\mathbf{u}_s + \mathbf{u}_s\cdot\underline{\boldsymbol{\Pi}}_s + \mathbf{h}_s] = q_s n_s\mathbf{u}_s\cdot\mathbf{E} + \sum_{t\neq s}\frac{\alpha_{s;t}\rho_s\rho_t}{m_s+m_t}\left[A_{s;t}k_B(T_t-T_s) + m_t(\mathbf{u}_t-\mathbf{u}_s)^2\right]$$
$$-\mathcal{E}_s n_e(I_s+R_s) + \frac{m_s}{m_{s-1}}n_e\mathcal{E}_{s-1}I_{s-1} + (n_e\mathcal{E}_{s+1} + n_{s+1}\mathcal{E}_e)R_{s+1}$$

$$q = \sum_s q_s n_s \qquad \mathbf{J} = \sum_s q_s n_s\mathbf{u}_s$$

$$\frac{1}{c^2}\partial_t\mathbf{E} - \nabla\times\mathbf{B} + \mu_0\mathbf{J} = \mathbf{0} \qquad \nabla\cdot\mathbf{E} = \frac{q}{\epsilon_0}$$
$$\partial_t\mathbf{B} + \nabla\times\mathbf{E} = \mathbf{0} \qquad \nabla\cdot\mathbf{B} = 0$$



Weak scaling physics-based solvers: Fully-ionized higher-density / pressure core expanding into magnetized plasma (collisionless).

Exploring High-order Discretizations and Scalable Solvers

Robust and high-order spatial discretizations with scalable iterative solution methods are important to BOUT++, PIXIE3D, and Drekar. These methods are critical for high-fidelity sims., on DOE leadership class next-gen architectures for reduced communication and increased local computational intensity.

- Exploring high-order FE reduced MHD solver based on MFEM discretizations, AMR, and extensions of our scalable physics-based preconditioners [1,2,5] (with FastMath SciDAC inst.) .
- Developed first high-order HDG FE resistive MHD formulation [11] and initial scalable multilevel solvers [12,13,14]. Demo on magnetic reconn., hydromagnetic Kelvin Helmholtz to P = 9.

Exploring in Memory Code Coupled Multiscale Transport/ Turbulence Modeling and Parallel IO for TDS apps.

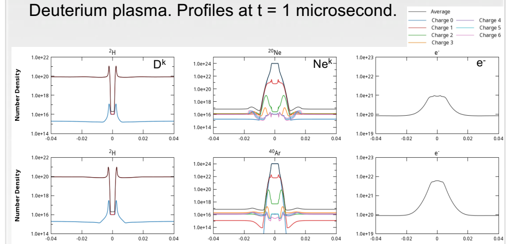
- Developed efficient in memory data transfer with Henson (RAPIDS SciDAC inst.) for multiscale coupling of TDS drift-MHD and transport codes for modeling ELM instabilities. Timing results indicate 100x speed up in data transfer time vs old file transfer method.
- VPIC kinetic particle-in-cell code now has efficient parallel IO implementation based on HDF5 (RAPIDS SciDAC inst).

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 channeled through runaway electrons.
- Complete avoidance is impractical
- Optimal scenario is to avoid runaway avalanche

- 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^{24} Ne^0, Ar^0 neutral gases expanding in a 100eV, n =10^{20} Deuterium plasma. Profiles at t = 1 microsecond.



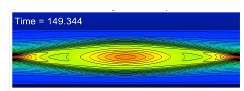
Highlight: Uncertainty Quantification

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

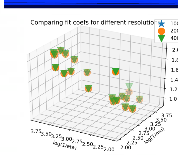
- Exploring multi-level and multi-fidelity methods to reduce the burden on high-fidelity models. (1) Highest-fidelity simulations can be prohibitive for use in UQ and only ~O(10) - O(100) might be possible, (2) Low fidelity "design" models often predictive of basic trends, (3) Plasma physics has a natural 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?

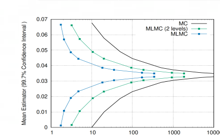
E.g. MLMC Methods for Efficient UQ

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 estimated statistical QoI. (with FASTMATH UQ SciDAC team)



Mesh	Normalized cost
400 x 400	1.0
200 x 200	0.1844
100 x 100	0.0307



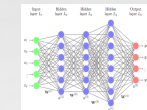


Estimator	N_{400}	N_{200}	N_{100}	Estimator StDev
MC	1000	-	-	1.128E-3
MLMC (2 levels)	4	5409	-	4.857E-4
MLMC	8	168	31381	2.085E-4

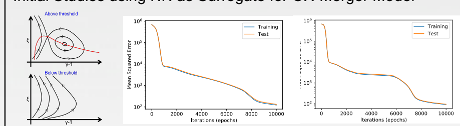
TABLE: Samples allocation per model and estimators' Standard Deviation for a total cost equivalent to 1000 high-fidelity realizations

Exploring the Utilization of Machine Learning (Deep NN) as Surrogate Models / ROM

- Deep Neural Networks (DNN) seek to detect and exploit low-dim structure
- Nonlinear ROM for evolution and QoI
- Current research: how to enforce physics constraints?



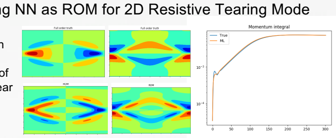
Initial Studies using NN as Surrogate for OX-Merger Model



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

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

Tearing mode simulation (velocities on right) and plot of QoI the L2 norm of momentum showing linear growth phase (left).



This very preliminary LSTM-ROM NN method uses a 2 stage learning process, (1) full-order temporal snapshots are to compute orthogonal POD bases, the coefficients at each time step are computed using a projection of the snapshots onto these bases, (2) the LSTM NN is then trained to reproduce the time series for the coefficients as well as the auxiliary QoIs at each time step. 3 POD modes are used. Run time PDEs: 250 sec on 72 cores; LSTM-ROM POD: 5 sec., NN training: 50 sec., NN ROM computation: 1 sec. (with RAPIDS SciDAC inst.)

Major Next Steps

- Carry out significant resistive and extended MHD stability computations using EFIT experimental equilibrium, study instabilities, breakdown of magnetic structure.
- Carry out initial INCITE-scale fast-reconnection and massive gas injection (MGI) 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 QoI surrogates, and ROM, and NN-ROM for dynamics of parameterized MHD / plasma codes

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