Tokamak Disruption Simulation (TDS) Center: Toward Robust 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:**

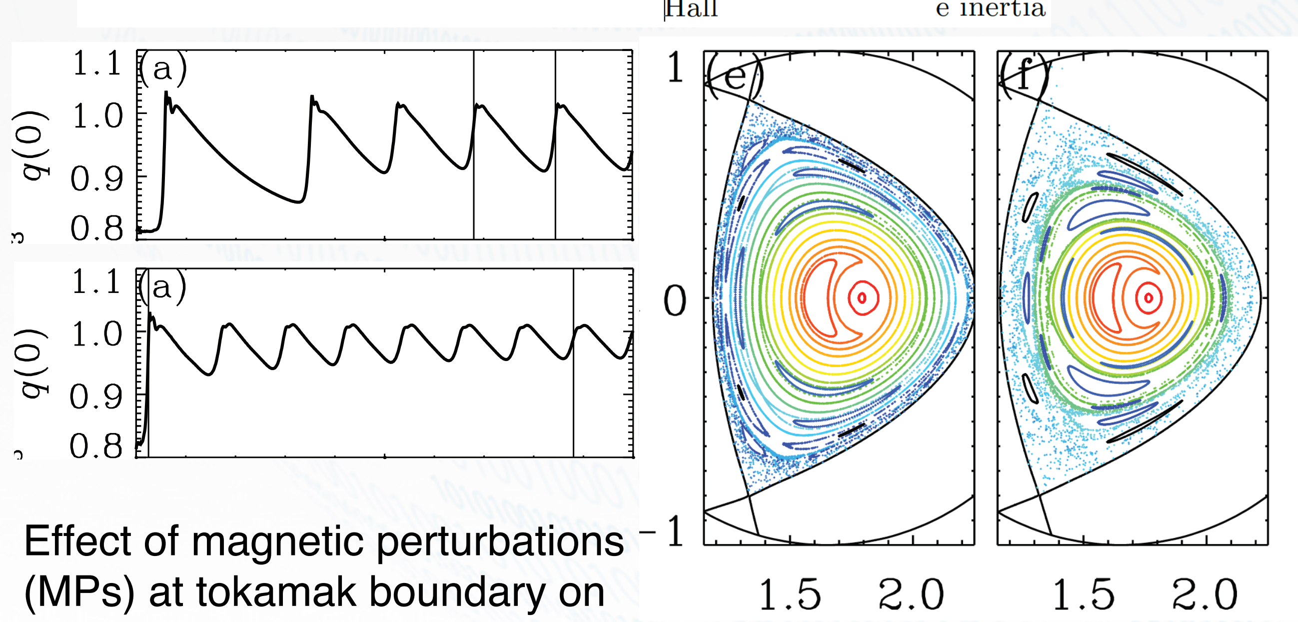
- Implicit/IMEX extended MHD and multifluid electromagnetic (EM) plasma formulations as continuum models and moment based accelerators for hybrid continuum/kinetic models.
- Iterative nonlinear/linear solvers, and physics-based block preconditioners, to enable optimal multigrid solvers for physics-compatible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

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].

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



Effect of magnetic perturbations (MPs) at tokamak boundary on sawtooth oscillation: Top left shows oscillation of q-profile at magnetic axis without MPs, bottom left with MPs. Right shows two Poincare snapshots in nonlinear phase with MPs (early (e), late(f)).

- 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 full multifluid plasmas, and accurate solution of multifluid in asymptotic MHD limits [7].

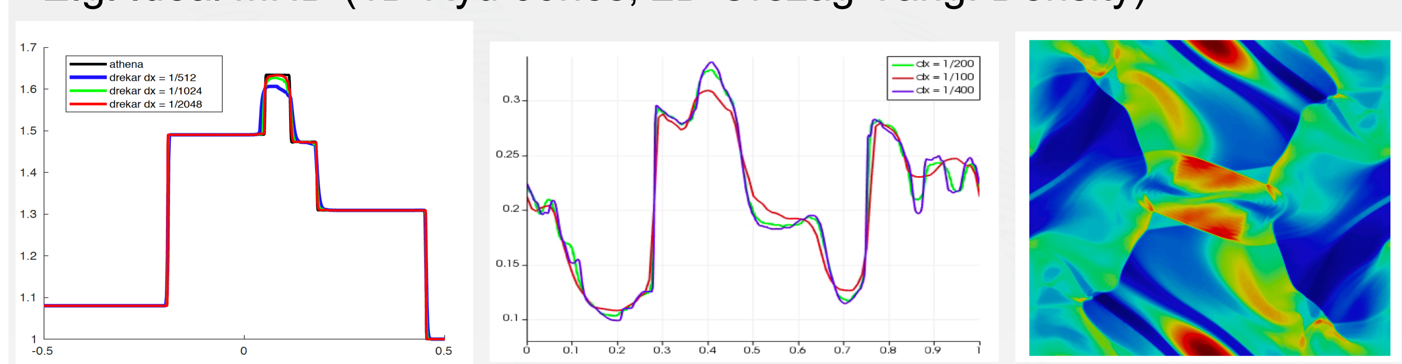
$$\frac{\partial \rho_a}{\partial t} + \nabla\cdot(\rho_a \mathbf{u}_a) = \mathcal{R}_{\rho_a}$$

$$\frac{\partial(\rho_a\mathbf{u}_a)}{\partial t} + \nabla\cdot(\rho_a\mathbf{u}_a\otimes\mathbf{u}_a + p_a I + \Pi_a) - q_a n_a(\mathbf{E} + \mathbf{u}_a\times\mathbf{B}) = \mathcal{R}_{\rho_a u_a}$$

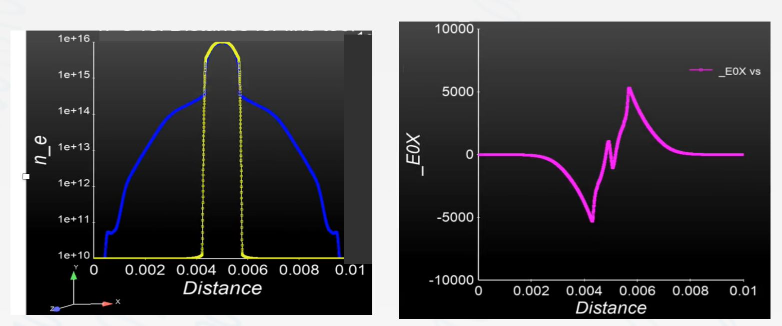
$$\frac{\partial \mathscr{E}_a}{\partial t} + \nabla\cdot((\mathscr{E}_a + p_a)\mathbf{u}_a + \Pi_a\cdot\mathbf{u}_a + \mathbf{h}_a) - q_a n_a \mathbf{u}_a\cdot\mathbf{E} + Q_a^{src} = \mathcal{R}_{\mathscr{E}_a}$$

$$\epsilon_0\frac{\partial\mathbf{E}}{\partial t} - \nabla\times\frac{1}{\mu_0}\mathbf{B} + \mathbf{J} = \mathbf{0};\quad \frac{\partial\mathbf{B}}{\partial t} + \nabla\times\mathbf{E} = \mathbf{0};\quad \mathbf{J} = \sum_k q_k n_k \mathbf{u}_k$$

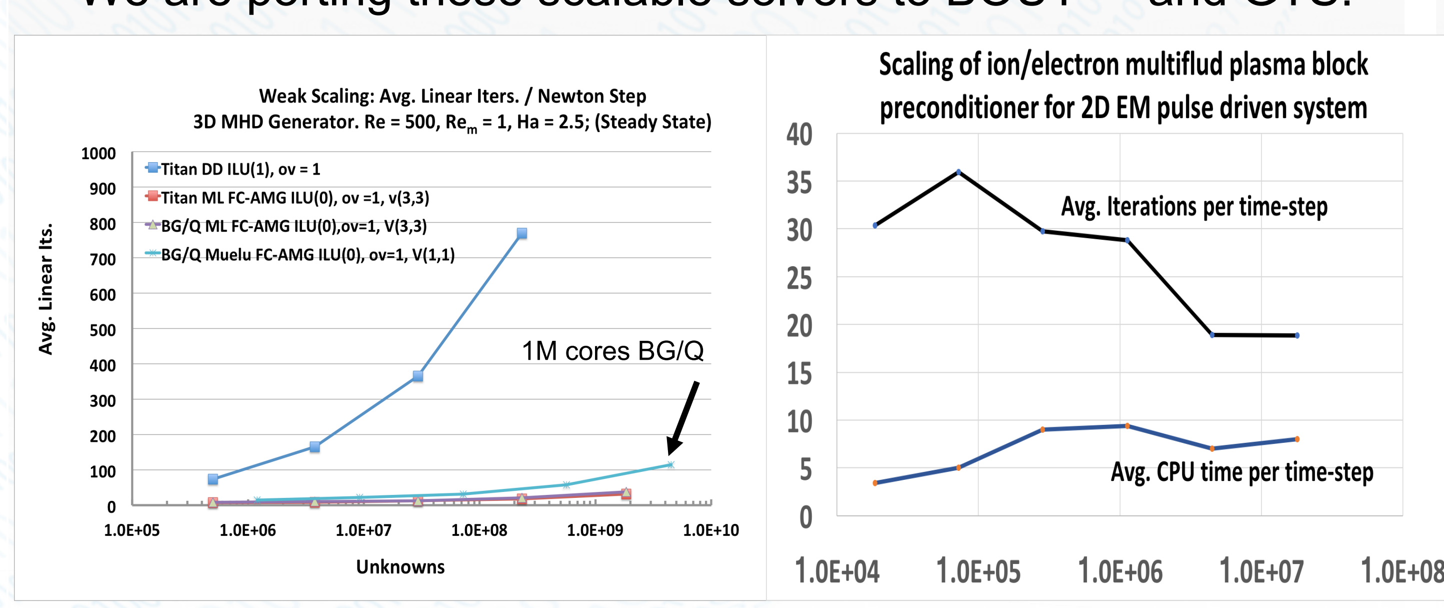
E.g. Ideal MHD (1D Ryu-Jones, 2D Orszag-Tang: Density)



E.g. Multifluid EM plasma. Expansion of initially neutral ion/electron plasma core into a low density environment. (Preliminary)



- Scalable MHD [1,4,5], extended MHD [2], and multifluid plasma [6,7] block preconditioners, have been developed. For the multifluid model these allow overstepping of EM waves, plasma & cyclotron frequency, and collisional time-scales, by > 10^4 for appropriate plasma problems [6,7].
- We are porting these scalable solvers to BOUT++ and GTS.



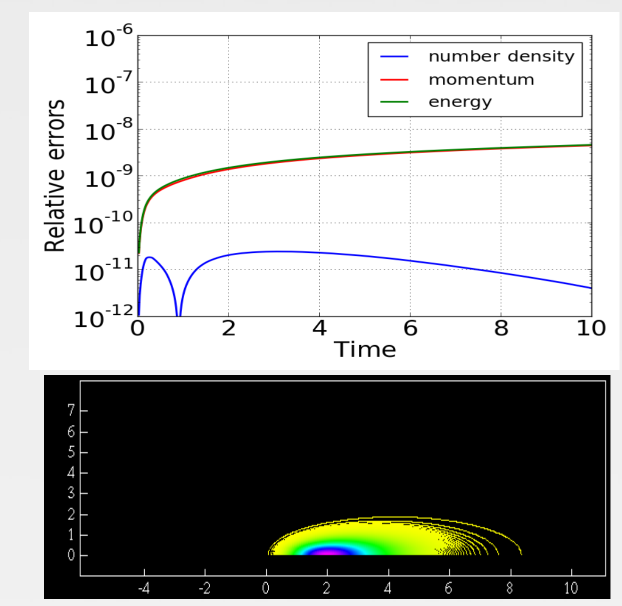
Weak scaling solvers: steady MHD (left), transient multifluid (right)

Highlight: Towards Fluid-kinetic Coupling with Runaway Electrons

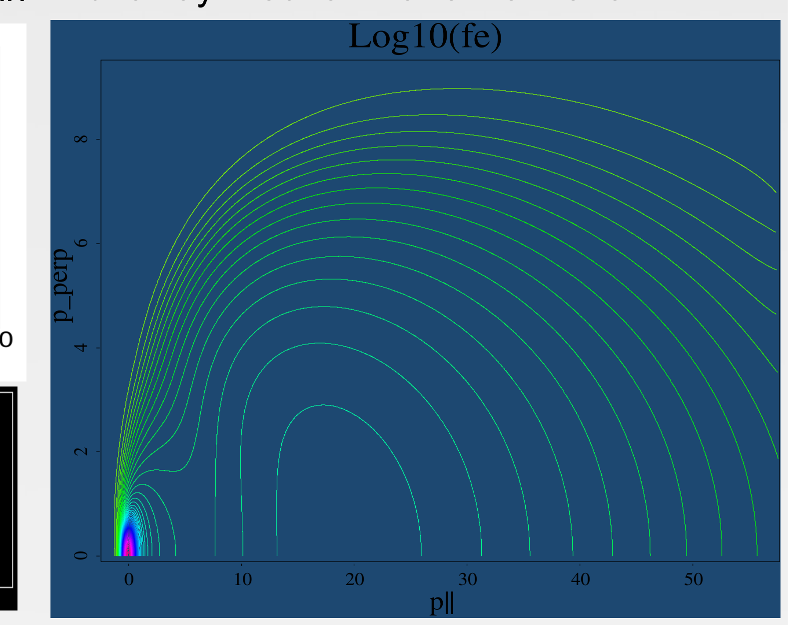
- Goal: to couple our fluid solvers with a novel relativistic Runaway Electron Fokker-Planck solver, featuring:

1. Exact conservation properties and preservation of positivity.
2. Optimal MG-based nonlinear solvers.
3. Adaptive meshing (under implementation).

Preservation of boosted Maxwellian



Runaway Electron Vortex formation

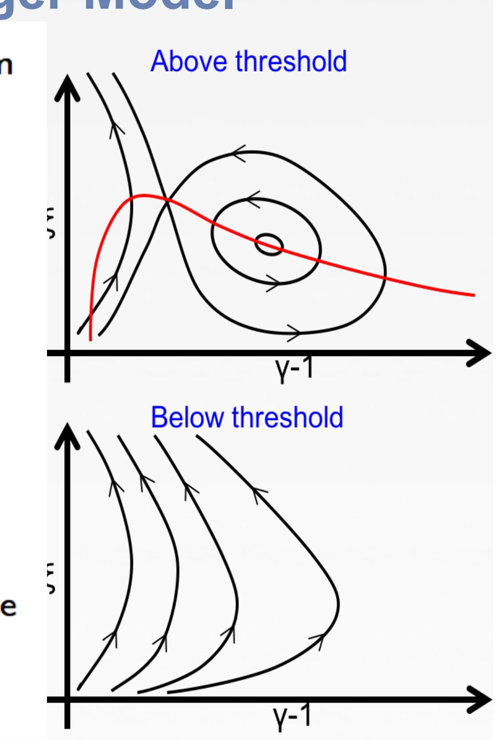


Highlight: Uncertainty Quantification

- Development of robust and efficient UQ and sensitivity analysis using efficient sampling, surrogate / reduced order modeling, and multifidelity approaches for sensitivities, forward UQ, and inverse UQ for data-informed model improvement.

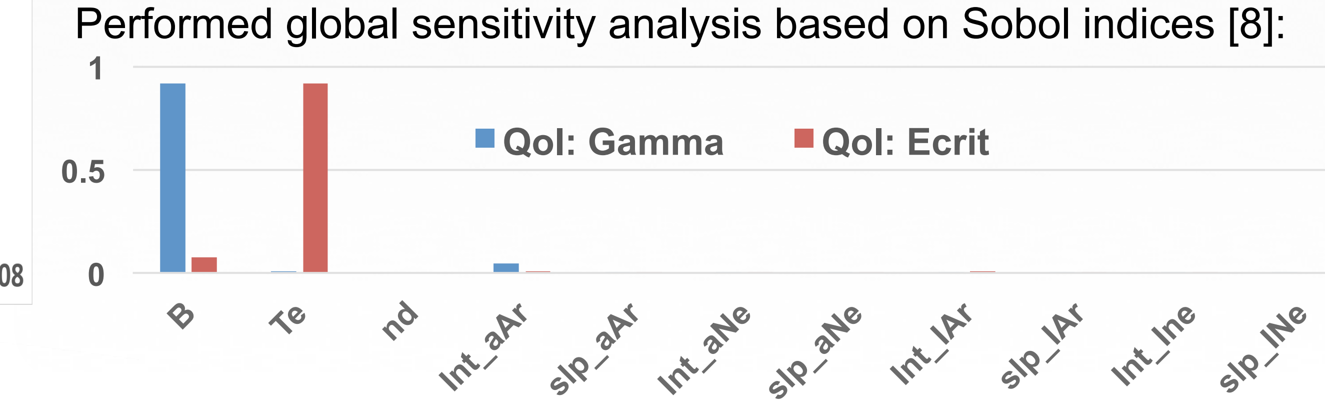
E.g. Initial Studies using OX-Merger Model

- 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
- Semi-analytic theory of the runaway threshold recently developed (McDevitt et al. 2018)
- Provides versatile tool for determining conditions under which a large runaway population can be avoided
- Depends on the strength of the magnetic field, the electron temperature and the charge state distribution of the impurity populations.



Sensitivity Analysis

Performed global sensitivity analysis based on Sobol indices [8]:

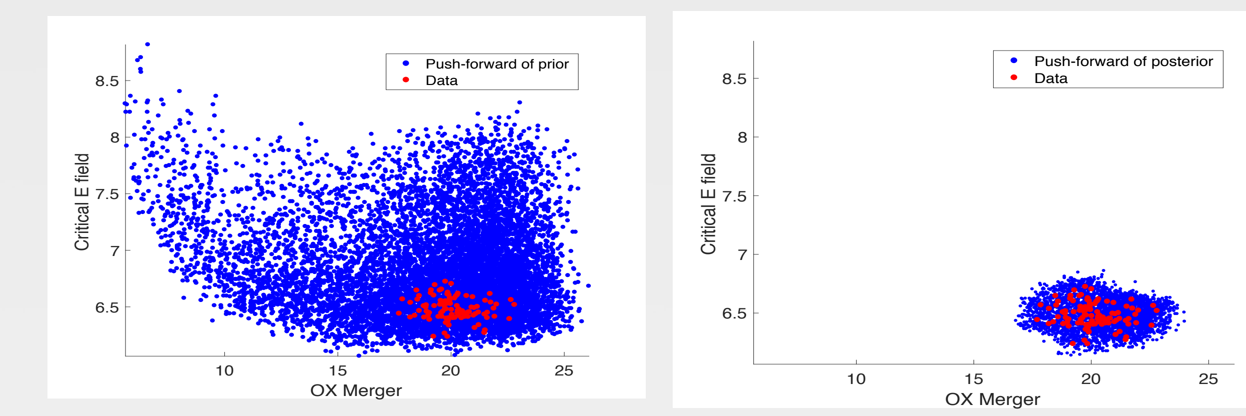


Stochastic Inversion

We combine measure-theoretic and Bayesian concepts to construct a consistent posterior [9] :

$$\pi_{\Lambda}^{\text{post}}(\lambda) = \pi_{\Lambda}^{\text{prior}}(\lambda)\frac{\pi_{\mathcal{D}}^{\text{obs}}(Q(\lambda))}{\pi_{\mathcal{D}}^{Q(\text{prior})}(Q(\lambda))},\quad \lambda\in\Lambda$$

Application to 0D OX-merger model: demonstrates that new method using inverse UQ better reproduces observed data.



Nonlinear ROM using empirical interpolation method

CPU time to solve incompressible Navier-Stokes equations [10]

# parameters	4	16	36	49
Solve full system	55.1s	53.6s	66.8s	57.1s
Solve reduced system	0.11s	1.76s	11.0s	24.8s

Major Next Steps

- Develop R&D version of PIXIE3D/Drekar with OMFIT capabilities, EFIT experimental equilibrium, study instabilities, breakdown of magnetic structure.
- Pursue initial INCITE-scale fast-reconnection and massive gas injection (MGI) type prototype problems
- Demonstrate high-order IMEX hybridized discontinuous Galerkin [11,12] 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 for dynamics of parameterized MHD / plasma codes

Incomplete List of References

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