

Verification and Validation of Extended-Magnetohydrodynamic Modeling of Disruption Mitigation

by

Brendan C. Lyons¹

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***See the author list of E. Joffrin et al. 2019 Nucl. Fusion 59 112021**

Virtually presented at the
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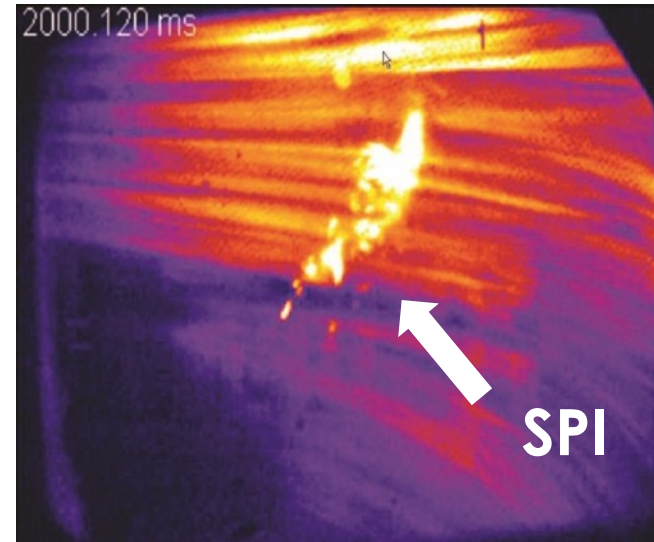
Many Grants Provide Opportunities of Synergistic Research

- **US DOE grants used for code validation & close collaboration with experiment**
 - GA Theory (DE-FG02-95ER54309) and DIII-D (DE-FC02-04ER54698)
 - CTTS SciDAC for MHD modeling (DE-SC0018109)
 - JET/KSTAR Disruption Mitigation Solution (DE-SC0020299)
- **EUROfusion Enabling Research project for JOREK code development and validation**
- **National Energy Research Scientific Computing Center for high-performance computing**



Studying of Disruption Dynamics and Mitigation Requires Multiphysics Models

- **Simulations validated against experiments are required to project mitigation techniques to future devices**
- **Integrated model is required to capture all relevant physics**
 - Magnetohydrodynamics (MHD) for macroscopic evolution of disruption dynamics
 - Atomic physics for impurity ionization/radiation
 - Drift-kinetics for runaway-electron (RE) evolution
- **Disparate spatial and temporal scales make numerical modeling particularly challenging**
- **M3D-C1¹, NIMROD^{2,3}, and JOEAK^{4,5} are rising to this challenge**
 - Different physics and numerical model provide robust verification opportunities
 - Multiple code permit parallel research efforts



DIII-D shattered pellet injection (SPI)
D. Shiraki, IAEA presentation 2016

¹S. C. Jardin, et al., *Comput. Sci. Discovery* 5, 014007 (2012)

²C. R. Sovinec et al., *J. Comput. Phys.* 195, 355 (2004)

³C. Sovinec & J. King, *J. Comput. Phys.* 229, 5803 (2008)

⁴G.T.A. Huysmans & O. Czarny, *Nucl. Fusion* 47, 659 (2007)

⁵O. Czarny & G. Huysmans, *J. Comput. Phys.* 227, 7423 (2008)

Outline and Major Results

- **Overview of code models**
- **Verification studies**
 - M3D-C1 & NIMROD show quantitative agreement in 2D, nonlinear benchmark, JOEREK differences likely due to its impurity model
 - M3D-C1 & NIMROD 3D nonlinear benchmarks
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M3D-C1 and NIMROD Extended-MHD Solvers are Coupled to Impurity Ionization/Radiation Models

- **Both codes solve full, nonlinear, 3D extended MHD equations**
 - M3D-C1 uses a complete C^1 finite-element representation
 - NIMROD uses finite elements in poloidal plane and Fourier modes toroidally
- **Both have been coupled to the KPRAD¹ impurity model**
 - Low-density, coronal non-equilibrium model based on ADPAK rate coefficients
 - Impurity & electron densities evolve according to ionization and recombination

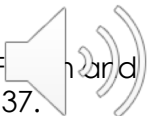
$$\frac{\partial n_z}{\partial t} + \nabla \cdot (n_z \mathbf{v}) = \nabla \cdot (D \nabla n_z) + \mathcal{I}_{z-1} n_{z-1} - (\mathcal{I}_z + \mathcal{R}_z) n_z + \mathcal{R}_{z+1} n_{z+1} + \mathcal{S}_z$$

- Thermal energy lost from plasma due to **ionization and radiation**
- NIMROD uses single-temperature, M3D-C1 uses single or two-temperature

$$n_e \left[\frac{\partial T_e}{\partial t} + \mathbf{v} \cdot \nabla T_e + \Gamma T_e \nabla \cdot \mathbf{v} \right] = (\Gamma - 1) (\eta J^2 - \nabla \cdot \mathbf{q}_e + Q_{ei} - \mathcal{P}_{rad}) - T_e \left(\frac{\partial n_e}{\partial t} + \mathbf{v} \cdot \nabla n_e \right)$$

$$n_{ti} \left[\frac{\partial T_i}{\partial t} + \mathbf{v} \cdot \nabla T_i + \Gamma T_i \nabla \cdot \mathbf{v} \right] = (\Gamma - 1) (-\nabla \cdot \mathbf{q}_i - Q_{ei} - \mathbf{\Pi} : \mathbf{v}) - T_i \left(\frac{\partial n_{ti}}{\partial t} + \mathbf{v} \cdot \nabla n_{ti} \right)$$

¹D.G. Whyte, et al., Proc. of the 24th Euro. Conf. on Controlled Fusion and Plasma Physics, Berchtesgaden, Germany, 1997, Vol. 21A, p. 1137.



JOREK Extended-MHD Solver Coupled to Coronal-Equilibrium Impurity Model

- **JOREK solves 3D nonlinear extended MHD equations**
[Huysmans and Czarny, NF 2007; Overview article: Hoelzl et al., in preparation; <https://www.jorek.eu/>]
 - 2D C^1 finite elements poloidally & Fourier modes toroidally
 - Fully implicit [Czarny and Huysmans, JCP 2008]
 - Free-boundary simulations with JOREK-STARWALL [Hoelzl et al., JPCS 2012]
 - Typically run in reduced MHD (including all simulations here)
- **Various extensions permit disruption mitigation modeling**
 - Neutrals [Fil et al., PoP 2015]
 - Shattered-pellet injection [Hu et al., NF 2018]
 - Impurities under coronal equilibrium [Hu et al., in preparation]
 - Impurities beyond coronal equilibrium is under development [Wieschollek et al.]
 - Runaway Electrons
 - Fluid model [Bandaru et al., Phys. Rev. E 2019]
 - Test particles [Sommariva et al., NF 2017 & 2018]



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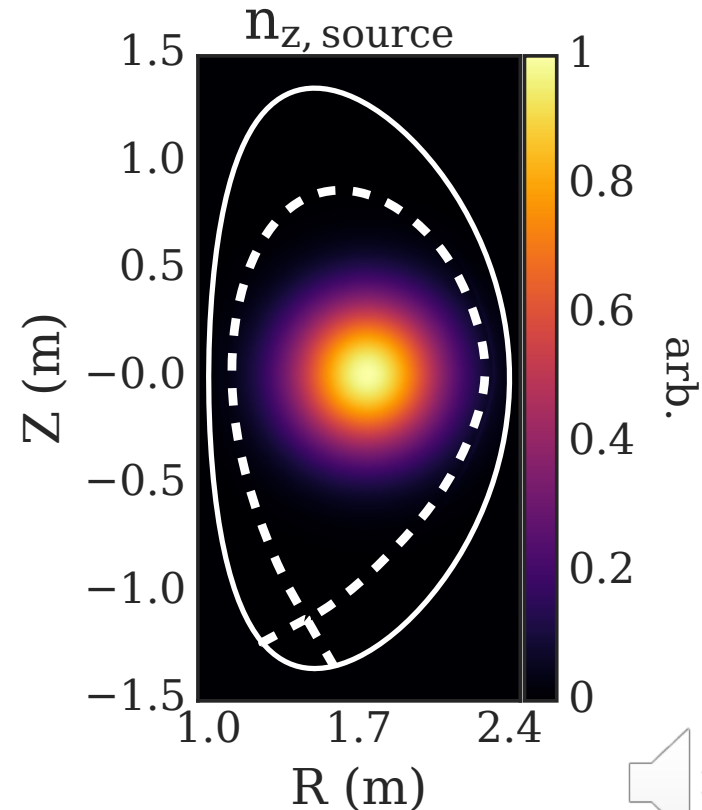
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- On-axis impurities induce inside-out thermal quench & hollowing of current
- After thermal quench, plasma forms expanding shell with core turbulence

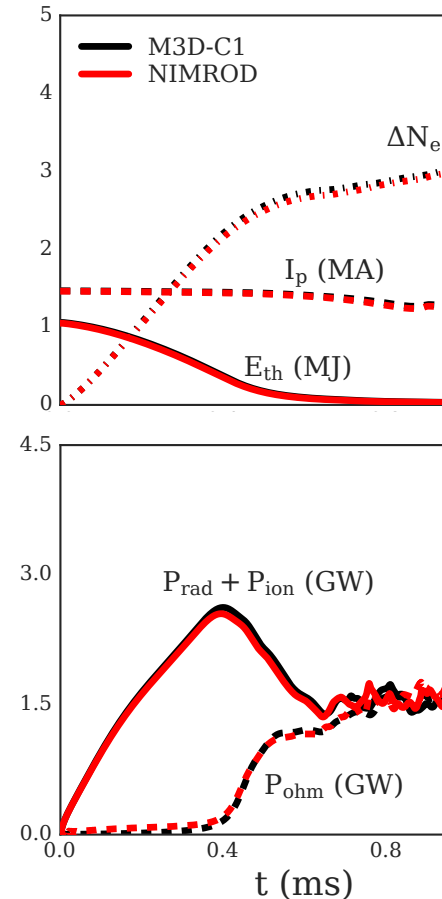
[†]B.C. Lyons et al., PPCF **61**, 6 (2019).
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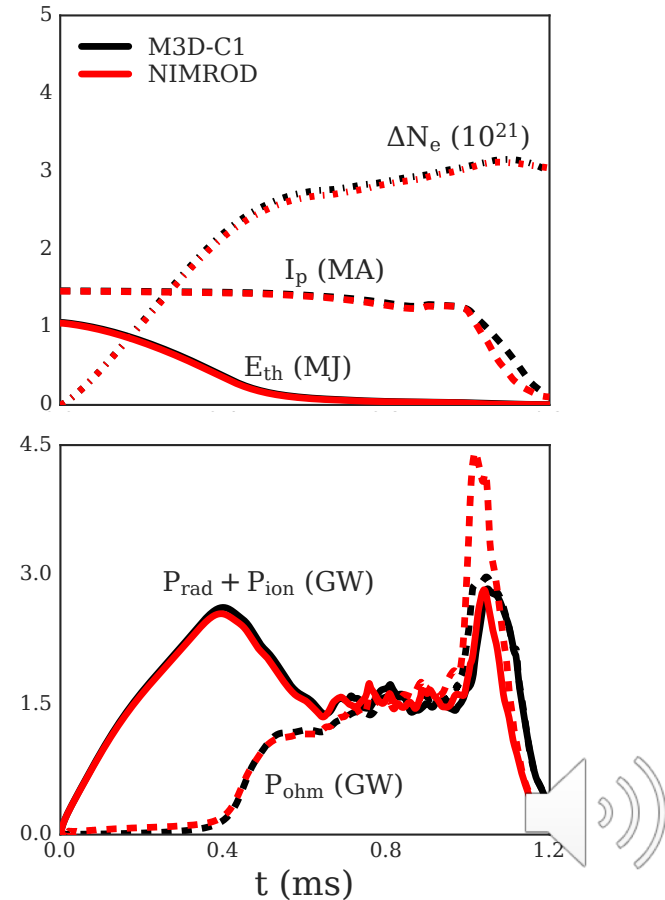
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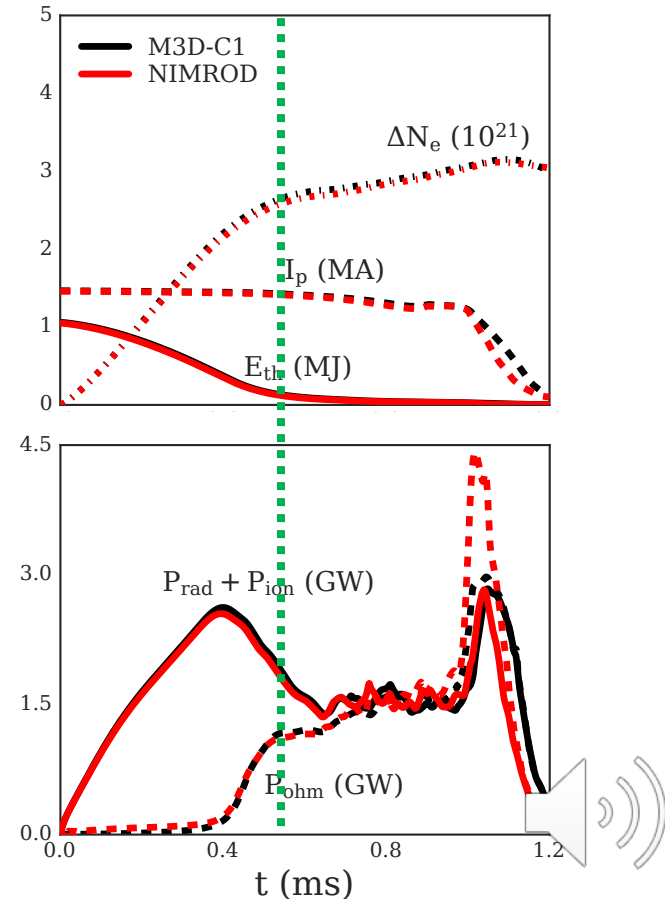
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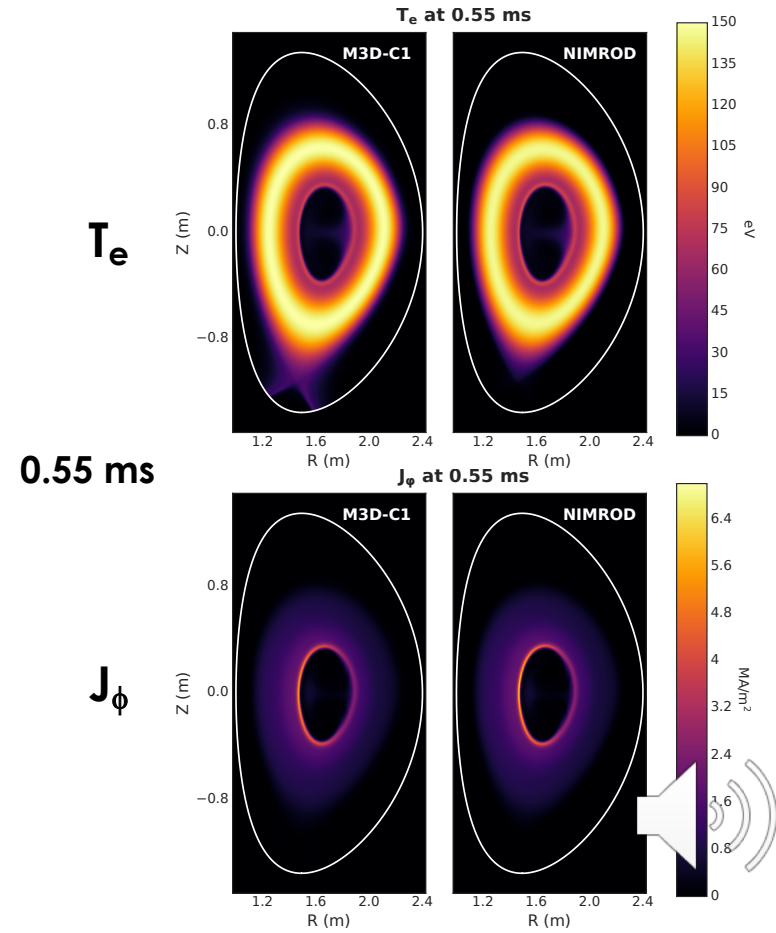
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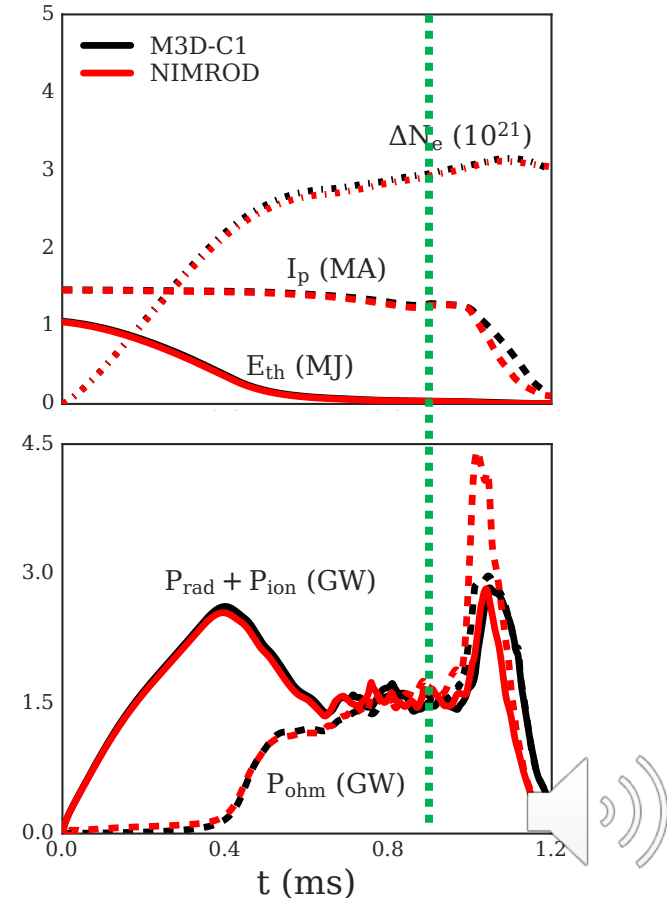
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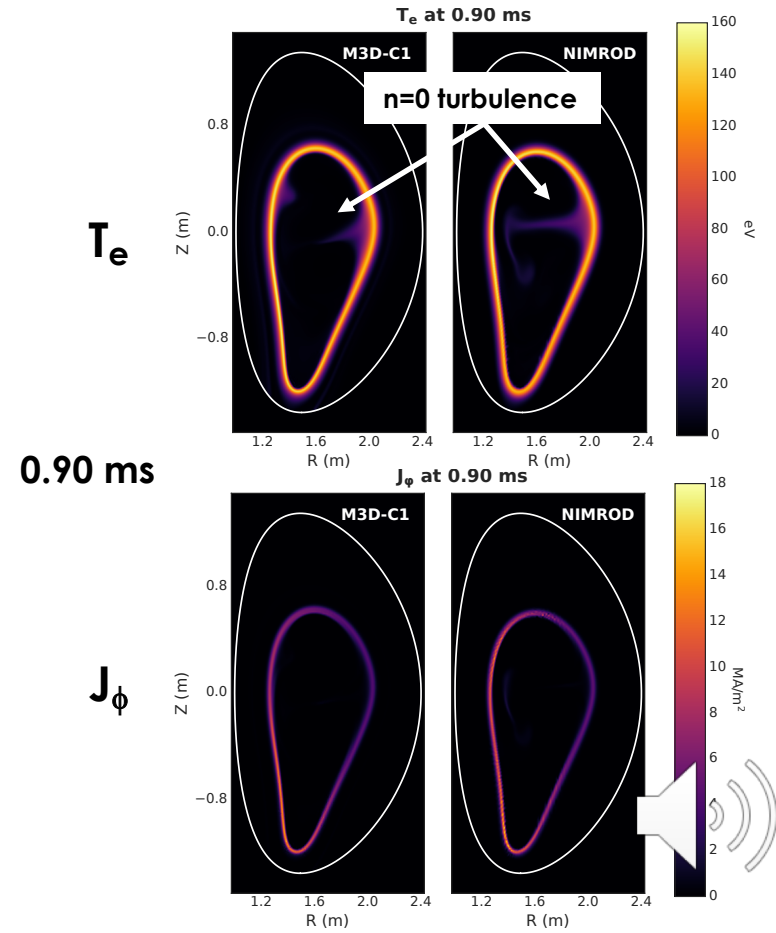
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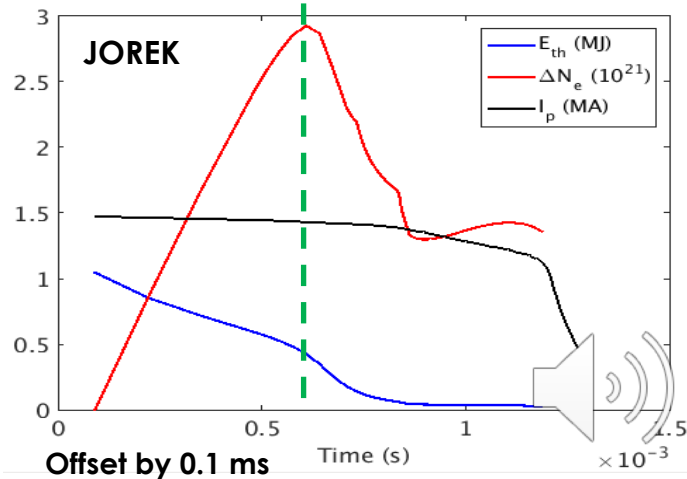
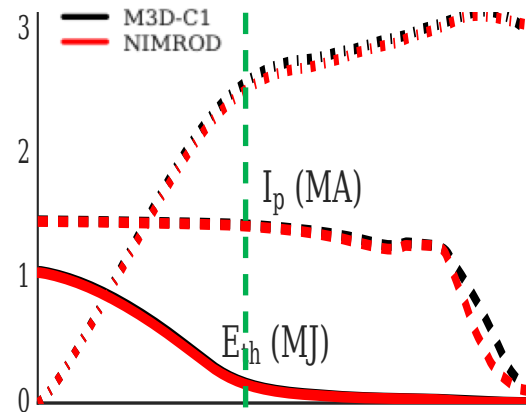
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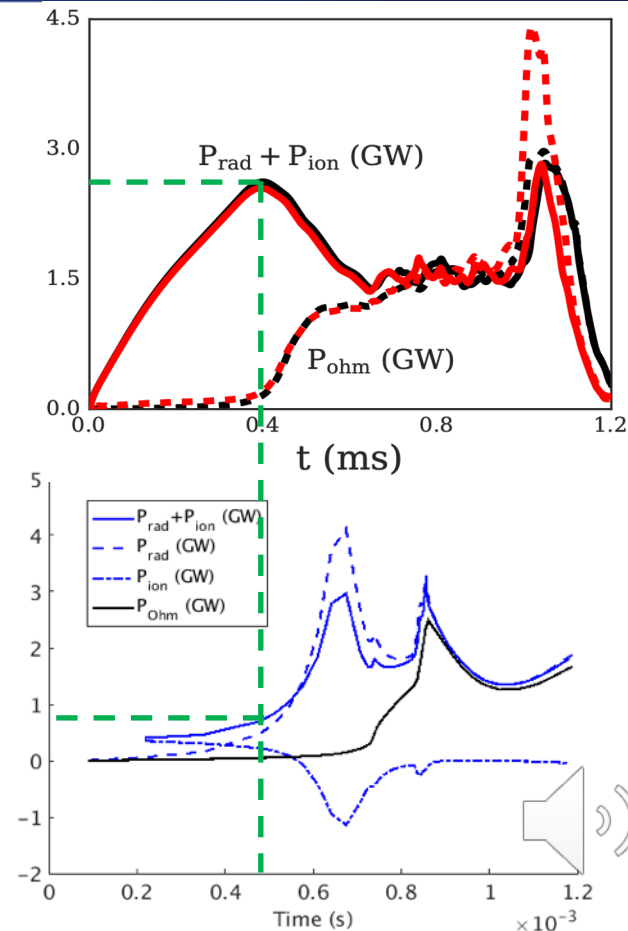
JOREK Modeling Shows Quantitative Differences Likely Due to Coronal-Equilibrium Impurity Model (Nardon)

- JOREK reduced-MHD simulation shows similar thermal quench timescale, though a bit slower
- Similar initial rate of density increase, but decreases in JOREK after thermal collapse
- Loss power rises more slowly in JOREK initially
- Likely due to crucial difference in impurity models
 - JOREK assume impurity charge states remain in coronal equilibrium
 - M3D-C1 & NIMROD use a coronal model, but allow each charge state to evolve in time
 - Motivates ongoing upgrade of JOREK impurity, and future work to move to collisional-radiative model in M3D-C1

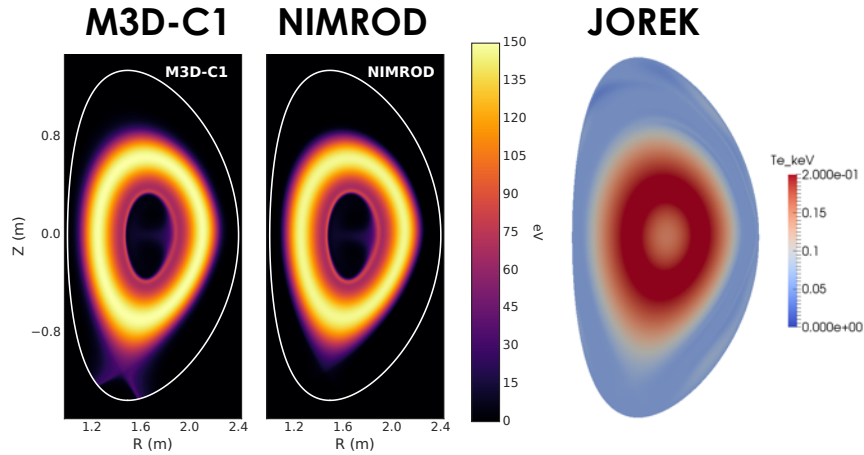


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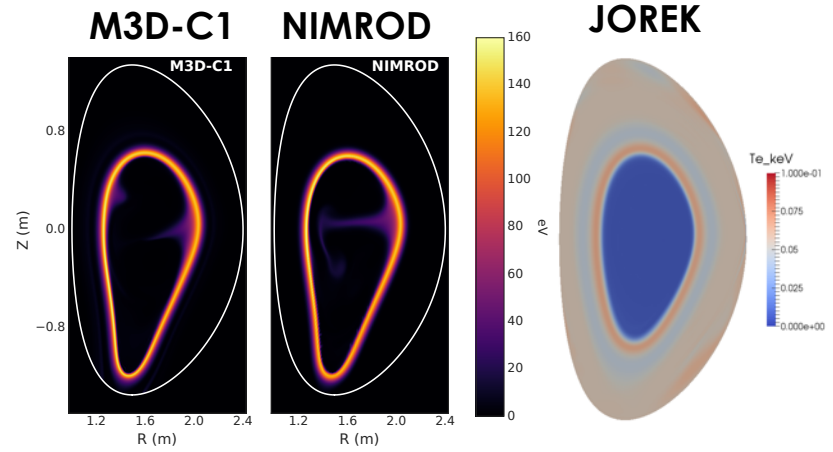
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JOREK Also Shows Inside-Out Thermal Quench and Evolving Plasma Sheet, but Differs Qualitatively (Nardon)



- T_e at ~ 0.55 ms after injection starts
- JOREK shows hollow profile, but less so



- T_e at ~ 1.0 ms after injection starts
- Sheet has formed in JOREK, but less shaping and no core turbulence



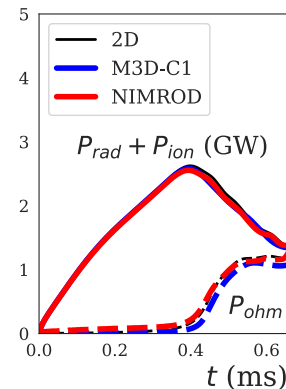
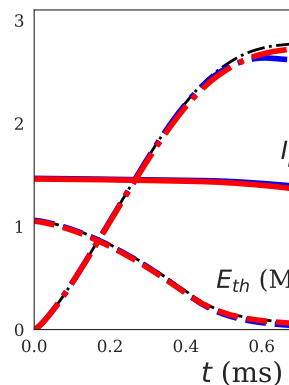
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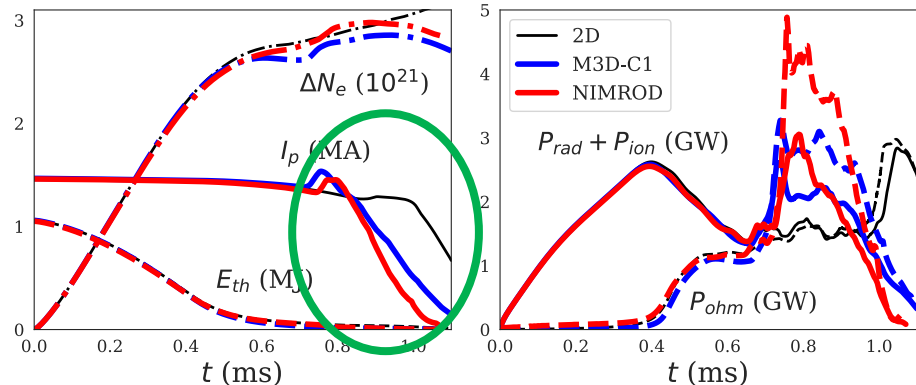
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 - Rapid current quench
 - Plasma sheet goes unstable after thermal quench
 - Mixing increases radiation & ohmic heating
- Prominent current spike*
 - 120-150 kA among largest seen in 3D, nonlinear MHD simulations
 - NIMROD spike slightly delayed and current quench is faster
 - Sensitivity to resistivity and boundary temperature under investigation



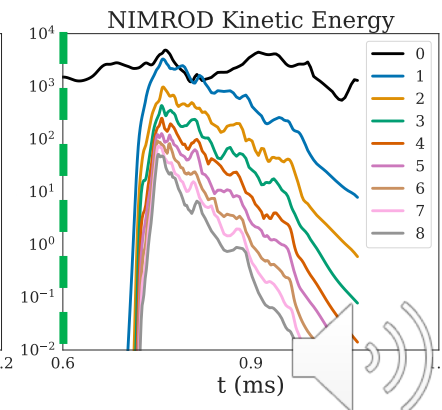
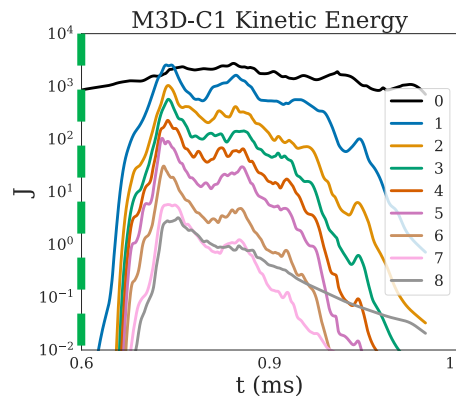
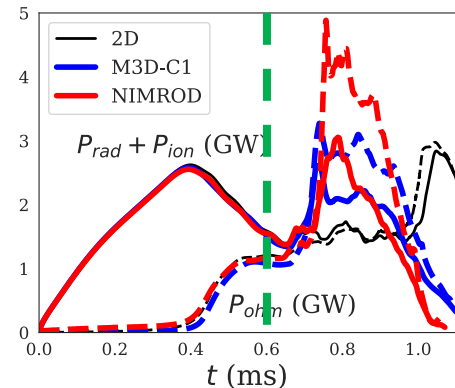
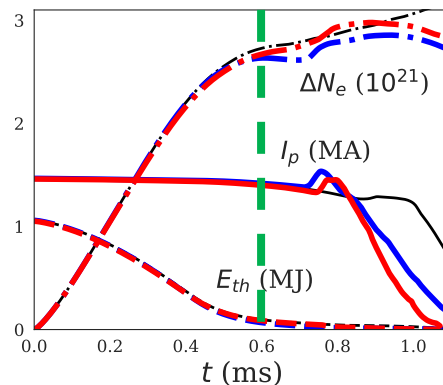
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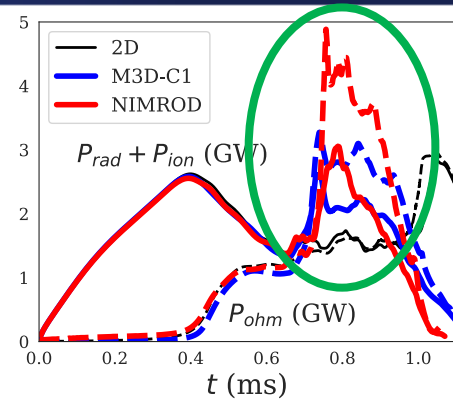
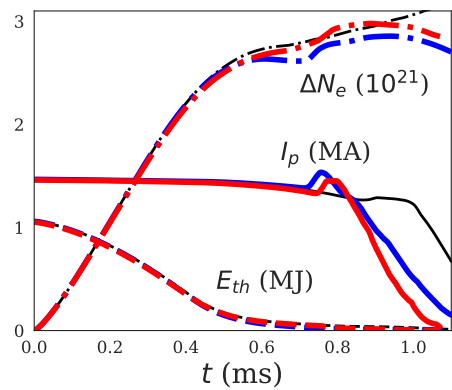
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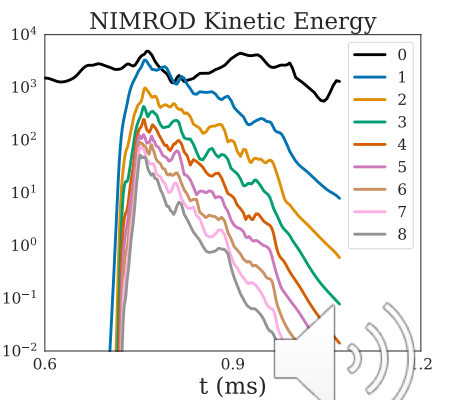
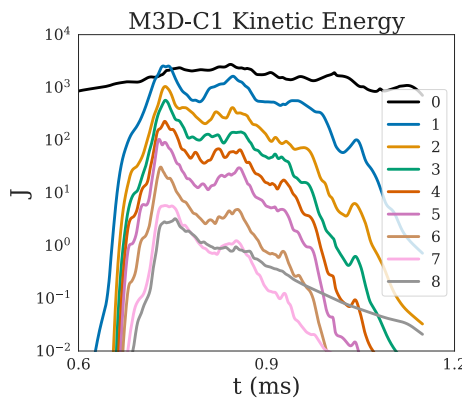


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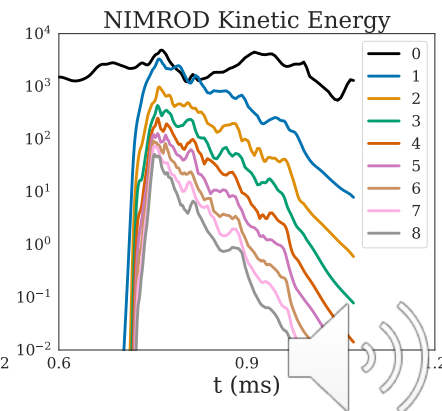
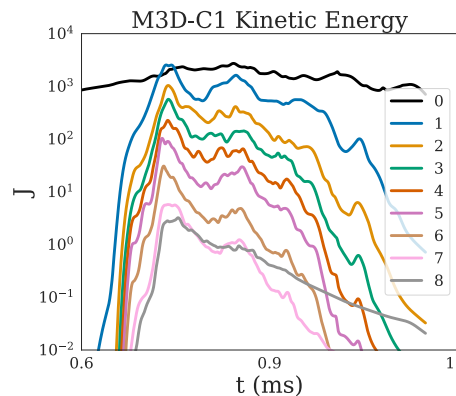
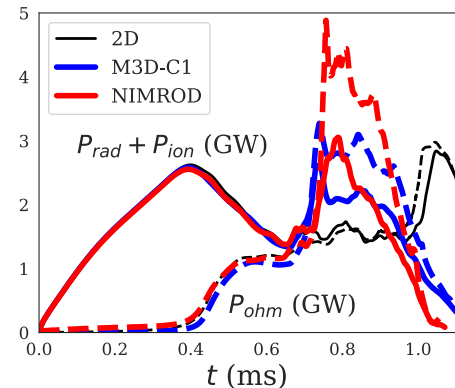
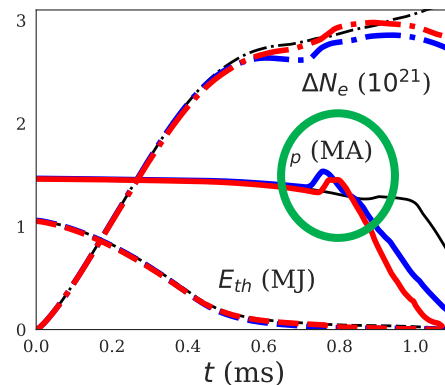
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*Letter on M3D-C1 current spike in preparation



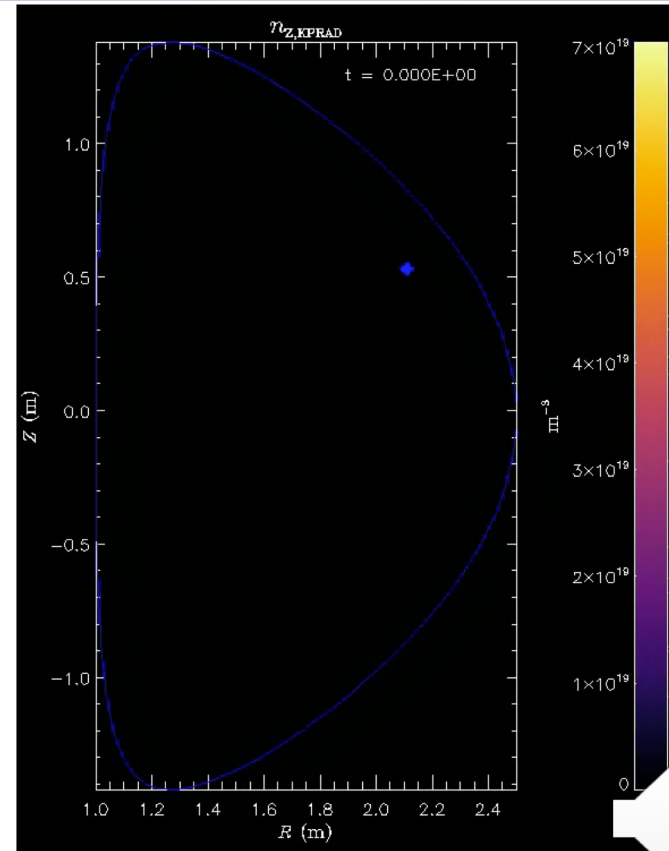
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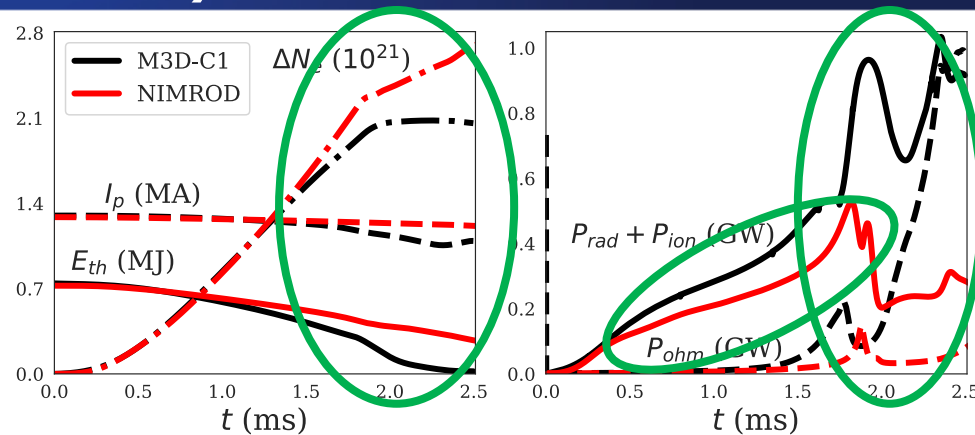
New 3D Benchmark between M3D-C1 & NIMROD with Injected, Ablating Pellet is Underway (Lyons, Kim)

- DIII-D 160606 @ 2990 ms: 0.7 MJ, 1.28 MA
- 3D nonlinear MHD with fixed boundary and single-temperature equation
- Pellet parameters
 - 3 mm radius, pure neon
 - 5 cm poloidal and 2.4 m toroidal deposition half-width
 - 200 m/s with realistic trajectory
- First results have obvious discrepancies
 - Early, quantitative agreement in number of electrons (i.e., ablation and ionization)
 - Both show strong MHD at ~1.8 ms but $n=3$ in M3D-C1 and $n=5$ in NIMROD
 - Induces rapid thermal quench in M3D-C1, but not in NIMROD
- Work to improve match will continue in earnest in near future



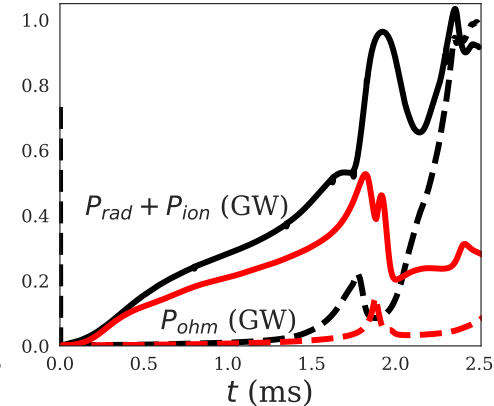
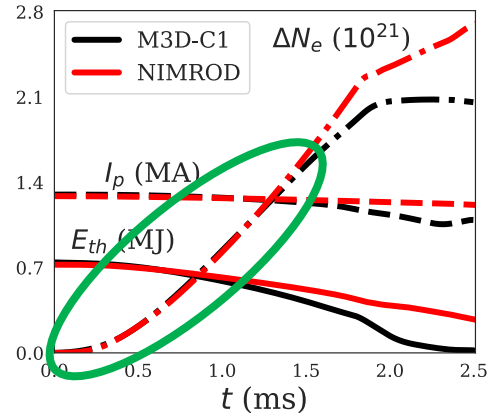
New 3D Benchmark between M3D-C1 & NIMROD with Injected, Ablating Pellet is Underway (Lyons, Kim)

- DIII-D 160606 @ 2990 ms: 0.7 MJ, 1.28 MA
- 3D nonlinear MHD with fixed boundary and single-temperature equation
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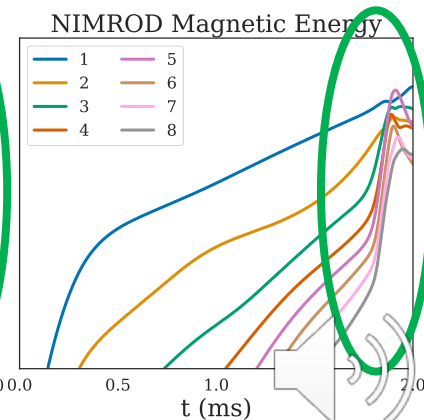
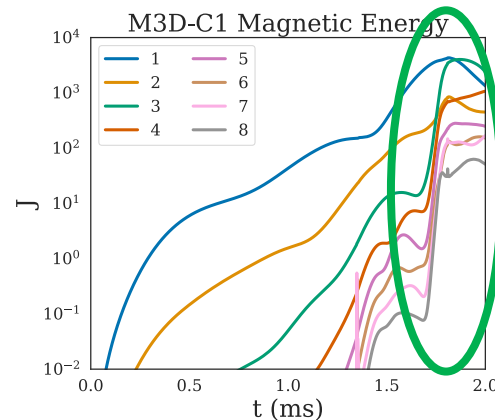
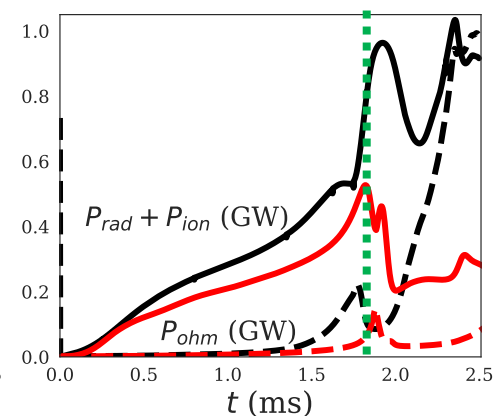
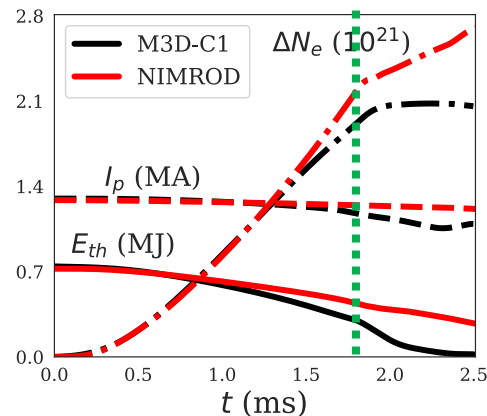
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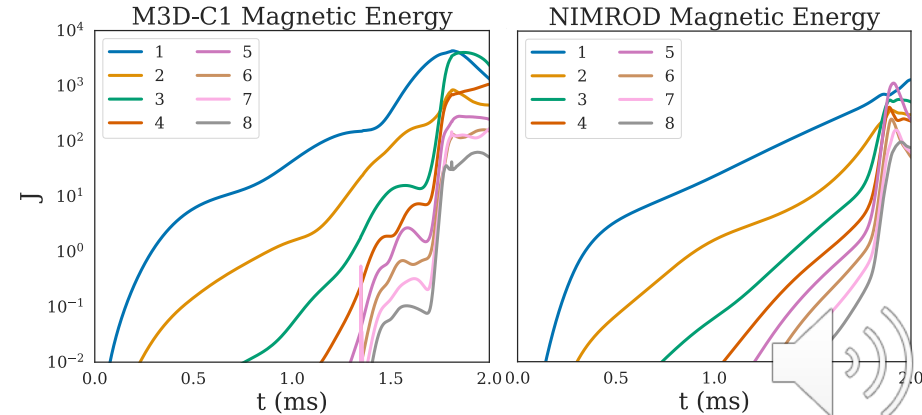
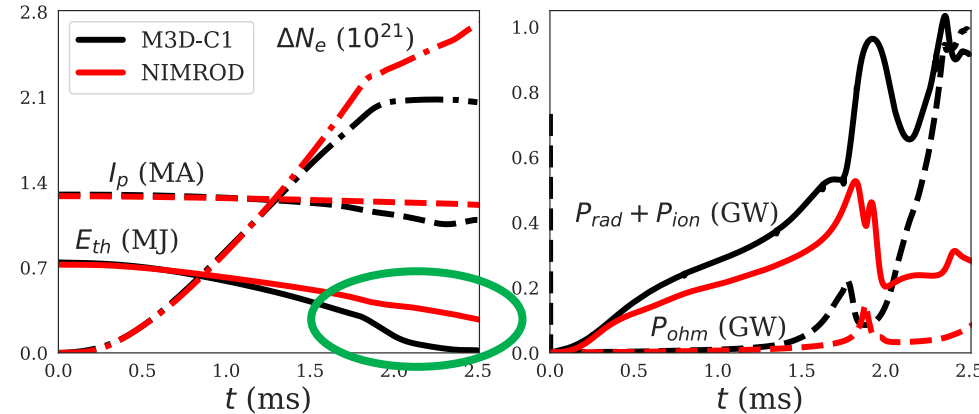
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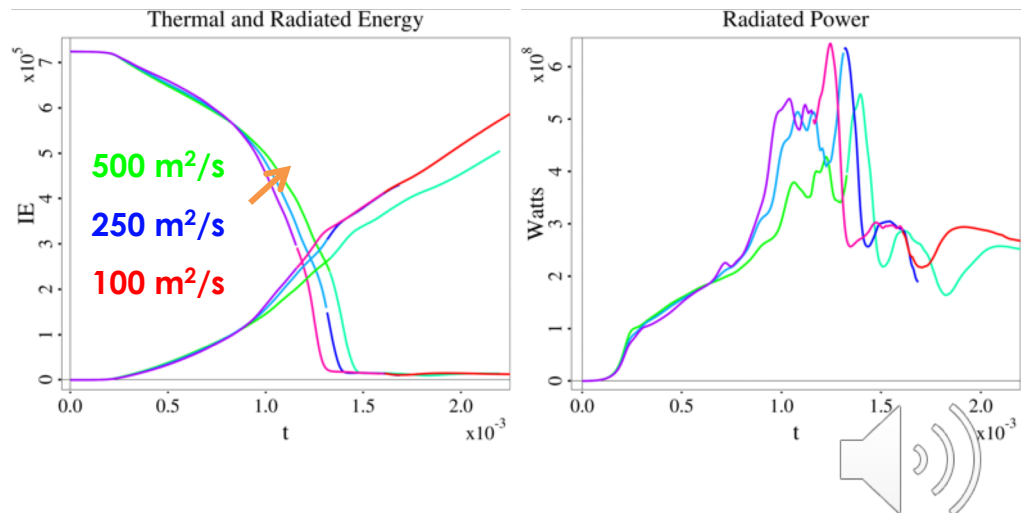
NIMROD Modeling Shows Lower Viscosity Leads to Shorter Thermal Quench due to Stronger Linear MHD Response (Kim)

viscosity	$d\phi/2\pi$	τ_{TQ} (ms)	P_{rad}^{peak} (GW)	E_{rad}/E_{th}	assim.
500 m ² /s	0.05	1.451	0.55	45%	34%
250 m ² /s	0.05	1.379	0.64	47%	38%
100 m ² /s	0.05	1.316	0.64	44%	41%

- Decreasing viscosity accelerates dynamics**

- Stronger linear response [(2,1),(3,2)] driven by ablating fragments
- Earlier nonlinear saturation but not necessarily larger amplitude

- Higher viscosity suppresses MHD activity, decreasing radiation



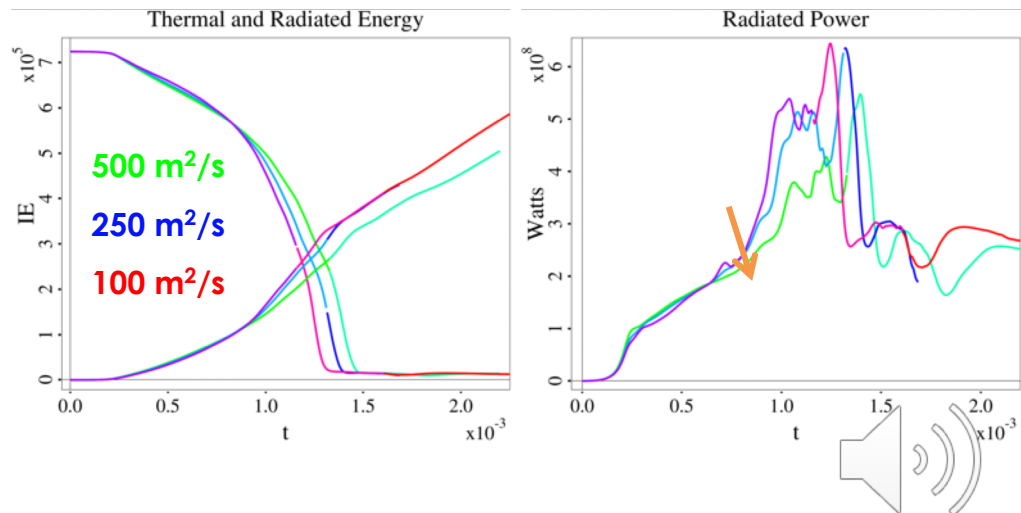
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NIMROD Modeling Shows Broader Toroidal Deposition Causes Shallower Penetration but Higher Assimilation (Kim)

viscosity	$d\phi/2\pi$	τ_{TQ} (ms)	P_{rad}^{peak} (GW)	E_{rad}/E_{th}	assim.
500 m ² /s	0.05	1.451	0.55	45%	34%
250 m ² /s	0.05	1.379	0.64	47%	38%
100 m ² /s	0.05	1.316	0.64	44%	41%
500 m ² /s	0.10	1.478	0.50	40%	42%
250 m ² /s	0.10	1.268	1.46	58%	66%
100 m ² /s	0.10	1.227	0.93	45%	61%

- **Overall, broader deposition causes**
 - Shorter thermal quench
 - Larger fraction of pellet ablated
- **Trends within broader deposition cases are less consistent, possibly due to nonlinear mixing from crossing of more flux tubes**



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M3D-C1 Validation with DIII-D Pellet Composition Shows Thermal Quench for Pure Neon Pellet Faster than Mixed Ne-D2 (Lyons)

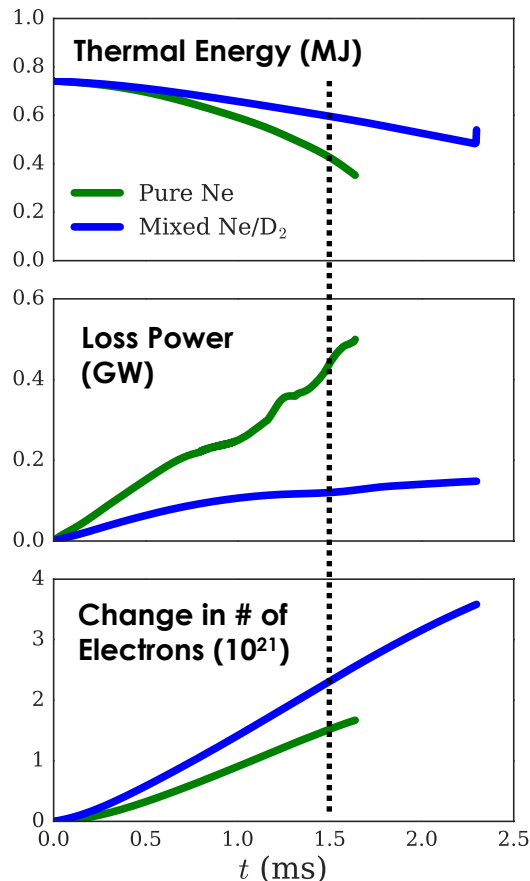
- **Simulations**

- DIII-D 160606
- Single, monolithic pellet
- Realistic velocity
- Half-widths: 10 cm pol.
3 m tor.

- **Radiative losses several times higher with pure neon than 10:1 D2:Ne**

- Trends are consistent with NIMROD modeling and experiment

- NIMROD agrees well with experiment
- Increased resolution improved results from publication*



Lyons IAEA Disruptions TM 2020



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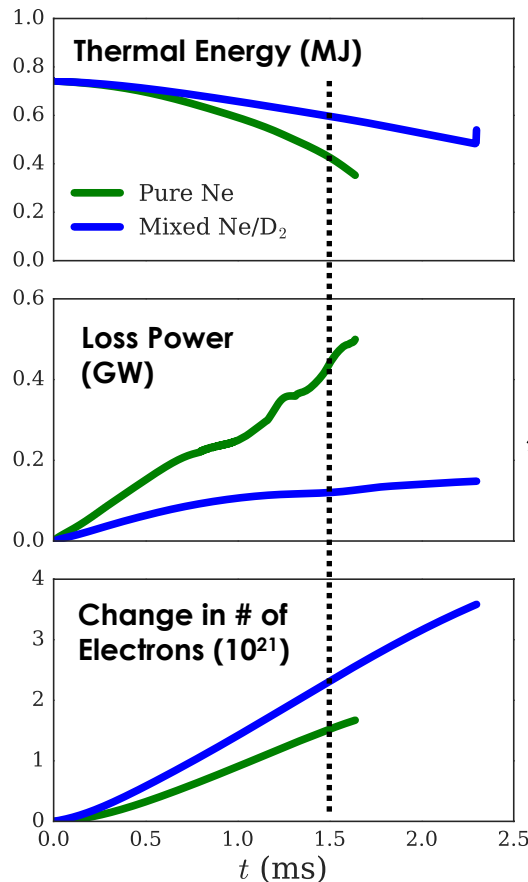
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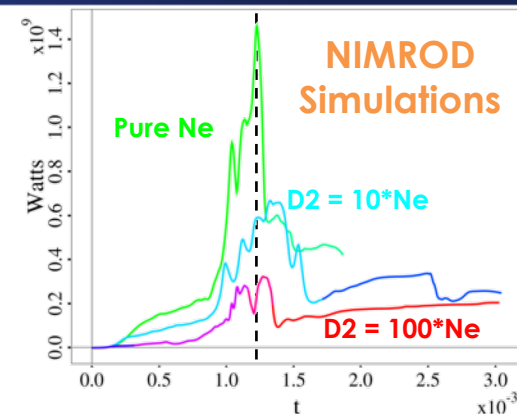
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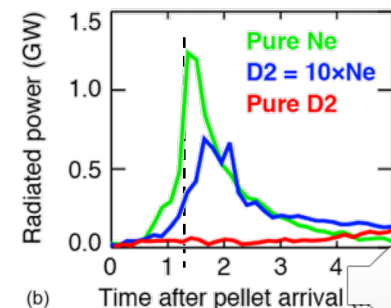
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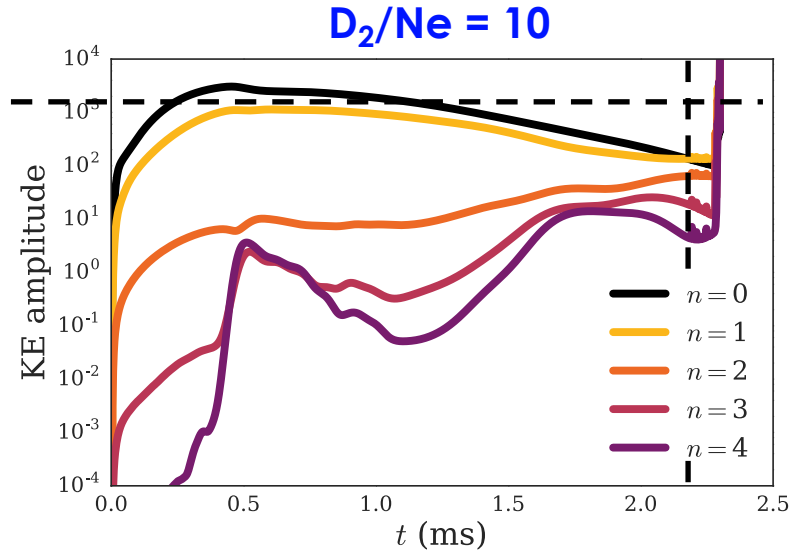
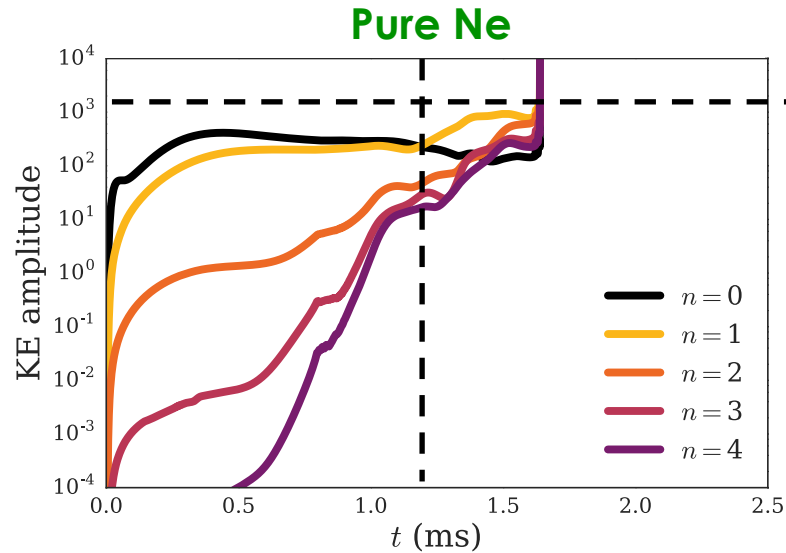
*Updated from C.C. Kim et al., Phys. Plasmas 26, 042510 (2019)



DIII-D Data

(b) D. Shiraki et al., Phys. Plasmas 23 (6), 062516

Pure Neon Pellet Induces Dominant $n=1$ Mode, Mixed Pellet Remains More Quiescent (Lyons)



- **Preliminary results: to be rerun with**
 - Higher toroidal resolution
 - Newer, more stable code version
- **Pure neon pellet drives linear instability**
- **Both go numerically unstable when plasma highly non-axisymmetric**



Outline and Major Results

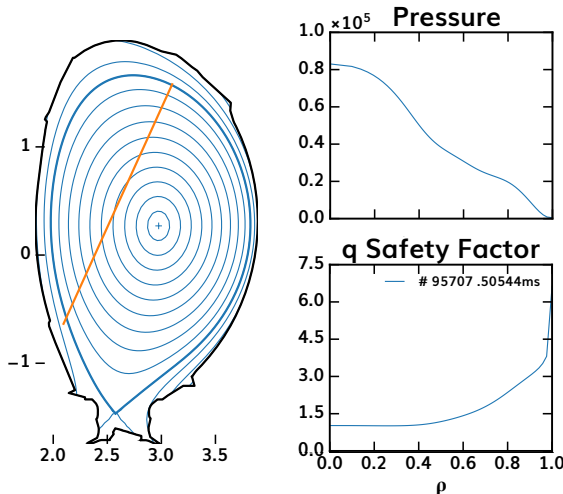
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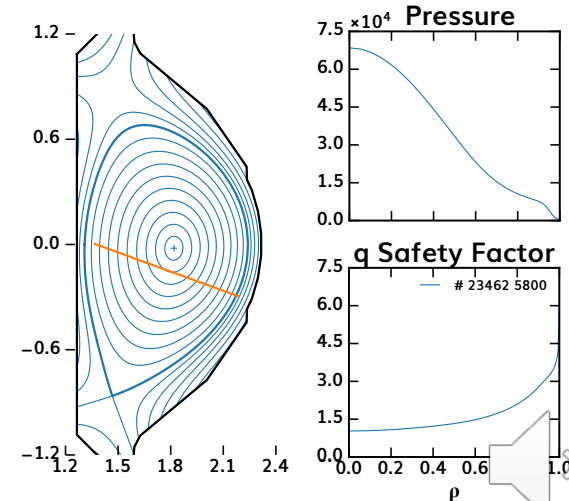
New International Collaboration will Validate M3D-C1 and NIMROD against Recent JET and KSTAR SPI Experiments

- **Modeling component of grant has several objectives**
 - Interpret recent mitigation experiments
 - JET, particular high thermal energy and radiation fraction/asymmetry
 - KSTAR, particularly dual, symmetric shattered-pellet injection
 - Develop cross-machine database to inform ITER disruption-mitigation system
 - Make predictions for additional experiments
- **Equilibria reconstructed with kinetic profiles acquired for recent experiments**

JET 95707
 $I_p = 2.4$ MA
 $W_{th} = 3.4$ MJ
(Scenario 1
High W_{th})



KSTAR 23462
 $I_p = 0.75$ MA
 $W_{th} = 0.40$ MJ



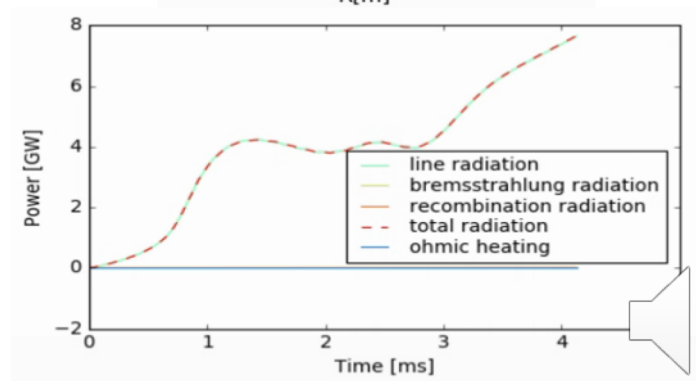
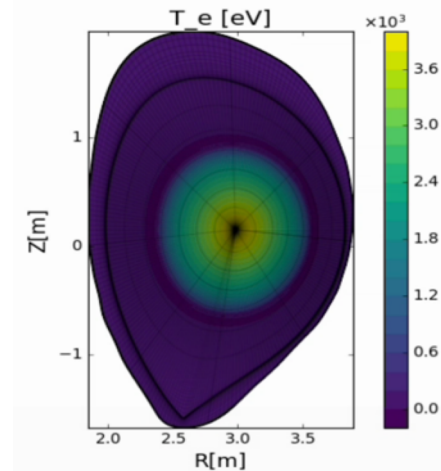
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 - Two different toroidal depositions, but varied diffusivity parameters
 - No significant MHD activity (beyond sawteeth) before numerical instability

- **M3D-C1 2D KSTAR modeling underway, 3D & NIMROD to follow**

- Dual injector simulations planned
- Multi-injector simulations demonstrated w/ NIMROD in DIII-D



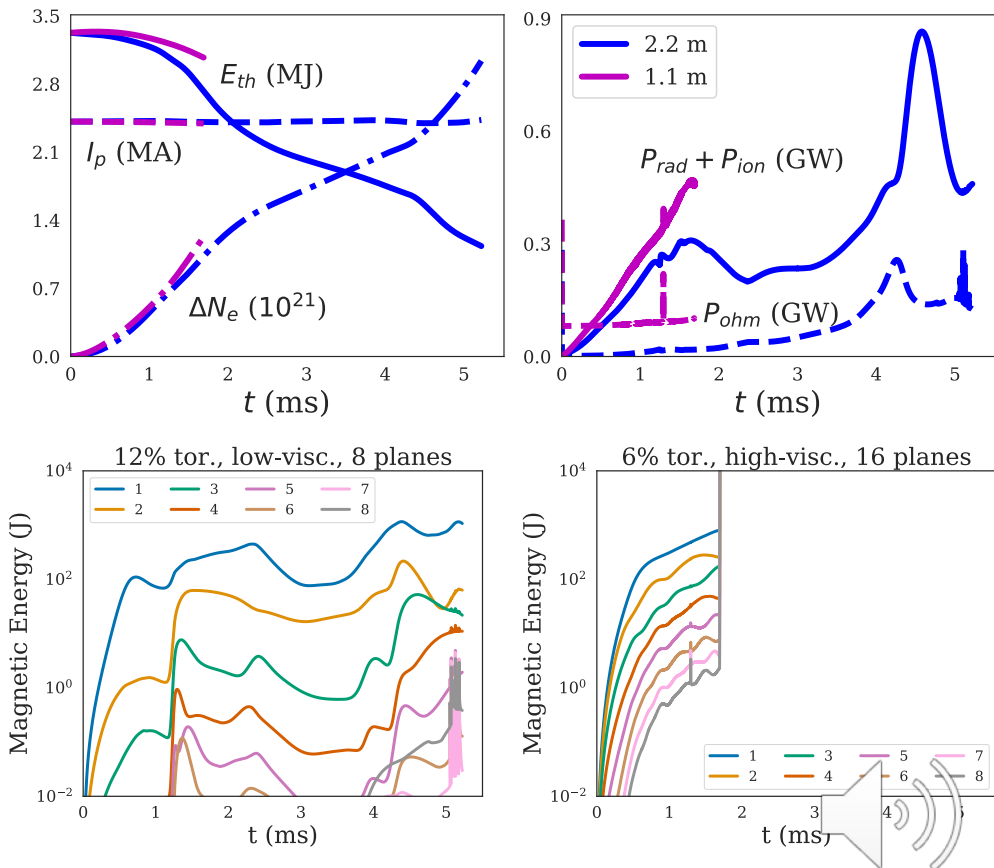
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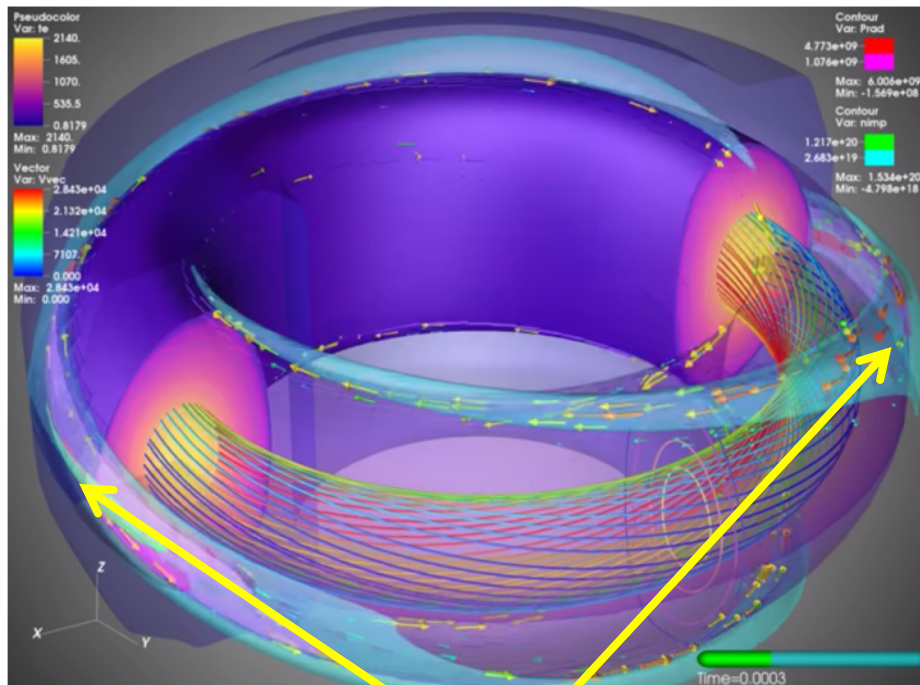
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NIMROD Dual Injection in DIII-D



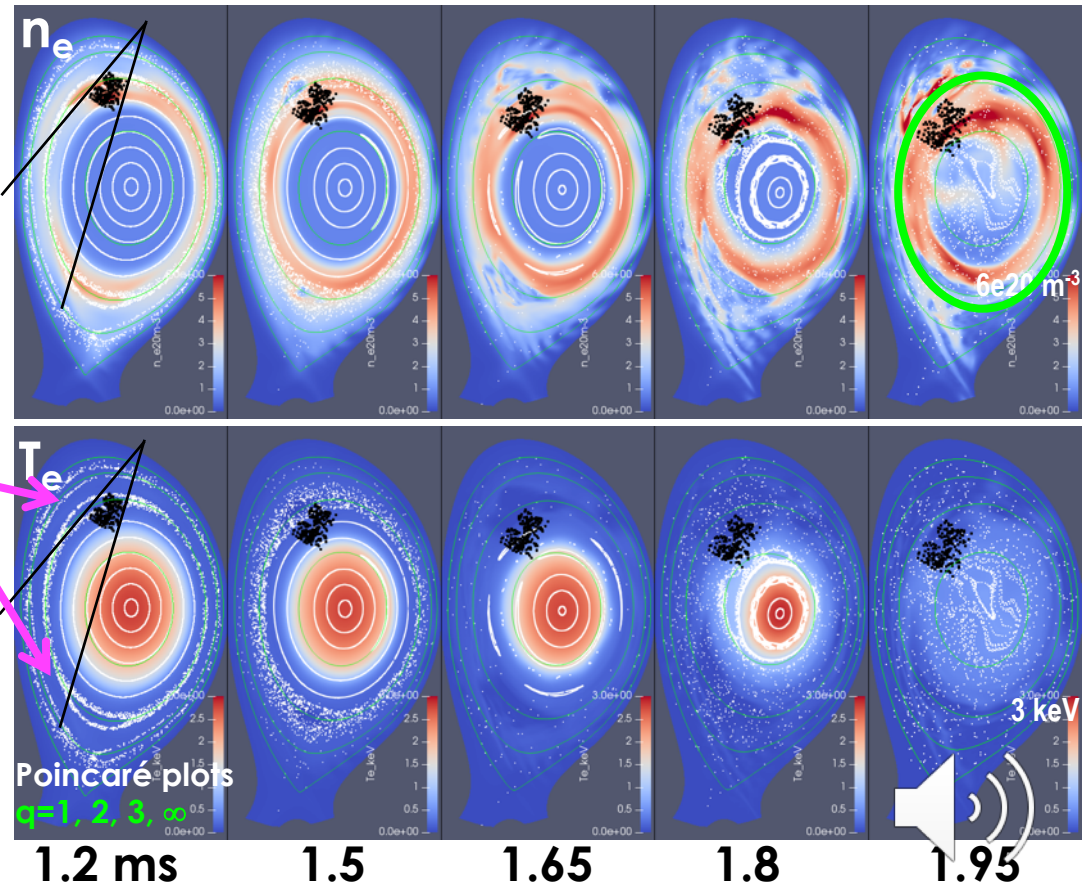
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JOEYK Modeling of JET Reference Scenario 1 Discharge Show MHD Driven Thermal Quench (Bonfiglio)

- **Shot 89800**
 - From earlier MGI experiment
 - Used for current Scenario 1
- **Pellet size and composition under active investigation**
 - 4.5 mm vs 8 mm
 - Pure Ne vs mixed Ne/D2
- **Example of 4.5 mm pure Ne**
 - MHD activity induced by $n=0$ current contraction and **helical cooling on rational surfaces**
 - Stochasticization causes thermal quench, but **core remains at low density** (potentially bad for runaway suppression)
- **Synthetic diagnostics are being implemented for experimental validation**



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Verification, Validation, and Predictive Modeling Will Continue

- **M3D-C1 and NIMROD**
 - Complete 3D benchmark this year
 - Extensive validation with experiment
 - DIII-D: dual SPI, thermal & magnetic energy
 - JET: high thermal energy and radiation fraction/asymmetry
 - KSTAR: dual, symmetric SPI
 - Model upgrades
 - Collisional-radiative impurity model
 - Coupling to detailed pellet ablation code
- **JOE**
 - Use synthetic diagnostics for JET validation
 - Upgrade to impurity model (ongoing) to complete 2D benchmark
- **All codes will make predictions for efficacy of ITER disruption-mitigation system**
 - Cross-machine, cross-code database will provide robust understanding of SPI dynamics
 - High-fidelity, 3D nonlinear modeling of relevant ITER scenarios



Acknowledgments and Disclaimers

- This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Fusion Energy Sciences, using the DIII-D National Fusion Facility, a DOE Office of Science user facility, under Awards DE-FG02-95ER54309, DE-FC02-04ER54698, DE-SC0018109, and DE-SC0020299.
- This research used resources of the National Energy Research Scientific Computing Center (NERSC), a U.S. Department of Energy Office of Science User Facility operated under Contract No. DE-AC02-05CH11231.
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- This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training program 2014-2018 and 2019-2020 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.



Additional slides

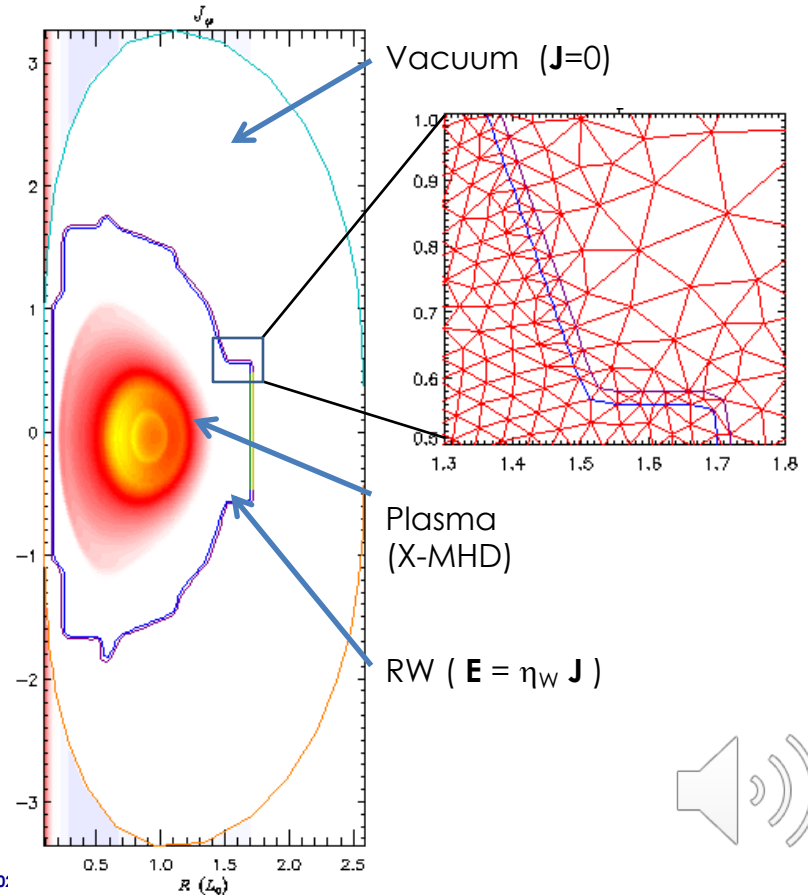


M3D-C1* Solves the Extended-MHD Equations

- Three-dimensional toroidal geometry
- Full (not reduced) MHD
- Solves for potential and stream-function fields for \vec{A} & \vec{v} ($\nabla \cdot \vec{B} = 0$ intrinsically)
- Includes resistivity, density diffusivity, viscosity, & thermal conductivity
- Two-fluid effects (optional)
- 3D high-order finite elements
 - Unstructured, triangular mesh in poloidal plane
 - Structured toroidally, but can pack planes
- Can solve with finite-thickness resistive wall in domain**

*S. C. Jardin, et al., *Comput. Sci. Discovery* 5, 014002 (2012).

**N.M. Ferraro, et al., *Phys Plasma* 23, 056114 (2016).



M3D-C1 Solves the Extended-MHD Equations

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{V}) = \nabla \cdot D_n \nabla n + S_n$$

Blue terms are 2-fluid

$$\frac{\partial \mathbf{A}}{\partial t} = -\mathbf{E} - \nabla \Phi, \quad \mathbf{B} = \nabla \times \mathbf{A}, \quad \mathbf{J} = \nabla \times \mathbf{B}, \quad \nabla_{\perp} \cdot \frac{1}{R^2} \nabla \Phi = -\nabla_{\perp} \cdot \frac{1}{R^2} \mathbf{E}$$

$$nM_i \left(\frac{\partial \mathbf{V}}{\partial t} + \mathbf{V} \cdot \nabla \mathbf{V} \right) + \nabla p = \mathbf{J} \times \mathbf{B} - \nabla \cdot \mathbf{\Pi}_i + \mathbf{S}_m$$

$$\mathbf{E} + \mathbf{V} \times \mathbf{B} = \frac{1}{ne} (\mathbf{R}_c + \mathbf{J} \times \mathbf{B} - \nabla p_e - \nabla \cdot \mathbf{\Pi}_e) - \frac{m_e}{e} \left(\frac{\partial \mathbf{V}_e}{\partial t} + \mathbf{V}_e \cdot \nabla \mathbf{V}_e \right) + \mathbf{S}_{CD}$$

$$\frac{3}{2} \left[\frac{\partial p_e}{\partial t} + \nabla \cdot (p_e \mathbf{V}) \right] = -p_e \nabla \cdot \mathbf{V} + \frac{\mathbf{J}}{ne} \cdot \left[\frac{3}{2} \nabla p_e - \frac{5}{2} \frac{p_e}{n} \nabla n + \mathbf{R}_c \right] + \nabla \cdot \left(\frac{\mathbf{J}}{ne} \right) : \mathbf{\Pi}_e - \nabla \cdot \mathbf{q}_e + Q_{\Delta} + S_{eE}$$

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$$\mathbf{V}_e = \mathbf{V}_i - \mathbf{J} / ne$$

$$\mathbf{R}_c = \eta ne \mathbf{J}, \quad \mathbf{\Pi}_i = -\mu \left[\nabla \mathbf{V} + \nabla \mathbf{V}^{\dagger} \right] - 2(\mu_c - \mu) (\nabla \cdot \mathbf{V}) \mathbf{I} + \mathbf{\Pi}_i^{GV}$$

$$\mathbf{\Pi}_e = (\mathbf{B} / B^2) \nabla \cdot \left[\lambda_h \nabla (\mathbf{J} \cdot \mathbf{B} / B^2) \right], \quad Q_{\Delta} = 3m_e (p_i - p_e) / (M_i \tau_e)$$

$$\mathbf{q}_{e,i} = -\kappa_{e,i} \nabla T_{e,i} - \kappa_{\parallel} \nabla_{\parallel} T_{e,i}$$



Ablation model for Ne-D2 pellets implemented in M3D-C1

- **Practical, analytic expression fit to more complex ablation model (Parks)**

$$G \text{ (g/s)} = \lambda(X) \left(\frac{T_e}{2000 \text{ eV}} \right)^{5/3} \left(\frac{r_p}{0.2 \text{ cm}} \right)^{4/3} \left(\frac{n_e}{10^{14} \text{ cm}^{-3}} \right)^{1/3}$$

λ is fitting function, depending on molar fraction of D2, X

- **M3D-C1 implementation**
 - Advance pellet location in time
 - Calculate number of particles ablated and pellet-surface recession at each time step
 - Deposit main ion and/or impurities onto arbitrary spatial distribution (e.g. 2D or 3D Gaussian)

