INL/CON-20-58673-Revision-1

Continued Validation Studies using the MOOSE Framework for Plasma Simulation with Electromagnetics

October 2020

Changing the World's Energy Future

Casey T Icenhour, Corey DeChant, Alexander D Lindsay, David Green, Steven Shannon

Idaho National Laboratory

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Casey Icenhour[1,2], Corey DeChant[1], Alexander Lindsay[2], David Green[3], Steven Shannon[1]

October 7, 2020

73rd APS Gaseous Electronics Conference

1. North Carolina State University, Raleigh, NC, USA
2. Idaho National Laboratory, Idaho Falls, ID, USA
3. Oak Ridge National Laboratory, Oak Ridge, TN, USA

Idaho National Laboratory

Oak Ridge National Laboratory

NSF

Outline

- Free and Open Source Software (FOSS) Multiphysics for LTP research → MOOSE Framework
  - Electromagnetics Library for Kinetics and fluids (ELK)
  - Zapdos + CRANE (plasma fluids and plasma chemistry reaction networks)
- Zapdos/ELK Coupling and Improvements
- Electrostatic Verification & Validation for 1D/2D CCPs
- Future Work
  - Electromagnetic CCP Simulation using Zapdos
  - Spark Plasma Sintering (SPS) using MOOSE thermo-mechanical models
- Summary / Acknowledgements

Why FOSS? Why MOOSE?

FOSS

- Free (as in no license fees)
- Free (as in freedom – all code is open, inspectable, and modifiable)
- Collaborative by nature
- Community focused

MOOSE

- Originally used for nuclear energy reactor research (neutronics, fluids, heat conduction) → **Multi-scale Multi-physics** [1]
- Modularity of code structure → **extensible and maintainable**
- NQA-1 certified development process for **code quality and testing** (vital for acceptance in nuclear certification)
- Demonstrated scalability to over 30K+ CPU cores [2]
- Already-established and vibrant community ecosystem

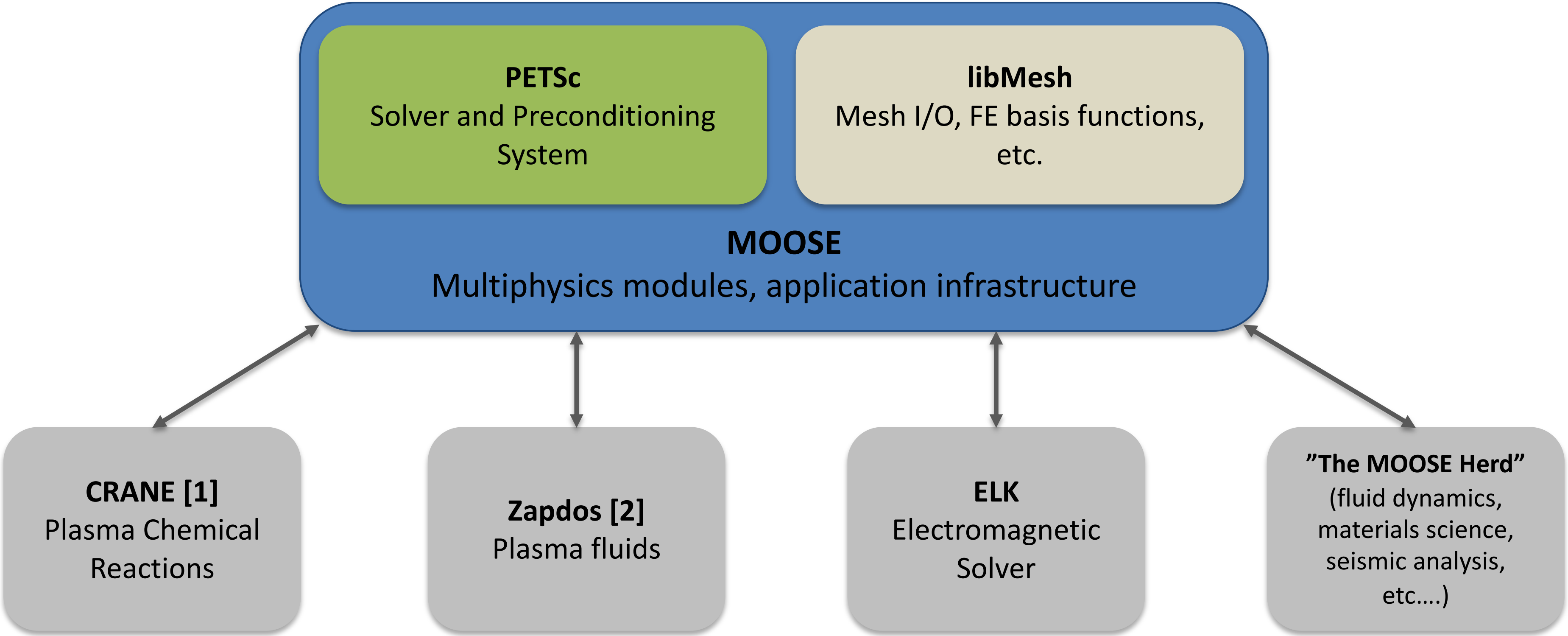
```
[Variables]
  [./T]
    initial_condition = 293.0 #in K
  [../]
  [./elec]
  [../]
[]

[Kernels]
  [./HeatDiff]
    type = HeatConduction
    variable = T
  [../]
  [./HeatTdot]
    type = HeatConductionTimeDerivative
    variable = T
  [../]
  [./HeatSrc]
    type = JouleHeatingSource
    variable = T
    elec = elec
  [../]
  [./electric]
    type = HeatConduction
    variable = elec
    diffusion_coefficient = electrical_conductivity
  [../]
[]
```

https://github.com/idaholab/moose/blob/next/modules/heat_conduction/test/tests/joule_heating/transient_jouleheating.i

[1] C. Permann *et al*. "MOOSE: Enabling massively parallel multiphysics simulation." *SoftwareX* **11** (100430). 2020.
[2] F. Kong *et al*. "A General-Purpose Hierarchical Mesh Partitioning Method with Node Balancing Strategies for Large-Scale Numerical Simulations." *2018 IEEE/ACM scalA. (2018)*

MOOSE + Apps Structure



[1] Keniley et al. APS GEC. Presentation. (2019)
[2] Lindsay et al. J. Phys. D: Appl. Phys. 49(23) 235204 (2016)

Electromagnetics Library for Kinetics and fluids (ELK)

- A general purpose electrostatic/electromagnetic solver tool within the MOOSE ecosystem.
- Base physics – Maxwell's Equations (in Helmholtz wave equation form)
- MOOSE Framework allows for coupling to other domains of physics and engineering
  - Heat Transfer
  - Materials Science
  - Chemistry
  - Fluid Dynamics
- What does this enable? **Self-consistent multiphysics + EM modeling within MOOSE**
  - Microwave Plasma Discharges
  - Wave Propagation Studies
  - Advanced Manufacturing Simulation
  - Next-generation reactor component design (molten liquid flow)
  - ……

ELK Base Physics Overview

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$ (Faraday's Law)

$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}$$ (Maxwell-Ampere Law)

$$\nabla \cdot \mathbf{D} = \rho$$ (Gauss's Law)

$$\nabla \cdot \mathbf{B} = 0$$ (Gauss's Law – magnetic)

$$\nabla \cdot \mathbf{J} = -\frac{\partial \rho}{\partial t}$$ (Continuity Equation)

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$$\mathbf{D} = \epsilon \mathbf{E}$$
$$\mathbf{B} = \mu \mathbf{H}$$
$$\mathbf{J} = \sigma \mathbf{E}$$

Constitutive Relations (describes the properties of the medium)

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$$\frac{\partial}{\partial t} \rightarrow j\omega$$

Time-harmonic Helmholtz Wave Equations

$$\nabla \times \left(\frac{1}{\mu} \nabla \times \mathbf{E} \right) - \omega^2 \epsilon \mathbf{E} = -j\omega \mathbf{J}$$

$$\mathbf{D} = \epsilon \mathbf{E}$$
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$$\nabla \times \left(\frac{1}{\epsilon}\nabla \times \mathbf{H}\right) - \omega^2 \mu \mathbf{H} = \nabla \times \left(\frac{1}{\epsilon}\mathbf{J}\right)$$

$$\mathbf{D} = \epsilon \mathbf{E}$$

$$\mathbf{B} = \mu \mathbf{H}$$

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$$\mathbf{D} = \epsilon \mathbf{E}$$

$$\mathbf{B} = \mu \mathbf{H}$$

$$\mathbf{J} = \sigma \mathbf{E}$$

Constitutive Relations (describes the properties of the medium)

Without this assumption…

Time-dependent Helmholtz Electric Field Equation (if $\mu=\mu_0$)

$$\nabla \times \nabla \times \mathbf{E} + \mu_0 \frac{\partial^2}{\partial t^2}(\epsilon \mathbf{E}) = -\frac{\partial}{\partial t}(\mu_0 \mathbf{J})$$

Zapdos Plasma System of Equations (current, electrostatic)

Drift - Diffusion Approximation

$$\frac{\partial n_j}{\partial t} + \nabla \cdot \Gamma_j = \sum_j S_{iz}$$

$$\Gamma_{e,i} = \mu_{e,i}(\nabla \mathrm{V}) n_{e,i} - D_{e,i} \nabla n_{e,i}$$

$$\Gamma_* = -\mathrm{D}_* \nabla n_*$$

Energy Conservation

$$\frac{\partial (n_e \varepsilon)}{\partial t} + \nabla \cdot \Gamma_\varepsilon$$

$$= -e\Gamma_e \cdot \nabla V - 3\frac{m_e}{m_i} n_e n_g k_{elastic} T_e - \sum_j E_j K_j$$

$$\Gamma_\varepsilon = \frac{5}{3}\varepsilon\Gamma_e - \frac{5}{3} n_e D_e \nabla n_e$$

Flux BC

$$\Gamma_i \cdot n = -\mu_i (\nabla V_{eff}) \cdot n n_i$$

$$\Gamma_e \cdot n = \frac{1}{4} v_{th,e} n_e \cdot n - \gamma \Gamma_i$$

$$\Gamma_\varepsilon \cdot n = \frac{1}{4} v_{th,e} \frac{5}{3} n_e \varepsilon \cdot n - \frac{5}{3} \varepsilon_{se} \gamma \Gamma_i$$

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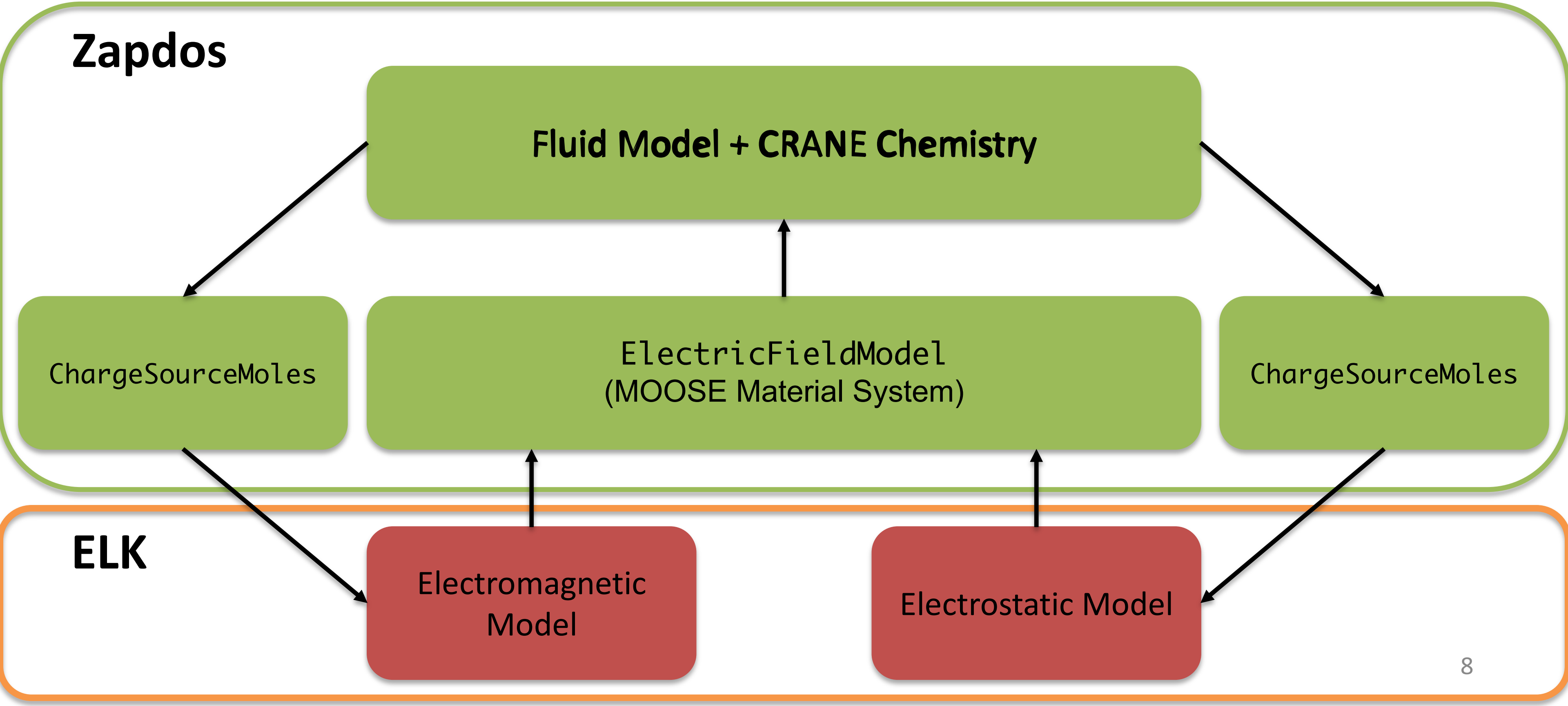
Plasma Interactions (CRANE)

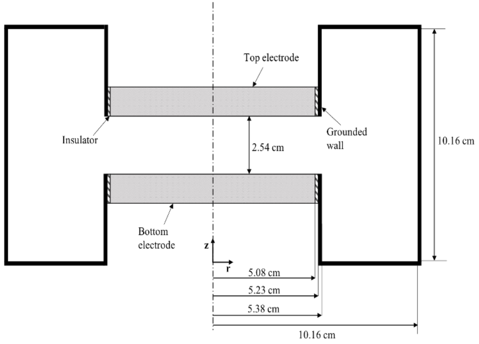
One Body	*Two Body*	*Three Body*
$S_{iz} = \nu k n_1$	$S_{iz} = \nu k n_1 n_2$	$S_{iz} = \nu k n_1 n_2 n_3$

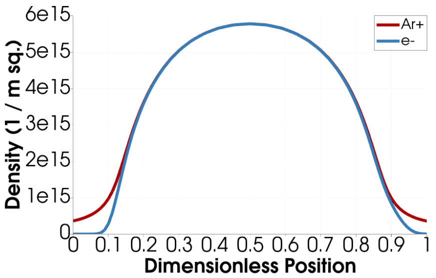
Simplified Code Coupling Scheme (Single Input File)

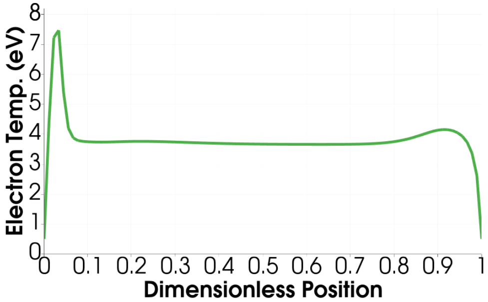


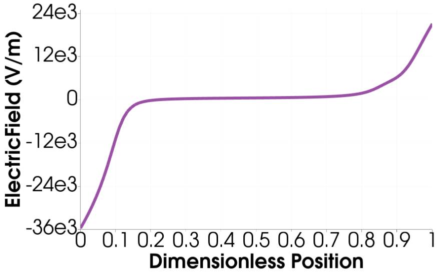
Initial Electrostatic Validation & Verification

- Following the simulation approach of Economou and Lymberopoulos [1, 2]
  - Argon discharge (e, ions, metastables)
  - press. = 100 mTorr
  - freq. = 13.56 MHz
  - Vpp = 100 V (single powered electrode)
- Previous 1D / 2D electrostatic results using only Zapdos showed very good agreement with the original work and serve as the basis for cross-code comparisons [3, 4]
- ELK + Zapdos can duplicate 1D results with similar runtime (without acceleration) and qualitative agreement.
  - T_e (Bulk) = ~4 eV
  - n_e (center) = 5.5e9 cm^{-2}
  - |E| (center) = 0.477 V/cm
- More work needs to be done to finalize and formalize these comparisons









[1] Lymberopoulos DP and Economou DJ, "Modeling and simulation of glow discharge plasma reactors," *J. Vac. Sci. Technol. A* **73** 1229 (1994)
[2] Lymberopolous DP and Economou DJ, "Two-dimensional Self-Consistent Radio Frequency Plasma Simulations Relevant to the Gaseous Electronics Conference RF Reference Cell," *J. Res. Natl. Inst. Stand. Technol.* **100** 473 (1995)
[3] DeChant C et al, APS GEC. Presentation. (2019)
[4] DeChant C et al, APS GEC. Presentation. (2020)

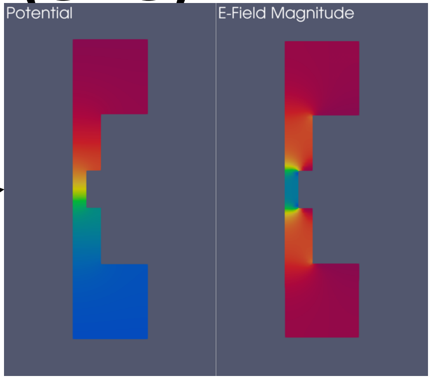
Future Work – Electromagnetic Plans

- Electromagnetic effects in CCPs with high frequencies
  - Relevant to the plasma processing industry
  - $f \gg 13.56$ MHz , $f \rightarrow \omega_p$
  - Plasma nonuniformities (ion fluxes, changing energy distribution functions)
  - Standing Waves
  - Surface Waves
  - Skin / Edge Effects

Ongoing Work – Spark Plasma Sintering (SPS)

- SPS is a manufacturing process that involves forming a solid mass from a metallic powder via Joule heating and pressure, without heating the material to a molten state.
- ELK, combined with a heat conduction module provided by MOOSE, is being used to solve the engineering scale electro-thermal problem

Electrostatic potential and electric field calculation in experimental graphite die geometry



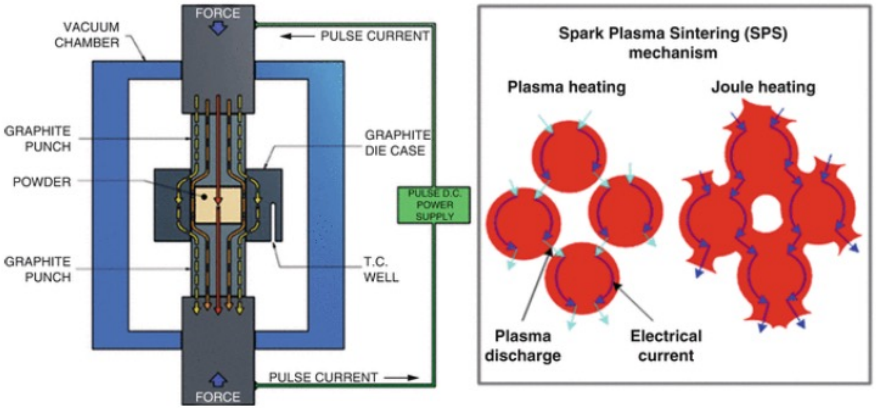
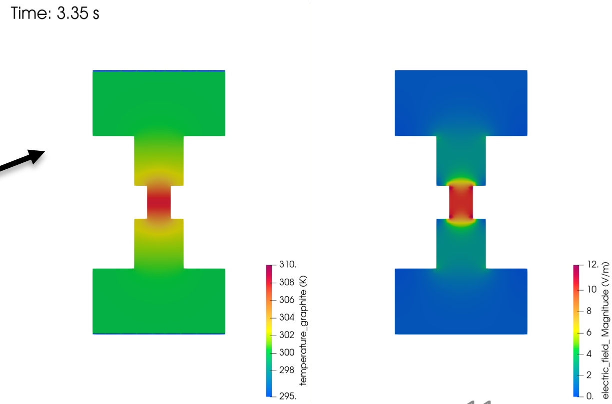


Figure: Yang K., et al. "Tuning Electrical Properties of Carbon Nanotubes via Spark Plasma Sintering." In: Bhushan B. (eds) Encyclopedia of Nanotechnology. Springer, Dordrecht (2015)

Calculated temperature (left) as a result of the applied electric field (right)



Summary

- FOSS projects can enable large, collaborative efforts within the LTP community to push the field forward.
- Established multiphysics projects, such as MOOSE, allow a jumping off point from a rigorous, proven platform that can run on workstations and supercomputers.
- Zapdos and ELK for plasma fluids and electromagnetics have been coupled to enable the addition of fully electromagnetic plasma simulation capabilities to the MOOSE ecosystem
- Initial validation of the coupling framework for 1D electrostatic problems has been promising, and the move to 2D and electromagnetic sample problems is on-going.

62nd Annual Meeting of the APS Division of Plasma Physics

Monday–Friday, November 9–13, 2020; Remote; Time Zone: Central Standard Time, USA

Session Index

Session NM10: Mini-Conference on Growing An Open Source Software Ecosystem For Plasma Science II

- Wednesday, November 11, 2020
- 9:30AM – 12:30PM CST

Acknowledgements

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  - The INL Graduate Fellowship Program – managed by Idaho National Laboratory, which is supported by the Office of Nuclear Energy of the U.S. Department of Energy under Contract No. DE-AC07-05ID14517
  - The National Science Foundation, under SI^2 Grant 1740300
  - The U.S. Department of Energy Office of Science Graduate Student Research program
- Special thanks to:
  - The MOOSE Framework Development Team
  - Oak Ridge Fusion and Materials for Nuclear Systems Division
  - Dr. Richard Martineau