An open source multi-physics platform to advance fundamental understanding of plasma physics and enable impactful application of plasma systems

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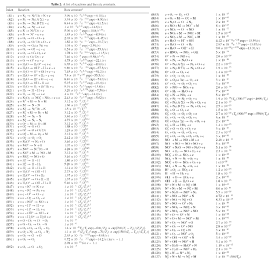
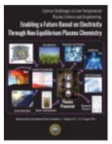
Enabling convergent research utilizing plasma science to enable impactful technology advances

Plasmas present an amazing complex multi-physics problem (field driven electrons producing novel chemistry through energy dependent impact and charge exchange in gas)

Plasmas provide solutions for several grand challenges

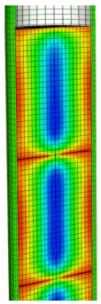


Sakiyama, Graves, et. al. JPD 45 425201 (2012)



A verified, validated, open source multi-physics framework will accelerate plasma-based solutions for societal need

The MOOSE open source platform



Originally developed for large scale simulation of nuclear reactor systems as part of the DOE Nuclear Energy effort. MOOSE and ALL associated tracked applications must meet NQA-1 requirements

FEA based, unstructured mesh with adaptivity, built around fluids, thermo-mechanics, neutron transport, heat transfer, mass transfer applications

Applications are built on the MOOSE framework, including ZAPDOS plasma module and ELK electromagnetic module developed under this SI² grant.

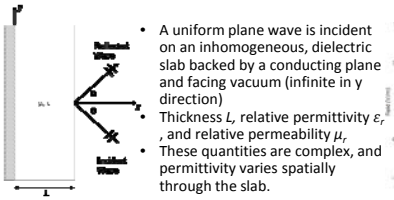
All applications tracked by MOOSE (including ZAPDOS and ELK) as well as changes to the framework must undergo review using GitHub Pull requests and pass a set of application regression tests before made available to users. >80% regression test code average maintained at all times.

We seek to add the necessary capability through plasma-based applications and enhancements to the MOOSE framework to enable plasma simulation.

Leverage the strict MOOSE SQP system to insure open source development with structured verification and validation processes

Electromagnetic Module:

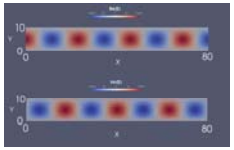
A. Modelling fields in lossy dielectric (typical plasma model)



- A uniform plane wave is incident on an inhomogeneous, dielectric slab backed by a conducting plane and facing vacuum (infinite in y direction)
- Thickness L, relative permittivity ε_r , and relative permeability μ_r
- These quantities are complex, and permittivity varies spatially through the slab.

B. Plane wave propagation in a waveguide (Field structure for plasma heating modes)

- Vacuum-filled waveguide with TM_{11} mode plane wave (amplitude = 1) being launched at Port (x = 0) and absorbed at Exit (x = L).
- Single-mode port boundary condition applied at x = 0, and first order absorbing boundary condition applied at x = L
- Sides of waveguide are conducting surfaces (E = 0)
- Future plans include creating formal Perfect Conductor curl conditions on the walls for multi-component solves.



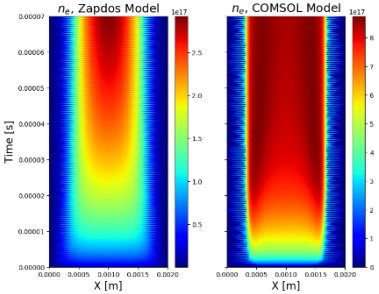
- f = 20 MHz
- L = 80m
- *Width* = 10m
- Compares well to textbook analytic solution for a TM_{11} mode.

Chemical Reaction Module:

Zapdos: Species densities (Drift-Diffusion Continuity Equations)

Chemical Reaction Module: Reaction Rate Equations (ZDPlasKin, MOOSE App, etc.)

Test Case: RF Discharge



Rate Equations:

$$\frac{d[N_i]}{dt} = \sum_{j=1}^{j_{max}} Q_{ij}(t)$$

$$aA + bB \rightarrow cC + dD$$

$$R_j = k_j[A]^a[B]^b$$

$$Q_A = -aR \quad Q_B = -bR$$

$$Q_C = cR \quad Q_D = dR$$

- *Zapdos* is being updated to include chemical reactions among an arbitrary number of species
- Currently treats Ar+, Ar*, and e- with 6 reaction pathways between them
- Includes capability for N species and any general two-body reactions

User Training and Workshops:

MOOSE/PetSc 3 day workshop to be held at Illinois May 15-17 (co-PI Curreli hosting)

2 Day plasma application focused workshop hosted by the collocated GEC / APS-DPP conference November 4-5 in Portland Oregon. Combined conference attendance approximately 2000

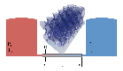
Facilities for 100+ person workshop provided as part of GEC workshop series. Live stream of workshop also planned.

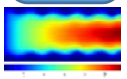
INL collaborators providing instructors as part of their annual MOOSE training nationwide. Co-PI's developing plasma based material around INL application development training format.

Derek Gaston (INL) hosts a MOOSE workshop at Penn State, 4 April 2017

2 day hands on application workshop using Darcy flow to introduce app development concepts

2 day hands on application workshop using validation efforts to introduce plasma app development (EM, chemistry, fluids, etc.)

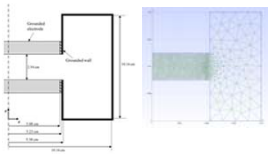




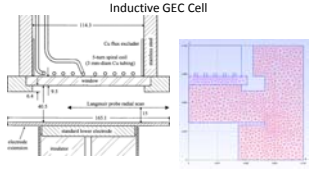
Validation plan:

use well established reference reactors employed by plasma community

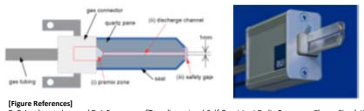
Capacitive GEC Cell



Inductive GEC Cell



COST APPJ



C-GEC – high field sheath simulation
I-GEC – high density conditions, EM coupling
COST – complex chemistry, high pressure discharges

[Figure References]
D. P. Lymberopolous and D. J. Economou, "Two-dimensional Self-Consistent Radio Frequency Plasma Simulations Relevant to the Gaseous Electronics Conference RF Reference Cell," *J. Res. Natl. Inst. Stand. Technol.*, vol. 100, p. 473, 1995.
P. A. Miller, G. A. Hebner, K. E. Greenberg, P. D. Pochan, and B. P. Aragon, "An inductively coupled plasma source for the Gaseous Electronics Conference RF Reference Cell," J. Res. Natl. Inst. Stand. Technol., vol. 100, p. 427—439, 1995.
Golda, Held, Redeker et. al., "Concepts and characteristics of the COST Reference Microplasma Jet", J. Phys. D. Appl. Phys. 49 (2016) 084003

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APS physics