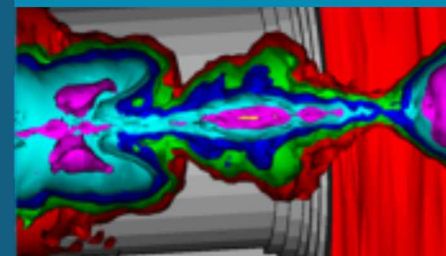
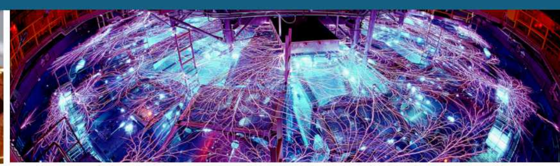
SAND2019-8647C

Multi-Scale, Multi-Physics Plasma Hybrid Algorithms, Modeling, and Simulations





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Goal of Initiative: address a need for multi-scale, multi-physics simulation capabilities that can treat real physics at the boundaries of plasma devices

Modern plasma physics devices, experiments, and problems of interest involve multiple physical processes occurring over a wide range of spatial, temporal, and plasma density scales:

- Often treated with a hierarchy of models to approximate the systems separately
- Have complex boundaries (i.e. plasmas coupled to electrodes)
- Involve non-equilibrium and non-Maxwellian plasma, not addressed in the fluid limit

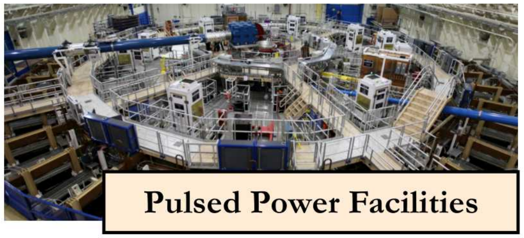
Electrode or wall boundaries are often approximated in simulations:

- Idealized (smooth, uniform, homogenous, passive, non-interacting, immobile)
- Do not include self-consistent particle or plasma evolution at the surface

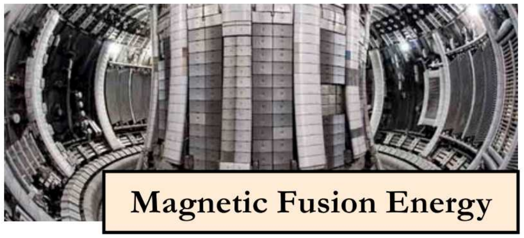
However, such boundary plasmas actually have a critical influence on the operation and performance of many plasma devices:

- Plasma containment systems (for magnetic fusion energy)
- High-energy particle accelerators, pulsed power facilities, etc.
- Industrial plasma technology, plasma arcs, etc.

We propose an initiative to develop multi-scale hybrid methods that simultaneously treat the transition from continuum (high density) to kinetic (low density) plasma regimes, resulting in a <u>plasma engineering design capability that would significantly advance the entire field</u>.



Pulsed Power Facilities



Magnetic Fusion Energy

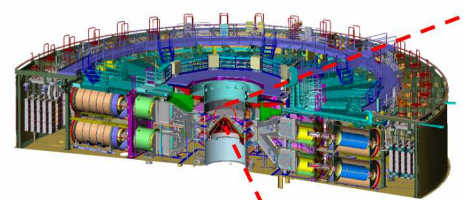
Accelerator Technology

Industrial Technology

Example: tera-watt class pulsed power machines generate electrode plasmas within the vacuum transmission lines

These electrode plasmas are:

- Non-thermal, non-neutral
- Relativistic, electromagnetic
- Three-dimensional, multi-scale



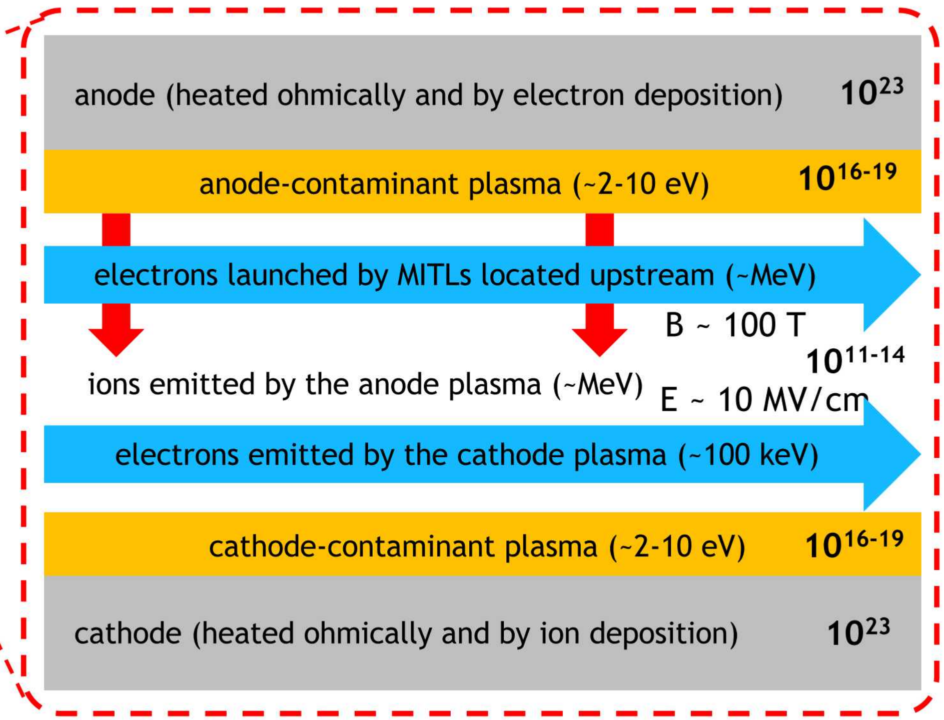
Simulations should account for:

- Energy deposition into the electrodes
- Neutral (contaminant) desorption and ionization
- Magnetization of the particles and plasmas
- Electron flow fraction and resulting loss
- Kinetic, MHD, and xMHD regimes, with collisions
- Electromagnetic waves

Validation experiments could measure:

- Coupled or transmitted current to the load
- Electrode heating; electron flow fraction and resulting loss; ion current
- Plasma onset, properties, and expansion; electric and/or magnetic fields

section of a “vacuum” transmission line at small radius



Example of multi-scale plasmas in a pulsed power accelerator crossing kinetic to continuum regimes

We propose an initiative that includes work to develop robust multi-scale plasma simulation approaches of general interest to the plasma community

Algorithm development to enable advanced plasma simulation:

- New algorithms to simultaneously simulate multi-fluid to kinetic density regimes; xMHD, asymptotic preserving
- Methods to reduce (or eliminate) the use of numerical density / conductivity floors
- Fast and scalable field preconditioners, solvers, and particle pushers
- Radiation transport, particle collisions, relativistic fluids, boundary layers, and plasma ionization kinetics

Multi-scale science for predicting electrode boundary effects:

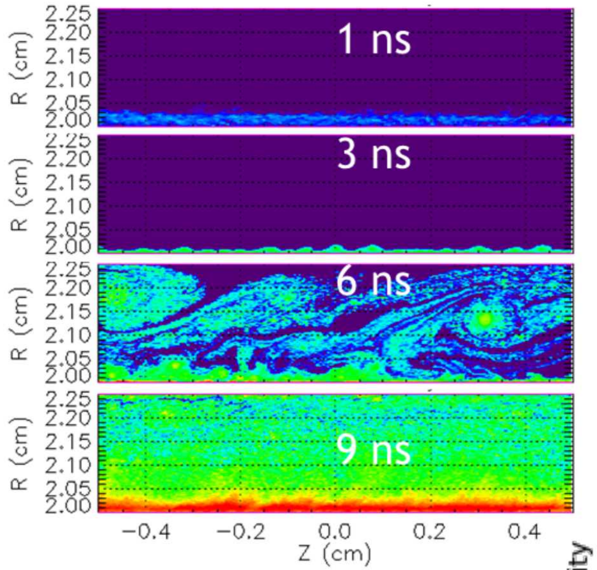
- Multi-material evolution with appropriate EOS (with of order 10 materials)
- Adaptive meshing to resolve boundary heating and energy deposition near surfaces
- DFT, MD, and/or GCMC techniques to improve understanding of contaminant desorption/wall vaporization
- Stimulated / thermal desorption from bulk/surface, melting / vaporization
- Ionization and recombination rate models to properly close physical models

Computational science and technology to ensure scalable simulation methods:

- Memory management techniques, including advanced particle merging methods
- Rapid meshing tools, including the ability to efficiently import CAD engineering models
- Zoning methods that smoothly treat complex device geometries
- Development of integrated research codes (and eventually production codes), born for next generation systems

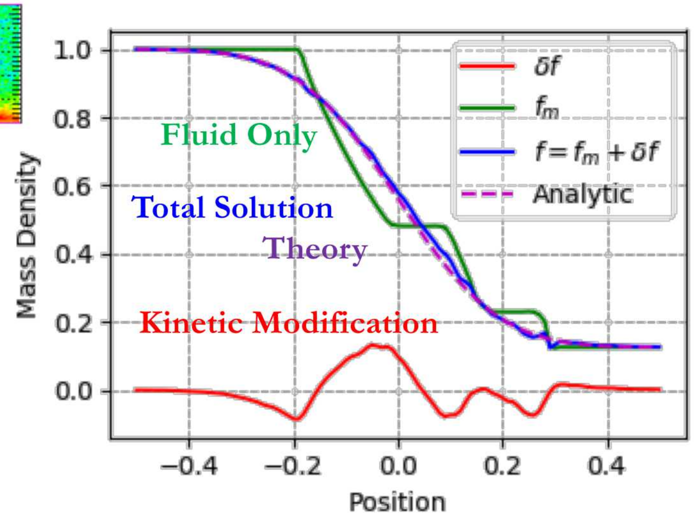
Sandia is funding a three-year "Grand Challenge" LDRD to stimulate lab-wide development of advanced plasma engineering models/codes

Desorbed neutral H_2, kinetic breakdown. 5 μm resolution.

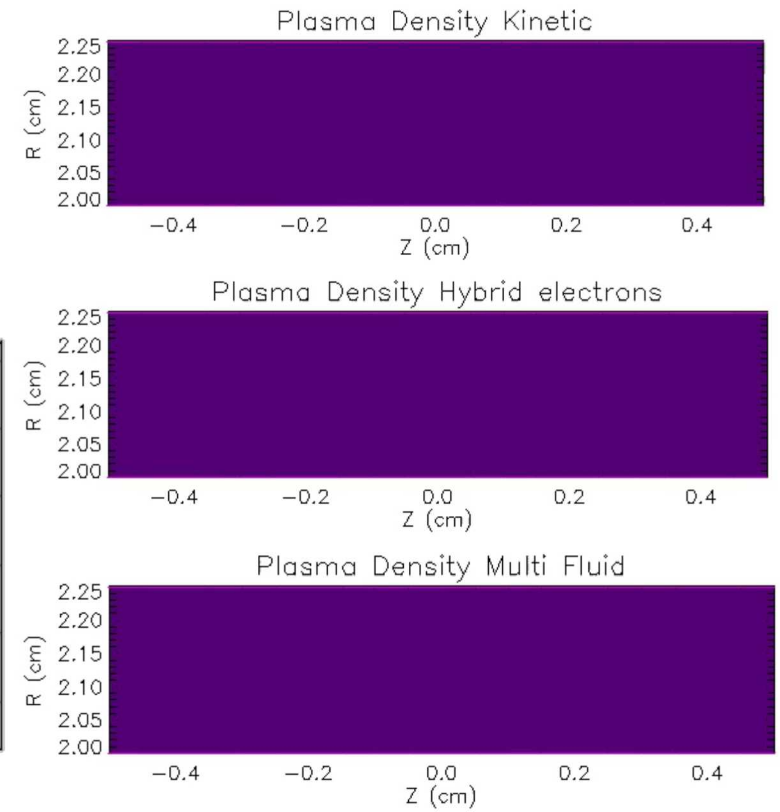


Evaluation of full kinetic breakdown models of electrode plasma using the CHICAGO research code Particle Migration Hybrid

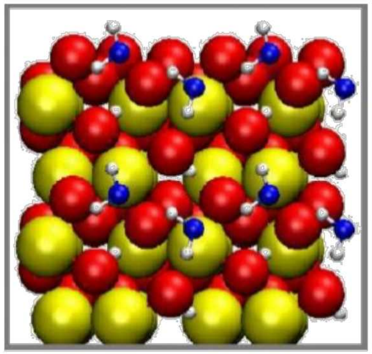
Calculation of an analytic shock problem using hybrid (δf) methods implemented in the EMPIRE research code



Evaluation of several simulation methods of electrode plasma growth using the CHICAGO research code Particle Migration Hybrid

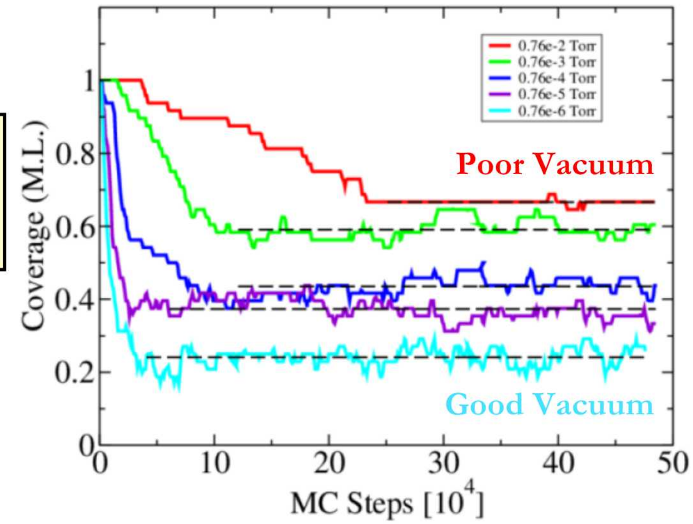


Sandia is funding a three-year "Grand Challenge" LDRD to stimulate lab-wide development of advanced plasma engineering models/codes



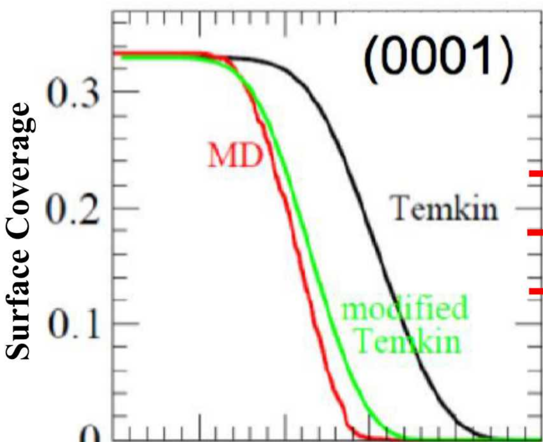
Density Functional Theory

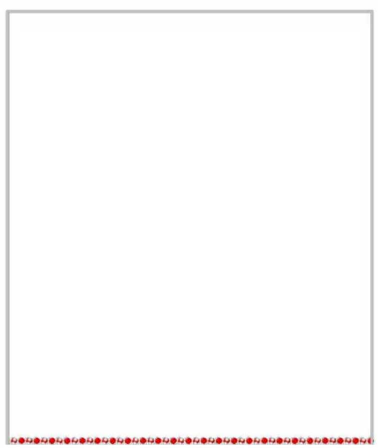
✓ Calculate the adsorption / desorption energies of contaminants (H_2O, CO_2, etc.) to steel surfaces (Fe_2O3, Cr_2O_3, etc.)



Grand Canonical Monte Carlo

✓ Calculate the amount of contaminant adsorption ("mono-layers") as a function of background vacuum

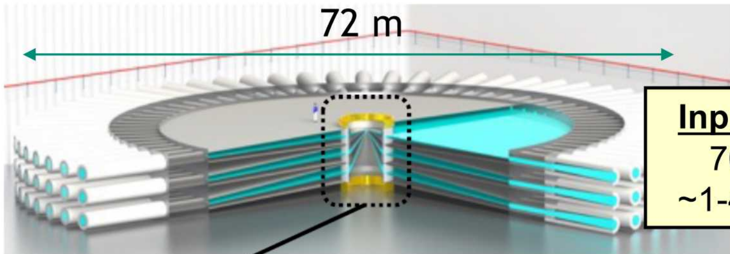


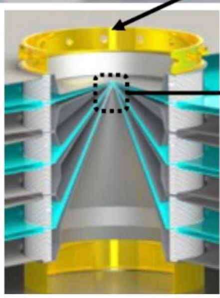


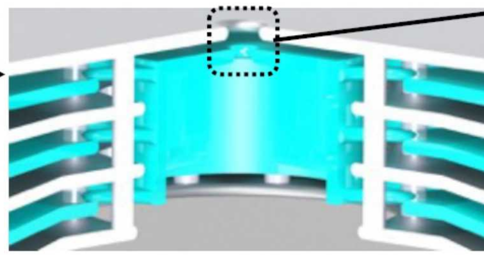
Molecular Dynamics

✓ Simulate the desorption of contaminants as a function of rapid current-induced surface heating ($2x10^9$ C/s)

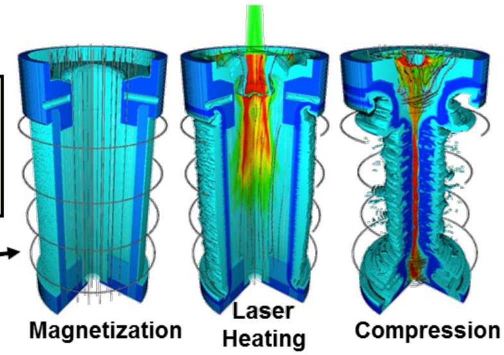
Example benefit: multi-scale simulation tools would enable improving the coupling of pulsed power drivers to HED targets for discovery science



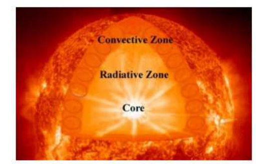




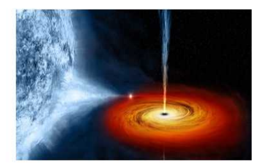
Input Conditions
70MA / 100ns
~1-4 PW Electrical



Output Conditions
30 PW D-T Neutrons
400 PW X-Rays

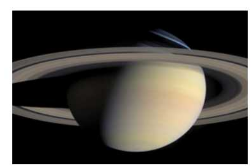


Discovery Science Experiments
- ✓ Fusion Ignition
- ✓ Astrophysics / Planetary Science
- ✓ Magnetized Plasmas
- ✓ X-Ray / Radiation Physics
- ✓ Dynamic Materials Science
- ✓ National Security Applications



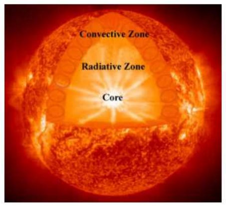
Driver / Source Design Principles
- ✓ Electromagnetics, Pulsed Power
- ✓ Mechanical / Electrical / Civil Engineering

Example Driver Uncertainties
- ✓ Electrode Plasma Formation / Expansion
- ✓ Current Loss



Pulsed Power Drivers are "Engines of Discovery": Five major discoveries in Astrophysics and Planetary Science within the Z Fundamental Science Program

Solar Model

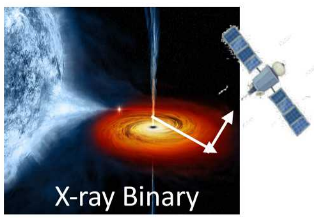


1 μg of stellar interior at R ~ 0.7Rsol

A higher-than-predicted measurement of iron opacity at solar interior temperatures

Jim Bailey, et. al., Nature **517**, 14048 (2015)

Black hole accretion



10^{-3} liters of accretion disk at R ~ 100 - 1000 km from black hole

Benchmark Experiment for Photoionized Plasma Emission from Accretion-Powered X-Ray Sources

G. P. Loisel, J. E. Bailey, et. al., Physical Review Letters **119**, 075001 (2017)

White dwarf photosphere

~0.1 liters of white dwarf photosphere

Laboratory Measurements of White Dwarf Photospheric Lines: Hβ

Ross Falcon, et. al., The Astrophysical Journal **806** (2015)

Planetary physics

2.5 - 7.5 μL (1.3 - 20 mg) shocked material

Implications for understanding Jupiter, Saturn, and thousands of exoplanets

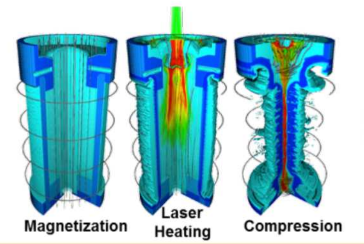
Direct observation of an abrupt insulator-to-metal transition in dense liquid deuterium

Marcus D. Knudson, Michael Desjarlais, et. al., Science **348**, 1455 (2015).

Impact vaporization of planetesimal cores in the late stages of planet formation

Richard D. Kraus, Seth Root, et. al., Nature Geoscience, DOI:10.1038/NGEO2369 (2015)

MagLIF
Magnetized Liner
Inertial Fusion



Experimental Demonstration of Fusion-Relevant Conditions in Magnetized Liner Inertial Fusion

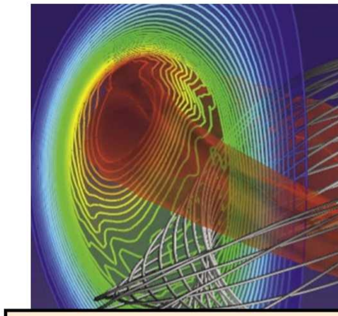
M. R Gomez, et al., Physical Review Letters 113, 155003 (2014)

30 nL of fusing magnetized plasma, B_zR>0.4 MGauss-cm, Te~3 keV

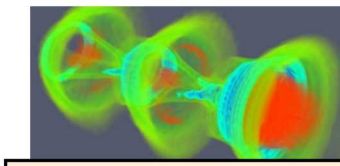
Example benefit: multi-scale simulation tools would be impactful to several areas of plasma technology development

Several reviews over the past decade have noted "multi-scale" or "hybrid" code technologies would be impactful:

- Magnetic Confinement (plasma/wall interactions, kinetic beam heating of fluid plasma, etc.)
  - 2010 NAS Report, "Plasma Science: Advancing Knowledge in the National Interest"
- Laser-Plasma Interactions (kinetic beam interactions with solid/plasma interface, etc.)
  - 2009 DOE OFES Advisory Committee Report, "Advancing HED Laboratory Plasmas"
- Low Temperature Plasmas (arc physics, industrial plasma processing, non-equilibrium, etc.)
  - 2012 J. Phys. D, "2012 Plasma Roadmap" (Review)
  - 2018 Plasma Sources Sci. Tech., "Foundations of Modelling Non-Equilibrium Plasmas" (Review)
- "Adaptive Kinetic-Fluid Models for Plasma Simulations on Modern Computer Systems", Kolobov and Deluzet, Frontiers in Physics, (2019)
- Applications to Accelerator Technology, Switching, High Voltage Engineering, etc.
- Fred Skiff, report Panel on Frontiers in Plasma Science on Tuesday, 7/23.
  - New algorithms, treating interfaces, and for multiple space and time scales
- Ellen Zwiebel, report Workshop on Opportunities in Plasma Astrophysics on Tuesday, 7/23.
  - Called for a plasma simulation computational effort on the scale of global climate modeling effort



Magnetic Confinement



Plasma / Beam Interactions

Industrial Plasma Applications

Requested funding, timeline, integration with exascale computing

Vision: A predictive plasma engineering design tool to enable more rapid progress than empirical approaches

- This is a large, decadal effort
- Existing and future DOE-funded exascale computing (on the floor in 5-10 years) would be used to develop these methods and simulations
  - simulations with scalable performance to encompass large fractions of future computing platforms
- Research and production codes tailored to a few large-scale problems of interest
- Requires multi-institution and multi-disciplinary collaborations to advance this research
  - funded via multi-institution proposals, $5-10 M/year total for up to 7-10 years
  - universities, national laboratories, industry partnerships
  - requires plasma physicists, mathematicians, computer scientists and engineering, nuclear engineers, materials science, chemists, atomic physics, etc.
  - validation experiments
- Also consider a Center for Computational Plasma Simulations ($3-5 M/year for 5 years, renewable once)

DOE National Laboratories

Industry Partnerships

University Collaborators

Flagship HPC Resources