Exceptional service in the national interest

SAND2016-1162PE

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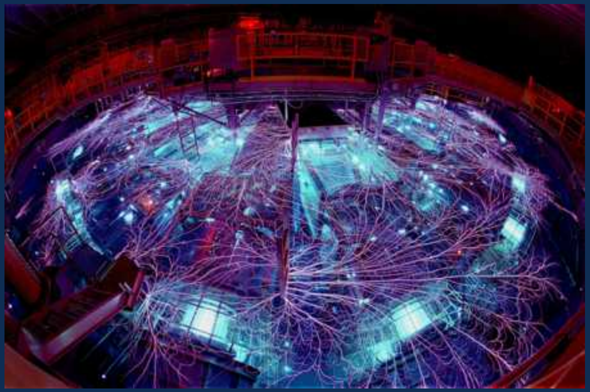

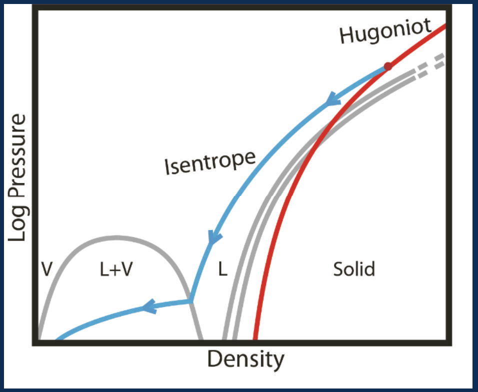

Sandia Interest and Capabilities in High Energy Density Physics

SAND2015- NNNNN C

Thomas Mattsson

Manager, HEDP Theory

2nd Joint Sandia-Georgia Tech Materials Workshop
Sandia National Laboratories Feb 10-11, 2016.

U.S. DEPARTMENT OF ENERGY · NNSA National Nuclear Security Administration

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MHD: currents and the corresponding magnetic fields can create high energy density matter

Current x magnetic field

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t}+(\mathbf{u}\cdot\nabla)\mathbf{u}\right)=\frac{\mathbf{J}\times\mathbf{B}}{c}-\nabla P\approx\frac{1}{4\pi}\mathbf{B}\bullet\nabla\mathbf{B}-\nabla\left(P+\frac{B^2}{8\pi}\right)$$

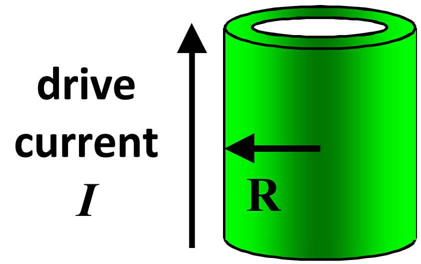
velocity field

Pressure

Magnetic field as scalar pressure

- Using pulsed power (current) as a source has advantages
  - *Can create high pressures without making material hot*
  - Generated over long time scales with control over the time history
  - Large samples and energetic sources (2 MJ to load of 20 MJ stored)
  - Low price - $4/Joule stored for refurbishment in 2007
- Integrated projects with theory/simulations/experiment
  - Develop, design, analyze, and optimize experiments

- 25 MA at 1cm radius is 1 Mbar
- 25 MA at 1mm radius is 100 Mbar



The current pulse on Z is tenfold compressed and then shaped depending on the experimental objective

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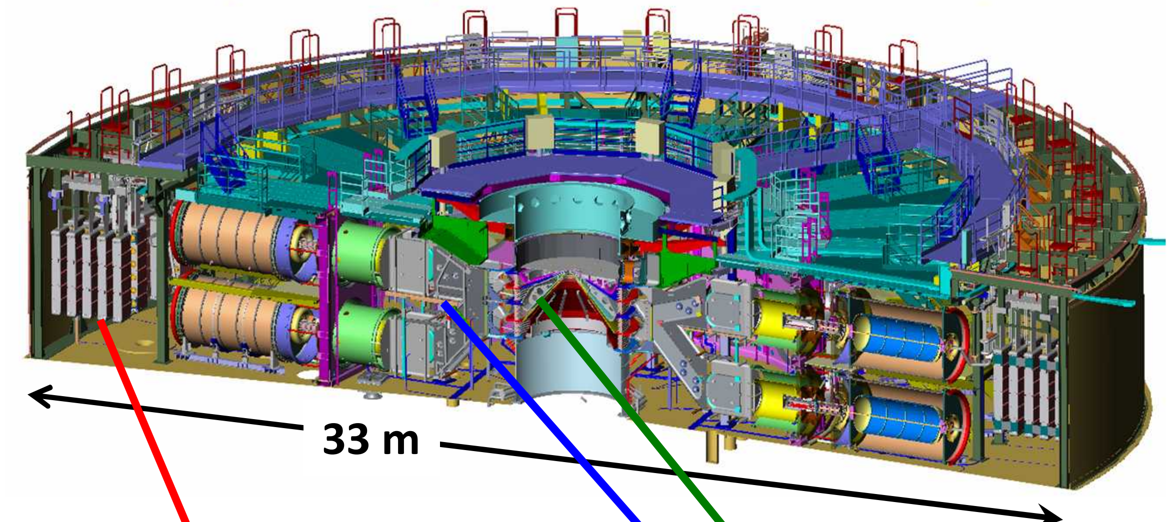
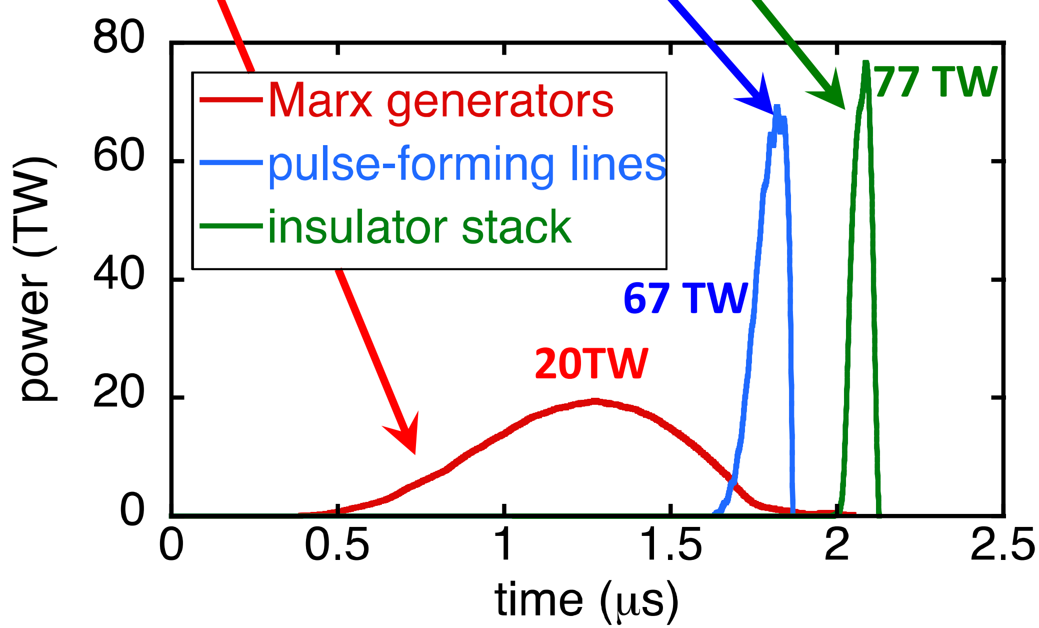


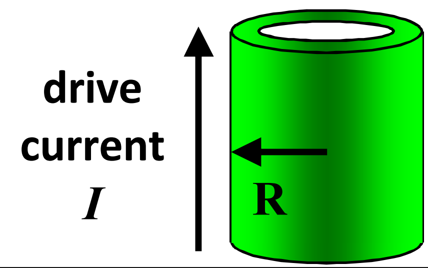
20 MJ stored on Z to:

0.5 MJ in MagLIF targets
0.1 MJ in DD fuel
1.5 MJ broad band x-ray
0.4 MJ Al K-shell x-ray



Magnetically Driven Implosion

$$P = \frac{B^2}{8\pi} = 105\left(\frac{I_{MA}/26}{R_{mm}}\right)^2 \text{ MBar}$$



100 MBar at 25 MA and 1 mm

We use magnetic fields to create HED matter in different ways for different applications

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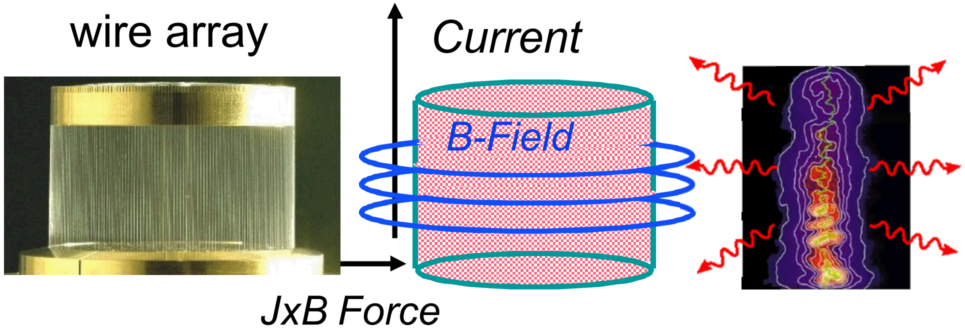
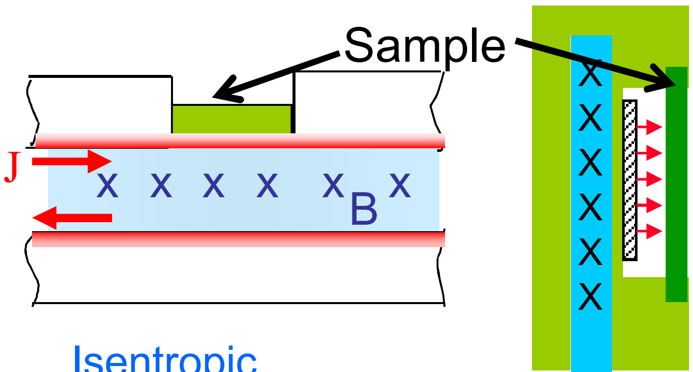
Radiation physics using Z-Pinch X-ray Sources



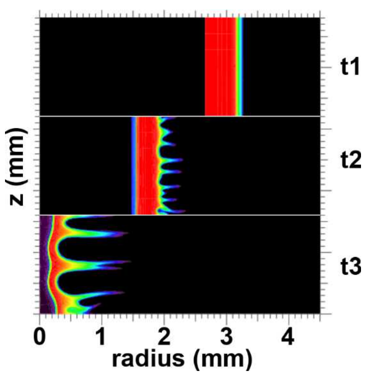
Materials Properties: EOS



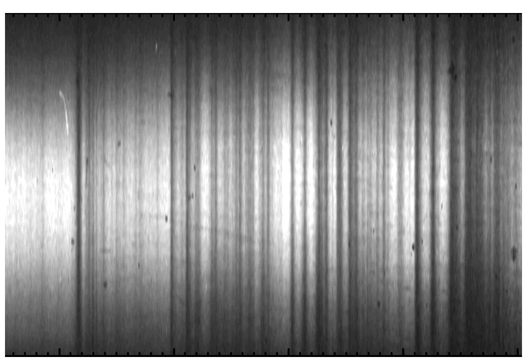
Isentropic Compression

Flyer Plate

Atomic- and plasma physics

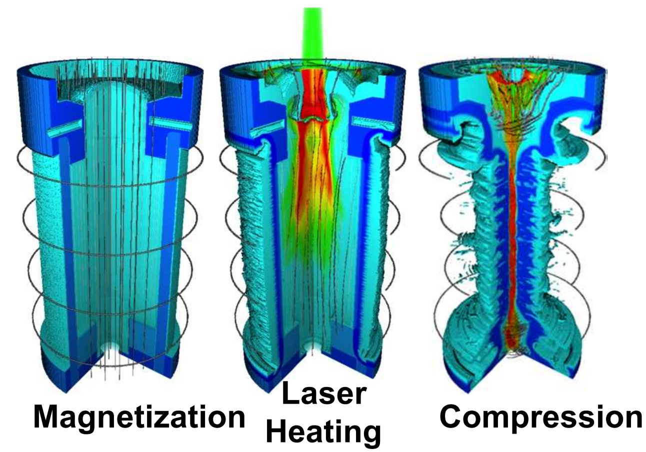


MRT instabilities



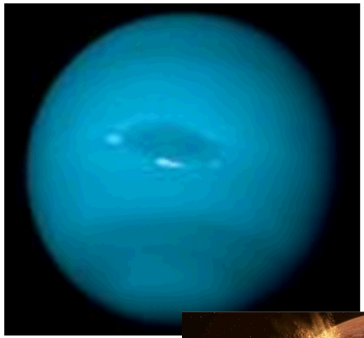
Iron spectrum

Inertial confinement fusion



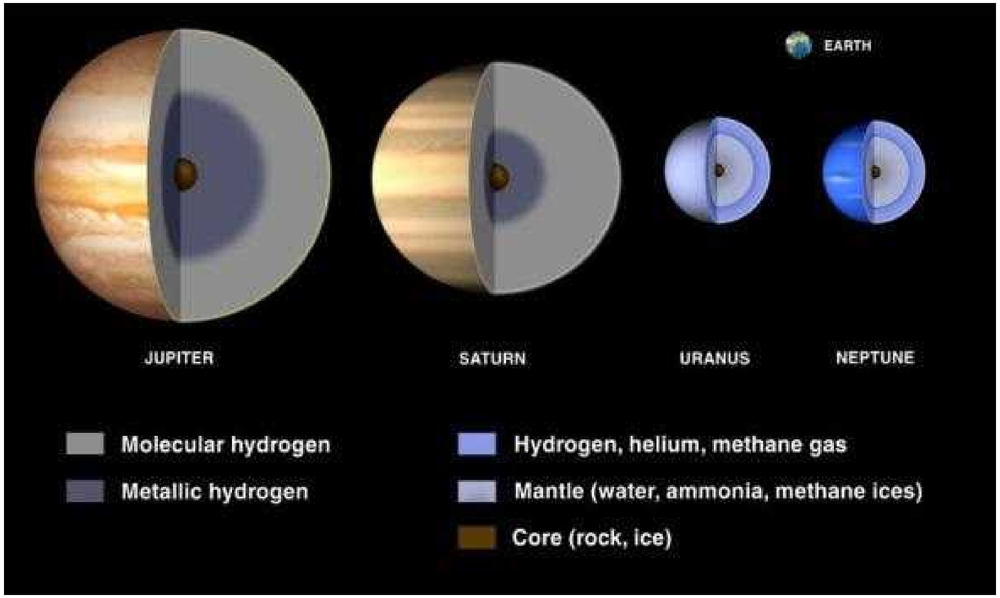
Properties of matter under HED (High Energy Density) conditions are important to many geophysical problems

- **Planetary science – Jupiter, Saturn, Uranus, Neptune, and exo planets [e.g. hot Neptunes]**
  - Water in 2005-2012: 2 Phys Rev Letts and 2 Phys Rev B
  - Metallization of hydrogen/deuterium: Science 2015
- **Planetary science – earths and super-earths**
  - Silicates, MgO (Phys. Rev. Lett. 2015), and iron/iron alloys
  - Determining the vaporization threshold for iron – and implications for planetary formation, Nature Geoscience 2015.
- **Materials for Stockpile Stewardship, HED and inertial confinement fusion (ICF)**
  - Investigating the periodic table from Aluminum to Zirconium: a broad range of materials are of interest - a talk in itself
  - *The programmatic work drives precision – we rely on the data!*



We have turned planetary science *quantitative* by high fidelity modeling and high-precision experiments

Understanding the properties of hydrogen is crucial for understanding giant planets



- **Present structure**
  - Layers of different composition while fulfilling observational constraints
- **Evolution**
  - Discrepancies in modeling the evolution of Jupiter and Saturn – the “Saturn age problem”
  - Why is Saturn so luminous?
- **Magnetic fields**
  - Origin of multi-polar fields in Neptune and Uranus

We have located the Liquid-Liquid Insulator-to-Metal Transition in deuterium to be a steep curve at 300 GPa

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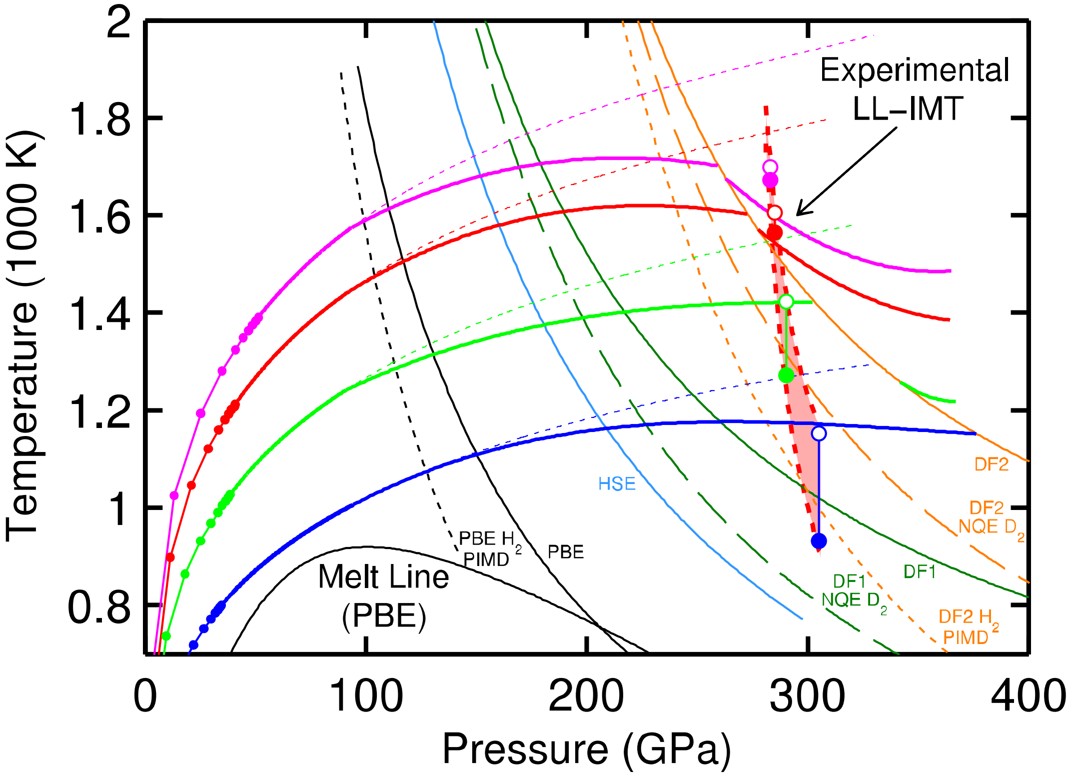
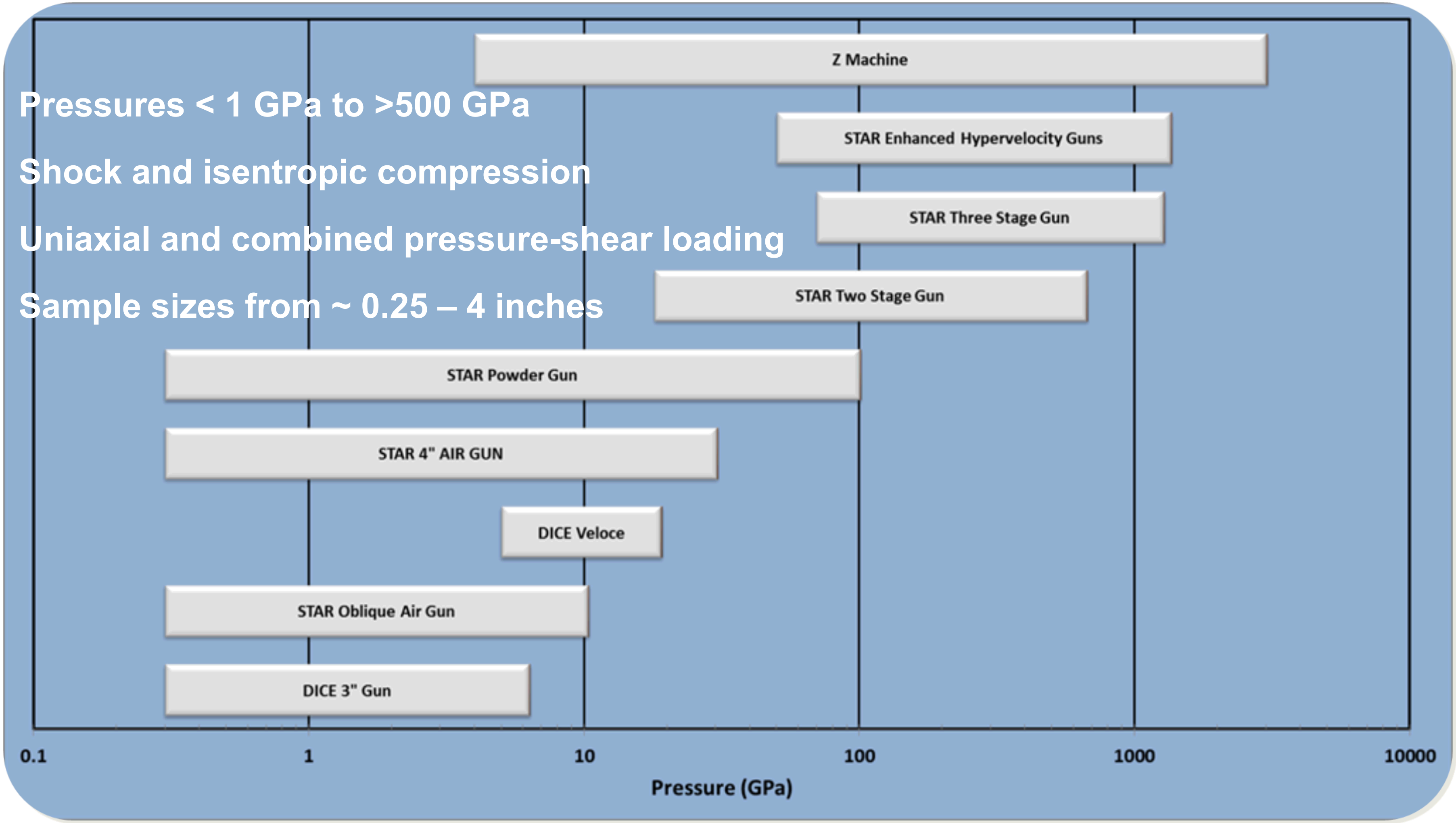


M.D. Knudson, M.P. Desjarlais, A. Becker, R.W. Lemke, K.R. Cochrane, M.E. Savage, D.E. Bliss, T.R. Mattsson, and R. Redmer, Science **348** 1455, 26 June 2015.

- **Experiments used a new shock + ramp drive to scan this space**
- ***Insensitivity to T suggests this is a ρ-driven transition***
  - ρ at the transition is inferred to be ~2-2.1 g/cc in deuterium
  - Qualitatively different transition than in shock experiments (T driven)
- **Broad team with expertise in diagnostics, pulse-shaping, experimental design, and first-principles simulations**
- **A project within the Z Fundamental Science Program**
  - Professor Ronald Redmer's group at University of Rostock

Sandia's dynamic material research facilities provide a wide range of compressive states

- Pressures < 1 GPa to >500 GPa
- Shock and isentropic compression
- Uniaxial and combined pressure-shear loading
- Sample sizes from ~ 0.25 – 4 inches



We seek a deep understanding of matter under extreme conditions – sets the research directions

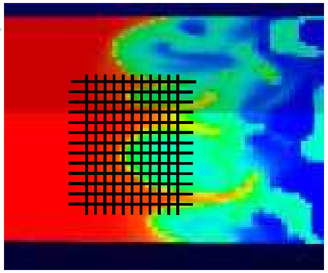
- **Multi-Mbar experiments on a broad range of materials**
  - **Shock- and ramp experiments**
    - **Shock – high temperature states**
    - **Ramp – quasi-isentropic compression**
  - **Diagnostics of HED conditions**
- **Modeling and simulations of materials and processes**
  - **Design, optimization, and analysis of experiments using multi-physics codes**
  - **First-principles simulations (Quantum Monte Carlo, Density Functional Theory, and more) for materials properties**
  - **Large-scale molecular dynamics of microphysics towards mesoscale**
  - **Development of material models – for use in multi-physics codes**

The strong integration between theory and experiments delivers a unique perspective

Backup slides

Magnetohydrodynamic simulations are coupled with experiments

Hydrodynamics

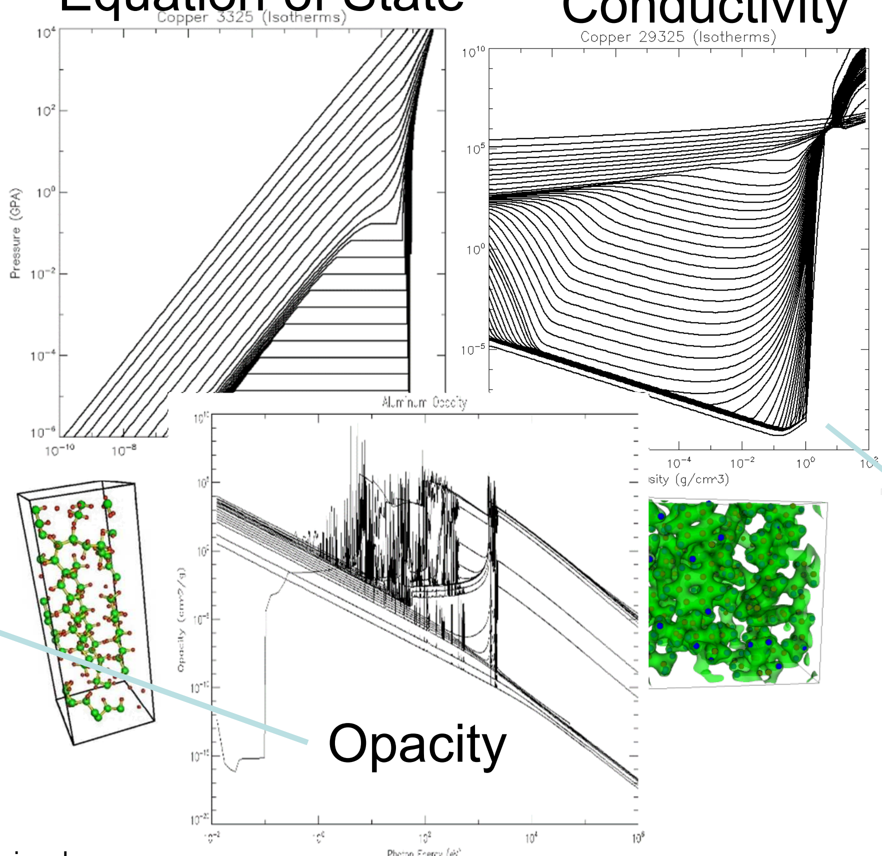


Tom Haill, SNL

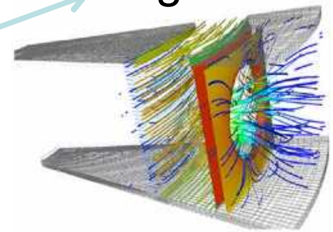
The hydrodynamics moves material based on the material properties.

Equation of State

Conductivity



Magnetics

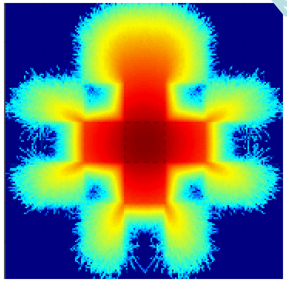


Chris Garasi, SNL

Conductivity determines magnetic
field diffusion.

Most simulation codes will tally the total energy in each cell and, based on that energy and the density, compute a new pressure and temperature in preparation for the next hydrodynamic step.

Radiation

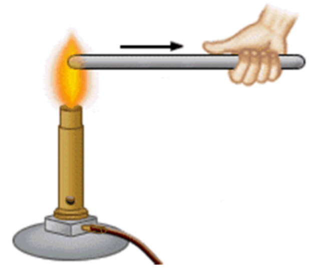


Tom Brunner, LLNL

Radiation is a key energy transfer mechanism in some systems

Opacity

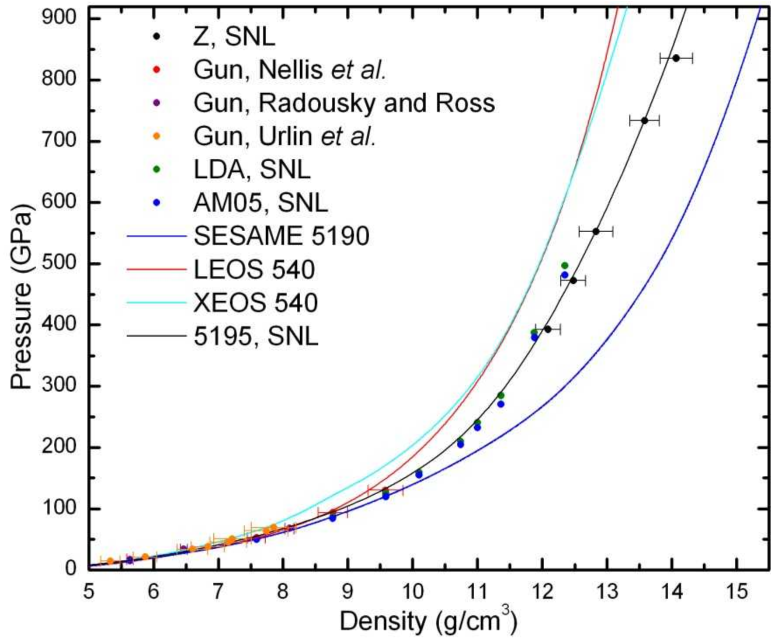
Conduction



Thermal conduction augments the movement of energy in a simulation.

Nuclear Mathematical and Computational Sciences: A Century in Review, A Century anew

We have seen tremendous scientific impact over the last ten years in combining high-fidelity theory/simulations/experiments



*Shock Hugoniot in xenon **predicted** by DFT/QMD (calculations by Rudy Magyar, experiments by Seth Root: PRL 2010)*

This DFT-MD based response of xenon were a true prediction – published before the experiments

- *Predictive* DFT-MD simulations are transforming the design and interpretation of Z experiments
  - SCIENCE **322**, 822-1825 (2008)
  - ICARUS **211**, 798 (2011)
  - Phys. Rev. Letts.
    - 2006, 2007, 2008, 2009, 2010, 2011, 2012, 2013, 2015
  - SCIENCE **348**, 1455 (2015)
  - Many articles in PRB, PoP, JAP, JCP, etc.

We perform multi-scale research – ranging from quantum mechanics to new advanced Magneto Hydrodynamics theory, -algorithms, and –codes.