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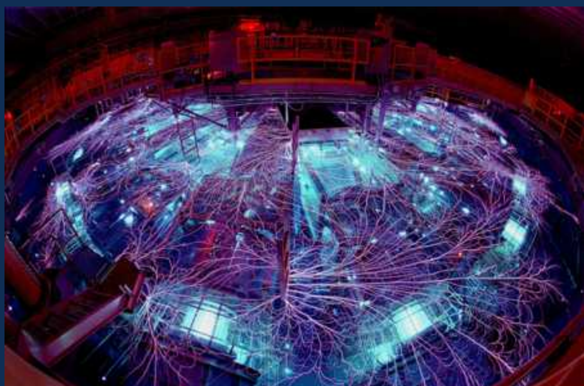
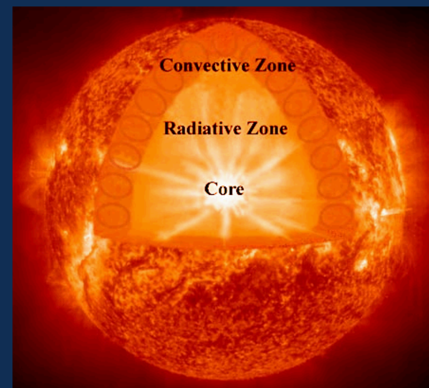
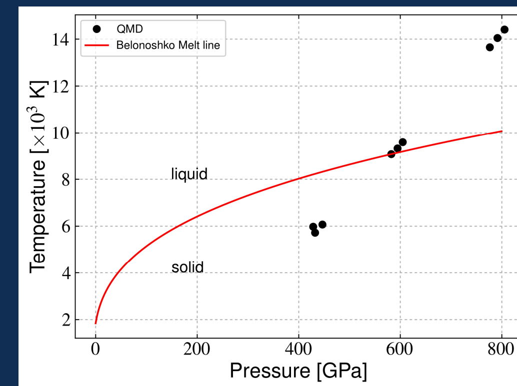






Leveraging Capabilities of the National Laboratories and Academia to Understand the Properties of Warm Dense $MgSiO_3$

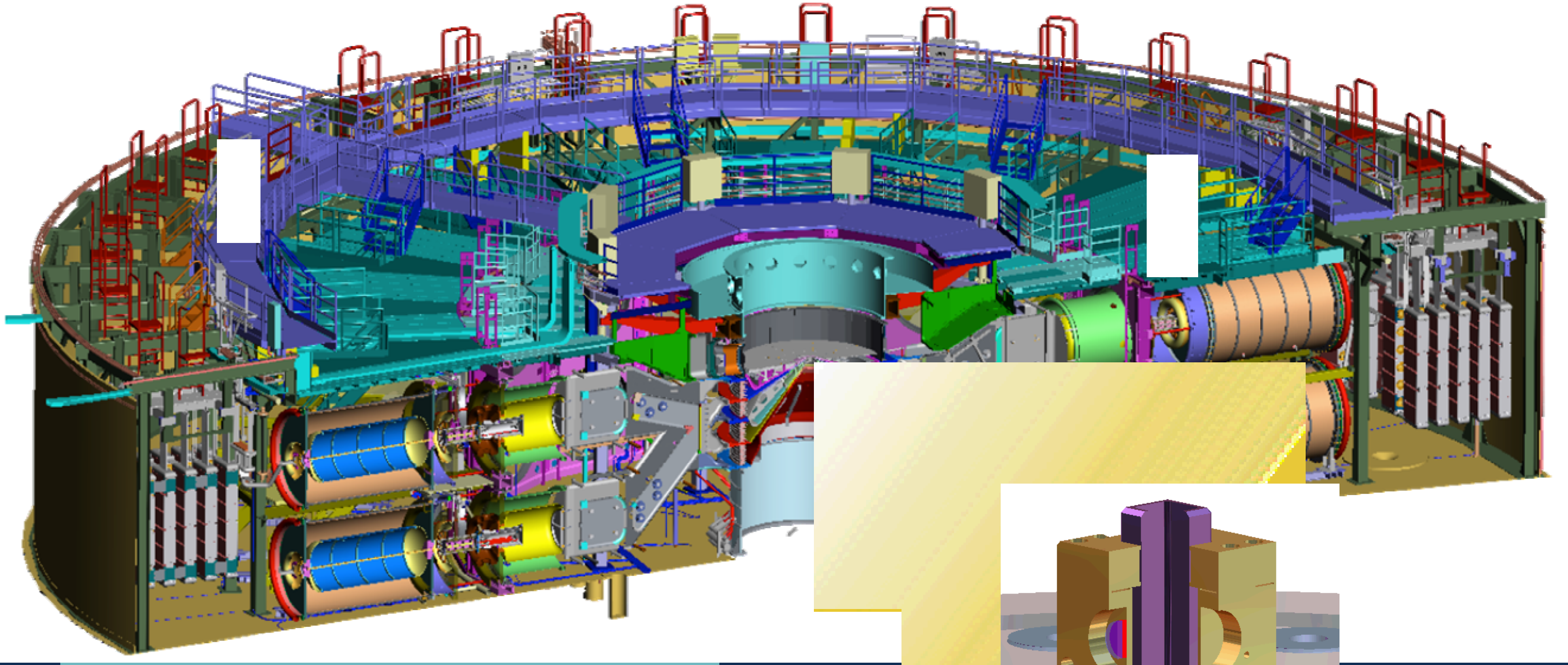
Thomas R. Mattsson, J. P. Townsend, L. Shulenburger, C.T. Seagle, M. Furnish (Sandia National Laboratories)

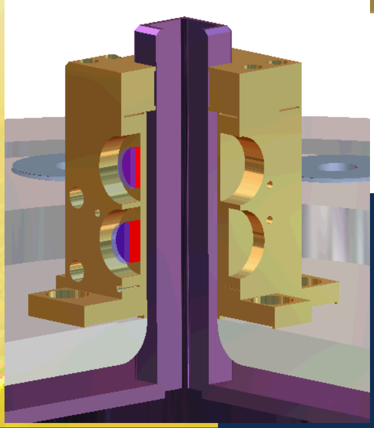
Y. Fei (Carnegie Institution of Washington)

SAND2017- C

Shock Compression of Condensed Matter 2017
St. Louis, MO

Sandia's Z Machine is a unique platform for multi-mission research on high energy density (HED) environments





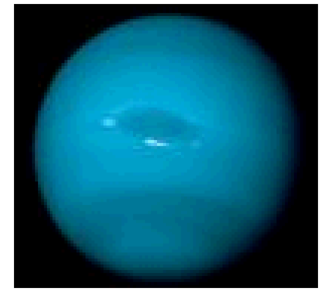
of State

- Pulsed Power Technology
- Magnetically Driven Implosions
- Inertial Confinement Fusion
- Dynamic Materials

I ~ 26 MA, τ ~100-1000 ns
X-ray power > 250 TW
X-ray energy > 2 MJ

Properties of matter under HED conditions are important to many geophysical problems – a focus of the Z Fundamental Science Program

- **Jovian planets and exo planets**
  - Water: 2 PRL and 2 PRB; hydrogen metallization (Science 2015).
- **Earth and super-Earths**
  - Silicates (MgO PRL 2015), and vaporization threshold for iron with implications for planetary formation (Nature Geoscience 2015).
- **Why study Bridgmanite?**
  - $MgSiO_3$ Magnesium silicate perovskite is an abundant mineral phase in the Earth and likely a most abundant silicate mineral in super-Earths
- **Project goals**
  - Obtain density and sound speed of pre-synthesized bridgmanite at super-Earth mantle conditions.
  - Integrate results from static and dynamic experiments to improve data accuracy and range.
  - Apply the results to understand the internal mantle structure of Earth and super-Earths.

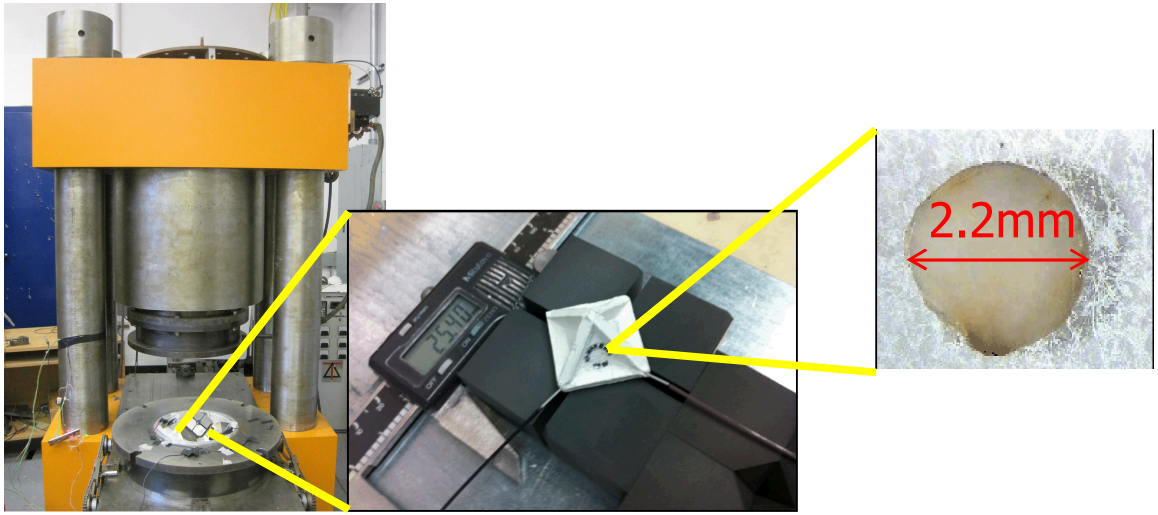


Our goal is to turn multi-Mbar planetary science quantitative by high fidelity modeling and high-precision experiments

Bridgmanite is meta-stable at normal pressure

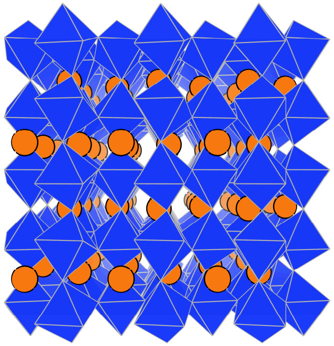
We use pre-synthesized bridgmanite to make target for Z-experiments to reach super-Earth conditions

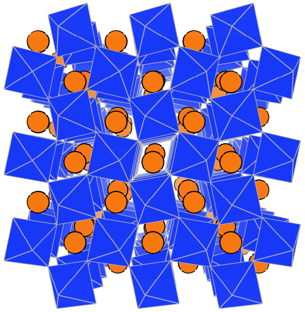
- Anvils: 1-in sintered diamond cubes
- Pressure: 25 GPa
- Temperature 1400 ˚C
- Sample size
  - 2.2mm in diameter
  - Adequate for Z experiments



Synthesis of bridgmanite in large-volume multi-anvil apparatus at Carnegie Institution of Washington, Washington DC.

Describing the electronic structure of materials from first principles – the power of DFT





Density Functional Theory (DFT)

- Quantum theory – Walter Kohn '98 Nobel prize in chemistry
- Molecular binding, ionization by pressure and/or temperature
- Now well-established in shock physics
  - Mike Desjarlais' work on D_2 in 2003 – *convergence is key*
  - Electrons with finite temperature k_BT and a Fermi distribution
- Efficient codes and big computers - hundreds of atoms for tens of ps

First-principles thermodynamics

- Internal energy, pressure, entropy, Hugoniot, sound speed, and structure/phases

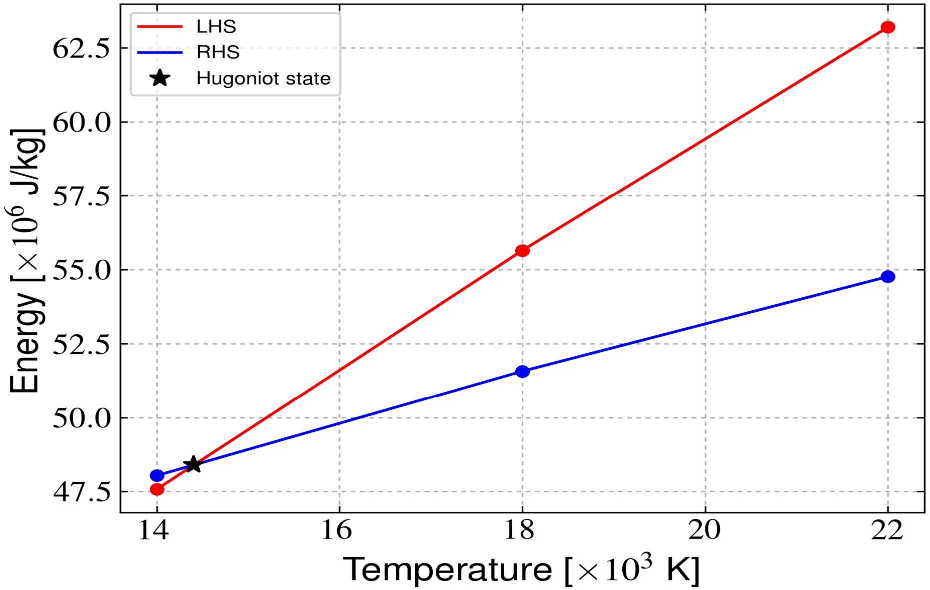
$$E - E_0 = \frac{1}{2}(P + P_0)(V_0 - V)$$ Hugoniot

$$C = V\sqrt{(P - P_0)\frac{\Gamma}{2V} + \left(\frac{dP}{dV}\right)_H\left[(V_0 - V)\frac{\Gamma}{2V} - 1\right]}$$ Sound speed

Calculate the internal energy and the pressure/volume relationship for the Hugoniot State

- **Computational details**
  - Initial state solid crystalline Bridgmanite at 4100 kg/m^3
  - Final state liquid
  - 160 atom unit cell
  - PBEsol exchange-correlation functional
  - Mean-value k-point (complex)
  - 800 eV plane-wave cutoff energy
  - PAW potentials
    - Mg $2p^6 3s^2$
    - Si $3s^2 3p^2$
    - O $2s^2 2p^4$
  - 1-5 picoseconds of simulations

$$E - E_0 = \frac{1}{2}(P + P_0)(V_0 - V)$$



Determining the Hugoniot state

Gruneisen parameter, dP/dV, and thus the sound speed is calculated as a finite difference

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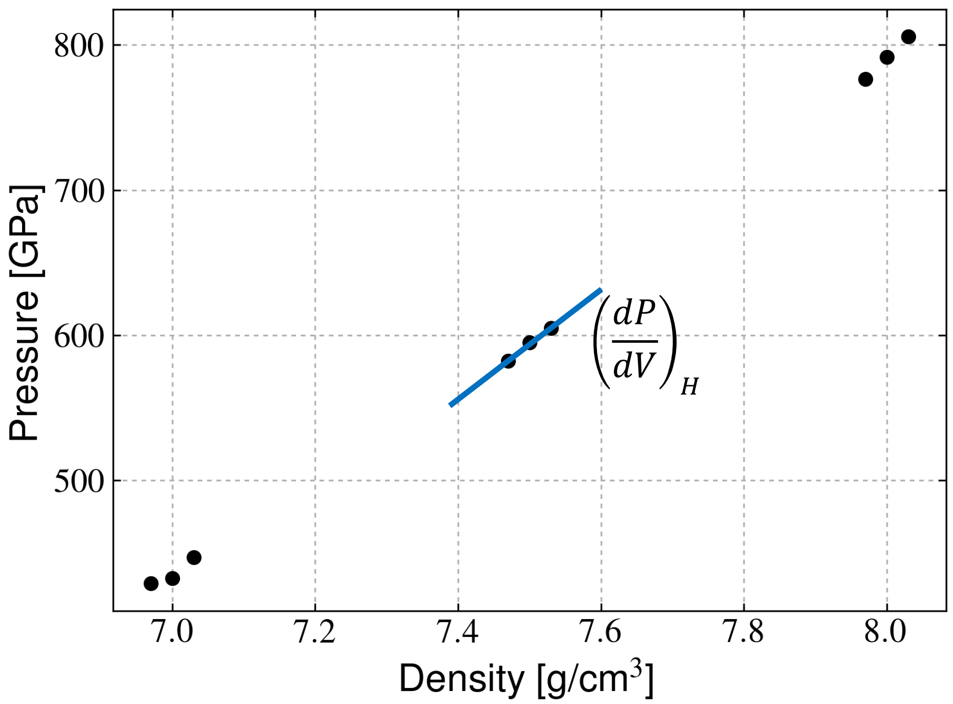

Calculating sound speed along the Hugoniot

Simulated Hugoniot points for Bridgmanite in the liquid phase predict the shock melting pressure

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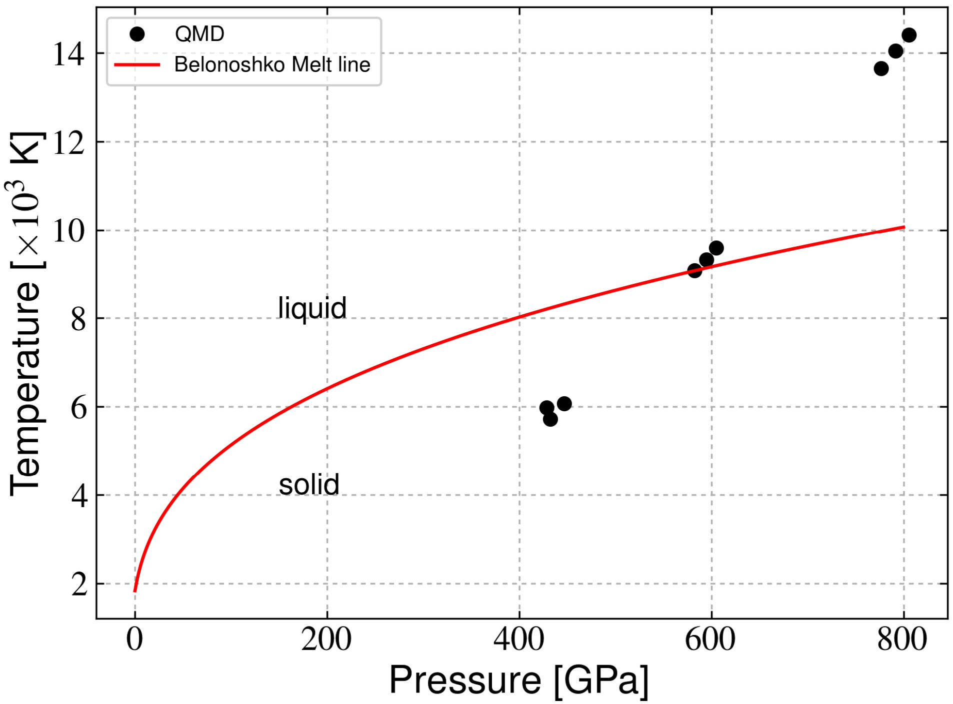
We predict melting along the Hugoniot at 600 GPa



Melt-line from A.B. Belonoshko et al PRL **94** 195701 (2005).

Calculated Hugoniot points for Bridgmanite in the liquid phase are in agreement with data

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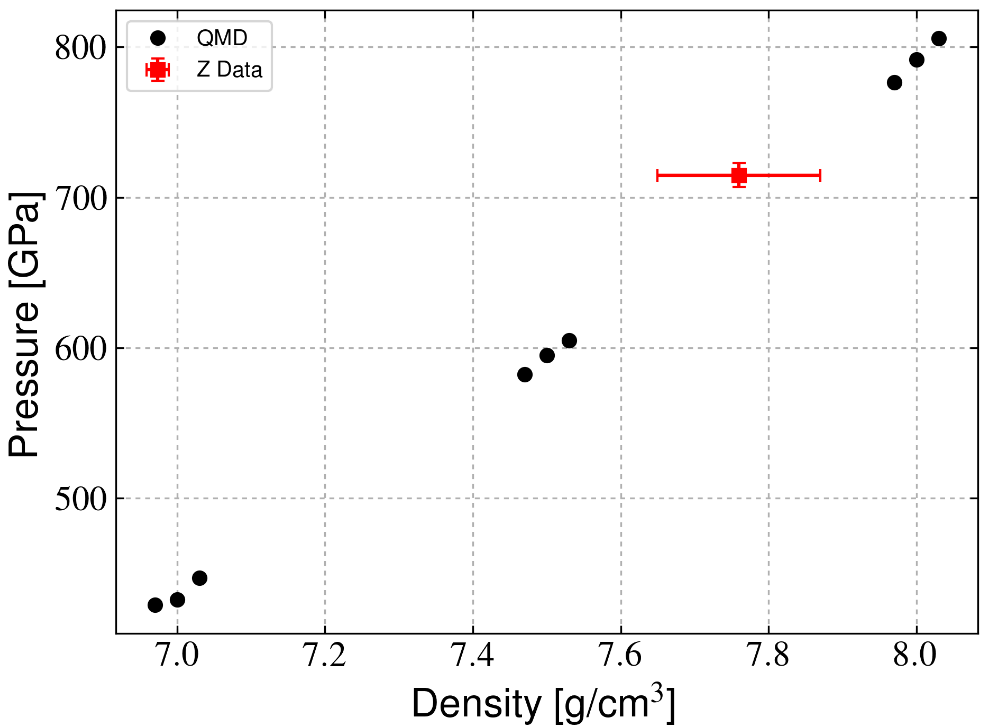
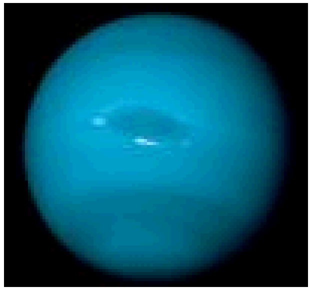
The first-principles results are in agreement with [preliminary] data from the Z-machine



Path forward – finalize experimental analysis and first-principles simulations, assess the impact on planetary structure



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Over the last 8 years, the Z Fundamental Science Program has developed into a key part of our research strategy

Timeline for the ZFSP

- 2009 – 1st IHEDS workshop in Santa Fe
- 2010 – 1st call for proposals
- 2013 – NNSA/NA-11 pause
- 2014 – Restart, review, and extension for 2015
- 2015 – 2nd call for proposals (2016 – 17)
- 2017 – 3rd call for proposals (2018 – 19)

- **Workshops**
  - 2009 – 2011, Santa Fe
    - IHEDS SNL/UT Austin – Alan Wootton
  - 2012, 14 – 17, Albuquerque
    - *"Research opportunities and user meeting"*

Call for proposals CY 18-19

The call is open and will close on September 15, 2017.

Contact me for details:
trmatts@sandia.gov

The Z Fundamental Science Program engages a broad international community and has advanced HED science

- **9 teams won shots on the 16-17 allocation**
  - Carnegie Institution of Washington
  - Lawrence Livermore National Laboratory
  - Sandia National Laboratories
  - UC Davis/ Harvard
  - University of Rostock, Germany
  - UN Reno
  - UT Austin x 2
  - Washington State University
- **Resources over 7 years**
  - 60+ dedicated ZFSP shots (5+ % of all Z shots)
  - Ride-along experiments on program shots
- **Science with far-reaching impact**
  - 1 Nature, 1 Nature Geoscience, 1 SCIENCE
  - 3 Phys. Rev. Lett, 3 PoP, PRA, PRB
- **Popular outreach**
  - National Public Radio, “All things considered”, Joe Palca 3/6/2014
  - Discover Magazine
    - Reportage 9/16/2012
    - *Iron rain #62 in top 100 Science stories in 2015*
  - Local TV coverage in 2015

Call for proposals CY 18-19

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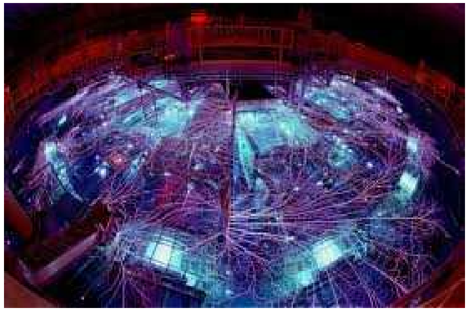
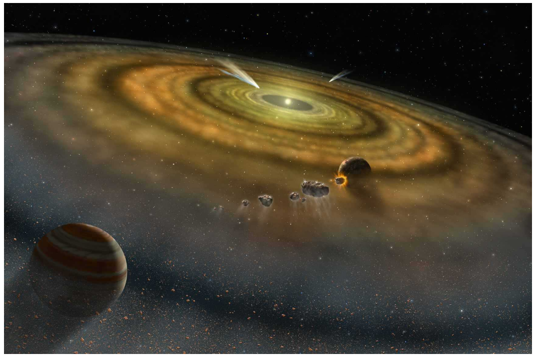
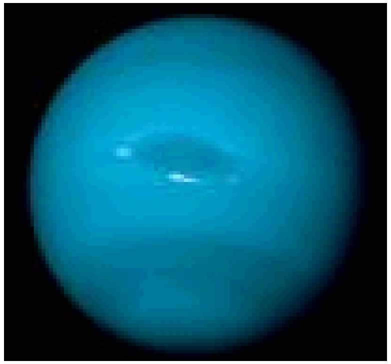
Pulsed power is exquisitely suited for HED science



- **Sandia's Z machine is ideal for Mbar material experiments**
  - Macroscopic samples and tens of ns timescale
  - Compression of solids and liquids
  - Obtain conditions of the interiors of gas giants, Earth, super-Earths, and other exoplanets



- **Strong integration between experiments, theory, and simulations**
  - From quantum mechanics to MHD and beyond



- ***Well-defined path for the future – decades of exciting HED Science research ahead***