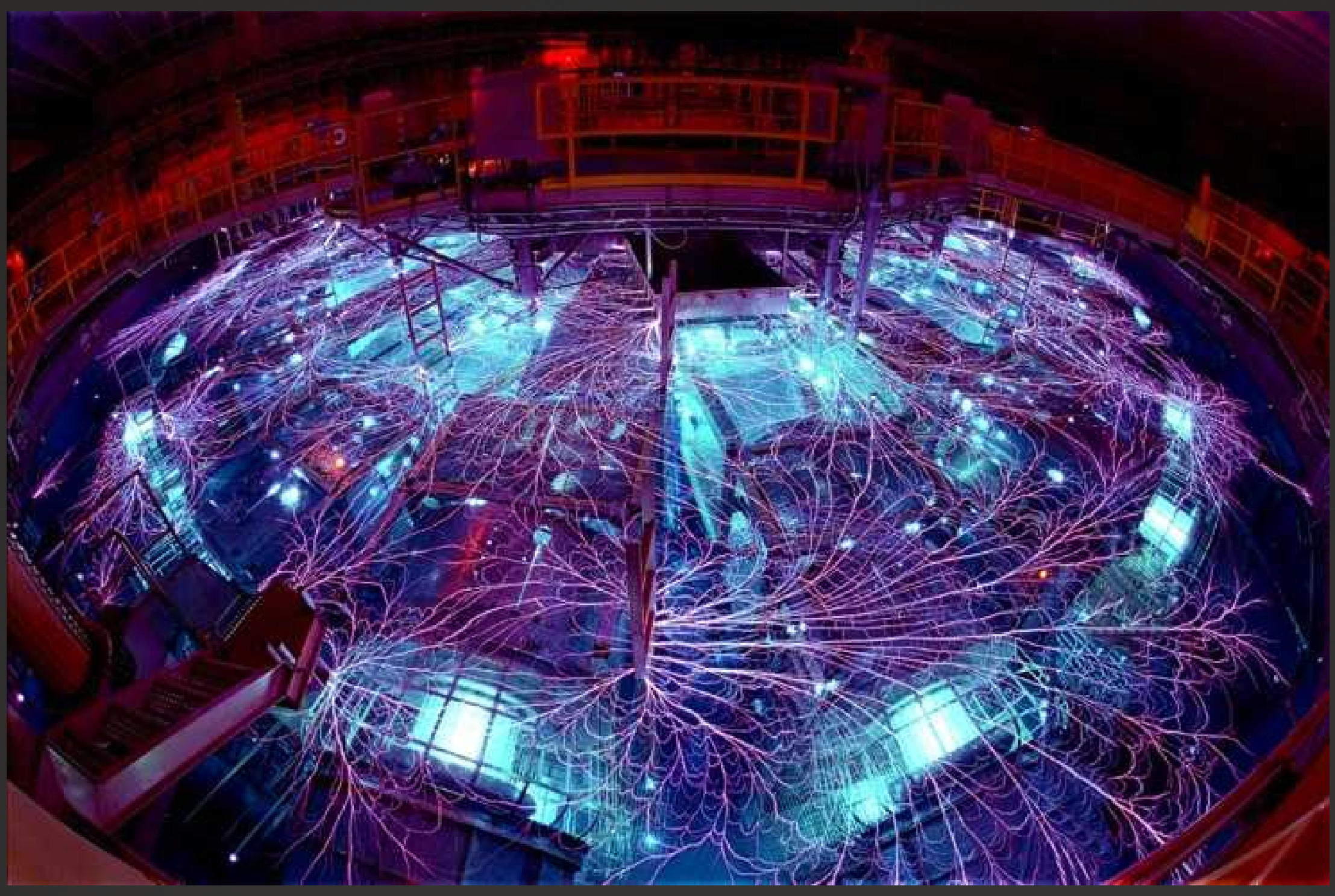
SAND2013-8184C

Quantum Molecular Dynamics Simulations of Materials



Many experiments are performed on Sandia National Laboratories' Z-Machine to understand materials or validate material models

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Thomas Haill, Ray Lemke,
Thomas R. Mattsson
Sandia National Laboratories

Resources: Chama, Pecos, Cielo, Redsky, Glory, Unity, Whitney

FUNDING AGENCY: Department of Energy

FUNDING ACKNOWLEDGEMENT: Office of Science of the U.S. Department of Energy under contract DE-AC02-06CH11357.

RESOURCE: chama, pecos, cielo, redsky, glory, unity, whitney

ALLOCATION: 10 Million Core-Hours

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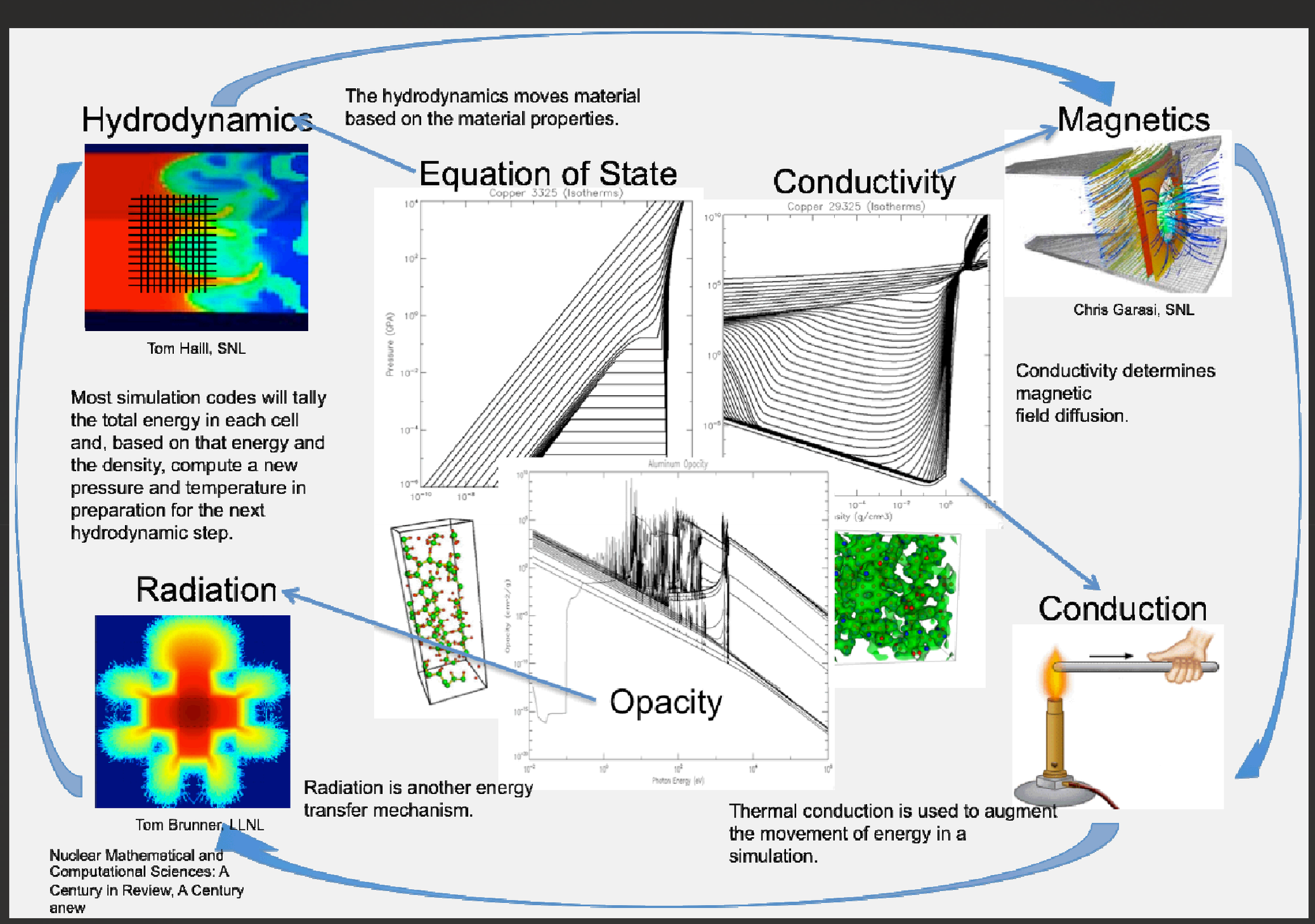
Using quantum molecular dynamics to build predictive equations of state



Radiation magnetohydrodyamics conduction codes and the split operator interaction with material models.

The importance of understanding materials and material models has become evident as experimental techniques have become more refined and our ability to interpret the results more astute. Until a few years ago, we could not predict even simple magnetically driven flyer plates[1]. However, by creating a more accurate Equation of State (EOS) and electrical conductivity model[2,3], ALEGRA was able to predict the velocity of an aluminum flyer with within 1% of its measured experimental value.

After this revelation, we have come to realize that the vast majority of our material models are inadequate outside of a few very narrow regimes, for example low pressure shocks or very high temperature, low density gasses. For some time, we used radiation magnetohydrodynamics conduction (Rad-MHD) codes to attempt to understand experimental behavior, but had limited success.

The increasing capability and capacity of computers has allowed us to begin calculating material properties using quantum molecular dynamics with a predictive accuracy (confirmed by subsequent experiments[4]), giving us confidence in our ability to create high fidelity material models that would allow Rad-MHD codes to also be more predictive. These models give us insight into the formation of giant planets, our moon, and capsules used at the National Ignition Facility (NIF) for fusion experiments.

[1] Lemke, Phys. Plasmas, vol 10, issue 4, 2003
[2] Desjarlais, Phys Rev. E, vol 66, issue 4, 2002
[3] Desjarlais, Contributions to Plasma Physicis, vol 41, issue 2-3, 2001
[4] Root, Phys Rev. B, vol 87, issue 22, 2013

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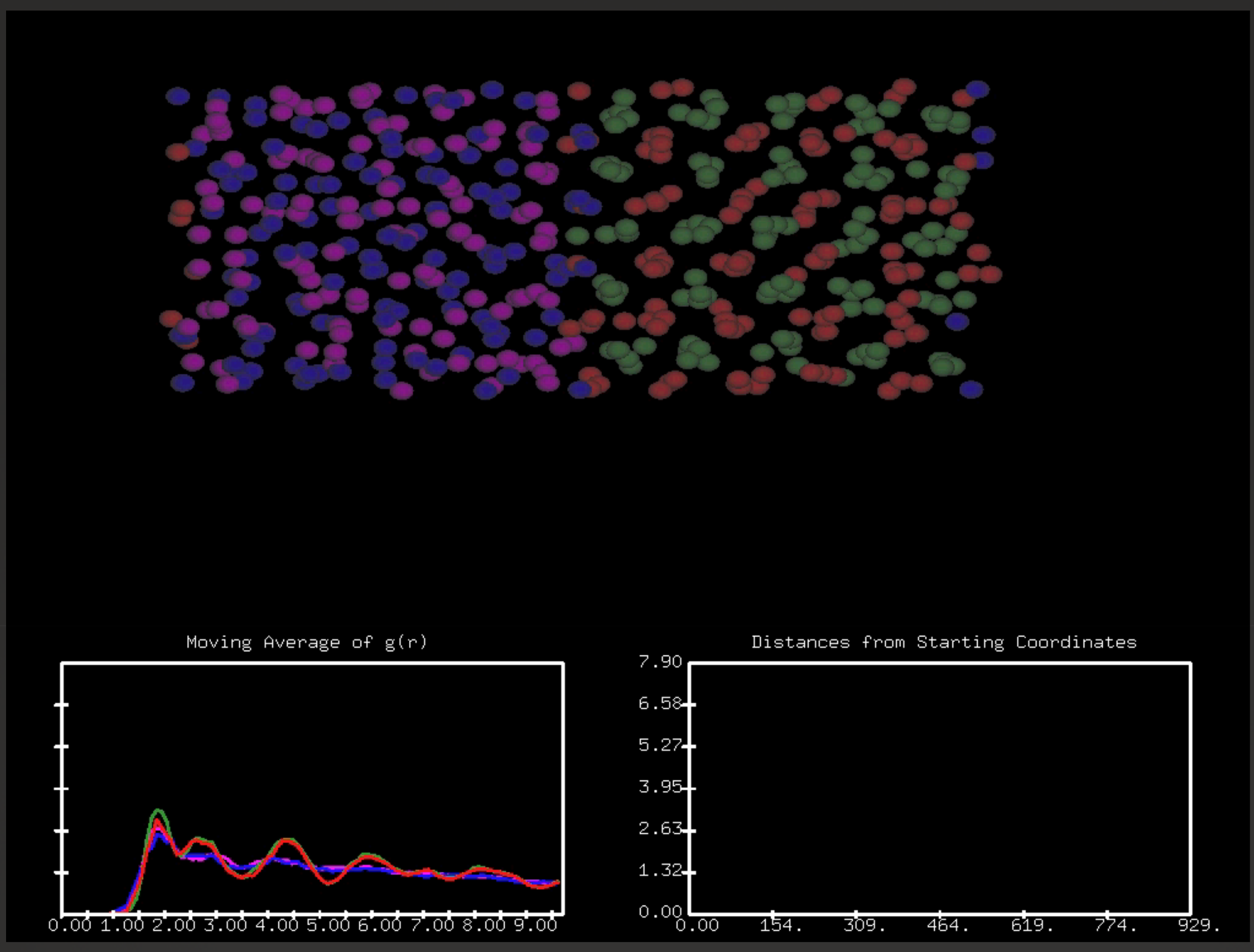
Quantum Molecular Dynamics: VASP



Two phase coexistence simulation of MgO. One side starts solid and the other liquid. Given time, one side will melt or the other solidify. Which of the two happens and the rate at which it does so can tell us a great deal about the melt transition.

The quantum molecular dynamics (QMD) code used in this analysis is Vienna Ab Initio Simulation Package (VASP)[5], where the Kohn-Sham equations[6] are solved in a plane-wave basis set. Projector augmented wave potentials[7] are used with LDA as the exchange and correlation functional. The molecular dynamics is performed in a two step process. VASP solves the Schrödinger equation for valence electrons and computes the stress tensor. The ions are represented by a potential and are point charges moved classically based on those forces. VASP then solves for the stress tensor again given the new positions. We continue to iterate until pressure and energy equilibrium is reached at which time we calculate the conductivity and opacity.

We can calculate a variety of material properties such as shock Hugoniot, isentropes, melt curve, critical point, cold curve, isotherms, conductivity, opacity, specific heat, bulk modulus, molecular dissociation, diffusion, viscosity, surface effects.

[5] Kresse, Phys Rev. B, vol 47, issue 1, 1993
[6] Kohn, Phys Rev., vol 140, 1965
[7] Blochl, Phys Rev. B, vol 50, issue 24, 1994

CO_2 shock Hugoniot calculation and experiments.The blue and red lines were the 2 previous equations of state designed from low pressure gas gun data. The green is the new equation of state based on QMD simulations which were validated by experiments.

Root, Phys Rev. B, vol 87, issue 22, 2013

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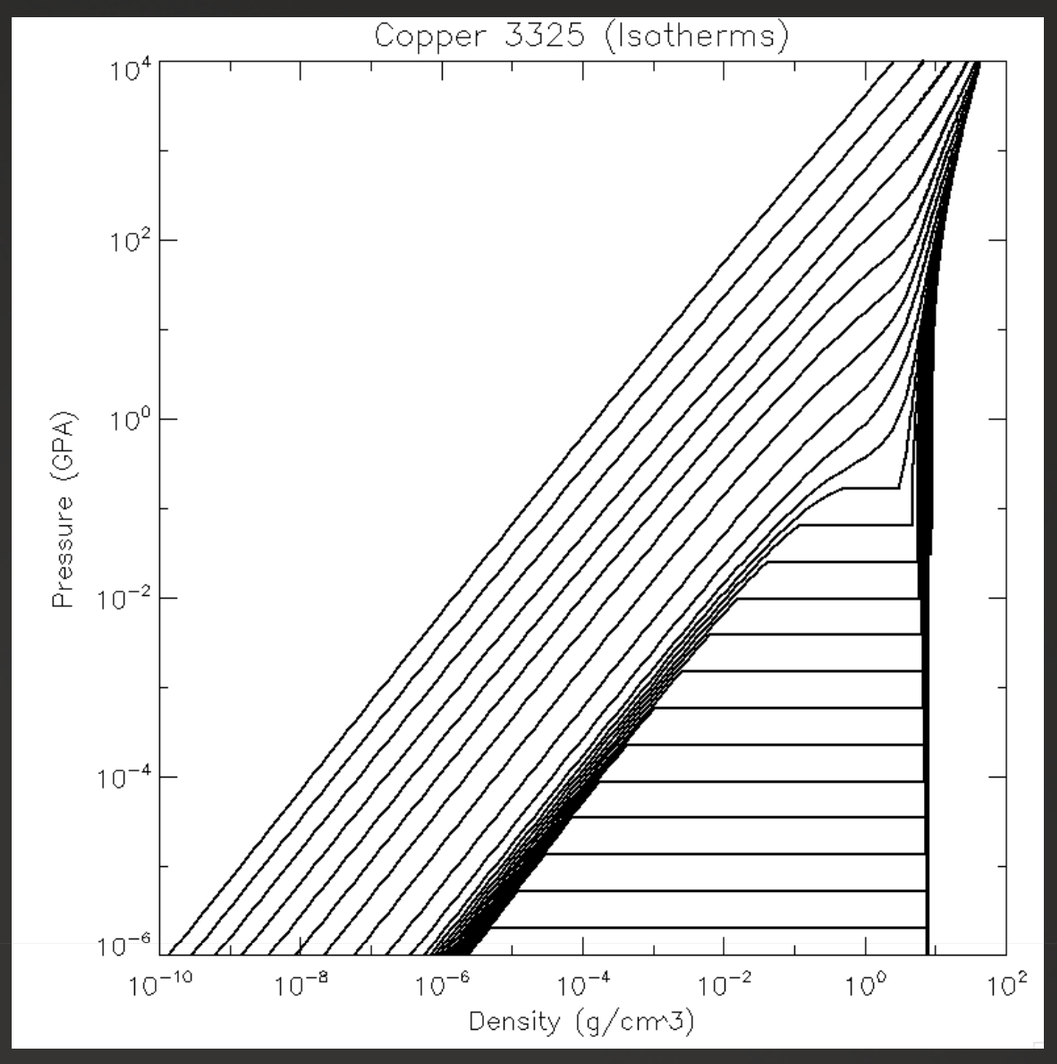
Creating material models takes millions of core hours each

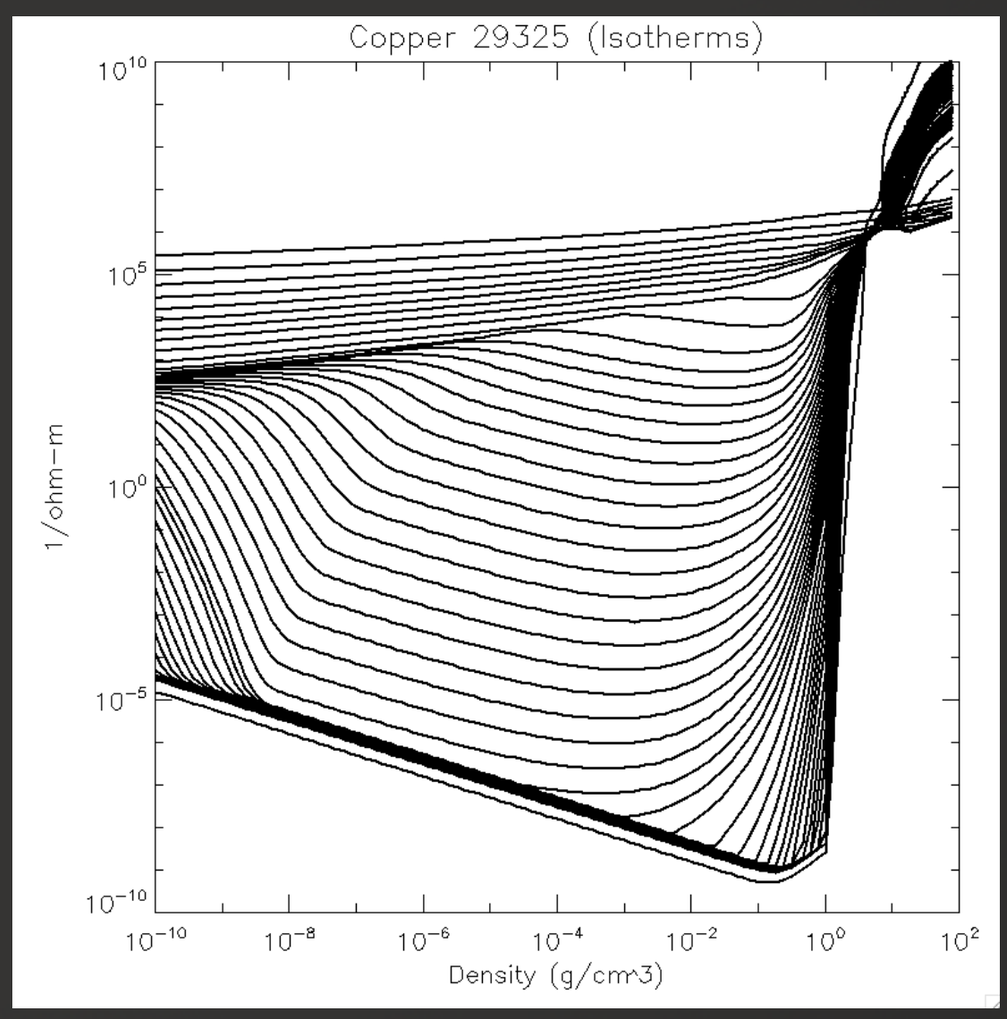
As seen in the previous slide, we can calculate material properties using VASP. However, to map out the minimum amount of phase space takes mullions of cpu hours. Each of the QMD points was between 50,000 and 100,000 cpu hours using between 500 and 100 cores. Melt curves are more difficult and take longer. As a general guideline, building one EOS or conductivity table used to take between 2M and 4M cpu hours and a years real time. With todays computers, we still need 2M to 4M cpu hours, but can now use that amount of time in only 3 to 6 months (depending on availability).

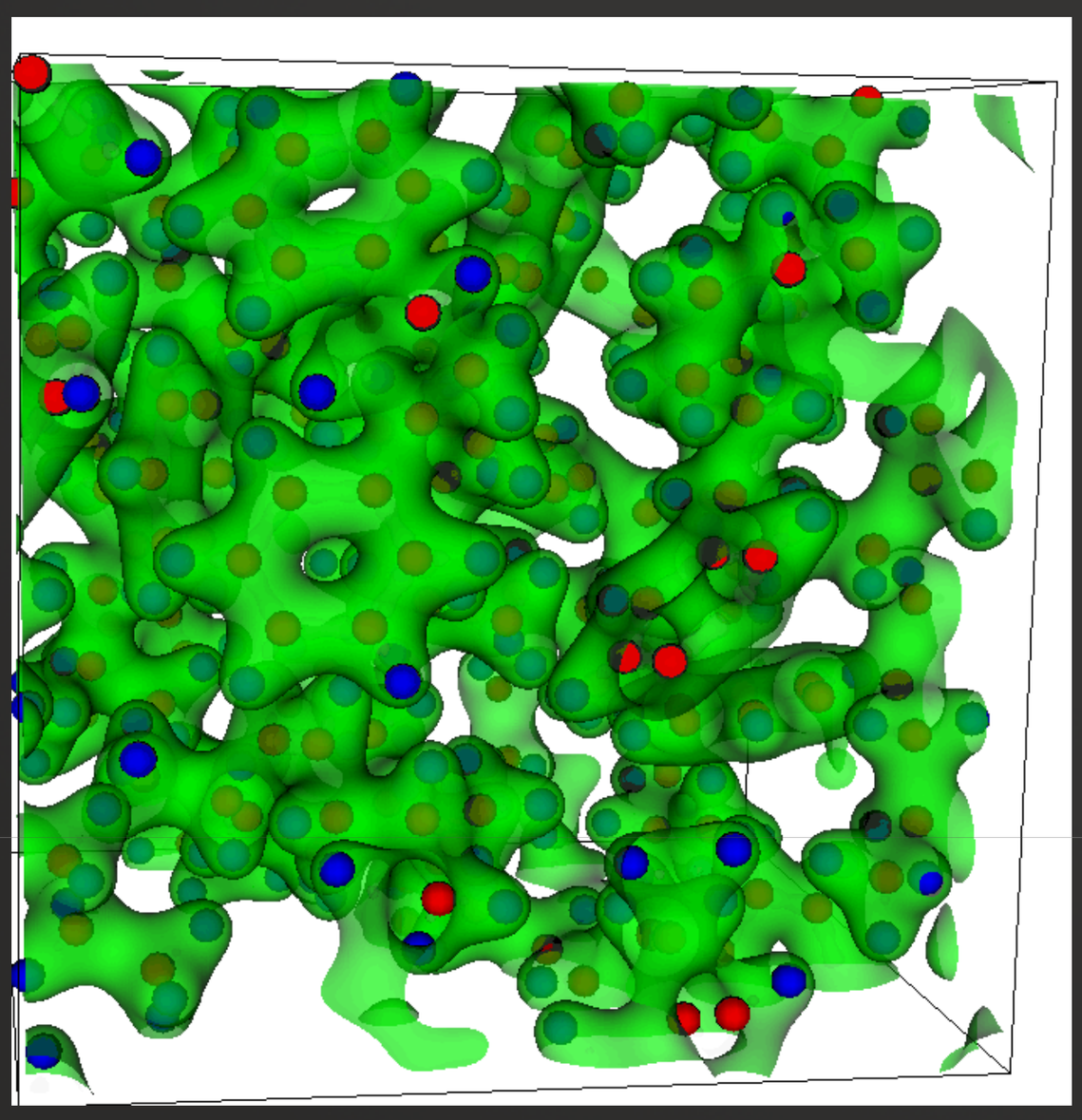
The larger capacity allows us to create multiple material models each year, and because of the speed, and communication (backplane) of these new computers, we can add more complexity to our simulations, allowing us to create material models that, only a decade ago, were more of a wish list.

One disadvantage is the cost of memory (RAM) for capacity computers. To bypass this problem, some of our simulations must be run with only half or a forth of the cores per node. So far, we have only needed to do this with some of our most difficult simulations and have gotten very good results. It is not optimal use of the machine, so we are selective on this type of simulation.



Above: Copper Equation of State. The lines are constant temperature lines mapping out pressure as a function of density. 3M cpu hours
Below: Copper conductivity isotherms. 4M cpu hours.





Isocharge surface of Glow Discharge Polymer (GDP) which is the material used in some fusion capsules. 1M cpu hours for the Hugoniot.

More complex materials take more time. Polymers in which we have to worry about chemistry require even more time because of the need to simulate chemistry time scales (picoseconds to nanoseconds) with a code that takes femtosecond time steps.

Also, we explore ever more difficult regions of phase space of increasingly exotic materials, our simulations require more RAM and time to ensure an acceptable level of understanding which we have come to expect for predictive material modeling.

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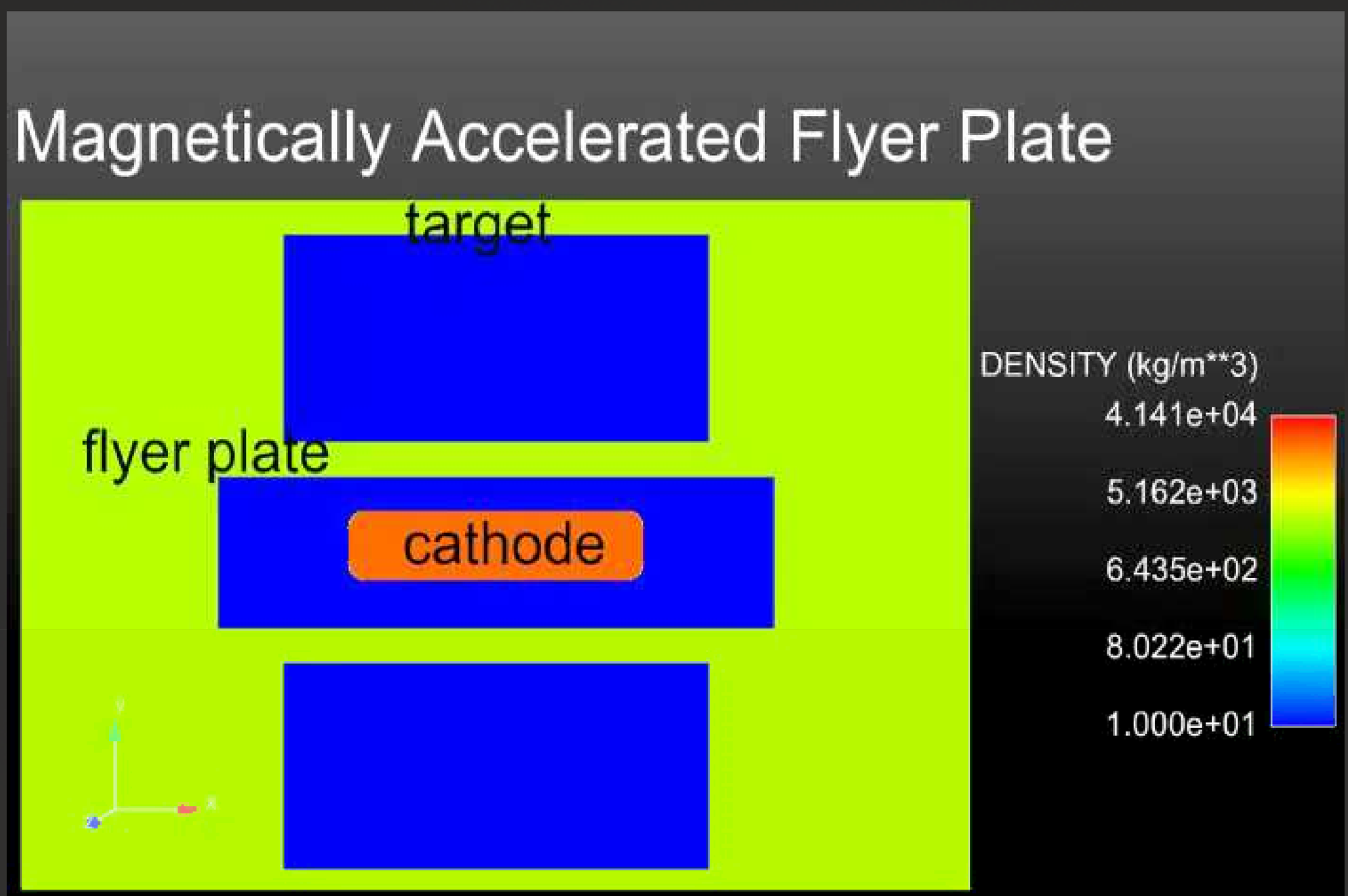
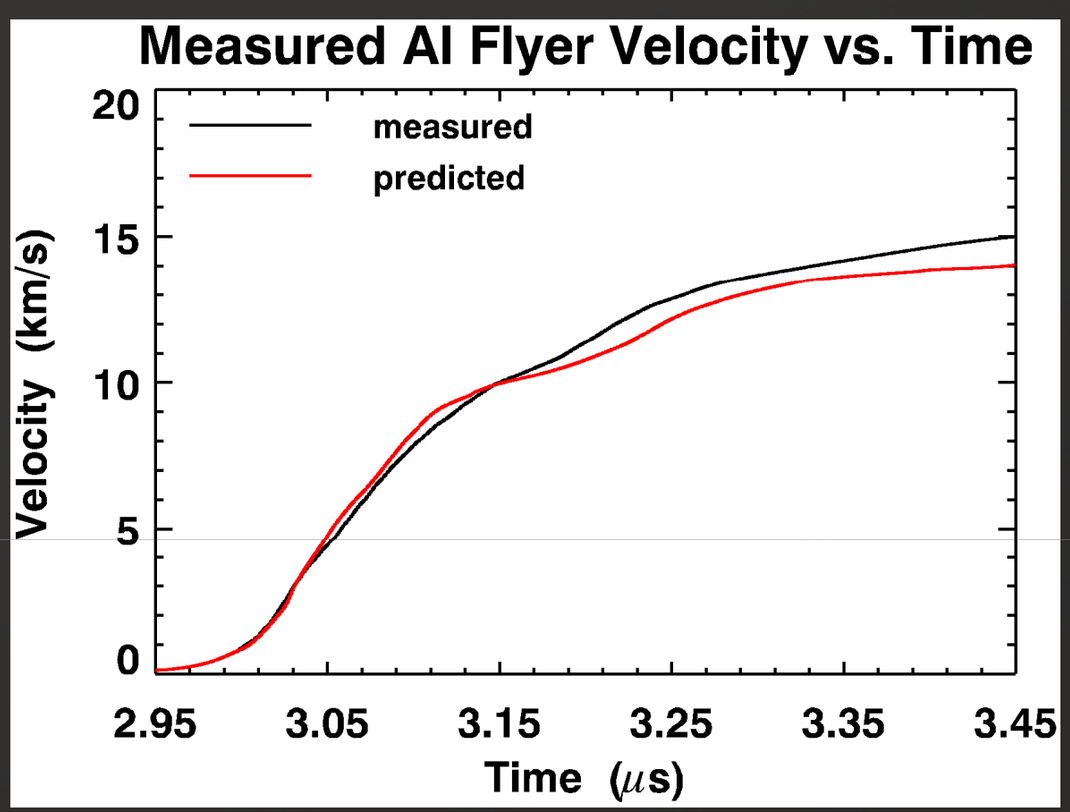
Accurate material models allow Rad-MHD codes to compute predictive results



Accurate material models allow the many years of Rad-MHD algorithm development to come to fruition. Equations of State give the properties which allow the codes to treat material correctly. Electrical conductivity models allow the right diffusion of magnetic field and the resultant Joule heating of the materials. Thermal energy is dispersed correctly via the thermal conduction algorithms. And finally, the opacity/radiaton is another mechanism for moving energy in the simulation.

The figure above is a cross section of a magnetically launched flyer plate. The Lorentz force pushes outward from the center and the moving material is the flyer. By adjusting how the current flows in the simulation so it is similar to the Z-Machine, we can determine the flyer's acceleration and velocity. It is important that the flyer doesn't melt before it impacts the far surface. A portion remains at solid density and room temperature. Because we know a great deal about the flyer material (usually aluminum), we can infer material properties of the target with high accuracy and use that information to validate our QMD simulations and the subsequent material models.

The figure to the right is the velocity measurement of a flyer from a simulation compared to experimental data. As can be seen, the new material models allowed ALEGRA-MHD to predict the flyer velocity to a few percent error.



Velocity profiles from an ALEGRA-MHD isentropically launched flier plate simulation compared with the experimental data. The difference is about 6%.

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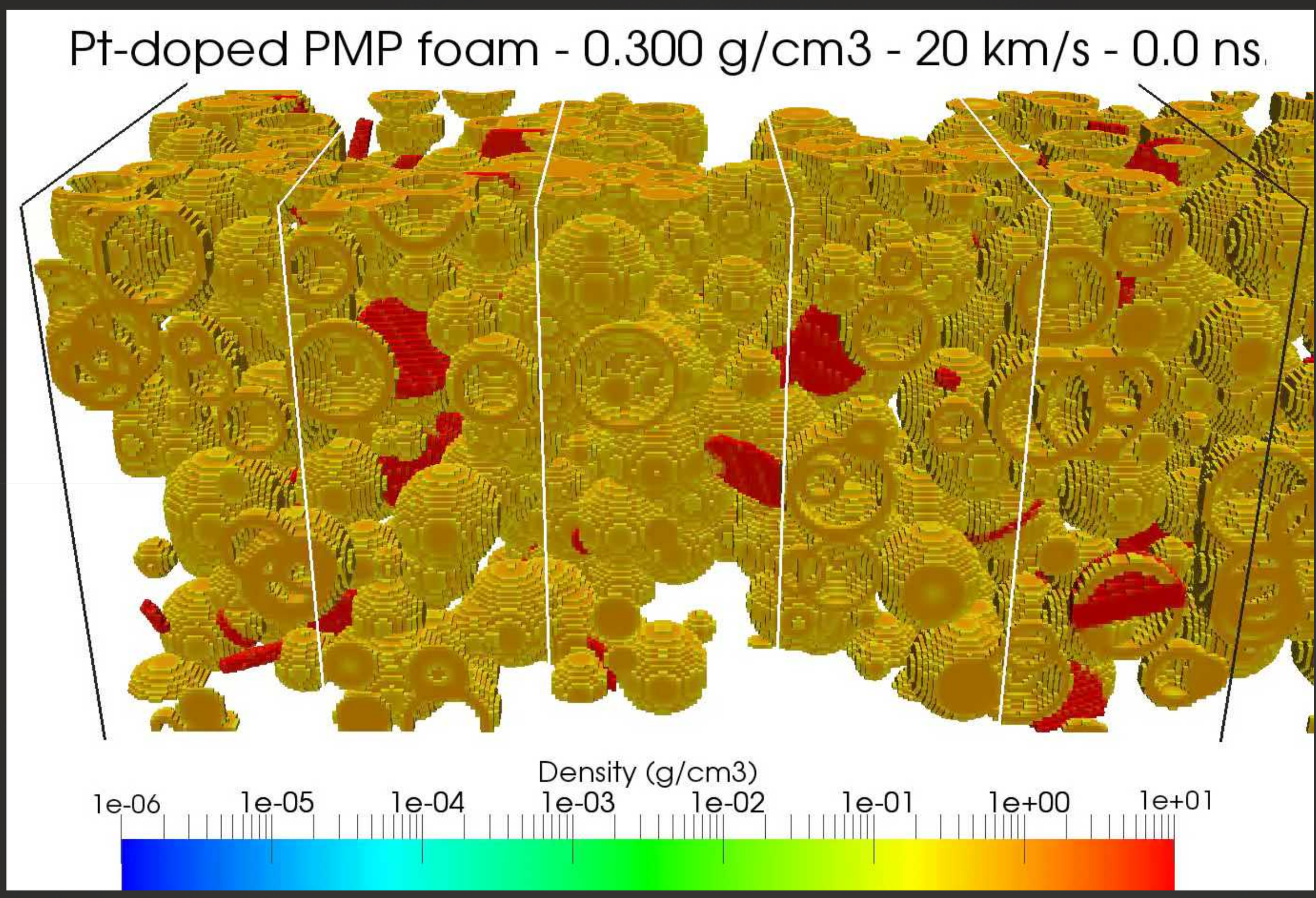
Better faster computers permit more complex materials



ALEGRA-MHD simulations of platinum PMP doped foam
Haill, Procedia Engineering, vol 58, pp 309-319, 2013

As computers increase in capability and capacity, we are able to do ever increasingly complex simulations which require more accurate and more intricate material models. We are coming to a time where we can begin model porous materials with some degree fidelity and build material models that can macroscopically represent a material that has microscopic information (surface energy for example). This is especially true for long chain polymers such as poly-(4-methyl-1-pentene) (PMP or TPX) foam where simulation space and number of atoms is beyond what we could dream of doing 5 years ago.

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