Message from the Assistant Deputy Administrator for Stockpile Stewardship, Chris Deeney

Our NNSA laboratories—Los Alamos National Laboratory, Lawrence Livermore National Laboratory, and Sandia National Laboratories—employ some of the most talented individuals working in the science, technology and engineering disciplines today. Read about some of their exciting technological innovations in the next column. Thanks to our academic partnerships and exciting hands-on mentoring programs, the caliber of the individuals we are able to recruit becomes more impressive each year. In this issue of the Stockpile Stewardship Quarterly, we introduce you to just a few of the extraordinary individuals, specifically some of the early career scientists, working on cutting edge technologies at our labs.

My management team and I had the pleasure of meeting and learning a little about the early career staff featured in this issue while on an in-depth management review of the NNSA laboratories in December. These individuals briefed us on the recent accomplishments and fascinating upcoming work to occur at their respective laboratories. I wanted to give you the chance to meet them too.

Enjoy the articles that follow, beginning with the article about exploring shock-induced chemistry on ultrafast timescales. As you read about the early career scientists and the quality of their work, you will no doubt be impressed. It is my hope that you will also be made aware of one very important fact: The Nuclear Security Enterprise will be in very good hands for decades to come!

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NNSA Labs Receive 2012 R&D 100 Awards

NNSA’s national laboratories claimed 12 of R&D Magazine’s prestigious R&D 100 Awards this year. Often called the “Oscars of Innovation,” the annual R&D 100 Awards recognize the most noteworthy technological advances at universities, private corporations and government labs around the world.

Lawrence Livermore National Laboratory (LLNL)

Los Alamos National Laboratory (LANL)
5. UTurn, a method that produces two new uranium iodide reagents and 6. Sequedex, revolutionary software package used for DNA analysis.

Sandia National Laboratories

Joint/Lab Site Awards

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I joined Los Alamos National Laboratory (LANL) as an undergraduate research assistant in 1999, working in the High Explosive Science and Technology group. The exciting research and exceptional mentoring that I received fostered my interest in performing research in a national lab setting and helped me choose my scientific specialization of physical chemistry.

Exploring Shock-Induced Chemistry on Ultrafast Timescales
A typical explosive detonation begins with a mechanical insult to the explosive, and that insult is eventually transformed from a mechanical impact into a self-sustaining chemical reaction. The intricacies of this transformation are not well understood and are an area of active research in the Shock and Detonation Physics group at LANL. This research provides understanding of the chemical processes that occur in the explosives in our stockpile and will result in designing explosive molecules with specific initiation properties and in the development of methods that can selectively initiate explosives through targeted breaking of the most vulnerable bonds in the molecule.

Over a decade ago, researchers at LANL began using ultrafast femtosecond (fs) laser to create supported shock waves in thin films of metals and polymers and, eventually, in liquids and explosives. Ultrafast lasers were selected to drive the shock events because it was recognized that observing the initial steps of chemical reaction in an explosive detonation requires synchronicity between the initiating event and diagnostics similar to the vibrational periods of molecular vibrations, namely tens of fs to ps. This synchronicity has been achieved through the use of a single ultrafast laser to both drive the shock waves and to probe the resulting material dynamics and reactive chemistry.

Ultrafast dynamic ellipsometry (UDE) is a form of chirped pulse spectroscopy that was developed as a single shot measurement to characterize both the motion of the shocked material and its changes in optical properties. UDE is similar to other interferometric shock diagnostics in that it provides velocities of the shocked materials to determine the equation of state. However, UDE also investigates the changes in the optical properties of the shocked materials by probing the sample at multiple angles of incidence and with both polarizations of light, and these changes can provide important insight into materials that are undergoing chemical reactions or phase transitions. Another benefit of using ultrafast lasers is the relative ease of integrating complex spectroscopic diagnostics with the shock event. Using non-linear optical processes, the fundamental frequencies of the ultrafast lasers have been transformed to infrared frequencies, which selectively probe the dynamics of the nitro-group chemistry in polyvinyl nitrate and to visible frequencies, which probe the broad absorptions in chemically reacting explosive crystals. The most recent spectroscopic developments have been focused on coherent Raman scattering (FSRS) techniques with picosecond time resolution as shown in Figure 1.

Figure 1. Vibrational temperature of two modes in single crystal calcite measured with the Raman loss to Raman gain intensity ratio of FSRS as a function of time after a flash-heating laser pulse.

References
Fascinated with the Aerodynamics of Flight

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I joined Sandia National Laboratories (SNL) in October 2010, following my doctoral work at the University of Colorado. I chose my career track because I have always been fascinated with the aerodynamics of flight. During my undergraduate years, I discovered that I enjoyed computational mechanics, and the combination of computational mechanics and aerodynamics ultimately led me down the path of an academic and professional career in high-speed aerodynamics and computational fluid dynamics.

Toward Exascale Simulation of Re-Entry Flight Environment

A need exists to better understand the re-entry aerodynamics of stockpile systems and fill in knowledge gaps associated with uncertainties in the flight environment. The leap in computational power when exascale computing platforms come into the picture presents an opportunity to gain a more fundamental understanding of re-entry physics through modeling and simulation. Research in this area is important for reducing cost and uncertainty associated with existing system modifications and future system design because flight data is generally unavailable until very late in a development cycle—long after most components have been designed. Moreover, flight data is too scarce to establish statistical significance of certain measured phenomena.

The primary focus of this work is aimed at improving predictive capabilities for the response of hypersonic re-entry vehicles; this involves modeling and simulation of random pressure loadings during re-entry, thermochemical nonequilibrium effects, aerodynamic response due to ablation of the thermal protection system, and laminar-to-turbulent boundary layer transition. Developing such a simulation capability is a significant challenge since many of these different physical phenomena are coupled and interact to produce the final response. For instance, surface pressure fluctuations are generated by the turbulent boundary layer in a given flight environment. Boundary layer transition is also a key physical phenomenon in random pressure loads on re-entry vehicles. Random loads are particularly severe when flow is transitional—where turbulent spots form in the boundary layer and convect downstream.

Direct numerical simulation (DNS) is a computational method that can simulate turbulent flow phenomena from first principles with few modeling restrictions. DNS is well suited for providing the highest accuracy predictions and gaining new physical insight for boundary layer transition and turbulent spot formation and migration. DNS comes at an extreme computational expense however, as the grid size required to directly resolve the turbulence is proportional to $Re^{1/4}$, where $Re$ is the Reynolds number. For realistic re-entry Reynolds numbers (on the order of $10^5$ - $10^6$), DNS is not expected to be a feasible approach for full system re-entry simulations even at exascale. However, exascale computing will enable sub-system scale simulations at Reynolds numbers previously unattainable with DNS. Reynolds-averaged Navier-Stokes (RANS) simulations, which entirely model the turbulent effects, are less accurate but are currently the standard approach for predicting turbulent behavior for full systems. Knowledge gained with sub-system scale DNS calculations can then be used to develop and calibrate RANS models used for full-scale re-entry simulation.

Large Eddy Simulation (LES) and hybrid RANS/LES methods lie between DNS and RANS from a turbulence modeling perspective. These methods model the smallest turbulent scales while directly simulating the larger turbulent eddies that can be resolved by the computational grid. LES and hybrid RANS/LES in particular can capture much of the turbulent physics while still remaining feasible from a computational cost perspective. For simulation of unsteady compressible turbulent flows for full systems, these methods are the clear choice and the future for design and qualification purposes.

Many challenges exist for making DNS and LES of re-entry problems viable on current computing platforms and future exascale architectures. Successful DNS and LES algorithms require higher-order, low numerical dissipation discretization methods to accurately characterize turbulent flows. Unstructured grid technology, which has been the standard for simulation of complex geometries, is challenging to extend to higher-order and is costly in terms of memory and parallel communication. Thus, this research is exploring low-dissipation schemes and efficient discretizations that minimize memory and communication costs while maintaining the flexibility to handle complex geometries. Investigation of explicit and hybrid implicit/explicit solver technology as well as exploring new scalable algorithms for implicit calculations is another focus area. All told, this research effort requires close integration between the numerical algorithms, programming models, and hardware architectures in order to make scalable re-entry simulations that are truly representative of actual flight a reality for tomorrow.
**Physics: A Way of Describing Nature**

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**Award**

Physics appealed to me from a young age as a way of describing nature. The promise of fusion energy and the coolness of astrophysics led me to study plasma physics.

Since coming to Lawrence Livermore National Laboratory (LLNL) in 2010, I’ve been learning about inertial confinement fusion (ICF) and stockpile stewardship. I love being able to apply my physics knowledge to real world applications in support of both basic science and national security.

**Probing ICF Plasmas**
The conditions at the center of an inertial fusion energy experiment are unlike anywhere else on Earth. The gas within the rapidly compressed capsule becomes plasma, in which the electrons and ions are no longer bound together. If the shock is strong and fast enough, the common assumption of local thermodynamic equilibrium (LTE) is violated, and the electrons and ions can have very different temperatures.

The National Ignition Facility (NIF) at LLNL presents a unique new capability to probe non-LTE plasmas and explore the nature of the electron-ion coupling. The goal of this research campaign is to field capsules with thin glass shells (~5µm thick, ~2mm diameter) in the Polar Direct Drive (PDD) configuration, in which NIF’s 192 lasers directly strike the capsule surface. This illuminates the surface with an intensity of ~10^15 W/cm², rapidly ablating the shell and driving a strong converging shock toward the center of the capsule. Ion temperatures of ~15 keV and electron temperatures of ~5 keV are reached. A small convergence ratio (~4) and rapidly ablated shell reduce susceptibility to hydrodynamic instabilities and lead to clean observations of the plasma. During the time of peak emission, the fairly flat radial temperature profiles mean that time-resolved measurements of the ion temperature (by neutron time-of-flight) and electron temperature (by x-ray spectroscopy using a Kr dopant) can be made without being overwhelmed by spatial gradients.

Extensive work has been done to examine the design space with 1-dimensional (1D) ARES Arbitrary Lagrangian-Eulerian Radiation Hydrodynamics simulations to find the most favorable capsule configurations. However, one of the major challenges of the PDD approach is achieving a spherically uniform implosion. The standard configuration at NIF is for Indirect Drive, where beams enter the ends of a cylindrical hohlraum to produce an x-ray drive. For PDD, each of the beams must be ‘re-pointed’ away from their nominal angles. Each beam can also have a separate power profile and focal length. Large ensembles of 2D simulations were run to probe the parameter space and find the optimal pointing resulting in the most spherical implosions. The amount of laser energy inevitably lost by beams missing the capsule as it implodes was measured with neutron time-of-flight and x-ray spectroscopy (using a Kr dopant) can be made without being overwhelmed by spatial gradients.

A Blind Study
Pino recently had the opportunity to participate in a Blind Study to assess the impact of a limited set of legacy data on the design process. A team of recently hired and relatively inexperienced WCI-AX Design Physicists i.e., Jesse Pino, Paul Demange, Kumar Raman, and Bryan Johnson, was tasked with attempting to design a weapon component with limited time and resources. After coming up with a proposed design, the team was given an additional amount of underground test data, and an assessment was made about how useful that data was in changing the proposed design or establishing confidence that it would perform.

The benefits of this exercise exceeded the primary goal; the reevaluation of the legacy data proved insightful in its own right. In addition, the exercise was educational for the participants, challenging them to think about the principles of design in ways that don’t often come up in traditional Stockpile Stewardship modeling.
**Enjoys High Pressure Situations**

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- NNSA Defense Programs Award of Excellence, 2010, Xenon Equation of State Team, Institute for Shock Physics  
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Growing up, I always had an interest in science: astronomy, paleontology, and blowing things up—normal kid interests. I knew from a young age that I would major in physics because that was where the big explosions happened. At a conference in 2001, I met Yogi Gupta who easily convinced me that experimental shock physics would be fun and interesting. After 5 years of challenging and exciting research at WSU, I graduated and came to Sandia National Laboratories (SNL).

I joined SNL in January 2008. I chose SNL because of the opportunity to do research on the Z machine. It is a unique facility where I can perform cutting-edge, significant research that contributes directly to our national security.

In addition to shock physics, I enjoy running, biking, swimming, and competing in triathlons. Go Big Red!

**Shock Physics**

At Sandia, I have been involved in a multitude of research projects. One of my primary projects has been working on the equations of state for cryogenically-cooled gases.

For several gases, such as xenon, krypton, argon, carbon dioxide (CO₂), the high-pressure, high-temperature equation of state (EOS) is unknown. Experimental data on these materials, initially in a cryogenic liquid state, are typically limited to 1 Mbar on the Hugoniot because of the limits of plate-impact launchers and the low impedance of the materials. The EOS models for the gases are able to replicate the cryogenic liquid Hugonions at low pressures. At pressures above where data exists, the EOS models rapidly diverge from one another, creating uncertainty in the high pressure-temperature response. Using the Sandia Z-machine, we measured the Hugonion state of the cryogenic liquids to multi-Mbar pressures. The experimental data are combined with density functional theory (DFT) simulations and the results are utilized to develop new EOS models.

In the Z experiments, the target load is designed so that the Z current pulse travels in a loop, creating a strong magnetic field. The resulting Lorentz force (J × B) produces an outward force capable of shocklessly accelerating solid flyer plates to 40 km/s. The cryo-targets (see Figure 1) consist of a copper cell with quartz front and rear windows. Quartz is used because it has been developed as a highly accurate impedance standard, which reduces uncertainties in the determined Hugonion state of the cryogenic liquids. A gas line attached to the target is used to fill the cell with high-purity gas, and the copper arm on the cell connects the target to the cryo-stat system. The required temperatures are 163 K (Xe), 118 K (Kr), 85 K (Ar), and 220 K (CO₂)—although the CO₂ requires significantly more gas pressure (130 PSI) to get to the liquid state. With this experimental setup, the maximum pressures attained were over 8 Mbar.

The results for liquid Xe were published in Physical Review Letters in 2010 (S. Root et al., PRL 105, 085501, 2010). The experimental data validated the predictions from the DFT simulations. The experimental and DFT results showed that the Xe EOS tables at that time bounded the true Hugoniot response. For liquid Kr, the resulting data also showed that the existing EOS tables bounded the true Hugoniot response. Ar, however, demonstrated that the EOS tables do not always bound the high-pressure Hugoniot. The experiments and DFT simulations on Ar conducted last summer showed significantly more compression than predicted by the prior EOS models. The experimental and DFT simulation results were shared with the other NNSA laboratories and have led to the development of new EOS models for these three noble gases and CO₂ which are now being used throughout the tri-labs.

Another research area has been in geological materials, such as MgO. MgO is abundantly found in the earth's mantle. Understanding its high P-T behavior is critical for modeling planetary interiors. On the Hugoniot, MgO should undergo a solid-solid phase transition and eventually melt. Using the Z machine, we have measured the Hugoniot with high precision from 3.3 Mbar up to 11 Mbar, investigating both phase transitions. The experimental data combined with DFT simulations have provided a more complete understanding of the MgO phase diagram.

![Figure 1. CO₂ cryogenic target. The CO₂ targets are connected to a liquid nitrogen cryo-stat through the copper cold arms. VISAR probes are mounted to the cryo-targets to measure velocities during the experiment. Below the cryo-targets are mounted MgO samples to measure the Hugoniot and release state of MgO.](image-url)
Early Fascination with Astronomy Sparks Passion for Physics

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• All-USA and All-California Academic First Team Scholarship, USA Today, 1997.

As a child, I was fascinated by astronomy. My parents, who are not scientists, encouraged a general interest in science, and astronomy became my favorite subject. When it came time to choose a university and a major, I decided to go into physics at the University of Nevada, Reno.

In 2005, I came to Los Alamos National Laboratory (LANL) as a graduate student to further my research, and the following year, I earned my Ph.D., working with Professor Roberto Mancini on “The Spectroscopic Characterization of Temperature, Density, and Mix in ICF Implosion Cores.” After graduating, I accepted a postdoctorate position at LANL. In 2008, I was converted to a staff scientist position in X Division.

Inertial Confinement Fusion
In the field of ICF, a major goal is to achieve a better understanding of factors that affect implosion quality. One such factor is the physical process of mixing between materials of different densities, such as the shell and fuel materials of an ICF capsule. The community’s understanding of mix has evolved substantially in the past several years due to an enhanced effort in this area; however, uncertainties remain. These uncertainties include variable density mix layer behavior when subjected to multiple strong shocks, and variable density mix associated with shear. These situations can arise in ICF capsules, as shock waves traverse capsule defects and initiate mix between shell and fuel materials, which results in degrading the yield.

At LANL, the BHR-2 turbulent mix model has been implemented into the RAGE radiation hydrodynamics code, a 1-dimensional (1D), 2D, and 3D code which is used to simulate the behavior of ICF capsules. Due to a lack of data in the strong shock regime and in shear flow, two laser-driven variable density mix experiments have been developed to provide detailed quantitative data to help validate and improve the BHR-2 mix model. The Reshock and Shear experiments are being performed at the University of Rochester’s Laboratory for Laser Energetics.

The Reshock experiment studies the Richtmyer-Meshkov-driven process of shocking and reshocking mix layers. The first laser-driven shock impacts a plastic ablator on one end of a 1.4 mm long Be tube, and drives a shock through a thin Al tracer disk which adjoins the ablator. As a result of the shock, the Al disk moves down the center of the cylinder, which is filled with low-density foam. When the Al mix layer is approximately in the center of the tube, it is reshocked by a laser-drive from the opposite end of the tube. The Al mix layer experiences a compression due to the counter-propagating shock, after which the layer continues to grow (see Figure 1, top). The radiographic data provides a measure of the mix width across the Al layer, and the results are compared to the widths extracted from simulated radiographs.

The comparisons are promising: BHR-2 accurately captures the evolution of the mix width.

The Shear experiment investigates shear-driven growth of a mix layer. In this experiment, one half-cylinder of a Be tube is filled with a low-density foam, while the other half-cylinder is filled with high-density foam. The two regions are separated by a thin Al plate. A single laser-driven shock from one side of the tube initiates hydrodynamic motion and produces a shear layer, which develops temporally and becomes more turbulent (see Figure 1, bottom). The area of the shear feature is extracted as a function of time from both the radiographic data and the simulated radiographs. Good agreement between the experimental data and the BHR-2 mix model is achieved.

The Reshock and Shear experiments are proving to be extremely useful in validation efforts for the BHR-2 mix model. Together, these experiments are answering some of the community’s questions as to the details of the physical mixing process as it occurs in ICF implosions.

Reference

Figure 1. The evolution of the reshock experiment shows the mix layer after the first shock has passed through it (8 ns), just after reshock during the compression phase (10 ns), and late in time as the mix layer becomes more turbulent (19 ns). (Bottom) The evolution of the shear experiment shows the initial shear growth and relative positions of the shocks in the low and high density foams (6 ns), the continued growth and widening of the shear feature (10 ns), and the late time development of turbulent features along the edge of the shear feature (14 ns).
A LOVE FOR MATH AND PHYSICS

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Awards and Honors
• Los Alamos Awards Program, Applications of Ignitions Projects Team, 2011.
• Graduated magna cum laude, UMB, 1997.
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I am a forth generation scientist/engineer. I have always enjoyed technical disciplines, particularly math and physics, but thanks to my parents also find great delight in literature, art and music.

After earning my Ph.D., I jumped at a great opportunity to join Los Alamos National Laboratory as a postdoctorate in 2007 and as a technical staff member in 2011.

Modeling Polar Direct Drive Implosions on NIF

The National Ignition Facility (NIF) provides a unique experimental platform to study high energy density physics, investigate the effects of mix during the implosion and advance our ultimate goal of inertial fusion energy. With NIF’s current configuration, efficiently utilizing available power is of crucial importance. The Polar Direct Drive (PDD) concept, extensively employed at the University of Rochester’s Laboratory for Laser Energetics and slated to be used on NIF in Defect-Induced Mix Experiment (DIME) this summer and in ignition studies in 2017, can provide a viable solution by allowing more energy to be coupled directly to the capsule. However, achieving significant fusion yield from an inertial confinement fusion capsule requires symmetric implosion of the capsule with less than 1% root mean square (rms) velocity variations over the capsule surface. For the direct-drive concept, symmetry is dependent upon the uniformity of laser illumination which must be maintained throughout the implosion. To optimize uniformity in PDD configuration, the individual beams must be re-pointed slightly away from the center of the capsule to increase the paucity of laser energy intercepting the equatorial region of the capsule.

To investigate the implosion symmetry of PDD NIF shots, 3-dimensional (3D) rad-hydro calculations were performed using HYDRA, which is a state-of-the-art, 3D arbitrary Lagrangian-Eulerian code. To date, these processes have been modeled in 2D incorporating 3D ray-tracing of azimuthally-symmetric annular laser beam cones. However, experimental studies on OMEGA (see Figure 1a) suggest that PDD capsule implosions require 3D modeling to accurately capture 3D geometry and energy deposition of the 192 NIF laser beams and predict the rad-hydro capsule evolution.

For this study, we simulated the implosion of an upper hemisphere of a 2.2-mm diameter, 30-micron thick CH capsule filled with 5.5 atm DT using a PDD NIF configuration with a total of 350kJ of laser energy delivered in approximately 2 ns. The simulations revealed a large mid-latitude perturbation in both the capsule radius and velocity at the end of acceleration phase that is directly correlated to the asymmetry observed in the absorbed power-density at its temporal peak. In an effort to improve the poloidal symmetry, we attempted to minimize these spatial variations by adjusting the laser pointings and spot shape. We were able to significantly improve the symmetry of the implosion, as well as decreasing the rms variations of the initial absorbed power-density by a factor of ~2 resulted in a reduction of asymmetries in shell radius and velocity by a factor of 6 and 2.5, respectively, while the neutron yield increased by 3.4%. Therefore, even moderate improvements in the spatial distribution of the power deposition during shock-transit time provide significant gains in the symmetry of the implosion.

Assessing azimuthal symmetry is a necessary and, to date, neglected aspect of direct drive implosions. We investigated it in the context of a study to determine the optimum method to remove a quad of laser beams to be used as an x-ray source for backlighting. The results of the clean capsule implosion (see Figure 1b) showed inherent variations in the capsule drive caused by the finite number of lasers used to drive the implosion, though they were much smaller than the poloidal ones. When one of the quads from the 50° ring was removed with its power being equally distributed between the remaining seven quads to ensure the same total laser drive energy, the azimuthal variations (see Figure 1c) increased by a factor of 10 to 15 resulting in the yield decrease by a factor of 2. Nonetheless, when the remaining quads in the 50° ring were repointed to restore the azimuthal symmetry the yield and the percent rms variations in the capsule radius and speed recovered to within 3.5% of the clean case.

References
A PSEUDO-RANDOM WALK FROM CHEMIST TO DESIGN PHYSICIST

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• LLNL Institutional Operational Excellence Award, 2009.
• Margaret Jorgenson Memorial Prize, Dept. of Chemistry, UC Berkeley, 2007.
• National Science Foundation Graduate Research Fellowship, 2002.
• Darleane Hoffman Award, Department of Chemistry, NMSU, 2002.

With a vague notion that I wanted to be a “research scientist,” I decided to major in chemistry. I was hired as an undergraduate to do Monte Carlo and molecular dynamics (MD) simulations. During this work, I became fascinated with modeling and simulation. Although I am a “chemist” by decree of my degrees, I minored in physics as an undergraduate, and studied the physics of superfluid helium as a graduate student. Ultimately, I wanted to use my education to address problems with practical applications, and that desire made working at LLNL a natural choice.

I joined LLNL as a postdoctorate in the Quantum Simulations Group in August 2007, was hired to the Physical and Life Sciences directorate in 2010, and moved to the WCI in 2011.

Developing Improved Physics Models for Predictive Simulations

High power laser facilities, such as the National Ignition Facility, and advanced diagnostics have enabled the determination of detailed properties of dense plasmas over unprecedented regimes. Developing modeling capabilities that adequately capture the physics of such plasmas, which may be partially degenerate and/or moderately coupled, represents a major challenge. A diverse multidisciplinary team is focused on applying classical MD simulations to address physics uncertainties in these systems. The strength of the MD method is that all the effects of collisions and strong inter-particle correlations are incorporated since all particles and their interactions are treated explicitly. They can thus serve as a complement to more traditional radiation-hydrodynamic simulations.

A critical element of these classical MD simulations is adequately capturing the quantum mechanical effects that are inherent to moderately and strongly coupled degenerate plasmas.

The incorporation of quantum mechanics into classical MD simulations is accomplished by using effective statistical potentials. Starting from the exact solution for a quantum two-body problem at finite temperature, one can calculate a diffractive Coulomb pair potential. This type of interaction potential accounts for quantum effects, which prevent the classical collapse of an attractive Coulomb system. The fermionic character of the electrons is handled via an effective Pauli potential which is derived from the pair correlation function for an ideal Fermi gas.

One way of validating these potentials is to make comparisons to available data from full quantum simulations. The approximations that are made in the construction of the statistical potentials and the simulation of electrons using classical MD become more accurate in the limit of high temperature, so initial validation efforts have focused on weakly coupled, nondegenerate hydrogen plasmas. A comparison of the pair correlation functions for a hydrogen plasma simulated with classical MD and hypernetted-chain (HNC) methods to the pair correlation functions computed with quantum path integral Monte Carlo (PIMC) is shown in Figure 1. The pair correlation functions calculated using statistical potentials are in good agreement with the PIMC results. The pair correlation function is of primary interest in determining how detailed interparticle correlation effects can modify the behavior of a plasma, so demonstrating that the classical simulations produce pair correlation functions in agreement with a full quantum simulation is an important step toward validating the use of the statistical potentials.

Current studies are focused on the construction of statistical potentials for partially ionized systems. These systems require particular care due to the presence of bound electrons around the nuclei. Interestingly, the types of potentials that provide the best agreement between MD and PIMC for the fully ionized hydrogen plasma predict non-physical formation of clusters in simulations of partially ionized beryllium. Work is underway to develop a methodology which incorporates feedback from quantum calculations of the electronic structure to construct more accurate statistical potentials for partially ionized systems.

References
Developing X-ray Sources for Extreme Radiation Environments on the Z Machine
by Brent Jones*, David J. Ampleford, Christopher A. Jennings, Stephanie B. Hansen, Michael E. Cuneo et al.
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When you flip the switch turning on a light bulb in your home, you activate a light source emitting about 6 watts of visible photons. When we turn on the Z Machine at Sandia National Laboratories (SNL) to conduct radiation effects experiments, we activate a source that is 5 trillion times more powerful. This power level in the tens of terawatts exceeds the average electrical power consumption of the entire planet. What’s more, these radiated photons are not visible with your eye (~3 eV), but rather in soft x-rays with 1-10 keV photon energies. For the few billionths of a second during which Z produces its x-ray pulse, an extremely intense radiation field is created, capable of simulating in the laboratory the hostile environment of a nuclear detonation. By studying the response of materials and systems under pulsed, radiation-driven stresses, Z serves a unique national role in Stockpile Stewardship.

The architecture of the Z pulsed power facility that enables these remarkable radiation environments is really a series of switches, each much more sophisticated than the familiar light switch. A set of laser-triggered gas switches and water switches precisely control the discharge of 20 MJ of stored electrical energy through transmission lines that compress the energy in time and space, converging with very high power density in the Z vacuum section. The final “switch” in the sequence is the magnetically-driven implosion of the load at the center of the machine. Figure 1(a) shows a typical nested stainless steel wire array load. Arrays are imploded over 100 ns, but produce their x-ray bursts in 2 to 10 ns, an extraordinary power pulse compression of up to 50:1. As the Z machine current approaches values exceeding 20 MA, the wires become plasma, and a strong magnetic field is generated surrounding the array. The resulting Lorentz force radially compresses the plasma into a hot, dense, radiating “z pinch” aligned with the axis of symmetry in the very heart of the machine.

Although such implosions are simple in principle, there are many outstanding questions surrounding their performance and operation. For one, does the plasma really accelerate to high velocities as implied by simulations? By measuring Doppler shifts in emitted x-ray lines, we have measured velocities of >700 km/s on Z as the magnetic field rapidly compresses the wire array plasma (see Figure 2). These velocities exist only briefly before the plasma collides and stagnates on the axis in a few nanoseconds, converting the accumulated kinetic energy to electron temperatures up to 5 keV (50 million degrees Celsius), hotter than the center of the sun.

These enormous temperatures are sufficient to strip materials with atomic numbers as high as copper to the K shell, meaning that only one or two bound electrons remain per atom. These atoms can then produce characteristic x-ray line radiation, as seen in Figure 3. The particular photon energies of the x-ray lines depend on the atomic number of the material that was imploded; as atomic number is increased, the x-ray photon energy of the source also increases. It is more energetically expensive to ionize to the K shell with increasing atomic number, and so x-ray yield tends to decrease. Nevertheless, the yields shown here represent the most energetic 1-10 keV x-ray sources presently realizable in any above-ground facility, thus enabling radiation effects experiments on Z in unique physical regimes.

Several experimental campaigns recently led by D.J. Ampleford optimized radiated outputs from aluminum and stainless steel (SS) wire arrays. In particular, the yields achieved from SS sources represent a 50% increase in output compared to those fielded for radiation effects studies prior to the completion of the Z refurbishment in 2007, and have shown excellent reproducibility of the spectrum and radiation pulse shape. While most of these sources are wire arrays, the argon x-ray source is achieved by pinching a supersonic jet of gas, a capability that is now being reestablished on Z for 2012 experiments. This system will also allow us to study krypton sources for the first time on Z, pushing the photon energies accessible at the facility up to 13 keV.

A second major question is how the structure of the imploding plasma evolves in space and in radiative emission properties as the z pinch implodes. We employ a variety of spectroscopic and imaging diagnostics to understand and optimize these sources. The z-pinch stagnation process is studied with a novel x-ray pinhole camera that combines filtered imaging of the K-shell emission above 1 keV with images of much lower 277 eV photons reflected from multilayer mirrors. As in Figure 4 for an aluminum wire array on Z, the composite images reveal cooler material (red) imploding onto and surrounding a hot core (yellow). It is apparent from these images that significant plasma instability is present. This originates from magnetic Rayleigh-Taylor instability growth that is seeded at the start of the wire array implosion at much larger radius. Designing and optimizing these x-ray sources involves a trade-off: large initial radius

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* Dr. Brent Jones is the 2012 IEEE Early Career Achievement Award recipient (see page 11).
is desired in order to achieve high final velocity and thus high temperature, but if the radius is too large then the Rayleigh–Taylor instability can begin to broaden the x-ray pulse and reduce the yield.

SNL has also pursued collaboration with NNSA-partnered universities on novel experiments to answer a number of other outstanding questions on physics of wire array implosions. At the University of Nevada, Reno, spectroscopic dopants were used to diagnose plasma conditions and track material flow. At Imperial College, we seeded perturbations in wire arrays in order to study Rayleigh–Taylor evolution in a controlled experiment.

The extensive data on wire array initiation, implosion structure, implosion velocity, and stagnation plasma properties are used to benchmark numerical simulations. Figure 1(b) shows density contours from a 3-dimensional magneto-hydrodynamic (3D MHD) simulation performed at SNL by C.A. Jennings. Such models are used to verify that the desired velocities can be achieved with adequate stability prior to performing Z experiments. They can also study array nesting techniques, which have been demonstrated experimentally to mitigate instability, improving radiation performance.

We are also now incorporating tabulated atomic emissivity and opacity models calculated by S.B. Hansen into the 3D MHD models, which allows for assessment of the K-shell x-ray power and yield. In collaboration with the Naval Research Laboratory, upcoming argon source experiments on Z have been designed and predictively modeled through numerical simulation which the experiments will soon test.

Such studies can challenge our theoretical understanding and the MHD codes used on Z for applications ranging from intense x-ray sources to studies of dynamic material properties under extreme pressures. With modeling capabilities and experimental platforms maturing, it is an exciting time for radiation physics research on Z.

References


Awards
DOE Early Career Research Award
Dr. Steven D. Pain of Oak Ridge National Laboratory, a former postdoctorate with Rutgers University through NNSA’s Stewardship Science Academic Alliances Program, received a 2012 DOE Early Career Research Award. He was selected for his research entitled “Nuclear Physics on the Road to FRIB: Enhancing Direct-Reaction Measurements Through High-Resolution Coincidence Experiments.” One of 68 scientists selected, he will share in $18.1 million in grants for researchers at universities and DOE’s national laboratories.

Pain was the lead postdoctorate in developing the Oak Ridge Rutgers University Barrel Array (ORRUBA) of silicon detectors. Now, as a co-principal investigator on the currently unfunded Low Energy Nuclear Science Center grant, he is leading the coupling of ORRUBA to the Gammasphere array of germanium gamma-ray detectors.

IEEE Early Career Achievement Award
Dr. Brent Jones of Sandia National Laboratories (SNL) was awarded the 2012 IEEE Nuclear and Plasma Sciences Society Early Achievement Award. Scientists who are within the first 10 years of their careers are eligible for this prestigious award intended “to recognize outstanding contributions to any of the fields making up nuclear and plasma sciences.” Jones will reach his 10-year milestone in August 2012.

Jones’ work has focused on understanding the physics of fast magnetic implosions on SNL’s Z machine and Saturn pulsed power facilities, as well as in collaborative university experiments. His contributions include studying the evolution of plasma instabilities through innovative wire array perturbation experiments, developing unique x-ray imaging and Doppler spectroscopic methods, and collaborating with scientists from SNL and other institutions on z-pinch sources for radiation effects testing. Jones has published three first-author articles on his z-pinch work in Physical Review Letters, including an assessment of a novel x-ray-driven hohlraum concept which was featured on the journal cover. Jones is a co-author of the article entitled “Developing X-ray Sources for Extreme Radiation Environments on the Z Machine” on pages 9-10.

Plasma Science & Applications (PSAC) Award
The IEEE Nuclear & Plasma Sciences Society presented the 2012 PSAC award to Dr. Andrew Ng, formerly of Lawrence Livermore National Laboratory, during the 2012 IEEE International Conference on Plasma Science held the week of July 9. Established in the 1980s, the award recognizes outstanding contributions to the field of plasma science in research or new applications. Ng received the honor for his “outstanding research and visionary leadership in plasma research, particularly in the area of warm dense matter, as well as his many contributions to the plasma science and applications community.”

Information Security Pitfalls
Protecting classified information is everyone’s responsibility. Beware of the three information security pitfalls below.

- **Overconfidence** - Only a Derivative Classifier (DC) with the proper guidance can be certain that information is or is not classified.
- **Incorrect Assumptions** - Do not assume that information in the public domain is not classified. The appearance of classified information in the public domain does not make it unclassified.
- **Poor Deliverable Planning** - Be sure to incorporate a classification review into your production schedule. Foregoing a classification review because you don’t have time is not an option.

When in doubt, consult a DC to verify the classification status of your product. A list of NNSA Classifiers, Declassifiers and UCNI Reviewers can be found on the NNSA HSO Website at http://hq.na.gov/hso.

Fundamental Science with Pulsed Power: Research Opportunities and User Meeting
Scheduled for August 5-8, 2012, this workshop will be the fourth of a series of yearly workshops held on fundamental science in extreme environments. The main objectives of it are (1) to discuss and outline future research directions in dynamic compression of matter using the Z Machine and a future 1 Mbar facility, and (2) to ensure that the collaborative user experiments undertaken on the machine are of the highest quality and impact. For more information, visit www.sandia.gov/pulsedpower/meeting/html.

Dr. Brent Jones, recipient of the 2012 IEEE Early Career Achievement Award, is pictured with the Z Machine’s multilayer mirror pinhole camera, a diagnostic that he developed. He is holding one of the multilayer mirrors that reflects 277 eV photons to create monochromatic self-emission images of the z-pinch implosion. The Figure 4 images on page 10 are data produced by this instrument.