



Stockpile Stewardship *Quarterly*

Defense Programs

Stockpile Stewardship in Action

Volume 1, Number 3

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

Thank you all for your excellent contributions in FY 2011. The Obama Administration and U.S. Congress supported additional dollars in science, technology and engineering, and we delivered on all the promises we made—and even more!

FY 2011 was phenomenal so we decided we should end the year with a *bang*. As you will read, the theme for this issue is high explosives (HEs). HE science is at the heart of stewardship, from predictive performance through safety, and is also a major area that our labs contribute to broader national security goals. This is evident in the 26-year-old Joint Munitions Program between the Department of Defense and Department of Energy. This program is an excellent example of two departments working together successfully, with the result being greater than the sum of the parts.

The technical articles herein demonstrate the important linkage between theory, advanced high performance computing, experiments and creativity. Dan Hook's article, for example, does not do justice to the enthusiasm and excitement he exudes when giving a talk on this subject. Maybe if you listen to Queen's *We Will Rock You* at full blast while reading his article, you will come close. The quality of the creativity and scientific excellence discussed in all our articles are tributes to the great people we have in our Nuclear Security Enterprise. I am committed to ensuring our

labs and university partners keep a pipeline of brilliant scientists and engineers coming to our enterprise.

It is also equally important to have a great team here at NNSA Headquarters. The crescendo of this year has been the completion of some excellent hiring. Brooke Samples is the new US/UK Program Coordinator. Already, her excellent organizational and communication skills are making a difference. Most recently, Dr. Jeff Quintenz joined us. Jeff is the new Director of the Office of Inertial Confinement Fusion. His insight and management experience will add significantly to our management team.

Major Eric Furman of the U.S. Air Force and Leah Kuchinsky, formerly of the Department of State, have also joined the office. Having new staff with diverse backgrounds has added to the depth of our discussions and deliberations. Strong and immediate technical support from our laboratory colleagues is key to our success so we are delighted to have Chris Werner, Aaron Koskelo and Bob Weaver, who will provide technical perspectives as we deliberate management and policy decisions through the next few years, which promise to be very exciting and unpredictable. The government has a number of challenges to work through so super-committees, deficit reductions and other such phrases will dominate the discourse. However, we are all working on an important mission so we must deliver, and if the technical excellence demonstrated in the articles in this issue remains our *modus operandi*, then we will deliver very well indeed! 🌟

New Director, Office of Inertial Confinement Fusion

Join the Office of Stockpile Stewardship in welcoming Dr. Jeff Quintenz to the role of Director, Office of Inertial Confinement Fusion. We look forward to Jeff's leadership and service to the ICF community and the stockpile stewardship team!



Quintenz

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Comments

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Simulation: A Window into the Detonation of High Explosives by Laurence E. Fried (Lawrence Livermore National Laboratory)

A high explosive (HE) releases chemical energy in an extremely short period of time. The release of energy is so fast that it creates a shock wave, called detonation, which travels at a typical speed of 8 km/s, or 18,000 miles per hour, much faster than the speed of sound, in the material. The power (i.e., rate of energy release) during detonation is around 8 gigawatts per cubic centimeter, 10 times the power output of a typical nuclear power plant. This high power is solely a consequence of the very rapid energy release. On a per-unit-mass basis, burning wood releases more energy than a HE does. At this energy release rate, detonating HEs reach enormous pressures and temperatures. When a typical HE detonates, it achieves pressures as high as 400,000 atmospheres (i.e., 6 million pounds per square inch), and temperatures reach more than 3,000 degrees Celsius (5,400 degrees Fahrenheit). Under these extreme conditions, the nature of the material chemistry is fundamentally changed.

NNSA scientists are investigating the mechanism of energy release in HEs. These investigations promise to enable the ever more precise predictions of the behavior of explosive materials across a wide range of conditions. Advances in computer power, coupled with advanced algorithms, have allowed NNSA scientists to simulate detonations on the scale of atoms. These simulations allow individual chemical reactions to be tracked and provide insight into the ways in which chemical behavior is modified at simultaneous extremes of pressure and temperature.

At Lawrence Livermore National Laboratory (LLNL), scientists are using the Blue-Gene/L supercomputer system to simulate and study the chemical behavior of PentaErythritol TetraNitrate (PETN) HE under conditions similar to those achieved in a detonation.¹ These scientists have found that water demonstrates an unusual catalytic action under extreme conditions, a behavior that is contrary to its behavior under ambient pressures and temperatures, where water usually behaves as an oxidizer or as a solvent. They also found that water dissociates and recombines at an extraordinarily high rate—up to 10^{14} times per second and that a majority of all reactions involve either H_2O or its dissociation products H and OH, as shown in Figure 1.

LLNL simulations also reveal that hydrogen atoms in HE material display significant non-molecular characteristics. If hydrogen atoms are bound tightly to other heavier elements (such as C, N, and O) in the HE, then they should diffuse at the same velocity as the heavy elements. Studies found that hydrogen atoms diffuse much more rapidly than heavy elements do. This indicates that hydrogen is becoming free of the heavy elements. The free nature of the H atom is a consequence of the extremely fast chemical reactivity of H and OH. In Figure 2, we show the position of H atoms and heavy atoms at the end of the simulation.

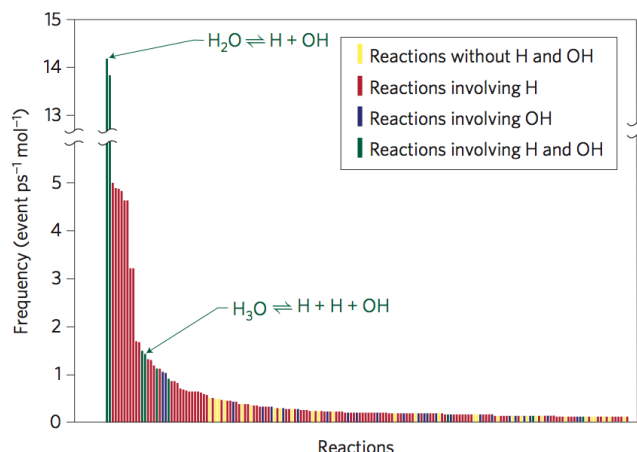


Figure 1: Reaction frequency for PETN high explosive is shown. Of the many thousands of reactions simulated, the vast majority involve H and OH.

Figure 2: H atoms in PETN (green) move further out of the initial simulation cell (yellow box) than C, N, or O atoms (red). This indicates significant non-molecular character of H under the conditions of detonation.

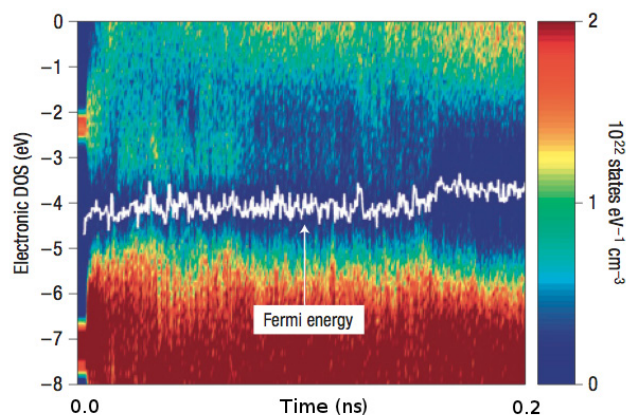
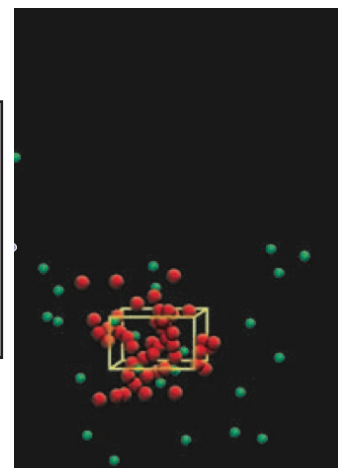


Figure 3: The density of electronic states for detonating nitromethane HE is shown. At the beginning of the simulation (0.0 ns), the system is insulating with little density of states near the Fermi energy. Between 0.01 and 0.05 ns, there are more states near the Fermi energy. We predict that nitromethane becomes a poor conductor.

H atoms (green) have moved further out of the initial simulation cell than heavier elements (red).

Other simulations at LLNL² have studied the electronic properties of detonating HEs. The studies of electronic properties demonstrated that HE molecules, which are electrical insulators at ambient conditions, become imperfect conductors for very short periods of time. This behavior is demonstrated in Figure 3, where the density of electronic states is shown as a function of time after the arrival of the shock front. These simulations used advanced algorithms developed at LLNL that speed up the simulations by more than five orders of magnitude.

These recent computational findings are being incorporated into NNSA codes that predict the detonation properties of

HEs. Improved versions of the codes will predict detonation properties with substantially enhanced accuracy over current versions. At the same time, experimental studies at LLNL and Los Alamos National Laboratory are testing the computational results using state-of-the-art ultrafast laser probes. As time goes on, the mystery of HE detonation will be more fully understood.

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Modeling of High-Explosive Detonation Performance by Mark Short (Los Alamos National Laboratory)

High explosives (HEs) are a key component of nuclear weapons. As part of the U.S. nuclear complex's role in stockpile stewardship, we conduct development and computational simulation of models for HE performance in both normal and off-normal conditions. HE performance involves accurate modeling of the energy delivery from a detonating explosive to a neighboring inert material, i.e., it relies on our ability to obtain both accurate detonation timing as well as spatial and temporal energy release for HE drive. The HE detonation is a supersonic shock wave supported by energy release due to chemical reactions that occur rapidly in a narrow region, a few hundreds of microns to a few millimeters wide, that is attached to the propagating shock. Typical detonation speeds in conventional and insensitive HEs are 6 to 9 km/s with pressures generated upward of several hundred thousand times that of the Earth's atmosphere.

In addition to performance modeling, stockpile stewardship involves the modeling of reaction dynamics that arise in HE safety and aging problems. HE safety involves the understanding of damage mechanisms of HE and the possible low-pressure slower-speed burning (deflagration) of HE brought about by weak mechanical and thermal stimuli (cook-off). However, deflagration can transition to detonation in an uncontrollable way, referred to as the deflagration-to-detonation transition (DDT). As a HE ages, material changes such as cracks and density variations may occur that could affect initiation and performance characteristics as well as HE sensitivity. The ability to model predictively these off-normal conditions is important.

In general, HE modeling is a tremendously challenging task having complications that arise from the multitude of varying flow physics that characterize both safety and performance problems. Add to that the multiple spatial and temporal evolution scales of HE reaction waves (e.g., the typical spatial scale of a detonation reaction zone is several orders of magnitude smaller than a typical explosive

geometry), we encounter a tremendous computational resolution challenge as well, the consequences of which have directly influenced the nature of existing and legacy HE models that have been developed. Also, since knowledge of the chemistry, equations of state and flow physics in extreme conditions is limited, most current and legacy HE models for performance and safety are empirically based, requiring extensive experimental recalibration for any changes in operating state. They possess limited predictive capability beyond the calibration conditions. The current thrust is towards the development of a new generation of credible, physics-based predictive HE models.

Focusing on HE performance, the two current performance modeling strategies include programmed burn and reactive burn models. The programmed burn model class was developed partly due to the lack of numerical resolution available to generate accurate performance results using reactive burn models. The programmed burn strategy involves a separate lower-dimensional, high-resolution calculation for detonation wave sweep (timing) and a low resolution calculation for the deposition of HE energy to the HE product gases that then push on the inert materials surrounding the HE. In contrast, reactive burn models describe the transition from reactants to products via a series of empirical, global reactant decomposition equations.¹ The progress of the shock is fully coupled to the modeling of the energy-releasing reactions. Accurate (numerical mesh independent) timing for reactive burn models can require upwards of 50 numerical points streamwise in the detonation reaction zone to obtain less than a 20 mm/ μ s timing error.

The timing component of the programmed burn model involves a surface wave calculation through the explosive geometry. Traditionally, this was done via a Huygens' construction, where the normal speed of the detonation is constant. For conventional high explosives (CHEs) like the HMX-based polymer-bonded explosives PBX-

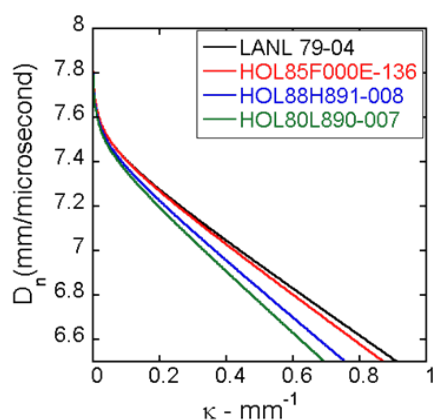


Figure 1: Normal detonation velocity variation with curvature for different lots of PBX 9502 obtained experimentally in a rate-stick configuration.

9501 or LX-14, that have a reaction zone thickness of the order of 100–200 microns, this is adequate. For the longer reaction zone insensitive high explosives (IHEs) like the triaminotrinitrobenzene-based PBX-9502 and LX-17, the Huygens' construction has been supplanted by the Detonation Shock Dynamics (DSD) timing model, developed by Bdzil and Stewart^{1,2} based on an earlier seminal paper by Bdzil.³ Basically, DSD evaluates the normal surface velocity as a function of the local shock surface curvature, a relationship typically obtained for each HE by experimental calibration. Figure 1 shows this variation for PBX-9502. Figure 2 shows a sample DSD calculation. In the Huygens and DSD cases, the timing calculation for a given geometry records the detonation arrival time in a computational cell (known as a burn table). Los Alamos National Laboratory (LANL) has developed a multi-material DSD surface propagation suite (LANLDSD) that utilizes narrow band and full-level set methods to propagate a DSD surface in 2-dimensional (D) and 3-D geometries.

The energy release calculation in a programmed burn approach begins by initializing burning in a computational cell according to the burn table. The traditional programmed burn model is designed to perform a nearly instantaneous burn from reactants to products over a few time steps, without aiming to capture the physical details of the reaction zone. For CHEs, accurate modeling/calibration of the product equations of state leads to good predictions of the HE drive. For the longer reaction zone IHEs, a Pseudo-Reaction-Zone (PRZ) model has been developed at LANL by Dey, Shaw and Wescott^{4,5} that adjusts the numerical reaction-zone length to be consistent with the variations in the local DSD detonation speed. The PRZ model transitions reactants to products by prescribing an expression for the burn fraction, and thus is reactive burn-like in nature. However, lower numerical resolution is required for PRZ than reactive burn as the highly resolution dependent detonation timing is precalculated. The main drawback of the programmed burn approach compared with a reactive burn approach is that it doesn't account for

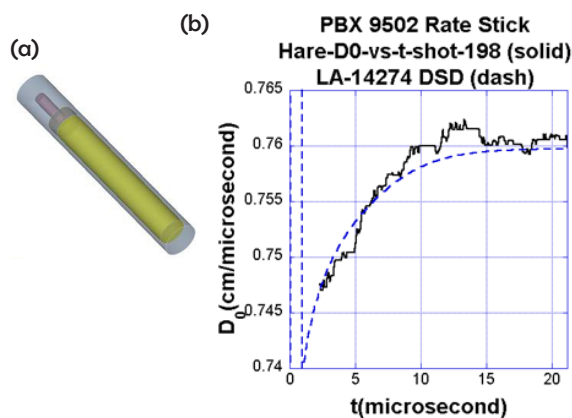


Figure 2: An example of a DSD timing calculation. (a) An explosive geometry is typically read from a hydrocode geometry setup. In this case, a rate-stick configuration is shown with PBX 9502 main charge (yellow), a PBX 9407 booster and detonator (red). A DSD timing calculation is conducted with LANLDSD. (b) Comparison of the DSD calculated centerline axial velocity (dashed curve) compared with results obtained experimentally by Hare et al.⁶ (solid curve) using an embedded fiber optic in the PBX 9502.

dynamic situations such as detonation initiation or for dead zone generation, regions where the HE does not detonate. However, it can be used for resolved 3-D calculations. Extensions to DSD/PRZ that can be applied to a wider range of conditions are currently being developed.

Looking forward, in the short term, the HE modeling effort needs development of enhanced predictive reactive burn and DSD/PRZ engineering models focused on physically based improvements in the chemistry, equations of state and flow physics models that can better account for off-normal conditions. In the mid-term (5 to 10 year horizon), improved predictive reactive flow modeling, in particular predictions for dead zone generation and propagation through cracked HE, require a new generation of models that homogenize the multi-phase physics of HE at the heterogeneous crystal microstructure level. In the long term, an understanding of explosive behavior at the HE crystal scale combined with large-scale molecular dynamics modeling has the potential to lead to a high-level predictive modeling capability. All these developments, however, will only occur through a close interaction between the experimental and modeling community, where novel experiments in extreme conditions need to be designed. Coupled with improvements in the HE models, computational strategies and platforms must also be designed that can adequately resolve the multiple spatial and temporal scales found in performance and safety problems.

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The Detonation Sandwich by Daniel E. Hooks (Los Alamos National Laboratory)

Take a slab of explosive, $\frac{1}{2} \times 6 \times 6$ inches, and begin a detonation along one edge. Confine the slab by placing similarly sized slabs of inert material on either side of the large surfaces, and you have the detonation confinement sandwich test. The explosive is the meat, and the confiners are the bread. You measure the rate of detonation through the slab with a series of pins, and you observe the detonation breakout shape at the end with a streak camera (an instrument for measuring the variation in a pulse of light's intensity with time). This simple arrangement, an idea conceived by Larry Hill and Tariq Aslam of Los Alamos National Laboratory, is providing some crucial data to test our understanding of detonation and our ability to efficiently model the process.

The analogy has significant limitations, but imagine that the flow of detonation in the explosive sandwich is like water in a river. The flow of the water is curved, primarily by the interaction of the flow with the riverbank and bottom. If the banks are deep and concrete, the flow remains fast and flow curvature isn't affected too much. With a shallow sandy bank, however, the flow is altered dramatically by the increased drag, giving increased curvature. In our detonation test, the sandwich is wide so that the cross-section where the measurement is made is two-dimensional, which is sort of like our simple view of the surface of the river. From this point, things get a little weird, but we'll come back to that in a moment.

In a detonation, the solid explosive converts to hot expanding gases ("products") through a series of chemical reactions at supersonic velocity or approximately 18,000 mph. To model this process, there should be a built-in system to account for the chemistry (which we don't understand in great detail) and resolution sufficient to capture the process (which is so fine it makes it extremely demanding computationally). This approach, called "reactive burn," is the approach of some models. On the other hand, detonation has been efficiently modeled by taking the process in two steps. First, ignoring the chemistry, the position of the detonation front is determined and tracked. In the second step, the energy of the chemical reactions is added by separate methods, which is not discussed here. A very good method to track the detonation utilizes the relationship between the curvature of the detonation front, the equations of state (EOSs) of the explosive material and its products, and the

boundary conditions of the detonation process. This is called the detonation shock dynamics (DSD) model.

DSD takes the EOS (or the thermodynamic equations describing the state of matter under a given set of physical conditions) of explosive and confining materials and defines a relationship where the detonation velocity is a function of the curvature of the front. This can then be converted, using a commonly employed trick of aerodynamicists, to a plot of pressure versus an angle at the edge of the detonation called the streamline deflection angle. On this "shock polar" diagram, confining materials can also be mapped, and one can deduce the boundary conditions for the detonation calculation, with the edge angle and confiner being important factors.

Now, if you have high confidence in the explosive and confining material EOS, sometimes the prediction of this angle is a simple matter. Because explosives tend to detonate with some stimulus pressure, it is tricky to measure the EOS at pressures nearing this point. So in most cases, these curves are extrapolations. Explosive and product EOS determinations are an active area of research for this reason, among others. However, we can also

approach the problem from the standpoint of the DSD theory, and simply measure the angles we need. This measurement delivers correct angles to the model and has the added benefit of validating the accuracy of the EOS. This is what the sandwich test is designed to do. Figure 1 shows a picture of an assembled sandwich test.

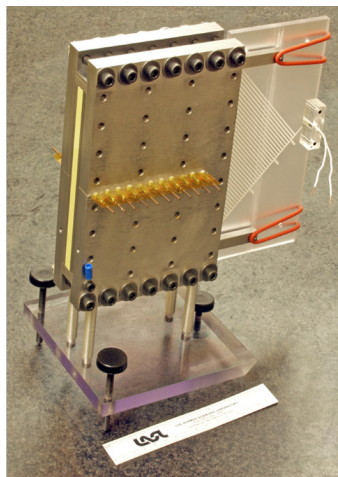


Figure 1: The sandwich test. The wires on the right are on the detonator, and the translucent plastic with white lines is a "line wave generator" that begins the detonation of the slab in a line. Visible along the center of the steel slabs are the connections for a row of timing pins. The yellow visible on the left is the edge of the PBX 9502 explosive slab. The camera records the shape of the detonation and the shock in confining slabs along this edge.

For “good” confining materials, the edge angles are just what you imagine. A heavy material is pushed away at some angle and the shock in the confining material trails behind the detonation front. This is the case for detonating insensitive explosive, PBX 9502, confined by tantalum as shown in Figure 2.

There are cases that can test the theory and stretch the imagination. Let’s consider three of them.

1. When the speed of sound in a confining material, or “sound speed,” is comparable to the explosive, then the shock in the confiner keeps pace with the detonation front, and might even lead the detonation on a small length scale (sound speed will generally increase with pressure). The confiner might be deflected into the flow like a rocket nozzle before bending away. DSD theory predicts that this result would arise in pairings like PBX 9502 confined by aluminum.

2. When a thin “poor” confiner is backed by a thick “good” confiner, theory predicts that the specific solution is dependent on the thickness of the layers, and the match to the good confiner might be a so-called “weak” solution. This might be the case for PBX 9502 confined by plastic backed by steel.

3. When the confiner has a sound speed that exceeds the detonation velocity of the explosive, the shock in the confiner would lead the detonation shock and influence the detonation process itself, except the detonation isn’t fast enough to shock the confiner. In the river analogy, the only close comparison is the forward curvature observed when water flows in a capillary tube. This is a poor analogy because in the supersonic detonation flow, what we expect is actually unsteady (turbulent) behavior. Thus, the DSD theory breaks down without higher order considerations. This seemingly unique situation is more easily constructed than you might think. Ammonium nitrate–fuel oil (ANFO)

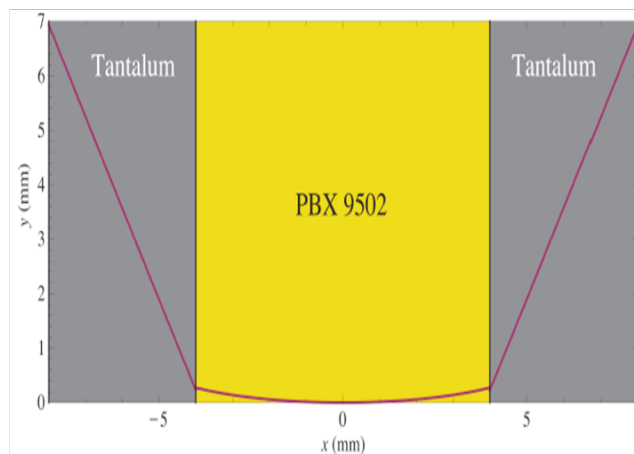


Figure 2: A detonation front from the streak camera data of a sandwich test.

confined by aluminum, and PBX 9502 confined by beryllium both fall into this category.

In cases 1 and 2, we’re not sure if we can resolve the small details to confirm the theory. In case 3, we don’t have the tools to measure a three-dimensional flow field with the needed time and spatial resolution. But in all of these cases, we expect there to be an “effective” deflection angle determined by the key features of the confinement, and depending on what we find out, we may be able to ignore the details the theory predicts in practical application.

Sandwich test results are giving these answers now. In the longer term, however, our scientific curiosity and rigorous validation of the theory demands tools that can resolve the details on the edge of detonation.

Speaking of curiosity, think this one over: how do you treat the interface if the confining material is itself another explosive?

Joint DoD/DOE Munitions Technology Development Program—High Explosives by Eric Mas (Los Alamos National Laboratory), Bruce Watkins (Lawrence Livermore National Laboratory), and Paul Butler (Sandia National Laboratories)

The Joint Department of Defense (DoD)/Department of Energy (DOE) Munitions Technology Development Program (IMP) is a cooperative, jointly funded effort of research and development to improve nonnuclear munitions technology. This program is enabled under a Memorandum of Understanding (MOU) between the DoD and DOE, approved in 1985, that tasks the nuclear weapons laboratories of the DOE to use their unique capabilities to gain scientific understanding and develop advanced technologies that can be used to solve problems common to both departments. This collaboration has proved to be of great benefit to both departments and has contributed to the development of technologies of critical importance in the life cycles of the nation’s nuclear and conventional weapons systems. Since the program’s inception, high explosives (HEs)

research has been one of the IMP’s most important thrusts. This article explores three HE topics currently under research: synthesis, modeling and simulation, and use of unique NNSA facilities to investigate HEs.

Synthesis

The DOE/NNSA weapon labs play a key role in our national effort to synthesize new HEs. The labs involvement with the IMP has lead to developing new materials that show promise for both NNSA and DoD applications. For instance, the materials diamino-dinitropyrazine oxide (LLM-105) (see Figure 1) and diamino-azoxyfurazan (DAAF) have explosive power similar to Research Department eXplosive (RDX), but are comparably much more thermally stable and insensitive to common insults. These traits allow a much wider safety margin when employed in munitions. The labs

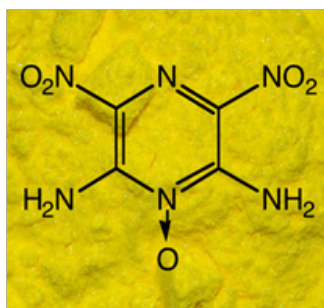


Figure 1: Molecular structure of LLM-105.

are also evaluating other materials such as melt-castable HEs that have high output power and low melting points.

JMP resources are also helping solve programmatic issues with existing materials. For example, the DoD overseas operations are placing increased demands for the insensitive high explosive triaminotrinitrobenzene (TATB), which is no longer produced domestically. To help the war effort, the DOE agreed to release some of its strategic stockpile of TATB to the DoD, and accelerated the effort to develop a new domestic source. The JMP and other interagency efforts identified several new synthesis routes that DOE and DoD are considering to ensure a reliable domestic source of TATB.

Modeling and Simulation

The ability to perform predictive simulations of HEs and weapon performance, target effects, and collateral damage has improved dramatically over the past decade. Using advanced computational tools developed by or with support from the JMP, the DoD is now able to design and develop many weapons on a computer, and then build and test small numbers of prototypes to verify the design; rather than using the historical, expensive, and time-consuming method of iteratively building and testing many units. For example, the hydrocode CTH, employed to model the dynamic response of materials and structures to impulse and impact, is the most used code on DoD high-performance computers, while the thermochemical code Cheetah, used by more than 500 licensed users, predicts the characteristics of every new HE for the DoD and NNSA. In addition, DoD engineers are increasingly using the hydrocode ALE3D and the SIERRA-Solid Mechanics suite of codes to design weapons and analyze systems' performance, vulnerability, and lethality. A DoD self-assessment determined that use of DOE codes saved DoD designers 6 to 12 months of development time and \$0.5M to \$2M per weapon system.

The ability to model the mechanical response and energetic performance of HEs is vital for designing new weapon systems and for evaluating the safety of an HE exposed to severe environments such as cold, heat, or nearby explosions. The large number of credible safety scenarios for the variety of materials, system configurations, and possible threats makes it impossible to rely solely on experimental

methods to evaluate a system. Computer codes such as CTH and ALE3D are commonly used to assess weapon safety in the event of thermal insults to energetic materials (EMs). For example, Figure 2 shows CTH simulations for a system containing an HE that is heated. In addition, these tools provide design support for critical EM safety components and subsystems.

These design and analysis tools require sophisticated models that accurately represent the important underlying physics, chemistry and materials properties for a wide range of weapon scenarios. New insights into EM behavior are now captured by CDAR-K and HERMES models (safety simulations); a multi-phase convective burn model (deflagration behavior); detonation shock dynamics and hot spot models (HE performance); and ViscoSCRAM (HE mechanical response), where ViscoSCRAM has been used by the U.S. Army and U.S. Air Force to assess weapon system survivability to bullet impact and by NNSA to close out a Significant Finding Investigation.

High performance computers and better diagnostics are enabling scientists to investigate the underlying physics and chemistry of HE response at ever smaller length and time scales. We currently run simulations on HE resolved to the micron scale (for comparison, the larger grains in our explosives are several hundred microns). Such simulations utilizing realistic material structures and properties are illuminating the complexities of the HE mechanical response, and those that combine ALE3D hydrodynamics with Cheetah thermochemistry and kinetics, provide unparalleled insight into the hot-spot initiation mechanisms of HEs.

NNSA Facilities to Investigate HEs

The MOU specifically states that unique capabilities at the NNSA labs should be used when appropriate to support JMP work. Premier facilities such as the Proton Radiography Facility (pRad), Dual Axis Radiographic Hydrotest Facility, ZR Facility, VELOCE pulsed power

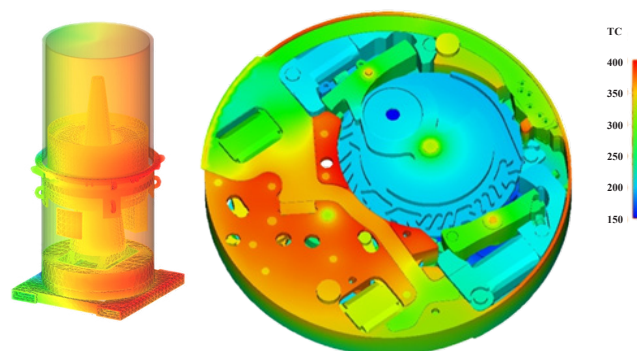


Figure 2: Weapons system model (left) for EM thermal insult assessments; board-level model (right) for critical EM safety design assessments.

generator, and the multi-headed x-ray diagnostic facility HYDRA use advanced diagnostics to observe and measure physical processes at the grain scale as the HE undergoes dynamic thermal and mechanical loading. Because our current models treat an HE as monolithic, they cannot capture the material behavior at these small-length scales. This is important because fracture, fragmentation, and ignition are often driven by the grain-scale structures. In order to treat these important phenomena in a predictive way, our next generation models will have to be informed by at least the mesoscale. It is unlikely that a systems-level simulation will resolve the explosive grains, but the effects of inhomogeneities and how they determine the bulk response must nevertheless be considered. For models to be predictive, these very important mesoscale responses will need to inform the macroscale models; which can be done using homogenization computational approaches. The JMP, accordingly, has several efforts working on next-generation HE homogenization models.

JMP scientists have developed and demonstrated methods to take proton radiographic images at pRad to measure the internal details of HE burning during a thermal explosion. Internal temperatures are monitored as the HE is heated and, when it is on the brink of igniting, it is initiated by a laser pulse, reliably causing the internal burning of the HE to be synchronized with the pRad beam. Using these techniques developed at the pRAD facility, JMP scientists have demonstrated that the radiographic observation of cracking, the propagation of density loss in the sample, and the measurement of the solid loss over time are precisely the observations necessary to understand the mechanisms of internal burning and reaction violence. This is illustrated in Figure 3, in which a cylindrical sample of PBX 9501 has been heated to ignition. The images show the evolution of a

crack pattern emanating from the point of thermal ignition, and the cylindrical case opening due to pressurization (see the vertical white feature at the cylinder midplane). In a collaborative effort, these techniques were applied at the HYDRA facility to enable x-ray radiography.

The contributions the JMP has made to HE science over the past 26 years are considerable, as demonstrated by the few examples presented here, but additional research will be required to create fully predictive computational tools. The ability to predict the fragmentation and inhomogeneous response of HEs, for example, will take considerable effort. Further, the breadth of the JMP goes far beyond HEs. The vision of the JMP is to conduct foundational research across a wide range of topics to address today's DOE and DoD

munitions science challenges while building capabilities that will enable innovative solutions to tomorrow's challenges. Additional JMP topics and accomplishments are available for discussion by contacting the three JMP Lab Managers.

Paul C. Butler, pcbutle@sandia.gov

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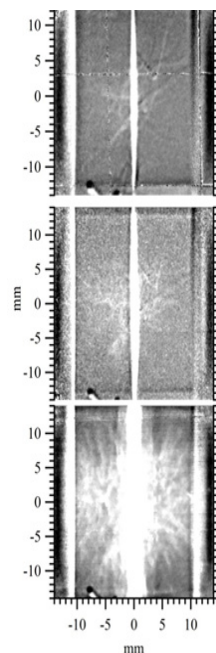


Figure 3: Proton transmission images of 1-inch diameter cylindrical experiment viewed side on with the axis of symmetry oriented horizontally. Frames are 10 μ s apart beginning 20 μ s after the TC trigger, progressing down.

2010 IEEE/NPSS Fusion Technology Award

Ulrickson of Sandia National Laboratories is the recipient of the 2010 Institute for Electrical and Electronic Engineers (IEEE)/Nuclear and Plasma Sciences Society (NPSS) Fusion Technology Award. Ulrickson received the award "for his outstanding and innovative technical leadership in the development of plasma facing components for fusion energy, for his leadership contributions to the ITER (International Thermonuclear Experimental Reactor) Blanket Integrated Product Team and to the United States ITER Domestic Agency, and for his many years of service to the fusion energy sciences community." Previously, Mike was recognized with a DOE Appreciation Award in 2007 for his leadership in the ITER Project and his service to the fusion energy sciences. His expertise in plasma facing components has been sought by many in the national and international communities.

2012 Tom W. Bonner Prize

Witek Nazarewicz, a distinguished theorist with broad expertise in nuclear physics, interdisciplinary many-body science, and computational physics, has been named the next recipient of the highly prestigious 2012 Tom W. Bonner Prize from the American Physical Society (APS). Nazarewicz will be awarded the Bonner Prize, which recognizes and encourages outstanding experimental research in nuclear physics, "for his foundational work in developing and applying nuclear Density Functional Theory, motivating experiments and interpreting their results, and implementing a comprehensive theoretical framework for the physics of exotic nuclei." The 2012 prize will be presented to Nazarewicz at a special ceremonial session during the APS meeting in Atlanta next spring. Nazarewicz is a Stewardship Science Academic Alliances grantee.

New Faces at the Office of Stockpile Stewardship

NNSA's Office of Stockpile Stewardship has welcomed several new professionals to its ranks over the past few months. Each brings impressive expertise and skillsets to our offices. The next time you're in town, stop by and say hello.

Major Eric Furman, an Air Force Fellow being sponsored by the Office of Advanced Simulation and Computing through June 2012, is a physicist/nuclear engineer from Air Force Headquarters, Strategic Deterrence and Nuclear Integration. He is here to gain an understanding of the NNSA structure, its capabilities and challenges, and its relationship with the Air Force and the rest of the Department of Defense.

Dr. Aaron Koskelo, a detailee from Los Alamos National Laboratory (LANL), where he served as Deputy Group Leader of the Plasma Physics Group, is providing expertise in the areas of analytical spectroscopy, instrumentation and imaging. He is also involved in related applications, including dynamic materials, remote sensing, and analytical chemistry. He will be supporting the Office of Defense Science and the Office of Nuclear Experiments through the end of April 2012.

Leah Kuchinsky is a Senior Project and Congressional Communications Manager with Science Applications International Corporation. She brings expertise in the areas of nuclear nonproliferation, weapons of mass destruction terrorism, and international security. Her responsibilities include drafting Congressional testimony and questions, preparing materials and briefings for Congressional members and staffers, and coordinating reports to Congress.



Furman

I am extremely happy that the Air Force has given me this opportunity to work with and learn from this NNSA team. I learn something new every day and I've enjoyed impressing my Air Force friends with all of the fabulous accomplishments you've done here and at the labs.



Koskelo

In uncertainty, there is opportunity. This is an excellent time to improve integration between the programs which drive our National Security mission. I am enjoying the challenge.



Kuchinsky

I am thrilled to be part of the NNSA team and excited to learn new things. I am eager to help further the vitally important Stockpile Stewardship mission.

Brooke Samples joined the Office of Defense Science as the United States (US)/United Kingdom (UK) Program Coordinator on August 29, 2011. Her areas of expertise include national security policy, international relations, and strategic planning. Among her major duties are overseeing all joint US and UK nuclear weapons research and development programs, technical weapons exchanges, and providing policy planning and program management expertise to evaluate and coordinate the exchange of nuclear weapons data under the Mutual Defense Agreement.

Dr. Robert (Bob) Weaver is a fellow from LANL with extensive experience in computing, large-scale computing, advanced simulation and computing (ASC) codes, and weapon design and weapon physics. As a detailee to the the Office of Advanced Simulation and Computing, he will examine exascale computing issues, including memory requirements of ASC codes to be aligned with the Predictive Capability Framework (PCF); detail emerging gap between current codes and architectures and probable machines in the 2018 and beyond timeframe. He will be at NNSA one week per month.

Dr. Chris Werner joined the Office of Defense Science as a science detailee from Lawrence Livermore National Laboratory's AX Division, where he worked in support of the ICF and secondary design community, investigating, developing and implementing algorithms. His areas of expertise include primary and secondary physics, Monte Carlo particle transport, radiochemistry, radiation transport, and nuclear data. He will work with the Office of Defense Science for the next 1-3 years.



Samples

I am excited about the opportunity to serve in this new role and look forward to continuing to expand and enhance collaborations between the US and UK on critical scientific and engineering programs.



Weaver

Having just started, I am extremely pleased to get to know all the people working in the Office of Stockpile Stewardship; I want to be a resource for anyone who would like to talk codes, computers, PCF and weapon physics. Please stop by.



Werner

Every day presents new challenges; decisions made here have national implications. I am thrilled to be a part of Defense Programs here at NNSA Headquarters.

Publication Highlights

This section highlights recent publications in high-impact scientific journals of research supported by the NNSA Office of Stockpile Stewardship.

Velocity and Timing of Multiple Spherically Converging Shock Waves in Liquid Deuterium, T.R. Boehly et al., Phys. Rev. Lett. 106, p. 19505, 2011.

The basic principle of inertial confinement fusion (ICF) is simple. Put enough energy into the fuel material fast enough to heat it to temperatures sufficiently high for significant fusion to occur during the brief time that its own inertia holds it more or less in place. The simplest way to do this would be to heat uncompressed spheres of fuel. Unfortunately, by the mid 1960s, theorists had already demonstrated that, to yield more fusion energy than the energy required to heat the fuel initially using such a scheme, it would be necessary to build laser drivers of orders of magnitude larger than the National Ignition Facility (NIF).

Eventually, scientists realized that driver energy requirements would be much lower if the fuel was first compressed to a very high density. This could best be done at a relatively low temperature. A small volume of the cold, compressed fuel material could then be heated to the temperature necessary for fusion ignition to occur by a strong, converging shock. Energetic alpha particles produced in these first fusion reactions would then propagate outward into the surrounding cold fuel, heating and igniting it, causing a burn wave to move outward, efficiently consuming the fuel. Unfortunately, a German physicist named Guderley had demonstrated as early as the 1940s that there are limits on the heating that can be achieved with a single shock, and that limit was too low for efficient fusion to occur.

By the early 1970s, scientists had devised an ignition scenario involving multiple, converging shocks that, in theory, should result in efficient burning of the fuel material. Those theories, which are currently being tested on the NIF, require extremely precise timing of the multiple, converging shocks. In this paper, an elegant series of experiments is described in which, for the first time, the effects on shock velocity of the convergence of multiple shocks in spherical geometry was directly observed for the first time. The experiments, performed on the OMEGA laser at the University of Rochester's Laboratory for Laser Energetics, point the way to the development of shock timing techniques that may well prove critical to the success of the National Ignition Campaign currently underway on the NIF.

Experimental Determination of Third-Order Elastic Constants of Diamond, J.M. Lang, Jr. et al., Phys. Rev. Lett. 106, p. 125502, March 2011.

Third-order elastic constants reflect the lowest-order anharmonic response of crystals and are important for understanding their thermomechanical and anisotropic response at extreme conditions. A minimum of six independent measurements are needed to determine the six third-

order elastic constants of a cubic crystal. Typically, acoustic measurements under both hydrostatic and uniaxial stress conditions provide the experimental data for determining these constants. However, due to the extreme stiffness and strength of diamond, only hydrostatic stress measurements are feasible and they provide only three results. To work around this limitation, the third-order elastic constants of diamond have been estimated to date from various theoretical models. The constants from these models show significant variations, demonstrating the need for relevant experimental data. The authors present a novel approach to obtain the requisite data using shock compression experiments on diamond.

In Figure 1, high purity, diamond single crystals were shock compressed along the [100], [110] and [111] crystallographic orientations to stresses ranging from 60 to 120 GPa, and the elastic response was carefully measured. The longitudinal stress-density results for each orientation were fit using finite strain theory to determine an "effective" third-order elastic constant for each of the three orientations. The shock wave compression results, along with published hydrostatic measurements, were used to determine the complete set of third-order elastic constants for diamond.

Some of the experimentally determined third-order constants agree somewhat with earlier theoretical work, but clear differences exist between experimental and calculated results. For the [110] and [111] orientations, the elastic response is measurably stiffer than predicted from theoretical calculations. Measurements on orientations other than those studied could show even larger differences, depending on the contributions from different third-order constants. The elastic response calculated using only second-order elastic constants deviates significantly from experimental results beyond 1% compression, showing the necessity to incorporate third-order elastic constants in understanding and modeling the anharmonic and anisotropic response of diamond at high stresses.

This work provides benchmark results to evaluate theoretical calculations on diamond at extreme conditions. The third-order elastic constants provide a starting point for understanding the high pressure solid-solid phase transition in diamond, the

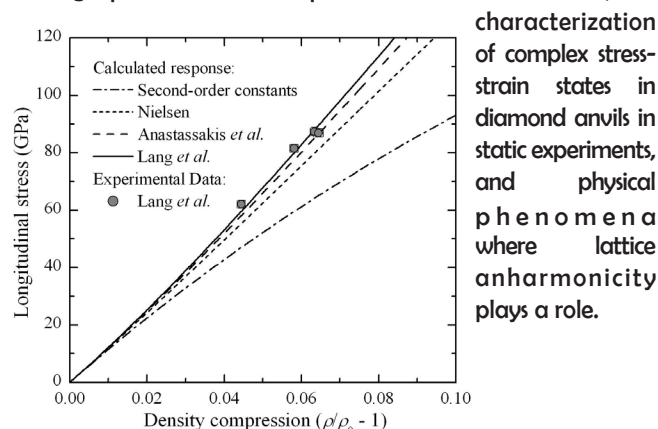
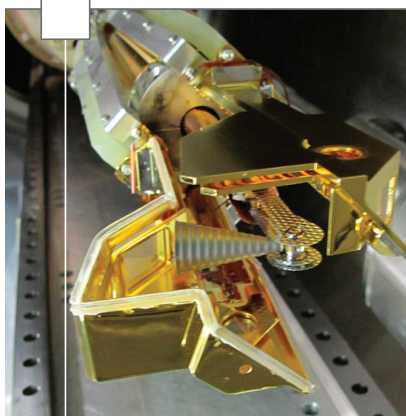
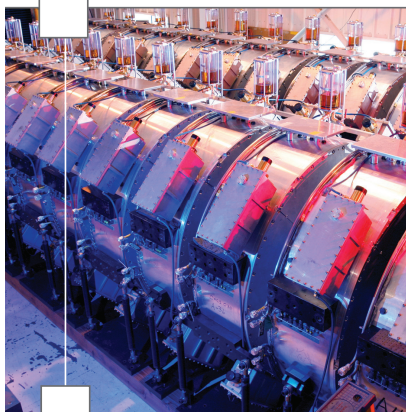
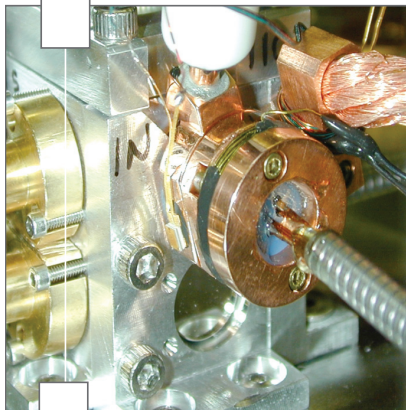


Figure 1: Calculated and measured response of diamond shock compressed along the [110] direction. Notice the deviation of the predictions using second-order elastic constraints.



APPLICATIONS DUE JANUARY 18, 2012

IMAGES TOP: At Sandia National Laboratories, high magnetic fields on the aluminum side of this magnetically launched aluminum/copper flyer drive it into diamond targets at tens of kilometers per second, generating enormous pressures and shock waves in the diamond.

MIDDLE: Circular aluminum structures create magnetic fields in Los Alamos National Laboratory's Dual Axis Radiographic Hydrodynamic Test accelerator, focusing and steering a stream of electrons.

BOTTOM: A "keyhole" target for a shock timing experiment is positioned on the ignition target insertion cryostat in the cryogenic target positioning system of the National Ignition Facility at Lawrence Livermore National Laboratory.

Images courtesy of respective laboratories.



Department of Energy National Nuclear Security Administration

Stewardship Science Graduate Fellowship

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- Yearly conferences
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- Renewable up to four years

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