Lawrence Livermore National Laboratory

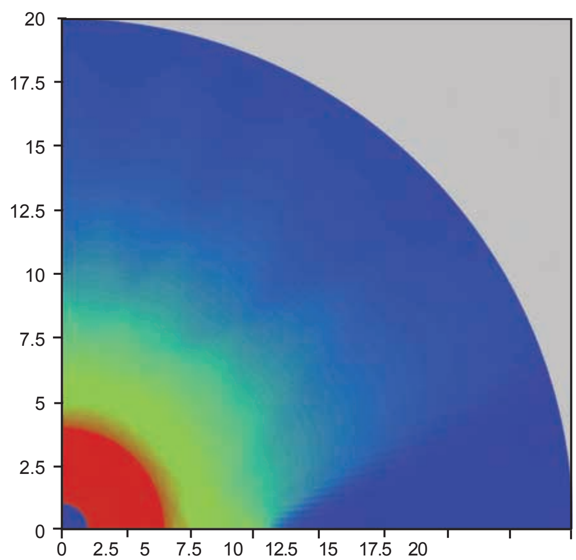
Development and Study of a Method Adaptive in Angle Variables for Solving 2D Transport Equation

Principal Investigators: Howard A. Scott (LLNL) and A. V. Alekseev (VNIIEF)

Project Description

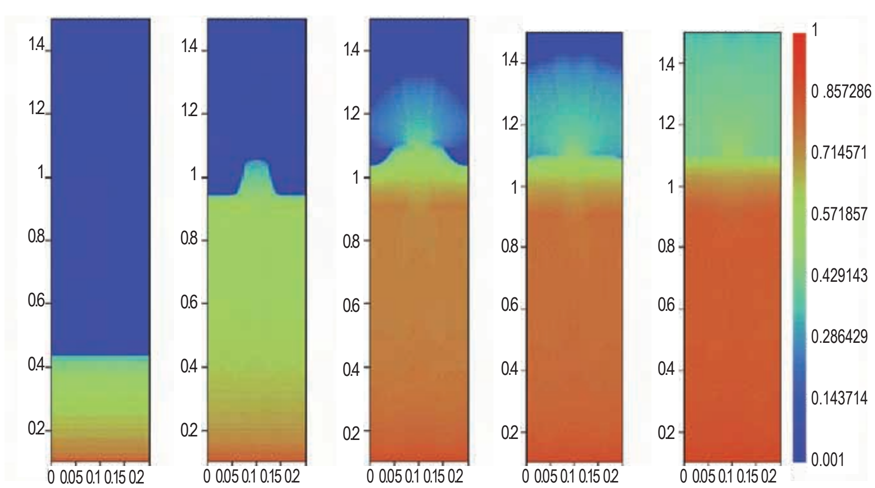
The objective of this project is to develop and demonstrate more efficient methods for solving radiation transport equations using adaptivity in angle variables. Conventional angular discretization methods require that the angular finite-difference grid be fine enough in any region. If the grid is too coarse, well-known "ray effects" appear. In addition, subdomains appear with a highly anisotropic particle flux distribution over directions where a very fine angular difference grid must be used, as well as subdomains where the distribution is nearly isotropic. In view of this, a promising approach to multidimensional transport solution efficiency enhancement using finite-difference approximations is one employing adaptive grids. Such adaptive methods are expected to resolve the "ray effect" problem in a cost-efficient manner.

The algorithm for solving the radiation transport equation using an angle-adaptive method with dynamic criteria for constructing the grid was evaluated using a set of benchmark test problems (pipe, slit, vacuum, and spherical).



The spatial distribution of radiation temperature, showing that geometric divergence is not accurately modeled by angular discretization in S_N transport algorithms, resulting in "ray effects."

Below: The radiation temperature distribution at five times. Radiation transport through a slit displays significant angular variations, including unphysical "ray effects."



Technical Purpose and Benefits

The simulation of multidimensional transport processes is an area of great interest. Deterministic methods, combined with improved discretization and acceleration techniques, hold the promise of accurate simulation of a variety of transport processes in complex geometries. However, the realization of this promise has proven to be very difficult, and further advances in algorithms are needed. One of the primary difficulties is that the number of variables required to model a given system can be extremely large, as the transport requires a description in six-dimensional phase space. Reduced dimensionality, using spatial symmetries, diffusive transport, or energy-averaged variables, is usually invoked to minimize the computational requirements, but each of these approximations has limited applicability. It remains true that resolved transport simulations of many physical systems remain beyond the reach of our most powerful computers. More efficient algorithms, such as the one demonstrated in this project, are needed. This adaptive approach may be contrasted to a complementary energy-adaptive approach investigated in project B541415.

Collaboration between Lawrence Livermore National Laboratory (LLNL), Livermore, CA, USA, and the Russian Federal Nuclear Center - All Russian Research Institute of Experimental Physics (RFNC-VNIIEF), Sarov, Russia

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Lawrence Livermore National Laboratory

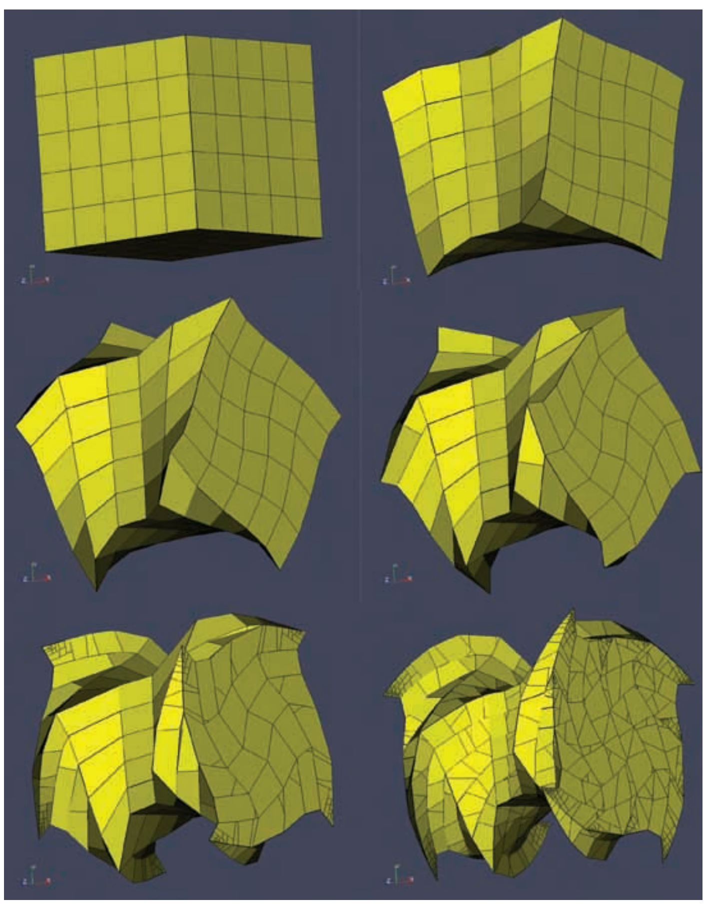
Mesh Refinement and Reconnection in Arbitrary Polyhedral Free-Lagrange Hydrodynamics Simulations

Principal Investigators: Douglas S. Miller (LLNL) and Vera Rasskazova (VNIIEF)

Project Description

The objective of this research is to develop and demonstrate a three-dimensional free-Lagrange hydrodynamics scheme incorporating mesh refinement to track shocks or material interfaces, allowing robust, high-quality hydrodynamic simulations. Mesh refinement allows many advantages: small-scale features in large-scale flows can be resolved, zones that are no longer needed to capture interesting physics can be deleted for efficiency, and dynamic features (such as shock waves) can be captured with many fewer zones than would be needed for equivalent accuracy with a Eulerian scheme.

A mesh refinement and coarsening algorithm was developed in a three-dimensional free-Lagrange code, with a detailed description of the method used to obtain solutions to the hydrodynamic equations and an explanation of the reconnection algorithm. The solution of a test problem defined by a rotating cone of zero viscosity fluid embedded in a stationary cube was used to demonstrate the algorithm and its efficiency.



The cube rotation problem: currently, the number of zones is 3500, compared to 125 zones initially.

Technical Purpose and Benefits

The accurate simulation of hydrodynamic and heat conducting flows requires significant computational resources. While a variety of adaptive mesh technologies exist, each has important drawbacks and inefficiencies. This project developed and demonstrated a three-dimensional free-Lagrange capability with arbitrary reconnection. This approach offers an alternative strategy to arbitrary Lagrangian-Eulerian and adaptive mesh refinement methods for simulating complex flows using the benefits of Lagrangian hydrodynamics extended to three dimensions.

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Lawrence Livermore National Laboratory

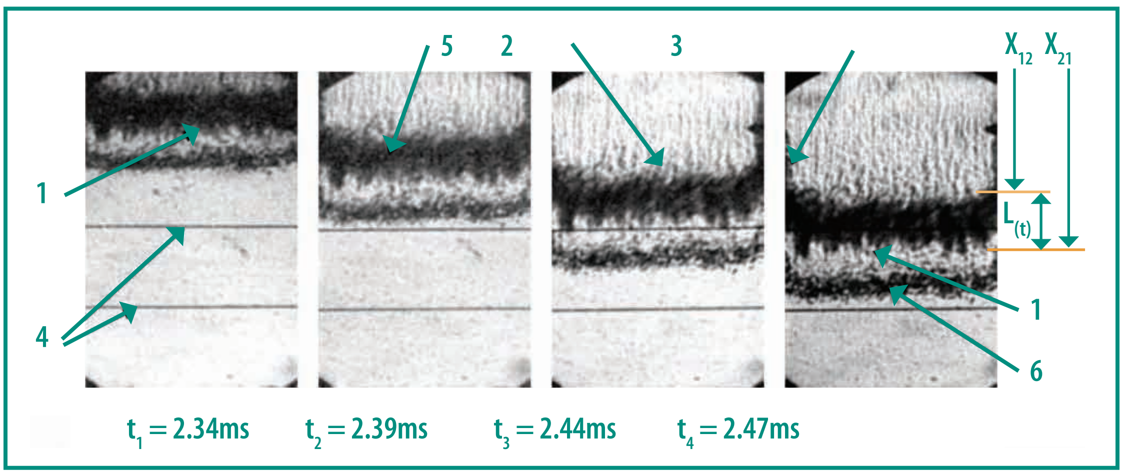
Multifunctional Shock Tube Experimental Investigation of Gravitational Instabilities Evolution

Principal Investigators: Oleg Schilling (LLNL) and Yury A. Kucherenko (VNIITF)

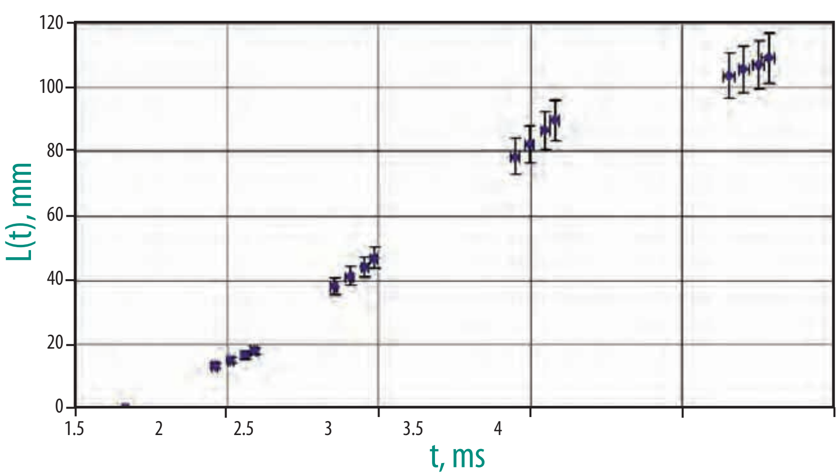
Project Description

The objective of this research is to experimentally determine the turbulent mixing properties under the combined action of the Richtmyer-Meshkov and Rayleigh-Taylor instabilities (which is characteristic of blast waves in supernovae) following the passage of a nonstationary shock wave through the interface separating two gases with different densities using the Multifunctional Shock Tube (MST) facility. The experiments were performed using gases with Atwood numbers $A = 0.21$ and $A = 0.82$ (air/carbon dioxide and helium/argon, respectively), where $A = (\rho_1 - \rho_2)/(\rho_1 + \rho_2)$. The Schlieren method was used to visualize the ensuing turbulent mixing of the gases. The time-evolution of the turbulent mixing layer width was determined in the light and heavy gases.

In this International Science & Technology Center (ISTC) Partner Project (Number 2716), the shock was explosively driven by detonating a mixture of hydrogen and oxygen, and a novel method of imposing perturbations on the thin nitrocellulose film separating the gases was used. The film was placed against a grid consisting of strong thin metal strings, and an electric current passing through the grid was used to destroy the film just as the shock arrived at the interface. Numerical simulations were performed to validate the design of the experiments.



Photographs of CO_2/He experiments: (1) mixing front in the light gas; (2) mixing front in the heavy gas; (3) wall flow; (4) scaled reference lines; (5) turbulent mixing layer; (6) fragments of nitrocellulose film.



Time-dependence of the average value of the turbulent mixing layer L(t). Error bars on the measurements are shown.

Technical Purpose and Benefits

This project carried out the first shock tube experimental investigation into the turbulent mixing evolution caused by the passage of a nonstationary shock wave through an interface separating two different density gases. The decaying shock wave accelerated the interface, thereby creating conditions for the development of both the Richtmyer–Meshkov and Rayleigh–Taylor instabilities. These experiments complement laser-driven experiments on blast wave instabilities by providing data on the qualitative structure of the mixing layer and the growth rate of the layer under a variety of conditions. Such experimental data can be used to validate numerical simulation codes that model Rayleigh–Taylor and Richtmyer–Meshkov instability-driven mixing.

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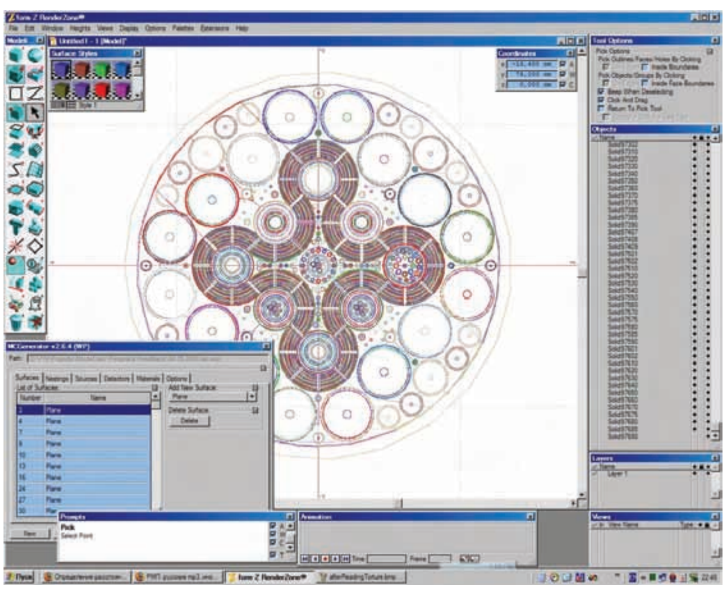
Monte Carlo Input Translators and Generator

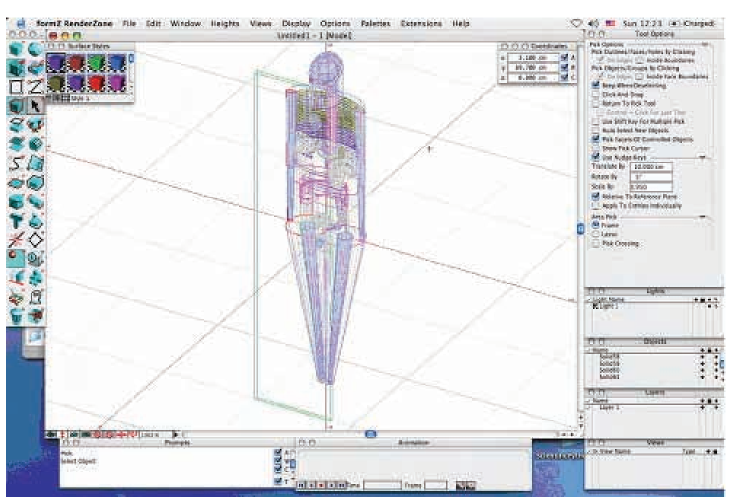
Principal Investigators: Kenneth E. Sale (LLNL) and Dmitry Mogilenskikh (Strela)

Project Description

The objective of this project is to develop plugins for three-dimensional modeling codes that read and write input file formats for three Monte Carlo radiation transport simulation codes: COG, TART, and MCNP. This represents the second stage of an effort to create a complete, unified generator (called MCGen) for the three transport codes. This stage focuses primarily on reading, writing, and translating the other input file definitions besides the geometry definition. The project delivers software in source code form.

The first stage of this project developed a minimal interface for the Windows and Macintosh converters using Python. A detailed analysis of the functionality of nested-space definitions in MCNP and COG was also performed, and unified format (UF) and conversions were implemented for UF ↔ COG and UF ↔ MCNP. The analysis and implementation of the process of conversion into TART geometry definitions were completed. The source definition syntax and semantics were analyzed for the three codes, and a unified format and conversions were implemented for UF ↔ COG, UF ↔ MCNP and UF ↔ TART. A set of Monte Carlo problem inputs with complex geometries was collected as a validation suite for the converter code.





The image on the top is from a FormZ model of a reactor system. The image on the bottom is a model of a radiation dose phantom.

Technical Purpose and Benefits

MCGen makes it possible to create faithful radiation transport models of very complicated objects far more quickly and reliably than has been possible previously. With the plugins developed in this project, these models can be developed using the powerful and sophisticated FormZ modeling interface and exported to a file that can be used as input to any of the major general purpose Monte Carlo radiation transport codes.

STRELA

Collaboration between Lawrence Livermore National Laboratory (LLNL), Livermore, CA, USA, and Strela, Snezhinsk, Russia

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Lawrence Livermore National Laboratory

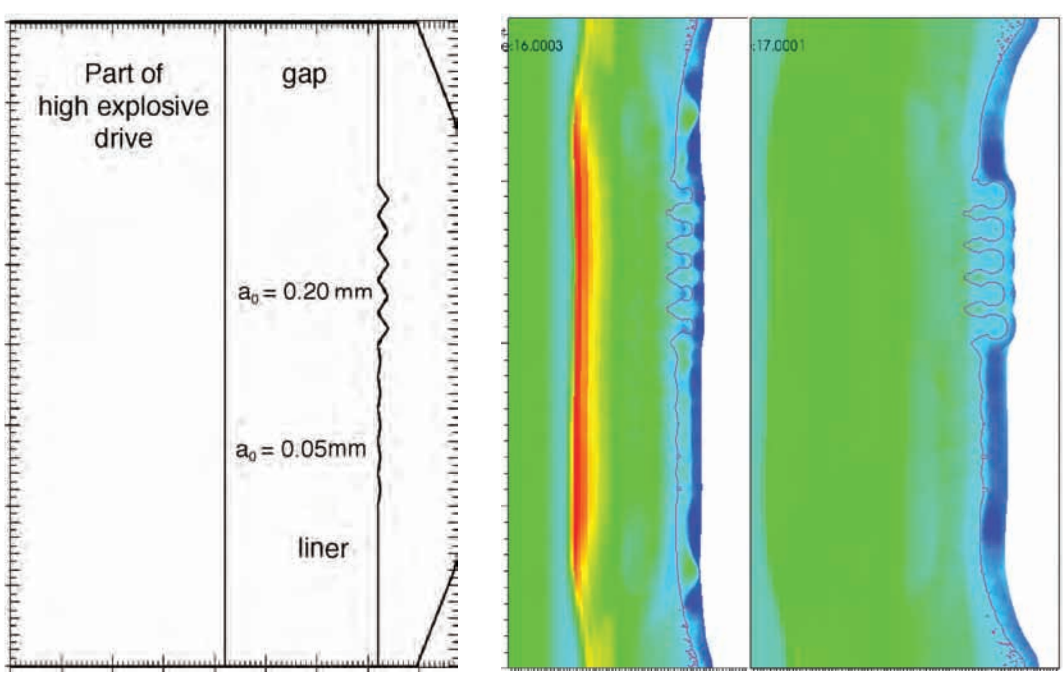
Vanadium Dynamic Strength Measurements

Principal Investigators: Patrick O. Egan (LLNL) and Victor Raevsky (VNIIEF)

Project Description

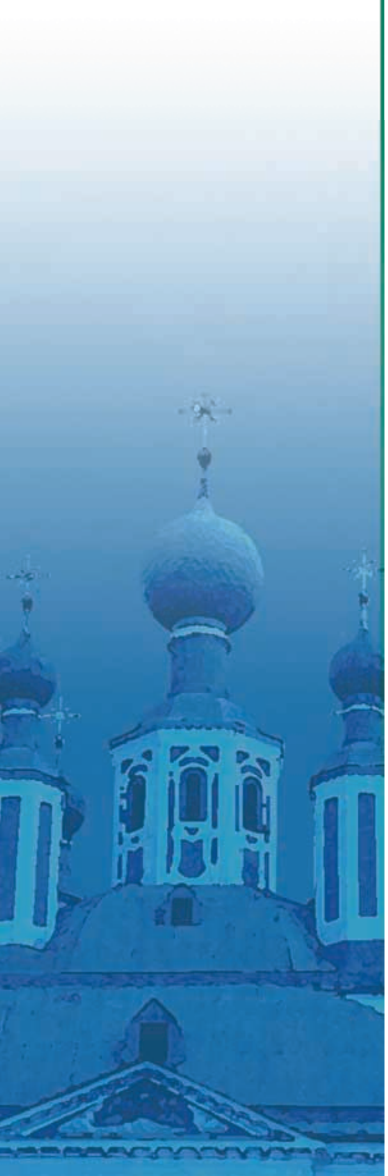
The objective of this research is to investigate the dynamic strength properties of vanadium under dynamic loading conditions. The experiments will be performed by shock-free loading vanadium samples to peak pressures of 600 kbar and strain rates in the range of 10^5 to 10^6 s^{-1}. The loading conditions will be characterized by velocimetry (VISAR) measurements. Observation of the growth (or lack thereof) of Rayleigh–Taylor instabilities in vanadium samples that are quasi-isentropically loaded by a high explosive system designed by VNIIEF will be observed using flash x-ray radiography. The vanadium metal used will be provided by LLNL so that the initial microstructures can be matched to materials used in LLNL experiments conducted at higher strain rates and shorter durations of peak pressures using laser-driven loading. These coupled experiments will allow systematic changes to be mapped out over an unprecedented range of conditions.

In the experimental design component, the drive conditions will be characterized using VISAR velocimetry measurements. A rippled perturbation will be machined on the vanadium surface and shown to be measured to ±10 microns. Numerical simulations of the proposed design will be performed as a means of validation. Ten experiments will be performed using two different grain sizes of vanadium (five shots per grain size), peak pressure to 600 kbar, and strain rates in the range 10^5 –10^6 s^{-1}. Each vanadium target will contain two zones of perturbations with different amplitudes. VNIIEF and LLNL will separately develop, validate, and update material strength models for vanadium.



Left: Initial configuration of a typical experiment, showing a schematic of the high explosive, gap, vanadium liner, and the machined perturbations with two different amplitudes.

Right: Simulated evolution of the Rayleigh–Taylor instability.



Technical Purpose and Benefits

Several dynamic strength models have been implemented in LLNL hydrocodes, including the Preston–Tonks–Wallace and Steinberg–Guinan models. The constitutive model parameters have been primarily set from Hopkinson-bar, Taylor impact, and shock-driven experiments. Traditional experimental techniques are not well suited to provide data at strain rates in the range 10^5–10^8 s^{-1}. The need for experiments to validate strength models, set parameters, and refine models at these conditions is imperative in order to provide the necessary confidence in our predictive capabilities. Previous VNIIEF experiments and LLNL laser experiments have indicated that the strength models inadequately represent the physical phenomena occurring under these conditions. The principal goal of these experiments is to address this uncertainty and to provide strength models that accurately represent the physics.

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The ACT-Electronic Project-Quantum Mechanical Simulation of Actinides

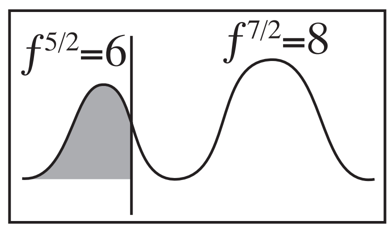
Principal Investigators: James G. Tobin (LLNL) and Andrey L. Kutepov (VNIITF)

Project Description

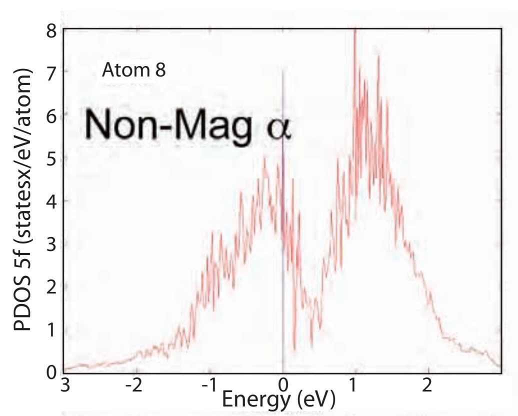
The objective of this project is to perform numerical quantum mechanical studies of material properties of selected actinides at or near ambient pressure (~1 atmosphere) and with temperatures in the range of T = 0 K to near room temperature (T = 300 K) to better understand the nature of highly correlated electron systems.

This project included a study of Np, including equilibrium geometry, total and partial density of states, magnetic moments, and differential with respect to energy magnetic moments. In addition, it provided comparison of the magnetic and electronic properties in the row U-Np-Pu-Am-Cm. Calculations of the total and partial density of states, and of the magnetic structure for Pu_3Al, Pu_3Ga and Pu_3In were performed. In addition, the formation energies for non-spin-polarized and spin-polarized cases were evaluated. Similar studies were performed for Am and Np alloys with Al, Ga, and In.

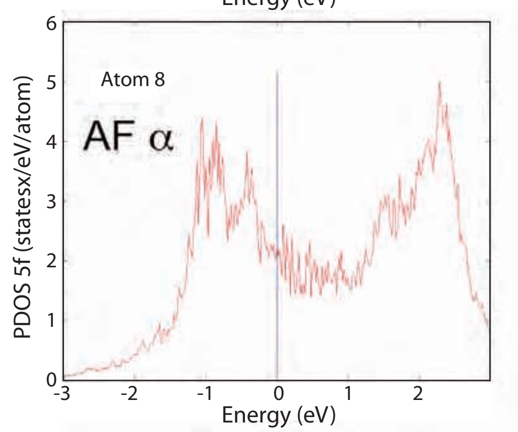
Simple picture derived from the spectroscopic analysis



Result of non-maganetic calculation, including spin-orbit in the Pu 5f's



Result of anti-ferromagnetic calculation, including spin-orbit in the Pu 5f's



Technical Purpose and Benefits

With the benefit of new experiments and quantum mechanical simulations, the electronic structure of Pu is finally being understood. In a series of experiments and linked theoretical modeling, the range of possible solutions for Pu electronic structure has been dramatically reduced. The work in this project demonstrated the absolute necessity of including spin-orbit splitting in the Pu 5f states in a direct and fundamental fashion, in both magnetic and non-magnetic calculations. The proper modeling of Pu electronic structure is key to predicting the behavior of Pu materials over time. This collaboration has led to a number of joint publications in leading physics journals:

J.G. Tobin, K.T. Moore, B.W. Chung, M.A. Wall, A.J. Schwartz, G. van der Laan, and A.L. Kutepov, "Competition Between Delocalization and Spin-Orbit Splitting in the Actinide 5f States," *Phys. Rev.* B 72, 085109 (August 2005).

J.G. Tobin, K.T. Moore, B.W. Chung, M.A. Wall, A.J. Schwartz, B.B. Ebbinghaus, M.T. Butterfield, N.E. Teslich Jr. , R.A. Bliss, S.A. Morton, S.W. Yu, T. Komesu, G.D. Waddill, G. van der Laan, and A.L. Kutepov, "Experimental Benchmarking of Pu Electronic Structure," *Matl. Res. Soc. Symp. Proc.* 893, 79 (2006).

J.G. Tobin, K.T. Moore, B.W. Chung, M.A. Wall, A.J. Schwartz, G. van der Laan, and A.L. Kutepov, "A Study of the Competition Between Delocalization and Spin-Orbit Splitting in the Actinide 5f States," in *Recent Advances in Actinide Science*, Royal Society of Chemistry, ed. R. Alvarez, N.D. Bryan and I. May, page 719 (2006).

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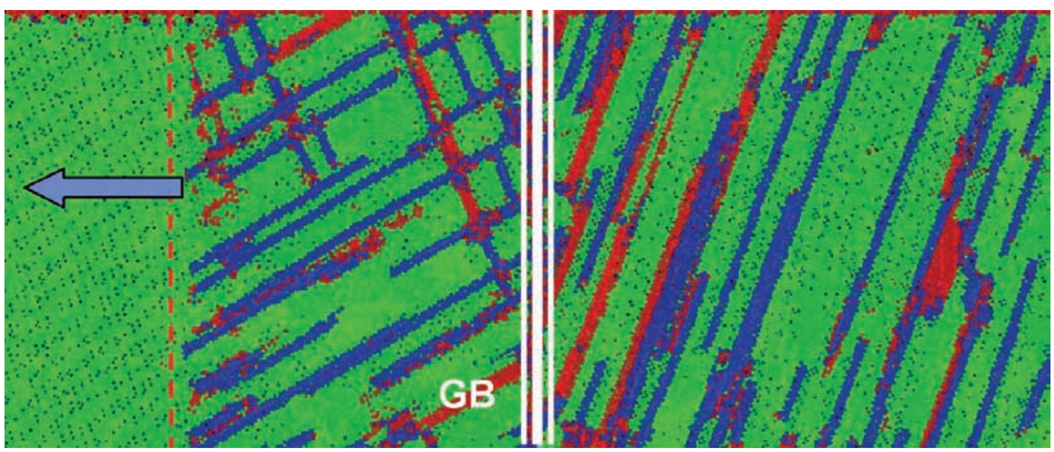
Molecular Dynamics Simulation of Elastic-Plastic and Spall Mechanisms in Cu when Dynamic Loading

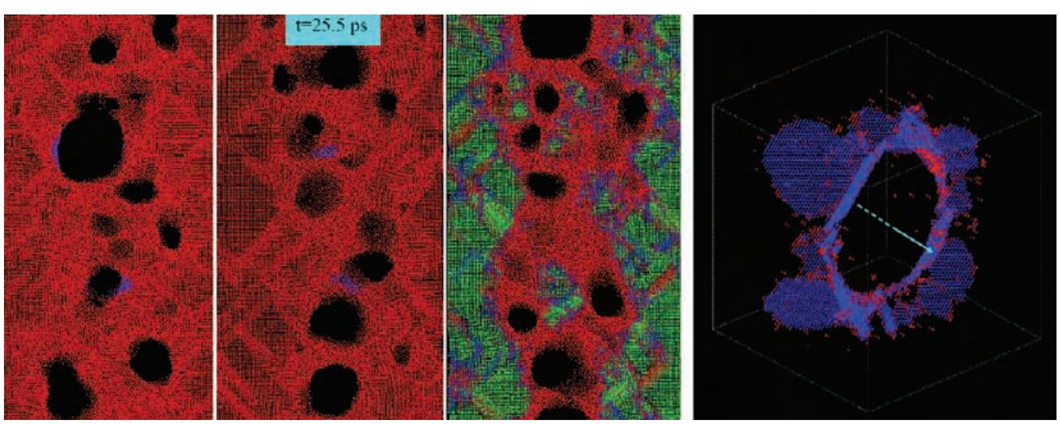
Principal Investigators: Eduardo M. Bringa (LLNL) and Vladimir V. Dryomov (VNIITF)

Project Description

The objective of this project is to perform molecular dynamics simulations of the interaction of shocks with crystal grain boundaries, dislocations, and inclusions to investigate elastic/plastic deformation of shock-loaded copper and to elucidate the influence of nano-inclusions in spall.

Typical simulations involve 10^7 atoms modeling a copper bicrystal. The EAM potential of Mishin was used. A set of simulations was performed with the grain boundary at five different angles with respect to the shock front (0, 30, 45, 65, and 90 degrees) and two different pressures. The simulations with loading involved four types of short pulses: square, triangular, Gaussian, and linear rise plus flat top. The spall simulations used randomly distributed nanoparticles (at least one near the spall plane) with a radius of 1 and 2 nm. The nanoparticles were simulated with the same potential, but changing the mass of the atoms. Two masses were considered: carbon-like and lead-like atoms.





Top: Molecular dynamics simulation showing a shock-grain boundary (GB) interaction. The blue arrow shows the shock propagation direction.

Bottom: The first, second, and third images are Cu+C, Cu+Pb, and Cu, respectively. Shock-induced spall is modified by nano-inclusions (blue). The fourth image shows a shock-dislocation loop interaction.

Technical Purpose and Benefits

The simulation of the interaction of shocks with highly symmetric grain boundaries will yield better understanding of experiments and simulations in polycrystals. The investigation into the elastic/plastic deformation of monocrystalline copper when shock loaded with short pulses of different shape yields improved understanding of the final microstructure in the shocked targets. Recent experiments have found nanoparticles at every void at the spall plane of copper targets: the investigation into the influence of nano-particles in spall may clarify whether nanoparticles act as stress concentrators, significantly decreasing the spall strength. All these contribute to the development and validation of improved constitutive models for shock-loaded polycrystalline materials.

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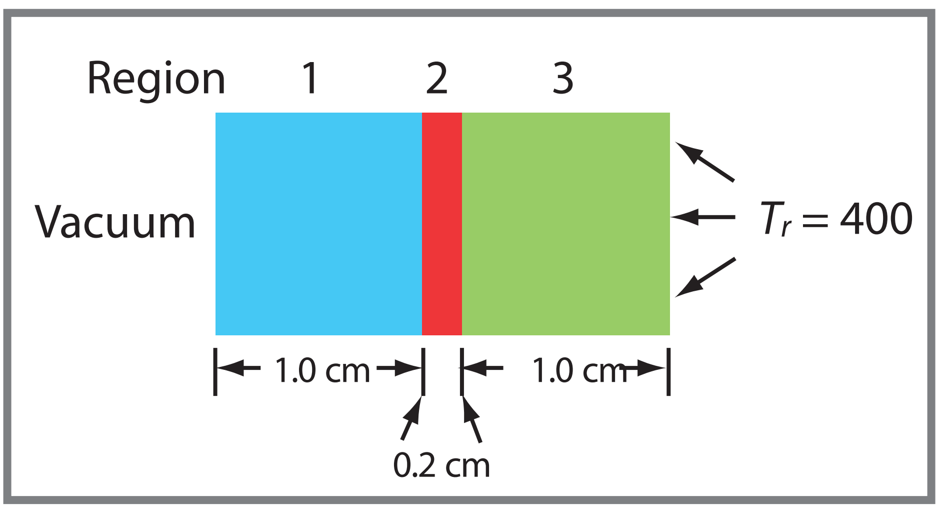
Development and Study of a Method Adaptive in Energy Variables for Solving the Radiation Transport Equation

Principal Investigators: Howard A. Scott (LLNL) and Alexander V. Gichuk (VNIIEF)

Project Description

The objective of this project is to develop and demonstrate more efficient methods for solving radiation transport equations using adaptivity in energy. Because the computational cost of a transport solution is roughly proportional to the number of energy groups used, minimizing the number of groups is desirable. However, energy discretizations of the transport equation necessarily approximate both material properties (opacities) and radiation spectra, so that the solution depends on the energy discretization. In addition, the solution may be sensitive to different spectral ranges in different regions of the domain. Adaptive techniques have the potential to address this issue, as well as to increase the accuracy and/or decrease the cost of a solution. This study addressed the need for increased efficiency by developing a numerical method using energy adaptivity.

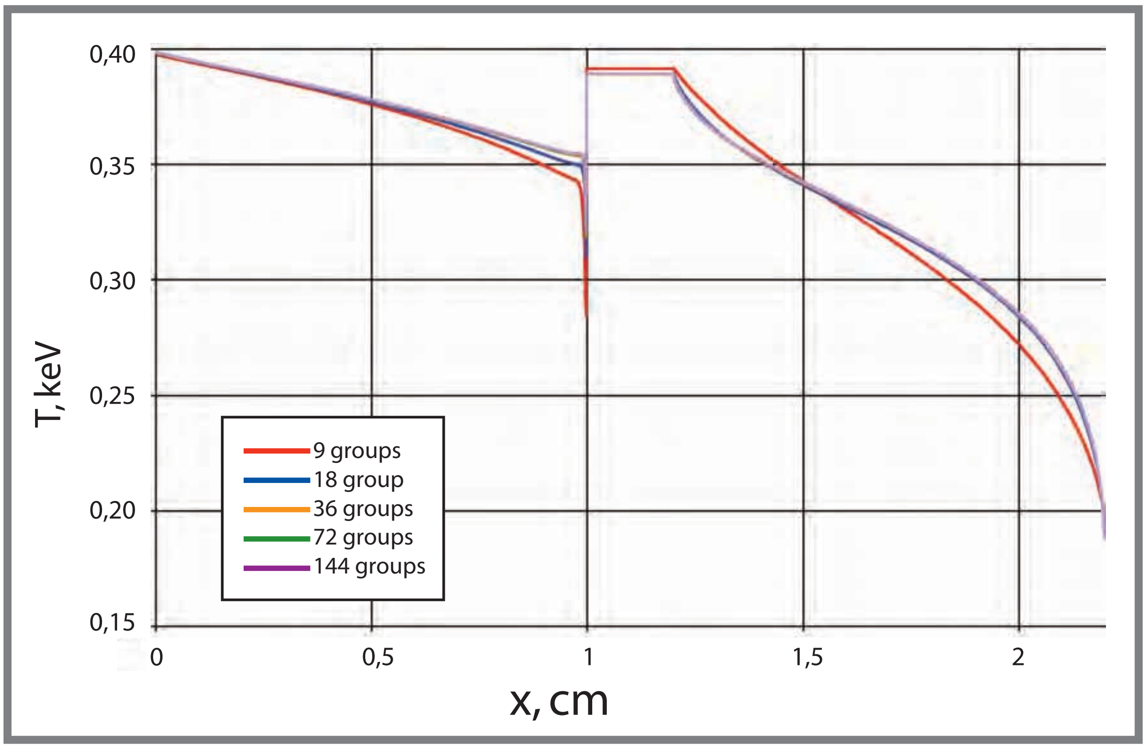
The algorithm for solving the radiation transport equation using an energy-adaptive method with dynamic criteria for constructing the energy grid was evaluated using a set of test problems. In addition to these problems, a test problem consisting of a planar one-dimensional system comprised of three regions, each with a uniform density and an initial temperature of 1 eV, was also used to test the algorithm. The transport coefficients were specified, and an isotropic radiation flux equivalent (400 eV blackbody) was incident on the boundary of region 3, with the boundary of region 1 being a free boundary. The diagnostic quantities of interest were the steady-state temperature profile and the temperature histories at positions throughout the three regions.



Schematic of test problem for energy adaptive studies.

Technical Purpose and Benefits

The simulation of multidimensional transport processes is an area of great interest. Deterministic methods, combined with improved discretization and acceleration techniques, hold the promise of accurate simulation of a variety of transport processes in complex geometries. However, the realization of this promise has proven to be very difficult, and further advances in algorithms are needed. One of the primary difficulties is that the number of variables required to model a given system can be extremely large, as the transport requires a description in six-dimensional phase space. Reduced dimensionality using spatial symmetries, diffusive transport, or energy-averaged variables is usually invoked to minimize the computational requirements, but each of these approximations has limited applicability. It remains true that resolved transport simulations of many physical systems remain beyond the reach of our most powerful computers. More efficient algorithms, such as the one demonstrated in this project, are needed.



Steady-state material temperature distribution for different numbers of groups.

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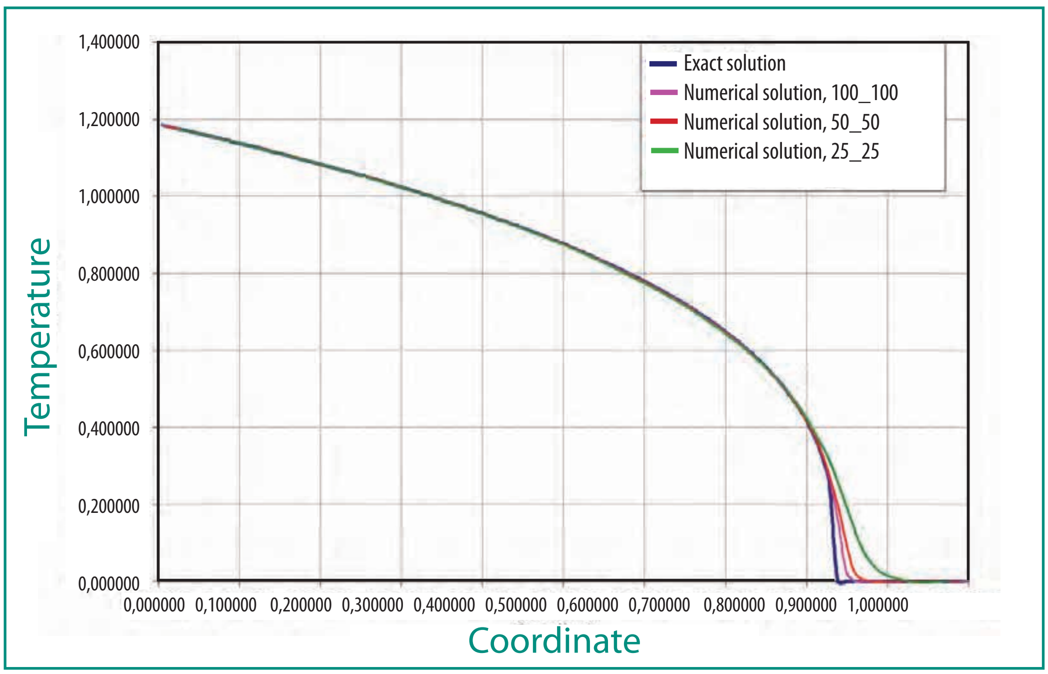
Structured/Unstructured Hybrid Mesh Hydrodynamics and Heat Conduction Studies

Principal Investigators: Howard A. Scott (LLNL) and Sergey I. Skrypnik (VNIIEF)

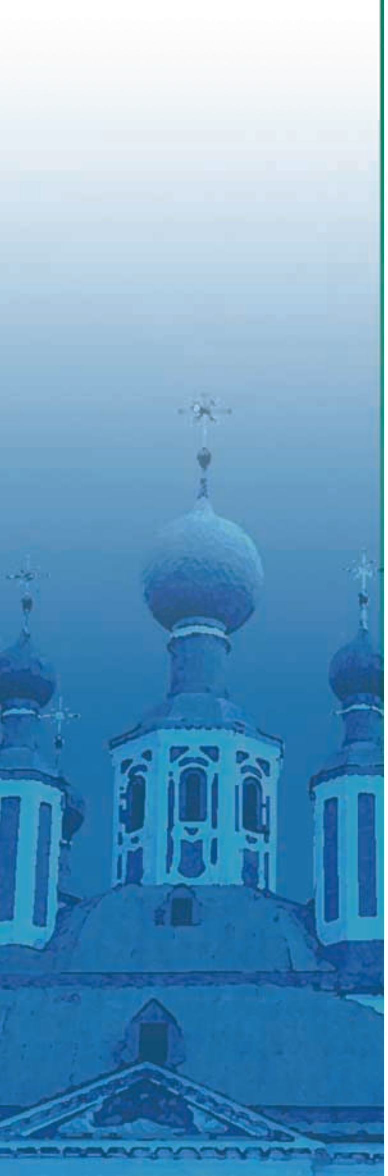
Project Description

The objective of this research is to develop and implement a methodology for two-dimensional hydrodynamics and heat conduction that allows the combined use of structured and unstructured meshes in the same simulation. The flexibility allowed by such "hybrid" meshes will expand the number of problem types that can be efficiently meshed and simulated. The algorithm is implemented in a benchmark code using analytical forms for all physical data such as the equation of state, heat conduction coefficients, etc. This project developed a serial version of the code, and a subsequent project develops a parallel version of the code.

Finite-difference equations were derived on combined grids using implicit difference schemes. A technique for transferring energy flow at the interface between grids was developed, together with a technique for the derivation of a simultaneous linear equation system and a solver for the single linear equation system. Algorithms were developed and implemented for the numerical solution of the equations using combined grids. The project also involved integrated debugging of the programs and test computations to verify the numerical implementation of the algorithms.

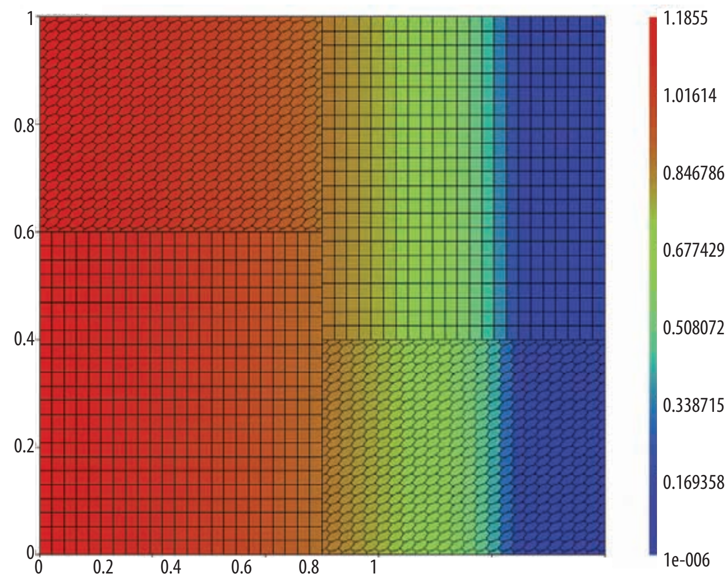


Temperatures for the exact and numerical solutions on grid 8.



Technical Purpose and Benefits

The accurate simulation of hydrodynamic and heat conducting flows requires significant computational resources. While a variety of adaptive mesh technologies exist, each has important drawbacks and inefficiencies. This project developed an adaptive hybrid mesh technology allowing the numerical solutions in different regions of a complex flow to be obtained using the most appropriate and computationally efficient mesh. In particular, a problem can be simulated using an unstructured grid in regions with complex boundaries and a structured grid in less geometrically complex regions.



Temperatures for the numerical solutions on grid 8.

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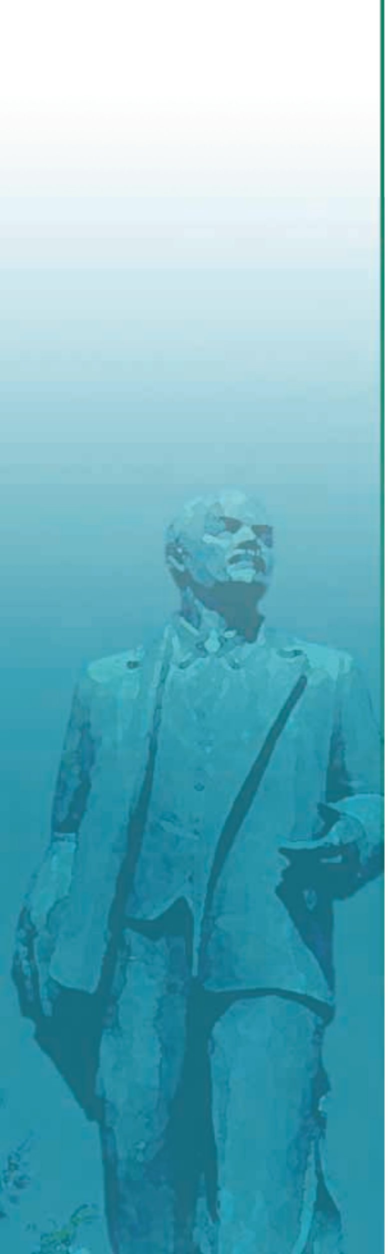
Analytical Solutions to Test Computer Codes Simulating Gas Dynamics and Radiation Transport Problems in Different Approximations

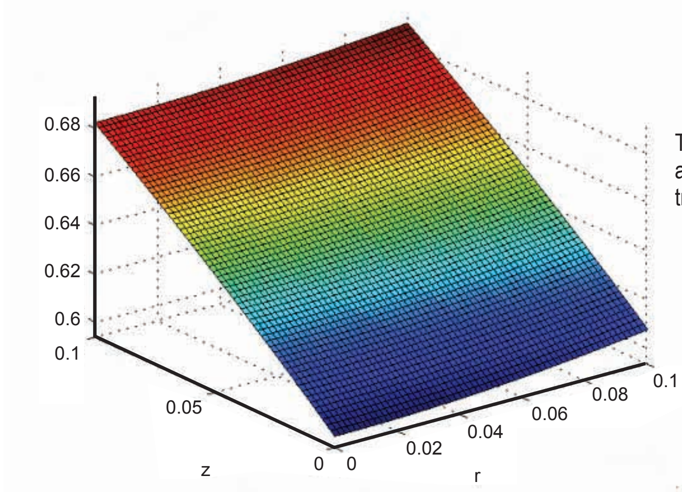
Principal Investigators: Howard A. Scott (LLNL) and Dmitry N. Bokov (VNIITF)

Project Description

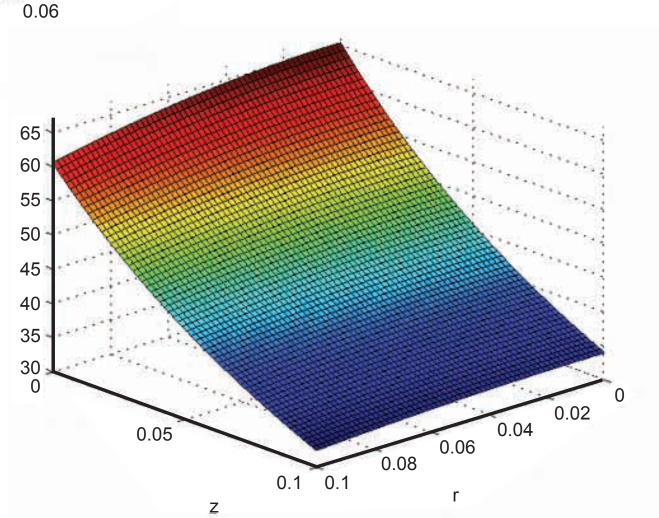
The objective of the project is to obtain new analytical solutions for problems in gas dynamics and radiation transport, as well as to compile a collection of analytical solutions on the basis of these new and already existing solutions. These analytical solutions can be very useful for estimating the accuracy of numerical methods and to test numerical simulation codes.

For radiation transport, these problems include the solution to the energy and radiation transport equations in the gray approximation for the one-dimensional, two-material configuration; the solution to the energy and radiation transport equations including the radiation spectrum in two-dimensional cylindrical geometry (motionless); the solution to the energy and radiation transport equations including the radiation spectrum in two-dimensional spherical coordinates (motionless); the solution to the spectral equations for energy and radiation transport in three-dimensional Cartesian coordinates (motionless); and the solution to the spectral equations for energy and radiation transport in three-dimensional Cartesian coordinates (with motion). For gas dynamics, these include solutions for problems with shock waves, pressure-driven gas motion at low initial surface curvature, strong discontinuities in the flows of plane and spatial double wave type, and an angle-shaped piston in a heterogeneous mixture of isothermal gases.





Temperature profile at $ct = 0.8$ for an analytical multi-frequency radiation transport problem.



Opacity profile at $ct = 0.8$ for an analytical multi-frequency radiation transport problem.

Technical Purpose and Benefits

Physical processes in space and time are described by systems of multidimensional partial differential equations. These systems are usually nonlinear and difficult to solve. To simulate different physical processes, numerical methods are used to enable computer codes to generate discrete solutions depending on spatial variables and time. There are a large number of techniques and codes for solving problems in gas dynamics and radiation transfer. To estimate the actual accuracy of a numerical method and computer code, problems with analytical solutions are very useful. This project collects a large set of different analytical solutions to problems in both gas dynamics and radiation transport that can be used in Validation and Verification assessments.

Collaboration between Lawrence Livermore National Laboratory (LLNL), Livermore, CA, USA, and the Russian Federal Nuclear Center - All Russian Research Institute of Technical Physics (RFNC-VNIITF), Snezhinsk, Russia

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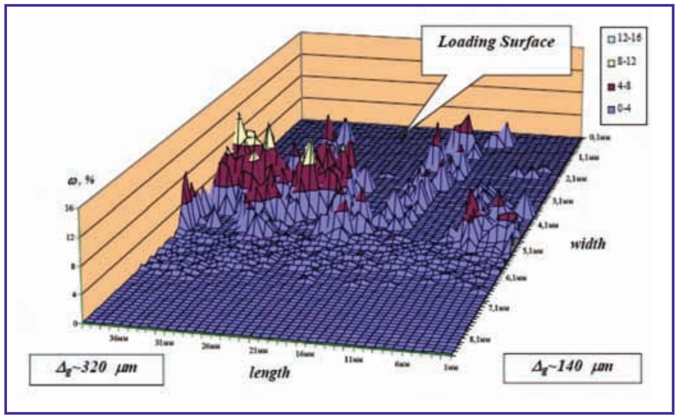
Experimental-Theoretical-Numerical Studies of Constitutive Behavior and Damage Mechanics

Principal Investigators: Marvin A. Zocher, Dean L. Preston, George T. Gray III (LANL), and Olga N. Ignatova (VNIIEF)

Project Description



Distribution of damage in sample subjected to variable-thickness gap test.

The formulation of mathematical models capable of predicting the behavior of materials when subjected to an arbitrary thermomechanical loading environment is an area of active research. It includes models for predicting the constitutive response of the material and the initiation and evolution of damage. Successful development of such predictive models inherently relies on experimental data obtained from laboratory tests carefully constructed to evaluate some particular thermomechanical response or mechanism. These experimental results then support the development of theoretical models, which can be implemented into a variety of numerical methods, thereby providing general-purpose predictive tools.

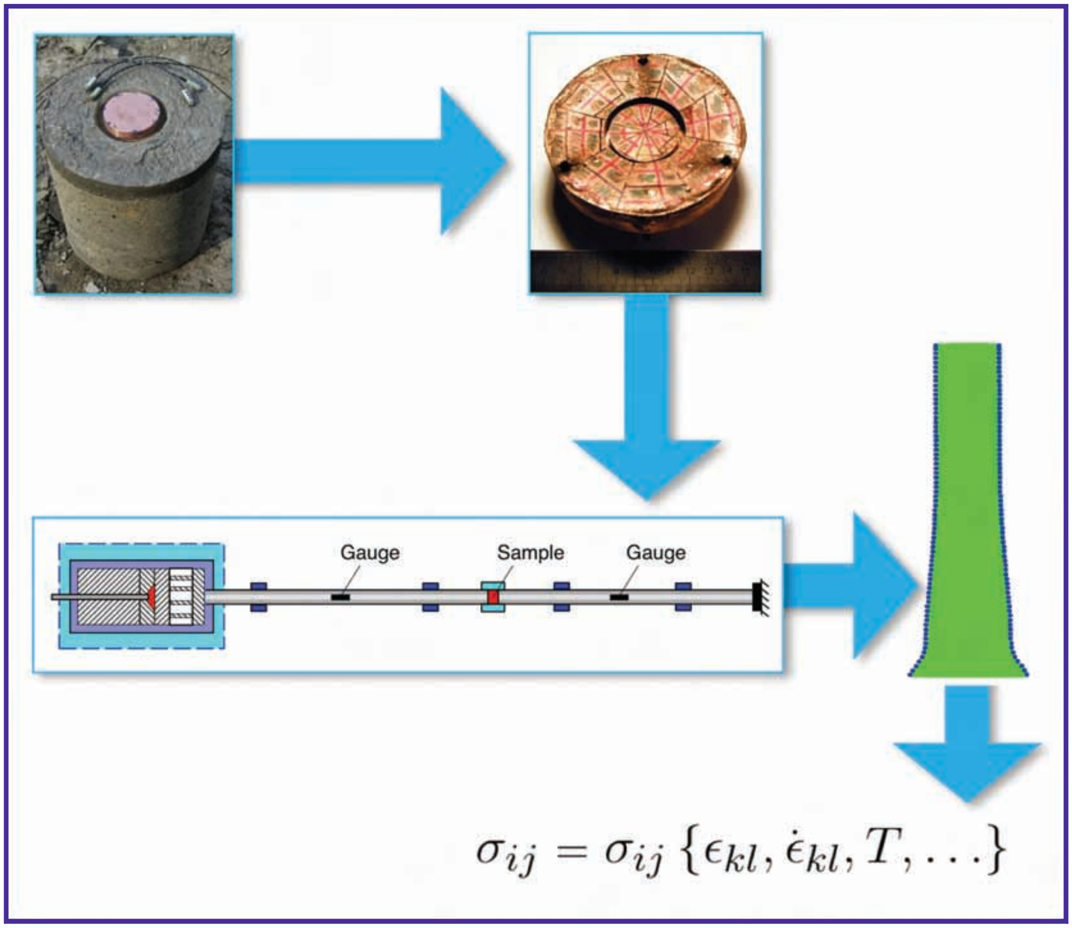
A variety of experimental techniques will be used in support of this work (e.g., split Hopkinson pressure bar, Taylor cylinder, flyer plate impact, and quasi-isentropic and shock loading by the expansion of HE detonation products).

Issues to be investigated include the effect of grain size on constitutive behavior and the mechanics of damage, the effect of deformation localization on constitutive behavior and the mechanics of damage, the evolutionary processes involved in both the time and spatial dependence of grain morphology and deformation localization, time scale effects related to transient thermal softening associated with deformation localization — both as it affects constitutive behavior and as it affects damage initiation and evolution, the mechanisms involved in damage compaction and the apparent "healing" of previously damaged materials, and the effects of such "healing" on subsequent constitutive behavior and sequel damage evolution.

Metallographic analysis will be used extensively to assess microstructural morphologies. Existing material models will likely be improved. It is possible that entirely new material models will be developed. Extensive numerical analysis will be conducted to assess the validity of numerical models.

Technical Purpose and Benefits

The development of better predictive capability is essential if LANL is to meet its obligations to NNSA and the country. Models that more accurately predict constitutive behavior and the mechanics of damage are of critical importance. Under this project, a number of new models have already been produced. Two examples are (1) a new constitutive model that accounts for evolving grain structure and (2) a new constitutive model that accounts for deformation localization and the effects thereof (extremely critical in high strain rate environments). The second of these two new models is nonlocal, accounting for issues of relaxation time and length scale. Some entirely new and unique damage experiments have been developed under this work, which are enabling the development of improved damage models. This work supports the objectives of the NNSA and both research institutions (LANL and VNIIEF) as they endeavor to improve their predictive capabilities in two critical areas — constitutive behavior and the mechanics of damage.



Preconditioning of material to alter its microstructure: one of the approaches being taken in the development of constitutive models that can account for evolving grain morphology and localization effects (in image on right) — green is predicted final shape; blue is measured final shape.

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Collaboration between Los Alamos National Laboratory (LANL), Los Alamos, NM, USA, and the Russian Federal Nuclear Center – All Russian Research Institute of Experimental Physics (RFNC-VNIIEF), Sarov, Russia

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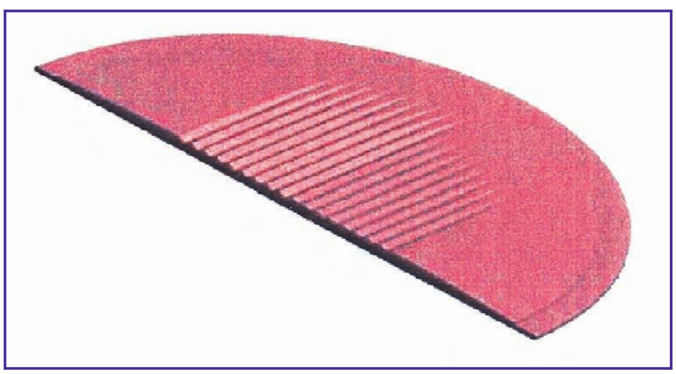
Influence of Dynamic Material Properties on Perturbation Growth in Solids

Principal Investigators: Ann M. Kaul, Marvin A. Zocher, Dean L. Preston, George T. Gray III (LANL), and Victor A. Raevsky (VNIIEF)

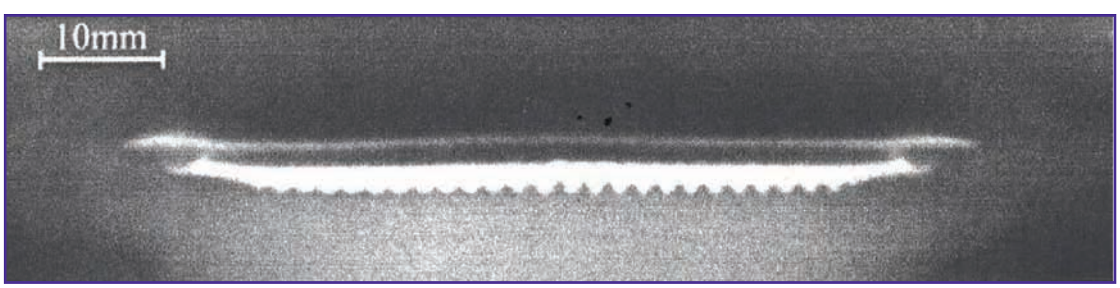
Project Description

The development of mathematical models capable of accurately predicting constitutive behavior over a wide range of strain rates (e.g., from quasistatic to 10^6 s^{-1}) is a particularly difficult task, and an area of active research today. A number of factors contribute to the difficulty, but two of the foremost are (1) constitutive theory demands a homogeneous field if one is to extract material properties from experimental results, and experimental methods that produce a homogeneous field have not been developed for strain rates above about 10^3 s^{-1} and (2) the fundamental mechanisms that govern material flow at high strain rates (i.e., on the order of 10^6 s^{-1}) are often different from those that are dominant under more modest strain rate conditions. To develop a constitutive model that is valid over a quasistatic to 10^6 s^{-1} strain rate regime, one must supplement material property tests (tests conducted at modest strain rates wherein homogeneity of the stress field is present) with specific experiments carefully designed to highlight high strain rate behavior. One of the most promising methods for evaluating constitutive behavior at high strain rates, especially at strain rates above about 10^5 s^{-1}, is the method of perturbation growth.

The method of perturbation growth relies on the Rayleigh-Taylor instability that occurs when a less-dense fluid (in this case, high-explosive detonation products) pushes on a pre-perturbed solid. Because of the instability, initial perturbations grow with time. Since the dominant factor governing perturbation growth is the constitutive behavior of the solid, this method is ideal for the evaluation of constitutive models in a high strain rate regime, especially in the 10^5 to 10^7 s^{-1} range. The researchers at VNIIEF are recognized leaders in applying this method.



Pre-perturbed sample.



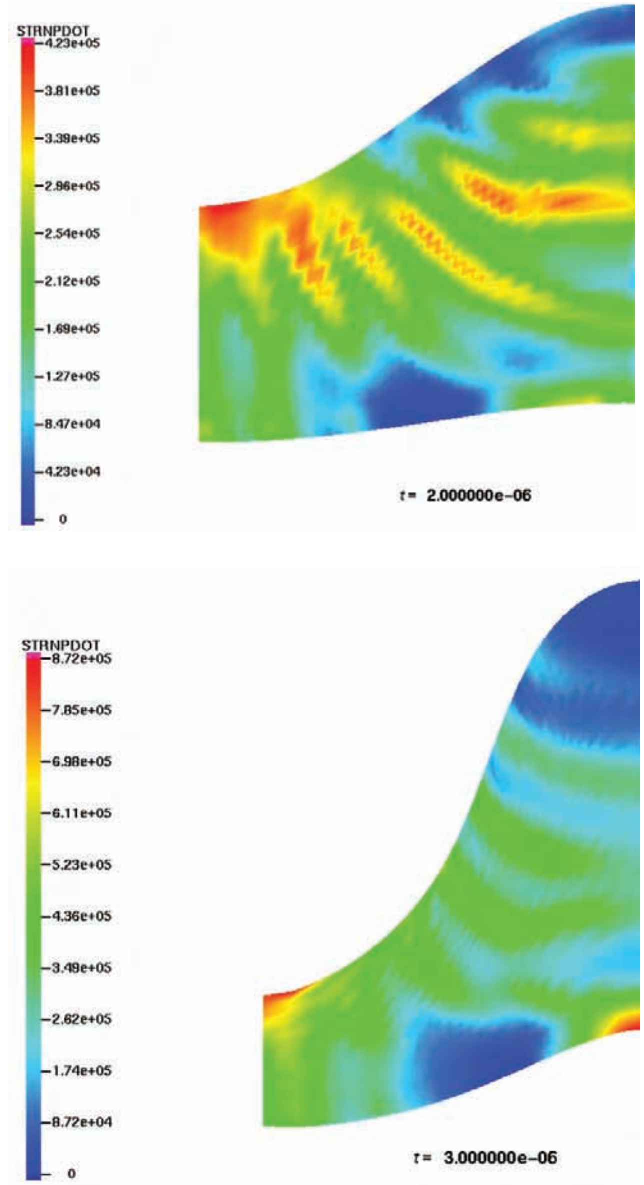
Radiograph showing perturbation growth.

The perturbation growth method will be applied for the purpose of developing constitutive models that are validated over a wide range of strain rate (quasistatic to 10^6 s^{-1}). As was alluded to earlier, the fundamental mechanisms that govern material flow at high strain rates are often different from those that are dominant under more modest strain rate conditions. It has been observed that phenomena such as heterogeneous deformation become extremely important at strain rates approaching 10^6 s^{-1}. Models that do not account for these phenomena will prove to be rather poor predictors of overall constitutive response under high strain rate conditions.

The fundamental objective of this work is the development of models that can be trusted over a wide strain rate regime. To achieve this end, these models must account for phenomena (such as localization) that are not accounted for in existing models.

Technical Purpose and Benefits

The development of better predictive capability is essential if LANL is to meet its obligations to NNSA and the country. Current constitutive models do a rather poor job of predicting high strain rate behavior because they do not account for some of the fundamental mechanisms that are responsible for material flow under these conditions. Under this project, new models are being developed. A new Relaxation Model has already been developed. This model incorporates a relaxation time that corresponds to a length scale associated with deformation localization. A new Two-Temperature model is under development. This model is nonlocal, and accounts for localization and the strong temporal heating associated with that localization. This work supports the objectives of the NNSA and both research institutions (LANL and VNIIEF) as they endeavor to improve their predictive capabilities in the area of high strain rate constitutive response, an area where existing capabilities are clearly lacking.



Simulation of perturbation growth at two different times.

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Shock Compression Studies of Phase Changing Materials with PVDF and Manganin Gauges

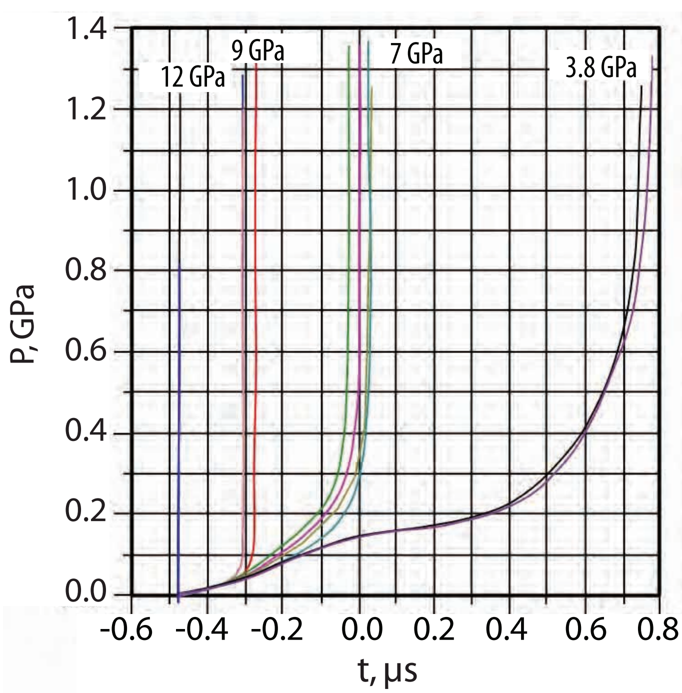
Principal Investigators: Frank J. Cherne III, Brian J. Jensen (LANL), and Mikhail V. Zhernokletov (VNIIEF)

Project Description

The development of an understanding of shock-induced phase transitions and models that describe these transitions is an area of active research. Included in this research is an evaluation of existing experimental techniques applied to materials that undergo large volume collapse as a result of phase transition. PVDF sensors will be employed to obtain sound velocities at shock conditions below which traditional photon emitting liquid sensors are applicable.

Under this project, experimental studies of the profiles of pressures, sound velocities, and temperatures for metals, organic and nonorganic compositions, which undergo phase transitions under shock compression and release, will be performed. This project is multi-faceted, including investigations of the shock-induced phase transition properties for three metals, namely, titanium, tin, and cerium. Contrary to expectation, preliminary results have shown that at the pressures under investigation, there is no indication of cerium metal reverting back to its low-pressure phase upon unloading. These preliminary studies included measurements of the sound speed of cerium under high pressure.

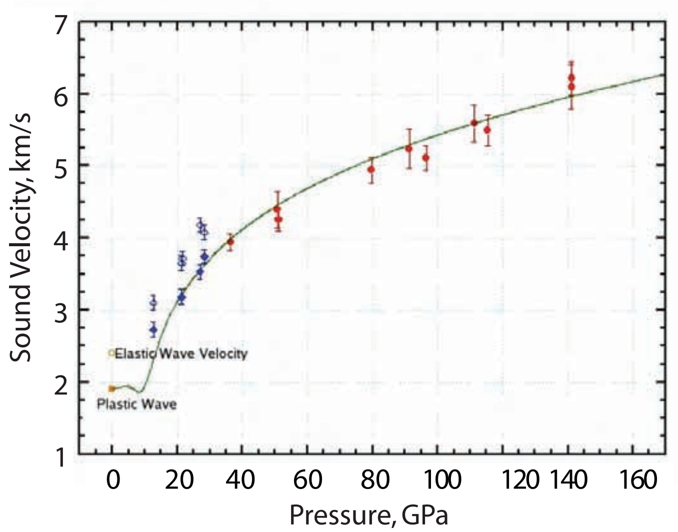
This project will include an investigation of the (γ–α) isomorphic solid-solid phase transition in cerium and the (α–ω) polymorphic solid-solid phase transition in titanium. Also to be investigated are the sound velocities in tin around the solid-liquid transition using the rarefaction overtake technique. The wave structure for these transitions will be thoroughly investigated, examining both the shock wave and its release wave structure. The gauges used for this work will be of the PVDF and Manganin variety. An additional necessary component of this research will be to examine the effect of temperature upon a variety of organic and inorganic compounds used during the study of phase transitions. With the data, we will be able to better understand the thermal effects produced during studies of shock-induced phase transitions.



Pressure versus time in cerium.

Technical Purpose and Benefits

The development of experimental techniques that foster the acquisition of data that can then be used to develop predictive models is essential if LANL is to meet its obligations to the NNSA and the country. Models that accurately describe the behavior of a material undergoing phase transition are of paramount importance in understanding the thermodynamic and kinetic states of the material. Useful measurements of the sound speed in cerium have already been obtained. In the conduct of these experiments, the overtake method was used with indicator liquids for higher pressures and with PVDF gauges for lower pressures. The lower pressure measurement technique utilized by VNIIEF was first applied to iron. The interest in the sound speed of cerium stems from the fact that sound speed is a more sensitive parameter for understanding the shocked state of the material. Aside from being able to extract the sound speed velocities using PVDF gauges, the gauges provide a time history of the shock wave, which can be used in the development of kinetic models for the various materials of interest.



Sound velocity as a function of pressure in cerium.

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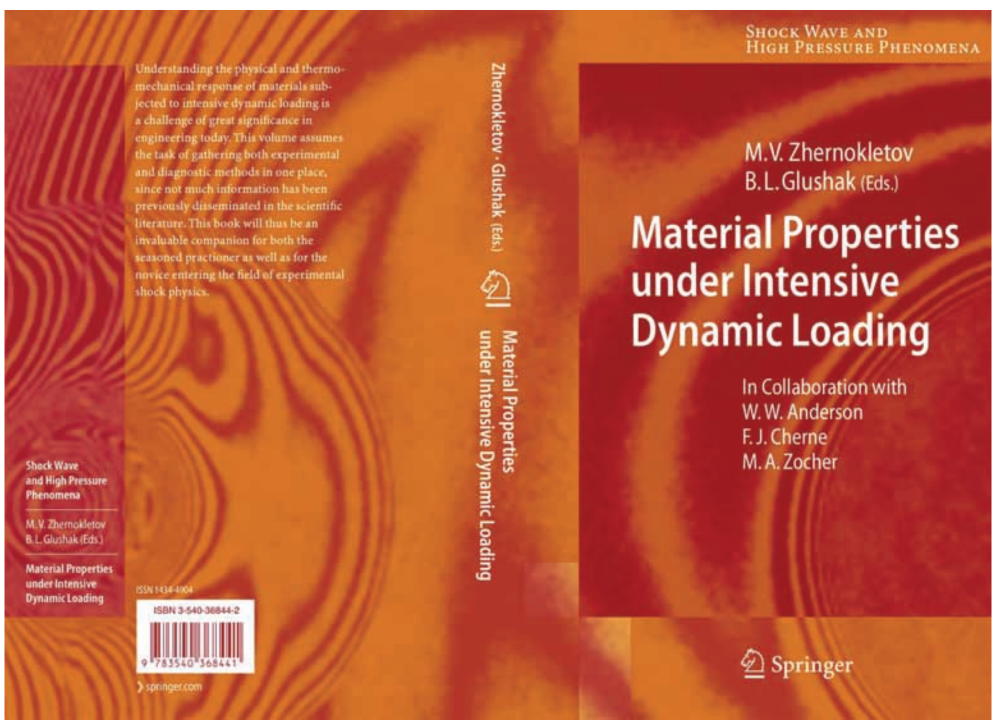
Publication of the Monograph Entitled "Methods for Study of Substance Properties Under Intense Dynamic Loading"

Principal Investigators: William W. Anderson (LANL), and Mikhail V. Zhernokletov (VNIIEF)

Project Description

Despite the high quality of the work being conducted under the US/Russian Science and Technology collaborations, the product of that work will inevitably be underutilized unless it is disseminated to the broader scientific community. In response to this realization, and with the objective of maximizing the benefit of the collaboration, the researchers involved in these collaborations often publish their work. This particular project has resulted in the publication (by Springer-Verlag) of an extensive (over 400 pages) book on the topic of shock physics.

The first line of the preface reads, "This book is the result of collaboration between the Russian Federal Nuclear Center – All Russian Scientific Research Institute of Experimental Physics (RFNC-VNIIEF) located in Sarov, Russia, and the University of California—Los Alamos National Laboratory (UC-LANL)." An excerpt from the preface that appears on the book cover reads, "Understanding the physical and thermomechanical response of materials subjected to intensive dynamic loading is a challenge of great significance in engineering today. This volume assumes the task of gathering both experimental and diagnostic methods in one place, since not much information has been previously disseminated in the scientific literature. This book will thus be an invaluable companion for both the seasoned practitioner as well as for the novice entering the field of experimental shock physics."



Technical Purpose and Benefits

The NNSA and LANL have an obligation to the country to maximize the benefit gained from the US/Russian Science and Technology collaborations. One key factor in achieving maximal benefit is the dissemination of the product of the collaborations to the broader scientific community. This major publication supports this objective.

Discussions in Moscow – Left to right: Dr. Frank J. Cherne III, Dr. Mikhail V. Zhernokletov, and Dr. Olga Tyupanova.

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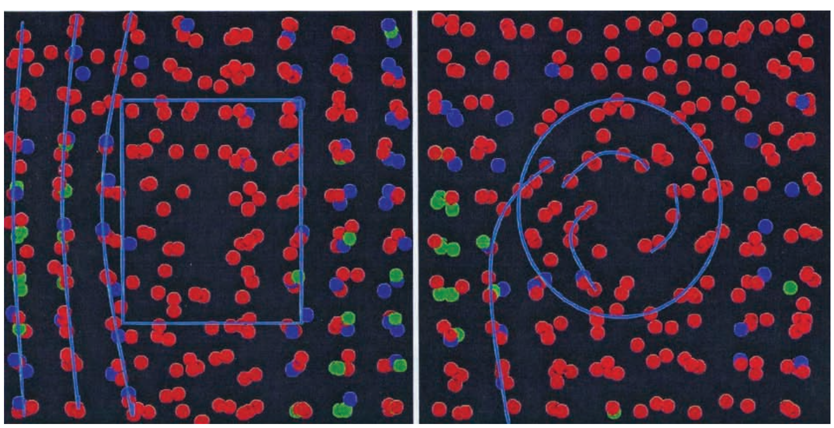
Molecular Dynamics Simulations of Shock-Induced Microstructure Evolution and Helium Bubble Diffusion in Metals

Principal Investigators: Dean L. Preston, Marvin A. Zocher (LANL), Vladimir V. Dremov, and Alexander V. Petrovtsev (VNIITF)

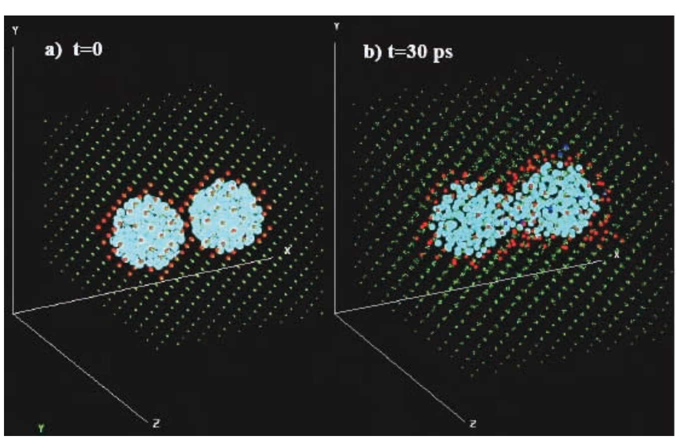
Project Description

The development of physically based mathematical models capable of predicting material response to arbitrary thermomechanical loading requires, in general, an understanding of physical mechanisms at multiple length scales. However, experimental capabilities for probing atomistic length scales under dynamic conditions are extremely limited. It is the goal of this project to compensate for this shortcoming in current experimental capabilities by carrying out a suite of molecular dynamics simulations to obtain numerical approximation of microstructural changes that take place in metals because of shock wave loading, and to investigate a number of issues related to the aging of plutonium.

With respect to microstructural changes that take place in metals due to shock wave loading, a number of issues are to be investigated. Examples include a determination of (1) the dominant mechanism for stress relaxation in polynanocrystalline metals and (2) the fundamental mechanisms involved in the initiation and evolution of damage in monocrystalline and polynanocrystalline metals. Preliminary results reveal that the dominant mechanism for stress relaxation in polynanocrystalline metals is through the



Damage initiation showing vortical atomic motion resulting in an approximately spherical void. (Phys. Rev. B, V74, No. 14, p144110)



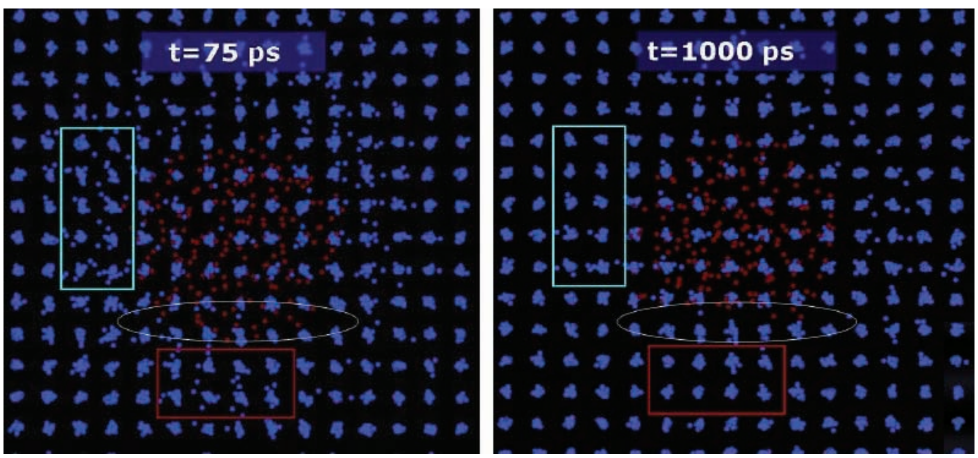
Simulation of bubble-bubble interaction.

production of stacking faults. Results obtained thus far on the initiation of damage reveal a tendency for damage to initiate in regions where stacking fault densities are high, especially at stacking fault intersections. Damage initiation is observed to proceed from the breaking of the first molecular bond to the formation of approximately spherical voids in a time span on the order of 0.2 ps. Vortical atomic motion, resulting in approximately spherical voids, is observed even in cases where the loading is approximately uniaxial.

One of the consequences of the aging of plutonium is an ever-increasing presence of helium trapped within the plutonium lattice. In order to predict the long-term effects of this, it is imperative that we gain a better understanding of the fundamental mechanisms involved in He-Pu interactions and the resultant effects of these interactions on macroscopic response. Issues to be investigated include the diffusion of He in a Pu lattice, He bubble formation, bubble-bubble interaction, the mechanics of self-irradiation damage in Pu already containing He bubbles, and He bubble diffusion.

Technical Purpose and Benefits

Much remains to be learned concerning the fundamental mechanisms that govern material constitutive response and the initiation and evolution of damage. This work supports the goals of the NNSA and the research institutions (LANL and VNIITF) for the development of more physically based mathematical models, models that are truer to the fundamental physical mechanisms at play, and models that account for more of the physics. Gaining a better understanding of the fundamental mechanisms involved in the aging of plutonium and in the consequences of that aging on the macroscopic response of the material is critical for LANL to meet its responsibilities to the NNSA and the country. This work supports the objectives of the NNSA and both research institutions (LANL and VNIITF) as they endeavor to improve their predictive capabilities with respect to plutonium aging and the consequences thereof.



Pu lattice in the vicinity of a He bubble (He to vacancy ratio 3:1; T = 600 K) at two different times – Pu atoms in blue; He atoms in red.

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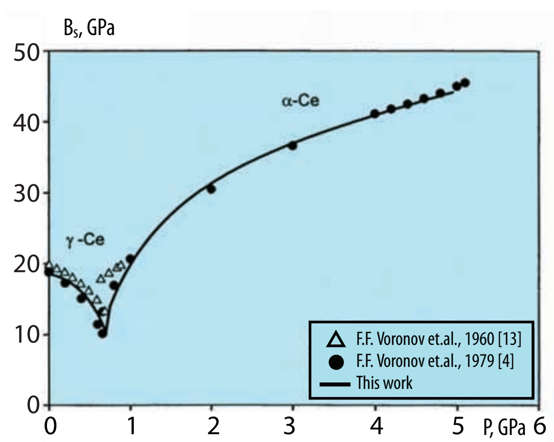
Phase Transition Kinetics and High-Rate Stress-Strain Response of Pure Cerium

Principal Investigators: George T. Gray III, Dean L. Preston, Marvin A. Zocher (LANL), Alexander V. Petrovtsev, and Evgeny A. Kozlov (VNIITF)

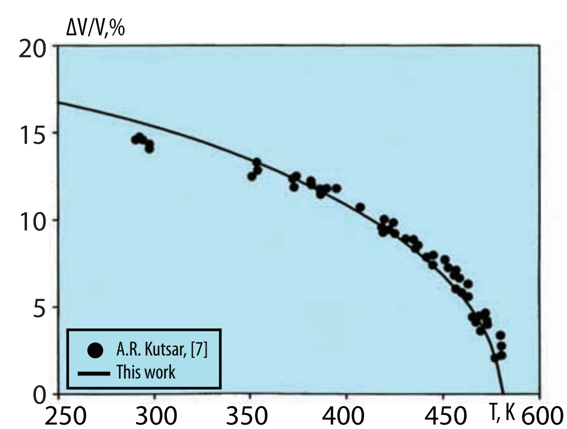
Project Description

Cerium has a very complex phase diagram. There are four solid phases at zero pressure, and at least three additional phases at elevated pressure. The γ phase (the stable room temperature zero pressure phase) exhibits an unusual hydrostatic constitutive behavior wherein the bulk modulus decreases with increasing pressure. Cerium is unique in that it is the only pure element possessing a solid-solid critical point. Perhaps the most interesting feature of cerium is the nature of the α–γ solid-solid phase transition, which occurs at about 0.75 GPa on the room temperature isotherm. This transformation is accompanied by a substantial (almost 15%) reduction in volume. This transition will have a profound effect on the dynamic response of cerium. The very large volume collapse has the effect of causing the temperature to increase at a rate much higher under dynamic compression than would be the case without the volume change. This should cause the pressure on the Hugoniot at which cerium melts to be much lower than that observed for many other metals. Cerium is thus an excellent choice of material for studies of shock-induced melting (and subsequent solidification). The complex phase structure of cerium also makes it an excellent material for studying phase stability and the kinetics of polymorphic phase transition.

A variety of experimental techniques will be used in this study. These include use of the Hopkinson split pressure bar, flyer plate impact, and the optical lever arm technique applied to wedge samples loaded by both sliding and normal detonation of high explosives. Issues to be investigated include phase stability and the kinetics of polymorphic phase transition, shock induced melting (and subsequent solidification), and



Adiabatic bulk modulus versus pressure (preliminary 2-phase EOS) compared to experimental data.

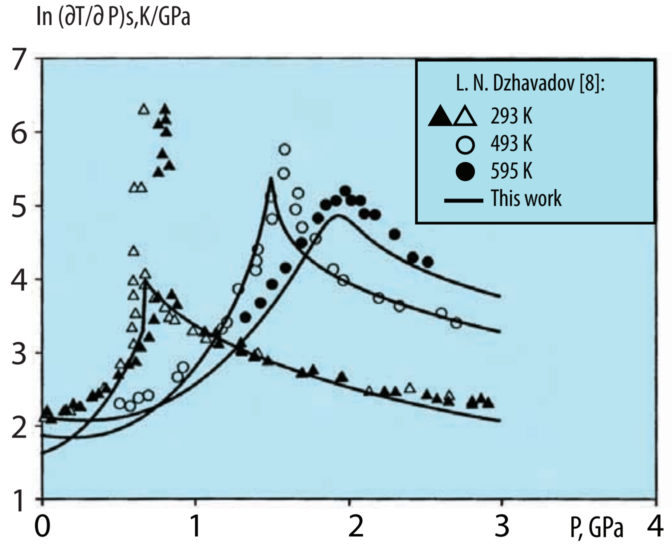


Volume change occurring with γ–α transition versus temperature (preliminary 2-phase EOS) compared to experimental data.

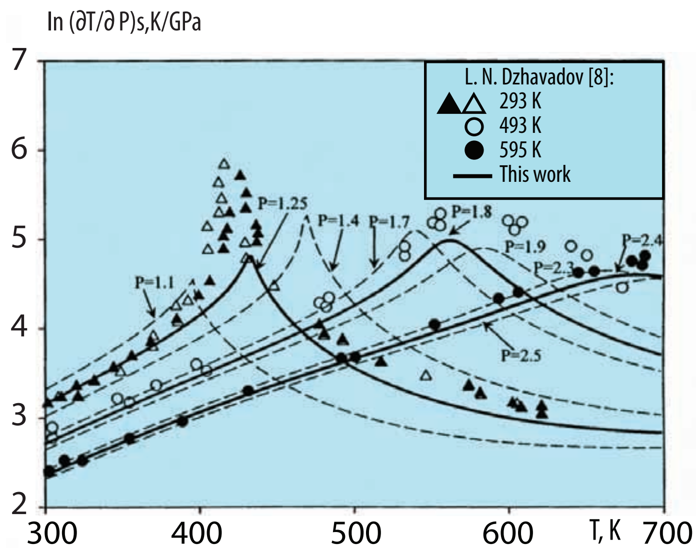
both hydrostatic and deviatoric constitutive behavior. Experimental results will be used in support of the development of a multiphase equation of state (EOS) and of an improved constitutive model for the deviatoric response of cerium.

Technical Purpose and Benefits

The development of better predictive capability is essential if LANL is to meet its obligations to NNSA and the country. One area where much remains to be understood, and where better understanding could be applied to the development of improved predictive capability, has to do with phase stability and the mechanics and kinetics of polymorphic phase transition. This work supports the objectives of the NNSA and both research institutions (LANL and VNIITF) as they endeavor to improve their predictive capabilities with respect to phase stability, polymorphic phase transition kinetics, multiphase equation of state, and deviatoric constitutive response of materials that are complex with respect to phase space.



Log (∂T/∂P)s versus pressure (preliminary 2-phase EOS) compared to experimental data.



Log (∂T/∂P)s versus temperature (preliminary 2-phase EOS) compared to experimental data.

Collaboration between Los Alamos National Laboratory, Los Alamos, NM, USA, and the Russian Federal Nuclear Center – All Russian Research Institute of Technical Physics (RFNC-VNIITF), Snezhinsk, Russia

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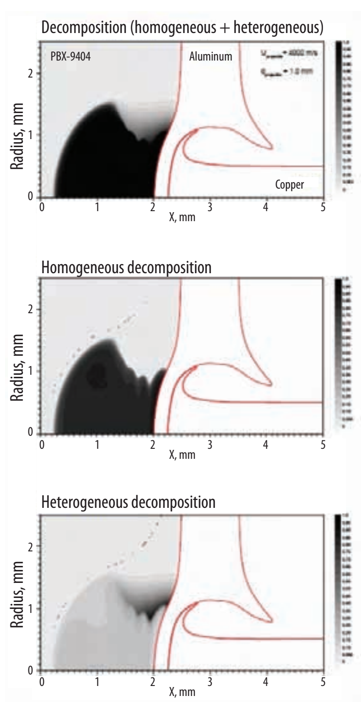
Development of an Improved Detonation Model

Principal Investigators: Marvin A. Zocher, Dean L. Preston, Yasuyuki Horie (LANL), and Vladimir Yu. Klimenko (ICP-RAS)

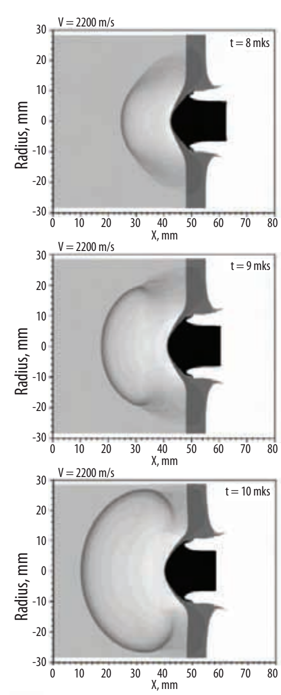
Project Description

The formulation of mathematical models capable of predicting the process of detonation of high explosives (HEs) is an area of active research. Analysis of recent experiments shows that HE decomposition occurs as the result of a complex mix of a number of fundamental decomposition mechanisms, each of which has its own domain of domination. The hot spot mechanism (heterogeneous mechanism) dominates in the pressure range from 30 kbar to 200 kbar. The homogeneous mechanism dominates at pressures > 300 kbar. In the intermediate region, 200–300 kbar, we have mixture of heterogeneous and homogeneous mechanisms. At very low pressures, P < 20 kbar, decomposition is governed by the so-called dislocation mechanism. It is necessary to emphasize that the stated values of boundary pressures — 30, 200 and 300 kbar — are qualitative and have concrete values for each explosive.

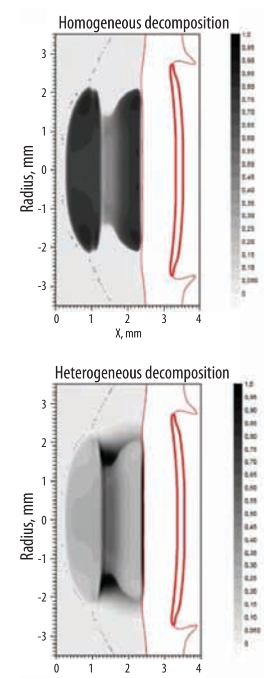
The primary goal of this project is to develop an improved model of detonation, one with accuracy on the order of 10% (existing models are considerably less accurate). The model will be applicable to standard PBX explosives and will be calibrated for PBX-9501 and PBX-9502.



Initiation of detonation in PBX 9404 shielded by aluminum for the impact of a copper rod traveling at 4000 m/s.



Initiation of detonation in Comp-B shielded by aluminum from the impact of a steel bullet traveling at 2200 m/s.



Initiation of detonation in PBX-9404 shielded by aluminum from the impact of a steel plate traveling at 1600 m/s.

The task will be performed in two stages. In the first stage (first year), it is planned to develop a numerical model with hot spot and homogeneous mechanisms of HE decomposition. This heterogeneous-homogeneous model (HH model) will be ready for precise calculations at pressures >20 kbar. In the second stage (second year), dislocation mechanisms will be incorporated into the HH model. The resultant heterogeneous-homogeneous-dislocation model (HHD model) will enable precise calculations at any pressure.

Technical Purpose and Benefits

The development of better predictive capability is essential if LANL is to meet its obligations to NNSA and the country. Models that more accurately predict the decomposition of high explosives are of critical importance to the NNSA and LANL. Under this project, a significant improvement in predictive capability may be made possible with the development of an HHD model for HE decomposition. Considerable progress has already been made, and preliminary results look quite promising. This work supports the objectives of the NNSA and both research institutions (LANL and RAS Inst. of Chemical Physics) as they endeavor to improve their predictive capabilities in the area of HE detonation.

Collaboration between Los Alamos National Laboratory, Los Alamos, NM, USA, and the Institute of Chemical Physics – Russian Academy of Science, Moscow, Russia

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Application and Study of the KM and VKL Methods on Flows with Interfaces

Principal Investigators: James R. Kamm, William J. Rider, Mikhail J. Shashkov (LANL), and Valentine Spiridonov (VNIIEF)

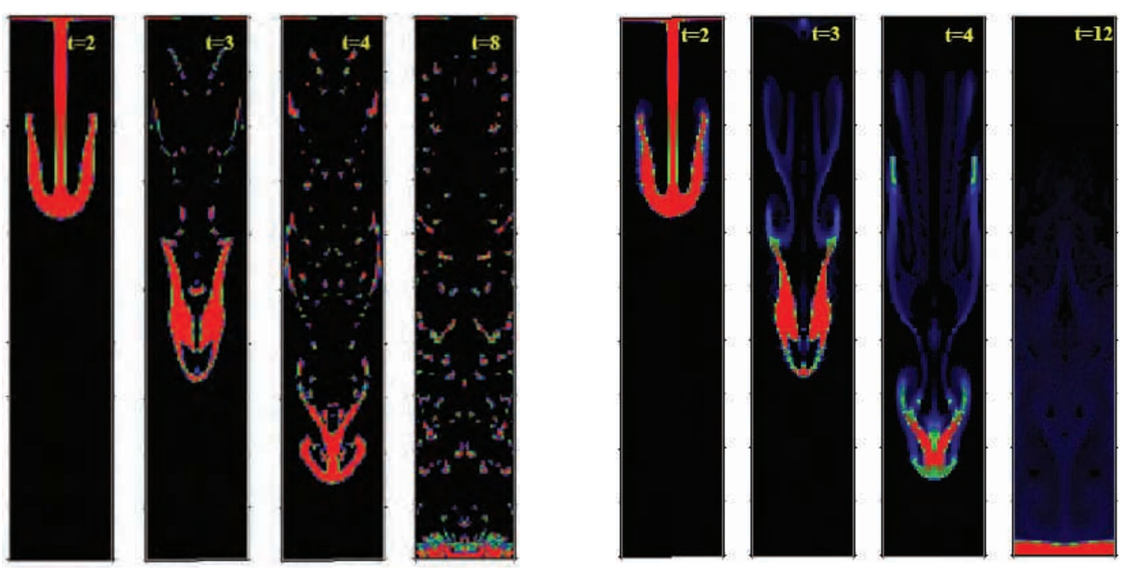
Project Description

A challenge in the computation of multidimensional, multimaterial gas dynamic flows is the simulation of severe material interface distortions. Highly distorted regions develop in many physical phenomena, including fluid instabilities leading to turbulent mixing. Engineering-scale flows presently cannot be simulated in a manner that is faithful to the fundamental physics at all length scales; consequently, interface or volume-tracking methods, in which computational cells contain several materials ("mixed cells"), must be employed. This topic is the focus of this project.

An initial study of these methods was completed under contract 377130133 in FY03, which covered the basic algorithms, simulations, and documentation of the methods in the VNIIEF LEGAK family of codes. That initial study described two techniques developed at VNIIEF: (1) the Concentration Method (KM) and (2) the Singled-Out Contact Lines (VKL) Method. The current project significantly extends these studies, providing understanding of the fundamental performance and characteristics of these algorithms on high-deformation fluid flow problems.

Technical Purpose and Benefits

This work supports the objectives of the NNSA and both research institutions (LANL and VNIIEF) by providing a critical, quantitative examination of multimaterial hydrodynamics algorithms used in VNIIEF simulation codes.



Comparison of late-time Rayleigh-Taylor simulation: left—using the method of concentrations (KM) without homogenization; right—using the homogenized three-fluid model.

Tasks to be completed during the first year of this project include (1) implementing high-resolution methods for the remap (advection) step of the algorithm and verifying this implementation in 1-D; (2) studying velocity smoothing on 2D test problems; and (3) computing, evaluating, and quantitatively assessing the accuracy of the KM and VKL methods on pure interface transport. Results have shown that (1) the particular advection method has a smaller effect than the interface treatment for hydrodynamic mixing; (2) velocity smoothing has a noticeable effect on small- and intermediate-scale structures in Rayleigh-Taylor flow; and (3) pure interface transport test problems clearly indicate that VNIIEF is using modern, high-resolution techniques.

Tasks to be completed in the second year of the project include work to (1) describe and implement algorithms for homogenization of disparate materials in the KM and VKL methods, providing evaluation of these approaches on specified test problems and (2) implement a tensor artificial viscosity in the Lagrangian step of the solution algorithm in LEGAK and quantitatively exercise these approaches on specified 2D problems. The outcome of this study included the following: (1) the so-called "three fluid" model used by VNIIEF is a unique method in multimaterial hydrodynamics that provides a novel approach to the homogenization problem with very good results and (2) edge- and projection-based tensor viscosities provide performance superior to the traditional Richtmyer-Neumann viscosity for both shock calculations and adiabatic flow problems.

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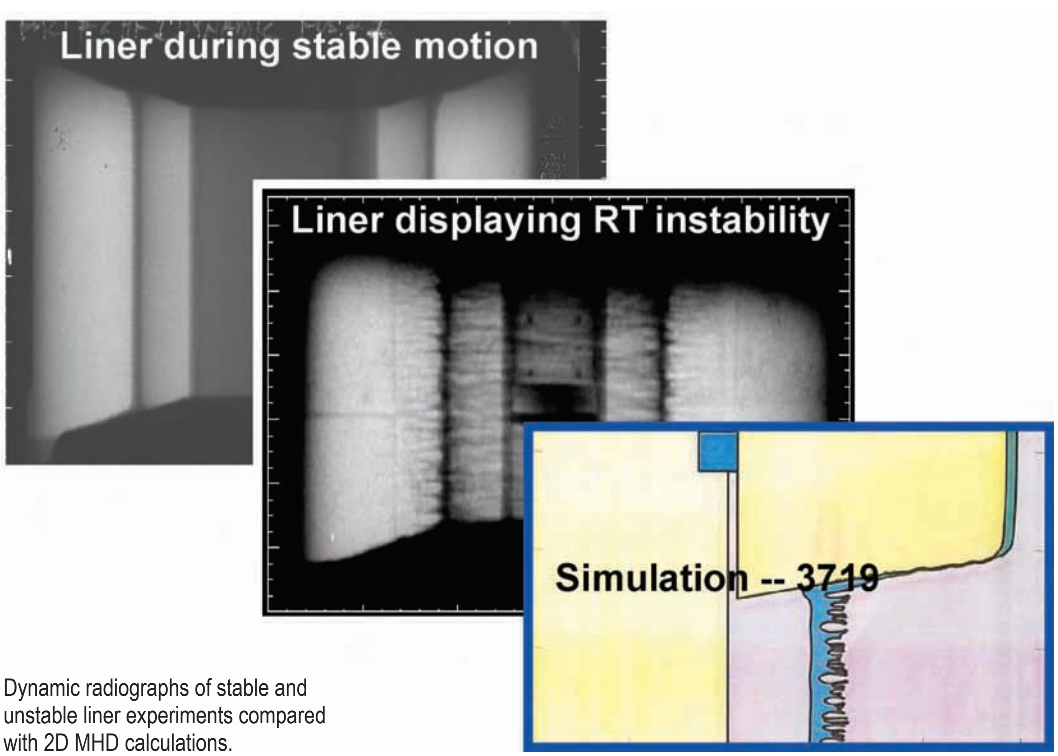
Liner Physics (LP) Experiments for Pulse Power Hydrodynamics

Principal Investigators: Walter L. Atchison, Robert E. Reinovsky (LANL), V.N. Mokhov, A. Buyko, V.B Yakubov, and S.F. Garanin (VNIIEF)

Project Description

The objective of this project is to test and improve MHD simulation capability in legacy codes and ultimately in ASC integrated codes by modeling magnetically driven, near-solid density, high precision, cylindrical imploding liner experimental data under a variety of initial conditions. These codes and models can extend the performance of magnetically imploded liners to higher drive energies and potentially higher implosion velocities, validating both hydrodynamics and materials models in the integrated codes for application to sophisticated dynamic systems. In the 1990s, an extended experimental series was conducted on the LANL Pegasus facility to study the "Liner Stability" (LS) problem (field/fluid/solid interfaces at the outer surface of cylindrical liner carrying very large electrical currents). Legacy US simulation codes with MHD capability, and Russian codes, were used, with some success, to simulate both bulk behavior of the implosion and to explore the details of interfacial behavior. In the late 1990s, the results from the LANL designed LS experiments were extended through a series of five VNIIEF-designed experiments (Russ 1-5) also exploring liner stability, but designed with both US and Russian simulation tools. Early in the series, the MHD stability of the field/metal interface was the focus of attention, and in later experiments, the behavior of liners after collision with a target was explored as well. In preparation for higher current experiments on Atlas, two experiments were conducted by VNIIEF (ALT 1,2) using a Russian pulse power system that duplicated the Atlas current waveform and provided insight into the problems to be expected at higher drive (Project: Atlas Liner Technology for Pulsed Power Hydrodynamics). By combining data from experiments and simulations, a model of liner behavior was held in fair confidence as Atlas operations began in Los Alamos in FY02. Of four "liner physics



Dynamic radiographs of stable and unstable liner experiments compared with 2D MHD calculations.

experiments" conducted in FY02, the results of the first two departed significantly from that predicted by the simulations, requiring short term modifications to both model and experiment to support the immediately following weapon physics experiments. These observations significantly challenged both the physics in the numerical models, especially the EOS models, and the ability of the integrated codes to describe a well defined, relatively simple implosion situation. Over the long-term, one or two Liner Physics (LP) experiments per year are planned to continue this investigation, and this task provides for VNIIEF participation in both simulation and experiment.

Technical Purpose and Benefits

The ability to accurately predict the dynamics of implosion systems is central to the NNSA mission to predict the behavior of complex systems. Highly detailed data from carefully controlled, magnetically driven liner experiments diagnosed with modern high precision, high resolution diagnostics, challenge current simulation capability, validating some hydrodynamic and some materials models, motivating improvements in others, and testing the ability of the integrated codes to model integrated problems.

Collaboration between Los Alamos National Laboratory (LANL), Los Alamos, NM, USA, and the Russian Federal Nuclear Center – All Russian Research Institute of Experimental Physics (RFNC-VNIIEF), Sarov, Russia

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Atlas Liner Technology (ALT) for Pulsed Power Hydrodynamics

Principal Investigators: R.E. Reinovsky, I.R. Lindemuth, R.J. Faehl, W.L. Atchison, G. Rodriguez (LANL), A. M. Buyko, A. A. Petrukhin, V.N. Mokhov, and V.K. Chernyshev (VNIIEF)

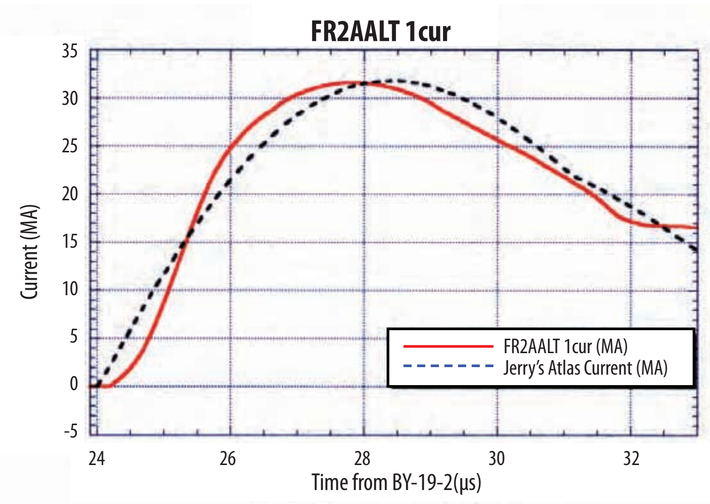
Project Description

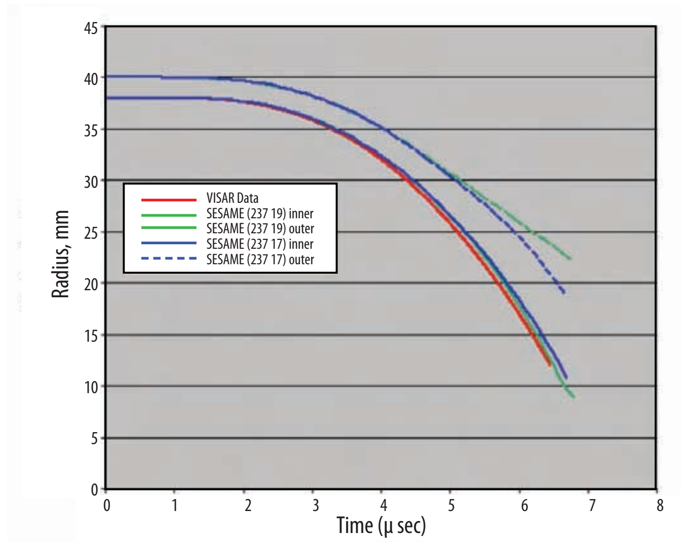
The Pulsed Power Hydrodynamics Program at Los Alamos National Laboratory (LANL) has constructed the Atlas capacitor bank (23 MJ, 30 MA, 240 kV) at the Nevada Test Site to magnetically drive high velocity implosions of cylindrical metal liners to obtain high-temperature and high-pressure conditions for high energy density physics impact experiments in a convergent geometry. The All-Russian Institute of Experimental Physics (VNIIEF) has developed pulsed power systems based on a multi-element disk explosive magnetic generator (DEMG) at similar current levels. A joint US/Russian series of advanced liner technology experiments at Atlas parameters (ALT-1, ALT-2) was conducted with the VNIIEF DEMG generator to simulate the performance of the Atlas capacitor bank and liner dynamics. Additionally, these experiments provided an opportunity to diagnose both generator performance and liner dynamics under extreme conditions involving effects such as melt, asymmetry, instability growth, drag, etc., that ultimately affect the fidelity of any liner implosion experiment. The ALT experiments were successfully conducted in 1999 (ALT-1) and 2001 (ALT-2) in Sarov, Russia. The VNIIEF DEMG generator and a foil opening switch were used to produce an electrical current waveform that reached peak values of over 32 MA and imploded aluminum liner velocities of 12 km/sec.

Photograph of the ALT-1 device on the firing point. The disk explosive generator (DEMG) is visible inside the heavy steel frame. Above the frame is the cylindrical transmission line, and above that is steel shielding surrounding the imploding liner experimental unit. Two radiographic x-ray sources are to the left of the shielding. Below the generator, not visible in this photograph, is the explosively driven helical electromagnetic generator (HEMG) that provides the seed current for the disk generator.

Technical Purpose and Benefits

Both laboratories (LANL and VNIIEF) seek to understand the technological issues of high-current magnetically-driven high velocity liners. This project mutually benefits both institutions by providing valuable liner performance information, leading to validation of MHD models. These MHD models, incorporated into integrated codes are used as design tools for experiments involving materials under high current and pressure conditions. The results of these early experiments affected design decisions and performance for subsequent Atlas and non-Atlas pulsed power physics experiments.





Results of ALT experiments designed to duplicate Atlas implosion conditions using VNIIEF DEMG system.

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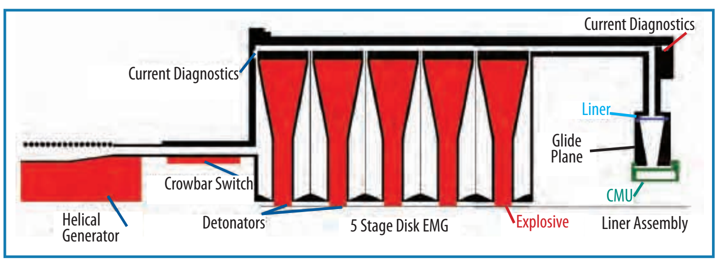
High-Energy Liner Experiment (HEL-1)

Principal Investigators: Robert E. Reinovsky (LANL), V.N. Mokhov, and V.K. Chernyshev (VNIIEF)

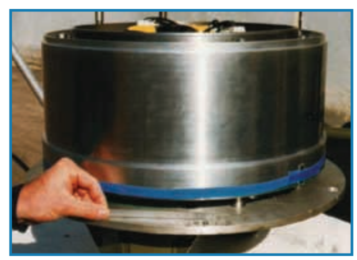
Project Description

Complementing the exploration of high performance liners at Pegasus (6-10 MA) and Atlas (15-25 MA) scale, a very High-Energy Liner implosion experiment (HEL-1) was conducted at 100 MA. The HEL-1 experiment was conducted in August 1996 by a team of scientists from Los Alamos National Laboratory (LANL) and the All Russian Scientific Research Institute of Experimental Physics (VNIIEF). The power supply for this experiment consisted of a disk explosive magnetic generator (DEMG) system delivering over 100 MA to an imploding liner experimental assembly. The DEMG consisted of five 1000 mm diameter disk generator elements, connected in series, with the seed current provided by a helical explosive generator. A preliminary test of this configuration, using a 5 nH static inductive load, produced 170 MA into a constant inductance load. Experiments reported by VNIIEF in the 1980s with this type of DEMG imploded copper and aluminum liners with masses up to 1200 grams. The aluminum HEL-1 liner was initially over 1600 grams.

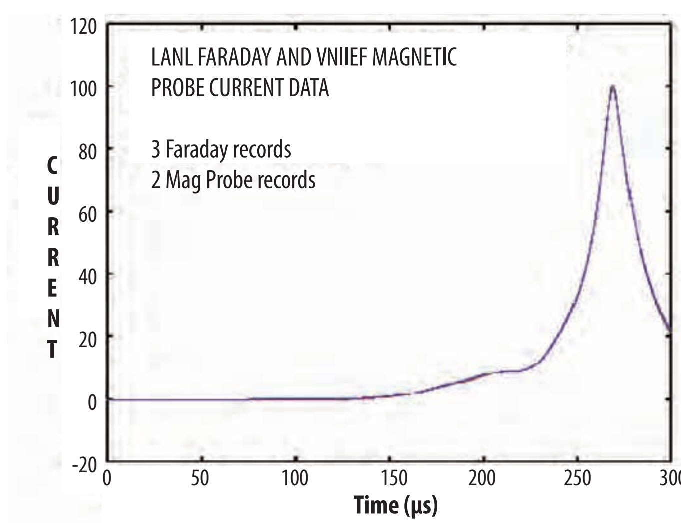
The objective of the experiment was to accelerate the aluminum liner to a kinetic energy of 20 MJ or greater and, through detailed diagnostics, determine the state of the liner when it arrived at the central measuring unit (CMU). The 100 MA current pulse produced by the DEMG imploded 1.6 kg, 4.0 mm thick aluminum alloy liner from an initial inner radius of 236 mm onto a target of radius 55 mm in a Z-pinch configuration. Both the end conductors (glide planes) and the target or central measurement unit contained an extensive array of diagnostics. Analysis of the experimental data from these diagnostics



Disk Explosive Magnetic Generator system.


HEL-1, 1.6 kg liner.


HEL-1 experimental assembly.



The DEMG produced >100 MA current to implode the liner.

showed that the inner surface of the liner reached a velocity between 6.8 and 8.4 km/s, consistent with detailed numerical calculations of the experiment using Legacy integrated codes. Those same calculations indicated that the liner was still substantially solid at the time of target impact and had a total kinetic energy of about 20 MJ. In virtually every way, the performance of the power supply, the transmission line, and the liner dynamics results agreed with calculations, usually to within 5%.

Technical Purpose and Benefits

The NNSA mission includes the need to validate sophisticated computer models of complex implosions at large scale and high velocity. Such implosions involve large amounts of kinetic energy, high pressures, high strains, and rates-of-strain in situations where detailed diagnostics are not always available. The magnetically imploded cylindrical liner provides a flexible, controllable, diagnosable source of data against which to validate both physics models and integrated codes. The successful execution of the HEL-1 experiment demonstrated the technology needed to produce such high precision data for validation and the capability to use high-energy liners to produce other high energy density environments for validating advanced physics models. Representative future applications include the generation of high pressures (100's of GPa) over relatively large areas (100-1000 mm^2) for material studies, the production of plasmas at near solid density for the study of warm, dense matter, the generation of high magnetic fields (1000 T and greater) in relatively large volumes (10's mm^3) for basic studies of the magnetic properties of matter, and the compression of a magnetized fusion plasma in Magnetic-Target Fusion (MTF). These applications are feasible only if the high-energy power supplies are reliable, their performance is predictable, and the energy can be efficiently delivered to loads. The HEL-1 experiment demonstrated that such an experiment can be designed using existing components and models, and that the system will perform as designed.

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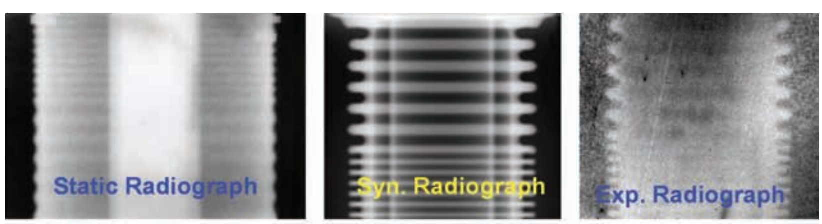
High Strain/High Strain Rate (HSR) Experiments

Principal Investigators: Walter L. Atchison (LANL), A. M. Buyko, and A. A. Petrukhin (VNIIEF)

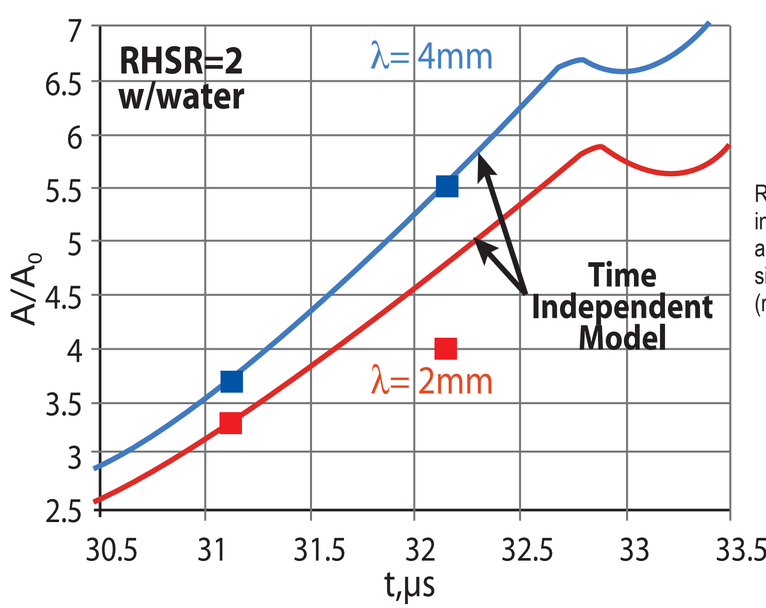
Project Description

Applying liner technology developed in previous LANL/VNIIEF technical efforts, the objective of this project is to obtain experimental data to validate existing models of the behavior of the strength of metals and polymers at high rates-of-strain in multi-dimensional strain fields and to motivate the development of new, extended strength models for use in integrated codes. A series of experiments, performed on laboratory capacitor bank facilities and on VNIIEF explosive pulsed power facilities, apply perturbation growth techniques to explore strength effects in reference metals (and possibly polymers) at conditions of high total strain and high rate of strain in converging geometry. This effort provides for the conceptual and engineering design, and for the fabrication, execution, and analysis of a series of experiments that will extend techniques first used in FY02 experiments on Atlas and demonstrated during a series of three joint LANL/VNIIEF DEMG experiments, designated R-HSR, conducted in FY03 and 04 at VNIIEF. The results of the new experiments will further expand the initial data set with the objective of quantitatively comparing Steinberg/Guinen (SG); Preston/Tonks/Wallace (PTW), MTS, and Gulschak models for strain-rate dependencies of material strength.

Conceptual design for the new series of experiments was completed in early FY03. Detailed engineering design was conducted and experiments begun in FY-04. Final analysis, completed in late FY-04 for the highly successful R-HSR-1,2 experiments reported two surprising results. The first result was a very substantial, and very unexpected, strengthening of a polymer (polyethylene) at high strain rates; and second, a similarly unexpected strengthening of M-1 copper at high strain rates. These results suggested



Static and dynamic radiographs of experimental system compared to predicted (synthetic) radiograph from simulation codes.



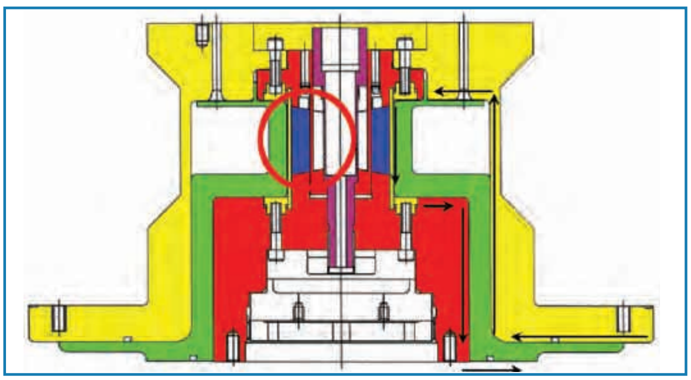
Results of FY03-04 experiments indicating good agreement between experiment and model at low strain rate (blue) but significant deviation at higher strain rates (red).

several changes to the technical approach for the new series, and a redesign of the experiments was completed in FY05 and 06 to, among other things, emphasize the effects of multidimensional strain fields that are present in the converging geometry but absent in earlier (separate) planar experiments. The new designs were technically reviewed in September 2005 and the final design report completed in FY06.

Uncertainties in the availability of the US Atlas platform in FY07 and beyond made it prudent to plan this task order to accommodate the possibility of executing the new series on Atlas or on an alternate experimental facility such as the Shiva Star system in Albuquerque or (again) using VNIIEF explosive pulsed power drive (as was demonstrated in FY03 and 04) . The additional complexity of creating final designs for two different experimental drivers has extended the time for the dual-design to late FY06 and tentatively means that the first experiments cannot be scheduled before early FY08.

Technical Purpose and Benefits

Validating material strength models under conditions of high-strain, imposed at high rates of strain, is important for accurately simulating the operation of dynamic systems. Furthermore, full-scale simulation of complex implosion experiments tests the capability of ASC codes, aids in the motivation of new and improved models, and similarly aids in code validation. Improved predictive capability is vital to the NNSA mission to achieve advanced predictive capability for sophisticated systems.



Configuration of "three layer liner" used in HSR experiments and the Atlas experimental platform at the Nevada Test Site.

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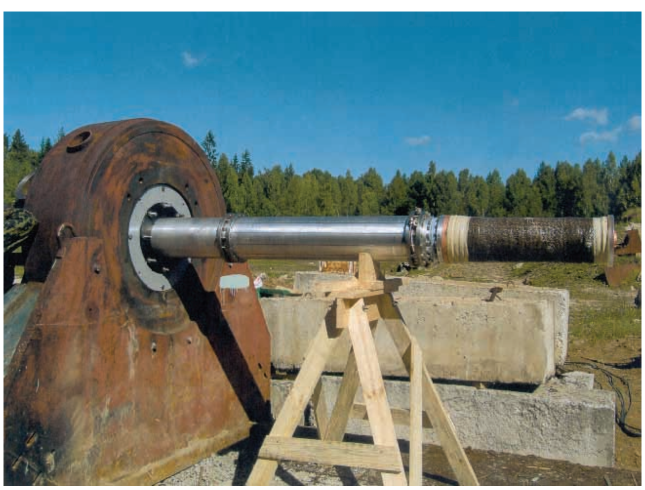
Exploration of Damage Mechanisms in Cylindrical Geometry

Principal Investigators: Ann M. Kaul (LANL) and Andre V. Ivanovsky (VNIIEF)

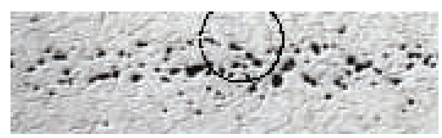
Project Description

Another application of liner technology is to explore spallation damage, a typical method of failure for ductile materials, resulting from the nucleation, growth, and coalescence of voids caused by high tensile stress. The development of mathematical models capable of accurately predicting the behavior of damage in metals in complex stress states has been an active research area for many years. While much progress has been made in this area (for example, the tensile elastic plastic, TEPLA, model), two major areas of research remain: (1) the mechanisms that control the onset of void formation and growth (damage initiation) and (2) the strength properties of a damaged material if the material is recompressed and the cracks closed. Additionally, while a significant body of data exists from one-dimensional experiments, very few experiments have been conducted in convergent configurations. Such data would allow experimental validation of the multidimensional aspects of existing models.

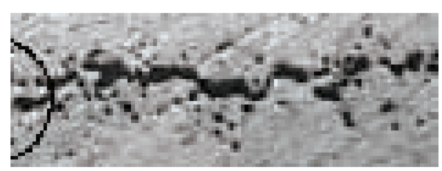
At the same time, a converging geometry allows access to non-one-dimensional stress states and the opportunity to explore void closure and material properties as the native material behind the damaged region is reaccelerated in the later stages of the cylindrical implosion. Magnetically driven implosions provide a degree of controllability and precision not available with other cylindrical implosion techniques. These experiments provide data in a convergent geometry that overlaps with and extends planar gas-gun damage data. VNIIEF researchers are acknowledged experts in the fielding of magnetically driven implosions. Additionally, recovery of the experimental sample is an important feature of these experiments, and VNIIEF has unparalleled expertise in recovery techniques for explosively powered experiments. Therefore, LANL designs and manufactures the experimental loads, while VNIIEF provides the system to power the experiment and protect the load. Diagnostic measurements are conducted jointly by both laboratories.



VNIIEF generator and load protection.



RD-1b, incipient spallation damage.



RD-1a, full crack formation.

The main objective of this effort is to obtain damage data in a (presumably) well understood material for development and validation of damage models; specifically, obtaining data near the damage initiation threshold and under conditions where voids close after damage. The first experimental series produced shocks with strengths near the damage initiation threshold, comparable to those produced in planar gas gun experiments, allowing comparison of material behavior in planar and cylindrical geometries. The second series of experiments demonstrated reacceleration and re-compaction, again near the damage threshold to investigate the behavior of recollected spallation-damaged material.

Data from these experiments are incorporated into the Tonks Ductile Failure Model (a research version of TEPLA). This model describes spallation situations with high tensile stresses and addresses the nucleation, growth, and coalescence of microvoids in ductile metals, which preferentially fail by this means. Future results will be used to develop the Tonks "Crush-up" Model, used to describe behavior of material re-collected after damage.

Technical Purpose and Benefits

The development of better predictive capability is essential if LANL is to meet its obligations to NNSA and the nation. Current damage models do not account for some of the fundamental mechanisms that lead to failure. Under this project, data are being produced to validate and improve damage models and to develop models of post-damage material behavior. This work supports the objectives of the NNSA and both research institutions (LANL and VNIIEF) as they endeavor to improve their predictive capabilities in the area of damage mechanics.

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Advanced Liner Technology Using VNIIEF Disk Explosive Magnetic Generators (DEMG)

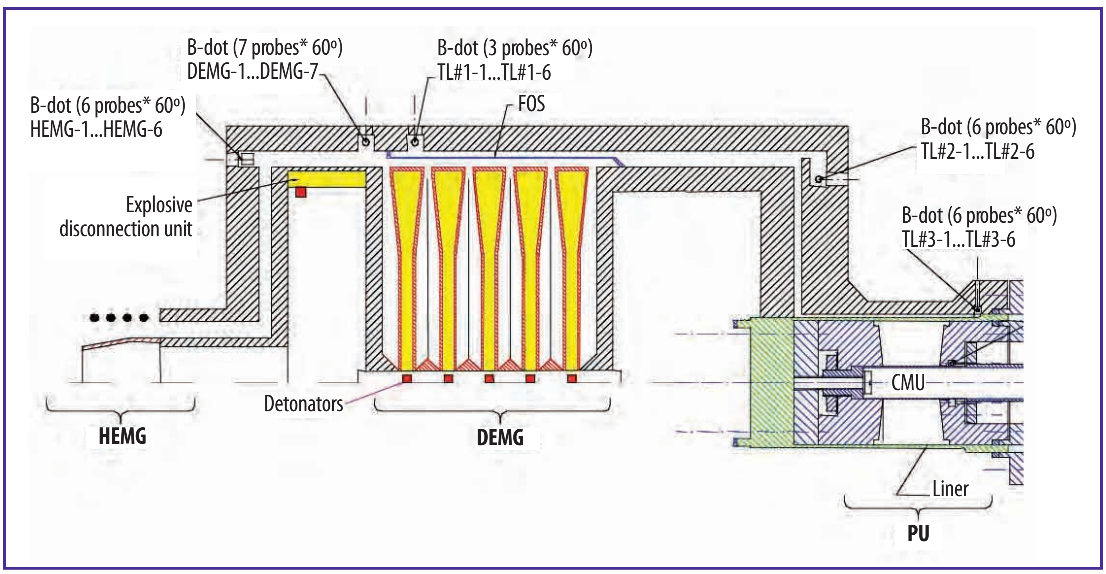
Principal Investigators: Robert E. Reinovsky (LANL), V.N. Mokhov, and Andre V. Ivanovsky (VNIIEF)

Project Description

The objective of this project is to make Russian Disk Explosive Magnetic Generator (DEMG) technology available for use in pulsed power hydrodynamics experiments conducted in the US. VNIIEF has made substantial investments in the intellectual property identified as DEMG technology, and DEMGs have been used in several joint LANL/VNIIEF experiments. The DEMG represents the highest current, most energetic high-performance pulsed power system available today. As the owner of the technology VNIIEF can either license the technology (at a substantial price) or enter into collaborative development efforts to apply their experience by designing a new DEMG system to meet specific technical needs. LANL and VNIIEF have adopted the latter approach, which has the additional advantage of advancing the concept of collaboration as VNIIEF brings technology worth far more than the token cost of the subtask, and LANL brings application experiments, diagnostics, and some advanced simulation techniques. Ultimately, the US can purchase DEMG hardware from VNIIEF as needed, probably at a cost that is significantly below that of comparable fabrication in the US and certainly far below the cost of independently developing the technology in the US.

DEMG system for ALT-1 Experiment.

A development contract, with incremental authorizations, was awarded in FY03 as a



Schematic of VNIIEF DEMG system for conducting imploding liner experiments.

multi-year effort planned in eight phases continuing into FY09 and10. The first phase of the effort was a conceptual design study exploring a variety of experimental applications including very high pressure shock applications, hydrodynamic instabilities, and quasi-isentropic compression applications to identify the general characteristics that will be required of a new pulsed power system. In the second phase, a more detailed experimental design report was prepared focusing on one application related to the high-strain, high-strain rate (HS-HSR) experiments. Work on this project was temporarily interrupted in FY05 and FY06 because of other program requirements. The next phase of design is planned for FY07 with the potential execution of a full-scale demonstration experiment beginning in FY08 and concluding in FY09. Separate programmatic funds for the application experiments would be required beyond the existing S&T program.

Technical Purpose and Benefits

A DEMG capability is needed for US experiments after FY07 to support pulsed power hydrodynamics experiments that cannot be conducted on Atlas or other laboratory facilities and that cannot be conducted in VNIIEF. The R-HSR series is an example a physics experiment that was conducted using VNIIEF DEMGs when Atlas was unavailable while being relocated to the DOE Nevada Test Site (NTS). Even if Atlas were available at the NTS, some experiments (e.g., ones involving special nuclear material) cannot be conducted jointly in VNIIEF and will be more economically executed in a consumable rather than a laboratory environment in the US. The DEMG capability also extends experiments to new parameters (higher energy and velocity). While a prototype experiment has been the initial design objective, the system issues are common to virtually any liner driven experiment.

ВНИИ VNIIEF

Collaboration between Los Alamos National Laboratory (LANL), Los Alamos, NM, USA, and the Russian Federal Nuclear Center – All Russian Research Institute of Experimental Physics (RFNC-VNIIEF), Sarov, Russia

Los Alamos NATIONAL LABORATORY

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Sandia National Laboratories

Numerical Simulation of Wire Array Implosions

Principal Investigators: Heath Hanshaw (SNL) and Igor V. Glazyrin (VNIITF)

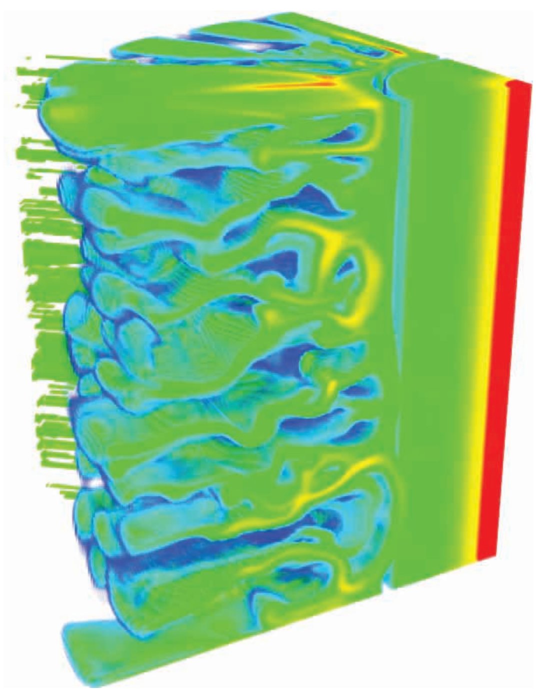
Project Description

Sandia implodes cylindrical arrays of wires on the pulsed power Z-machine to produce radiation for inertial confinement fusion (ICF) and other related experiments. The individual wires are quickly heated (exploded) by electrical energy and form an unstable plasma liner that is driven to collision on axis at very high velocity. Sandia Advanced Simulation & Computing (ASC) has a magnetized High Energy Density Physics (HEDP) modeling program to design and understand wire array physics, but these problems are inherently 3-D and extremely challenging. In many cases, the physics is unknown, and modeling is used as an exploration tool to understand what is missing. In particular, the physics of wire initiation and ablation into a plasma shell is not well understood.

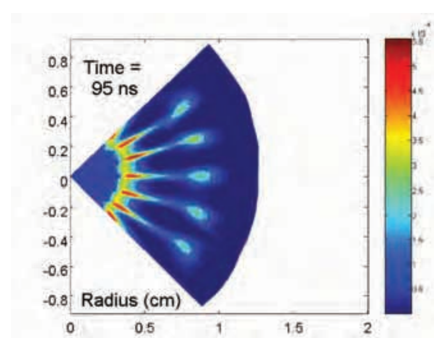
VNIITF also has a sophisticated magnetized HEDP modeling program and works with experimentalists at High Current Electronics Institute (HCEI, Tomsk), VNIIEF (S-300 at Sarov), and TRINITI (Angara V at Moscow), as well as with Sandia and Imperial College, London, England. In particular, VNIITF is making progress incorporating kinetic effects in HEDP simulations through hybrid models performing high-order Eulerian adaptive mesh simulations, whereas Sandia's efforts are in Lagrangian ALE codes. As part of this contract, VNIITF will use its codes to simulate wire array implosion phenomena.

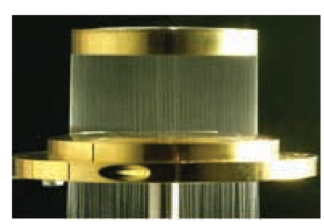
Five tasks will be performed at the discretion of the Sandia principal investigator:

- Develop a modeling plan: physics, algorithms, numerical methods;
- Perform simulations using an existing MHD code, refining the code as necessary to capture specific physics of wire explosions and wire array compression;
- Perform verification and validation tests, including comparison of material models and comparison with Sandia codes;
- Add advanced MHD terms to the code;
- Implement adaptive gridding.



Simulations using 3-D radiation-MHD capability in ALEGRA-HEDP provide understanding to scale to ZR.





40mm diameter array of 240, 7.5 - µm-diameter wires.

Technical Purpose and Benefits

The governing factor for this collaboration is the need to explore the impact of a variety of physics and modeling choices on wire array physics to verify and validate modeling choices used for experiment and machine design. Neither Sandia nor VNIITF has a complete understanding of wire array physics, yet each has areas of complementary expertise. The benefit of this collaboration will be an increased understanding of wire array physics, and specifically a greater understanding of the validity of modeling choices.

Collaboration between Sandia National Laboratories (SNL), Albuquerque, NM, USA, and the Russian Federal Nuclear Center – All Russian Research Institute of Technical Physics (RFNC-VNIITF), Snezhinsk, Russia

Sandia National Laboratories

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Sandia National Laboratories

Development of Hybrid Codes for Modeling Petawatt Laser Interactions with Dense Matter

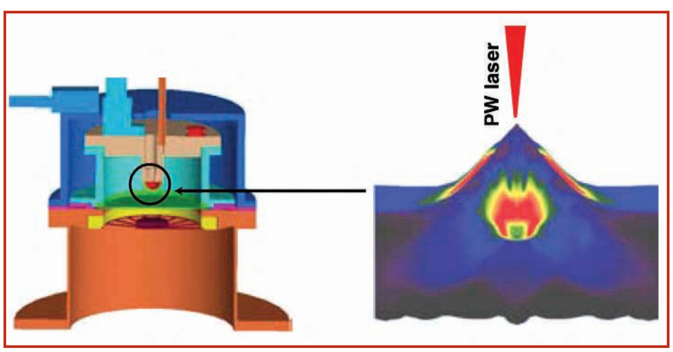
Principal Investigators: Heath Hanshaw (SNL) and G.V. Baydin (VNIITF)

Project Description

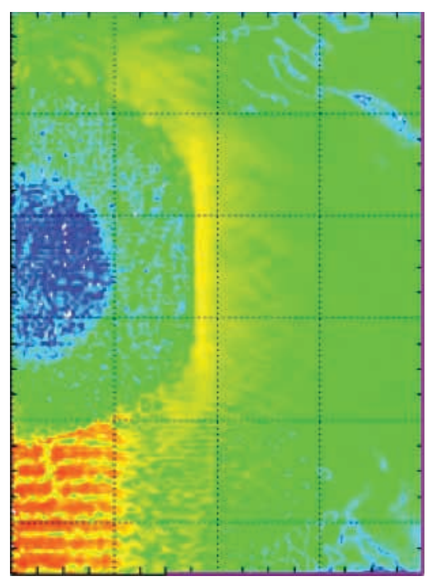
Accurate modeling of dense plasma physics is an extreme challenge, particularly in the case of short pulse petawatt (PW) lasers (like Z-PW at Sandia) used for creating pulsed electron, ion, or x-ray beams for inertial confinement fusion (ICF) experimental diagnostics or for fast ignition studies. Both Sandia and VNIITF have been pursuing state-of-the-art hybrid (Particle in Cell plus fluid) implicit code development projects.

Voss Scientific (formerly MRC), a Sandia contractor, has developed with Sandia the implicit hybrid code LSP, which can simulate most of the physics of PW-laser plasma interactions, a unique capability within the three U.S. defense laboratories. Sandia plans to bring LSP technology in-house, to integrate it with other Sandia code capabilities, to verify and validate the capability, and to use it to design experiments using Z-PW for ICF and other applications.

For this prospective code project to be successful, it is crucial to critically examine modeling approaches, from included physics to equations to numerical approaches. For example, simultaneous multiscale modeling of fine-scale spatial effects, like the Weibel instability, remains beyond LSP's capabilities (except when run as a standalone simulation whose results are modeled grossly as an anomalous resistivity in a large-scale simulation). Yet these small-scale physics can have drastic effects on beam evolution. Like Sandia, VNIITF is also combining several code capabilities into a hybrid implicit plasma code, and they also plan on using algorithms developed and previously published jointly by Voss and Sandia. One of the most interesting features of VNIITF's plan is to implement its hybrid implicit code in an adaptive mesh (AMR) setting, which could potentially aid modeling of this instability's effects (and those of other instabilities) on beam generation, allowing greatly improved experimental designs.



Fast ignition simulation.



Log of proton density accelerated from the rear side of a thin foil by electric fields generated by petawatt laser irradiation of the front surface.

Under this contract, VNIITF will complete development of a hybrid implicit code using adaptive mesh refinement and use that code to simulate the interaction of a short pulse PW laser with dense matter for cases of interest like fast ignition.

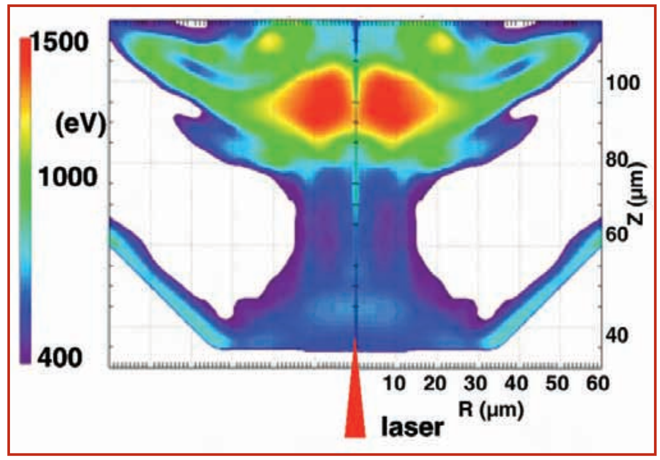
Five tasks will be performed at the discretion of the Sandia principal investigator:

- Develop models and test problems of different stages of laser plasma interaction;
- Simulate test problems and perform code comparisons with Sandia's;
- Develop initial 2-D AMR hybrid implicit code;
- Perform validation simulations of beam experiments and compare with Sandia's;
- Simulate the "fast-ignition" problem.

Technical Purpose and Benefits

A major inducement is utilizing the expertise resident at VNIITF in employing hybrid codes to model petawatt laser-plasma interactions for application at Sandia. Because this work represents cutting edge research, both institutions benefit, particularly in the area of comparing alternative modeling and techniques. The primary benefit lies in gaining validated modeling tools to effectively utilize Sandia's Z-beamlet-petawatt laser.

Technologist Benjamin Thurston examines the debris shield that protects the giant Z-Beamlet laser's final focusing lens from flying debris when the Z-accelerator fires.



Simulation of "fast-ignition."

Collaboration between Sandia National Laboratories (SNL), Albuquerque, NM, USA, and the Russian Federal Nuclear Center – All Russian Research Institute of Technical Physics (RFNC-VNIITF), Snezhinsk, Russia

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Numerical Magneto-Hydrodynamic Simulation of Z- and Z-θ Pinches at Pulsed Power Facilities at Sandia National Laboratories

Principal Investigators: Heath Hanshaw (SNL) and Andrey P. Orlov (VNIIEF)

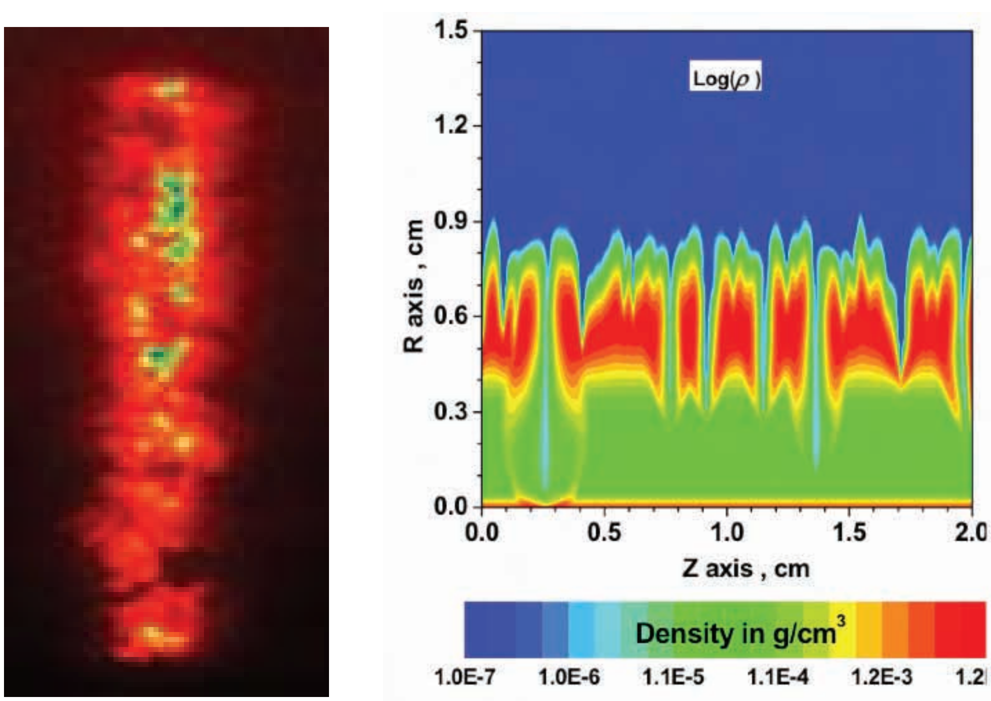
Project Description

Sandia has an ongoing effort to model and design Z-pinch radiation sources. Z-pinches achieve High Energy Density conditions, but low density kinetic effects and instabilities are important in their evolution. Though many elements of Z-pinch physics are not captured by fluid approximations, a fluid radiation magneto-hydrodynamic (RMHD) approach is the simplest and cheapest for design calculations. Approximate models are used in attempts to capture the missing physics. The Orlov group at VNIEEF is using a similar approach to model Z-pinches and explosively driven magnetic compression generators, but has made some different modeling choices, such as the choice of low density resistivity models, relativistic effects, and vacuum wave terms.

The goal of this effort is to validate numerical 2-D and 3-D RMHD models of Z-pinch experiments performed at Sandia. An existing VNIIEF 2-D code, FLUX-rz, will be used to axisymmetrically model Z-machine wire array shots, where the array is modeled as a liner including axial perturbations. Subsequently, more elaborate physics models including Hall effects will be performed in 2.5-D and 3-D simulations.

Three tasks will be performed at the discretion of the Sandia principal investigator:

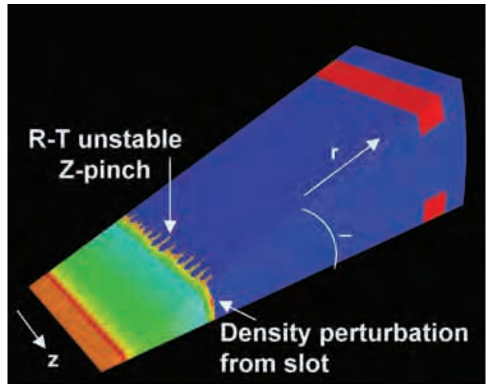
- Validate 2-D (*r-z*) numerical simulation of annular Z-pinches against Z-machine shots.
- Expand to 2.5-D (*r-z*) numerical simulations and evaluate Hall effects.
- Add radiation to FLUX-3-D code, and perform simulations to assess 3-D effects.



Measured time integrated thermal x-ray emission from a stagnating wire array on Z, showing the imprint of the Rayleigh Taylor instability. Right: Simulation of Z-shot 48 by Andrey Orlov of VNIIEF, showing how different Rayleigh Taylor bubbles stagnate at different times to produce axially varying x-ray radiation.

Technical Purpose and Benefits

Numerical 2-D and 3-D radiation magneto-hydrodynamic simulation is one of the tools to get a more detailed understanding of, and a quantitative description for, physical phenomena occurring in the imploding plasma loads. Using this numerical simulation of existing experimental results on pulse generation and magnetic field compression could lead to optimizing the Z- and Z-θ Pinches in future experiments. Prediction of liner loads using RMHD models is urgent because of the possible passage to longer Z-pinch implosion times at Sandia.



3D ALEGRA-HEDP simulation of a periodic cylindrical wedge of the slotted anode can wire array implosion, showing the imprint of the diagnostic slots on the implosion.

View of a cylindrical wire array and foam target through the oval diagnostic slots of the outer anode can.

Collaboration between Sandia National Laboratories (SNL), Albuquerque, NM, USA, and the Russian Federal Nuclear Center – All Russian Research Institute of Experimental Physics (RFNC-VNIIEF), Sarov, Russia

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Sandia National Laboratories

Atomistic Study of Phonon Generation and Evolution by Laser Excitation

Principal Investigators: E.P. (Tony) Chen (SNL) and Alexander Belyaev (IPME)

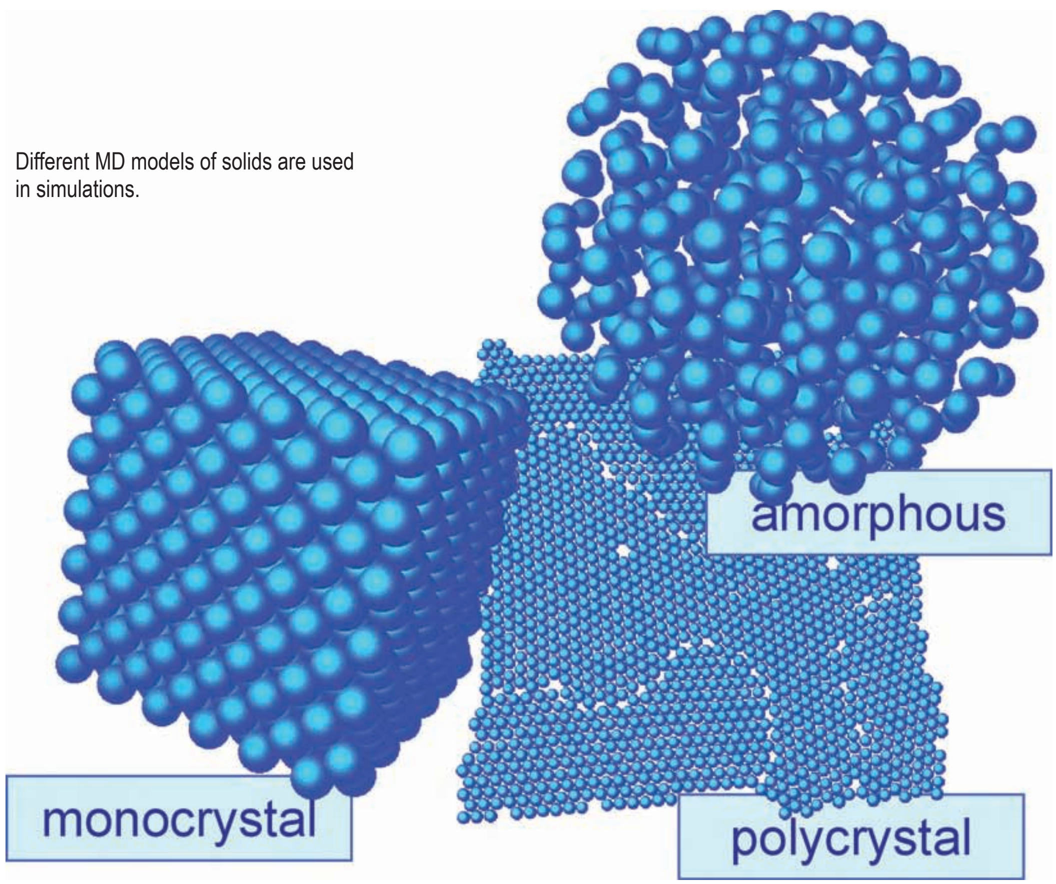
Project Description

An atomistic study of thermal transport by a concentrated energy source will be conducted, including molecular dynamics (MD) simulations. Experiments measuring the transport of heat introduced by laser excitation provide data for guiding and validating numerical results.

Four tasks will be performed at the discretion of the Sandia principal investigator:

- Construct structural-rheological model of a two-component solid appropriate for description of its atomic-corpuscular nature; derive boundary-value problem for a medium with a complex structure; construct nonlinear model for phonon build-up in silicon monocrystal subjected to various conditions; simulation of heat propagation in monocrystal solid.
- Derive dynamical equations and constitutive laws for 3-D solid; model transfer of energy to higher vibratory modes, construct coupled nonlinear equations for low-frequency and high–frequency acoustic field and thermal field interacting with excitons; propagation of heat in polycrystal solid.
- Model ballistic phonon transport.
- Model the characteristics that influence material structure on phonon transport.

Different MD models of solids are used in simulations.



Technical Purpose and Benefits

The use of atomistic simulation brings high fidelity physics into materials modeling. At atomic length and time scales, classical continuum approaches for describing the transport of energy and for differentiating heat from elastic waves become questionable. In atomistics, it is expected that energy transport will be affected by the individual and group behavior of phonons. This project proposes an atomistic study of thermal transport from a concentrated energy source. The goal is to characterize the transport of energy in an atomic lattice including the effects of phonon dispersion, interaction, and decay.

The project will aid in characterizing the distribution and evolution of phonon spectra, density states, decay, and dispersion for dynamic atomistic simulations of the thermomechanical deformation of solids. It will examine the effect of quasi-diffusion on heat transport in dynamic atomistic simulations and investigate the validity of classical continuum approaches for describing thermal conductivity and energy transport in solids. The results are essential to the development of fracture and failure prediction capabilities by providing physical understanding of the energy dissipation and transport processes, for example, at the crack tip.

Signing contract in St. Petersburg—From left to right: Dr. Tony Chen, Ms. Patty Jojola, Professor Belyaev, and Professor Dimitry Indeitsev.

Collaboration between Sandia National Laboratories (SNL), Livermore, CA, USA, and IPME (Research Institute of Mechanical Engineering Problems), St. Petersburg, Russia

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Atomistic Study of Phonon Generation and Evolution During Dynamic Crack Propagation

Principal Investigators: E.P. (Tony) Chen (SNL) and Alexander Selezenev (VNIIEF)

Project Description

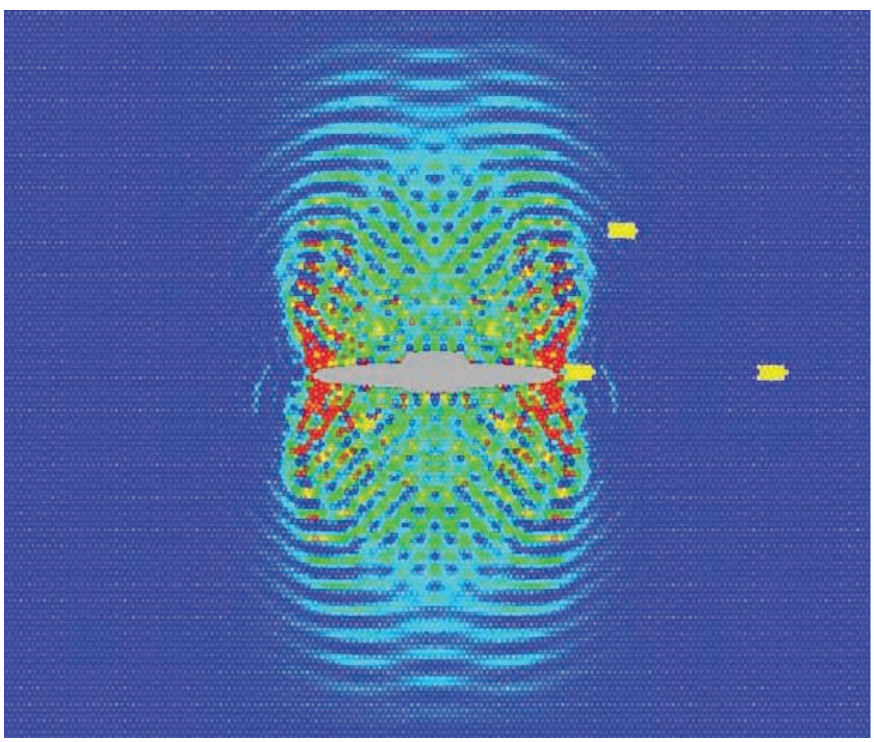
This project involves conducting molecular dynamics (MD) simulation of micro-crack propagation in materials. It will use MD simulation to study phonon generation mechanisms during initiation and propagation of a micro-crack; the MD simulation will be performed in 2-D and 3-D geometries.

Initially 2-D and 3-D crystal structures will be built using parallel computers. SageMD code will be parallelized and used in MD simulations. Details of the MD simulations will be defined.

With MD simulation, the sample will be loaded with boundary conditions specified under which initially the crack extension proceeds in the direction perpendicular to the crack plane. The temperature behavior of the quantities under study will be investigated, using a different temperature ensemble during the MD simulation.

Four tasks will be performed at the discretion of the Sandia principal investigator:

- Generating crystal structures;
- Conducting MD simulation in 2-D of crack propagation in crystal structures;
- Conducting MD simulation in 3-D of crack propagation in crystal structures;
- Analyzing and summarizing results.



Results of MD simulation of crack propagation.

Technical Purpose and Benefits

The understanding of material fracture mechanisms is an important phase in developing new materials with tailored responses. The crack propagation dynamics is an important mechanism responsible for prescriptive material responses. Despite the long history of the research into this effect, it is as yet not well understood.

This project proposes an atomistic study of the phonon generation and interactions that occur during dynamic crack propagation. The crack tip acts as a focal point at which stored strain energy is released upon the breaking of bonds. In the continuum point of view, this energy is converted to heat and elastic waves, whereas the atomic framework models the converted energy strictly as phonons. The evolution of these emitted phonons in atomistics plays an important role in governing the limiting speed and the onset of dynamic crack tip instabilities, although the exact processes are unknown. Also unknown is how this energy conversion differs when crack propagation is accompanied by the creation of material defects, such as dislocations.

We hope to gain from this collaboration a better understanding of fracture mechanisms—an essential gradient in developing predictive simulation capabilities.

Discussions in Vienna—From left to right: Dr. Robert Thomas, Dr. Tony Chen, and Dr. Alexander Selezenev.

Collaboration between Sandia National Laboratories (SNL), Livermore, CA, USA, and the Russian Federal Nuclear Center – All Russian Research Institute of Experimental Physics (RFNC-VNIIEF), Sarov, Russia

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Sandia National Laboratories

Performance and Reliability Modeling of MEMS: Modeling the Effects of Mechanics and Chemistry on Material Damage and Failure

Principal Investigators: E.P. (Tony) Chen (SNL) and Alexander Belyaev (IPME)

Project Description

Factors will be studied in this project that affect the performance of microElectroMechanical Systems (MEMS) from two perspectives:

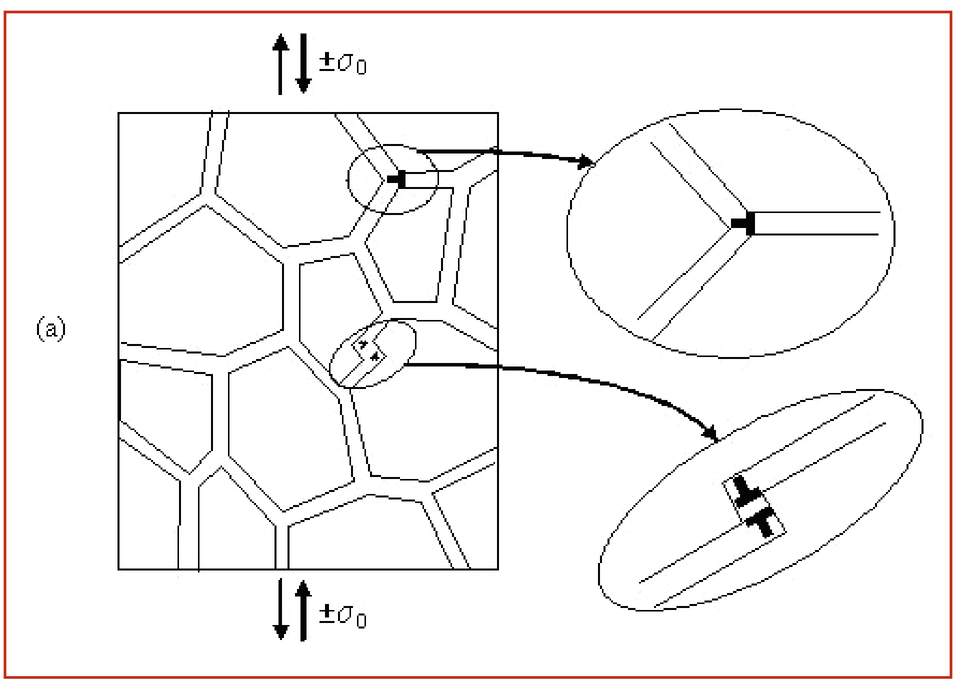
- Creep and recrystallization in relatively low-cycle, thermally activated devices
- Fatigue in high-cycle devices

Four tasks will be performed at the discretion of the Sandia principal investigator:

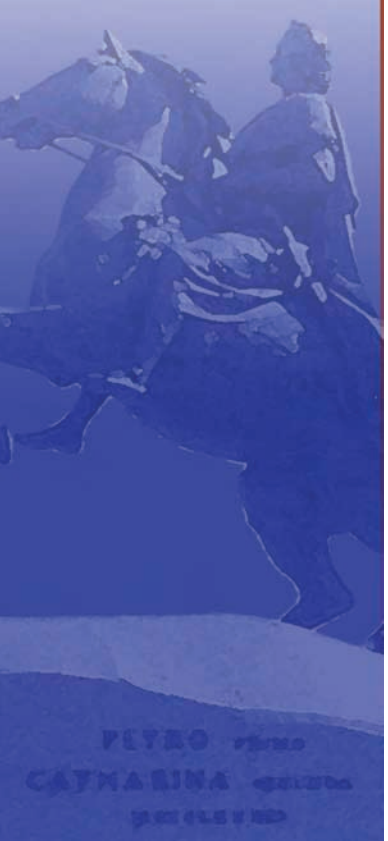
- Construct nonlinear model with drastically changing lattice structure under temperature and stress field; model crack interaction localized phase transforming area; produce theoretical model of mechanisms for nucleation and growth of fatigue cracks in polysilicon materials; molecular dynamics modeling of low-cycle high-amplitude loading of a monocrystal material with defects.
- Derive nonlinear equations of catastrophic deformations and fatigue crack growth; model grain growth in polysilicon materials under thermal treatment and creep.
- Model couple interaction between crack growth, stress-assisted diffusion, and chemical reactions.
- FEM and molecular numerical simulation of damage evolution in polycrystalline solids.

Technical Purpose and Benefits

Microsystems fail not only by catastrophic modes, in which devices sustain severe damage, but also by more subtle modes that result in a loss of functionality, though the devices remain largely intact. The catastrophic modes tend to involve a complete breakdown in any



Nucleation of nanoscale cracks/nanovoids in polysilicon under fatigue load.



one of the thermal, mechanical, or electrical properties of the device, such as the fracture of a structural member. The more subtle failure modes tend to involve a coupling of electron-thermomechanical responses such as a creep leading to a change in electrical resistivity and thermal conductivity causing the force or range of motion in an actuator to fall outside design tolerances. Accurate life predictions require material property evolution to be included in coupled-physics device simulation in order to assess how all these factors affect device performance over time. This contract studies factors affecting the performance and reliability of MEMS from two perspectives: (1) creep and recrystallization in relatively low-cycle, thermally activated devices and (2) fatigue in high-cycle devices.

The results of this project will improve our understanding of the performance and reliability characteristics of MEMS so as to allow the adaptation of this cutting edge technology in the stockpile.

Meeting in St. Petersburg—From left to right: Dr. John Aidun, Academician Nikita Morozov, and Dr. Tony Chen.

Collaboration between Sandia National Laboratories (SNL), Livermore, CA, USA, and IPME (Research Institute of Mechanical Engineering Problems), St. Petersburg, Russia

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Sandia National Laboratories

Development of a Platform-Independent Molecular Builder and Visualizer

Principal Investigators: John Aidun (SNL) and Alexander Selezenev (VNIIEF)

Project Description

A Unix/Linux based, platform-independent molecular builder and visualizer (MBV) was developed as a preprocessor and postprocessor for atomistic simulations. This project drew on the substantial experience and accomplishment of the VNIIEF team in this area. Developments were selected, in particular, to enable atomistic simulations of crystal defects, grain boundaries, and *material interfaces*, which are topics of active interest at Sandia and VNIIEF and in the wider materials science and solid state physics communities. Joint research was conducted to identify how to define the atomistic configurations of material interfaces in the geometric (unrelaxed) approximation, which include both grain boundaries and heterogeneous *material interfaces*. Specific capabilities for constructing grain boundaries and *material interfaces* were then implemented in the MBV. The resulting capability is being deployed at both labs to enhance productivity of analyses and investigations with atomistic methods.

Eight of nine contracted tasks have been performed to date. Highlights of the MBV capabilities are as follows:

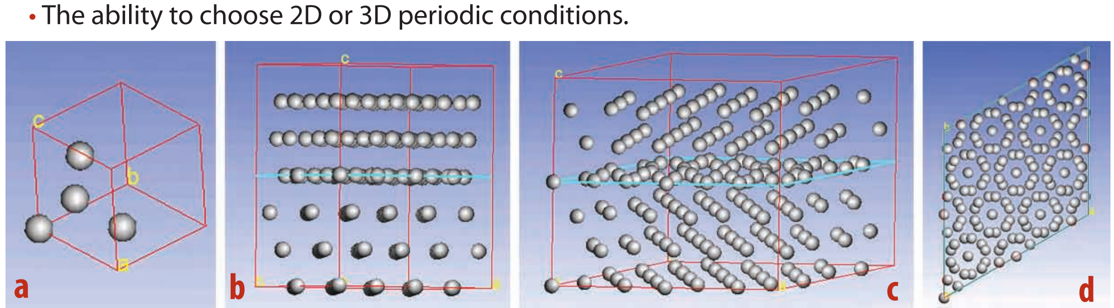
The basic, GUI-driven capability supports construction of single crystal atomistic configurations of any space group symmetry with the option of specifying a super cell for the simulation by replicating the unit cell. Included in this is the ability to easily modify the atom configurations, locally, to output several formats, and to visualize results from a variety of atomistic simulation codes. Additional modules include the capability to cleave a bulk crystal and to add molecules or atoms onto the cleaved surface; to construct grain boundary (GB) configurations that form commensurate interfaces, in the geometric (unrelaxed) approximation; to construct an arbitrary bi-crystal slab material interface structure composed of atoms or molecules of the user's choice and having periodic boundary conditions (PBCs) in two orthogonal directions in the plane of the interface. Bi-crystal and material interface configuration can each be altered by interactively selecting and shifting, removing, or adding particular atoms.

Under development is the capability to build supercells of crystals with polyatomic unit cell bases. The specific aim is to enable construction of molecular solids.

Delivered with each task are the MBV software, installation procedure instructions, and the updated Users' Manual.

The capability to construct material interfaces is fairly general, though constrained by the requirement that the resulting systems admit periodic boundary conditions in the directions in the plane of the interface. The capability comprises:

- Enumeration of the symmetrical tilt GBs;
- Enumeration of the symmetrical twist GBs;
- The possibility to remove atoms closer than a specified distance from boundary plane;
- The ability to specify the width of crystals on either side of boundary plane;
- User specification of translations on either side of the interface;
- The ability to manipulate atoms to add impurities or create defects;
- The ability to apply labels to surface layer portions of atoms;
- The ability to choose 2D or 3D periodic conditions.



Example of grain boundary (GB) construction: symmetric twist GB in aluminum. (a) Aluminum unit cell. (b)-(d) Three projections of the symmetrical twist grain boundary with angle θ = 81,78680, Plane (111) and planar Σ=7.

Technical Purpose and Benefits

Molecular builders and visualizers are an enabling technology for atomistic simulation methods. They can substantially increase a materials researcher's productivity in performing atomistic numerical simulations. A number of commercial products are available, but an MBV that can be readily modified, is platform independent, and is freely available to computational scientists at DOE laboratories and other government research laboratories is highly desirable. The MBV produced in the present project also includes an efficient and easy to use graphical user interface (GUI) to enable local modifications of the atomic structures. Moreover, it has a unique capability to construct (unrelaxed) grain boundaries and material interfaces, as illustrated in the table and figure. Such configurations are the needed starting point for investigating the challenging questions of how material microstructure influences material properties and how processing details determine microstructure. These investigations are important contributors toward the long term goal of *designing* materials to have specified properties to meet NNSA mission needs.

In the near term follow-on tasks, we will transition toward using the MBV to facilitate particular computational materials research endeavors while still adding to the MBV capabilities and providing for any needed maintenance or bug fixes to the utility. The chosen research topic is the response of molecular crystals to shock wave loading. This basic science area is of interest to RusAtom and NNSA laboratories for its relevance to high explosive safety.

Futures \ Visualizers	MolDraw	ACD/Structure Drawing Applet	MW3D Crystal Lab	Crystal Studio	Crystal Maker	CaRIne Crystallography	MBV
Platform, OS	Windows	Multiplatform	Multiplatform	Windows	Windows XP Mac OS	Windows Linux	Multiplatform
3D visualization (OpenGL)	–	–	+	+	+	+	+
3D Tools (zoom, rotation…)	+	–	+	+	+	+	+
Geometrical Tools	+	+	–	+	+	+	+
Lattice builder	+	–	–	+	+	+	+
Simulation/ Animation	+/–	–/–	–/–	+/+	+/+	+/+	+/+
Surface cleaving	–	–	–	+	–	+	+
RDF/ MSD/ Temperature calc.	–/–/–	–/–/–	–/–/–	–/–/–	–/–/–	+/–/–	+/+/+
Multi-windows support	–	–	–	+	+	+	+
X-Ray diffraction patterns	–	–	–	+	–	+	–
Defects, dislocations	–	–	–	+	+	+	+
Surface builder	–	–	–	+	–	+	+
GB Construction	–	–	–	–	–	–	+
Export formats	Gaussian, CRYSTAL 98, GULP, EXAFS, MOLPLOT, Phio-78, PLUTON, Shakal, XMOL, POV-Ray	MDL molfile	PDB	CIF, CSV, XYZ, XRD, POV-Ray	CCL, Chem3D, CIF, CSSR, FDAT, ICSD, PDB, SHELX, Struplo, MacMolecule	N/A	CERIUS, MOPAC, VASP, PDB, XYZ, CIF
Import formats	Gaussian, Crystal 2000, ADF, Mopac, HyperChem, XTL, EXAFS, CSD, PDB, XMOL, CIF	MDL molfile	PDB	CIF, CSV, XYZ, XRD, POV-Ray	Chem3D, CIF, PDB, MacMolecule	N/A	CERIUS, MOPAC, VASP, PDB, XYZ, CIF
Price	free	free	free	1398$	429-1899	795-5895	free

Comparison of Available Visualization Utilities.

Sandia National Laboratories

Collaboration between Sandia National Laboratories (SNL), Livermore, CA, USA, and the Russian Federal Nuclear Center – All Russian Research Institute of Experimental Physics (RFNC-VNIIEF), Sarov, Russia

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Sandia National Laboratories

Extending Non-Equilibrium Molecular Dynamics Simulation Methods

Principal Investigators: John Aidun (SNL) and Genri Norman (JIHT)

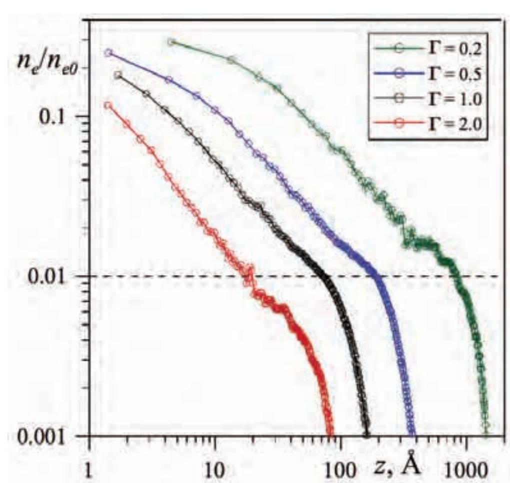
Project Description

Novel nonequilibrium molecular dynamics (NEMD) simulation methods are being extended and applied in four areas of mutual interest to Sandia and Joint Institute for High Temperatures, Russian Academy of Sciences (JIHT RAS). NEMD is being applied to (1) understanding relaxation and equilibration in non-ideal, nondegenerate plasmas; (2) characterizing melting or cavitation of condensed matter systems that are super-heated or under hydrostatic tension; (3) devising classical interaction potentials that can represent changing bonding character as a system evolves; and (4) investigating the mechanisms of shock-induced plasticity and fracture in metals.

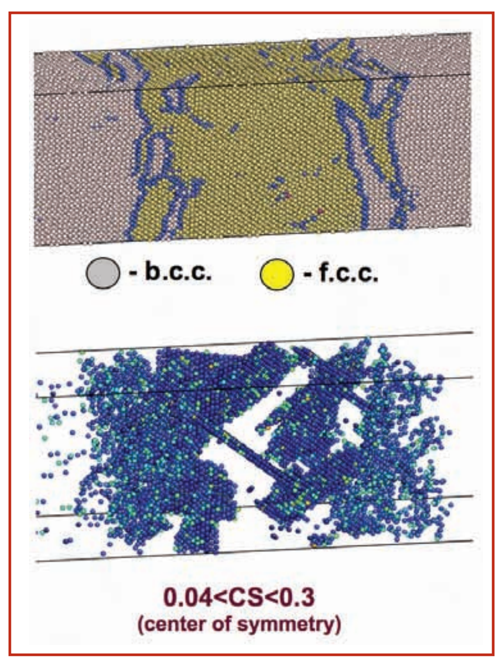
Three tasks were performed in CY06:

- Investigation of interacting, drifting, nonideal plasmas;
- Investigation of melting in super-heated condensed matter;
- Development of reactive potentials for material interfaces using the Cluster Multi-Range Interpolation (CMRI) scheme.

Follow-on work in each of the four areas is being pursued in CY07. In the area of nonideal plasmas, JIHT is studying the role of bound, high energy, quasi-classical electron-ion pairs on the relaxation of nonideal plasmas. Algorithms are being developed for identifying such bound states in MD simulations. The fraction of the bound states, their energies, and lifetimes will be studied for the nonideal plasmas simulated in CY06. The formation process for the bound states will be determined, and the recombination time will be compared with characteristic times of the different relaxation processes observed in the CY06 simulations. JIHT will also compare the results from CY06 with existing continuum models of plasma equilibration to assess the agreement in various regimes defined by the set of values of nonideality parameter; ion and electron temperatures; and ion mass and charge. Finally, JIHT is developing a new simulation technique for more accurate treatment of close particle collisions. The approach being used is to separate the interaction potential into short-ranged cluster binding models and long-ranged classical pair-wise force field. The antisymmetrized wave packet MD will be used to describe the



Formation of the Double Layer-Relaxed density profiles of electrons depending on the plasma nonideality.



Structural changes in the rarefaction wave in an initially BCC single crystal.

particle collisions or bound states of a small number of electrons and ions for the cluster model. The CMRI scheme will be applied to combine individual cluster binding models and long-ranged force field into a single set of dynamic equations for electrons and ions. In the area of highly nonequilibrium condensed matter, JIHT will study cold crystal lattice stability in the presence of "hot" electrons (~10 eV) using *ab initio* MD based on the finite temperature density functional theory. The *ab initio* simulations will be used to validate the quality of the description of interatomic interactions in the two-temperature states considered by classical (many-body) potentials. A procedure will be proposed for development of temperature dependent classical potentials suitable for describing the two-temperature systems considered.

JIHT is using the CMRI scheme to fit empirical potential parameters to quantum chemistry (QC) data. In particular, they are pursuing development of an automated procedure for construction of combined potentials: fitting the parameters of two functionally different empirical potentials in different atom environments and fitting the CMRI-specific interpolation parameters to the QC data in the transition between the two empirical potentials.

JIHT is also pursuing several related tasks in the area of shock-induced plasticity and fracture. This includes investigating the mechanisms of structural transformations, spall, and fracture in solids under high rate impulse loading. They are developing a kinetic nucleation-and-growth model to represent the results obtained from the NEMD simulations in hydrodynamic simulations of shock wave spall experiments. Lastly, they will attempt to use the CMRI scheme to construct an interatomic potential that switches smoothly between fast nonreactive potential and the more accurate, computationally demanding reactive potential ReaxFF developed by van Duin and Goddard.

Technical Purpose and Benefits

This project will enhance both our understanding and our capabilities for investigating the dynamic response of multiple types and states of materials under a variety of loading conditions. This understanding finds application in weapons performance, weapons effects, ICF, high energy density physics (HEDP), and advanced nuclear energy reactors.

Possible future applications of the more accurate treatment of close particle collisions in nonideal plasma simulation are plasmas at low temperatures, mixtures of molecules, atoms and multiple charged ions.

The interpolated, combined force fields should find useful application in simulating nonequilibrium systems of atoms. The demonstration simulation will treat graphite oxidation reactions. The hybrid force field incorporating ReaxFF will be demonstrated in simulating cracking in silicon and, if that is successful, applied to study spontaneous decay of distended silicon near its stability boundary.

Understanding the mechanisms of shock-induced plasticity and fracture in metals is a long time, outstanding problem in shock wave physics. JIHT's innovative approaches stand to make significant contributions in this area.

Signing the agreement. Clockwise from left: Ms. Patty Jojola (SNL buyer), Dr. John Aidun (SNL PI), Dr. Genri Norman (JIHT PI), and Dr. Vladimir Zeigarnik (JIHT).

JIHT

Collaboration between Sandia National Laboratories, Albuquerque, NM, USA, and JIHT RAS (Joint Institute for High Temperatures, Russian Academy of Sciences), Moscow

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Sandia National Laboratories

Scalability Assessment for Parallel Algorithms of Numerical Simulation: Gas Dynamics and Heat Conduction (Diffusion)

Principal Investigators: Robert Benner (SNL) and Yuri Bartenev (VNIIEF)

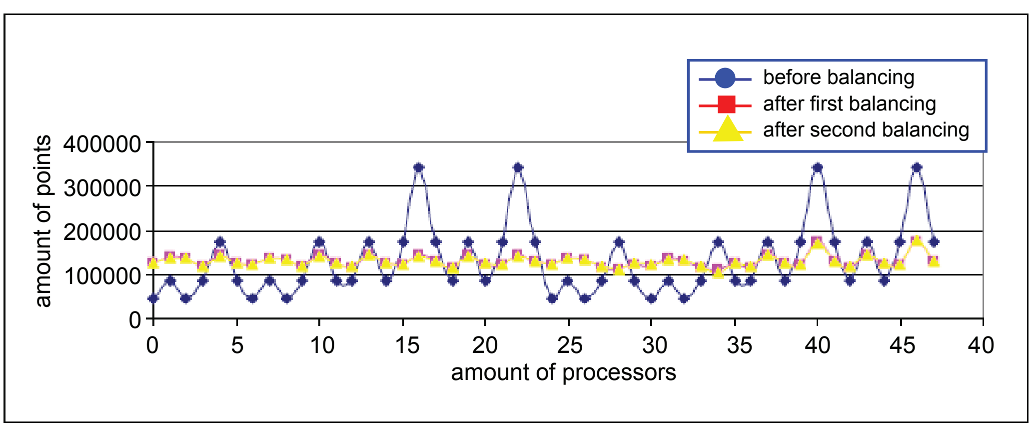
Project Description

The scalability of 3-D solutions to gas dynamics and diffusion equations on parallel computers will be researched. The work is conducted within several software requirements, such as minimization of redundant computations, minimization of interprocessor communications, and optimization of transfer lengths. Furthermore, there are three sources of load imbalance to be considered: the physical terms of the governing equations, mathematical sources of imbalance, such as local iterations and software optimizations, and the hardware itself and associated system software.

Using an analytical approach, validated by 3-D simulations, VNIIEF will obtain formulas for the runtime of algorithms based on problem and parallel computer parameters. This will permit prediction of the scalability of applications on future high-performance computers (e.g., those created by ASC or VNIIEF).

Twelve tasks will be performed at the discretion of the Sandia principal investigator, and as of December 2006, the first six tasks have been completed:

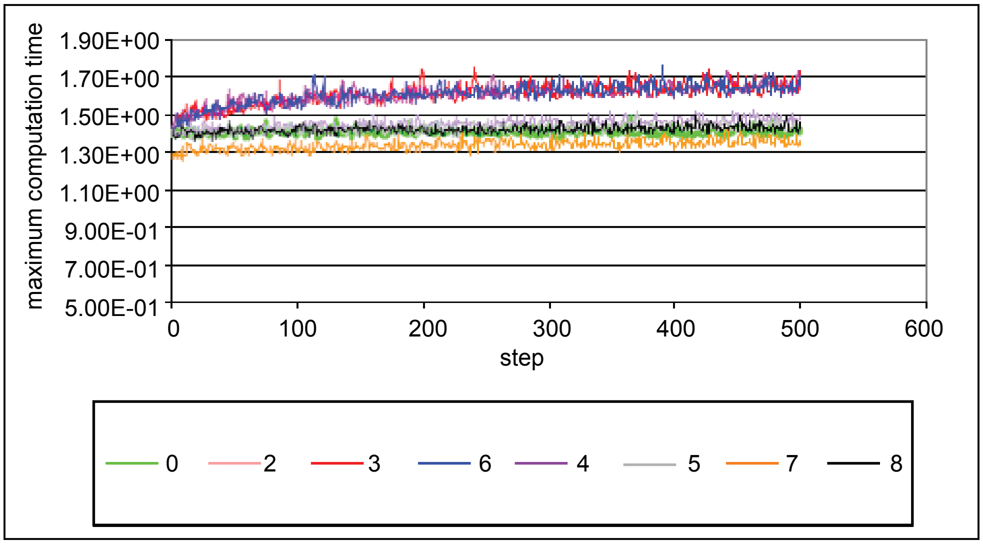
- Provide a description of Trek+++.
- Develop a set of dynamic problem examples as test cases for Trek+++.
- Develop and implement the analytical runtime formula for the Eulerian approach for gas dynamics problems.
- Develop analytical runtime formula for diffusion problems and validate gas dynamics and diffusion runtime formulas for Eulerian approach.
- Improve scalability of algorithms for gas dynamics.
- Improve scalability of algorithms for gas dynamics as well as coupled gas dynamics and diffusion problems.
- Enhance analytical runtime formula and calculator.
- Improve model of computational scheme for adaptive grid refinement of gas dynamic problems to enhance scalability.
- Improve model of computational scheme for adaptive grid refinement of gas diffusion problems to enhance scalability; develop diffusion and dynamic models.
- Enhance analytical runtime formula and analytical formula calculator incorporating adaptive grid refinement algorithms.
- Present at an international conference in St. Petersburg, Russia.



Distribution of points over the processors, 48 processors.

Technical Purpose and Benefits

Both Sandia and VNIEFF are major supercomputer users on behalf of their governments. It is of mutual interest to both organizations for their use of supercomputers to be efficient and predictable. By modeling hypothetical supercomputer operations, it can be determined whether particular algorithms will be successful and whether changes need to be made in the supercomputer design. Software styles with good performance over many hypothetical computer designs can be recommended for use.



Maximum computation time on one processor versus computational step on 48 processors.

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Modified for the Web

Sandia National Laboratories

Development of Fast High Current Linear Transformer Drivers for the Next Generation of Z-pinch Fusion Drivers.

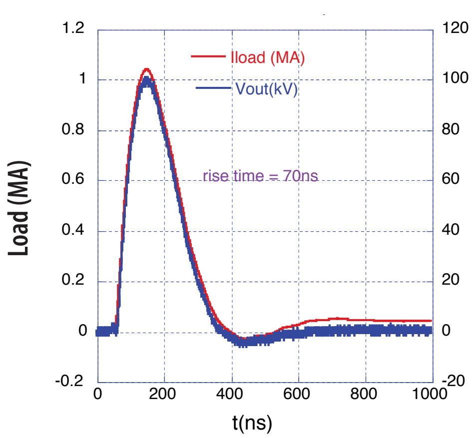
Principal Investigators: Michael G. Mazarakis (SNL) and Alexander Kim (HCEI)

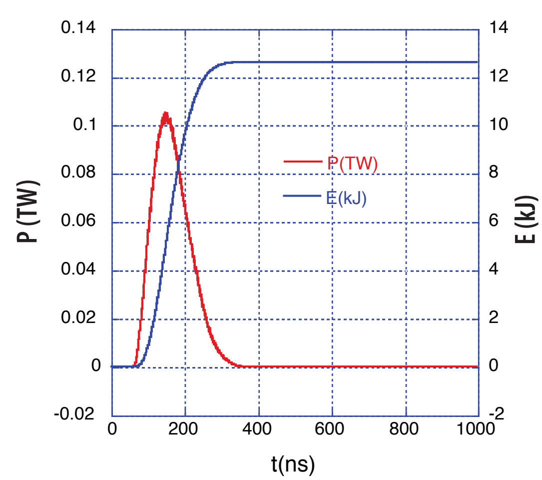
Project Description

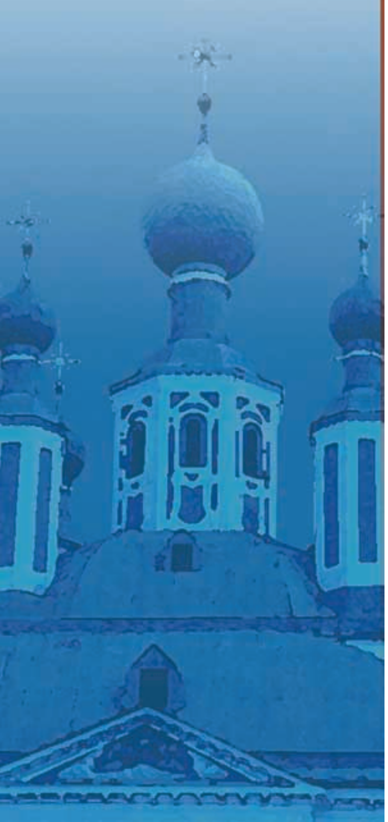
This project constitutes a revolutionary approach to pulsed power that eliminates Marx generators' high voltage switches, oil and water tanks of the conventional Z-pinch drivers. Sandia and the High Current Electronics Institute (HCEI) at Tomsk, Russia are the leaders in developing a new type of very compact, high current, high voltage, voltage adders of short 70-100-ns pulses based on the Linear Transformer Driver (LTD) technology. The salient feature of the new technology is switching and inductively adding the pulses at low voltage straight out of the capacitors through low inductance transfer and ferromagnetic core isolation. High voltage is obtained by inductively adding many stages in series like in our voltage adder–HERMES III–accelerator. MultiMegamp currents can be achieved by connecting many voltage adders in parallel.

This collaborative effort, which started in 2004, involves the development and building of 1-MA, 100-kV, 1-TW LTD stages. Our near-term goal is to build a number of those LTD pulsers, stack them together and test them in a voltage adder configuration similar to that of our HERMES III pulsed power accelerator. Our ultimate goal is to utilize these devices as building blocks for the next generation of Z-pinch drivers.

Although the project has several tasks, there are three that are primary. The first involves the production of a detailed design of the oil-filled LTDZ stage suitable for vacuum tight serial connection in the module. This includes a detailed design of all the support tools needed to assemble and test separate stages, and to install 10 such stages in series into the module. The second involves the fabrication and assemblage of two LTDZ stages, the support tools, trigger and pre-magnetizing systems, air and oil communications for the whole module. The third involves performing electrical tests of the LTDZ stages, measuring and recording critical voltages and currents in the stages. Further optional effort could involve the production, assemblage and testing of some number of additional identical LTDZ stages to be installed into the same module. HCEI shall design and produce the vacuum diode load and the center conductor for tests of the module with matched diode load.







Technical Purpose and Benefits

This project studies transport problem computations in multiple-layer systems of various optical thickness using both space decomposition and decomposition in energy variables. Published mathematical tasks will be used for analysis. Two independent combinations of the two parallelization algorithms are assumed, and the efficiency of combining parallelization in energy groups with parallelization in space will be considered.

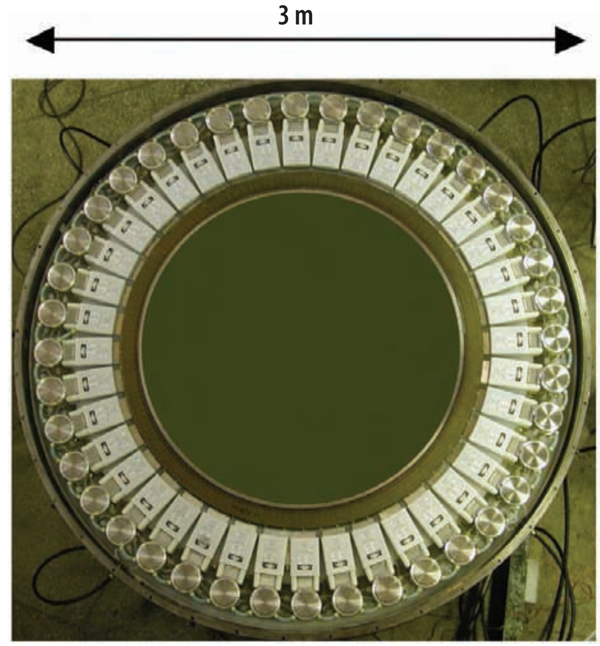


Figure 1. 1-MA, LTD stage top cover removed.

HCEI

Collaboration between Sandia National Laboratories (SNL), Albuquerque, NM, USA, and High Current Electronic Institute (HCEI), Tomsk, Russia.

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Modified for the Web

Measurement of Time Instability (Heterogeneity) of Parallel Computer and Its Impact on Parallel Algorithm Scalability

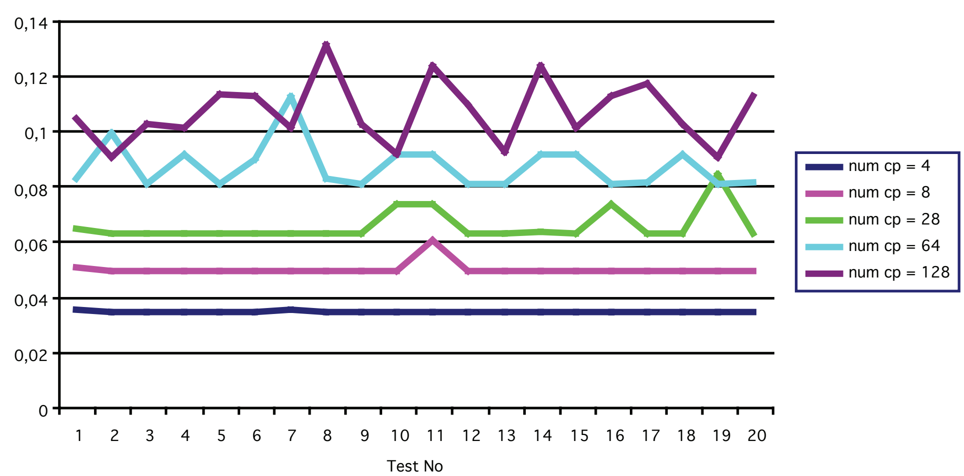
Principal Investigators: Robert Benner (SNL), A.M. Vargin, and Yuri Bartenev (VNIIEF)

Project Description

Timing instabilities diminish the efficiency of supercomputers. Timing instabilities of interest include unequal central processing unit speeds, unequal memory speeds, operating system noise, and message contention on interprocessor interconnects. This project seeks to characterize these timing instabilities though a measurement program. The project will develop a parallel software program to measure and report timing instabilities on a parallel computer, including validation that the program's results are accurate, release of the program as general tool with "open source" license, and publication of a scientific paper.

Six tasks will be performed at the discretion of the Sandia principal investigator. The first three tasks have been completed as of December 2006. The remaining tasks are scheduled for completion by September 2007, with successive tasks being completed at 3 or 4 month intervals:

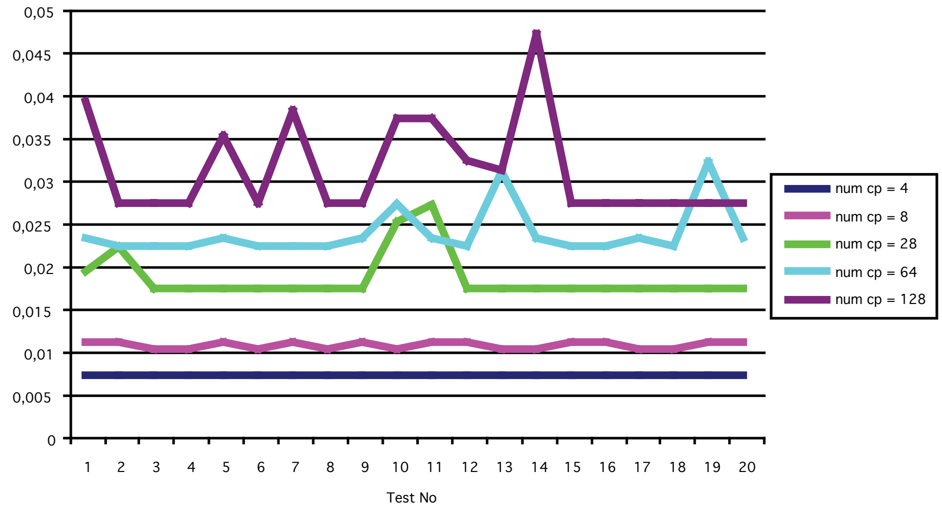
- Development of proposals, project specifications, and prototyping of activities.
- Develop measurers of noise on a single cluster node.
- Develop the measurers of noise on all cluster noted and regular scalable communication operation instability.
- Develop the measurers of cluster regular communication instabilities on algorithms possessing weak scalability degradation, including testing and reduction of tests to a complex with limited shell possibilities and verification on parallel clusters.
- Develop measurers of regular communication instabilities in a part of a cluster in a random communication system load with communication and I/O operations on the side of the other part of the cluster, including testing and reduction of tests to a complex.
- Develop full-value shell and perform complex testing of project. Verify measurer on actual parallel clusters and develop follow-on proposals.



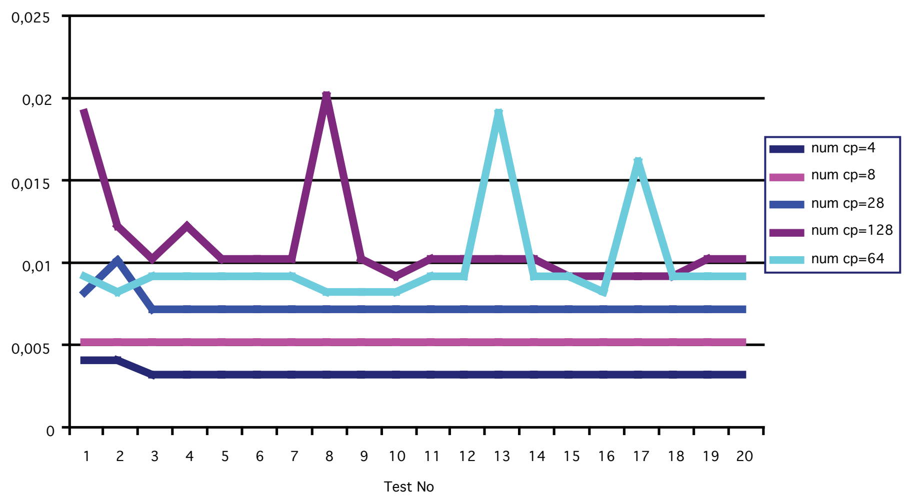
Runtime of solver Bicgstab with preconditioner block Gauss-Seidel.
Approximation template = 7. Number iterations = 1.
Local size of matrix = 1000 rows. Number of calls = 40.

Technical Purpose and Benefits

As a result of this work, the measurement program will run loops on all processors of a supercomputer to identify small timing differences. Then the measurement program will process the data into parameters for a model of timing instabilities. The program can be used in purchasing computers to select those with better timing stability. It can be used as a diagnostic tool for improving hardware and software, and it can help to assess the feasibility of increasing the size of a supercomputer or parallel applications. In particular, the measurement and characterization of operating system noise would lead to improvements in the runtime performance and scalability of these systems as well as future systems and the applications that run on them.



Runtime of function Matvec. Approximation template = 27. Matrix size = 1000 rows. Number of calls = 40.



Runtime of function Matvec. Approximation template = 7. Matrix size = 1000 rows. Number of calls = 40.

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Sandia National Laboratories

Scalability Studies for Simulation Codes Based on Varying Models of Interprocessor Communications

Principal Investigators: Robert Benner (SNL), A.M. Vargin, and Yuri Bartenev (VNIIEF)

Project Description

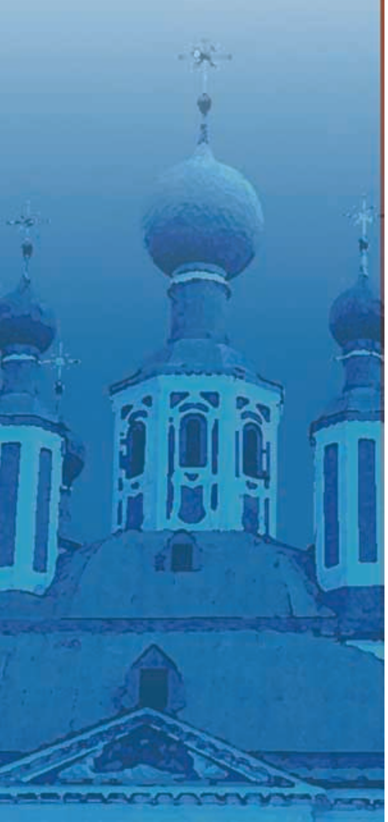
To write supercomputer simulation codes that will run well on future supercomputers, research in this project is directed towards implementing simulation algorithms, with a specific emphasis on interprocessor communications. The effectiveness of interprocessor features for simulation algorithms is evaluated. Models of the subsystems of future supercomputers will determine how well codes will scale up to run on future computers and help to develop codes with minimal degradation in the event of faults. The project focuses on communication features and coordinates with other projects focusing on other features. Existing simulation codes are used in the project.

Seven tasks will be performed at the discretion of the Sandia principal investigator; the first two tasks were completed in early 2006, and the rest are awaiting approval/revision:

- Develop a draft and final project plan, including a statement of the problem, technical issues, approach, research tasks, and duration and level of effort.
- Host meeting for follow-on work and produce meeting notes.
- With regard to the environments with different topologies: (1) develop data exchange algorithms for global exchanges, (2) develop estimates of exchange durations given different mechanisms of data delivery parameterized by the numbers of processing elements, channel bandwidths, and delays, and (3) determine the maximum number of processing elements for certain parameters.
- Investigate scalability (clusterization) variants for multiprocessor environments with different topologies and communication mechanisms, as well as variants for different forms of data exchange and external memory, and investigate communication parameters of the multiprocessor environments.
- Investigate the means of ensuring high multiprocessor environment reliability by adding redundant elements to the basic elements as a fail-safe.
- Determine main design parameters of multiprocessor environments with different topologies and conduct investigations of their hardware complexity.
- Provide final report with final results analysis and proposals for further study.

Technical Purpose and Benefits

Understanding how older and existing codes will run on future supercomputers is necessary because future supercomputers will have greater parallelism and shifts in the nature of some subsystems. Accurate and predictable mathematical models will permit developers to ensure that algorithms will run on petaFLOPS-class supercomputers with perhaps a hundred thousand to a million processors. Algorithms need to be formulated that work, even if processors are faulty or a node is removed, and if possible, they need to be friendly to low-cost, high-performance computers, such as clusters.



Estimation of time complexity for global exchange algorithms

	Environ-ment	Com-muni-cation type	A^1_ω / γ	A^ω_ω / γ	A^S_ω / γ	A^ω_1 / γ	A^T_ω / γ	Note
1	2	3	4	5	6	7	8	9
1	1D	1	$\frac{1}{2}\frac{Q}{V}\omega$ 1	$\frac{1}{2}\frac{Q}{V}\omega$ 1	$\frac{1}{2}\frac{Q}{V}\omega$ 1	$\frac{1}{2}\frac{Q}{V}\omega$ 1	$\frac{1}{2}\frac{Q}{V}\omega^2$ ω	$\gamma = \frac{T(A^i_j)}{T_{\lim}}$
		2	$T_c\omega + \frac{Q}{V}\log\omega$ 1	$T_c\omega^2 + \frac{Q}{V}\omega\log\omega$ logω	$\frac{1}{4}T_c\omega^2 + \frac{Q}{V}\omega$ 1	$\frac{1}{4}T_c\omega^2 + \frac{Q}{V}\omega$ 1	$\frac{1}{8}T_c\omega^3 + \frac{1}{2}\frac{Q}{V}\omega^2$ ω	
		3	$\frac{1}{2}T_c\omega + \frac{Q}{V}$ 1	$\frac{1}{2}T_c\omega^2 + \frac{1}{2}\frac{Q}{V}\omega$ 1	$\frac{1}{8}T_c\omega^2 + \frac{1}{2}\frac{Q}{V}\omega$ 1	$\frac{1}{8}T_c\omega^2 + \frac{1}{2}\frac{Q}{V}\omega$ 1	$\frac{1}{8}T_c\omega^3 + \frac{1}{2}\frac{Q}{V}\omega^2$ ω	
2	2D	1	$\frac{Q}{V}\sqrt{\omega}$	$\frac{1}{2}\frac{Q}{V}\omega$ 2	$\frac{1}{2}\frac{Q}{V}\omega$ 2	$\frac{1}{2}\frac{Q}{V}\omega$ 2	$\frac{1}{2}\frac{Q}{V}\omega^2$ 2ω	
		2	$2T_c\sqrt{\omega} + \frac{Q}{V}\log\omega$	$2T_c\omega + \frac{1}{2}\frac{Q}{V}\omega\log\omega$ 2logω	$K_1T_c + \frac{Q}{V}\omega$ 4	$K_1T_c + \frac{Q}{V}\omega$ 4	$\frac{1}{2}T_c\omega^{\frac{3}{2}} + 2\frac{Q}{V}\omega^{\frac{3}{2}}$ $8\omega^{1/3}$	$K_1 = \frac{1}{4}\omega^{\frac{3}{2}} + \frac{3}{4}\omega + \frac{1}{2}\sqrt{\omega}$
		3	$\frac{1}{4}T_c\omega + \frac{Q}{V}$	$\frac{1}{2}T_c\omega^2 + \frac{1}{2}\frac{Q}{V}\omega$ 2	$\frac{1}{8}T_c\omega^{\frac{3}{2}} + \frac{1}{2}\frac{Q}{V}\omega$ 2	$\frac{1}{8}T_c\omega^{\frac{3}{2}} + \frac{1}{2}\frac{Q}{V}\omega$ 2	$\frac{1}{4}T_c\omega^{\frac{3}{2}} + \frac{Q}{V}\omega^{\frac{3}{2}}$ $4\omega^{1/3}$	

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Sandia National Laboratories

Thermal Decomposition of Polymeric Materials

Principal Investigators: Ken Erickson (SNL), Andrey Sviridov and Vladimir Sirenko (VNIIA)

Project Description

In March 2004, Sandia National Laboratories (SNL) and the All Russian Research Institute of Automatics (VNIIA) initiated a material-science project to study thermal decomposition of polymeric materials pertinent to weapons safety analyses and numerical modeling.

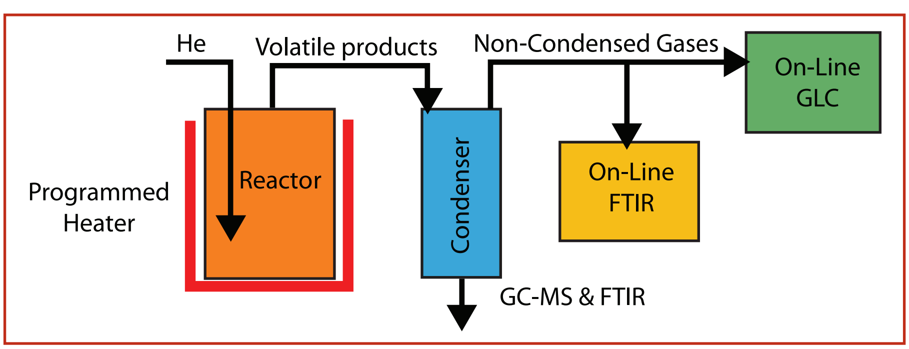
The project includes tasks for both experiments (Tasks 1-3 and Task 7 subtasks) and modeling (Tasks 4, 5, and Task 7 subtask). The initial objectives of the project were to: (1) determine chemical mechanisms and kinetics controlling thermal decomposition of polymers subjected to heating rates between 5ºC/min and 10,000ºC/min and (2) develop submodels for thermal decomposition, based on kinetics and physical properties, which could be incorporated into numerical models for safety analyses. A third objective, agreed to by SNL and VNIIA during FY06 was to develop models for heat transfer and pressure growth caused by thermal decomposition of polymer foams in closed containers in fire environments. (Experimental work is specified in Option Tasks 10 and 11 for FY08. Modeling work is specified in Tasks 8 and 9 authorized in FY07 and Option Task 11 for FY08.)

The project is now in its fourth year and has been primarily funded by Defense Programs (experimental work) and by ASC (modeling work). The first three years of the project were very successful. During FY05, thermal decomposition experiments were completed with epoxies and polyurethanes at heating rates ranging from 5ºC/min to 10,000ºC/min. The materials were similar to, but not identical to, those studied by Erickson et al. at Sandia using complementary techniques. During FY06, experiments were completed that involved quantitative chemical analyses of the solid, liquid, and gas-phase products from constant-temperature decomposition of 20 to 40 gram samples. Joint experiments were done at SNL (April 2006) and VNIIA/Mendeleev Institute (June 2006) involving complementary capabilities. Several low-molecular weight gas-phase products were quantitatively determined, which provided needed data for refining decomposition mechanisms and kinetics. Submodels for decomposition of the materials studied were developed from the experimental data.

The objective of new work in FY07 is to develop models for heat transfer and pressure growth caused by thermal decomposition of polymer foams in closed containers in fire environments. This work has direct application to Directed Stockpile Work's (DSW's) assured safety issues of foam decomposition and pressurization, for which C6 and ASC (PEM) projects currently exist.

Technical Purpose and Benefits

This work will produce submodels that will be useful for determining the chemical reaction mechanisms and kinetics controlling thermal decomposition of selected polymer materials subjected to a large range of relevant heating rates. This work will further produce models for heat transfer and pressure growth caused by thermal decomposition of polymer foams in closed containers in fire environments.



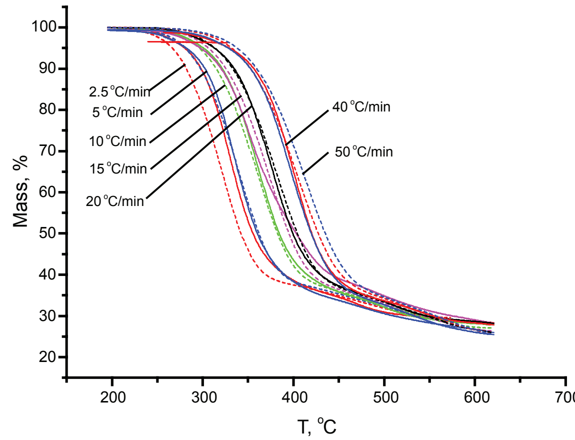
Schematic large sample thermal decomposition.

The project has significantly benefited US/DP, ASC, and the Russian Federation, and the data exchange between laboratories has been mutually beneficial. The project has contributed to quantitative understanding of polymer behavior in accident and fire scenarios. Results have contributed to engineering analyses supporting systems safety and structural vulnerability studies based on accident and fire scenarios. Specific examples include:

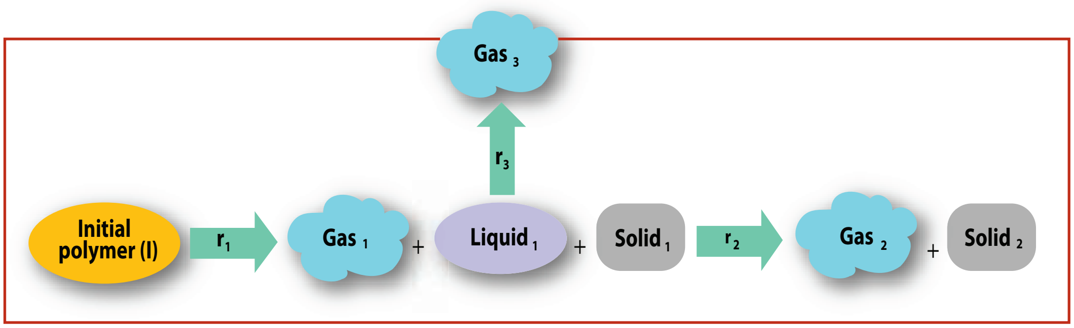
(1) Results from high-heating rate decomposition experiments showed that mechanisms change little below heating rates of about 800 °C/min. This supported theoretical arguments made by Erickson as part of the FY04 Level I V&V milestone, during which the external panel expressed concerns about the effect of heating rate on the adequacy of rate expressions used in the numerical simulations of validation experiments.

(2) From recent work, the quantitative analyses of low-molecular-weight decomposition products will provide input for determining equations-of-state for use with models for predicting pressurization of sealed containers in fire environments.

(3) The decomposition submodels that were developed support engineering analyses for systems safety studies and provide a basis for the new work to develop models for heat transfer and pressure growth caused by thermal decomposition of polymer foams in closed containers in fire environments.



Predicted and experimentally observed mass loss during TGA experiments with polyurethane foam at a variety of heating rates. Solid lines are experimental results, and dotted lines are predicted results.



$d[I]/dT = -r_1/B$;
$d[Solid_1]/dT = (r_1\alpha_1\alpha_2 - r_2)/B$;
$d[Liquid_1]/dT = r_1\alpha_1(1 - \alpha_2)/B - r_3$;
$d[Solid_2]/dT = r_2\beta_1/B$;
$d[Mass]/dT = (-r_1(1 - \alpha_1) - r_2(1 - \beta_1))\ B - r_3$;

where

$B = dT/dt$ = sample heating rate.
t = time
T = sample temperature
$r_1 = k_1{*}\exp(-E_1/(T+273)){*}[I]$
$r_2 = k_2{*}\exp(-E_2/(T+273)){*}[Solid_1]$
$r_3 = B{*}k_3{*}\exp(-E_3/(T+273)){*}[Liquid_1]$,
k_1, k_2, k_3 = pre-exponential multipliers;
E_1, E_2, E_3 = the activation energies, referred to gas constant;
α_1 = mass of ($Solid_1$ + $Liquid_1$) formed per unit mass of initial polymer consumed by r_1
α_2 = mass of $Solid_1$ formed per unit mass of ($Solid_1$ + $Liquid_1$) formed by r_1
β_1 = mass of $Solid_2$ formed per unit mass of solid1 consumed by r_2

For polyurethane foam:

r_1 = decomposition rate of urethane groups with formation of CO_2 (Gas_1), aromatic amines and isocyanates ($Liquid_1$), and secondary polymer ($Solid_1$)
r_2 = decomposition of secondary polymer ($Solid_1$) with formation of H_2O, CO_2, olefines, propylene glycols (Gas_2) and coke ($Solid_2$)
r_3 = rate of evaporation of aromatic amines and isocyanates (Gas_3).

Collaboration between Sandia National Laboratories, Albuquerque, NM, USA, and All Russian Research Institute of Automatics (RFNA-VNIIA), Moscow, Russia

Sandia National Laboratories

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Sandia National Laboratories

Z-Theta Plasma Compression Experiments

Principal Investigators: Kenneth W. Struve (SNL); Pavel Repin and Andrey Orlov (VNIIEF)

Project Description

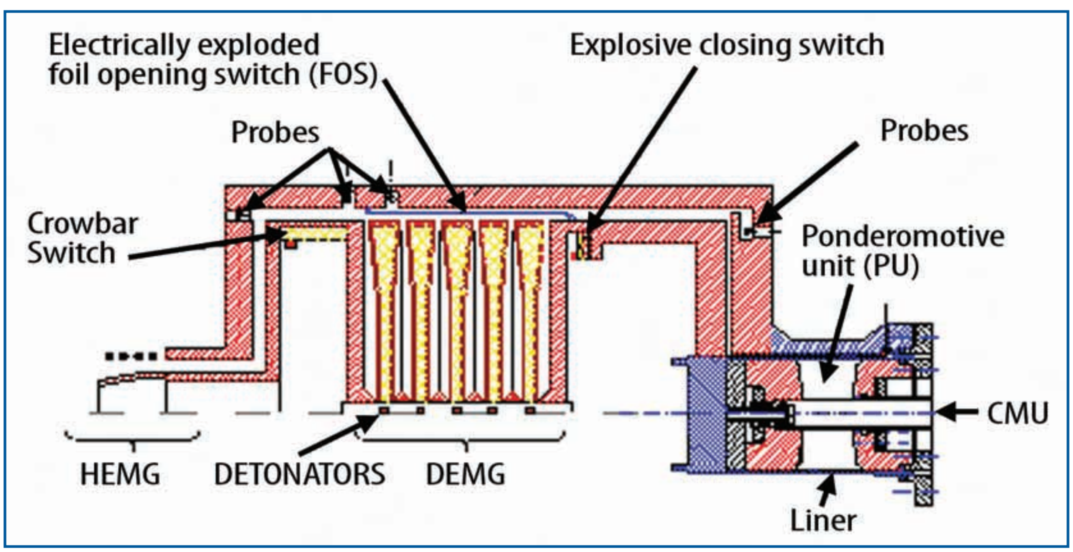
The purpose of this project is to prepare and perform joint U.S.-Russian Z-machine experiments on compression of longitudinal magnetic field using a collapsing z-pinch based on multi-wire arrays.

The possibility of longitudinal magnetic field compression with a hollow gas jet in a z-pinch configuration has been shown experimentally. The longitudinal magnetic field suppresses instabilities in the plasma, which allows radical compression of a liner 15 to 30 times. Similar experiments have been performed at currents with amplitude less than 10MA. At high currents, it is necessary to use liners with higher linear mass, which can be achieved with liners formed from multi-wire arrays. The work should address the question of efficiency of axial magnetic flux compression by plasma liners based on multi-wire arrays. Preliminary calculations show the possibility of obtaining and recording ultra-high magnetic fields (>50 MG).

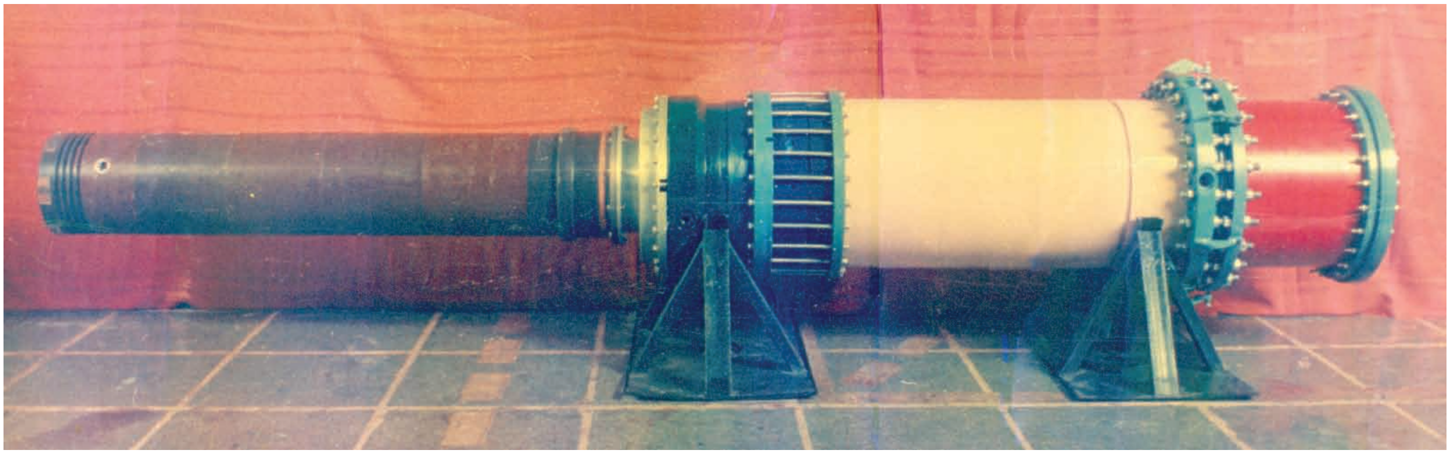
This work will include calculations and theoretical studies, preliminary experiments on the Saturn accelerator at Sandia National Laboratories, explosive generator shots at VNIIEF, and preparation and participation in similar experiments on the Z accelerator at Sandia if experiments in Russia are successful.

Technical Purpose and Benefits

This work evaluates an alternate plasma compression scheme that could lead to record-level magnetic field generation, and which could be a new fusion technique. This is a new effort based on proposals by the group at VNIIEF. It is expected that this effort will also relate to work on explosive generators at VNIIEF, and provide insight on Russian explosive generator technology. NNSA benefits by allowing the evaluation of a promising alternate plasma compression scheme for similar efforts, before committing resources and time on U.S. accelerators. Sandia researchers benefit by learning experimental techniques and plasma compression schemes from the Russians that broaden their capabilities and focus in an area of specific fusion expertise. The Russian experiments provide unique, complementary approaches to high-current z-pinch driver.



Russian Electromagnetic Pulse Generator



Russian Electromagnetic Pulse Generator

Collaboration between Sandia National Laboratories (SNL), Albuquerque, NM, and the Russian Federal Nuclear Center – All Russian Research Institute of Experimental Physics (RFNC-VNIIEF), Sarov, Russia

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