Summary of LLNL Russian Projects

O. Schilling

January 22, 2007
Disclaimer

This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor the University of California nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or the University of California, and shall not be used for advertising or product endorsement purposes.

This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.
Project: Development and Study of a Method Adaptive in Angle Variables for Solving 2D Transport Equation

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

Contract Number: B526462

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, the 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 multi-dimensional 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).

Technical Purpose and Benefits

The simulation of multi-dimensional 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. However, 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.
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”.

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

Contact Information:

Howard A. Scott
Lawrence Livermore National Laboratory
P. O. Box 808, L-18
Livermore, CA 94550
925 423-1530 (phone)
925 422-5112 (fax)
E-mail: hascott@llnl.gov

Alexander V. Alexeev
Russian Federal Nuclear Center—All Russian Research Institute of Experimental Physics
Mira Avenue, 37
Sarov, Nizhnyi Novgorod Region
607190, Russia
831 30-42912 (phone)
831 30- 54565 (fax)
E-mail: gichuk@md08.vniief.ru
Project: Analytical Solutions to Test Computer Codes Simulating Gas Dynamics and Radiation Transport Problems in Different Approximations

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

Contract Number: B513835

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 problems 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.

Technical Purpose and Benefits

Physical processes in space and time are described by systems of multi-dimensional 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.
Temperature profile at $ct = 0.8$ for an analytical multi-group radiation transport problem.

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

Contact Information:

Howard A. Scott
Lawrence Livermore National Laboratory
P. O. Box 808, L-18
Livermore, CA 94550
925 423-1530 (phone)
925 422-5112 (fax)
E-mail: hascott@llnl.gov

Dmitry N. Bokov
Russian Federal Nuclear Center—All Russian Research Institute of Technical Physics
P.O. Box 245
Snezhinsk, Chelyabinsk region
456770, Russia
351 72-547-30 (phone)
351 72-551-18 (fax)
E-mail: d.n.bokov@vniitf.ru
**Project:** Molecular Dynamics Simulation of Elastic-Plastic and Spall Mechanisms in Cu when Dynamic Loading

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

**Contract Number:** B541414

**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 were 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 pulse. The spall simulations used randomly distributed nano-particles (at least one near the spall plane) with radius 1 and 2 nm. The nano-particles were simulated with the same potential, but changing the mass of the atoms. Two masses were considered: carbon-like and lead-like atoms.

**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 nano-particles act as stress concentrators, significantly decreasing the spall strength. All of these contribute to the development and validation of improved constitutive models for shock-loaded polycrystalline materials.
Molecular dynamics simulation showing a shock-grain boundary (GB) interaction. The blue arrow shows the shock propagation direction.

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.

Contact Information:

Eduardo M. Bringa  
Lawrence Livermore National Laboratory  
P. O. Box 808, L-367  
Livermore, CA 94550  
925 423-5724 (phone)  
925 423-0785 (fax)  
E-mail: bringa1@llnl.gov

Vladimir V. Dryomov  
Russian Federal Nuclear Center—All Russian Research Institute of Technical Physics  
P.O. Box 245  
Snezhinsk, Chelyabinsk region  
456770, Russia  
351 723-2930 (phone)  
351 723-2919 (fax)  
E-mail: v.v.dryomov@vniitf.ru
Project: Development and Study of a Method Adaptive in Energy Variables for Solving the Radiation Transport Equation

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

Contract Number: B541415

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. As 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.

Technical Purpose and Benefits

The simulation of multi-dimensional 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. However, 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.
Absorption coefficient vs. energy in the three regions of the test problem.
Project: Multifunctional Shock Tube Experimental Investigation of Gravitational Instabilities Evolution

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

Contract Number: B533350

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 non-stationary 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 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.

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 non-stationary 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.
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.

Contact Information:

Oleg Schilling  
Lawrence Livermore National Laboratory  
P. O. Box 808, L-23  
Livermore, CA 94550  
925 423-6879 (phone)  
925 423-0925 (fax)  
E-mail: schilling1@llnl.gov

Yury A. Kucherenko  
Russian Federal Nuclear Center—All Russian Research Institute of Technical Physics  
P.O. Box 245  
Snezhinsk, Chelyabinsk region  
456770, Russia  
351 72 511-38 (phone)  
351 72 320-77 (fax)  
E-mail: kucherenko@five.ch70.chel.su
Project: The ACT-Electronic Project—Quantum Mechanical Simulation of Actinides

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

Contract Number: B541413

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 \( (T = 300 \text{ K}) \) 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\(_3\)Al, Pu\(_3\)Ga, and Pu\(_3\)In 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.

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 such as Physical Review Letters and Physics Letters B.
Simple Picture derived from the spectroscopic analysis

Result of non-magnetic calculation, including spin-orbit in the Pu 5f’s

Result of antiferromagnetic calculation, including spin-orbit in the Pu 5f’s

Contact Information:

James G. Tobin
Lawrence Livermore National Laboratory
P. O. Box 808, L-23
Livermore, CA 94550
925 422-7247 (phone)
925 423-7040 (fax)
E-mail: tobin1@llnl.gov

Andrey L. Kutepov
Russian Federal Nuclear Center—All Russian Research Institute of Technical Physics
P.O. Box 245
Snezhinsk, Chelyabinsk region
456770, Russia
351 723-2930 (phone)
351 723-2919 (fax)
E-mail: A.L.Kutepov@vniitf.ru
Project: Monte Carlo Input Translators and Generator

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

Contract Number: B533364

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 was 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.

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

Contact Information:

Kenneth E. Sale  
Lawrence Livermore National Laboratory 
P. O. Box 808, L-186  
Livermore, CA  94550  
925 423-0686 (phone)  
925 423-2759 (fax)  
E-mail: sale1@llnl.gov

Dmitry Mogilenskikh  
Strela  
U1, 13 Vasilyeva  
Snezhinsk, Chelyabinsk region  
456770, Russia  
351 723-2930 (phone)  
351 723-2919 (fax)  
E-mail: d.v.mogilenskikh@strela.snz.ru
Project: Vanadium Dynamic Strength Measurements

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

Contract Number: B539547

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 $10^5$ 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.

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 $10^5$–$10^6$ 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 which accurately represent the physics.
Simulated evolution of the Rayleigh–Taylor instability.

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

Contact Information:

Patrick O. Egan
Lawrence Livermore National Laboratory
P. O. Box 808, L-97
Livermore, CA 94550
925 423-5144 (phone)
925 422-0779 (fax)
E-mail: egan1@llnl.gov

Victor A. Raevsky
Russian Federal Nuclear Center—All Russian Research Institute of Experimental Physics
Mira Avenue, 37
Sarov, Nizhnyi Novgorod Region
607190, Russia
831 304-5009 (phone)
831 304-4558 (fax)
E-mail: root@gdd.vniief.ru
**Project:** Mesh Refinement and Reconnection in Arbitrary Polyhedral Free-Lagrangian Hydrodynamics Simulations

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

**Contract Number:** B530330

**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-Lagrangian 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 an Eulerian scheme.

A mesh refinement and coarsening algorithm was developed in a three-dimensional free-Lagrangian 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.

**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-Lagrangian 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.
The cube rotation problem: at the latest time, the number of zones is 3500 compared to 125 zones initially.

Contact Information:

Douglas S. Miller
Lawrence Livermore National Laboratory
P. O. Box 808, L-38
Livermore, CA 94550
925 424-4738 (phone)
925 423-9208 (fax)
E-mail: miller18@llnl.gov

Vera Rasskazova
Russian Federal Nuclear Center—All Russian Research Institute of Experimental Physics
Mira Avenue, 37
Sarov, Nizhnyi Novgorod Region
607190, Russia
831 30-40995 (phone)
831 30-53808 (fax)
E-mail: rassvv@md08.vniief.ru
Project: Structured/Unstructured Hybrid Mesh Hydrodynamics and Heat Conduction Studies

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

Contract Number: B541416

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 conveniently 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.

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 exact and numerical solutions on grid 8.

Contact Information:

Howard A. Scott
Lawrence Livermore National Laboratory
P. O. Box 808, L-18
Livermore, CA 94550
925 423-1530 (phone)
925 422-5112 (fax)
E-mail: hascott@llnl.gov

Sergei I. Skrypnik
Russian Federal Nuclear Center—All Russian Research Institute of Experimental Physics
Mira Avenue, 37
Sarov, Nizhnyi Novgorod Region
607190, Russia
831 30-40995 (phone)
831 30-53808 (fax)
E-mail: ssi@vniief.ru
Project: Russian-US Workshop on Fundamentals of Pu Science

Collaboration between the Lawrence Livermore National Laboratory (LLNL), Livermore, CA and Los Alamos National Laboratory (LANL), Los Alamos, NM, and the Rosatom Laboratories, VNIITF, VNIIEF, and VNIINM

Conference Organizers: Michael Fluss (LLNL), Sigfried Hecker (prior to 2006) and Luis Morales (LANL), Boris Nadykto (VNIIEF), Lidia Timofeeva (VNIINM), Alexander V. Petrovtsev (VNIITF)

Project Description

The first Russian-US Workshop on Fundamentals of Pu Science was held in 2001 at VNIIEF, Sarov, Russia. Sig Hecker (LANL) and Boris Nadykto (VNIIEF) were the organizers. Subsequently, the participation in this workshop was expanded to include scientists from three Rosatom Laboratories (VNIITF, VNIIEF, and VNIINM) and two NNSA Laboratories (LLNL and LANL). Both LLNL and LANL have underwritten these meetings when held in the US. The Rosatom Laboratories have also provided underwriting for the meetings held in Russia. The program consists of oral papers amplified by several poster sessions. Considerable time is provided for discussions both in a formal setting and informally as well. Each workshop results in a book of extended abstracts in both English and Russian, which serves to document the meetings and provide for further interactions during the following year. The host Laboratory provides for simultaneous or sequential translations during presentations, and makes available interpreters during the poster sessions.

Technical Purpose and Benefits

Workshop photos from 2002, 2004, and 2005 showing the increasing attendance of both Russian and US scientists.
These meetings have broadened the understanding of the nature and focus of Russian research into the fundamental properties of plutonium and plutonium alloys. The workshops permit specialists to compare ideas and approaches and receive unique critical evaluation from experts in their respective fields. The participating Laboratories have utilized these annual meetings to strengthen and to initiate new relationships with many of the participating Russian scientists. The program topics cover subjects in the areas of radiation damage in plutonium, plutonium phase diagrams and phase stability, and the fundamental physical properties of plutonium such as electronic structure, magnetism, and heat capacity.

History of Meetings

2001 Sarov
2002 Sarov
2003 LANL, held in conjunction with the Plutonium Futures International Conference, 2003, Albuquerque, NM
2004 Sarov
2005 Snezhinsk
2006 LLNL, held in conjunction with the Plutonium Futures International Conference, 2006, Pacific Grove, CA.
2007 Planned for Sarov

While the attendance at the early meetings was modest, the most recent meetings have involved over one hundred scientists from the five laboratories. Figure 1 shows the Workshop photographs from the 2002, 2004, and 2005 meetings. Note the increase in participants. The Sixth Workshop (see Figure 2) held at LLNL continued this trend and provided amplification for focused topics discussed earlier in the week at the International Conference, Pu Futures—The Science, 2006 in Pacific Grove, CA.