Sandia National Laboratories (SNL)
Current Projects with the Russian Federation

Project Title:	Development of Models of Energy Transfer in Nanostructured Materials.
Russian Institute:	Institute for Problems in Mechanical Engineering, Russian Academy of Sciences (IPME RAS), St. Petersburg.
Brief Description:	To develop modeling approaches and simulations to examine energy transport and transfer in materials with structural features at the nanoscale. Tasks include developing such a model for thin crystal structures subjected to short duration laser excitation, and using atomic-scale simulations to evaluate microscopic expressions for stress and heat flux in crystals containing defects such as vacancies, dislocations and bi-material interfaces.
Purpose of Work/Research:	This research benefits Sandia's interest in designing energy storage and generation materials, and provides insight on the unique behavior at small scales that will be vital in future technologies.
Publications or Papers Presented:	1. V.A. Kuzkin, A.M. Krivtsov, "Equivalent thermo-mechanical parameters for perfect crystals," *IUTAM Symposium on the Vibration Analysis of Structures with Uncertainties*, Vol. 27, pp. 403– 416 (2011), http://dx.doi.org/10.1007/978-94-007-0289-9 2. V.A. Kuzkin, A.M. Krivtsov, R.E. Jones, J.A. Zimmerman, "Equivalent stress tensor for discrete systems: problems and solutions", in preparation (2012).
Project Principal Investigators:	Jonathan Zimmerman, (SNL). Alexander K. Belyaev, (IPME RAS).

Project Title:	Molecular Dynamics Estimates of Thermal Conductivity of Semiconductors
Russian Institute:	All-Russian Research Institute of Experimental Physics (VNIIEF), Sarov
Brief Description:	Thermal conductivity of semiconductor materials has a significant influence on their performance in electronic devices. The thermal conductivity is, in large part, mediated by lattice vibrations, as opposed to the flow of electrons. Molecular dynamics (MD), a computational technique well suited to representing phonons and scatterers of phonons (such as point defects and free surfaces), is the primary computational tool being developed and used in this research. Graphene has become a material of great technological interest due to its unique electrical and thermal properties.
Purpose of Work/Research:	The thermal characteristics of graphene and other 2D structures are of great interest to the developing graphene electronics industry. Graphene as an electronic material has many unique advantages but its ability to dissipate waste heat is a crucial consideration. This work will characterize the thermal conductance of graphene as a function of number of layers, interlayer bonding, etc., in order to facilitate the application of this novel material.
Publications or Papers Presented:	A.A. Seleznev, A.Yu. Aleynikov, P.V. Ermakov, N.S. Ganchuk, S.N. Ganchuk, R. Jones, "Molecular dynamics calculation of the thermal conductivity coefficient of the Germanium single crystal," *Physics of the Solid State*, **54**, 462–467 (2012).
Project Principal Investigators:	Reese Jones, (SNL). Alexander A. Seleznev (VNIIEF).

Project Title:	Application of Models for Chemical Material Damage
Russian Institute:	Institute for Problems in Mechanical Engineering, Russian Academy of Sciences (IPME RAS), St. Petersburg
Brief Description:	Mechano-chemistry is at the heart of many processes important to the national laboratories. Specifically, oxidation, corrosion and infiltration by molecular gases can greatly enhance fracture and failure of structural metal parts.
Purpose of Work/Research:	This work is focused on well-founded models of stress-assisted corrosion. This research will help us model the shape and mobility of corrosion fronts in order to prevent component failure
Publications or Papers Presented:	1. E.N. Vilchevskaya, I.K. Korolev, A.B. Freidin, "On phase transitions in the domain of material inhomogeneity. II. Interaction between a crack and an inclusion undergoing phase transition," *Mechanics of Solids*, **46**, pp. 683-691 (2011), http://dx.doi.org/10.3103/S0025654411050049 2. A.B. Freidin, "Modeling of kinetics of phase and chemical transformations in deformable solids," *Herald of the Lobachevsky University of Nizniy Novgorod*, 2011. Special issue, No. 4(5) (in Russian, the issue devoted to the 10th All-Russian Congress on Fundamental Problems of Theoretical and Applied Mechanics). 3. A.B. Freidin, E.N. Vilchevskaya, "Stress-assist chemical reactions front propagation in axially symmetric problems," *Int. J. Engineering Sci*., in review (2012). 4. A.B. Freidin, "On a chemical affinity tensor and chemical reactions front propagation in elastic solids," *Doklady Physics*, to appear (2012). 5. E.N. Vilchevskaya, I.K. Korolev, A.B. Freidin, "On chemical reactions front propagation in elastic solids," *Doklady Physics*, to appear (2012). 6. E. Vilchevskaya, A.B. Freidin, I.K. Korolev, "Surface Chemical Reactions Kinetics in Elastic Solids," to be presented at the 8th European Solid Mechanics Conference, July 9-13, 2012, Graz, Austria, http://www.esmc2012.tugraz.at/

7. A.B. Freidin, E.N. Vilchevskaya, I.K. Korolev, D.O. Volkova, “On Kinetics of Interface Boundaries and Chemical Reactions Fronts in Elastic Solids,” to be presented at the 8th European Solid Mechanics Conference , July 9-13, 2012, Graz, Austria, http://www.esmc2012.tugraz.at/

Project Principal Investigators: Reese Jones, (SNL).
Alexander B. Freidin, (IPME RAS).

Project Title:	Extending Non-Equilibrium Molecular Dynamics Simulation to Model Extreme States of Matter
Russian Institute:	Joint Institute for High Temperature, Russian Academy of Sciences (JIHT RAS), Moscow (http://jiht.ru/en/)
Brief Description:	The goal of this project is to establish theory and develop methods for applying Non-Equilibrium Molecular Dynamics to study shock deformation of solids, non-ideal warm dense matter, electrical behavior of new devices, and electrical response of materials to radiation. This project is a continuation of a collaboration begun in September 2006, since which time the JIHT team has developed connections with Sandia staff who pursue computational modeling of material response under high pressure or high energy loading conditions. Recent efforts have been on collaborative efforts to characterize JIHT results in MD-based simulations of diffusion, which was recognized at Sandia as anomalous diffusion, a topic of active basic theoretical research at Sandia..
Purpose of Work/Research:	Resulting methods facilitate understanding of a wide variety of shockwave, high energy density physics phenomena, and radiation effects. Additionally, JIHT's demonstrated applications of these methods are themselves scientific investigations in these same subject areas.
Publications or Papers Presented:	1. I.V. Morozov, I.A. Valuev. "Improvement of Wave Packet Molecular Dynamics using Packet Splitting," *Contributions to Plasma Physics*, **52**, 140–144, 2012, http://dx.doi.org/10.1002/ctpp.201100105 2. I.V. Morozov, I.A. Valuev, "Application of the Wave Packet Molecular Dynamics to Simulation of Nonideal Plasmas at Moderate Temperatures," International Conference on Strongly Coupled Coulomb Systems, Budapest, Hungary, July 24-29, 2011, http://www.sccs2011.net(oral presentation). 3. I.V. Morozov, I.A. Valuev, "Simulations of Nonideal Plasmas by the Method of Split Wave Packet Molecular Dynamics," Scientific-Coordination Session on "Non-ideal Plasma Research", Moscow, Russia, November 23-24, 2011, http://www.ihed.ras.ru/npp2011(oral presentation).

4. N.A. Kazeev, I.V. Morozov, "Solution of the Equations of Motion with Variable Time Step in the Method of Wave Packet Molecular Dynamics," 54th Scientific Conference of Moscow Institute of Physics and Technology, Dolgoprudny, Moscow Region, Russia, November 25-26, 2011, http://mipt.ru/nauka/54conf (oral presentation).

5. I.V. Morozov, S.G. Semenov, "Effective Implementation of Complex Error Function for the Method of Wave Packet Molecular Dynamics," 54th Scientific Conference of Moscow Institute of Physics and Technology, Dolgoprudny, Moscow Region, Russia, November 25-26, 2011, http://mipt.ru/nauka/54conf(oral presentation).

6. I.V. Morozov, I.A. Valuev, "The Method of Molecular Dynamics with Wave Packet Splitting for Simulation of Electron-Ion Nonideal Plasmas," XXXIX Zvenigorod International Conference On Plasma Physics And Controlled Fusion, Zvenigorod, Russia, February 6–10, 2012, http://www.fpl.gpi.ru/Zvenigorod/XXXIX/Zven_XXXIX_e.html (oral presentation).

7. I.V. Morozov, I.A. Valuev, "Improvement of Wave Packet Molecular Dynamics using Packet Splitting," // XXVII International Conference on Equations of State for Matter, Elbrus, Kabardino-Balkaria, Russia, March 1-6, 2012, http://www.ihed.ras.ru/elbrus12 (oral presentation).

8. S.V. Starikov, V.V. Stegailov, G.E. Norman, V.E. Fortov, M. Ishino, M. Tanaka, N. Hasegawa, M. Nishikino, T. Ohba, T. Kaihori, E. Ochi, T. Imazono, T. Kavachi, S. Tamotsu, T.A. Pikuz, I.Yu. Skobelev, A.Ya. Faenov, "Laser ablation of gold: Experiment and atomistic simulation," *JETP Letters*, **93**, 642–647, http://dx.doi.org/10.1134/S0021364011110129

9. G.E. Norman, S.V. Starikov, V.V. Stegailov, "Atomistic modelling of laser ablation of gold: effect of electron pressure relaxation," *JETP Letters*, **114**, April 2012 (in press), http://www.jetp.ac.ru/cgi-bin/r/index/r/141/4/38910?a=list

10. G. Norman, S. Starikov, V. Stegailov, V. Fortov, I. Skobelev, T. Pikuz, A. Faenov, S. Tamotsu, Y. Kato, M. Ishino, M. Tanaka et al., "Nanomodification of gold surface by picosecond soft X- ray laser pulse," *J. Appl. Phys.* (in review, 2012).

11. P.A.Zhilyaev, V.V.Stegailov, "Ab-initio molecular dynamics: perspectives of multi-CPU and hybrid supercomputers deployment," *Numerical Methods and Programming* (in press) http://num-meth.srcc.msu.su/english/index.html

12. S.V. Starikov, G.E. Norman,V.V. Stegailov, "Atomistic simulation of laser ablation of gold films," XXVI International Conference on Interaction of Intense Energy Fluxes with Matter, Elbrus, Kabardino-Balkaria, Russia, March 1–6, 2011 (oral presentation).

13. V.V.Stegailov, S.V. Starikov: "Atomistic simulation of laser ablation in gold: the influence of electronic excitation on mechanical properties," 9th Workshop "Complex systems of charged particles and their interaction with electromagnetic radiation," Moscow, Presidium RAS, April 13–14, 2011 (oral presentation).

14. S.V. Starikov, V.V. Stegailov, G.E. Norman, "Atomistic simulation of laser ablation of gold: the effects of electronic pressure," International Workshop on Warm Dense Matter 2011 (WDM2011), Pacific Grove, CA, USA, June 5–8, 2011 (oral presentation).

15. G.E. Norman, S.Yu. Skobelev, V.V. Stegailov, "Excited states of warm dense matter," International Workshop on Warm Dense Matter 2011 (WDM2011), Pacific Grove, CA, USA, June 5–8, 2011 (poster presentation).

16. V.V. Stegailov, S.V. Starikov, G.E. Norman, "Atomistic simulation of laser ablation of gold: the 7effects of electronic pressure," The 2011 APS Conference on Shock Compression of Condensed Matter (SCCM2011), Chicago, IL, USA, June 26–July 1, 2011 (oral presentation).

17. S.V. Starikov, V.V. Stegailov, G.E. Norman, O.V. Sergeev, P.A. Zhilyaev, "Ab initio study of mechanic, thermodynamic and transport properties of gold after electronic excitation," The 2011 APS Conference on Shock Compression of Condensed Matter (SCCM2011), Chicago, IL, USA, June 26–July 1, 2011 (oral presentation).

18. P.A. Zhilyaev, V.V. Stegailov, "First-principles conductivity calculations for metal with hot electrons," 54th Scientific conference of Moscow Institute of Physics and Technology, Dolgoprudny, Moscow Region, Russia, November 25–26, 2011 (oral presentation).

Project Principal Investigators: John Aidun, (SNL).
Genri E. Norman, (JIHT RAS).

Project Title: International Shock Wave Database (ISWdb)

Russian Institute: Joint Institute for High Temperatures, Russian Academy of Sciences (JIHT/RAS), Moscow (http://jiht.ru/en/).

Brief Description: This project aims to develop an on-line, unclassified database of shock-wave experimental data and associated models and analysis tools as an open resource to the international shockwave and high-pressure physics communities. It builds on the experience of the principal investigator and the project team in collecting data and producing the RusBank on-line database (http://www.ficp.ac.ru/rusbank).

Purpose of Work/Research: The purpose of this activity is to make available thermodynamic and mechanical properties of materials under conditions of shock -wave and other dynamic loadings, selected related quantities of interest, and the meta-data that describes the provenance of the experimental measurements and material models through an open, web- based interface. The database, which will be installed on two, mirrored internet servers (one in Russia and the other in the U.S.), will be a resource to the international shock-wave and high pressure physics communities, free for non-commercial use. The goal is for the experimentalist to both use the database and to contribute to their archival and new unclassified data, on an on-going basis.

Publications or Papers Presented:

P.R. Levashov, I.V. Lomonosov, J.B. Aidun, *International Shock-Wave Database Project: Report of the Requirements Workshop*, Sandia Technical Report, SAND2012-1888 (2012).

I.V. Lomonosov, K.V. Khishchenko, P.R. Levashov, D.V. Minakov, A.S. Zakharenkov, J.B. Aidun, "International shock-Wave data base," 9th New Models and Hydrocodes for shock Wave Processes, London, UK, April 23-27, 2012. http://www3.imperial.ac.uk/shockphysics/nmh (oral presentation).

Project Principal Investigators: John Aidun, (SNL).
Igor V. Lomonosov, (JIHT RAS).

Project Title:	Thermally-Driven Foam Decomposition and Container Pressurization
Russian Institute:	All-Russian Institute of Automatics (VNIIA), Moscow (http://vniia.ru/eng/)
Brief Description:	The purpose of this research is to demonstrate and evaluate advanced computational tools for analysis of this thermally-driven foam decomposition and its effect on pressurization of sealed containers.
Purpose of Work/Research:	Previous research enabled collaborative work that determined the mechanisms and kinetics for decomposition of polyurethane and epoxy foams. Those results provide the foundation of the current research, in which alternative approaches to modeling these complex phenomena will be evaluated.
Publications or Papers Presented:	**1.** V.S. Sirenko, R.A. Koslovskiy, E.I. Popova, S.G. Mulyashow, K.L. Erickson, "Use of Multiple Experimental Techniques to Study Thermal Decomposition of Polyurethane Foam," *Proceedings of SAMPE 2007*, Baltimore, MD, June 2007. **2.** K.L. Erickson, A. B. Dodd, E. C. Quintana, "Physical Behavior and Container Pressurization During Thermal Decomposition of Polyurethane Foams," *Proceedings of the 22nd Annual Conference on Recent Advances in Flame Retardancy of Polymeric Materials*, Stanford, CT, 23-25 May 2011, ISBN: 978-1-61839-469-9. **3.** K.L. Erickson, A. B. Dodd, R. E. Hogan, K.J. Dowding, "Heat Transfer, Foam Decomposition, and Container Pressurization: Comparison of Experimental and Modeling Results," *Proceedings of Interflam 2010: 12th International Conference on Fire Science and Engineering*, Nottingham, UK, 5-7 July 2010, pp. 521-532, ISBN: 978-0-9556548-7-9. **4.** K.L. Erickson, A. B. Dodd, R. E. Hogan, "Modeling Pressurization Caused by Thermal Decomposition of Highly Charring Foam in Sealed Containers," *Proceedings of BCC 2010*, Stamford, CT, 24-26, May 2010, ISBN: 9781617823282.
Project Principal Investigators:	Roy Hogan and Amanda Dodd, (SNL). Andrey S. Sviridov, (VNIIA).

Project Title:	Scalability of Hybrid Processor Systems
Russian Institute:	All-Russian Research Institute of Experimental Physics (VNIIEF), Sarov (http://en.vniief.ru/)
Brief Description:	Modern computer systems are characterized by increasing numbers of processing elements and increasing architectural complexity. The particular focus, as the drive towards the Exascale era proceeds, is hybrid systems composed of universal processors (MIMD components) and arithmetic accelerators (SIMD components). This work will model the efficiency/scalability of such systems, as well as propose and develop methods for improving the efficiency. Methods that will be examined include application-specific environments, reconfigurable processing elements (e.g., FPGAs), and recursive applications of the MIMD, SIMD and reconfigurable components.
Purpose of Work/Research:	The objective of this research is to quantify the effect of diverse hybrid node architectures upon supercomputer application performance.
Publications or Papers Presented:	One goal of this project is to complete and publish a book, tentatively titled "Scalability Studies for Simulation Codes Based on Varying Models of Interprocessor Communications," in English and Russian, based on this research.
Project Principal Investigators:	Robert Benner, (SNL). Sergey A. Stepanenko, (VNIIEF).

Project Title:	Implementation, Study, and Tests of 3D Computational Schemes for MHD Equations in Lagrangian-Eulerian Variables for Multi-Component Compressible Materials
Russian Institute:	All-Russian Research Institute of Experimental Physics (VNIIEF), Sarov (http://en.vniief.ru/)
Brief Description:	The numerical simulation of multi-material compressible magneto hydrodynamic (MHD) flows in the ALE (Arbitrary Lagrangian-Eulerian) framework is associated with several challenges. In particular, there is the difficulty of assigning hydrodynamic and magnetic parameters of the separate materials in a mixed cell. A second difficulty is associated with accurate solution of the equations of advection and diffusion. Many issues remain open regarding the relation of different modeling approaches for these problems.
Purpose of Work/Research:	The comparison of algorithms on well-codified test problems provides a defensible basis for evaluating the different models. This project describes in detail the numerical methods used to solve equations of 3D heterogeneous compressible MHD flows in Lagrangian-Eulerian variables, conducts quantitative analysis of the these codes, and develops new problems for multi-material MHD flows.
Publications or Papers Presented:	This project is new in FY12, so there are no publications yet. The result of previous collaboration examining multi-component hydrodynamics resulted in the publication: Yuriy.V. Yanilkin, E.A. Goncharov, V.Yu. Kolobyanin, V.V. Sadchikov, J.R. Kamm, M.J. Shashkov, W.J. Rider "Multi-Material Pressure Relaxation Methods for Lagrangian Hydrodynamics" *Computers and Fluids* (in review, 2012).
Project Principal Investigators:	Allen C. Robinson, John H. Niederhaus, and James R. Kamm, (SNL). Yuriy V. Yanilkin, (VNIIEF).