Title:

**MULTISCALE SCIENCE FOR SCIENCE-
BASED
STOCKPILE STEWARDSHIP**

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Multiscale Science for Science-Based Stockpile Stewardship (LDRD Project 97601)

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Abstract

This is the final report of a three-year, Laboratory-Directed Research and Development (LDRD) project at the Los Alamos National Laboratory (LANL). The goal of this project has been to develop and apply the methods of multiscale science to the problems of fluid and material mixing due to instability and turbulence, and of materials characterization. Our specific focus has been on the SBSS (science-based stockpile stewardship) issue of assessing the performance of a weapons with off-design, aged, or remanufactured components in the absence of full-scale testing. Our products are physics models, based on microphysical principles and parameters, and suitable for implementation in the large scale design and assessment codes used in the nuclear weapons program.

Background and Research Objectives

Essentially all of the US stockpile has been designed using simulation programs that combine physics and phenomenological models. This approach has been very successful when the nuclear test program was operating to support the phenomenological models and to provide full system testing. With the cessation of testing, the country has adopted a strategy of improving the predictability of the design codes by enhancing the fidelity of the physics models through a combination of theory and small scale experiments; this strategy is termed SBSS (science-based stockpile stewardship). Even though there are presently no new-design weapons systems being designed, a predictive capability is considered essential to understand the possible consequences of aging of materials, remanufacture of key components, etc., on performance and safety.

One longstanding issue in nuclear design is the role of fluid instability and turbulence leading to material mix. A second longstanding issue is the formulation of constitutive models for solid dynamic behavior, including brittle and ductile fracture, friction, plasticity, etc.

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The underlying physical phenomena occur at length and time scales that are much too small to be resolved in the design codes. Thus one is forced to introduce models to represent the effects of the unresolved physical processes. In these terms, our research objective is to develop a scalable theory based on the microscopic physics, whose parameters can be rigorously related to the resolved scales of the simulation.

Importance to LANL's Science and Technology Base and National R&D Needs

Stockpile stewardship is a core mission of LANL; our project attempts to bridge the gap between fundamental research and practical implementation of results into the design tools. The problems that we focus on---turbulence, fluid instability, and material characterization---have a fundamental character that makes them interesting to the broad scientific community, and at the same time represent issues of great concern to the nuclear weapons program. Our ability to publish some of our results in the open literature gives added credibility to the strength of the parts of the program that must remain classified.

Scientific Approach and Accomplishments

Our research has been organized into three general areas. First, we have studied the evolution of interfacial fluid instabilities (Rayleigh-Taylor, Kelvin-Helmholtz, Richtmyer-Meshkov) and the resulting interpenetrative mix of materials. We have developed new closures for two-pressure two-phase flow, and investigated the nature of the boundary conditions at the edges of the mixing layer, which are based on drag and buoyancy laws. We have validated our front tracking code (FronTier) by comparing simulations of Richtmyer-Meshkov instability growth with other codes, with data, and with a new nonlinear analytic theory. We have taken moments of the spectral equations that describe the distribution of fluctuating energy across the entire spectrum of length scales, rederiving the usual transport equations plus one new extension---a nonlocal transport of length scale from the middle of the mixing layer to beyond its outer edges. We have completed a characteristic analysis of our hybrid multifluid turbulent-mix model. We have continued our development of a model for crenulative instability and applied it to the spherical convergence of an incompressible fluid with a nonhomogeneous distribution of kinematic viscosity.

Second, in the area of the formation of surface ejecta from a shocked metal-gas interface and subsequent transport, we have continued our development of a model for metals by implementing contact forces (Hertzian and frictional) and bonding into a smooth particle hydrodynamics code (SPH). The model is based on the distinct element technique, where the material is represented as a discrete set of grains rather than as a continuum; thus the effects of discontinuous microstructure are accounted for in the formation of the ejecta. Preliminary studies show that several processes contribute to the formation of ejecta, including the intragranular fracture of individual grains and intergranular fracture leading to small clusters of grains. We have tested the implementation by simulating shock wave propagation and plate impact experiments. We began to develop interaction laws between the solid particles (interacting through contact forces) and fluid particles (interacting through potential forces), leading ultimately to a discrete model for particle suspensions.

Third, in the area of predicting material properties (i.e., effective elastic moduli, yield strength, friction coefficient) based on microstructure, we have extended our study of the spallation process in ductile metals due to void growth in uranium and tantalum. We have included the effects of damage clustering and void linking, and made extensive comparisons with experimental data. We have used molecular dynamic simulations to study the atomic level processes leading to interfacial friction. We have studied the intermixing of light and heavy constituents in a hot dense plasma environment, and also the penetration of fast charged particles into plasmas.

We have participated in the implementation and testing of several of the above models into both classified legacy and ASCI design codes.

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