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Fully Atomistic Simulations of Hydrodynamic Instabilities and Mixing

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Abstract

The large-scale computational capabilities at LLNL make it possible to develop seamless connections from processes at the atomic scale to complex macroscopic phenomena such as hydrodynamic instabilities and turbulent mixing. Traditionally, these connections have been made by combining results from different scientific fields. For gases and fluids, atomic and molecular scattering cross sections must first be obtained and incorporated into Boltzmann transport equations. Their solution yields then transport coefficients which are input parameters for the Navier-Stokes equations for fluid dynamics. The latter are solved numerically with hydro-codes. For visco-elastic solids, on the other hand, atomistic simulations must first provide constitutive laws for the mobility and multiplication of dislocations and other crystalline defects. In turn, these laws are utilized to construct meso-scale models for plastic deformation. These models are then incorporated into hydro- and finite element codes to predict the macroscopic behavior of solid materials. Many of these intermediate steps can be bypassed with large-scale molecular dynamics simulations. For this purpose, codes have been developed in which trajectories of atoms or molecules are mapped onto continuum field descriptions for mass density, mass flow, stresses, and for temperature. It is now possible to compare directly and quantitatively atomistic simulations with predictions from hydro- and finite element codes and with experimental results.

Mission Relevance

LLNL missions in stockpile stewardship, and in national and homeland security require the computational analysis of complex phenomena utilizing hydro- and finite element codes. The validation of the fundamental properties and of dynamic processes in materials must be traced back to first principles at the atomic level. The research has demonstrated that a direct validation can be accomplished with large-scale molecular simulations utilizing high-fidelity interatomic potentials.

Accomplishments and Results

We have developed a large suite of computer codes, from the construction of simulation supercells with arbitrary density gradients and for different shock loading, to those for analysis and post-processing of raw molecular dynamics output to calculate the time- and space-averaged flow and vorticity fields, mixing layer growth rate, interface power spectrum and dominant wavelength, and temperature and stress distributions. In addition,

various tools for visualization have also been developed to allow direct comparison with predictions from hydro- and finite element codes.

Instability growth rates for the linear and nonlinear regimes of the classical Rayleigh-Taylor instability have been computed in large 3-D MD simulations starting with given interface perturbations. These results were used to validate hydrodynamic growth models. Additional simulations were performed in which no perturbation is pre-imposed on the initial interface. Rather, the interface roughness is brought about by thermal fluctuations. From these simulations, the mixing layer thickness and the power spectrum of the interface were obtained as a function of simulation time for this system.

The collapse of bubbles containing a fluid less dense than the surrounding fluid was investigated when a planar shock wave propagated through the medium. The evolution of the bubble shape compared well with experimental results.

Helium bubbles with diameters of 3 nm in solid aluminum were subject to strong planar shocks that resulted in melting. Surprisingly, the bubbles deformed little and quickly resumed their spherical shape after passage of the shock front. The high surface tension of a liquid metal suppresses the Rayleigh-Taylor instability.

The growth of a sinusoidal interface between solid aluminum and liquid xenon was simulated under an acceleration of 10^{12} ms^{-2}. Massive stacking faults and dislocations are generated in the troughs and spread deep into the crystal solid as well as into the lateral directions, forming a plastically deformed surface layer with a thickness of about twice the wavelength of the initial interface perturbation.

The computer codes developed in this project were also employed to extract dynamic strength values, the Hugoniot, and plastic heating from shock compression simulation of aluminum. A comprehensive comparison with results from gas gun experiment demonstrated excellent agreement.

Publications

Kubota, A. et al. (2005). Effects of aging on shock and isentropic compression response in Face-centered-cubic metals. 14th Am. Phys. Soc. Topical Conf. Shock compression of Condensed Matter, Baltimore, MD, July 31-Aug. 3, 2005.

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