Molecular dynamics investigations of the ablator/fuel interface during early stages of laser driven inertial confinement fusion[1]

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The National Ignition Facility focuses 192 high-powered laser beams into a volume smaller than a AAA battery. The 500 trillion watts of energy heat the inside of the gold-plated volume to generate copious x-rays that bathe an even smaller spherical target, which is compressed and heated to temperatures that generate fusion reactions. A critical issue in this campaign is the understanding of the mix of the fuel/ablator interface during the heating and compression of the fuel. Mixing occurs at various length scales, including atomic-scale inter-species mixing and hydrodynamic scale Rayleigh-Taylor instability mixing. Because the ablator fuel interfaces is preheated by energy from the incoming shock, it is important to understand the dynamics of the interface before the shock arrives. The interface is in the warm dense matter phase with a deuterium-tritium fuel mixture on one side and a plastic (H, C, and O) mixture on the other. We would like to understand various aspects of the evolution of this warm dense mixture, including the state of the interface when the main shock arrives, the role of electric field generation at the interface, and the character and time scales for diffusive-like mixing. For example, does the electric field at the interface drive kinetic transport processes? And, how does the microphysics at this scale ultimately seed larger-scale hydrodynamic instabilities?

In this talk I will describe a MD approach we are developing to model these processes. In the current model the ions are treated as classical point particles whose dynamics is accurately treated through the computation of their trajectories. Because we must reach extremely large length (many microns) and time scales (many picoseconds), we have developed a simplified electronic structure model. Furthermore, because of the non-equilibrium nature of the processes under investigation, our electronic density must be "reactive" to some degree. In our electronic model we include time-varying ionization levels, external heating, heat conduction, and electron-ion energy exchange. I will describe the physics models, code implementations of the models, issues associated with executing these models on machines such as Vulcan and Sequoia, and results from our recent simulations. Finally, I will discuss improvements to the models that are underway.

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