MAR14-2014-020742

Abstract for an Invited Paper
for the MAR14 Meeting of
the American Physical Society

Integrating Simulation and Data for Materials in Extreme Environments

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We are using large-scale molecular dynamics (MD) simulations to study the response of nanocrystalline metals such as tantalum to uniaxial (e.g., shock) compression. With modern petascale-class platforms, we are able to model sample sizes with edge lengths over one micrometer, which match the length and time scales experimentally accessible at Argonne's Advanced Photon Source (APS) and SLAC's Linac Coherent Light Source (LCLS). I will describe our simulation predictions and their recent verification at LCLS, as well as outstanding challenges in modeling the response of materials to extreme mechanical and radiation environments, and our efforts to tackle these as part of the multi-institutional, multi-disciplinary Exascale Co-design Center for Materials in Extreme Environments (ExMatEx). ExMatEx has initiated an early and deep collaboration between domain (computational materials) scientists, applied mathematicians, computer scientists, and hardware architects, in order to establish the relationships between algorithms, software stacks, and architectures needed to enable exascale-ready materials science application codes within the next decade. We anticipate that we will be able to exploit hierarchical, heterogeneous architectures to achieve more realistic large-scale simulations with adaptive physics refinement, and are using tractable application scale-bridging proxy application testbeds to assess new approaches and requirements. The current scale-bridging strategies accumulate (or recompute) a distributed response database from fine-scale calculations, in a top-down rather than bottom-up multiscale approach. I will demonstrate this approach and our initial assessments, using the newly emerging capabilities at new 4^{th} generation synchrotron light sources as an experimental driver.