Scale-Bridging Modeling of Material Dynamics: Petascale Assessments of the Road to Exascale

TIMOTHY GERMANN, Los Alamos National Laboratory, EXMATEX TEAM — Within the multi-institutional, multidisciplinary Exascale Co-design Center for Materials in Extreme Environments (ExMatEx), we are engaging 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. Our focus has been on scale-bridging strategies that accumulate (or recompute) a distributed response database from fine-scale calculations, in a top-down rather than bottom-up multiscale approach. To evaluate and exercise the task-based programming models, databases, and runtime systems required to perform such many-task computation workflows, we are carrying out petascale demonstrations in 2015 which I will describe in this talk.

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