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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 (Ex-MatEx), 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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