Computational Co-Design for Materials in Extreme Environments

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Summary: Given the increasing complexity of high-performance computing systems (architectures, software stack, and application codes), *computational co-design* is recognized to be critical as we move from current petascale (10^{15} operations/second) to exascale (10^{18} operations/second) supercomputers over the next 5-10 years. Our recently launched Exascale Co-design Center for Materials in Extreme Environments (ExMatEx) intends to do this by initiating an early and extensive collaboration between computational materials scientists, computer scientists, and hardware manufacturers, to develop a multiphysics exascale simulation framework for modeling materials subjected to extreme mechanical and radiation environments.

Introduction

Exascale computing will transform computational materials science by enabling the pervasive embedding of microscopic behavior into meso- and macroscale materials simulation. This transformation requires exploring and adopting fundamentally new algorithmic approaches that are targeted at the emerging high performance computing (HPC) software and hardware environment of greatly increased levels of concurrency, heterogeneity, and flop/byte ratios. The objective of the Exascale Co-design Center for Materials in Extreme Environments (ExMatEx) is to establish this interrelationship between algorithms, system software, and hardware required to develop a multiphysics exascale simulation framework for modeling materials subjected to extreme mechanical and radiation environments. Such a simulation capability will play a key role in solving many of today's most pressing problems, including producing clean energy, extending nuclear reactor lifetimes, and certifying the aging nuclear stockpile. This will be accomplished via a focused effort in four primary areas:

- Scale-bridging algorithms: Our science strategy is an uncertainty quantification (UQ)-driven *adaptive physics refinement* in which coarse-scale simulations dynamically spawn tightly coupled and self-consistent fine-scale simulations as needed [1]. This strategy is crucial for capturing how the macroscale, bulk response is influenced by microstructural detail. Thus, in a high strain-rate loading problem, a finite element method calculation may spawn finer-scale crystal plasticity or atomistic models as needed when the available empirical constitutive model is inadequate, for instance in the vicinity of a shock front (Fig. 1). Such a procedure may be carried through multiple levels of refinement, or applied to the time domain, e.g., using *ab initio* techniques to compute activation energies for a rate theory or kinetic Monte Carlo model.
- Programming models: This multi-program, multi-data (MPMD) *task-based* scale-bridging approach leverages the extensive concurrency and heterogeneity expected at exascale while enabling novel data models, power management, and fault tolerance strategies within applications. The programming models (e.g., domain specific languages (DSLs) that raise the application level of abstraction) and the approaches developed to achieve this will be broadly applicable to a variety of multiscale, multiphysics applications beyond the materials science ones addressed here.

- Proxy applications: *Proxy apps* and kernels play a key role in our co-design process, as they are the main mechanism for exploring algorithm design space and communicating the application workload to the hardware architects and system software developers. Proxy apps for single-scale single-program, multi-data (SPMD) applications (e.g., molecular dynamics) will be used to assess node-level data structures, memory and power management strategies, while system-level data movement, fault management, and load balancing techniques will be evaluated via the asynchronous task-based MPMD scale-bridging proxy apps.

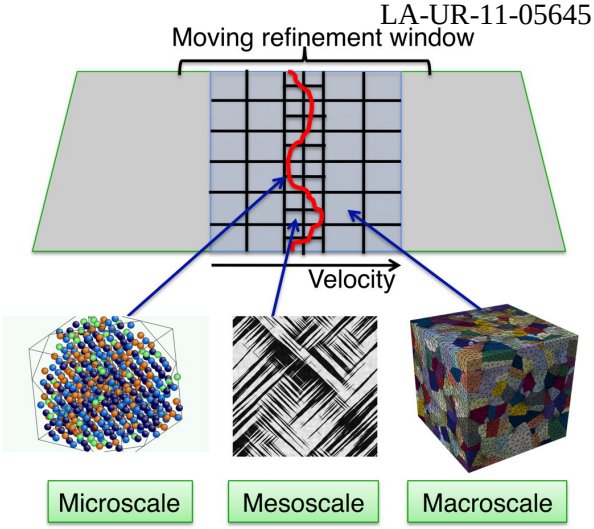

Figure 1. Adaptive physics refinement approach for the case of a high strain-rate loading problem in which a shock wave traverses a material. A coarse-scale model at the continuum level spawns lower length-scale simulations at the polycrystal and single crystal levels as needed. The highly nonequilibrium environment in the immediate vicinity of the shock front may further be probed in a 3-scale bridging approach, as indicated schematically.

- Co-design analysis and optimization: We will establish and execute a continuous modeling, evaluation, optimization, and synthesis loop, including optimization of algorithms and architectures for performance, memory and data movement, power, and resiliency. Proxy applications and performance models/simulators (from node- to system-level, including exascale complexity) will be used to introduce a realistic domain workload into the exascale hardware and software stack development process at an early stage, and together with scalable analysis tools will inform a *co-optimization loop* to address the challenges of power, resiliency, concurrency, and heterogeneity that will characterize exascale platforms.

Although targeted at the domain science challenges of modeling materials in extreme environments, the techniques, tools, and solutions that we develop will benefit a much larger class of multiscale, multiphysics applications across numerous scientific areas.

References

[1] N.R. Barton, J.V. Bernier, J. Knap, A.J. Sunwoo, E.K. Cerreta, and T.J. Turner, "A call to arms for task parallelism in multi-scale materials modeling," *Int. J. Numer. Meth. Engng.* **86**, 744–764 (2011).

Acknowledgements

This work is supported by the U.S. Department of Energy, Office of Science, Advanced Scientific Computing Research (ASCR) program.

Los Alamos National Laboratory is operated by the Los Alamos National Security, LLC, for the National Nuclear Security Administration of the U.S. Department of Energy under Contract DE-AC52-06NA25396.