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Exascale computing and what it means for shock physics[1]

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The U.S. Department of Energy is preparing to launch an Exascale Computing Initiative, to address the myriad challenges required to deploy and effectively utilize an exascale-class supercomputer (i.e., one capable of performing 10^{18} operations per second) in the 2023 timeframe. Since physical (power dissipation) requirements limit clock rates to at most a few GHz, this will necessitate the coordination of on the order of a billion concurrent operations, requiring sophisticated system and application software, and underlying mathematical algorithms, that may differ radically from traditional approaches. Even at the smaller workstation or cluster level of computation, the massive concurrency and heterogeneity within each processor will impact computational scientists. Through the multi-institutional, multi-disciplinary Exascale Co-design Center for Materials in Extreme Environments (ExMatEx), we have 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. In my talk, I will discuss these challenges, and what it will mean for exascale-era electronic structure, molecular dynamics, and engineering-scale simulations of shock-compressed condensed matter. In particular, we anticipate that the emerging hierarchical, heterogeneous architectures can be exploited to achieve higher physical fidelity simulations using adaptive physics refinement.

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