Bridging scales in materials simulation in the exascale era

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Exascale systems promise unprecedented spatial, temporal, and fidelity reach for materials simulations—but that promise is conditional on algorithms that fit the machines we actually have: heterogeneous nodes, deep memory hierarchies, limited bandwidth, and high synchronization costs. Using case studies drawn from large-scale atomistic simulations of materials, I will discuss how these hardware realities reshape the scaling path of standard methods and, in turn, the scientific questions we can tackle. I will then use these examples to illustrate the challenges and opportunities offered by the exascale and show how the combination of novel simulation methodologies, machine learning, and new hardware architectures make possible simulations that were just a dream only a few years ago.