 ICCES, vol.16, no.4, pp.125-125

Petascale Molecular Dynamics Simulations of Photo-mechano-chemistry

Aiichiro Nakano, Rajiv K. Kalia, and Priya Vashishta

Summary

We have developed a metascalable (or "design once, scale on new architectures") parallelization scheme to perform large spatiotemporal-scale molecular dynamics (MD) simulations of materials on peta-to-exaflops computers based on embedded divide-and-conquer algorithms. The scheme has achieved parallel efficiency well over 0.95 on 212,992 IBM BlueGene/L processors for 218 billion-atom MD and 1.68 trillion electronic degrees-of-freedom quantum-mechanical MD in the framework of density functional theory. Simulation results reveal intricate interplay between photoexcitation, mechanics, flow, and chemical reactions at the nanoscale. Specifically, we will discuss atomistic mechanisms of: (1) mechanically enhanced reaction kinetics in nanobubbles and nanojets; (2) rapid hydrogen production from water catalyzed by metallic nanoclusters; and (3) rapid transport of photoexcited electrons in light-harvesting molecules. This work was done in collaboration with Fuyuki Shimojo and Satoshi Ohmura (Kumamoto, Japan) and Ken-ichi Nomura (USC).