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Simulating long time behavior of materials: a case study of sintering of nanoparticles AMIT SAMANTA, SELIM ELHADJ, JEFF BUDE, TAMMY OLSON, JON LEE, JAE HYUCK YOO, Lawrence Livermore National Laboratory — Physical processes in nature exhibit disparate time-scales, for example time scales associated with processes like phase transitions, various manifestations of creep, sintering of particles etc. are often much higher than time the system spends in the metastable states. The transition times associated with such events are also orders of magnitude higher than time-scales associated with vibration of atoms. Thus, atomistic simulations of such transition events is a challenging task. In this talk, I will present a method to overcome the time-scale problem and efficiently explore the free energy surface of a complex system. I will discuss how this method can be used to gain quantitative atomic-scale insights into the sintering of nanoparticles. The simulations suggest that processes like interfacial and bulk diffusion along with grain rotation play an important role during sintering. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. LLNL-ABS-664253

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