Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Order parameter aided efficient phase space exploration under extreme conditions[1] AMIT SAMANTA, Lawrence Livermore Natl Lab — 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, an atomistic simulation of such transition events is a challenging task. Consequently, efficient exploration of configuration space and identification of metastable structures in condensed phase systems is challenging. In this talk I will illustrate how we can define a set of coarse-grained variables or order parameters and use these to systematically and efficiently steer a system containing thousands or millions of atoms over different parts of the configuration. This order parameter aided sampling can be used to identify metastable states, transition pathways and understand the mechanistic details of complex transition processes. I will illustrate how this sampling scheme can be used to study phase transition pathways and phase boundaries in prototypical materials, like SiO2 and Cu under high-pressure conditions.

[1]This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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Date submitted: 09 Nov 2016 Electronic form version 1.4