“Parallelizing Time”: Decreasing the Wall-clock Time to Reach Equilibrium in Materials Simulations

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We often employ molecular dynamics or Monte Carlo computer simulations to study systems at equilibrium. Normally, we use a single long run (SLR) to analyze the system’s observables and detect the attainment of equilibrium. However, as we will discuss, such runs can take a long time. In this talk, we use a new method called swarm relaxation, in which a large number of independently initialized runs is analyzed in order to detect the onset of equilibrium within a much shorter wall-clock time than is possible in a SLR. The efficiency of this method is analyzed for a liquid water system in which a small cluster of ice has been introduced. We show that the “swarm relaxation” method works exceedingly well, compressing the wall-clock time required to detect the onset of equilibrium by a factor of at least 100.