Freezing by Monte Carlo Phase Switch

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ABSTRACT

We describe a Monte Carlo simulation procedure [1] that allows sampling of the disjoint configuration spaces associated with crystalline and fluid phases, within a single simulation. The method utilised biased sampling techniques to enhance the probabilities of gateway states (in each phase) which are such that a global switch (to the other phases) can be implemented [2, 3]. Equilibrium freezing point parameters can be determined directly; statistical uncertainties prescribed transparently; and finite-size effects quantified systematically [4, 5]. The method is potentially quite general; we apply it to the freezing of hard spheres.

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