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Finite Size Scaling of the First Order Transition of Molecular Systems KA MING TAM, BRIAN NOVAK, NICHOLAS WALKER, DOREL MOLDOVAN, MARK JARRELL, Louisiana State University — The calculation of the melting temperature remains an important challenge in the simulation of molecular systems. The conventional method based on stabilizing the co-existence of liquid and solid phases requires rather large system sizes. This is problematic for ab-initio simulations as they are often restricted to small systems of a couple hundreds of atoms. The first order transition, which melting is a prominent example, has been studied in the context of other statistical physics models. We employ some of these techniques to predict the melting point. A key concept of understanding the phase transition is in the energy distribution. We study the energy distribution of molecular systems by calculating the ratios of different cumulants. They show behaviors expected for the first order transition and thus finite size scaling can be used to extract the transition temperature. In contrast to the conventional co-existence method, large system sizes are not necessary. The prediction can be systematically improved by better sampling of the energy distribution, and efficiently utilizes parallel simulations.

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