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Monte Carlo simulation study of simple two-dimensional systems MICHAEL HUGHES, Grinnell College — The relationship between the two-particle interaction potential in a system and the macroscopic observables that result is a key issue in statistical mechanics. To explore this relationship, Monte Carlo simulations are performed on a variety of two-dimensional systems including hard disks and a 2-D Lennard-Jones system. For hard disks, we were not able to confirm the prediction that there is a phase transition containing a region where the pressure is constant with increasing density, although there is evidence that a solid forms under certain conditions as expected. We are also able to produce a pressure-density plot at a constant temperature for the Lennard-Jones model, which shows evidence of a fluid-solid phase transition around $kT/\epsilon = 0.82$. Also, Monte Carlo calculations are performed directly in the Gibbs ensemble by allowing fluctuations in the volume and particle number, and the phase boundary lines are located more expediently than they are by using traditional canonical ensemble Monte Carlo calculations.

Michael Hughes Grinnell College

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