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Multi-Grand, Multi-Canonical, Flat Histogram, Monte Carlo Simulations for the Square Well Fluid. CADE TROTTER, Oregon State University — Currently micro-canonical at histogram simulations are used to give properties of the micro-canonical ensemble at all temperatures of a system with a constant number has recently developed a grand-canonical at histogram capable of giving thermodynamic properties at any number of atoms in a system with a given temperature. While both micro-canonical and grand-canonical work very well, we have combined the two methods to create a multi-grand, multi-canonical at histogram, Monte Carlo simulation. Our newly proposed method functions by allowing for a simulation to change in energy, and number of atoms at any temperature. By allowing for so many degrees of freedom we are able to produce the entire equation of state from just one simulation.

> Cade Trotter Oregon State University

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