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Molecular Dynamics and the Melting Transition: A Computational Modeling Approach for Building Intuition DEREK OSTROM, GUS HART, Brigham Young University — Even simple models, like Lennard-Jones particles, can show remarkably realistic physics and exhibit important phenomena. Using a Lennard-Jones model and molecular dynamics simulations using a simple Verlet algorithm for generating dynamics, melting/freezing transitions can be observed, ground state structures can be discovered, and the Maxwell-Boltzmann distribution emerges spontaneously. These simulations can be an intuitive starting point for building intuition and spring-boarding to simulations of more complex representations of real materials.

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