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Tuning the Metropolis algorithm SPENCER HART, DEREK OSTROM, GUS HART, Brigham Young University — The Metropolis algorithm is a method for simulating equilibrium states of systems. Metropolis Monte Carlo simulations are commonly used to explore material properties, such as transition temperatures. For complex systems, statistical convergence can be hard to achieve, making the results ambiguous. Increasing your sample size will increase the likelihood of convergence, but if the simulation already takes 20 days, increasing the runtime by an order of magnitude is impractical. In an effort to find the best ways to improve simulation results without just increasing runtime, we explored the effects of various computational parameters on a test case, 2D binary alloy model. These parameters include the number of random samples (called Monte Carlo steps), lattice size, and temperature step-size. We hope to use these results to improve simulations of more complex systems in the future.

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