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Stephen H. Harnish* (harnishs@bluffton.edu). *MD simulations of acoustically-controlled defect dynamics: An analog of Born's law in QM*. Preliminary report.

As a mentor for the 2018-19 National Computational Science Institute's Blue Waters Student Internship Program I am guiding code development for simulations on the University of Illinois' Blue Waters supercomputer system. These molecular dynamics simulations track vacancies and interstitials in face-centered cubic and diamond cubic Lennard-Jones lattices. By simulating induced acoustic standing waves in these solids, we test the prediction that defects are more likely at acoustic wave antinodes than nodes and that the long-term PDF for defects are proportional to the square of the amplitudes of the acoustic standing waves. A kinetic Monte Carlo model and its associated eigenvalue/eigenvector analysis supports this hypothesis, which offers close analogies to Born's law in quantum mechanics. The goal of this year-long project is to further test this hypothesis via MD simulations. Aspects of code development and benefits of parallelization will be presented along with the preliminary report of these simulations. (Received September 25, 2018)