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Stephen H. Harnish* (harnishs@bluffton.edu). *Modeling wave velocity and frequency spectra in low-temperature, compressed LJ lattices: HPC simulations, mathematical theory and applications to acoustic metrics.* Preliminary report.

Analysis of wave velocities and vibrational spectra of solids often start with simplifying assumptions of isotropic homogeneous media with harmonic interatomic potentials. In these models the velocity of a longitudinal wave is proportional to the square root of the ratio of Young's elastic modulus and the density of the medium, while the natural angular frequency of a harmonic oscillator is the square root of Hooke's constant divided by the mass. These introductory models can explain many wave phenomena of solids. Yet a careful analysis of real material systems often requires more subtlety. For instance, in anharmonic oscillators the resonant frequency shifts are proportional to the square of the oscillation amplitude. We'll report our computational and theoretical research on an intermediate level model of the temperature dependence of wave velocity and frequency spectra in compressed LJ lattices. The high performance simulations were performed on the Glenn cluster of the Ohio Supercomputer Center and with the assistance of an undergraduate Petascale intern, sponsored by the National Computational Science Institute. We'll end with a preliminary report on applications to acoustic metrics in analogue models of relativity. (Received September 23, 2011)