Lattice-gas models of interatomic forces

Our collaborator Jeffrey Yepez (Phillips Laboratory, Hanscom Field, MA) is exploring lattice-gas models of matter in which interatomic distances can vary in a continuous way in response to changes in pressure, temperature, etc. Such features are a prerequisite for the realistic modeling of molecular organization. The picture shows liquid/solid phase transition; shear and compressional waves have been observed in the crystalline phase.

CAM-8 simulation on 512×512×512 (≈1/8 billion) sites