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Virtual X-Ray and Electron Diffraction Patterns from Atomistic Simulations on Heterogeneous Computing Platforms[1] SHAWN COLEMAN, Department of Mechanical Engineering, University of Arkansas, YANG WANG, Pittsburgh Supercomputing Center, Carnegie Mellon University, LUIS CUEVA-PARRA, Mathematics Department, Auburn University Montgomery, DOUGLAS SPEAROT, Department of Mechanical Engineering, University of Arkansas — Electron and X-ray diffraction are well-established experimental methods used to explore the atomic scale structure of materials. In this work, a computational algorithm is developed to produce virtual electron and X-ray diffraction patterns directly from atomistic simulations. In this algorithm, the diffraction intensity is computed via the structure factor equation over a 3-dimensional mesh of {hkl} points in reciprocal space. To construct virtual selected area electron diffraction (SAED) patterns, a thin hemispherical slice of the reciprocal lattice map lying near the surface of the Ewald sphere is isolated and viewed parallel to a specified zone axis. X-ray diffraction 2θ line profiles are created by virtually rotating the Ewald sphere around the origin of reciprocal space, binning intensities by their associated scattering angle. The diffraction code is parallelized using a heterogeneous mix of MPI and OpenMP. The atom positions are distributed via MPI while the reciprocal space mesh is parallelized using either OpenMP threads launched on regular CPU cores or offloaded to MIC hardware. The complexity of heterogeneous MPI/OpenMP parallelization on mixed hardware will be discussed.

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