

Abstract Submitted
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Feature detection for large-scale molecular dynamics simulations

HYOUNGKI PARK, Ohio State University, DAVID RICHIE, Stone Ridge Technology, JEONGNIM KIM, University of Illinois at Urbana-Champaign, JOSEPH GORSE, Battelle Memorial Inst, JOHN WILKINS, Ohio State University — Advances in computer hardware and numerical methods compound the analysis of complex, large-scale evolutionary phenomena. Progress comes from just-in-time analysis and data compression. Real-time multiresolution analysis (RTMRA) on dynamical quantities (e.g., positions and local energies of atoms) – based on simple Haar wavelets – compresses data more than 100-fold while retaining 0.1 Å.m.s. resolution. Further, RTMRA techniques enable a sophisticated event detection scheme capable of identifying meta-stable structures and detecting infrequent events, e.g., structural transitions, in the presence of thermal noise. As an example, the dynamics over a broad temperature range of silicon defect systems yields visually clear diffusion mechanisms for small silicon interstitial clusters (single-, di-, and tri-interstitial), and initiating growth of extended defects such as the extended 311 defects.

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