Freud: a software suite for high-throughput simulation analysis ERIC HARPER, MATTHEW SPELLINGS, JOSHUA ANDERSON, SHARON GLOTZER, Univ of Michigan - Ann Arbor — Computer simulation is an indispensable tool for the study of a wide variety of systems. As simulations scale to fill petascale and exascale supercomputing clusters, so too does the size of the data produced, as well as the difficulty in analyzing these data. We present *Freud*, an analysis software suite for efficient analysis of simulation data. Freud makes no assumptions about the system being analyzed, allowing for general analysis methods to be applied to nearly any type of simulation. Freud includes standard analysis methods such as the radial distribution function, as well as new methods including the potential of mean force and torque and local crystal environment analysis. Freud combines a Python interface with fast, parallel C++ analysis routines to run efficiently on laptops, workstations, and supercomputing clusters. Data analysis on clusters reduces data transfer requirements, a prohibitive cost for petascale computing. Used in conjunction with simulation software, Freud allows for smart simulations that adapt to the current state of the system, enabling the study of phenomena such as nucleation and growth, intelligent investigation of phases and phase transitions, and determination of effective pair potentials.

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