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Building Modern Cloud Accessible Tools for Materials Simulations

Nicholas J. Finan, Saaketh Desai, Samuel Reeve, Alejandro Strachan
Department of Materials Engineering, Purdue University

ABSTRACT

In recent years, commercial computer systems have grown more user friendly, allowing for new users to quickly and easily make contributions. Unfortunately, this trend is not as apparent in the field of computational materials simulations. The tools used by researchers in this field have remained just as esoteric as the systems of the past. While the methods used in materials simulations continue to grow in complexity and accuracy, the user experience has been neglected entirely. This project aims to eliminate the need for hours spent adjusting file formats and searching for preexisting code, and instead allow researchers to focus on analyzing outputs. Such an endeavor requires the use of online repositories, nanoHUB simulations, and various analysis tools demonstrating materials simulations and making use of molecular dynamics, density functional theory and continuum simulations. Given input files following current LAMMPS standards, this tool can calculate the Radial Distribution Function, X Ray Diffraction, and Vibrational Density of States of the system in question while anticipating issues that will lead to erroneous results. Rather than leaving the user to decide much of the fine customization that goes into these types of analysis, the tool implements a series of robust defaults that provide valid results for most systems. While the tool does not provide the user with This tool also offers a high degree of modularity, allowing for easy integration of additional analysis code.

KEYWORDS

LAMMPS, Rappture, Jupyter, nanoHUB, NCN, Molecular Dynamics, DFT, ab initio