Utilities To Execute Pipelines (UTEP)

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Abstract

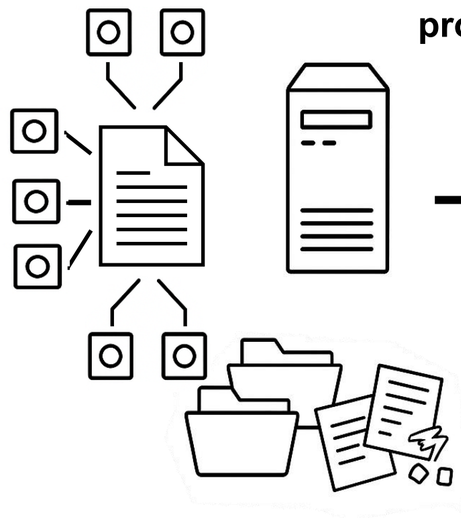
Python framework that automates the creation, submission, and execution of large-scale simulation datasets, reducing human error and saving time when managing hundreds or thousands of jobs. Deployed on the Perlmutter supercomputer at NERSC, it has proven efficient, accurate, and adaptable to other computing platforms.

Objectives

- Efficiently manage big data on supercomputers, saving time and storage.
- Minimize human error in simulation workflows.
- Adaptable to many software packages.

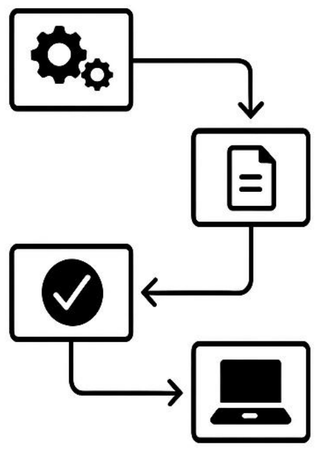
Statement of the Problem

Embarrassingly parallel simulations.

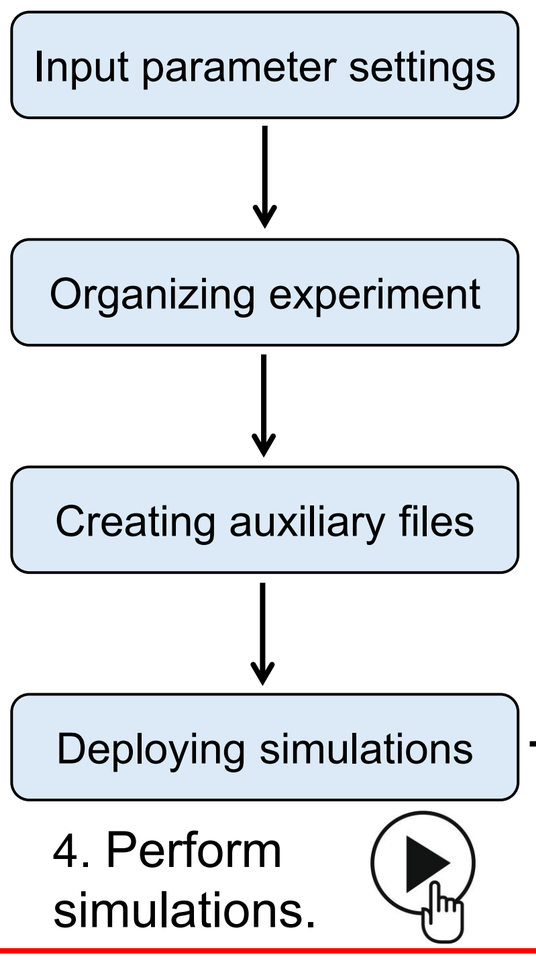


Manual job + self-management = time-consuming + error prone.

UTEP automates and organize pipelines and analyzes



Methodology



1. Define experiment parameters.

2. Construct a hierarchically organized directory structure.

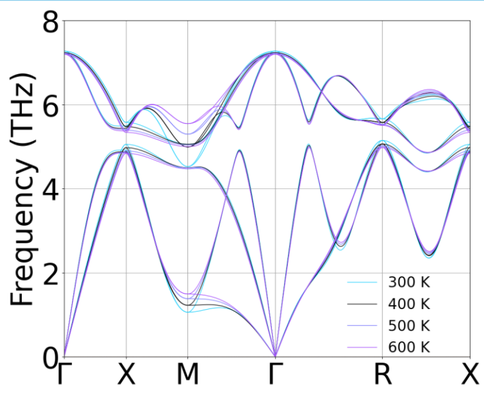
3. Generate supporting files.

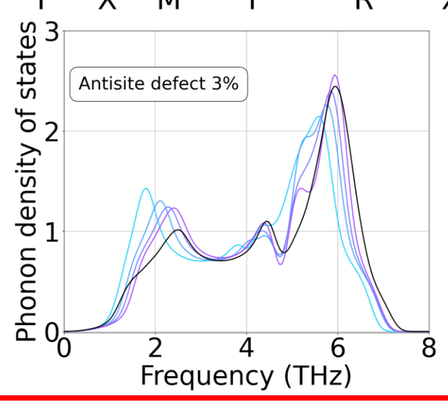
4. Perform simulations.

5. Data visualization and data collection.

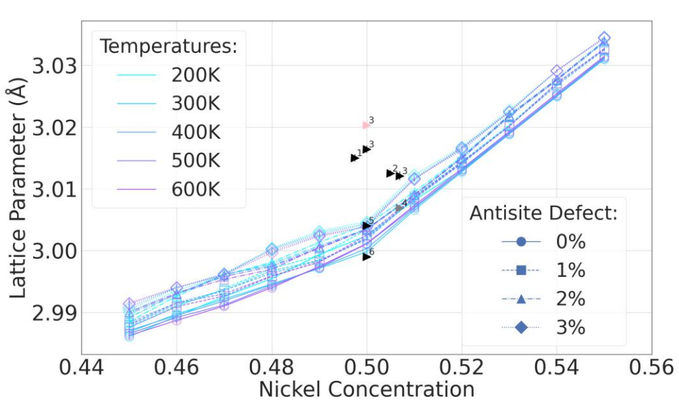
Results from Simulation Tools Deployed with UTEP

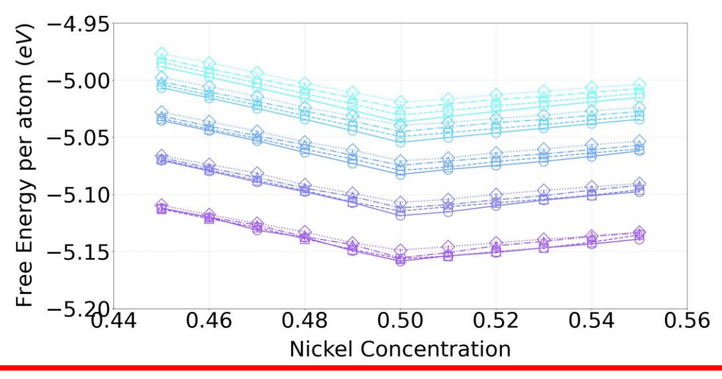
Harmonic Ensemble Lattice Dynamics



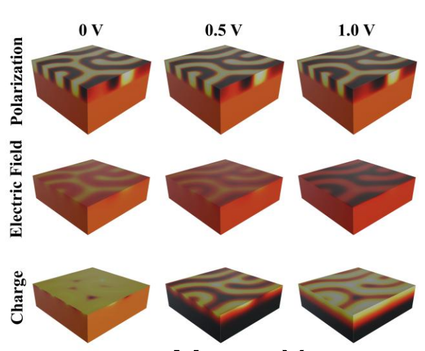


Temperature-Dependent Harmonic Model

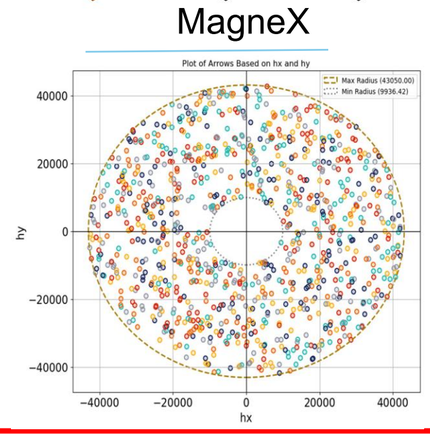




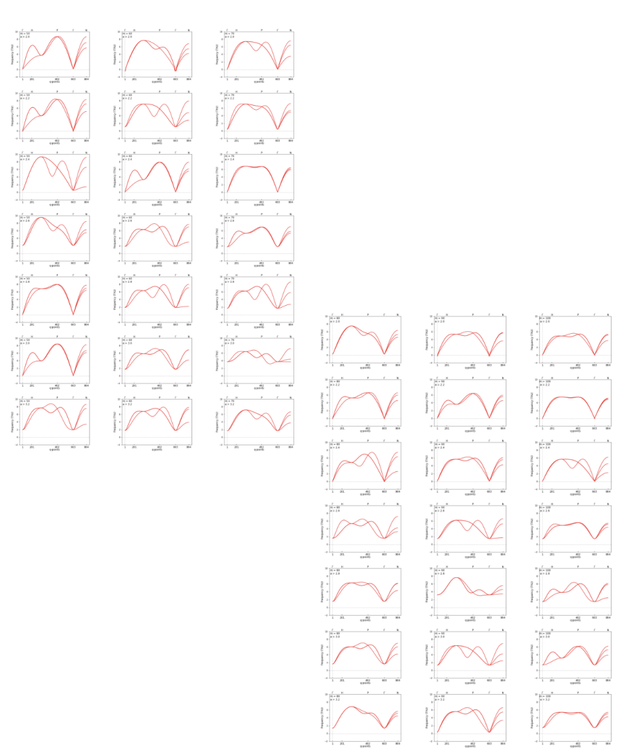
FerroX



MagneX



Stability map for BCC crystal using MOGA



References: