

ASIMTools: A lightweight framework for scalable and reproducible atomic simulations

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Summary

Atomic SIMulation Tools (ASIMTools) is a lightweight workflow and simulation manager for reproducible atomistic simulations on Unix-based systems. Within the framework, simulations can be transferred across computing environments, DFT codes, interatomic potentials and atomic structures. By using in-built or user-defined python modules (called asimmodules) and utilities, users can run simulation protocols and automatically scale them on slurm based clusters or locally on their console. The core idea is to separate the dependence of the atomistic potential/calculator, the computing environment and the simulation protocol thereby allowing the same simulation to be run with different calculators, atomic structures or on different computers with just a change of one parameter in an input file after initial setup. This is increasingly necessary as benchmarking Machine Learning Interatomic Potentials has become a core part of computational materials science. Input and output files follow a simple standard format, usually yaml, providing a simple interface that also acts as a record of the parameters used in a simulation without having to edit python scripts. The minimal set of requirements means any materials science codes can be incorporated into an ASIMTools workflow in a unified way.

Statement of need

Atomic simulations are a key component of modern day materials science in both academia and industry. However, simulation protocols and workflows used by researchers are typically difficult to transfer to systems using different inputs, codes and computing environments. It often involves rewriting entire scripts in different languages to change from one type of atomistic potential or atomic structure to another. This leads to poor reproducibility and inefficient transfer of code from one researcher to the next. In addition, there exists a zoo of tools and packages for atomic simulation with more being developed every day (Walsh, 2024). There is however no unifying framework that can encompass all these tools without significant software development effort. Significant effort should not be necessary because while the source of the fundamental outputs of atomistic potentials such as energy, forces etc. may differ, simulation protocols built on these outputs should converge towards the most accurate and computationally efficient. ASIMTools focuses on this last aspect by introducing asimmodules which are simply Python functions that act as simulation protocols which have no dependence on a specific atomistic potential or computational environment or atomic structure. Through iteration and community input, these simulation protocols will hopefully converge towards best practice and ensure reproducibility of simulation results.

ASIMTools is for users interested in performing atomistic calculations on UNIX-like operating systems and/or on slurm-based High Performance Computing clusters. By defining simulation protocols as "asimmodules", they can be easily added to the library of provided asimmodules

42 and iterated on. The flexibility of ASIMTools allows integration of any kind of simulation
43 tools such as the heavily used Atomic Simulation Environment (Larsen et al., 2017) pymatgen
44 (Ong et al., 2013), LAMMPS (Thompson et al., 2022) etc. with examples provided. With the
45 asimmodules defined, users only need to provide a set of inputs in the form of yaml files that
46 define the parameters used for each simulation and are therefore a concrete record of used
47 parameters.

48 State of the Field

49 There exist a number of popular workflow tools for atomistic simulations such as Aiiida (Huber
50 et al., 2020), Fireworks (Jain et al., 2015) and many more. These tools provide frameworks for
51 constructing complex workflows with different underlying principles. Some managers enforce
52 strict rules that ensure that data obeys FAIR principles and emphasizes data provenance and
53 reproducibility. These methods however tend to be fairly large packages with steep learning
54 curves. ASIMTools provides a simple interface as a starting point that can transform any code
55 into ASIMTools compatible code by simply wrapping it in a function that returns a Python
56 dictionary. Any such code can work in ASIMTools and with a few extra steps, the protocol
57 can be made to support an arbitrary calculator and input atomic structure.

58 In some workflow managers, such as Atomic Simulation Recipes (Gjerding et al., 2021), once
59 workflows are built, it can often be difficult to quickly change and iterate over key parameters
60 such as the choice of atomistic calculator or structure as they are intrinsically built into the
61 code. This is particularly challenging in an age where machine learning models are becoming
62 more popular. Workflows involving machine learning interatomic potentials tend to require
63 the ability to repeat the same calculations on different examples, using different calculators
64 on different hardware iteratively. This is where the value of ASIMTools lies in contrast to
65 more established workflows. ASIMTools is not designed to replace the more powerful workflow
66 managers but rather to supplement them. This is achieved by providing unified inputs that
67 can be easily integrated into, for example, Aiiida as Python functions/asimmodules while also
68 being a stand-alone lightweight workflow manager for simpler cases.

69 Usage To-Date

70 ASIMTools has been used in the benchmarking Machine Learning Interatomic Potentials
71 (Phuthi, Yao, et al., 2024) and creating a workflow for calculation of vibrational properties of
72 solids calculations (Phuthi, Huang, et al., 2024).

73 Conclusion and Availability

74 The ASIMTools package is a powerful tool for building and executing atomic simulation
75 protocols locally and at scale on slurm-based HPC infrastructure. The code is hosted on
76 a public Github repository (<https://github.com/BattModels/asimtools>) with a number of
77 examples. Asimmodules for common calculations are also implemented with examples. Interested
78 users are encouraged to submit issues, contact developers and make pull requests, particularly
79 for adding new simulation protocols to the library.

80 Author Contribution Statement

81 Conceptualization by Keith Phuthi. Coding and development by Keith Phuthi and Emil
82 Annevelink. Paper writing by Keith Phuthi. Project management by all.

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