

foamlib: A modern Python package for working with OpenFOAM

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Summary

foamlib is an open-source Python package that provides a high-level, modern, object-oriented programming interface for working with OpenFOAM cases and their files. It is designed to simplify the development of workflows that involve running OpenFOAM simulations, as well as pre- and post-processing steps. foamlib understands OpenFOAM's file formats and case structures, and provides an ergonomic, Pythonic API for manipulating cases and files, including a full parser and in-place editor for the latter. It also includes support for running OpenFOAM cases asynchronously and on Slurm-based HPC clusters.

Statement of need

foamlib is a Python package that offers a high-level programming interface for manipulating OpenFOAM cases and files, including a full standalone parser and in-place editor for the latter. It is not a thin wrapper library around existing OpenFOAM commands, nor does it provide Python bindings for OpenFOAM's C++-based code. Except for workflows that specifically involve running OpenFOAM solvers or utilities, foamlib can be used by itself without requiring an installation of OpenFOAM, e.g., allowing for pre- or post-processing steps to be performed on a different system than is used to run the simulations.

Dealing with OpenFOAM simulations from Python can be challenging, as (i) OpenFOAM uses its own non-standard file format that is not trivial to parse, and (ii) actually running OpenFOAM cases programmatically can require substantial boilerplate code for determining the correct commands to use, and then invoking said commands while accounting for other relevant considerations such as avoiding oversubscription of CPU resources when executing multiple cases at the same time. foamlib aims to address these challenges by providing a modern Python interface for interacting with OpenFOAM cases and files. By abstracting away the details of OpenFOAM's file formats, case structures, and recipes for execution, foamlib makes it easier to create Python-based workflows that involve running OpenFOAM simulations, as well as their pre- and post-processing steps. The ultimate goal of foamlib is that code for common OpenFOAM workflows, such as running parallel or HPC-based optimization loops, can be easily written in a concise, readable, and composable manner.

The closest existing software to foamlib is PyFoam (Gschaider, 2023), which is an established package that provides an alternative approach for working with OpenFOAM from Python. We believe that foamlib offers several advantages over it, notably including compatibility with current versions of Python, transparent support for fields stored in binary format, a more Pythonic fully type-hinted API with PEP 8—compliant naming, as well as support for other modern Python features such as asynchronous operations. We would also like to mention here



other Python packages with similar functionality—most notably including the ability to parse OpenFOAM output files—: fluidfoam (CyrilleBonamy et al., 2025), fluidsimfoam (Augier & Danaeifar, 2025) and Ofpp (Xianghua, 2023).

Features

Requirements and installation

foamlib is published on PyPI and conda-forge, meaning that it can be easily installed using either pip or conda. The only prerequisite is having an installation of Python 3.7 and later, with 3.7 being chosen due to the fact that many high-performance computing (HPC) environments do not provide more up-to-date Python versions. However, in contrast with PyFoam, which is not currently compatible with Python releases newer than 3.11, foamlib works and is tested with all supported Python versions up to the current Python 3.13.

Besides the recommended packaged installs, official Docker images are also made available (with variants with or without OpenFOAM provided).

Rationale for building a standalone library

foamlib is designed to be a standalone library that can be used independently of OpenFOAM itself. Notably, it does not expose or use the OpenFOAM C++ API itself. This allows foamlib to avoid any kind of dependence on any version or distribution of OpenFOAM, which is especially relevant considering that OpenFOAM is available in two major, incrementally diverging distributions. This design choice also allows for the development of workflows that involve OpenFOAM simulations to be performed on a different system than the one used to run the simulations. The major disadvantage of this approach is that foamlib needs to maintain its own implementation of an OpenFOAM file parser. However, this is mitigated by the fact that OpenFOAM's file formats are not expected to change frequently, and that foamlib's parser is designed to be flexible and easily extensible.

OpenFOAM distribution support

foamlib is tested with both newer and older OpenFOAM versions from both major distributions (i.e., openfoam.com and openfoam.org). Nevertheless, as mentioned before, OpenFOAM itself is not a required dependency of foamlib, being only necessary for actually running OpenFOAM solvers and utilities.

OpenFOAM case manipulation

foamlib provides an object-oriented interface for interacting with OpenFOAM cases. The main classes for this purpose are FoamCaseBase, FoamCase, AsyncFoamCase, and AsyncSlurmFoamCase; all of which are presented below.

FoamCaseBase class

The FoamCaseBase class is the base class for all OpenFOAM case manipulation classes in foamlib. It takes the path to an OpenFOAM case on construction, and provides methods for inspecting and manipulating the case structure, whether before, during or after running the case. FoamCaseBase behaves as a sequence of FoamCaseBase.TimeDirectory objects, each representing a time directory in the case. FoamCaseBase.TimeDirectory objects themselves are mapping objects that provide access to the field files present in each time directory (as FoamFieldFiles—read below for information on file manipulation). Note, as of now, even in the case of a decomposed case, the TimeDirectory object will iterate over the reconstructed time directories.



FoamCase class

The FoamCase class is a subclass of FoamCaseBase that adds functionality for running Open-FOAM cases. It is meant to be the default class used for interacting with OpenFOAM cases in foamlib. The following methods are present in FoamCase objects:

- run(): runs an OpenFOAM case
- clean(): removes files generated during the case run
- copy(): copies the case to a new location
- clone(): makes a clean copy of the case (equivalent to copy() followed by clean()—but may be more efficient)

Notably, the run() method can automatically determine how to run a case based on inspecting its contents and applying some heuristics. If a run or Allrun (or Allrun-parallel) script is present in the case directory, it will be used to run the case. Otherwise, the run() method can execute blockMesh, invoke an Allrun.pre script, restore the "0" directory from a backup, run decomposePar, and/or run the required solver (as set in the case's controlDict) in serial or parallel mode, as required by the case. The behavior can be customized by passing specific arguments to the run() method.

By default, the run() method creates log files in the case directory that capture the output of the invoked commands. Besides being included within the log files, the contents of the standard error stream (stderr) are also stored in memory so that they can be shown in the exception message if a command fails, for easier debugging.

The clean() method removes all files generated during the case run. It uses a clean or Allclean script if present, or otherwise invokes logic that removes files and directories that can be re-created by running the case.

foamlib is also designed in a way that it can be directly used within Python-based (All)run and (All)clean scripts, without risk of calls to run() and clean() causing infinite recursion.

Besides being usable as regular methods, both copy() and clone() also permit usage as context managers (i.e., with Python's with statement), which can be used to create temporary copies of a case, e.g., for testing or optimization runs. Cases created this way are automatically deleted when exiting the relevant code block.

AsyncFoamCase class

AsyncFoamCase is an alternative subclass of FoamCaseBase that provides an asynchronous interface for running OpenFOAM cases. It is designed to work with Python's asyncio library, allowing for the execution of multiple OpenFOAM cases concurrently in a single Python process.

In AsyncFoamCase, all of the run(), clean(), copy(), and clone() methods are asynchronous coroutines, which can be simply awaited from other asynchronous code. These methods otherwise retain the same semantics as their synchronous counterparts in FoamCase.

In order to avoid oversubscription of the available computational resources, AsyncFoamCase defines a mutable class attribute named max_cpus (defaulting to the number of available CPUs) that limits how many cases can be run concurrently. If a run() call being awaited requires more CPUs than are available, the case will not be executed immediately but will rather wait until enough CPUs are freed up by the completion of other run() calls.

Besides its obvious use to orchestrate parallel optimization loops, AsyncFoamCase can also be used to speed up testing workflows that involve running multiple OpenFOAM cases by running them concurrently. For instance, it can be used in conjunction with the pytest (Krekel et al., 2004) framework and the pytest-asyncio-cooperative (Thiart, 2024) plugin, as the authors of this paper currently do to test several OpenFOAM-based projects (Gerlero et al., 2021, 2024; Gerlero, 2024; Gerlero & Kler, 2024).



AsyncSlurmFoamCase class

AsyncSlurmFoamCase is a direct subclass of AsyncFoamCase that adds support for running OpenFOAM cases on Slurm-based HPC clusters. When using this class, every call to run() by default will run the case by submitting one or more Slurm jobs to the cluster. An optional fallback keyword argument can be set to True to run the case locally if Slurm is not available, allowing for seamless local and cluster-based execution.

OpenFOAM file manipulation

foamlib also provides an object-oriented interface for reading from and writing to OpenFOAM files. The main classes for this purpose are FoamFile and FoamFieldFile, which are described below

FoamFile class

The FoamFile class offers high-level facilities for reading and writing OpenFOAM files, providing an interface similar to that of a Python dict. FoamFile understands OpenFOAM's common input/output file formats, and is able to edit file contents in place without disrupting formatting and comments. Most types of OpenFOAM "FoamFile" files are supported, meaning that FoamFile can be used for both pre- and post-processing tasks.

OpenFOAM data types stored in files are mapped to built-in Python or NumPy (Harris et al., 2020) types as much as possible, making it easy to work with OpenFOAM data in Python. Table 1 shows the mapping of OpenFOAM data types to Python data types with foamlib. Also, disambiguation between Python data types that may represent different OpenFOAM data types (e.g., a scalar value and a uniform scalar field) is resolved by foamlib at the time of writing by considering their contextual location within the file. The major exception to this preference for built-ins is posed by the FoamFile.SubDict class, which is returned for sub-dictionaries contained in FoamFiles, and allows for one-step modification of entries in nested dictionary structures—as is commonly required when configuring OpenFOAM cases.

For clarity and additional efficiency, FoamFile objects can be used as context managers to make multiple reads and writes to the same file while minimizing the number of filesystem and parsing operations required.

Finally, we note that all OpenFOAM file formats are transparently supported by foamlib, including ASCII, double- and single-precision binary formats, as well as compressed files.

Table 1: Mapping of OpenFOAM data types to Python data types with foamlib.

2 52414	foamlib (accepts and	
OpenFOAM	returns)	foamlib (also accepts)
scalar	float	
vector/tensor	numpy.ndarray	Sequence[float]
	list[float]	
label	int	
switch	bool	
word	str	
string	str (quoted)	
multiple tokens	tuple	
list	list	Sequence
dictionary	FoamFile.SubDict dict	Mapping
dictionary entry	tuple	
uniform field	float numpy.ndarray	Sequence[float]
non-uniform	numpy.ndarray	Sequence[float]
field		<pre>Sequence[Sequence[float]]</pre>



OpenFOAM	foamlib (accepts and returns)	foamlib (also accepts)
dimension set dimensioned	FoamFile.DimensionSet FoamFile.Dimensioned	Sequence[float] numpy.ndarray

FoamFieldFile class

FoamFieldFile is a convenience subclass of FoamFile that simply adds properties for accessing data expected to be present in files that represent OpenFOAM fields, such as internal_field, dimensions, and boundary_field.

Documentation and examples

Examples of foamlib usage are provided in the README file of the project. Additionally, Sphinx-based documentation covering the entirety of the public API is available at foamlib.readthedocs.io.

Implementation details

Type hints

foamlib is fully typed using Python's type hints, which makes it easier to understand and use the library, as well as enabling automatic checks for type errors using tools like mypy (Lehtosalo, 2024).

Parsing

foamlib contains a full parser for OpenFOAM files, which is able to understand and write to the different types of files used by OpenFOAM. The parser is implemented using the pyparsing (McGuire, 2024) library, which provides a powerful and flexible way to define parsing grammars.

A special case parser is internally used for non-uniform OpenFOAM fields, which can commonly contain very large amounts of data in either ASCII or binary formats. The specialized parser uses regular expressions to extract these data, which results in greatly improved parsing performance—a more than 25x speedup versus PyFoam, as measured on a MacBook Air (Apple Inc., Cupertino, Calif., USA) with an M1 processor and 8 GB of system RAM—, while not sacrificing any of the generality of the parsing grammar. For extra efficiency and convenience, these fields map to NumPy arrays in Python.

Asynchronous support

Methods of FoamCase and AsyncFoamCase have been carefully implemented in a way that greatly avoids duplication of code between the synchronous and asynchronous versions by factoring out the common logic into a helper intermediate class.

Continuous integration

Continuous integration of foamlib is performed automatically using GitHub Actions, and includes:

- Testing with all supported Python versions (currently 3.7 to 3.13)
- Testing with multiple OpenFOAM distributions and versions (currently 9, 12, 2006 and 2406)
- Testing on a Slurm environment
- Code coverage tracking with Codecov



- Type checking with mypy
- Code linting and formatting with Ruff
- Package building with uv

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