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SOFTWARE METAPAPER

FluidSim: Modular, Object-Oriented Python Package for High-Performance CFD Simulations

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The Python package `fluidsim` is introduced in this article as an extensible framework for Computational Fluid Mechanics (CFD) solvers. It is developed as a part of FluidDyn project [2], an effort to promote open-source and open-science collaboration within fluid mechanics community and intended for both educational as well as research purposes. Solvers in `fluidsim` are scalable, High-Performance Computing (HPC) codes which are powered under the hood by the rich, scientific Python ecosystem and the Application Programming Interfaces (API) provided by `fluiddyn` and `fluidfft` packages [11]. The present article describes the design aspects of `fluidsim`, which includes use of Python as the main language; focus on the ease of use, reuse and maintenance of the code without compromising performance. The implementation details including optimization methods, modular organization of features and object-oriented approach of using classes to implement solvers are also briefly explained. Currently, `fluidsim` includes solvers for a variety of physical problems using different numerical methods (including finite-difference methods). However, this metapaper shall dwell only on the implementation and performance of its pseudo-spectral solvers, in particular the two- and three-dimensional Navier-Stokes solvers. We investigate the performance and scalability of `fluidsim` in a state of the art HPC cluster. Three similar pseudo-spectral CFD codes based on Python (Dedalus, SpectralDNS) and Fortran (NS3D) are presented and qualitatively and quantitatively compared to `fluidsim`. The source code is hosted at Bitbucket as a Mercurial repository bitbucket.org/fluiddyn/fluidsim and the documentation generated using Sphinx can be read online at fluidsim.readthedocs.io.

Keywords: Fluid dynamics; Python; FFT; simulations

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(1) Overview

Introduction

Designed as a specialized package of the FluidDyn project for computational fluid mechanics (CFD), `fluidsim` is a comprehensive solution to address the needs of a fluid mechanics student and researcher alike – by providing scalable high performance solvers, on-the-fly postprocessing, and plotting functionalities under one umbrella. In the open-science paradigm, scientists will be both users and developers of the tools at the same time. An advantage of `fluidsim` is that, most of the users just have to read and write Python code. `fluidsim` ensures that all critical modules, classes and functions are well documented – both as inline comments and as standalone documentation, complete with examples

and tutorials. For these reasons `fluidsim` can become a true collaborative code and has the potential to replace some in-house pseudo-spectral codes written in more conventional languages.

Balance between runtime efficiency and cost of development

In today's world where clusters are moving from petascale to exascale performance, computing power is aplenty. In most research scenarios, it becomes apparent that *man-hours are more expensive than computing time*. In other words, the cost of development outweighs the cost of computing time. Therefore, developers should be willing to make small sacrifices in efficiency, to improve development time, code maintainability and

clarity in general. In exceptional cases when computing time become more expensive, one can still use existing optimized and performance-tuned compiled libraries implemented in native languages as the core, and rely on high level programming languages to extend them for specific applications.¹

For the above reasons, majority of `fluidsim`'s code-base, in terms of line of code, is written using pure Python syntax. However, this is done without compromising performance, by making use of libraries such as `Numpy`, and optimized compilers such as `Cython` and `Pythran`.

`Numpy` functions and data types are sufficient for applications such as initialization and postprocessing operations, since these functions are used sparingly. Computationally intensive tasks such as time-stepping and linear algebra operators which are used in every single iteration must be offloaded to compiled extensions. This optimization strategy can be considered as the computational equivalent of the Pareto principle, also known as the 80/20 rule.² The goal is to optimize such that "80 percent of the runtime is spent in 20 percent of the code" [10]. Here, `Cython` [3] and `Pythran` [8] compilers comes in handy. An example on how we use `Pythran` to reach similar performance than with Fortran by writing only Python code is described in the companion paper on `fluidfft` [11].

The result of using such an approach is studied in the forthcoming sections by measuring the performance of `fluidsim`. We will demonstrate that a very large percentage of the elapsed time is spent in the execution of optimized compiled functions and thus that the "Python cost" is negligible.

Target audiences

`fluidsim` is designed to cater to the needs of three kinds of audience.

- *Users*, who run simulations with already available solvers. To do this, one needs to have very basic skills in Python scripting.
- *Advanced users*, who may extend `fluidsim` by developing customized solvers for new problems by taking advantage of built-in operators and time-stepping classes. In practice, one can easily implement such solvers by changing a few methods in base solver classes. To do this, one needs to have fairly good skills in Python and especially object-oriented programming.
- *Developers*, who develop the base classes, in particular, the operators and time stepping classes. One may also sometime need to write compiled extensions to improve runtime performance. To do this, desirable traits include good knowledge in Python, `Numpy`, `Cython` and `Pythran`.

This metapaper is intended as a short introduction to `fluidsim` and its implementation, written mainly from a user-perspective. Nevertheless, we also discuss how

`fluidsim` can be customized and extended with minimal effort to promote code reuse. A more comprehensive and hands-on look at how to use `fluidsim` can be found in the tutorials,³ both from a user's and a developer's perspective. In the latter half of the paper, we shall also inspect the performance of `fluidsim` in large computing clusters and compare `fluidsim` with three different pseudo-spectral CFD codes.

Implementation and architecture

New features were added over the years to the package whenever demanded by research interests, thus making the code very user-centric and function-oriented. This aspect of code development is termed as YAGNI, one of the principles of agile programming software development method, which emphasizes not to spent a lot of time developing a functionality, because most likely *you aren't gonna need it*.

Almost all functionalities in `fluidsim` are implemented as classes and its methods are designed to be modular and generic. This means that the user is free to use inheritance to modify certain parts to suit one's needs, and avoiding the risk of breaking a functioning code.

Package organization

`fluidsim` is meant to serve as a framework for numerical solvers using different methods. For the present version of `fluidsim` there is support for finite difference and pseudo-spectral methods. An example of a finite difference solver is `fluidsim.solvers.ad1d` which solves the 1D advection equation. There are also solvers which do not rely on most of the base classes, such as `fluidsim.base.basilisk` which implements a 2D adaptive meshing solver based on the CFD code Basilisk. The collection of solvers using pseudo-spectral methods are more feature-rich in comparison.

The code is organized into the following sub-packages:

- `fluidsim.base`: contains all base classes and a solver for the trivial equation $\partial_t \mathbf{u} = 0$.
- `fluidsim.operators`: specialized linear algebra and numerical method operators (e.g., divergence, curl, variable transformations, dealiasing).
- `fluidsim.solvers`: solvers and postprocessing modules for problems such as 1D advection, 2D and 3D Navier-Stokes equations (incompressible and under the Boussinesq approximation, with and without density stratification and system rotation), one-layer shallow water and Föppl-von Kármán equations.
- `fluidsim.util`: utilities to load and modify an existing simulation, to test, and to benchmark a solver.

Subpackages `base` and `operators` form the backbone of this package, and are not meant to be used by the user explicitly. In practice, one can make an entirely new solver for a new problem using this framework by simply writing one or two importable files containing three classes:

- an `InfoSolver` class,⁴ containing the information on which classes will be used for the different tasks in the solver (time stepping, state, operators, output, etc.).
- a `Simulation` class⁵ describing the equations to be solved.
- a `State` class⁶ defining all physical variables and their spectral counterparts being solved (for example: u_x and u_y) and methods to compute one variable from another.

We now turn our attention to the simulation object which illustrates how to access the code from the user's perspective.

The simulation object

The simulation object is instantiated with necessary parameters just before starting the time stepping. A simple 2D Navier-Stokes simulation can be launched using the following Python script:

```
from fluidsimsolvers.ns2d.solver import Simul
params = Simul.create_default_params()
# Modify parameters as needed
sim = Simul(params)
sim.time_stepping.start()
```

The script first invokes the `create_default_params` classmethod which returns a `Parameters` object, typically named `params` containing all default parameters. Modifications to simulation parameters

```
from fluidsims import load_sim_for_plot
# in the directory of the simulation
sim = load_sim_for_plot()
# or with the path of the simulation
# sim = load_sim_for_plot("~/Sim_data/NS2D.strat_240x240_S8x8_2018-04-20_13-45-54")

# to retrieve the value of a parameter
print(f"viscosity = {sim.params.nu_2}")

# to plot the space averaged quantities versus time
sim.output.spatial_means.plot()
# to load the corresponding data
data = sim.output.spatial_means.load()

# for a 2d plot of the variable "b"
sim.output.phys_fields.plot("b", time=2)
# to save a 2d animation
sim.output.phys_fields.animate("b", tmin=1, tmax=5, save_file=True)
```

Figure 1 demonstrates how an user can access different objects and its associated methods through the simulation object for the solver `fluidsim.solvers.ns3d`. Do note that the object and method names are similar, if not same, for other solvers. The purpose of the objects are listed below in the order of instantiation:

- `sim.params`: A copy of the `params` object supplied by the user, which holds all information critical to run the simulation and generating the output.
- `sim.info_solver`: Contains all the subclass information, including the module the class belongs to.
- `sim.info`: A union of the `sim.info_solver` and the `sim.params` objects.

are made after this step, to meet the user's needs. The simulation object is then instantiated by passing `params` as the only argument, typically named `sim`, ready to start the iterations.

As demonstrated above, parameters are stored in an object of the class `Parameters`, which uses the `ParamsContainer` API⁷ of `fluiddyn` package [2]. `Parameters` for all possible modifications to initialization, preprocessing, forcing, time-stepping, and output of the solvers is incorporated into the object `params` in a hierarchical manner. Once initialized, the "public" (not hidden) API does not allow to add new parameters to this object and only modifications are permitted.⁸ This approach is different from conventional solvers reliant on text-based input files to specify parameters, which is less robust and can cause the simulation to crash due to human errors during runtime. A similar, but less readable approach to `ParamsContainer` is adopted by `OpenFOAM` which relies on dictionaries to customize parameters. The `params` object can be printed on the Python or IPython console and explored interactively using tab-completion, and can be loaded from and saved into XML and HDF5 files, thus being very versatile.

Note that the same simulation object is used for the plotting and post-processing tasks. During or after the execution of a simulation, a simulation object can be created with the following code (to restart a simulation, one would rather use the function `fluidsim.load_for_restart`):

- `sim.oper`: Responsible for generating the grid, and numerical methods such as FFT, IFFT, dealiasing, divergence, curl, random arrays, etc.
- `sim.output`: Takes care of all on-the-fly post-processing outputs and functions to load and plot saved output files. Different objects are assigned with tasks of loading, plotting and sometimes computing:
 - `sim.output.print_stdout`: the mean energies, time elapsed and time-step of the simulation printed as console output.
 - `sim.output.phys_fields`: the state variables in the physical plane. It relies on `sim.state` to load or compute the variables into arrays.
 - `sim.output.spatial_means`: mean quantities such as energy, enstrophy, forcing power, dissipation.

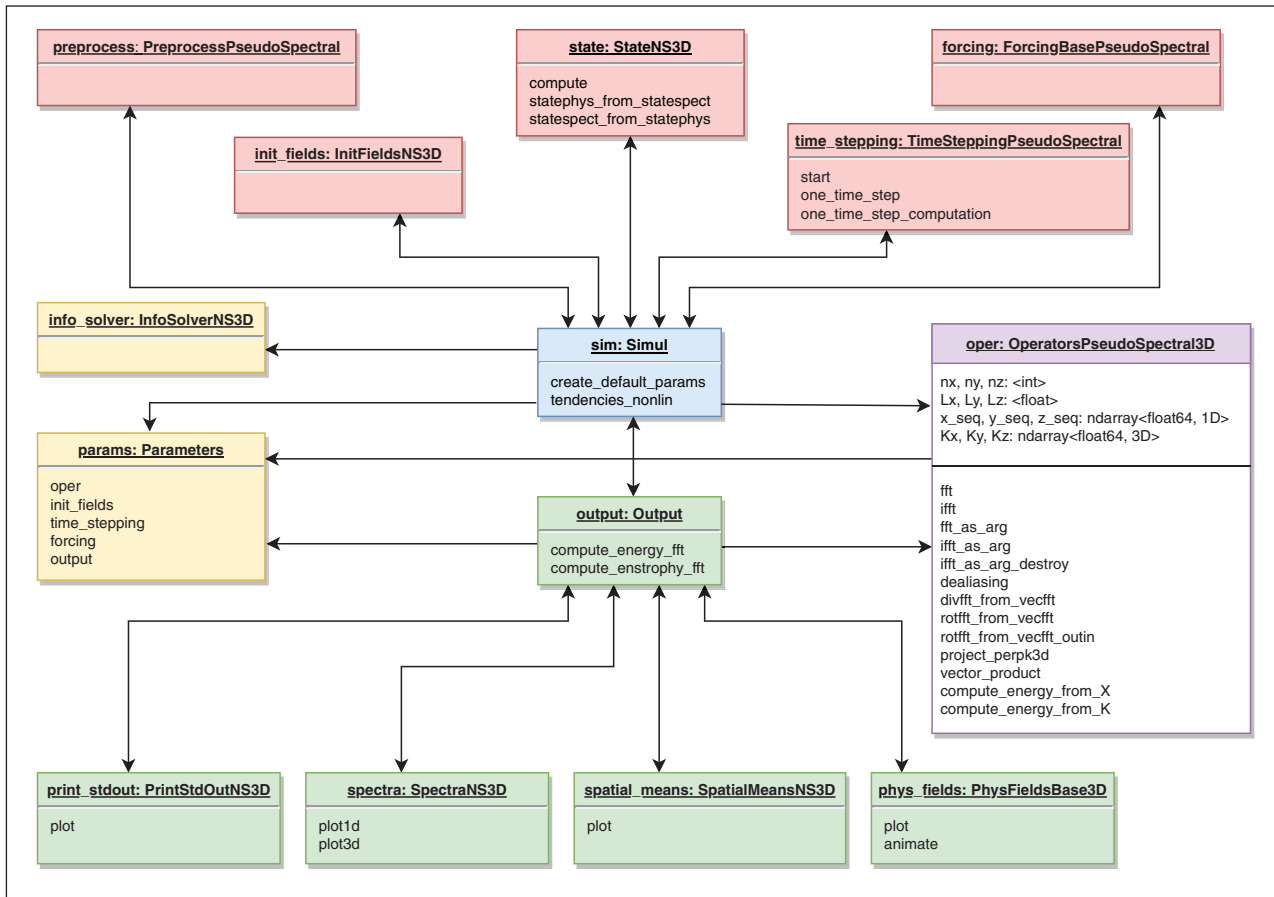


Figure 1: UML diagram of the simulation object (`sim`) for the solver `fluidsim.solvers.ns3d`. Each block represents an object or instance of a class, and the object name and the class name are written as headings. The solid arrows show how objects are associated with each other. Methods and variables of significance to the user are displayed in the body of each object block.

- `sim.output.spectra`: energy spectra as line plots (i.e. as functions of the module or a component of the wavenumber).
- `sim.output.spect_energy_budg`: spectral energy budget by calculating the transfer term.
- `sim.output.increments`: structure functions from physical velocity fields.
- `sim.state`: Defines the names of the physical variables being solved for and their spectral equivalents, along with all required variable transformations. Also includes high-level objects, aptly named `sim.state.state_phys` and `sim.state.state_spect` to hold the arrays.
- `sim.time_stepping`: Generic numeric time-integration object which dynamically determines the time-step using the CFL criterion for specific solver and advances the state variables using Runge-Kutta method of order 2 or 4.
- `sim.init_fields`: Used only once to initialize all state variables from a previously generated output file or with simple kinds of flow structures, for example a dipole vortex, base flow with constant value for all gridpoints, grid of vortices, narrow-band noise, etc.
- `sim.forcing`: Initialized only when `params.forcing.enable` is set as `True` and it computes

the forcing variables, which is added on to right-hand-side of the equations being solved.

- `sim.preprocess`: Adjusts solver parameters such as the magnitude of initialized fields, viscosity value and forcing rates after all other subclasses are initialized, and just before the time-integration starts.

Such a modular organization of the solver's features has several advantages. The most obvious one, will be the ease of maintaining the code base. As opposed to a monolithic solver, modular codes are well separated and leads to less conflicts while merging changes from other developers. Secondly, with this implementation, it is possible to extend or replace a particular set of features by inheriting or defining a new class.

Modular codes can be difficult to navigate and understand the connection between objects and the classes in static languages. It is much less a problem with Python where one can easily decipher this information from object attributes or using IPython's dynamic object information feature.⁹ Now, `fluidsim` goes one step further and one can effortlessly print the `sim.info_solver` object in the Python/IPython console, to get this information. A truncated example of the output is shown below.

```

>>> sim.info_solver
<fluidsim.solvers.ns3d.solver.InfoSolverNS3D object at 0x7fb6278263c8>

<solver class_name="Simul" module_name="fluidsim.solvers.ns3d.solver"
  short_name="ns3d">
  <classes>
    <OperatorsPseudoSpectral3D
      module_name="fluidsim.operators.operators3d"/>

    <State class_name="StateNS3D" keys_computable="['rotz']"
      keys_linear_eigenmodes="['rot_fft']" keys_phys_needed="['vx', 'vy',
        'vz']" keys_state_phys="['vx', 'vy', 'vz']"
      keys_state_spect="['vx_fft', 'vy_fft', 'vz_fft']"
      module_name="fluidsim.solvers.ns3d.state"/>

    <TimeStepping class_name="TimeSteppingPseudoSpectralNS3D"
      module_name="fluidsim.solvers.ns3d.time_stepping"/>

    <InitFields class_name="InitFieldsNS3D"
      module_name="fluidsim.solvers.ns3d.init_fields">
      <classes>
        <from_file class_name="InitFieldsFromFile"
          module_name="fluidsim.base.init_fields"/>

        <from_simul class_name="InitFieldsFromSimul"
          module_name="fluidsim.base.init_fields"/>

        <in_script class_name="InitFieldsInScript"
          module_name="fluidsim.base.init_fields"/>

        <constant class_name="InitFieldsConstant"
          module_name="fluidsim.base.init_fields"/>

        <!--truncated output-->
      </classes>
    </InitFields class_name="InitFieldsNS3D"
      module_name="fluidsim.solvers.ns3d.init_fields">
  </classes>
</solver>

```

Note that while the 3D Navier-Stokes solver relies on some generic base classes, such as `OperatorsPseudoSpectral3D` and `TimeSteppingPseudoSpectral`, shared with other solvers for other purposes there are solver-specific classes. The latter is often inherited from the base classes in `fluidsim.base` or classes available in other solvers – this made possible by the use of an object-oriented approach. This is particularly advantageous while extending existing features or creating new solvers to use class inheritance.

Performance

Performance of a code can be carefully measured by three different program analysis methods: profiling, micro-benchmarking and scalability analysis. Profiling traces various function calls and records the cumulative time consumed and the number of calls for each function. Through profiling, we shed light on what part of the code consumes the lion's share of the computational time and observe the impact as number of processes and MPI communications increase. Micro-benchmarking is the process of timing a specific portion of the code and comparing different implementations. The aspect is addressed in greater detail in the companion paper on `fluidfft` [11]. On the other hand, a scalability study measures how the speed of the code improves when it is deployed with multiple CPUs operating in parallel. To do this, the walltime required by the whole code is measured to complete a certain number of iterations, given a problem size. Finally, performance can also be studied by comparing different codes on representative problems. Since such comparisons should not focus only

on performance, we present a comparison study in a separate section.

The profiling and scaling tests were conducted in a supercomputing cluster of the Swedish National Infrastructure for Computing (SNIC) namely Beskow (PDC, Stockholm). Relevant details regarding software and hardware which affect performance are summarised in **Table 1**. Note that no hyperthreading was used while carrying out the studies. The code comparisons were made on a smaller machine. Results from the three analyses are systematically studied in the following sections.

Profiling

It is straightforward to perform profiling with the help of the `cProfile` module, available in the Python standard library. For `fluidsim`, this module has been conveniently packaged into a command line utility, `fluidsim-profile`. Here, we have analyzed both 2D and 3D Navier-Stokes solvers in Beskow, and plotted the results in **Figures 2** and **3** respectively. Functions which consume less than 2% of the total time are displayed within a single category, *other*.

In **Figure 2** both sequential and parallel profiles of the 2D Navier-Stokes solver shows that majority of time is spent in inverse and forward FFT calls (`ifft_as_arg` and `fft_as_arg`). For the sequential case, approximately 0.14% of the time is spent in pure Python functions, i.e. functions not built using `Cython` and `Pythran`. `Cython` extensions are responsible for interfacing with FFT operators and also for the time-step algorithm. `Pythran` extensions are used to translate most of the linear algebra operations into optimized,

statically compiled extensions. We also see that only 1.3% of the time is not spent in the main six functions (category *other* in the figure). With 8 processes deployed in parallel, time spent in pure Python function increases to 1.1% of the total time. These results show that during the optimization process, we have to focus on a very small number of functions.

From **Figure 3** it can be shown that, for the 3D Navier-Stokes solver, majority of time is attributed to FFT calls.

The overall time spent in pure Python function range from 0.001% for 512³ grid points and 2 processes to 0.46% for 128³ grid points and 8 processes. This percentage tends to increase with the number of processes used since the real calculation done in compiled extensions take less time. This percentage is also higher for the coarser resolution for the same reason. However, the time in pure Python remains for all cases largely negligible compared to the time spent in compiled extensions.

Table 1: Specifications of the supercomputing cluster and software used for profiling and benchmarking.

Cluster	Beskow (Cray XC40 system with Aries interconnect)
CPU	Intel Xeon CPU E5-2695v4, 2.1GHz
Operating System	SUSE Linux Enterprise Server 11, Linux Kernel 3.0.101
No. of cores per nodes used	32
Maximum no. of nodes used	32 (2D cases), 256 (3D cases)
Compilers	CPython 3.6.5, Intel C++ Compiler (icpc) 18.0.0
Python packages	fluiddyn 0.2.3, fluidfft 0.2.3, fluidsims 0.2.1, numpy (OpenBLAS) 1.14.2, Cython 0.28.1, mpi4py 3.0.0, pythran 0.8.5

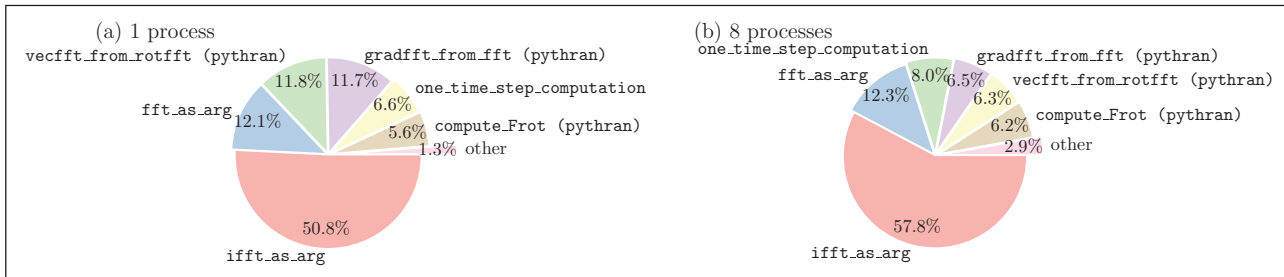


Figure 2: Profiling analysis of the 2D Navier-Stokes (`fluidsim.solvers.ns2d`) solver using a grid sized 1024 × 1024 **(a)** in sequential with `fft2d.with_fftw1d` operator and **(b)** with 8 processes with `fft2d.mpi_with_fftwmpi2d` operator.

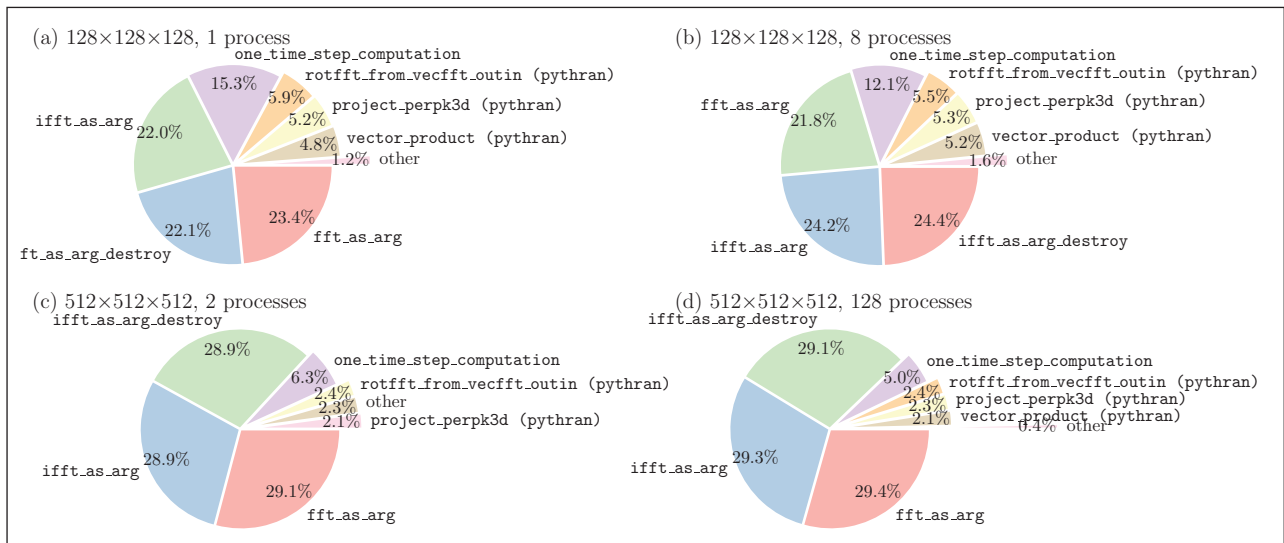


Figure 3: Profiling analysis of the 3D Navier-Stokes (`fluidsim.solvers.ns3d`) solver. Top row: grid sized 128 × 128 × 128 solved **(a)** sequentially using `fft3d.with_fftw3d` operator and **(b)** with 8 processes using `fft3d.mpi_with_fftwmpi3d` operator. Bottom row: grid sized 512 × 512 × 512 using `fft3d.mpi_with_fftwmpi3d` operator **(c)** with 2 processes and **(d)** with 128 processes.

Scalability

Scalability can be quantified by speedup S which is a measure of the time taken to complete N iterations for different number of processes, n_p . Speedup is formally defined here as:

$$s_\alpha(n_p) = \frac{[\text{Time elapsed for } N \text{ iterations with } n_{p,\min} \text{ processes}]_{\text{fastest}} \times n_{p,\min}}{[\text{Time elapsed for } N \text{ iterations with } n_p \text{ processes}]_\alpha} \quad (1)$$

where $n_{p,\min}$ is the minimum number of processes employed for a specific array size and hardware, α denotes the FFT class used and “fastest” corresponds to the fastest result among various FFT classes. In addition to number of processes, there is another important parameter, which is the size of the problem; in other words, the number of grid points used to discretize the problem at hand. In *strong scaling* analysis, we keep the global grid-size fixed and increase the number of processes. Ideally, this should yield a speedup which increases linearly with number of processes. Realistically, as the number of processes increase, so does the number of MPI communications, contributing to some latency in the overall time spent and thus resulting in less than ideal performance. Also, as shown by profiling in the previous section, majority of the time is consumed in making forward- and inverse-FFT calls, an inherent bottleneck of the pseudo-spectral approach. The FFT function calls are the source of most of the MPI calls during runtime, limiting the parallelism.

2D benchmarks

The Navier-Stokes 2D solver (`fluidsim.solvers.ns2d`) solving an initial value problem (with random fields) was chosen as the test case for strong scaling analysis here. The physical grid was discretized with 1024×1024 and 2048×2048 points. Fourth-order Runge-Kutta (RK4) method with a constant time-step was used for time-integration. File input-output and the forcing term has been disabled so as to measure the performance accurately. The test case is then executed for 20 iterations. The time elapsed was measured just before and after the `sim.time_stepping.start()` function call, which was then utilized to calculate the average walltime per iteration and speedup. This process is repeated for two different FFT classes provided by `fluidfft`, namely `fft2d.mpi_with_fftw1d` and `fft2d.mpi_with_fftwmpi2d`.

Although the FFT classes are different for sequential and parallel runs, for the sake of comparison, we have tabulated the actual walltime elapsed in **Table 2**. Clearly due to the differences in the implementations, for `fftw1d`-based classes it takes a performance hit with parallelization, while for classes based on `fftw2d` the performance improves.

In **Figure 4** we have analyzed the strong scaling speedup S and walltime per iteration. The fastest result for a particular case is assigned the value $S = n_p$ as

Table 2: Elapsed times (in seconds) for twenty time steps of 1024×1024 case with the 2D Navier-Stokes 2D (`fluidsim.solvers.ns2d`) solver.

FFT class	Time ($n_p = 1$)	FFT class	Time ($n_p = 2$)
<code>fft2d.with_fftw1d</code>	6.63	<code>fft2d.mpi_with_fftw1d</code>	7.63
<code>fft2d.with_fftw2d</code>	5.59	<code>fft2d.mpi_with_fftwmpi2d</code>	3.91

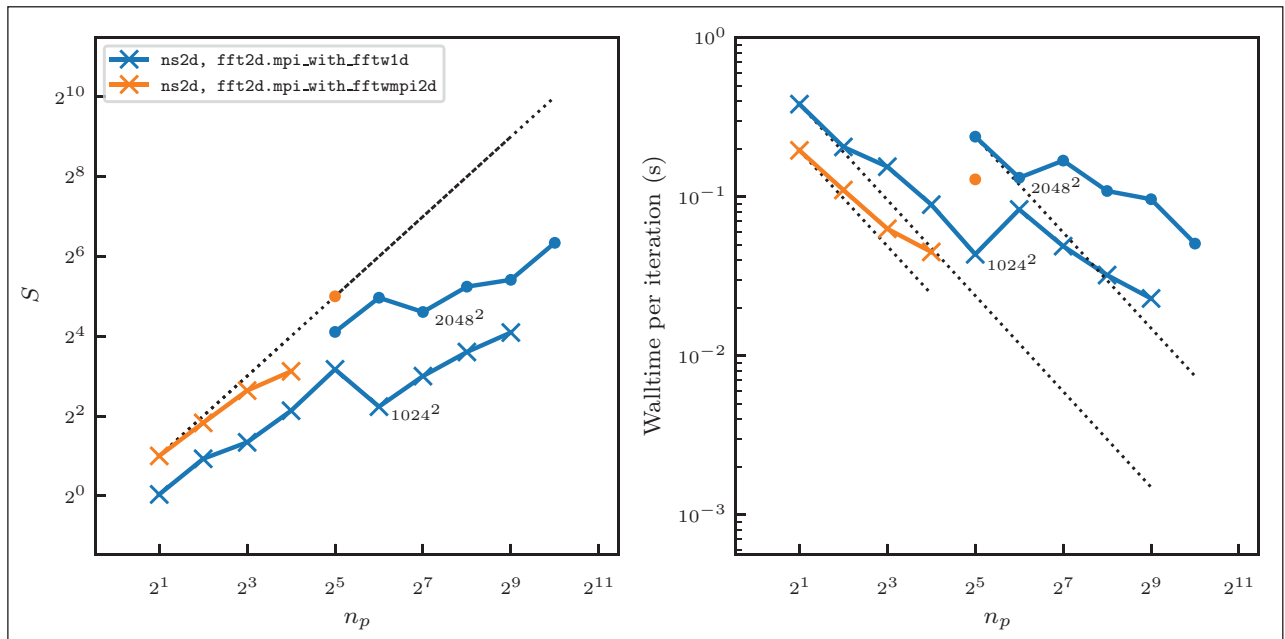


Figure 4: Strong scaling benchmarks of the 2D Navier-Stokes (`fluidsim.solvers.ns2d`) solver. The number of cores n_p goes from 2 to $2^{10} = 1024$. Crosses and dots correspond to 1024×1024 and 2048×2048 grid points, respectively.

mentioned earlier in Eq. 1. Ideal speedup is indicated with a dotted black line and it varies linearly with number of processes. We notice that for the 1024×1024 case there is an assured increasing trend in speedup for intra-nodes computation. Nevertheless, when this test case is solved with over a node ($n_p > 32$); the speedup drops abruptly. While it may be argued that the speedup is impacted by the cost of inter-node MPI communications via network interfaces, that is not the case here. This is shown by speedup for the 2048×2048 case, where speedup increases from $n_p = 32$ to 64, after which it drops again. It is thus important to remember that a decisive factor in pseudo-spectral simulations is the choice of the grid size, both global and local (per-process), and for certain shapes the FFT calls can be exceptionally fast or vice-versa.

From the above results, it may also be inferred that superior performance is achieved through the use of `fft2d.mpi_with_fftwmpi2d` as the FFT method. The `fft2d.mpi_with_fftw1d` method serves as a fallback option when either FFTW library is not compiled using MPI bindings or the domain decomposition results in zero-sized arrays. The latter is a known issue with the current version of `fluidfft` and `fluidsim` and requires further development.¹⁰ This is the reason why the scalability of `fft2d.mpi_with_fftwmpi2d` seems to be restricted in **Figure 4**, whereas in reality it can be scalable as `fft2d.mpi_with_fftw1d`. To the right of **Figure 4**, the real-time or walltime required to perform a single iteration in seconds is found to vary inversely proportional to the number of processes, n_p . The walltime per iteration ranges from 0.195 to 0.023 seconds for the 1024×1024 case, and from 0.128 to 0.051 seconds for the 2048×2048 case. Thus it is indeed feasible and scalable to use this particular solver.

3D benchmarks

Using a similar process as described in the previous section, the Navier-Stokes 3D solver (`fluidsim.solvers.ns3d`) is chosen to perform 3D benchmarks. As demonstrated in **Figure 5** two physical global grids with $128 \times 128 \times 128$ and $1024 \times 1024 \times 1024$ are used to discretize the domain. Other parameters are identical to what was described for the 2D benchmarks.

Through `fluidfft`, this solver has four FFT methods at disposal:

- `fft3d.mpi_with_fftw1d`
- `fft3d.mpi_with_fftwmpi3d`
- `fft3d.mpi_with_p3dfft`
- `fft3d.mpi_with_pfft`

The first two methods implements a 1D or *slab* decomposition, i.e. the processes are distributed over one index of a 3D array. And the last two methods implement a 2D or *pencil* decomposition. For the sake of clarity, we have restricted this analysis to the fastest FFT method of the two types in this configuration, namely `fft3d.mpi_with_fftwmpi3d` and `fft3d.mpi_with_p3dfft`. A more comprehensive study of the performance of these FFT methods can be found in [11].

In **Figure 5** the strong scaling speedup and walltime per iteration are plotted from 3D benchmarks in Beskow. The analysis here is limited to single-node and inter-node performance. For both grid-sizes analyzed here, the `fft3d.mpi_with_fftwmpi3d` method is the fastest of all methods but limited in scalability because of the 1D domain decomposition strategy. To utilize a large number of processors, one requires the 2D decomposition approach. Also, note that for the $1024 \times 1024 \times 1024$ case, a single-node measurement was not possible as the size of

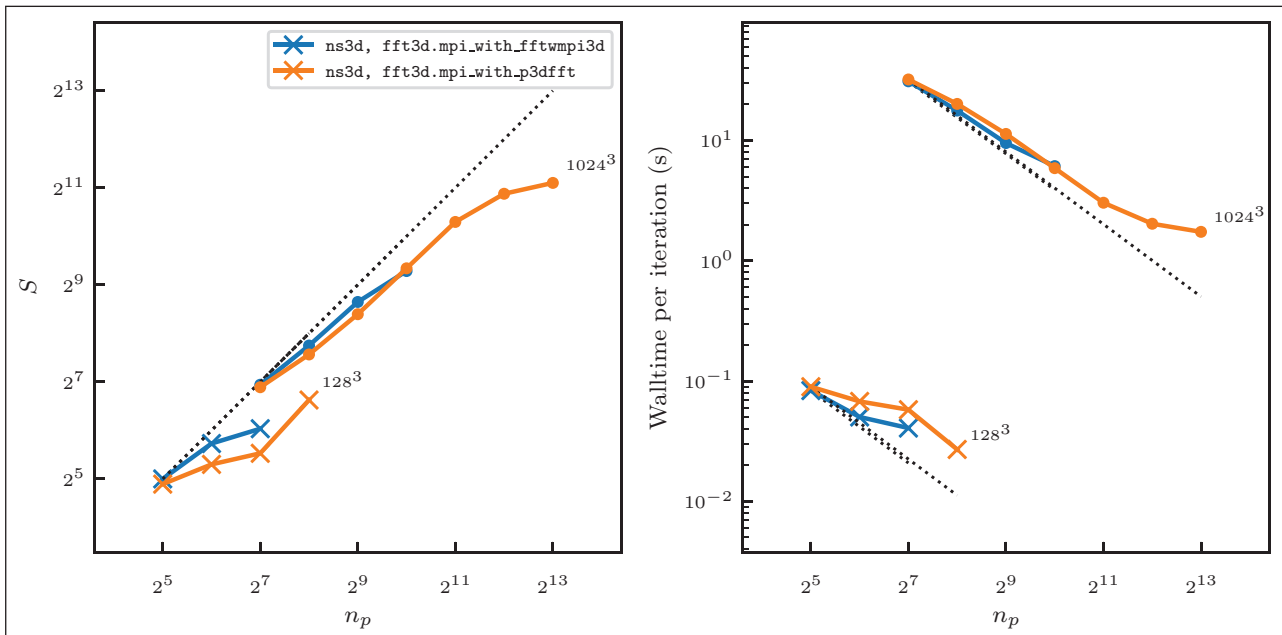


Figure 5: Strong scaling benchmarks of the 3D Navier-Stokes (`fluidsim.solvers.ns3d`) solver in Beskow. The number of cores n_p goes from $2^5 = 32$ to $2^{13} = 8192$. Crosses and dots correspond to 128^3 and 1024^3 grid points, respectively.

the arrays required to run the solvers exceeds the available memory. For the same case, a speedup reasonably close to linear variation is observed with `fft3d.mpi_with_p3dfft`. It is also shown that the walltime per iteration improved from 0.083 to 0.027 seconds for the $128 \times 128 \times 128$ case, and from 31.078 to 2.175 seconds for the $1024 \times 1024 \times 1024$ case.

CFD pseudo-spectral code comparisons

As a general CFD framework, `fluidsim` could be compared to OpenFOAM (a CFD framework based on finite-volume methods). However, in contrast to OpenFOAM, the current version of `fluidsim` is highly specialized in pseudo-spectral Fourier methods and it is not adapted for industrial CFD.

In this subsection, we compare `fluidsim` with three other open-source CFD pseudo-spectral codes¹¹:

- Dedalus [5] is “a flexible framework for spectrally solving differential equations”. It is very versatile and the user describes the problem to be solved symbolically. This approach is very different than the one of `fluidsim`, where the equations are described with simple Numpy code. There is no equivalent of the `fluidsim` concept of a “solver”, i.e. a class corresponding to a set of equations with specialized outputs (with the corresponding plotting methods). To run a simulation with Dedalus, one has to describe the problem using mathematical equations. This can be very convenient because it is very versatile and it is not necessary to understand how Dedalus works to define a new problem. However, this approach has also drawbacks:
 - Even for very standard problems, one needs to describe the problem in the launching script.
 - There is a potentially long initialization phase during which Dedalus processes the user input and prepares the “solver”.
 - Even when a user knows how to define a problem symbolically, it is not simple to understand how the problem is solved by Dedalus and how to interact with the program with Python.
 - Since solvers are not implemented out-of-the-box in Dedalus, specialized forcing scheme or outputs are absent. For example, the user has to implement the computation, saving and plotting of standard outputs like energy spectra.
- SpectralDNS [12] is a “high-performance pseudo-spectral Navier-Stokes DNS solver for triply periodic domains. The most notable feature of this solver is that it is written entirely in Python using Numpy, MPI for Python (`mpi4py`) and `pyFFTW`.”

Therefore, SpectralDNS is technically very similar to `fluidsim`. Some differences are that SpectralDNS has no object oriented API, and that the user has to define output and forcing in the launching script¹², which are thus usually much longer than for `fluidsim`. Moreover, the parallel Fourier transforms are done using the Python package `mpiFFTW4py`, which is only able to use the FFTW library and not other libraries as with `fluidfft` [11].

- NS3D is a highly efficient pseudo-spectral Fortran code. It has been written in the laboratory LadHyX and used for several studies involving simulations (in 3D and in 2D) of the Navier-Stokes equations under the Boussinesq approximation with stratification and system rotation [7]. It is in particular specialized in stability studies [4]. NS3D has been highly optimized and it is very efficient for sequential and parallel simulations (using MPI and OpenMP). However, the parallelization is limited to 1D decomposition for the FFT [11]. Another weakness compared to `fluidsim` is that NS3D uses simple binary files instead of HDF5 and NetCDF4 files for `fluidsim`. Therefore, visualization programs like Paraview or Visit cannot load NS3D data.

As with many Fortran codes, Bash and Matlab are used for launching and post-processing, respectively. In terms of user experience, this can be a drawback compared to the coherent framework `fluidsim` for which the user works only with Python.

Description of the test. We have formulated the benchmarks tests that all the aforementioned codes solve the Navier-Stokes equations expressed in the

- stream function-vorticity ($\psi - \zeta$) formulation for the bidimensional simulations,

$$\begin{aligned}\partial_t \hat{\zeta} &= -(\widehat{\mathbf{u} \cdot \nabla \zeta}) - \nu \kappa^2 \hat{\zeta} \\ -\kappa^2 \hat{\psi} &= \hat{\zeta} \\ \hat{\mathbf{u}} &= i \mathbf{k} \times \hat{\mathbf{e}}_{k_z} \hat{\psi}\end{aligned}$$

where the hat (^) notation signifies spectral quantities, \mathbf{u} , ν is the viscosity, and \mathbf{k} represents the velocity and wavenumber vectors, and $\kappa = |\mathbf{k}|$ (See `fluidsim.solvers.ns2d` solver documentation).

- rotational form for the tridimensional simulations,

$$\partial_t \hat{\mathbf{u}} = P_{\perp} (\widehat{\mathbf{u} \times \zeta}) - \nu \kappa^2 \hat{\mathbf{u}}$$

where the P_{\perp} operator projects the vector field onto a divergence free plane (see `fluidsim.solvers.ns3d` solver documentation and [6]) and is equivalent to a pressure correction step.

We compare the code with a very simple and standard task, running a solver for ten time steps with the Runge-Kutta 4 method. The solvers in `fluidsim` relies on `fluidfft` to perform the dealiasing operation applied to the non-linear terms (say, $\hat{\mathbf{N}}$) to ensure that no aliasing errors emerge in the course of the simulation. This is implemented by setting zeros according to this expression.

$$\hat{\mathbf{N}}(k_x, k_y) = 0 \text{ if } (k_x > C_d k_{max} \vee k_y > C_d k_{max})$$

where C_d stands for the coefficient of dealiasing and has a typical value of 2/3. Other codes, such as spectralDNS and Dedalus allows instead to zero-pad the spectral arrays with typically 3/2 times more modes along each wavenumber axis, an optimization which can potentially save significant

computation time.¹³ For quantitative comparisons and for the sake of simplicity, we limit ourselves to compare only sequential runs. We have already discussed in detail, the issue of the scalability of pseudo-spectral codes based on Fourier transforms in the previous section and in the companion paper [11].

In contrast to the framework `fluidsim` for which it is easy to define a new solver for a new set of equations, NS3D is specialized in solving the Navier-Stokes equations under the Boussinesq approximation. Using NS3D to solve a new set of equations would require very deep changes in many places in the code.

Note that Dedalus does not implement the standard fully explicit RK4 method¹⁴. Thus for Dedalus, we use the most similar time stepping scheme available, RK443, a 4-stage, third-order mixed implicit-explicit scheme described in [1]. Note that in the other codes, part of the linear terms are also treated implicitly. Also note that in several cases, the upper bound of time step is not first limited by the stability of the time scheme, rather by other needs (to resolve the fastest wave, accuracy, etc.), so these benchmarks are representative of elapsed time for accurate real-life simulations.

Bidimensional simulations. We first compare the elapsed times for two resolutions (512^2 and 1024^2) over a bidimensional space. The results are summarized in **Table 3**. The results are consistent for the two resolutions. `fluidsim` is the fastest code for these cases. Dedalus

Table 3: Elapsed times (in seconds) for ten RK4 time steps for two bidimensional cases and the four CFD codes.

	<code>fluidsim</code>	Dedalus	SpectralDNS	NS3D
512^2	0.51	1.53	0.92	0.82
1024^2	2.61	8.00	3.48	3.96

is three times slower than `fluidsim` but as discussed earlier, the time stepping method is different. Another notable issue of Dedalus is a long initialization time (more than 3 min for 1024^2 compared to approximately 5 s for `fluidsim`). Also note that Dedalus has been optimized for bounded domains with Chebyshev methods. The two other codes SpectralDNS and NS3D have similar performance: slightly slower than `fluidsim` and much faster than Dedalus. The Fortran code NS3D is slower (by 47%) than the Python code `fluidsim`. This can be explained by the fact that there is no specialized numerical scheme for the 2D case in NS3D, so that more FFTs have to be performed compared to SpectralDNS and `fluidsim`. This highlights the importance of implementing a well-adapted algorithm for a class of problems, which is much easier with a highly modular code as `fluidsim` than with a specialized code as NS3D.

Tridimensional simulations. We now compare the elapsed times for ten RK4 time steps for a tridimensional case with a resolution 128^3 . Dedalus is slow and does not seem to be adapted for this case so we do not give exact elapsed time for this code. SpectralDNS is slightly slower (11.55 s) than the two other codes (9.45 s for `fluidsim` and 9.52 s for NS3D). This difference is mainly explained by the slower FFTs for SpectralDNS.

Figure 6 presents a more detailed comparison between NS3D (blue bars) and `fluidsim` (yellow bars). The total elapsed times is mainly spent in five tasks: FFTs, Runge-Kutta 4, curl, vector product and “projection”. The times spent to perform these tasks are compared for the two codes.

We see that FFTs in NS3D are very fast: the FFT execution is 0.55 s longer for `fluidsim` (nearly 9% longer). This difference is especially significant for sequential run for which there is no communication cost involved in the FFT computation, thus making it the least favorable case

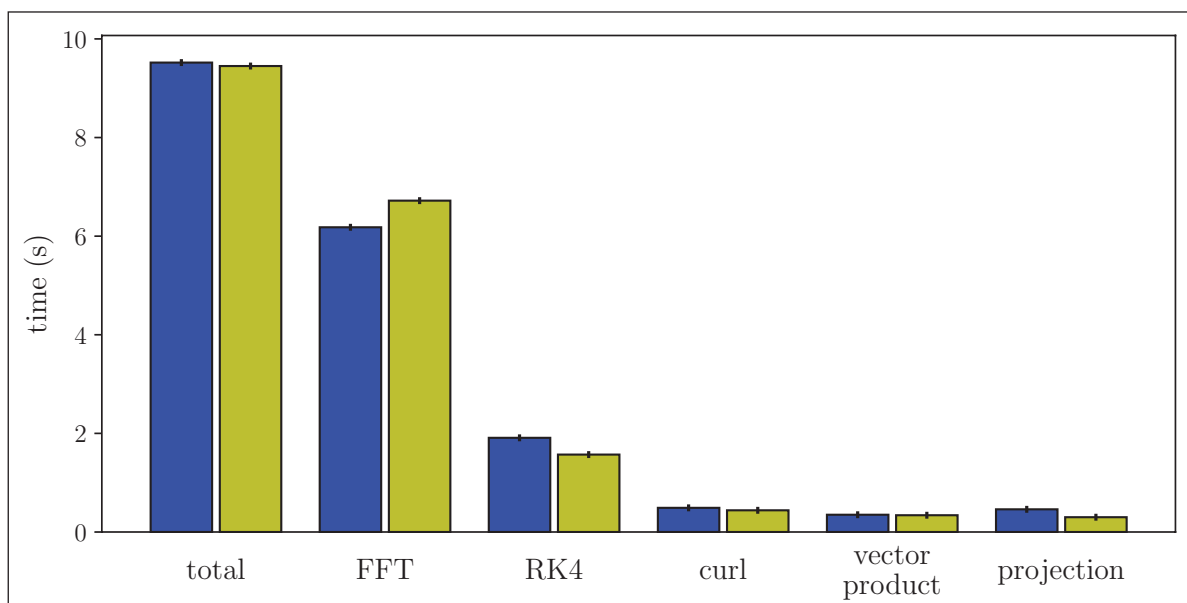


Figure 6: Comparison of the execution times for a 3D case (128^3 , 10 time steps) between NS3D (blue bars) and `fluidsim`. The first two bars correspond to the total time and the others to the main tasks in terms of time consumption, namely FFT, Runge-Kutta 4, curl, vector product and “projection”.

for `fluidsim`. Indeed, MPI communications are input-output bounded tasks which are not faster in Fortran than in Python.

This difference can partially be explained by the fact that in NS3D, all FFTs are in-place (so the input can be erased during the transform). On one hand, this choice is good for performance and for a lower memory consumption. On the other hand, since the same variables are used to store the fields in real and in Fourier spaces, it makes the code harder to write, to understand and to modify. Since memory consumption in clusters is much less of a problem than in the past and that code simplicity is highly important for a framework like `fluidsim`, we choose to use out-of-place FFTs in `fluidsim`. Another factor is that the flag `FFTW_PATIENT` is used in NS3D which leads to very long initialization and sometimes faster FFTs. Since we did not see significant speed-up by using this flag in `fluidsim` and that we also care about initialization time, this flag is not used and we prefer to use the flag `FFTW_MEASURE`, which usually leads to similar performance.

Time stepping in NS3D is significantly slower than in `fluidsim` ($0.34 \text{ s} \approx 20\%$ slower). We did not find a performance issue in NS3D. The linear operators are slightly faster in `fluidsim` than in the Fortran code NS3D. This is because this corresponds to Pythran functions written with explicit loops (see [11]).

Although the FFTs are a little bit faster for NS3D, the total time is slightly smaller (less than 1% of the total time) for `fluidsim` for this case.

These examples do not prove that `fluidsim` is always faster than NS3D or is as fast as any very well optimized Fortran codes. However, they do demonstrate that our very high-level and modular Python code is very efficient and is not slower than a well-optimized Fortran code.

Quality control

`fluidsim` also packages unit tests to go alongside the related modules. Throughout the development process it is made sure that all tests pass on a priority-basis, especially prior to a release, to ensure that new changes to package does not damage existing functionality.

A part of the unit tests checks the solvers for verifiable conservation laws such as, enstrophy and energy conservation due to non-dissipative terms in the governing equations. Thus we ensure the accuracy of the solutions and also to some degree prevent arithmetic and logic errors. The remainder of tests are meant to verify the robustness of the code for example, to avoid passing unexpected inputs between functions. These tests can prevent common error types such as syntax errors, I/O errors, run time errors and compilation errors (for the extensions).

It is also important to quantify the completeness of the tests, and this is done by calculating the code coverage. Code coverage is the ratio of the number of lines tested by unit tests over the total number of lines in the whole package. For the present version of `fluidsim` the code coverage is valued at approximately 70%. For `fluidsim`, the code coverage results are displayed at Codecov. `fluidsim` has also been checked by comparing its results for well-known verification problems, as for example the

Taylor-Green vortices for the incompressible Navier-Stokes equations.¹⁵ We also try to follow a consistent code style as recommended by PEP (Python enhancement proposals) 8 and 257. This is also inspected using lint checkers such as `flake8` and `pylint` among the developers. The code is regularly cleaned up using the Python code formatter `black`.

All the above quality control techniques are implemented within the continuous testing solutions, Travis CI and Bitbucket Pipelines. Instructions on how to run unit tests, coverage and lint tests are included in the documentation.

(2) Availability

Operating system

Any POSIX based OS, such as GNU/Linux and macOS.

Programming language

Python 2.7, 3.4 or above. For the next versions, we will drop Python 2.7 support and Python ≥ 3.6 will be required.

Dependencies

- **Minimum:** `fluiddyn`, `Numpy`, `h5netcdf`, `fluidfft` (and FFT libraries, see [11]).
- **Optional:** `Scipy`, `mpi4py`, `Cython` and `Pythran`, `pulp`.

List of contributors

- Ashwin Vishnu Mohanan (KTH): Development of the shallow water equations solver, `fluidsim.solvers.swll`, testing, continuous integration, code coverage and documentation.
- Cyrille Bonamy (LEGI): Extending the sub-package `fluidsim.operators.fft` (currently deprecated) into a dedicated package, `fluidfft` used by `fluidsim` solvers.
- Miguel Calpe (LEGI): Development of the 2D Boussinesq equation solver, `fluidsim.solvers.ns2d.strat`.
- Pierre Augier (LEGI): Creator of `fluidsim` and Fluid-Dyn project, developer of majority of the modules and solvers, future-proofing with Python 3 compatibility and documentation.

Software location

Archive

Name: PyPI

Persistent identifier: <https://pypi.org/project/fluidsim>

Licence: CeCILL, a free software license adapted to both international and French legal matters, in the spirit of and retaining compatibility with the GNU General Public License (GPL).

Publisher: Pierre Augier

Version published: 0.2.2

Date published: 02/07/2018

Code repository

Name: Bitbucket

Persistent identifier: <https://bitbucket.org/fluiddyn/fluidsim>

Licence: CeCILL

Date published: 2015

Emulation environment

Name: Docker

Persistent identifier: <https://hub.docker.com/r/fluiddyn/python3-stable>

Licence: CeCILL-B, a BSD compatible French licence.

Date published: 02/10/2017

Language

English

(3) Reuse potential

fluidsim can be used in research and teaching to run numerical simulations with existing solvers. Its simplicity of use and its plotting capacities make it particularly adapted for teaching. fluidsim is used at LEGI and at KTH for studies on geophysical turbulence (see for example [9]). Since it is easy to modify any characteristics of the existing solvers or to build new solvers, fluidsim is a good tool to carry out other types of simulations for academic studies. The qualities and advantages of fluidsim (integration with the Python ecosystem and the FluidDyn project, documentation, reliability – thanks to unit tests and continuous integration –, versatility, efficiency and scalability) make us think that fluidsim can become a true collaborative code.

There is no formal support mechanism. However, bug reports can be submitted at the Issues page on Bitbucket. Discussions and questions can be aired on instant messaging channels in Riot (or equivalent with Matrix protocol)¹⁶ or via IRC protocol on Freenode at #fluiddyn-users. Discussions can also be exchanged via the official mailing list.¹⁷

Notes

¹ See [13] for a similar discussion.

² See [3], wiki.haskell.org/Why_Haskell_matters.

³ See fluidsim.readthedocs.io/en/latest/tutorials.html.

⁴ Inheriting from the base class `fluidsim.base.solvers.info_base.InfoSolverBase`.

⁵ Inheriting from the base class `fluidsim.base.solvers.base.SimulBase`.

⁶ Inheriting from the base class `fluidsim.base.state.StateBase`.

⁷ See fluiddyn.readthedocs.io/en/latest/generated/fluiddyn.util.paramcontainer.html.

⁸ Example on modifying the parameters for a simple simulation: fluidsim.readthedocs.io/en/latest/examples/running_simul.html.

⁹ See ipython.readthedocs.io.

¹⁰ See FluidFFT issue 4.

¹¹ For the sake of conciseness, we limit this comparison to only four codes. We have also found the Julia code `FourierFlows.jl` to demonstrate interesting performance for 2D sequential runs, but without support for 3D cases and MPI parallelization.

¹² See the demo scripts of SpectralDNS.

¹³ See FluidFFT issue 21.

¹⁴ See the Dedalus issue 38.

¹⁵ An demonstration is documented as an example in the online FluidSim documentation.

¹⁶ <https://matrix.to/#/#fluiddyn-users:matrix.org>.

¹⁷ <https://www.freelists.org/list/fluiddyn>.

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Competing Interests

The authors have no competing interests to declare.

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