**automan**: a simple, Python-based, automation framework for numerical computing

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February 6, 2018

**Abstract**

We present an easy-to-use, Python-based framework that allows a researcher to automate their computational simulations. In particular the framework facilitates assembling several long-running computations and producing various plots from the data produced by these computations. The framework makes it possible to reproduce every figure made for a publication with a single command. It also allows one to distribute the computations across a network of computers. The framework has been used to write research papers in numerical computing. This paper discusses the design of the framework, and the benefits of using it. The ideas presented are general and should help researchers organize their computations for better reproducibility.

1 Introduction

It is well known that reproducibility is a cornerstone of science. Clearly, reproducibility (or repeatability) is vitally important for computational science as well. Barba [1] provides a succinct overview of some of the most important articles on reproducibility. Ensuring repeatability in computational work takes additional effort. Unfortunately, there are not many immediate or direct incentives for a researcher to invest time in building systems that ensure repeatability. Further, as discussed in [5], there can be significant challenges involved in carefully repeating and replicating numerical experiments.

In this paper we discuss how we automated a computational research paper. We believe that this is a very important step in facilitating reproducible research. The approach used in our automation framework is fairly general and could be of use to other researchers. Our implementation is open source and available at [http://github.com/pypr/automan](http://github.com/pypr/automan). What is perhaps more important is that we discovered that repeatability can be very profitable to the researcher. This is important since it provides an incentive for one to invest time in making computational research repeatable. It is our hope that the ideas discussed in the current work and our framework are of general use and facilitate greater reproducibility in computational science.

Many computational science papers tend to involve the following tasks:

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run several computations, each requiring several hours to complete. The programs executed are typically compiled programs written in a low-level language like FORTRAN, C, or C++. Sometimes these may be implemented in a higher-level language like Python or MATLAB. Regardless of the choice of programming language, researchers often need to run different programs with various parameters.

- compare results generated by different computational methods and compare computational results with theoretical or experimental data.

- collate these results into a variety of plots, tables, and other forms suitable for sharing in the form of a publication.

Once these plots and tables are generated, the authors can complete a manuscript describing the novelty of the study along with the results of the study.

Our automation framework, called automan, was used to automate the computations performed during the development of a Smoothed Particle Hydrodynamics (SPH) scheme that we implemented called the “Entropically Damped Artificial Compressibility SPH” [8], the scheme is henceforth called EDAC-SPH.

SPH is a particle-based scheme that can be used to simulate a wide variety of problems (see [6] for a review). There are many SPH “schemes” in the literature. In our work, we needed to compare our results with established SPH schemes as well as known exact solutions and experimental data. The framework allowed us to:

- run all simulations and produce all the figures for the manuscript with a single command.

- incrementally add, modify, and rerun simulations.

- easily plot and compare a variety of similar simulations.

- modify and update any of the figures and plots without needing to re-run the long-running simulations.

- distribute our simulations on a collection of other idle desktop computers on the network.

The framework is implemented entirely in Python [14]. There are several automation frameworks that already exist. We had initially used pydoit [11] and later luigi [2]. Both of these tools are certainly very useful and many of the ideas used in the current framework are inspired from there. Lancet [13] provides very interesting abstractions of how to parametrize, and specify simulations, however, it does not offer any task management or automation facilities.

The venerable ReDoc [12] offers a general strategy to automate tasks using a Makefile with a small amount of custom rules that they provide. These allow a scientist to create, view, delete any figures produced and also clean any intermediate results produced. They also suggest that researchers segregate their files into three different categories of files based on how easy they are to recreate. The ideas provided by ReDoc are very important,
however, the details of the implementation are not always optimal for long running computations on loosely distributed computers. Make is best suited for compiling programs and the execution and scheduling of the tasks is not easy to control or modify. Further, ReDoc does not help abstract key tasks that are important when analyzing computational simulations. Our framework attempts to address some of these.

Sumatra \[\text{3}\], takes a more comprehensive approach by providing a suite of commands to capture the details of all computational experiments including the versions of the dependent packages that are used to run every command. This provides a much more comprehensive framework. Our framework is orthogonal to the goals of Sumatra and makes it easier to manage a collection of tasks. We do not capture the entire environment or track the results themselves. As such, it is possible to use the sumatra framework with ours.

Nextflow \[\text{4}\] is a very powerful package for reproducibility. It provides a domain specific language for specifying, and executing computational pipelines. It can optionally use docker containers to provide repeatability in computational simulations. It interfaces well with existing pipelines written in other scripting languages. Our approach is much simpler, and completely implemented in Python. Given that our analysis and post-processing code is written in Python, our framework is a more natural fit for us. In addition our framework provides some general abstractions to group and split the simulations and avoid repetitive code.

Our framework provides the following core features:

- the ability to define arbitrary tasks and their dependencies in Python. This is exactly similar to what is provided by the luigi package \[\text{2}\] mentioned above.
- the ability to perform post-processing using the convenience of Python. The framework provides several convenient abstractions that make this easier to do.
- minimize repetitive code for comparison of similar computational schemes.
- control the scheduling and execution of tasks, including running tasks on remote computers.

We point out several common patterns and abstractions that were useful in implementing our framework. These ideas are general and could allow other researchers to better organize their own computations for reproducibility.

In the following, we use examples from our computations in order to demonstrate the automation framework. The remainder of the paper is organized as follows. We provide a brief, high-level background of our research paper in order to provide a context for the automation framework. We then discuss the overall design of our framework. We discuss how the framework allowed us to distribute the computations across generic Linux/MacOS computers on the network accessible via `ssh`. We discuss how our implementation provided features that were not readily available in many other tools and discuss possible future directions of the framework.
2 Background

As mentioned in the introduction, computational work often requires executing programs that run for a long period of time. This can be anywhere from a few hours to several days and sometimes weeks. The programs are often to be run with different initial conditions or parameters in order to explore a variety of questions. After these simulations are run, researchers need to compare the results of these computations and produce plots and tables that are assembled into a manuscript.

Typically these individual simulations are run manually, thereafter, plots and tables are made manually and then added to a manuscript. This workflow does not scale and does not lend itself for easy reproducibility. The recommendations of Wilson et al. [15] and Sandve et al. [10] provide very general guidelines to make this workflow more productive, reliable, and reproducible.

In this paper we use the Smoothed Particle Hydrodynamics method as a typical example of a numerical method. As with any established numerical method, there are different variants of the basic method. In the following we use the term “scheme” to denote a variant of a basic numerical method. In our research work [8], a new SPH scheme called EDAC-SPH was being developed to simulate incompressible fluid flow problems. This scheme was compared with an established scheme called the Weakly-Compressible SPH formulation (WCSPH) as well as a recent SPH formulation called the Transport-Velocity Formulation (TVF).

The entire implementation of the WCSPH, TVF, and new schemes was made using the PySPH framework [7, 9]. The PySPH framework allows users to write the SPH schemes and programs in the Python programming language. Each program solving a benchmark problem, written using PySPH, supports a variety of command line arguments to configure various parameters. Users are encouraged to add their own command line options to their scripts. While all of the examples in this work use Python, it is important to note that one may use any executable program or script with automan.

A simple workflow for performing the necessary numerical simulations would involve the following steps:

1. Break-up each benchmark problem into several command line program invocations that can be executed independently. Each of these simulations is typically called a “case”.

2. For each benchmark problem, execute each of the simulations (cases).

3. Once the simulations are completed, gather the post-processed data or perform additional post-processing and create any plots or tables.

4. Assemble the relevant plots for the manuscript.

The above workflow works best when the programs support command line arguments to setup various parameters. This can be extended to cases which require specific input files as well. The framework requires that each case produce any output files in a specified and configurable directory.
We consider a few example problems to clarify the above. In the case of our research, one of the problems we simulated is the Taylor-Green-Vortex problem (TGV) which has a known exact solution. We needed to simulate several cases of this problem with nine different variants of SPH schemes. These results needed to be compared. The command line programs for these would typically be of the following form:

- Use the WCSPH scheme as implemented in the pysph package (note that the command "pysph run" executes a standard PySPH example):

  $ pysph run taylor_green --scheme wcsph --nx 50 -d wsph

- Use the WCSPH scheme and add a tensile correction with the default value of nx:

  $ pysph run taylor_green --scheme wcsph --tensile-correction -d tc

- Use the TVF scheme (the code is a Python script in this case):

  $ python taylor_green.py --scheme tvf --nx 50 -d tvf

The "-d path" argument ensures that the results are written to the specified path. Once each of these commands complete, the results of the simulation along with any post-processing are made available inside the respective directories. Typically, PySPH scripts create a results.npz file which contains any post-processed results in raw form. The .npz extension is used to store standard NumPy arrays. These results then need to be compared and plotted. Sometimes new post-processing is necessary for the purposes of a manuscript that may not be relevant to the case itself. This represents part of a single benchmark problem being explored. There will typically be many more cases and benchmark problems to simulate.

Clearly, command line arguments are used extensively here. If the user has to create different input files to run these simulations, that could also be supported by the framework. However, having extensive command line argument support greatly facilitates the automation of the simulations.

In the next section we describe how the new framework can be used to automate the execution and post-processing of these simulations.

3 Design of the automation framework

The general approach to using the framework is as follows:

- Each set of related simulations are grouped into what is called a “Problem”. Each problem also contains Python code for producing different plots from these simulations. Users create subclasses of a base “Problem” class to customize the required simulations and analysis for that particular problem. This is illustrated in Fig 1. The post-processing generates content that can be immediately used in a manuscript.
• Each simulation to be run can be created as either an instance of a “Simulation” class or specified as a command string to be executed. The simulation class makes it very easy to abstract common plotting tasks for a given kind of simulation.

• All the problem classes are collected and passed to an “Automator” instance which is given two directory paths, one for the simulation outputs and one for the final manuscript figures. This object checks if the final outputs are already made, if not, it runs any necessary simulations (if their output is not already created) and the Python code for producing the plots. The simulations can be run either on the local machine or distributed across a cluster of machines. This is done by delegating them to a task runner which in turn delegates the actual execution to a scheduler. This is illustrated in Fig 2.

![Diagram of problem encapsulating simulations and post-processing](image)

Figure 1: Sketch illustrating how a Problem encapsulates several simulations and some post-processing which produces content for the manuscript.

3.1 Simple example

We consider a simple example to elaborate the design discussed in section 3. Listing 1 shows the outline of the contents of a file, automate.py, illustrating the use of the automation framework.

Listing 1: automate.py illustrating the automation framework.

```python
def in automan.api import Problem, Simulation, Automator
```
Figure 2: Sketch of the overall design of the automator which manages several problems and executes the simulations.

```python
3 class TaylorGreen(Problem):
4     def get_name(self):
5         return 'taylor_green'
6
7     def setup(self):
8         pysph_cmd = 'pysph run taylor_green'
9         self.cases = [
10             Simulation(
11                 root=self.input_path('std_sph'),
12                 base_command=pysph_cmd,
13                 job_info=dict(n_core=1, n_thread=2),
14                 scheme='wcsph', nx=50
15             ),
16             Simulation(
17                 root=self.input_path('std_sph_tensile_correction'),
18                 base_command=pysph_cmd,
19                 job_info=dict(n_core=1, n_thread=2),
20                 scheme='wcsph', nx=50, tensile_correction=None
21             ),
22             # ...
23         ]
24
25     def run(self):
26         self.make_output_directory()
27         self._plot_decay_error_all()
28         self._plot_decay_error()
29```
automator = Automator(
    simulation_dir='outputs',
    output_dir='manuscript/figures',
    all_problems=[TaylorGreen]
)
automator.run()

We start by looking at the automator object (lines 30–34). It is passed two directory names, 'outputs' and 'manuscript/figures' as well as a list of Problem classes. The outputs directory will contain the outputs generated by the simulations and the other will contain the final plots for the manuscript. The automator instance has a run method that is executed to perform the automation. Several things can be noted in the TaylorGreen class (starting at line 3) which is a subclass of the Problem class.

- The get_name method (lines 4-5) returns a name which is a sub-directory containing all relevant outputs for this particular problem. When this problem is executed, all the simulation outputs will be inside outputs/taylor_green/. The figures will be inside manuscript/figures/taylor_green/.

- The setup method (lines 7-23) simply creates a collection of cases. Each case is an instance of a Simulation class. Each simulation is given a root path and a basic command along with some information on the number of cores and threads desired. The n_core argument is used to distribute the load to different machines depending on the availability of free cores. The number of threads is a parameter used by OpenMP. All subsequent keyword arguments are converted to command line arguments automatically.

  The simulation instances are passed additional options explicitly as keyword arguments in Python instead of in the command string to make it easy to filter cases for post-processing. For example, it is possible to easily filter all the cases which have nx=50 and scheme='wcsph'. This is discussed later.

- The run method (lines 25–28) performs any post-processing of the outputs in order to produce the final figures for the manuscript. The details of the methods self._plot_decay_error_all() etc. (lines 27, 28) are not discussed here. They are simple functions that make any necessary plots. The simulation instances make it easy to refer to files within the simulation output.

The automate.py completely specifies the simulations. The plotting code is routine Python (and not shown in the listing). To use the automation script, a user runs:

$ python automate.py

The automator first checks if manuscript/figures/taylor_green directory exists. If it does not, all the simulations are executed and the plotting code is called automatically after the simulations complete.

It is often necessary to modify or change the plots without re-running the simulations, this can be achieved by executing:
To re-run completed simulations, one must explicitly delete the appropriate directories in the `outputs` directory. On the other hand, if the simulation code itself fails, one may simply correct the simulation code and re-run the automation script, and the corrected code will be executed again.

In similar fashion, a user could create any number of `Problem` classes and all of their simulations and post-processing will be executed if these classes are passed to the automator (see line 33 in Listing 7).

When the `automate.py` script is executed, it simulates all problems by default. This is sometimes inconvenient when one wishes to only create the plots for a particular problem, this can be done by specifying the particular problem, for example:

```
$ python automate.py -f TaylorGreen EllipticalDrop
```

will execute only the Taylor-Green and elliptical drop problems. The name of the problem specified is not case sensitive.

When working actively on research, there are times when one may wish to run just one particular simulation out of the many for a problem. In this case, one can do the following:

```
$ python automate.py TaylorGreen -m "*tensile*"
```

This will run just a specific set of simulations that match the criterion, and in this case it will run the `std_sph_tensile_correction` case. It will not execute the post-processing code since the other cases may not have been run. This is particularly useful if one only wants to run a few simulations without generating all the plots for the problem. The search criterion is matched using standard Unix `fnmatch` patterns to make it easy to select specific cases to run.

### 3.2 More details on simulations and problems

The `Simulation` and `Problem` classes are clearly important in the above example and these classes provide some convenient functionality. Creating a `Simulation` object is generally done as follows:

```
>>> s = Simulation(root_dir, base_command, job_info, **kw)
```

The simulation object stores a path (`root_dir`) to where the simulation output should be generated and is given a basic command line to run. The argument `job_info` is optional and helps specify the execution context in terms of number of cores and threads needed by the simulation. Any additional keyword arguments are converted into command line arguments using the `get_command_line_args` method of the class. This makes it easy to customize the command line arguments. There are other methods provided to facilitate convenient access to the data generated by the simulation and making plots from the outputs. These are illustrated by way of an example below (on an interactive Python interpreter):
Listing 2: Illustration of Simulation class usage and behavior.

```python
>>> s = Simulation(
...   'outputs/sph',
...   'pysph run elliptical_drop',
...   job_info=dict(n_core=1, n_thread=2),
...   timestep=0.005,
...   tensile_correction=None
... )

>>> s.name
'sph'

>>> s.command
'pysph run elliptical_drop --timestep=0.005 --tensile-correction'

>>> s.get_command_line_args()
'--timestep=0.005 --tensile-correction'

>>> s.input_path('results.npz')
'outputs/sph/results.npz'

>>> s.data.fid
<open file 'outputs/sph/results.npz' ...>

>>> s.render_parameter('tensile_correction')
'tensile_correction'

>>> s.get_labels(['timestep'])
'timestep=0.005'
```

Note that each simulation has a name which is the name of directory in which the output is generated. The command property has automatically converted the parameters timestep, tensile_correction to suitable command line arguments. It is important to note again that the commands that are executed such that one may configure the output directory in which they will generate output using a command line argument. In the present case, this additional command line argument is added by the PySPHTask discussed later below. If a user wishes to specify this in the simulation one could use the special string $output_dir to specify the directory and this will be automatically substituted. For example one could specify the simulation as follows:

```python
>>> s = Simulation('outputs/sph', 'command -d $output_dir')
```

Here, the $output_dir will be substituted with the actual directory name when the simulation is executed by a task.

The input_path method makes it easy to refer to a path inside the output directory. The render_parameter method returns a string for each parameter given to it. This is convenient when one wishes to ensure that when a legend is rendered for a parameter (say alpha which is to be rendered as $) that it uses a suitable LaTeX label. A user
may choose to configure it to their needs. The \texttt{get\_labels}, renders out multiple such parameters suitable for a legend.

The class also provides a \texttt{data} property that returns the data loaded from a \texttt{results.npz} file generated by many PySPH examples. Clearly, this will need to be configured to suit other packages. This property makes it easy to plot post-processed results.

When many plots needed to be made from a given kind of simulation, it is convenient to create a customized subclass of the \texttt{Simulation} class. For the paper in [8], there were around 45 Taylor-Green simulations to make. This required a custom subclass as below:

Listing 3: Example illustrating a custom subclass of the \texttt{Simulation}.

```python
1 class TGV(Simulation):
2     def get_command_line_args(self):
3         # ...
4     def render_parameter(self, param):
5         # ...
6     def l1(self, **kw):
7         import matplotlib.pyplot as plt
8         data = self.data
9         plt.plot(data[‘t’], data[‘l1’], **kw)
10        plt.xlabel(‘t’); plt.ylabel(r’$L_1$ error’)
```

This implementation overrides the default to customize how the command line arguments are generated. The parameter rendering is also changed from the default. Several convenient plotting methods are implemented and we show only one \texttt{l1} (line 6 above). This method plots the $L_1$ error using \texttt{matplotlib}.

Since the parameters of interest are passed to a simulation as additional keyword arguments, it is possible to filter out specific cases for comparison. The automation framework provides a few convenient functions. For example, take the case where we wish to plot the $L_1$ error for cases with different numerical schemes but where \texttt{nx=50}. Recall that the actual plots are made by the \texttt{Problem} class, in our example, this is the \texttt{TaylorGreen} class in listing 1 and the code for the plots would be:

Listing 4: Example illustrating convenient functions for post-processing simulations.

```python
1     def _plot_decay_error_all(self):
2         import matplotlib.pyplot as plt
3         cases = filter_cases(self.cases, nx=50, perturb=0.2)
4         plt.figure()
5         compare_runs(cases, ‘l1’, labels=[‘scheme’])
6         plt.legend(loc=’upper left’)  
7         plt.savefig(self.output_path(‘l1_error_all.pdf’))
8         plt.close()
```

There are two new functions introduced here:

- \texttt{filter\_cases}: this function is given a sequence of cases and any additional parameters (see line 4 above). It filters out the cases that satisfy the particular parameters.
In the code above, all the cases with \texttt{nx}=50 with \texttt{perturb}=0.2 are returned.

- \texttt{compare_runs}: calls the given method name ('\texttt{l1}' in line 7 above) for all the cases and labels them with the given set of labels to be indicated in the plot. It can also be passed a method name for an exact solution plot. Instead of method names, any callable function can be passed. When this function is called, it is passed the simulation instance.

An additional convenience function is \texttt{filter_by_name} which picks the cases given particular names.

These methods make it easy to manage many simulation instances and quickly produce a publication-ready plot comparing various aspects of the simulations. In our case, we had one \texttt{Problem} class with 16 instances of the \texttt{TGV} simulation object and another with 29. The plotting code is not repeated as it is abstracted out in the \texttt{TGV} class. The filtering functions along with the \texttt{compare_runs} function allows us to compare any number of specific simulations very easily. This greatly reduces the repetitive plotting code for a large number of plots.

The \texttt{Problem} class has been used in listing 1 and collects various \texttt{Simulation} instances and specifies how the simulations are compared to produce a variety of outputs. The problem class has the following important features:

- A problem class is always passed the simulation directory and the output directory. In our example above, this would correspond to ’\texttt{outputs}’ and ’\texttt{manuscript/figures}’ respectively. Instantiating the class does not result in any computations being executed.

- The \texttt{get_name} method is used to specify the directory for this particular problem which collect both the simulation outputs and the figures.

- The \texttt{setup} method is used to define the various simulation cases. We have already seen this method used in the initial example, Listing 1.

- The \texttt{run} method is used to compare the simulations and produce the necessary output. This has also been seen earlier.

- The \texttt{input_path} and \texttt{output_path} methods are convenience methods to help find files in the input and output directories.

- The \texttt{get_commands} method returns a list of commands to execute in order to run the simulations.

- The \texttt{get_requires} method returns a list of tasks to execute in order to run the simulations. Tasks are discussed in the next section and allow the user to define the commands to be executed in a powerful way. By default, the tasks are automatically created from the commands. Users may overload this method to create tasks in other ways.
The Simulation and Problem classes thus allow the user to specify the simulations to be executed and how these are to be compared. This is sufficient information to start using the framework. The next sections discuss the execution of the tasks as well as the simple cluster management that is available.

3.3 Scheduling and execution of tasks

The automation framework provides a simple design for tasks inspired by the elegant design of Luigi’s [2] tasks. A task has three important methods:

- **complete**: this indicates if the task has successfully completed. This method should raise an exception if there is an error while running the task.

- **run**: this executes the task.

- **requires**: this produces a sequence of other tasks that should be completed before this task may be run.

This design allows one to create complex pipelines with dynamic task generation and dependencies. A PySPHTask class subclasses the Task class and provides methods that make it easy to execute a PySPH simulation, and check if a simulation has completed. It also adds a suitable command line argument to the command in order to have PySPH generate its output in the correct directory. A more general CommandTask is available which can be used by users who are not using PySPH.

A simple WrapperTask is provided which is complete when all of its required tasks are complete. A SolveProblem task subclass generates the tasks required to simulate a particular problem and runs the problem’s run method when all the simulations are complete. A RunAll wrapper task instantiates and executes the given problem classes using the SolveProblem instances. This is illustrated in Fig 3.

A TaskRunner class executes the various tasks in the correct order such that the required tasks are completed first. The tasks are not directly executed by the TaskRunner. Instead, the execution is passed on to a Scheduler. A Job class encapsulates the command that needs to be executed, this includes the environment variables, the number of cores to use, the output directory etc. A Worker class encapsulates a computer that may execute the job. A LocalWorker handles local executions and a RemoteWorker handles remote executions via ssh. A Scheduler manages these workers and is configured using a simple configuration file. Each time a PySPH task executes, it creates a Job instance and passes it to the scheduler. The scheduler checks for any free workers (by checking the CPU load of the computer) and submits the job to the worker. While tasks are pending or running, TaskRunner polls the current tasks every so often to see if they are completed. As soon as tasks are completed, any remaining tasks are scheduled for further execution. The TaskRunner and Scheduler are illustrated crudely in the Fig 3.

In this fashion, the tasks are separated from the actual execution of the programs. This allows one to run the jobs locally or remotely. The outputs generated on remote computers is copied to the computer where the automate script is executed. Currently, only local execution and execution via SSH is supported but it is relatively easy to extend this to support other kinds of execution contexts.
Figure 3: Sketch illustrating the TaskRunner and the Scheduler. Also shown is the RunAll task which manages all the given Problem instances.

It is important to note that the expectation from the user is that they have an executable or script that is configurable via command line arguments and furthermore that we can specify where it should generate its output files. We believe that this is not too much to ask from a user. By doing this, we are able to schedule and execute a large number of simulations and automatically perform any analysis on the results.

3.4 Cluster management

As discussed, the automation framework can transparently execute simulations on remote machines. The remote machines should be accessible via password-less SSH. This is easy to do and requires the user to setup an SSH key-pair. The remote machine should also have the minimum requirements for running PySPH (or whatever software package one is interested in). For PySPH this requires a C++ compiler and a basic Python installation on the remote machine. Given these, the user may easily add new remote nodes by running:

$ python automate.py -a remote_host

This will copy the necessary files from the local computer to the remote computer and setup everything on the remote machine. The configuration is saved to a config.json file. The scripts for setting up and updating the remote host will be placed in a .automan directory and can be edited if the remote machines require a different setup.

Once a new computer is added, when one runs the automate.py script it will automatically distribute the computations across all the workers and the local machine. If for
some reason one does not wish to use a particular worker, one can remove the entry from the config.json file.

If the source code for the simulations is edited, one can update it on all the nodes by running:

```
$ python automate.py -u
```

This updates the sources on all workers, rebuilds PySPH, and runs any problems specified.

4 Discussion

The framework discussed above is fairly simple. The example provided in section 3.1 in Listing 1 shows that a user can quickly put together a problem which simulates a variety of cases and perform some post-processing on the results. The automation framework ensures the execution of the code in the correct order. Since the script is written in Python, users may perform any kind of post-processing. The approach of specifying parameters as keyword arguments allows users to filter the cases based on the choice of parameters. This facilitates easy comparison of numerical schemes. By separating the cases being run and the plotting code, we allow users to compare the cases very easily with little or no repetition of code. These features are unique to our automation framework.

The Task based infrastructure makes it possible to extend the framework to other situations with complex dependencies. The task executor (TaskRunner) and scheduler may also be customized if needed. Most users are likely to not need this.

As discussed in the introduction, there are many other tools that could have also been used to perform the dependency and task management. While the other tools provided inspiration for our implementation, they do not explicitly provide the additional conveniences that our framework provides. We consider a few of these tools in the following and discuss why we preferred to implement our own.

- Luigi [2] is designed to specify and execute tasks that have complex dependencies. It is used to process large amounts of data and is very general purpose. While our initial attempts used luigi and some of our own design is directly inspired by luigi, we found that it was much easier to write our own implementation than use luigi. In particular,
  - the default luigi scheduler made it difficult to run multiple jobs in parallel in a distributed fashion.
  - the command line arguments had many additional options that we found were confusing to the average user.

- Doit [11] is a very general task management and automation tool. However, we found that its scheduler did not always make it easy to hierarchically build tasks on demand. On the other hand luigi allowed for such an approach. Moreover, it was not clear how a user could to change the scheduler easily.
Lancet [13] provides general abstractions to decompose running a suite of programs into a parametrization of options, specification of the actual commands to run, and how to actually execute the task. Unfortunately, this does not include any task management or automation of tasks and their dependencies.

Our framework takes some of the best ideas in these tools to do what we require. We wish to emphasize that our intention is not to claim that our solution is universal or necessarily unique. On the other hand, the ideas discussed are general, related to many other tools, and relatively easy to implement in a high-level programming language like Python.

ReDoc[12] uses GNU Make which is more well suited to managing compilation of sources rather than long-time execution and distribution of tasks. Sumatra [3] as discussed in the introduction, is a more general and comprehensive framework. Nextflow [4] is also very comprehensive and offers many excellent advantages including support for execution via docker and extensive support for other tools. Nextflow could have perhaps been used to manage our tasks, however our approach to break up the simulations and post-processing into Simulation instances and Problem instances is still useful and could be used with either of these tools.

It is important to note that the automan framework suggests the following key recommendations,

• the programs that need to be run should be configurable using command line arguments (it is always possible to do this or write wrapper scripts for existing programs that do this);

• the program should be able to generate output into a specified and configurable directory.

• if the programs also perform part of the post-processing, it is often a good idea for the post-processing data to be saved into an easy to load format for comparison with other executions of the program.

As mentioned earlier, spending time on automating our results was very beneficial. In [8] a new SPH scheme was developed and in order to test the performance of the new scheme, 11 benchmark problems were simulated [7]. The results of these were compared with exact solutions (where available), the results produced by the WCSPH and TVF implementations, and sometimes compared with results produced by other numerical methods. This resulted in about 75 different simulations that required more than 7 days of computational time on a recent quad-core desktop machine with an Intel i7-4770 CPU at 3.40GHz. The work progressed over the course of a year while the author had the usual academic workload with a large amount of time fragmentation. As the work progressed, issues were discovered that were fixed and several simulations needed to be re-run. Some issues were major and some were minor but all of these required some re-running of these simulations. The manuscript was also written incrementally. Once submitted the

1 The code and manuscript for the publication is available at https://gitlab.com/prabhu/edac-sph/.
reviewer responses were also addressed, sometimes requiring further generation of plots and additional simulations. Our framework made it very easy to handle this despite the typical fragmentation of time in academia.

automan is still a very young package and there are some additional features that are not yet supported. For example, it does not yet support executing simulations using a batch processing system like torque or slurm. It has also not been tested with other computational tools apart from PySPH. Our implementation is open source. Depending on user interest, these features may be added in the future.

5 Conclusion

In this paper we present a simple automation framework called automan that we use to manage multiple long-running simulations and generate results suitable for publication. The framework is open source and makes it possible to run all simulations and generate the figures for publication with one command. The simulations can be optionally distributed to other computers on a shared network. An important contribution is a simple abstraction of separating the different computations into individual problems. Each problem may require multiple simulations called cases. By explicitly specifying the parameters of a simulation, we are able to filter and select different cases. This minimizes repetitive code. The framework helps make a researcher more productive and facilitates reproducibility.

Acknowledgments

We are grateful to Prof. M. Ramakrishna for providing valuable feedback on this manuscript.

References

[1] Lorena A. Barba. Barba-group reproducibility syllabus, October 2016. URL https://hackernoon.com/barba-group-reproducibility-syllabus-e3757ee635cf [Online; posted 30-October-2016.

[2] Erik Bernhardsson, Elias Freider, et al. Luigi, 2012–. URL https://github.com/spotify/luigi Online; accessed 11-October-2016.

[3] A. P. Davison, M. Mattioni, D. Samarkanov, and B. Teleńczuk. Sumatra: A Toolkit for Reproducible Research. In V. Stodden, F. Leisch, and R. D. Peng, editors, Implementing Reproducible Research, chapter 3, pages 57–78. Chapman & Hall, 2014. ISBN 978-1-4665-6159-5.

[4] Paolo Di Tommaso, Maria Chatzou, Evan W. Floden, Pablo P. Barja, Emilio Palumbo, and Cedric Notredame. Nextflow enables reproducible computational workflows. Nature Biotechnology, 35(4):316–319, April 2017. ISSN 1087-0156. doi:10.1038/nbt.3820. URL http://dx.doi.org/10.1038/nbt.3820
[5] O. Mesnard and L. A. Barba. Reproducible and replicable Computational Fluid Dynamics: It’s harder than you think. *Computing in Science Engineering*, 19(4): 44–55, 2017. ISSN 1521-9615. doi: 10.1109/MCSE.2017.3151254.

[6] J. J. Monaghan. Smoothed Particle Hydrodynamics. *Reports on Progress in Physics*, 68:1703–1759, 2005.

[7] Prabhu Ramachandran. PySPH: a reproducible and high-performance framework for smoothed particle hydrodynamics. In Sebastian Benthall and Scott Rostrup, editors, *Proceedings of the 15th Python in Science Conference*, pages 127 – 135, 2016.

[8] Prabhu Ramachandran and Kunal Puri. Entropically damped artificial compressibility for SPH. *Under review*, 2017.

[9] Prabhu Ramachandran, Kunal Puri, et al. PySPH: a python-based SPH framework, 2010–. URL http://pypi.python.org/pypi/PySPH/.

[10] Geir Kjetil Sandve, Anton Nekrutenko, James Taylor, and Eivind Hovig. Ten simple rules for reproducible computational research. *PLOS Computational Biology*, 9(10): 1–4, 10 2013. doi: 10.1371/journal.pcbi.1003285. URL https://doi.org/10.1371/journal.pcbi.1003285.

[11] Eduardo Schettino. DoIt automation tool, 2008–. URL http://pydoit.org Online; accessed 11-October-2016.

[12] M. Schwab, N. Karrenbach, and J. Claerbout. Making scientific computations reproducible. *Computing in Science Engineering*, 2(6):61–67, Nov 2000. ISSN 1521-9615. doi: 10.1109/5992.881708.

[13] Jean-Luc R Stevens, Marco Elver, and James A Bednar. An automated and reproducible workflow for running and analyzing neural simulations using Lancet and IPython Notebook. *Frontiers in neuroinformatics*, 7(44), 2013. doi: 10.3389/fninf.2013.00044. URL http://dx.doi.org/10.3389/fninf.2013.00044

[14] Guido van Rossum et al. The Python programming language, 1991–. URL http://www.python.org/ Online; accessed: 11-October-2016.

[15] Greg Wilson, D. A. Aruliah, C. Titus Brown, Neil P. Chue Hong, Matt Davis, Richard T. Guy, Steven H. D. Haddock, Kathryn D. Huff, Ian M. Mitchell, Mark D. Plumbley, Ben Waugh, Ethan P. White, and Paul Wilson. Best practices for scientific computing. *PLOS Biology*, 12(1):1–7, 01 2014. doi: 10.1371/journal.pbio.1001745. URL https://doi.org/10.1371/journal.pbio.1001745.