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Abstract

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COFFEE—An MPI-parallelized Python package for the numerical evolution of differential equations



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ABSTRACT

COFFEE (Conformal Field Equation Evolver) is a Python package primarily developed to numerically evolve systems of partial differential equations over time using the method of lines. It includes a variety of time integrators and finite differencing stencils with the summation-by-parts property, as well as pseudo-spectral functionality for angular derivatives of spin-weighted functions. Some additional capabilities include being MPI-parallelisable on a variety of different geometries, HDF data output and post processing scripts to visualize data, and an actions class that allows users to create code for analysis after each timestep.

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Code metadata

| | |
|--|--|
| Current code version | v1 |
| Permanent link to code/repository used for this code version | https://github.com/ElsevierSoftwareX/SOFTX_2019_93 |
| Legal Code License | GNU General Public License (GPL) |
| Code versioning system used | git |
| Software code languages, tools, and services used | Python 2.7, C, MPI, HDF5, numpy, spinsfast, libfftw3 |
| Compilation requirements, operating environments | Dependencies: mpi4py with compatible MPI implementation, h5py with compatible HDF implementation, numpy, scipy, Gnuplot, matplotlib and a variety of standard Python modules (e.g. abc, logging and math). |
| If available Link to developer documentation/manual | documentation provided in the code and the repository |
| Support email for questions | maintainers are contactable via the gitlab repository |

1. Motivation and significance

We present a software package, the Conformal Field Equation Evolver or COFFEE for short, that implements techniques suitable for numerical solution of time dependent systems of differential equations (DEs) via the method of lines. COFFEE is primarily implemented in Python. It imposes very few requirements on users and was written with PEP8 [1] as the guiding philosophy. Although COFFEE cannot compete with some existing numerical integrators for speed, it offers a low barrier for use and substantial flexibility.

COFFEE was specifically developed to compute solutions to a system of hyperbolic partial differential equations (PDEs) that represent Friedrich's conformal field equations [2]. It has been used in eight research projects to numerically study the conformal properties of general relativity, [3–10]. As an illustration of the capabilities of COFFEE, in [10] it was used to solve a system of PDEs in the form of an Initial Boundary Value Problem (IBVP) containing 46 variables and 45 constraints on two different high performance clusters using up to 200 processes. It evolved the system in time for a range of resolutions, approximated spatial derivatives in a number of ways, stably imposed user-given boundary conditions and stored the data in HDF files. Post-processing scripts demonstrated convergence and stability of the computed solution and produced visualizations of the

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output. COFFEE contains the tools necessary to rigorously investigate the numerical evolution of a system of time dependent PDEs.

COFFEE is unique in that, there is no computational PDE software designed with the philosophy of user-friendliness and flexibility that has been used to solve complex and challenging systems of equations, for example those derived from Einstein's field equations. This contrasts COFFEE with existing software like Cactus [11], Chombo [12] or PETSc [13].

2. Software description

COFFEE was designed to significantly reduce the amount of work needed to write code to solve systems of equations. Thus, despite its numerical nature, COFFEE is implemented in Python and relies heavily on `numpy`, `mpi4py`, `hdf5` and custom C code. Implementation in Python has obvious disadvantages. For example; as Python is an interpreted language syntax can have a large impact on speed of execution (compare for loops to list comprehensions), there are structural issues with interpreted languages (in the case of Python this is the reason for the GIL), additional overhead in the translation of Python script to Python byte code and then to machine instructions, and a lack of the compile time checks that are found in strongly typed languages. Nevertheless the papers [3–10] demonstrate that COFFEE is capable of solving technically challenging and computationally intensive systems of PDEs.

Implementation in Python also has advantages. Of particular note is duck typing, dynamic introspection and code injection, which reduces the need for the user to conform to strict programming patterns and understand the “COFFEE way of doing things”. Conforming to the philosophy of Python, COFFEE evaluates code as given and fails fast, i.e. stops the simulation rather than continuing with a potential flaw. Before each iteration of the simulation, a collection of “actions” are run. Each action is an arbitrary piece of user code that has complete access to all data at the current time step and almost all objects performing the simulation. This gives users substantial complete control over the simulation.

The COFFEE code base has been written for readability over performance (except for code dealing with the MPI and HDF API's). The code contains plenty of comments highlighting trickier portions of code, why certain algorithms were chosen and portions of code that are bug prone under change. As a general point, we believe that code should not be viewed as an immutable body of work but rather like working on a whiteboard: added to and altered as needed. Hence, we expect users to directly alter COFFEE's code based whenever more convenient than other methods of changing the simulation; e.g. run time control can be exercised in actions or in system objects described in Section 2. Due to the technicalities of working with MPI and HDF API's, however, caution should be exercised when editing the `mpi`, `actions.hdf_output` and `io.simulation_data` modules.

The core functionality of COFFEE is an MPI-enabled implementation of the method of lines with code to support spectral and finite difference techniques for spatial derivatives over clusters of computers. Thus it is an implementation of the numerical methods required for evolving time dependent systems of ODEs and PDEs, e.g. parabolic and hyperbolic systems. Of particular note, COFFEE includes code for the simultaneous approximation (SAT) method [14] for imposing stable boundary conditions, the papers [15–17] for summation-by-parts finite difference operators, and [18] for fast spin-weighted spherical harmonic transforms for numerical implementation of the $\bar{\partial}$ -calculus (eth-calculus), see for example [19]. IO uses HDF5 for data storage. It has been run on desktop workstations, on a cluster of computers at the University of Otago and on the New Zealand eScience Infrastructure's high performance computing cluster.

For the rest of this section, it may be helpful for the reader to refer to the UML sequence diagram of COFFEE, as shown in Fig. 1.

The `IBVP` class represents an initial boundary value problem. To initialize this class objects behaving similarly to a “Solver”, a `System` object, and a `Grid` object must be provided. The solver describes how steps along the lines of the simulation are performed. The system calculates the time derivative of the functions being simulated. The grid object describes the domain of the functions and manages the MPI API. Additional options, which have sensible defaults, at initialization are a list of actions to be performed during simulation (e.g. data reduction, visualization, error calculation, and so on), the maximum number of iterations and a minimum time step.

Solvers are objects that know how to integrate one dimensional ODEs. An abstract base class is provided along with implementations of the Euler (explicit and implicit), the 4th order Runge Kutta method and a variation of the 4th order Runge Kutta method that incorporates boundary data for intermediate steps. An adaptive 4th order Runge Kutta method has been implemented but not tested sufficiently for this release of COFFEE. The code for this will eventually be included in the repository.

System objects represent the system of differential equations to be solved using the method of lines. An abstract base class is provided as a form of documentation of the otherwise implicitly assumed API provided by custom classes filling the role of a system object. System classes must have a method that returns what the next timestep is to be (this allows for adaptive simulation), a method (`evaluate()`) that calculates the time derivative at a particular point in time, and methods that give initial and boundary values.

To make life easier for the user a number of numeric (spatial) derivative operations have been implemented. Instances of these have been used in the `evaluate()` method in published papers. Code for the following operators is provided:

- 11 finite difference stencils,
- 9 different implementations using the fast Fourier transform,
- The Geroch–Held–Penrose operators $\bar{\partial}$ and $\bar{\partial}'$,
- 7 summation by parts finite difference operators with 3 supporting dissipation operators.

The Geroch–Held–Penrose operators are supported by a module, `swsh`, which can calculate and manipulate spin-weighted spherical harmonics.

The `Grid` object represents the domain of the functions being calculated. To instantiate a grid object the number of data points in each dimension, the bounds for the values of coordinates on the data points, an `MPIInterface` object, and an object describing the “boundary data” must be provided. The `MPIInterface` object wraps an instance of `MPI_COMM` itself wrapped by the `mpi4py` module (COFFEE has been tested against both MPICH and Open MPI). COFFEE `MPIInterface` objects understand how to communicate sufficient data to neighbouring processes to allow simulation to continue when simulation is performed over multiple processes via MPI.

The abstract base class for boundary data, `ABCBoundary`, represents the information needed to determine what data has to be sent between sub-grids on different processes via a subclass of `MPIInterface`. The `ABCBoundary` objects draw a distinction between sub-grid “edges” that are internal and external to the full grid as represented by the `Grid` object. Each internal and external edge can, in principle, have differing numbers of ghost points and points on the “boundary” region that will be communicated. This data is communicate via the `boundary_slices()` method.

Once simulation is started COFFEE enters a “main” loop contained in the `ibvp` class. First, the next timestep is determined.

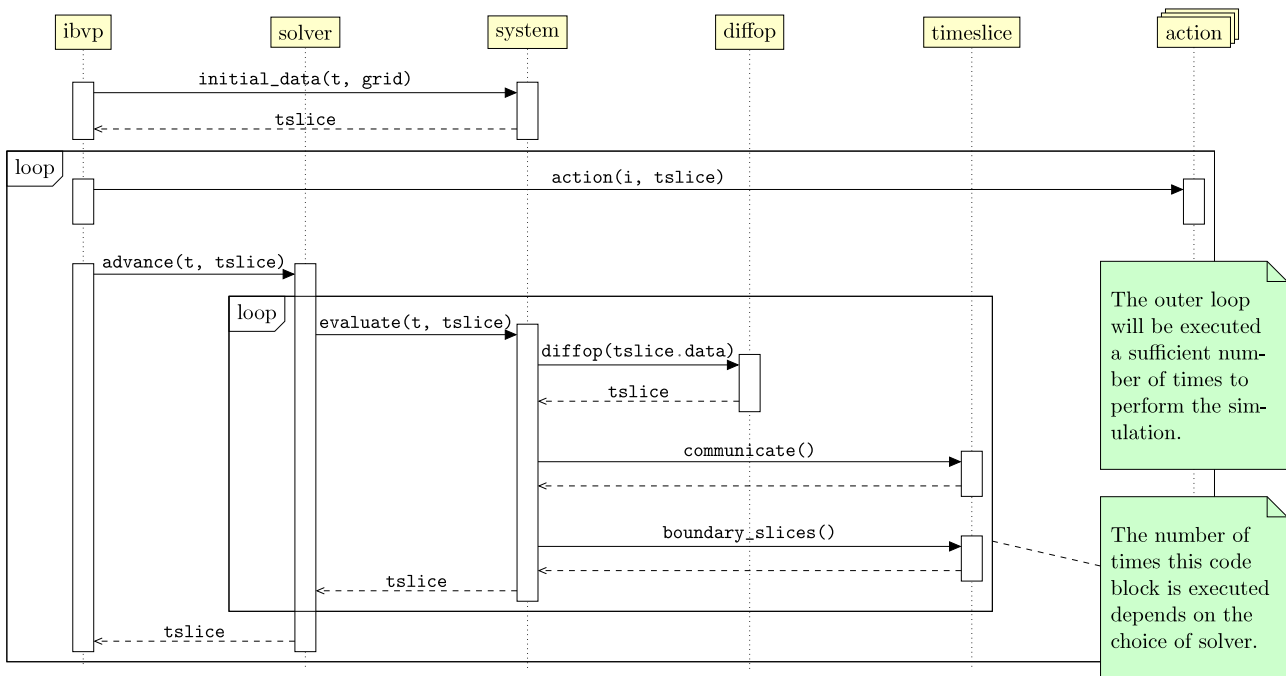


Fig. 1. A UML sequence diagram of COFFEE. The names of function calls and variables have been preserved in the diagram, t is the current time, $tslice$ is a time slice of function data (passed in the `advance()` and `evaluate()` methods and created in the `initial_data()` call) or derivatives of function data (returned in the `diffop()` call) or values of functions at intermediate times (returned from the `evaluate()` call), i is the values of the function at the current time. Note that the lifetime of the $tslice$ object is strictly speaking incorrect as different time slices are used in each of the inner fragment loops. The Solver is responsible for creation of new time slices between each fragment evaluation. We have left this off the diagram as it only serves to complicate it.

Second, each action in the action list is performed. Third, the values of the function at the current time plus the time step are calculated. Fourth, the process is repeated until an exception is raised, e.g. an overflow occurs, or the final time is reached.

All data in each iteration of the main loop is stored in a time slice object. Each time slice contains the function data, the grid, and the current time.

The last major portion of COFFEE worth discussing is actions. An action is a piece of code that does something with a `timeslice`. Actions are user definable and can contain references to any object available at runtime. When called an action is passed the current `timeslice`. Actions have complete freedom and therefore are able to dynamically affect the simulation. An action should subclass the `actions.Prototype` class and at least implement the function `_doit()`.

COFFEE is supported by additional scripts that work on the resulting `hdf` files to produce the normal array of secondary derived information, such as the calculation of convergence rates, errors, visualization, and manipulation of data in `hdf` files.

There are only a few requirements that need to be met before COFFEE can be used to compute solutions, see Section 3 for an example or refer to one of the more detailed examples provided in the COFFEE repository. Users must provide:

1. an object with a method that returns the next time step Δt and a method that computes the time derivative of the system at a given point in time (which we call “the system”),
2. select an object which can solve ordinary differential equations (ODEs) or provide their own (“the solver”), and
3. specify the domain of the solution to be computed and what discretization to use (“the grid”).

Once these components have been selected from libraries within COFFEE, or have been custom written, they are passed as arguments during object initialization to the `ibvp` class. The simulation can now be run by calling the `ibvp.run()` method.

There are an array of additional options that can be specified involving IO, MPI topology and data communication, methods for calculation of spatial differences, length of simulation and forced evaluation at specific times, and real time visualization.

To run a simulation the user must instantiate objects that behave like the COFFEE provided `System`, `Grid`, `Solver` and `IBVP` classes. COFFEE has existing implementations of `Grid`, `Solver` and `IBVP` classes that are sufficient for most simulations. Since the `System` class represents the system of DEs to be solved this is left to the user for implementation. Collectively these classes contain all information needed to perform a simulation. In the research projects cited above initialization of these classes and the start of simulation has been collected in what we call a setup file. See Listing 2 for a minimal example of a setup file. The COFFEE repository contains more detailed examples. For use in research, the Otago numerical relativity group included a plethora of runtime command line customizations in setup files, but this is not required. Typical options in a setup file involve: logging, differential operators, solvers, output settings, “action lists” and settings related to real time generation of visualizations.

2.1. Software architecture

In keeping with Python’s philosophy COFFEE’s architecture is flat, except where interaction with MPI or HDF API’s is needed. As a consequence explicit code dependencies are either obvious, e.g. the IO system relies on `h5py`, or explicitly stated, e.g. `Grid` objects use instances of the `ABCBoundary` class which is in the `grid.grid` module along with the `Grid` class. In order to document the implicit dependencies which result from Python’s reliance on duck typing numerous abstract base classes are provided. These classes document the otherwise implicit assumptions made about class API’s. We encourage users to subclass abstract base classes, though this is not required.

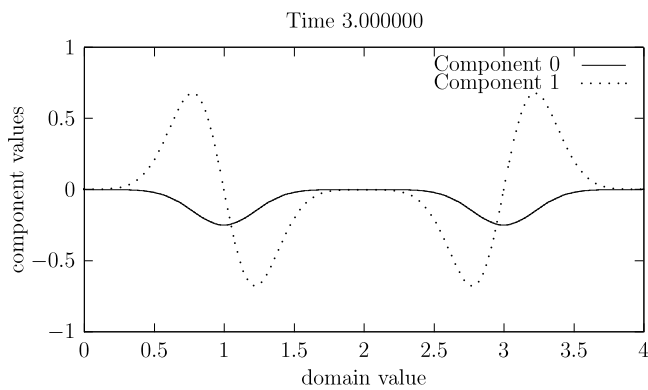


Fig. 2. A graph of the function computed by Listings 1 and 2. Component 0 is the value of the function that solves the wave equation specified in Listing 1, while component 1 is its derivative. The time has been chosen to show the function after the first reflection off both boundaries but before the separate wave packets merge for the first time. You can replicate this graph by using the `gpl_plotter` action to run only at time 3.0.

Since the implicit dependencies are the most likely to cause issues for new users we briefly describe them. Fig. 1 describes the expected flow of data during initialization of the data and one iteration of the simulation and therefore presents a schematic view of the implicit dependencies internal to COFFEE.

3. Illustrative examples

We give an example of code that solves the one dimensional wave equation in the code Listings 1 and 2 (also see Fig. 2). Code from these listings can be found in the COFFEE repository. The first file, given in Listing 1 defines the system object. It specifies what spatial differential operator to use, how to calculate a time step, the initial data and how to calculate the time derivatives of the solution. The second file, given in Listing 2, initializes the objects necessary for simulation and hands them to an IBVP object which manages the main simulation loop.

4. Impact

There are only a few other packages currently available that incorporate a similar set of features to COFFEE. Each of these has different philosophies, structure and goals. For example, the Cactus code [11,20] is a very large, community-driven project developed over many years. However the philosophy of Cactus and that of COFFEE differ greatly; Cactus is extremely optimized, written mostly in Fortran and C, and is very strict on how things are done and what the user can do. COFFEE on the other hand is written in Python and is designed for ease-of-use and flexibility. These properties make COFFEE and Cactus natural complements of each other and useful in their own right. In particular, COFFEE, although powerful enough to satisfy advanced programmers, is also aimed at users from a variety of different fields that may have limited programming skills. These users want a simple way to numerically evolve systems of ODEs or PDEs and are not necessarily worried about speed.

To help reduce runtime, COFFEE is MPI-parallelized: The computational domain is split into smaller domains, each having its own memory and dedicated core. The performance increase using MPI is exemplified with the strong scaling test results given in Table 1. It is seen that increasing the number of MPI processes decreasing runtime up to around 32 cores, after which increasing MPI processes starts to increase computational time again. This is expected as the total gridsize is fixed, and the point at which increasing the number of MPI processes stops decreasing runtime

Table 1

A strong scaling test, using the one-dimensional system of symmetric hyperbolic PDEs described in [8], with: 12801 equi-distant spatial gridpoints between $z = -1$ and $z = +1$, spatial stepsize Δz , CFL of 0.5, temporal stepsize of $CFL * \Delta z$, spatial derivatives approximated with a fourth-order finite differencing operator with the summation-by-parts property [17] and boundary conditions implemented with the SAT method [14]. The simulations were run on New Zealand eScience Infrastructure's Mahuika cluster which has 8,136 cores in 226 \times Broadwell (E5-2695v4, 2.1 GHz, dual socket 18 cores per socket) compute nodes.

| # of processes | 1 | 2 | 4 | 8 | 16 | 32 | 64 | 128 |
|----------------|-------|-------|-------|------|------|------|------|------|
| Runtime (s) | 256.6 | 190.4 | 117.7 | 71.9 | 61.3 | 54.5 | 54.8 | 58.4 |

will increase with an increased total gridsize. For a sufficiently large number of MPI processes, communication between each subgrid has increased to a point where the communication itself is now the bottleneck.

User interaction with MPI in COFFEE is minimal, only a few lines of Python code are needed in the setup file, detailing: the dimension of the grid, the periodicity (if any), and the topology (e.g. Cartesian). A few more lines communicating data between processes in the system file may also be needed, e.g. for spatial derivative approximations. Examples of how to do the above are given in COFFEE's repository, see Code metadata table.

Further, COFFEE contains an implementation of spin-weighted spherical harmonics using the optimized transform algorithm of [18]. Current research involving COFFEE involves a modified version of [18] which is optimized for axi-symmetry. This code is not released in this version of COFFEE but will be included after sufficient testing has been completed. This specialized spin-weighted spherical harmonic code was used in [10,21].

The COFFEE package is extremely versatile as it presupposes very little about the system that the user inputs. Thus if a process can be modelled over time by a differential equation or a system of differential equations then it can be numerically evolved in COFFEE. Of course whether or not a numerical solution can be found will depend on the specifics of the system of equations and the chosen numerical methods.

5. Conclusions

COFFEE is a user-friendly Python package for the numerical evolution of (a system of) ODEs and PDEs. It contains a wide variety of numerical algorithms for marching in time, approximating spatial derivatives and stably imposing boundary conditions as well as being MPI-parallelized by the splitting of the computational domain. It has been rigorously tested during multiple research projects and has functionality through the *actions class* for performing user-defined tasks during the evolution. COFFEE is ideally suited to users that hold user-friendliness above absolute speed and want flexibility to tailor the code to their particular problem.

CRedit authorship contribution statement

Georgios Doulis: Software. **Jörg Frauendiener:** Software. **Chris Stevens:** Software. **Ben Whale:** Software.

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```

1 # file name: OneDwave.py
2 import numpy as np
3
4 from coffee.tslices import tslices
5 from coffee.system import System
6 from coffee.diffop.sbp import sbp
7
8 class OneDwave(System):
9
10     def __init__(self):
11         self.D = sbp.D43_2_CNG()
12
13     def timestep(self, u):
14         return 0.4 * u.domain.step_sizes[0]
15
16     def initial_data(self, t0, grid):
17         axis = grid.axes[0]
18         rv = 0.5 * np.exp(-10 * (axis - axis[int(axis.shape[0] / 2)]))**2)
19         return tslices.TimeSlice([rv, np.zeros_like(rv)], grid, t0)
20
21     def evaluate(self, t, Psi):
22         f0, Dtf0 = Psi.data
23         DxXf = np.real(self.D(f0, Psi.domain.step_sizes[0]))
24         DtDtf = DxXf
25         DtDtf[-1] = 0.0
26         DtDtf[0] = 0.0
27         return tslices.TimeSlice([Dtf0, DtDtf], Psi.domain, time=t)

```

Listing 1: A code listing for the file that defines the `system` object representing the one dimensional wave equation with Dirichlet boundary conditions.

```

1 # file name: OneDwave_setup.py
2 from coffee import ibvp, solvers, grid
3 from coffee.actions import gp_plotter
4
5 from OneDwave import OneDwave
6
7 system = OneDwave()
8 solver = solvers.RungeKutta4(system)
9 grid = grid.UniformCart((200,), [(0, 4)])
10 plotter = gp_plotter.Plotter1D(
11     system,
12     'set yrange [-1:1]',
13     'set style data lines'
14 )
15
16 problem = ibvp.IBVP(solver, system, grid=grid, action=[plotter])
17 problem.run(0, 50)

```

Listing 2: The listing for the file that initiates simulation. Objects representing the system, a solver and a grid over which the solution will be calculated are initialized. The grid is chosen to have 200 steps over the interval (0,4). The simulation runs over the time interval (0,50). The `ibvp` object plots the output using gnuplot.

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Declaration of competing interest

The authors declared that they had no conflicts of interest with respect to their authorship or the publication of this article.

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