

Simplifying Parallelization of Scientific Codes by a Function-Centric Approach in Python

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Abstract.

The purpose of this paper is to show how existing scientific software can be parallelized using a separate thin layer of Python code where all parallel communication is implemented. We provide specific examples on such layers of code, and these examples may act as templates for parallelizing a wide set of serial scientific codes. The use of Python for parallelization is motivated by the fact that the language is well suited for reusing existing serial codes programmed in other languages. The extreme flexibility of Python with regard to handling functions makes it very easy to wrap up decomposed computational tasks of a serial scientific application as Python functions. Many parallelization-specific components can be implemented as generic Python functions, which may take as input those functions that perform concrete computational tasks. The overall programming effort needed by this parallelization approach is rather limited, and the resulting parallel Python scripts have a compact and clean structure. The usefulness of the parallelization approach is exemplified by three different classes of applications in natural and social sciences.

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1. Introduction

Due to limited computing power of standard serial computers, parallel computing has become indispensable for investigating complex problems in all fields of science. A frequently encountered question is how to transform an existing serial scientific code into a new form that is executable on a parallel computing platform. Although portable parallel programming standards, such as MPI and OpenMP, have greatly simplified the programming work, the task of parallelization may still be quite complicated for domain scientists. This is because inserting MPI calls or OpenMP directives directly into an existing serial code often requires extensive code rewrite as well as detailed knowledge of and experience with parallel programming.

The hope for non-specialists in parallel computing is that many scientific applications possess high-level parallelism. That is, the entire computational work can be decomposed into a set of individual (and often collaborative) computational tasks, each of coarse grain, and can be performed by an existing piece of serial code. Depending on the specific application, the decomposition can be achieved by identifying a set of different parameter combinations, or (fully or almost) independent computations, or different data groups, or different geometric subdomains. For a given type of decomposition, the parallelization induced programming components, such as work partitioning, domain partitioning, communication, load balancing, and global administration, are often generic and independent of specific applications. These generic components can thus be implemented as reusable parallelization libraries once and for all. This is what we exemplify in the present paper.

It is clear that a user-friendly parallelization approach relies on at least two factors: (1) The existing serial code should be extensively reused; (2) The programming effort by the end user must be limited. To achieve these goals we suggest to use Python to wrap up pieces of existing serial code (possibly written in other languages), and implement the parallelization tasks in separate and generic Python functions.

Python [1] is an extremely expressive and flexible programming language at its core. The language has been extended with numerous numerical and visualization modules such as NumPy [2] and SciPy [3]. The two requirements of a user-friendly parallelization mentioned above are actually well met by Python. First of all, Python is good at inter-operating with other languages, especially Fortran, C, and C++, which are heavily used in scientific codes. Using wrapper tools such as F2PY [4], it is easy to wrap up an existing piece of code in Fortran and C and provide it with a Pythonic appearance.

Moreover, among its many strong features, Python is extremely flexible with handling functions. Python functions accept both positional arguments and keyword arguments. The syntax of a variable set of positional and keyword arguments (known as “`(*args,**kwargs)`” to Python programmers) allows writing libraries routines that work with any type of user-defined functions. That is, the syntax makes it possible to call a Python function without revealing the exact number of arguments.

It is also straightforward to pass functions as input arguments to a Python function

and/or return a function as output. A callable class object in Python can be used as if it were a stand-alone function. Such a construction, or alternatively a closure (known from functional programming), can be used to create functions that carry a state represented through an arbitrarily complex data structure. The result is that one can express the flow of a scientific code as a Python program containing a set of calls to user-defined Python functions. These user-defined functions can be ordinary functions or classes that wrap pieces of the underlying scientific code. This is what we call a *function-centric* representation of the scientific code. With such a function-centric approach, we can build a general framework in Python for almost automatic parallelization of the program flow in the original scientific code. Later examples will convey this idea in detail.

Performance of the resulting parallel application will closely follow the performance of the serial application, because the overhead of the parallelization layer in Python is just due to a small piece of extra code, as we assume the main computational work to take place in the Python functions that call up pieces of the original scientific code. In the parallelization layer, good performance can be ensured by using efficient array modules in Python (such as `numpy` [2]) together with light-weight MPI wrappers (such as `pypar` [5]). For examples of writing efficient Python code segments for some standard serial and parallel numerical computations, we refer the reader to Cai et al. [6].

Related Work. In C++, generic programming via templates and object-oriented programming has been applied to parallelizing serial scientific codes. Two examples can be found in [7] and [8], where the former uses C++ class hierarchies to enable easy implementation of additive Schwarz preconditioners, and the latter uses C++ templates extensively to parallelize finite element codes. Many scientific computing frameworks have also adopted advanced programming to incorporate parallelism behind the scene. In these frameworks (see, e.g., [9, 10, 11, 12, 13]) the users can write parallel applications in a style quite similar to serial programming, without being exposed to many parallelizing details. Likewise are frameworks that are specially designed to allow coupling of different serial and parallel components, such as Cactus [14] and MpCCI [15]. The Python programming language, however, has not been widely used to parallelize existing serial codes. The Star-P system [16] provides the user with a programming environment where most of the parallelism is kept behind the scene. Hinsien [17] has combined Python with BSP to enable high-level parallel programming. In addition, quite a number of Python MPI wrappers exist, such as `pyMPI` [18], `pypar` [5], `MYMPI` [19], `mpi4py` [20, 21], and `Scientific.MPI` [22]. Efforts in incorporating parallelism via language extensions of Python can be found in [23, 24, 25].

The contribution of the present paper is to show by examples that a function-centric approach using Python may ease the task of parallel scientific programming. This result is primarily due to Python's flexibility in function handling and function arguments. As a result, generic tasks that arise in connection with parallelization can often be programmed as a collection of simple and widely applicable Python functions,

which are ready to be used by non-specialists to parallelize their existing serial codes.

This paper contains three examples with different algorithmic structures. A wide range of problems in science can be attacked by extending and adapting the program code in these examples. Moreover, readers whose problems are not covered by the examples will hopefully from these examples understand how we solve programming problems by identifying the principal, often simplified, underlying algorithmic structure; then creating generic code to reflect the structure; and finally applying the generic code to a specific, detailed case. Our approach is much inspired by the success of mathematics in problem solving, i.e., detecting the problem's principal structure and devising a generic solution makes complicated problems tractable. With Python as tool, we demonstrate how this strategy carries over to parallelization of scientific codes.

The remainder of the paper is organized as follows. We give in Section 2 a simple but motivating example, explaining the principles of splitting a problem into a set of function calls that can easily be parallelized. Generic parallelization of three common types of real scientific applications are then demonstrated in Section 3. Afterwards, Section 4 reports the computational efficiency of the suggested parallelization approach applied to specific cases in the three classes of scientific problems. Some concluding remarks are given in Section 5.

2. A Motivating Simple Example

2.1. Serial Version

Suppose we want to carry out a parameter analysis that involves a large number of evaluations of a multi-variable mathematical function $f(a_1, \dots, a_q)$. The Python implementation of f may use p positional arguments and k keyword arguments such that the total $p + k$ arguments contain at least the variables a_1, \dots, a_q (i.e., $q \leq p + k$). As a very simple example, consider the parabola $f(x, a, b, c) = ax^2 + bx + c$ with the following Python implementation ($q = 4, p = 1, k = 3$):

```
def func(x, a=0, b=0, c=1):
    return a*x**2+b*x+c
```

Suppose we want to evaluate `func` for a particular set of input parameters chosen from a large search space, where x , a , b , and c vary in specified intervals. The complete problem can be decomposed into three main steps: (1) initialize a set of arguments to `func`; (2) evaluate `func` for each entry in the set of arguments; (3) process the set of function return values from all the `func` calls.

Step (1) calls a user-defined function `initialize` which returns a list of 2-tuples, where each 2-tuple holds the positional and keyword arguments (as a tuple and a dictionary) for a specific call to `func`. Step (2) iterates over the list from step (1) and feed the positional and keyword arguments into `func`. The returned value (tuple) is stored in a result list. Finally, step (3) processes the result list in a user-defined function `finalize` which takes this list as input argument.

A generic Python function that implements the three-step parameter analysis can be as follows:

```
def solve_problem(initialize, func, finalize):
    input_args = initialize()
    output = [func(*args, **kwargs) for args, kwargs in input_args]
    finalize(output)
```

Note that the use of *list comprehension* in the above code has given a very compact implementation of the `for`-loop for going through all the evaluations of `func`. The `initialize`, `func`, and `finalize` functions are passed to `solve_problem` as input arguments. These three user-defined functions are independent of `solve_problem`.

As an example, assume that \mathbf{x} is a set of n uniformly distributed coordinates in $[0, L]$, and we vary a and b in $[-1, 1]$ each with m values, while c is fixed at the value 5. For each combination of a and b , we call `func` with the vector \mathbf{x} as a positional argument and the a , b , c values as keyword arguments, and store the evaluation results of `func` in a list named `output`. The objective of the computations is to extract the a and b values for which `func` gives a negative value for one or several of the coordinates $x \in [0, L]$. For this very simple example, the concrete implementation of the `initialize` and `finalize` functions can be put inside a class named `Parabola` as follows:

```
class Parabola:
    def __init__(self, m, n, L):
        self.m, self.n, self.L = m, n, L

    def initialize(self):
        x = numpy.linspace(0, self.L, self.n)
        a_values = numpy.linspace(-1, 1, self.m)
        b_values = numpy.linspace(-1, 1, self.m)
        c = 5

        self.input_args = []
        for a in a_values:
            for b in b_values:
                func_args = ([x], {'a': a, 'b': b, 'c': c})
                self.input_args.append(func_args)
        return self.input_args

    def func(self, x, a=0, b=0, c=1):
        return a*x**2+b*x+c

    def finalize(self, output_list):
        self.ab = []
        for input, result in zip(self.input_args, output_list):
            if min(result) < 0:
                self.ab.append((input[0][1], input[0][2]))
```

Now, to find the combinations of a and b values that make $ax^2 + bx + c < 9$, we can write the following two lines of code (assuming $m = 100$, $n = 50$, and $L = 10$):

```
problem = Parabola(100, 50, 10)
solve_problem(problem.initialize, problem.func, problem.finalize)
```

Note that the desired combinations of a and b values will be stored in the list `problem.ab`. Also note that we have placed `func` inside class `Parabola`, to have all

pieces of the problem in one place, but having **func** as stand-alone function or a class method is a matter of taste.

Despite the great mathematical simplicity of this example, the structure of the **solve_problem** function is directly applicable to a wide range of much more advanced problems. Although **initialize** and **finalize** are Python functions with very simple arguments (none and a list, respectively), this is not a limitation of their applicability. For example, the **initialize** step in our simple example needs values for m , n , and L , the a and b interval and so on, which can not be specified in the generic **solve_problem** function. To overcome this limitation, the information of m , n , and L can be hard-coded (not recommended), or transferred to **initialize** through global variables (not recommended in general) or carried with **initialize** as a state, either as class attributes or as a surrounding scope in a closure. We have chosen the class approach, i.e., class attributes store user-dependent data structures such that the **initialize** and **finalize** methods can have the simple input argument structure demanded by the generic **solve_problem** function. Alternatively, a closure as follows can be used instead of a class (this construct requires some knowledge of Python's scoping rules):

```
def initialize_wrapper(m, n, L):
    def initialize(self):
        x = numpy.linspace(0, L, n)
        a_values = numpy.linspace(-1, 1, m)
        ...
        return input_args
    return initialize
```

Now, the returned **initialize** function will carry with it the values of m , n , and L in the surrounding scope. The choice between the class approach and the closure approach, or using global variables in a straightforward global **initialize** function, is up to the programmer. The important point here is that **initialize** must often do a lot, and the input information to **initialize** must be handled by some Python construction. Similar comments apply to **finalize**.

2.2. Parallel Version

Let us say that we want to utilize several processors to share the work of all the **func** evaluations, i.e., the **for**-loop in the generic **solve_problem** function. This can clearly be achieved by a task-parallel approach, where each evaluation of **func** is an independent task. The main idea of parallelization is to split up the **for**-loop into a set of shorter **for**-loops, each assigned to a different processor. In other words, we need to split up the **input_args** list into a set of sub-lists for the different processors. Note that this partitioning work is generic, independent of both the **func** function and the actual arguments in the **input_args** list. Assuming homogeneous processors and that all the function evaluations are equally expensive, we can divide the **input_args** list into **num_procs** (number of processors) sub-lists of equal length. In case **input_args** is not divisible by **num_procs**, we adjust the length of some sub-lists by 1:

```
def simple_partitioning(length, num_procs):
```

```

    sublengths = [length/num_procs]*num_procs
    for i in range(length % num_procs): # treatment of remainder
        sublengths[i] += 1
    return sublengths

def get_subproblem_input_args(input_args, my_rank, num_procs):
    sub_ns = simple_partitioning(len(input_args), num_procs)
    my_offset = sum(sub_ns[:my_rank])
    my_input_args = input_args[my_offset:my_offset+sub_ns[my_rank]]
    return my_input_args

```

Using the above generic `get_subproblem_input_args` function, each processor gets its portion of the global `input_args` list, and a shorter `for`-loop can be executed there. Note that the syntax of Python lists and `numpy` arrays has made the function very compact.

The next step of parallelization is to collect the function evaluation results from all the processors into a single global output list. Finally, we let `finalize(output)` run only on the master processor (assuming that this work does not require parallelization). For the purpose of collecting outputs from all the processors, the following generic Python function can be used:

```

def collect_subproblem_output_args(my_output_args, my_rank,
                                   num_procs, send_func, recv_func):
    if my_rank == 0: # master process?
        output_args = my_output_args
        for i in range(1, num_procs):
            output_args += recv_func(i)
        return output_args
    else:
        send_func(my_output_args, 0)
        return None

```

The last two input arguments to the above function deserve some attention. Both `send_func` and `recv_func` are functions themselves. In the case of using the `pypar` wrapper of MPI commands, we may simply pass `pypar.send` as the `send_func` input argument and `pypar.receive` as `recv_func`. Moreover, switching to another MPI module is transparent with regard to the generic function named `collect_subproblem_output_args`. It should also be noted that most Python MPI modules are considerably more user-friendly than the original MPI commands in C/Fortran. This is because (1) the use of keyword arguments greatly simplifies the syntax, and (2) any picklable (marshable) Python data type can be communicated directly.

Now that we have implemented the generic functions `get_subproblem_input_args` and `collect_subproblem_output_args`, we can write a minimalistic parallel solver as follows:

```

def parallel_solve_problem(initialize, func, finalize,
                           my_rank, num_procs, send, recv):
    input_args = initialize()
    my_input_args = get_subproblem_input_args(input_args,
                                              my_rank, num_procs)

    my_output = [func(*args, **kwargs) \
                  for args, kwargs in my_input_args]

```

```

output = collect_subproblem_output_args(my_output, my_rank,
                                       num_procs, send, recv)

if my_rank == 0:
    finalize(output)

```

We remark that the above function is generic in the sense that it is independent of the actual implementation of `initialize`, `func`, and `finalize`, as well as the Python MPI module being used. All problems that can be composed from independent function calls can (at least in principle) be parallelized by the shown small pieces of Python code.

As a specific example of using this parallel solver, we may address the problem of evaluating the parabolic function (`func` and class `Parabola`) for a large number of parameters. Using the `pypar` MPI module and having the problem-dependent code in a module named `Parabola` and the general function-centric tools in a module named `function_centric`, the program becomes as follows:

```

from Parabola import func, Parabola
from function_centric import parallel_solve_problem

problem = Parabola(m=100, n=50, L=10)
import pypar
my_rank = pypar.rank()
num_procs = pypar.size()
parallel_solve_problem(problem.initialize,
                      func,
                      problem.finalize,
                      my_rank, num_procs,
                      pypar.send, pypar.receive)

pypar.finalize()

```

To the reader, it should be obvious from this generic example how to parallelize other independent function calls by the described function-centric approach.

3. Function-Centric Parallelization

We have shown how to parallelize a serial program that is decomposable into three parts: `initialize`, calls to `func` (i.e., a set of independent tasks), and `finalize`. In this section, we describe how the function-centric parallelization is helpful for three important classes of scientific applications: Markov chain Monte Carlo simulations, dynamic population Monte Carlo simulations, and solution of partial differential equations. We use Python to program a set of simple and generic parallelization functions.

3.1. Parallel Markov chain Monte Carlo Simulations

The standard Markov chain Monte Carlo algorithms are embarrassingly parallel and have exactly the *same* algorithmic structure as the example of parameter analysis in Section 2. This means that the functions `initialize`, `func`, and `finalize` can easily be adapted to Monte Carlo problems. More specifically, the `initialize` function prepares the set of random samples and other input parameters. Some parametric model is

computed by the `func` function, whereas `finalize` collects the data returned from all the `func` calls and prepares for further statistical analysis.

Function-centric parallelization of Markov chain Monte Carlo applications closely follows the example in Section 2. We can reuse the three generic functions named `get_subproblem_input_args`, `collect_subproblem_output_args`, and `parallel_solve_problem`, assuming that all the `func` evaluations are equally costly and all the processors are equally powerful so there is no need for more sophisticated load balancing.

In Section 4.1, we will look at a real-life Markov chain problem from political science (Appendix Appendix A gives its mathematical description).

3.2. Population Monte Carlo with Dynamic Load Balancing

A more advanced branch of Monte Carlo algorithms is population Monte Carlo, see [26]. Here, a group of walkers, also called the *population*, is used to represent a high-dimensional vector and the computation is carried out by a random walk in the state space. During the computation some of these walkers may be duplicated or deleted according to some acceptance/rejection criteria, i.e., the population is dynamic in time. Population Monte Carlo algorithms have been proven useful in a number of fields, spanning from polymer science to statistical sciences, statistical physics, and quantum physics.

Unlike the examples so far, where the computational tasks were totally independent and of static size, population Monte Carlo algorithms may be viewed as an iteration in time where we repeatedly do some work on a dynamic population, including moving the walkers of the population and adjusting the population size, which in a parallel context calls for dynamic load balancing.

3.2.1. Serial Implementation A serial implementation of the time integration function can be as follows:

```
def time_integration(initialize, do_timestep, finalize):
    walkers, timesteps = initialize()
    output = []
    for step in range(timesteps):
        old_walkers_len = len(walkers)
        output.append(do_timestep(walkers))
        walkers.finalize_timestep(old_walkers_len, len(walkers))
    finalize(output)
```

The input arguments to the generic `time_integration` function are three functions: `initialize`, `do_timestep`, and `finalize`. This resembles the three-step structure discussed in Section 2. The `do_timestep` function can have a unified implementation for all the variants of population Monte Carlo algorithms. The other two input functions are typically programmed as methods of a class that implements a particular algorithm (such as diffusion Monte Carlo in Section 4.2). Here, the `initialize` method sets up a population object `walkers` (to be explained below) and determines the number of

time steps the walkers are to be propagated. The `finalize` method can, e.g., store the output for later analysis.

The purpose of the `do_timestep` function is to implement the work for one time step, including propagating the walkers and adjusting the population. An implementation that is applicable for all population Monte Carlo algorithms may have the following form:

```
def do_timestep(walkers):
    walkers.move()
    for walker in range(len(walkers)):
        if walkers.get_marker(walker) == 0:
            walkers.delete(walker)
        elif walkers.get_marker(walker) > 1:
            walkers.append(walker, walkers.get_marker(walker)-1)
    return walkers.sample_observables()
```

The above implementation of `time_integration` and `do_timestep` assumes that `walkers` is an object of a class, say with name `Walkers`, that has a certain number of methods. Of course, the flexibility of Python allows that the concrete implementation of class `Walkers` be made afterwards, unlike C++ and Java that require class `Walkers` be written before implementing `time_integration` and `do_timestep`. Here, we expect class `Walkers` to provide a generic implementation of a group of walkers, with supporting methods for manipulating the population. The most important methods of class `Walkers` are as follows:

- `move()` carries out the work of moving each walker of the population randomly according to some rule or distribution function.
- `get_marker(walker)` returns the number of copies belonging to a walker with index `walker`, where 0 means the walker should be deleted, 2 or more means that clones should be created.
- `append(walker, nchilds)` and `delete(walker)` carry out the actual cloning and removal of a walker with index `walker`.
- `sample_observables()` returns the observables at a given time step, e.g., an estimate of the system energy.
- `finalize_timestep(old_size, new_size)` does some internal book keeping at the end of each time step, such as adjusting some internal variables. It takes as input the total number of walkers before and after the walker population has been adjusted by the `do_timestep` function.
- `__len__` is one of Python's special class methods and is in our case meant to return the number of walkers. A call `len(walkers)` yields the same result as `walkers.__len__()`.

For a real application, such as the diffusion Monte Carlo algorithm (see Section 4.2 and Appendix Appendix B), the concrete implementation of the methods should reflect the desired numerical algorithm. For example, the `move` method of diffusion Monte Carlo uses diffusion and branching as the rule to randomly move each walker, and the `finalize_timestep` method adjusts the branching ratio.

3.2.2. *Parallelization* Parallelism in population Monte Carlo algorithms arises naturally from dividing the walkers among the processors. Therefore, a parallel version of the `time_integration` function may be as follows:

```
def parallel_time_integration(initialize, do_timestep, finalize,
                             my_rank, num_procs, send, recv, all_gather):
    my_walkers, timesteps = initialize(my_rank, num_procs)
    old_walkers_len = sum(all_gather(numpy.array([len(my_walkers)])))
    my_output = []
    for step in range(timesteps):
        # do what is required at this time step and measure CPU time
        t_start = time.time()
        results = do_timestep(my_walkers)
        my_output.append(results)
        task_time = time.time() - t_start

        # redistribute walkers and get walker size per process
        num_walkers_per_proc = dynamic_load_balancing(\
            my_walkers, task_time, my_rank, num_procs,\
            send, recv, all_gather)

        # finalize task for this time step
        new_walkers_len = sum(num_walkers_per_proc)
        my_walkers.finalize_timestep(old_walkers_len, new_walkers_len)
        old_walkers_len = new_walkers_len
    my_output = collect_subproblem_output_args(my_output, my_rank,
                                                num_procs, send, recv)

    if my_rank == 0:
        finalize(my_output)
```

In comparison with its serial counterpart, the `parallel_time_integration` function has a few noticeable changes. First, the input arguments have been extended with five new arguments. The two integers `my_rank` and `num_procs` are, as before, meant for identifying the individual processors and finding the total number of processors. The other three new input arguments are MPI communication wrapper functions: `send`, `recv`, and `all_gather`, which can be provided by any of the Python wrapper modules of MPI. The only exception is that `pypar` does not directly provide the `all_gather` function, but we can easily program it as follows:

```
def all_gather (input_array):
    array_gathered_tmp = pypar.gather (input_array, 0)
    array_gathered = pypar.broadcast (array_gathered_tmp, 0)
    return array_gathered
```

Second, we note that the `initialize` function is slightly different from the serial case, now accepting `my_rank` and `num_procs` as input. This is because initial division of the walkers is assumed to be carried out here, giving rise to `my_walkers` on each processor. Third, a new function `dynamic_load_balancing` is called during each time step. This function will be explained below in detail. Fourth, unlike that the serial counterpart could simply pass the size of its walkers to `finalize_timestep`, the parallel implementation needs to collect the global population size before calling `finalize_timestep`. We remark that each local population knows its own size, but not the global population size. For this purpose, the `dynamic_load_balancing` function returns the individual local population sizes as a `numpy` array. Last, the

`collect_subproblem_output_args` function from Section 2.2 is used to assemble all the individual results onto the master processor before calling the `finalize` function.

As mentioned before, parallelization of population Monte Carlo algorithms has to take into account that the total number of walkers changes with time. Dynamic redistribution of the walkers is therefore needed to avoid work load imbalance. The generic `dynamic_load_balancing` function is designed for this purpose, where we evaluate the amount of work for each processor and, if the work distribution is too skew, we move the excess walkers from a busy processor to a less busy one. The function first checks the distribution of local population sizes. If the difference between the smallest number of walkers and the largest number of walkers exceeds some predefined threshold, `dynamic_load_balancing` finds a better population distribution and redistributes the walkers:

```
def dynamic_load_balancing(walkers, task_time, my_rank, num_procs, \
                           send, recv, all_gather):
    walkers_per_proc = all_gather(numpy.array([len(walkers)]))
    if imbalance_rate(walkers_per_proc) > walkers.threshold_factor:
        timing_list = all_gather(numpy.array([task_time]))
        rebalanced_work = find_optimal_workload(timing_list,
                                                walkers_per_proc)

        walkers = redistribute_work(walkers,
                                    walkers_per_proc,
                                    rebalanced_work,
                                    my_rank, num_procs, send, recv)

    return walkers_per_proc
```

Two helper functions `find_optimal_workload` and `redistribute_work` are used in the above implementation. Here, `find_optimal_workload` finds the optimal distribution of work, based on how much time each local population has used. The `redistribute_work` function carries out the re-shuffling of walkers. A straightforward (but not optimal) implementation of these functions goes as follows:

```
def find_optimal_workload(timing_list, current_work_per_proc):
    total_work = sum(current_work_per_proc)
    C = total_work/sum(1./timing_list)
    tmp_rebalanced_work = C/timing_list
    rebalanced_work = numpy.array(tmp_rebalanced_work.tolist(), 'i')
    remainders = tmp_rebalanced_work-rebalanced_work
    while sum(rebalanced_work) < total_work:
        maxarg = numpy.argmax(remainders)
        rebalanced_work[maxarg] += 1
        remainders[maxarg] = 0
    return rebalanced_work

def redistribute_work(my_walkers, work_per_proc, rebalanced_work,
                     my_rank, num_procs, send, recv):
    difference = work_per_proc-rebalanced_work
    diff_sort = numpy.argsort(difference)
    prev_rank_min = diff_sort[0]
    while sum(abs(difference)) != 0:
        diff_sort = numpy.argsort(difference)
        rank_max = diff_sort[-1]
        rank_min = diff_sort[0]
        if rank_min == prev_rank_min and rank_max != diff_sort[1]:
            rank_min = diff_sort[1]
```

```

    if my_rank==rank_max:
        send(my_walkers.cut_slice(rebalanced_work[my_rank]),\
             int(rank_min))

    elif my_rank==rank_min:
        my_walkers.paste_slice(recv(int(rank_max)))
    difference[rank_min] += difference[rank_max]
    difference[rank_max] = 0
    prev_rank_min = rank_min
    return my_walkers

```

Careful readers will notice that two particular methods, `my_walkers.cut_slice` and `my_walkers.paste_slices`, provide the capability of migrating the work load between processors in the `redistribute_work` function. These two methods have to be programmed in class `Walkers`, like the other needed methods described earlier: `move`, `get_marker`, `append`, `delete`, and so on. The `cut_slice` method takes away excess work from a local population and the `paste_slice` method inserts additional work into a local population. Note that the input argument to the `cut_slice` method is an index threshold meaning that local walkers with indices larger than that are to be taken away. The returned slice from `cut_slice` is a picklable Python object that can be sent and received through MPI calls.

The generic `redistribute_work` function deserves a few more words. Among its input arguments is the ideal work distribution, `rebalanced_work`, which is calculated by `find_optimal_workload`. The `redistribute_work` function first calculates the difference between the current distribution, `work_per_proc`, and the ideal distribution. It then iteratively moves walkers from the processor with the most work to the processor with the least work until the difference is evened out.

This load balancing scheme is in fact independent of population Monte Carlo algorithms. As long as you have an algorithm repeatedly doing a task over time and where the amount of work in the task varies over time, this scheme can be reused. The only requirement is that an application-specific implementation of class `Walkers`, in terms of method names and functionality, should match with `dynamic_load_balancing` and `redistribute_work`. It should be noted that the given implementation of the latter function is not optimal.

The algorithm of diffusion Monte Carlo, described in Appendix Appendix B, is a typical example of a population Monte Carlo algorithm. The implementation is described in Section 4.2 and Appendix Appendix B.

3.3. Parallel Additive Schwarz Iterations

From the perspective of communication between processors, parallelization of the Monte Carlo algorithms is relatively easy. Parallel Markov chain Monte Carlo algorithms only require communication in the very beginning and end, whereas parallel population Monte Carlo algorithms only require communication at the end of each time step. Actually, our function-centric approach to parallelization can allow more frequent communication. To show the versatility of function-centric parallelization, we apply

it to an implicit method for solving partial differential equations (PDEs) where communication is frequent between processors.

More specifically, many PDEs can be solved by an iterative process called *domain decomposition*. The idea is to divide the global domain, in which the PDEs are to be solved, into n overlapping subdomains. The PDEs can then be solved in parallel on the n subdomains. However, the correct boundary condition at the *internal* subdomain boundaries are not known, thus leading to an iterative approach where one applies boundary conditions from the last iteration, solves for the n subdomain problems again, and repeats the process until convergence of the subdomain solutions (see e.g. [27, 28]). This algorithm is commonly called additive Schwarz iteration and can successfully be applied to many important classes of PDEs [29, 30, 31]. The great advantage of the algorithm, especially from a software point of view, is that the PDE solver for the global problem can be reused for each subdomain problem. Some additional code is needed for communicating the solutions at the internal boundaries between the subdomains. This code can be implemented in a generic fashion in Python, as we explain later.

Let us first explain the additive Schwarz algorithm for solving PDEs in more detail. We consider some stationary PDE defined on a global domain Ω :

$$\mathcal{L}(u) = f, \quad x \in \Omega, \quad (1)$$

subject to some boundary condition involving u and/or its derivatives. Dividing Ω into a set of overlapping subdomains $\{\Omega_s\}_{s=1}^P$, we have the restriction of (1) onto Ω_s , for all s , as

$$\mathcal{L}(u) = f, \quad x \in \Omega_s. \quad (2)$$

The additive Schwarz method finds the global solution u by an iterative process that generates a series of approximations u_0, u_1, u_2 and so on. During iteration k , each subdomain computes an improved local solution $u_{s,k}$ by locally solving (2) for $u = u_{s,k}$ with $u_{s,k} = u_{k-1}$ as (an artificial) boundary condition on Ω_s 's non-physical internal boundary that borders with neighboring subdomains. All the subdomains can *concurrently* carry out the local solution of (2) within iteration k , thus giving rise to parallelism. At the end of iteration k , neighboring subdomains exchange the latest local solutions in the overlapping regions to (logically) form the global field u_k . The subdomain problems (2) are of the same type as the global problem (1), which implies the possibility of reusing an existing serial code that was originally implemented for (1). The additional code for exchange of local solutions among neighbors can be implemented by generic communication operations, independently of specific PDEs.

A generic implementation of parallel additive Schwarz iteration algorithm can be realized as the following Python function:

```
def additive_Schwarz_iterations(subdomain_solve, communicate,
    set_BC, max_iter, threshold, solution,
    convergence_test=simple_convergence_test):
    iter = 0; not_converged = True    # init

    while not_converged and iter < max_iter:
```

```

iter += 1
solution_prev = solution.copy()
set_BC(solution)
solution = subdomain_solve()
communicate(solution)
not_converged = not convergence_test(\
    solution, solution_prev, threshold)

```

In the above function, `max_iter` represents the maximum number of additive Schwarz iterations allowed, and `subdomain_solve` is a function that solves the subdomain problem of form (2) and returns an object `solution`, which is typically a `numpy` array containing the latest subdomain solution $u_{s,k}$ on a processor (subdomain). However, `solution` may well be a more complex object, say holding a collection of scalar fields over computational grids, provided that (i) the object has a `copy` method, (ii) `convergence_test` and `communicate` can work with this object type, and (iii) `subdomain_solve` returns such an object. This flexibility in choosing `solution` reflects the major dynamic power of Python and provides yet another illustration of the generality of the examples in this paper.

Given an existing serial code, for example in a language like Fortran or C/C++, the `subdomain_solve` function is easily defined by wrapping up an appropriate piece of the serial code as a Python class (since `subdomain_solve` does not take any arguments, the function needs a state with data structures, conveniently implemented as class attributes as explained in Section 2.1).

The `communicate` argument is a function for exchanging the latest local solutions among the subdomains. After the call, the `solution` object is updated with recently computed values from the neighboring subdomains, and contents of `solution` have been sent to the neighbors. The `communicate` function is problem independent and can be provided by some library. In our implementation, the implementation is entirely in Python to take advantage of easy programming of parallel communication in Python. The `set_BC` argument is a function for setting boundary conditions on a subdomain's internal boundary. This function depends on the actual serial code and is naturally implemented as part of the class that provides the `subdomain_solve` function.

The `convergence_test` function is assumed to perform an appropriate convergence test. The default generic implementation can test

$$\max_{1 \leq s \leq P} \frac{\|u_{s,k} - u_{s,k-1}\|^2}{\|u_{s,k}\|^2}$$

against a prescribed threshold value. An implementation reads

```

def simple_convergence_test(solution, solution_prev, threshold=1E-3):
    diff = solution - solution_prev
    loc_rel_change = vdot(diff,diff)/vdot(solution,solution)
    glob_rel_change = all_reduce(loc_rel_change, MAX)
    return glob_rel_change < threshold

```

We remark that `all_reduce` is a wrapper of the MPI `MPI_Allreduce` command and `vdot` computes the inner product of two `numpy` arrays.

Unlike the three-component structure described in Sections 3.1 and 3.2, the main ingredients for parallel additive Schwarz iterations are the functions of `subdomain_solve`, `communicate`, `set_BC`, and `convergence_test`. In other words, it is not natural to divide the work of solving a PDE into `initialize`, `func`, and `finalize`. Nevertheless, function-centric parallelization is also here user-friendly and gives a straightforward implementation of `additive_Schwarz_iterations` as above. The `convergence_test` function shown above is clearly generic, and so is the `communicate` function in the sense that it does not depend on the PDE. Both functions can be reused for different PDEs. The other two functions are PDE dependent, however, `subdomain_solve` normally wraps an existing serial code, while the implementation of `set_BC` is typically very simple.

4. Applications and Numerical Experiments

In this section we will address three real research projects involving the three classes of algorithms covered in Section 3. The projects have utilized our function-centric approach to parallelizing existing codes. That is, we had some software in Fortran, C++, and R performing the basic computations needed in the projects. The serial software was wrapped in Python, adapted to components such as `initialize`, `func`, `do_timestep`, `finalize`, `subdomain_solve`, `communicate`, `set_BC`. Parallelization was then carried out as explained in previous sections. An important issue to be reported is the parallel efficiency obtained by performing the parallelization in a Python layer that is separate from the underlying serial scientific codes.

The Python enabled parallel codes have been tested on a Linux cluster of 3.4 GHz Itanium2 processors, which are interconnected through 1Gbits ethernet. The purpose is to show that the function-centric parallelization approach is easy to use and that satisfactory parallel performance is achievable.

4.1. Parallel Markov Chain Monte Carlo Simulations

The first case is from political science and concerns estimating legislators' ideal points by the Markov chain Monte Carlo (MCMC) method. For a detailed description of the mathematical problem and the numerical method, we refer the reader to Appendix Appendix A. This application fits into the setup in Section 3.1. The statistical engine is provided by the PSCL library [32] in R [33], for which there exists a Python wrapper.

To use the function-centric parallelization described in Section 3.1, we have written a Python class named PIPE. In addition to the constructor of the class (i.e., the `__init__` method), there are three methods as follows:

- `initialize` sets up the functionality of the PSCL library through the Python wrapper of R (named `rpy`), and prepares the input argument list needed for `func`.

- **func** carries out the computation of each task by invoking appropriate functions available through **rpy** (in short, **func** is a Python wrapper to the R function **ideal** from the PSCL library).
- **finalize** summarizes the output and generates an array in R format.

The resulting parallel Python program is now as short as

```
from function_centric import parallel_solve_problem
import pypar
my_rank = pypar.rank()
num_procs = pypar.size()

from pypipe import PIPE
problem = PIPE("EP1.RData", "rcvs", "NULL", "NULL")
parallel_solve_problem(problem.initialize, problem.func, problem.finalize,
                      my_rank, num_procs, pypar.send, pypar.receive)
pypar.finalize()
```

The practical importance of a parallel MCMC code is that large and computationally intensive simulations are now easily doable. More specifically, data from the European Parliament between 1979 and 2004 [34] are used for simulation. During the five year legislative terms, the European Parliament expanded the size of the membership as well as the number of votes taken. (This trend has continued since 2004.) It is hence increasingly computationally intensive to estimate the ideal point model without reducing the length of the Markov chain. We examined the parallel performance by comparing the computing time for each of the five legislatures, running the parallelized code on 32 CPUs. The results are reported in Table 1. When comparing the results, the reader should note that we have not made any attempts to optimize the **ideal** code (called by our **func** function) for the purpose of parallelization. This makes it straightforward to switch to new versions of the **ideal** function. We ran 100,000 MCMC iterations. The parallel efficiency was about 90%.

Table 1. Speedup results associated with voting analysis.

Legislature	Votes	Members	1 CPU	32 CPUs	Efficiency
1979 - 1984	810	548	287m 32.560s	10m 13.318s	87.91%
1984 - 1989	1853	637	783m 59.059s	26m 58.702s	91.06%
1989 - 1994	2475	597	1006m 59.258s	33m 26.140s	94.11%
1994 - 1999	3603	721	1905m 0.930s	66m 0.068s	90.20%
1999 - 2004	5639	696	2898m 45.224s	102m 7.786s	88.70%

4.2. Parallel Diffusion Monte Carlo Simulations

As an example of population Monte Carlo methods, we will now look at parallel Diffusion Monte Carlo (DMC) computations (see Appendix Appendix B for a detailed numerical description), which is used here to simulate Bose-Einstein condensation. We recall from Section 3.2 that dynamic load balancing is needed in connection with the parallelization,

and can be provided by the generic `dynamic_load_balancing` function. To utilize the parallel time integration function `parallel_time_integration` from Section 3.2, we need to program a parallel version of the `initialize` function. The `do_timestep` function from Section 3.2 can be used as is.

```
def initialize(my_rank, num_procs):
    nwalkers = 1000
    nspacedim = 3
    stepsize = 0.1
    timesteps = 200
    walkers_per_proc = simple_partitioning(nwalkers, num_procs)
    my_walkers = Walkers(walkers_per_proc[my_rank], nspacedim, stepsize)
    my_walkers.threshold_factor = 1.1
    return my_walkers, timesteps
```

This `initialize` function is quite similar to its serial counter part. As noted in Section 3.2, it takes as input `my_rank` and `num_procs`. The `simple_partitioning` function is called to partition the walker population. A `my_walkers` object is assigned to each processor, and a threshold factor is prescribed to determine when load balancing is needed.

Together with the `parallel_time_integration` function from Section 3.2, the above `initialize` function is the minimum programming effort needed to parallelize a serial population Monte Carlo code. For the particular case of our parallel Diffusion Monte Carlo implementation, we also need to know the global number of walkers in every timestep to be able to estimate its observables globally. Moreover, the load balancing scheme needs the time usage of each processor during each time step.

A class with name `Walkers` needs to be implemented to match with the implementations of `parallel_time_integration`, `dynamic_load_balancing`, and the above `initialize` function. The essential work is to provide a set of methods with already decided names (see Section 3.2), such as `move`, `append`, `delete`, `finalize_timestep`, `cut_slice`, and `paste_slice`. A concrete example of the `Walkers` class is described with more details in Appendix Appendix B.

We report in Table 2 the timing results of a number of parallel DMC computations. The parallel efficiency was about 85%. We increased the total number of walkers when more processors were used in the simulation, such that the number of walkers assigned to each processor remained as 200. Such a use of parallel computers for DMC simulations mimics the everlasting wish of quantum physicists to do larger computations as soon as more computing resource becomes available. Note that in this scaled scalability test, good speedup performance is indicated by an almost constant time usage independent of the number of processors.

4.3. Parallel Boussinesq Simulations

Simulating the propagation of ocean waves is the target of the our third and final concrete case. The reader is referred to Appendix Appendix C for the mathematical model and the numerical method. The involved equations can be solved in parallel by the additive Schwarz algorithm of Section 3.3.

Table 2. Timing results of the parallel DMC simulations where each processor is constantly assigned with 200 walkers, all moved in 5000 time steps.

CPU's	Time	Efficiency
1	37m10.389s	N/A
5	42m32.359s	87.39%
10	42m00.734s	88.48%
20	42m29.945s	87.47%
30	42m33.895s	87.33%
40	43m30.092s	85.45%
50	43m39.159s	85.16%

Our starting point for parallelization is a 25 years old legacy Fortran 77 code consisting of a set of subroutines. More specifically, the most important subroutines are `KONTIT` and `BERIT`, which target the two semi-discretized equations (C.3) and (C.4) of the mathematical model (see Appendix Appendix C). These two Fortran 77 subroutines contain intricate algorithms with nested layers of do-loops, which are considered to be very difficult to parallelize by directly inserting MPI calls in the Fortran code. Performing the parallelization outside the Fortran code is therefore much more convenient. Using the proposed framework in the present paper the parallelization is a technically quite straightforward task.

The subdomain solver consists of calls to the subroutines `KONTIT` and `BERIT`. The implementation of the Python function `subdomain_solve` (see Section 3.3) requires a Python interface to `KONTIT` and `BERIT`, which can easily be produced by the F2PY software. Since a subdomain solver needs to set artificial boundary conditions at non-physical boundaries, we have programmed two light-weight wrapper subroutines in Fortran, `WKONTIT` and `WBERIT`, which handles the boundary conditions before invoking `KONTIT` and `BERIT`. We then apply F2PY to make `WKONTIT` and `WBERIT` callable from Python. Since the Fortran subroutines have lots of input data in long argument lists and `subdomain_solve` takes no arguments, we have created a class where the Fortran input variables are stored as class attributes:

```
import f77 # extension module for the Fortran code

class SubdomainSolver:
    def __init__(self, ...):
        # set input arguments to the Fortran subroutines as class attributes
        # (nbit,F,YW,H,QY,WRK,dx,dy,dt,kit,ik,gg,alpha,eps,
        # lower_x_neigh,upper_x_neigh,lower_y_neigh,upper_y_neigh)

    def continuity(self):
        self.Y, self.nbit = f77.WKONTIT(\
            self.F, self.Y, self.YW, self.H, self.QY, self.WRK,
            self.dx, self.dy, self.dt, self.kit, self.ik,
            self.gg, self.alpha, self.eps, self.nbit,
            self.lower_x_neigh, self.upper_x_neigh,
            self.lower_y_neigh, self.upper_y_neigh)
```

```

def bernoulli(self):
    # similar to the continuity method

sd = SubdomainSolver(...)
subdomain_solve1 = sd.continuity
subdomain_solve2 = sd.bernoulli

```

Note that since there are two PDEs (C.3) and (C.4), we have created two functions: `subdomain_solve1` and `subdomain_solve2`. The main computation of the resulting parallel program is in the following while loop:

```

t = 0
while t < t_stop:
    t = t+dt
    additive_Schwarz_iterations(subdomain_solve1, communicate,
                                set_BC, 10, 1E-3, sd.Y)
    additive_Schwarz_iterations(subdomain_solve2, communicate,
                                set_BC, 10, 1E-3, sd.F)

```

The `additive_Schwarz_iterations` function from Section 3.3 can be placed in a reusable module. The `communicate` function is borrowed from a Python library for mesh partitioning and inter-subdomain communication. The `set_BC` function actually does not do anything for this particular application.

Speedup results are reported in Table 3, for which the global solution mesh was fixed at 1000×1000 , and the number of time steps was 40. The results show that we can handle a quite complicated mathematical problem in a black-box Fortran code with our suggested simple framework and obtain a remarkable good speedup, with just a trivial extension of the Fortran code.

Table 3. The speedup results of the Python enabled parallel Boussinesq simulations.

CPUs	Time	Speedup	Efficiency
1	166.66s	N/A	N/A
2	83.61s	1.99	99.67%
4	44.45s	3.75	93.73%
8	20.16s	8.27	103.33%
16	11.43s	14.58	91.13%

5. Conclusion

We have shown how serial scientific codes written in various common languages, including Fortran, C, C++, and Python, can be parallelized in a separate, small software unit written in Python. The advantage of such an approach is twofold. First, the existing, often complicated, scientific high-performance code remains (almost) unchanged. Second, the parallel algorithm and its inter-processor communication are conveniently implemented in high-level Python code.

This approach to parallelization has been implemented in a software framework where the programmer needs to implement a few Python functions for carrying out the

key steps in the solution approach. For example, our first application involves doing a set of independent tasks in parallel, where a small Python framework deals with the parallelism and demands the user to supply three functions: `initialize` for preparing input data to the mathematical model, `func` for calling up the serial scientific code, and `finalize` for processing the computational results. Some more functions must be supplied in more complicated problems where the algorithm evolves in time, with a need for dynamic load balancing and more parallel communication.

Our simple software frameworks outlined in this paper are applicable to many different scientific areas, and we have described some common classes of problems: parameter investigation of a mathematical model, standard Monte Carlo simulation, Monte Carlo simulation with need for dynamic load balancing, and numerical solution of partial differential equations. In each of these cases, we have outlined fairly detailed Python code such that most technical details of the parallel implementations are documented. This may ease the migration of the ideas to new classes of problems beyond the scope of this paper.

In particular, the shown frameworks have been used to parallelize three real scientific problems taken from our research. The problems concern Markov Chain Monte Carlo models for voting behavior in political science, Diffusion Monte Carlo methods for Bose-Einstein condensation in quantum mechanics, and additive Schwarz and finite difference methods for simulating ocean waves by a system of partial differential equations. The results of our investigations of the parallel efficiency are very encouraging: In all these real science problems, parallelizing serial codes in the proposed Python framework gives almost optimal speedup results, showing that there arises no significant loss due to using Python and performing the parallelization “outside” the serial codes.

As a conclusion, we believe that the ideas and code samples from this paper can simplify parallelization of serial codes greatly, without significant loss of computational efficiency. This is good news for scientists who are non-experts in parallel programming but want to parallelize their serial codes with as small efforts as possible.

Appendix A. Voting in Legislatures

In the spatial model of politics, both actors' preferences over policies (ideal points) and policy alternatives are arranged geometrically in a low-dimensional Euclidean space. An actor receives the highest possible utility if a policy is located at her ideal point; she gains or loses utility as the policy moves towards or away from her ideal point [35]. We adopt the Bayesian approach proposed by Clinton, Jackman and Rivers [36]. Assume there are n legislators who vote on m proposals. On each vote $j = 1, \dots, m$, legislator $i = 1, \dots, n$ chooses between a "Yea" position ζ_j and a "Nay" position ψ_j located in the policy-space \mathbb{R}^d , where d is the number of dimensions. Then, we have $y_{ij} = 1$ if legislator i votes "Yea" on roll call j , and $y_{ij} = 0$ if she votes "Nay". The model assumes quadratic utility functions. The ideal point of legislator i is $x_i \in \mathbb{R}$, while η_{ij} and v_{ij} are stochastic elements whose distribution is jointly normal. The variance of the stochastic elements is $(\eta_{ij} - v_{ij}) = \sigma_j^2$. Denote the Euclidean norm by $\|\cdot\|$, utility maximising implies that legislator i votes "Yea" on vote j if

$$U_i(\zeta_j) = -\|x_i - \zeta_j\|^2 + \eta_{ij} > U_i(\psi_j) = -\|x_i - \psi_j\|^2 + v_{ij} \quad (\text{A.1})$$

and "Nay" otherwise. Clinton, Jackman and Rivers [36] show that the model can be understood as a hierarchical probit model:

$$P(y_{ij} = 1) = \Phi(\beta_j' \mathbf{x}_i - \alpha_j), \quad (\text{A.2})$$

where $\beta_j = 2(\zeta_j - \psi_j)/\sigma_j$, $\alpha_j = (\zeta_j' \zeta_j - \psi_j' \psi_j)/\sigma_j$, $\Phi(\cdot)$ is the standard normal function, β_j is the midpoint between the "Yea" and "Nay" positions on proposal j , and \mathbf{x}_i is the legislator's ideal point. The direction of α_j indicates the location of the status quo relative to the proposal. If α_j is positive, the new proposal is located higher on the dimension than the status quo. If α_j is negative, the new proposal is located lower on the dimension than the status quo.

The MCMC Algorithm. In the Markov Chain Monte Carlo (MCMC) algorithm for the statistical analysis of voting behavior [36], the difference between utilities of the alternatives on the j th vote for the i th legislator is given by $y_{ij}^* = \beta_j' \mathbf{x}_i - \alpha_j + \epsilon_{ij}$, where β_j and α_j are model parameters, \mathbf{x}_i is a vector of regression coefficients and ϵ_{ij} are standard normal errors. If we know β_j and α_j , \mathbf{x}_i can be imputed from the regression of $y_{ij}^* + \alpha_j$ on β_j using the m votes of legislator i and vice versa. If we know \mathbf{x}_i , we can use the votes of the n legislators on roll call j to find β_j and α_j . Given \mathbf{x}_i , β_j and α_j (either from priors or from the previous iteration), we can find y_{ij}^* by drawing ϵ_{ij} randomly from a normal distribution subject to the constraints implied by the actual votes, i.e., if $y_{ij} = 0$, $y_{ij}^* < 0$ and if $y_{ij} = 1$, $y_{ij}^* > 0$.

The goal is to compute the joint posterior density for all model parameters β_j and α_j , $j = 1, \dots, m$ and all coefficient vectors x_i , $i = 1, \dots, n$. The MCMC algorithm forms a Markov chain to explore as much as possible of this joint density, i.e., letting t index an MCMC iteration,

- (i) find $y_{ij}^{*,t}$ from \mathbf{x}_i^{t-1} , β_j^{t-1} and α_j^{t-1} ,

- (ii) sample β_j^t and α_j^t using \mathbf{x}_i^{t-1} and $y_{ij}^{*,t}$,
- (iii) find \mathbf{x}_i^t from β_j^t , α_j^t and $y_{ij}^{*,t}$.

This process must then be repeated until convergence, i.e., that the samples have moved away from the priors to the neighborhood of the posterior mode before samples are drawn.

Clinton, Jackman and Rivers [36, p. 369] find that the computation time is increasing in nmT , where n is the number of legislators, m is the number of votes and T is the number of MCMC iterations. Although they argue that very long runs are normally not necessary, they nevertheless advise long runs to ensure that the MCMC algorithm has converged. It is increasingly time-consuming to estimate the model on a standard desktop computer as the size of the legislature and the number of votes increase.

Appendix B. Bose-Einstein Condensation

The famous experiment of Anderson et al. [37] was about cooling 4×10^6 ^{87}Rb down to temperatures in the order of 100 nK for observing Bose-Einstein condensation in the dilute gas. To model this fascinating experiment in the framework of Quantum Monte Carlo, so that numerical simulations can be extended beyond the physical experiments, we may use the governing Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{R}, t) = H \Psi(\mathbf{R}, t). \quad (\text{B.1})$$

The most important parts of the mathematical model are a Hamiltonian H and a wave function Ψ , see [38]. The Hamiltonian for N trapped interacting atoms is given by

$$H = -\frac{\hbar^2}{2m} \sum_{i=1}^N \nabla_i^2 + \sum_{i=1}^N V_{\text{ext}}(\mathbf{r}_i) + \sum_{i < j}^N V_{\text{int}}(|\mathbf{r}_i - \mathbf{r}_j|). \quad (\text{B.2})$$

The external potential V_{ext} corresponds to the trap used to confine the ^{87}Rb atoms, and was in the experiment in the order of \mathbf{r}^2 . The two-body interaction $V_{\text{int}}(|\mathbf{r}_i - \mathbf{r}_j|)$ can be easily described by a hard-core potential of radius a in a dilute gas. We have however, for the sake of simplicity, neglected these interactions in our example implementation of class `Walkers`.

The Method of Diffusion Monte Carlo. In the Diffusion Monte Carlo (DMC) method [39], the Schrödinger equation is solved in imaginary time,

$$-\frac{\partial \psi(\mathbf{R}, t)}{\partial t} = [H - E] \psi(\mathbf{R}, t). \quad (\text{B.3})$$

The formal solution of (B.3) is

$$\psi(\mathbf{R}, t) = e^{-[H-E]t} \psi(\mathbf{R}, 0), \quad (\text{B.4})$$

where $e^{[-(H-E)t]}$ is called the *Green's function*, and E is a convenient energy shift.

The wave function $\psi(\mathbf{R}, t)$ in DMC is represented by a set of random vectors $\{R_1, R_2, \dots, R_M\}$, in such a form that the time evolution of the wave function is actually represented by the evolution of a set of walkers. This feature gives rise to task parallelism. The wave function is positive definite everywhere, as it happens with the ground state of a bosonic system, so it may be considered as a probability distribution function.

The DMC method involves Monte Carlo integration of the Green's function by every walker. The time evolution is done in small time steps τ , using the following approximate form of the Green's function:

$$e^{-(H-E)t} = \prod_{i=1}^n e^{-(H-E)\tau}, \quad (\text{B.5})$$

where $\tau = t/n$. Assume that an arbitrary starting state can be expanded in the basis of stationary,

$$\psi(\mathbf{R}, 0) = \sum_{\nu} C_{\nu} \phi_{\nu}(\mathbf{R}), \quad (\text{B.6})$$

we have

$$\psi(\mathbf{R}, t) = \sum_{\nu} e^{-(E_{\nu}-E)t} C_{\nu} \phi_{\nu}(\mathbf{R}), \quad (\text{B.7})$$

in such a way that the lowest energy components will have the largest amplitudes after a long elapsed time, and in the limit of $t \rightarrow \infty$ the most important amplitude will correspond to the ground state (if $C_0 \neq 0$)[‡].

The Green's function is approximated by splitting it up in a diffusional part,

$$G_D = (4\pi D\tau)^{-3N/2} \exp\{-(\mathbf{R}' - \mathbf{R})^2/4D\tau\}, \quad (\text{B.8})$$

which has the form of a Gaussian and a branching part,

$$G_B = \exp\{-(V(\mathbf{R}) + V(\mathbf{R}'))/2 - E_T\tau\}. \quad (\text{B.9})$$

While diffusion is taken care of by a Gaussian random distribution, the branching is simulated by creation and destruction of walkers with a probability G_B . The idea of DMC computation is quite simple; once we have found an appropriate approximation of the short-time Green's function and determined a starting state, the computation consists in representing the starting state by a collection of walkers and letting them independently evolve in time. That is, we keep updating the walker population, until a large enough time when all other states than the ground state are negligible.

[‡] This can easily be seen by replacing E with the ground state energy E_0 in (B.7). As E_0 is the lowest energy, we will get $\lim_{t \rightarrow \infty} \sum_{\nu} \exp[-(E_{\nu} - E_0)t] \phi_{\nu} = C_0 \phi_0$.

Algorithm 1 Diffusion Monte Carlo

```

for step in range( 0, timesteps ):
    for i in range( 0, Nwalkers ):
        Diffusion;
        propose move  $\mathbf{R}' = \mathbf{R} + \xi$ 
        Branching;
        calculate replication factor  $n$ :
             $n = \text{int}(\exp\{-(V(\mathbf{R}) + V(\mathbf{R}'))/2 - E_T\}\tau)$ 
        if  $n = 0$ :
            mark walker as dying
        if  $n > 0$ :
            mark walker to make  $n - 1$  clones
        Remove dead walkers and make new clones;
        Update walker population  $N_{\text{walkers}}$  and adjust trial energy;
        Sample contributions to observable.

```

The Implementation. In Algorithm 1 we summarize the DMC algorithm corresponding to (B.8)-(B.9). In the algorithm ξ is a Gaussian with zero mean and a variance of $2D\tau$ corresponding to (B.8). The deleting and cloning of walkers are, as mentioned in Section 3.2, performed by the `do_timestep` function, repeated here for clarity:

```

def do_timestep(walkers):
    walkers.move()
    for walker in range(len(walkers)):
        if walkers.get_marker(walker) == 0:
            walkers.delete(walker)
        elif walkers.get_marker(walker) > 1:
            walkers.append(walker, walkers.get_marker(walker)-1)
    return walkers.sample_observables()

```

The main computational work of the DMC algorithm at each time step is implemented in the `move` function inside class `Walkers`, together with a helper function `branching`:

```

class Walkers:
    ...

    def branching(self, new_positions):
        old_potential = potential(self.positions)
        new_potential = potential(new_positions)
        branch = numpy.exp(-(0.5 * (old_potential + new_potential)
                                - self.adjust_branching) * self.stepsize)
        self.markers = numpy.array(branch +
                                    numpy.random.uniform(0,1,branch.shape), 'i')

    def move(self):
        displacements = numpy.random.normal(0, 2*self.stepsize,
                                             self.positions.shape)
        new_positions = self.positions + displacements
        self.branching(new_positions)

```

```

    self.positions = new_positions
    ...

```

The `move` function first generates a set of Gaussian (normal) distributed random numbers, corresponding to (B.8). Next, it calls the `branching` function, which calculates a potential $V(\mathbf{r}) = \mathbf{r}^2$ for the old and the new positions[§]. These potentials are used to calculate G_B following (B.9) and create an integer array `self.markers` with its average value equal to G_B (stored in the `branch` variable). This array is of the same length as the number of walkers (stored in `self.positions`) and marks the walkers as dying or clone-able.

It is worth noticing that if the new potential of a walker is much higher than that in the previous time step (i.e., the walker is far from the center of the trap), the value of `branch` will be close to 0 and the walker will be deleted. However, if the new potential is much lower (i.e. closer to the center of the trap), `branch` will be greater than 1 and the walker will be cloned. As long as the two-body interaction is ignored, the walkers will only be encouraged to move towards the center of the trap, thus yielding a lower energy than seen in real experiments.

Appendix C. Ocean Wave Propagation

The following two PDEs, normally termed as the Boussinesq water wave equations [40], can be used to model wave propagation:

$$\frac{\partial \eta}{\partial t} + \nabla \cdot \left((H + \alpha \eta) \nabla \phi + \epsilon H \left(\frac{1}{6} \frac{\partial \eta}{\partial t} - \frac{1}{3} \nabla H \cdot \nabla \phi \right) \nabla H \right) = 0, \quad (\text{C.1})$$

$$\frac{\partial \phi}{\partial t} + \frac{\alpha}{2} \nabla \phi \cdot \nabla \phi + \eta - \frac{\epsilon}{2} H \nabla \cdot \left(H \nabla \frac{\partial \phi}{\partial t} \right) + \frac{\epsilon}{6} H^2 \nabla^2 \frac{\partial \phi}{\partial t} = 0. \quad (\text{C.2})$$

The primary unknowns of (C.1)-(C.2) are the water surface elevation $\eta(x, y, t)$ and the depth-averaged velocity potential $\phi(x, y, t)$. The symbol H denotes the water depth as a function of (x, y) . The advantage of the above Boussinesq wave model, in comparison with the standard shallow water equations, is its capability of modeling waves that are weakly dispersive ($\epsilon > 0$) and/or weakly nonlinear ($\alpha > 0$), see [41]. Therefore, the Boussinesq water wave equations are particularly adequate for simulating ocean wave propagation over long distances and large water depths.

Discretization of the Boussinesq water wave equations (C.1)-(C.2) normally starts with a temporal discretization as follows:

$$\begin{aligned} & \frac{\eta^\ell - \eta^{\ell-1}}{\Delta t} + \nabla \cdot \left(\left(H + \alpha \frac{\eta^{\ell-1} + \eta^\ell}{2} \right) \nabla \phi^{\ell-1} + \right. \\ & \left. \epsilon H \left(\frac{1}{6} \frac{\eta^\ell - \eta^{\ell-1}}{\Delta t} - \frac{1}{3} \nabla H \cdot \nabla \phi^{\ell-1} \right) \nabla H \right) = 0, \end{aligned} \quad (\text{C.3})$$

[§] In a more optimized implementation, the old potential would have been stored from the previous move and not calculated every time.

$$\begin{aligned} & \frac{\phi^\ell - \phi^{\ell-1}}{\Delta t} + \frac{\alpha}{2} \nabla \phi^{\ell-1} \cdot \nabla \phi^{\ell-1} + \eta^\ell - \\ & \frac{\epsilon}{2} H \nabla \cdot \left(H \nabla \left(\frac{\phi^\ell - \phi^{\ell-1}}{\Delta t} \right) \right) + \frac{\epsilon}{6} H^2 \nabla^2 \left(\frac{\phi^\ell - \phi^{\ell-1}}{\Delta t} \right) = 0, \end{aligned} \quad (\text{C.4})$$

where we use ℓ to denote the time level, and Δt denotes the time step size. The basic idea of computation at each time step is to first compute η^ℓ based on $\eta^{\ell-1}$ and $\phi^{\ell-1}$ from the previous time step, and then compute ϕ^ℓ using the new η^ℓ and the old $\phi^{\ell-1}$. To carry out the actual numerical computation, we need a spatial discretization of (C.3)-(C.4), using e.g. finite differences or finite elements, so we end up with two systems of linear equations that need to be solved during each time step.

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