Compmake: Minimal Effort Parallelization and Job Management for Python Applications

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***Abstract*—Compmake is a jobs-oriented Python library that provides Make-like functionality to Python applications. The user minimally modifies its program, so that now it describes the computation as a jobs graph. Once that is done, Compmake provides for free a series of features including parallelization, caching, failure tolerance, dependencies handling, job scheduling, and a console interface to inspect the results.**

I. Introduction

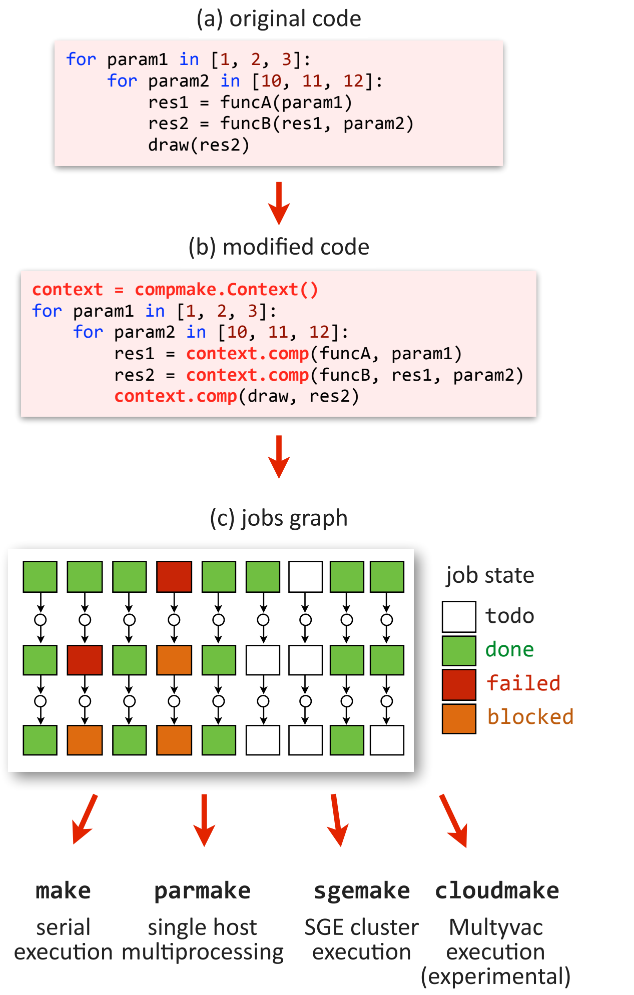
Compmake is a Python library that provides Make [1]-like facilities for Python applications. To use Compmake, the user minimally modifies their Python script to turn function calls into "jobs" definition, so that Compmake can understand the processing layout and the opportunities for parallelization (Fig. 1).

Once this is done, Compmake provides several features:

- **Parallelization**: Jobs can be executed in parallel, both on a single host, on a cluster using SGE, and, experimentally, in the cloud using Multyvac.
- **Caching:** The computation can be interrupted (CTRL-C) and restarted without losing the results of the jobs already executed.
- **Selective computation**: The user can choose to execute only part of the jobs.
- **Failure tolerance:** If a job fails by throwing an exception, the error is recorded, and processing continues for jobs continues processing the jobs that do not depend on the failed one.
- **Console**: Familiar commands (`make` , `clean` , `ls` , etc.) are available for scheduling job processing and inspecting completions, failures, and resources usage.

Compmake's design goal is to have the most functionality while imposing little burden on the programmer. Parallelization is the most obvious benefit, but not the only one. Compmake helps immensely the development process.

Compmake allows creating applications that are structured in "jobs" which create a "job graph" (Fig. 1*b*). The jobs graph is dynamic. Jobs that can depend on other jobs, and spawn other jobs recursively. Once the jobs are defined, there are several options for running them. They can be run serially or in parallel, either all in the same process or spawning a different process. Several backends for parallel processing are available, including single-machine multiprocessing, and cluster processing using the Sun Grid Engine (SGE) interface [2].


(a) original code

```
for param1 in [1, 2, 3]:
    for param2 in [10, 11, 12]:
        res1 = funcA(param1)
        res2 = funcB(res1, param2)
        draw(res2)
```

(b) modified code

```
context = compmake.Context()
for param1 in [1, 2, 3]:
    for param2 in [10, 11, 12]:
        res1 = context.comp(funcA, param1)
        res2 = context.comp(funcB, res1, param2)
        context.comp(draw, res2)
```

Figure 1. The user minimally modifies the program, so that Compmake can understand its processing layout and the opportunities for parallelization. The same program can be run serially, in parallel using single-host multiprocessing, or on a cluster.

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II. Why using Compmake

There are many reasons to use Compmake. Perhaps the most evident is the support for parallelization. This sections explains the other less obvious benefits of Compmake, especially during development.

Suppose that you are working on the simple program below:

```
for param1 in [1, 2, 3]:
    for param2 in [10, 11, 12]:
        res1 = funcA(param1)
        res2 = funcB(res1, param2)
        draw(res2)
```

For every value of the parameters, there is an invocation of the functions `funcA()`, `funcB()`, followed by `draw()`, which depends on the results of the other two. The following are probable scenarios that occur during development in which Compmake can help.

Suppose you are working on improving the function `draw()`. You find yourself running the whole program again and again to check the results of that function. This is a waste because `funcA()` and `funcB()` did not change. It's obvious that some caching mechanism is needed. You can implement one in different ways. You can explicitly dump the intermediate results to a file using *pickling* [3], then write code to read that file if it exists. But now your 5 lines program has become a buggy 30 lines program.

Compmake helps by implementing automatic caching of the results.

Suppose there is a bug for one combination of values of the parameters, say `param1=2` and `param2=11`. Therefore you want to re-run processing only for that combination of the parameters. Without Compmake the best way to do this is perhaps to comment out the two `for` loops, which is easy enough…Eventually, the source code becomes a mess of commented and decommented lines.

Compmake helps by implementing selective execution. The user can choose which jobs to execute.

You left the computation running for the night. When you check it out in the morning, you discover that there is one combination of `param1` and `param2` that makes `funcB()` throw an exception. Your program terminated around 1am. The fix is easy enough and you have to start again from the beginning.

Compmake helps by working around the failure of part of your jobs.

What about parallelization? Yes, the *multiprocessing* module [4] seem quite easy to use. You just need to add a few lines of code. But wait, there is a nested loop. You probably have to write different functions… and, where exactly can you parallelize?

Compmake helps by automatically discovering the possible parallelization opportunities in your program.

No, really, what you want is running your computation on the large university cluster. You do have an account. Of course, the code using the multiprocessing module cannot be directly adapted to run on the cluster.

Compmake helps by separating the frontend (job definition) and the backend (job execution). There are several backends available: you can try your program on your computer with multiprocessing, and then run the same program, unchanged, on an SGE cluster.

In short, writing computationally intensive batch processes presents a series of common problems. In isolation, each of them could be overcome by writing *ad hoc* code. Compmake helps by solving each of these problems (and more) in a robust way, once and for all.

III. When *not* to use Compmake

Compmake has been designed for relatively long computational expensive batch jobs. Currently, Compmake is not well suited for:

- Applications consisting of very small jobs (say < 0.1 s of CPU time per job), because of the overhead.
- Applications containing more than ~50,000 jobs. That is the level for which you can have a responsive console with the filesystem storage backend.
- Applications for which all the intermediate results are too big to be stored on disk.

See also Section VIII, which describes Compmake's limitations from a more technical point of view.

A. Alternatives

Depending on what you need to do, there are many other products that might be used:

- There are libraries that focus on performance instead of generality and are optimized for specific dataflows. One example is Spark [5].
- Hadoop [6] can be used for *MapReduce* [7] dataflows.
- Celery [8] is a popular distributed task queue.
- Scoop [9] is a recent Python library that shares some of Compmake's philosophy.

Both Celery and Scoop could be used to serve as "backend" for Compmake (just like Multyvac and SGE).

IV. A Compmake Tutorial

(See also the screencast at purl.org/censi/compmake-basics)

A. Installation

The simplest way to install Compmake is using `easy_install`:

```
$ easy_install -U compmake
```

Alternatively, you can use `pip`:

```
$ pip install -U compmake
```

You can also clone the *Git* repository:

```
$ git clone https://github.com/AndreaCensi/compmake.git
$ cd compmake
$ python setup.py develop
```

If you plan to make your own changes to Compmake, first fork the repository at github.com/AndreaCensi/compmake so that you can easily do pull requests.

B. Creating jobs

Compmake makes a Python program parallelizable through a simple change in the code.

A function invocation like

```
function(param)
```

is modified in an invocation of the kind

```
context.comp(function, param)
```

where `context` is a `compmake.Context` object.

This and a couple of lines of initialization are all that is needed to make a program parallelizable.

The invocation `context.comp(function, param)` does not actually run the computation `function(param)`, but rather it creates a corresponding “job” in the job database. It returns, immediately, a “promise” (or “future”) representing the result of calling that function. This value can be used successive calls to `context.comp()`. In this way, Compmake learns the computational structure of your program.

For example, suppose this is the original code:

```
res = function(param)
function2(param2, res)
```

In Compmake you would write:

```
p = context.comp(function, param)
# p is a placeholder for function(param)
assert isinstance(p, compmake.Promise)
# use p as you would use the result
context.comp(function2, param2, p)
```

When the snippet is executed two jobs are created. The result of the first function will be passed to the second function.

example.py

```
import time

# A few functions representing a complex workflow
def funcA(param1):
    print('funcA(%s)' % param1)
    time.sleep(1) # ... which takes some time
    return param1

def funcB(res1, param2):
    print('funcB(%s, %s)' % (res1, param2))
    time.sleep(1) # ... which takes some time
    return res1 + param1

def draw(res2):
    print('draw(%s)' % res2)

if __name__ == '__main__':
    from compmake import Context
    context = Context()
    # A typical pattern: you want to try
    # many combinations of parameters
    for param1 in [1,2,3]:
        for param2 in [10,11,12]:
            # Simply use "y = comp(f, x)" whenever
            # you would have used "y = f(x)".
            res1 = context.comp(funcA, param1)
            # You can use return values as well.
            res2 = context.comp(funcB, res1, param2)
            context.comp(draw, res2)

    # Now, a few options to run this:
    # 1) Call this file using the compmake program:
    #  $ python example.py
    #  and then run "make" at the prompt.
    # 2) Give the command on the command line:
    #  $ python example.py "make"
    import sys
    if len(sys.argv) == 1:
        print('Presenting an interactive console')
        context.compmake_console()
    else:
        print('Running the computation in batch mode')
        cmd = " ".join(sys.argv[1:])
        context.batch_command(cmd)
```

Figure 2. A complete example

C. A complete example

To write a complete example, there are a couple of lines of initialization needed to initialize Compmake’s “context”.

Fig. 2 gives a complete example of a Compmake program (`example.py`). Above the source code there is a download link.

If you run this program:

```
$ python example.py
```

You will see a prompt:

```
Compmake 3.3  (27 jobs loaded)
@:
```

This prompt, starting with “`@:`” is the prompt for Compmake’s console.

Run `make` at the prompt:

```
@: make
```

This will execute all jobs serially.

D. Using the console

Compmake's console is used for listing, executing, cleaning jobs.

1) Listing jobs: The command `ls` gives a list of the jobs together with their status:

```
@: ls
    draw    todo
    draw-2  todo
    draw-3  todo
    draw-4  todo
[...]
```

The possible states are given in Table I.

Table I
COMPMAKE JOBS STATES

state	*meaning*
`todo`	The job was not executed yet.
`done`	The job was successfully executed.
`failed`	The job was executed and failed.
`blocked`	The job cannot be executed because one of its dependencies failed or is blocked.

2) Making jobs: The command `make [<jobs>]` runs the computation in series:

```
@: make
```

The first time you run this, you will see the names of the jobs being executed scrolling by. However, the second time, the output will be something like:

```
@: make
Nothing to do.
```

because Compmake has cached the results of the computation.

After making, use `ls` to see the results:

```
@: ls
    draw   done
    draw-2 done
    draw-3 done
    draw-4 done
    draw-5 done
[...]
```

3) Cleaning up: Use the command `clean` to *clean* all jobs:

```
@: clean
```

4) Selective re-make: You can selectively remake part of the computations. For example, suppose that you modify the `draw()` function, and you want to rerun only the last step. You can achieve that by

```
@: remake draw*
```

Compmake will reuse the computations (`funcA()` and `funcB()`) but it will redo the last step.

The same effect can be obtained using `clean` and `make` :

```
@: clean draw*
@: make draw*
```

E. Naming jobs

Each invocation of the `context.comp()` function produces one "job". Each job is described by a unique ID. By default, the ID is generated by the name of the function, with a progressive number postponed. You can use the command `ls` to obtain a list of the jobs. For this example, the output would be:

```
@: ls
      draw     todo
      draw-2   todo
      draw-3   todo
      draw-4   todo
      draw-5   todo
      draw-6   todo
[...]
```

As you can see, the jobs are named `funcA` -n, `funcB` -n, `draw` -n.

It is very useful to have distinctive names for the jobs. Compmake provides two mechanisms to that effect. The first is the function `context.comp_prefix()` which takes a string used as a prefix for the job ids generated. That command is particularly useful in scenarios like the example where one want to group the functions by the parameters:

using_compmake2.py

```
from mycomputations import funcA, funcB, draw

if __name__ == '__main__':
    from compmake import Context
    context = Context()

    for param_a in [1, 2, 3]:
        for param_b in [10, 11, 12]:
            # Add a prefix to the job ids for easy reference
            prefix = 'a%s-b%s' % (param_a, param_b)
            context.comp_prefix(prefix)

            res1 = context.comp(funcA, param_a)
            res2 = context.comp(funcB, res1, param_b)
            context.comp(draw, res2)

    context.compmake_console()
```

Now the `ls` command gives:

```
@: ls
      a1-b10-draw   todo
      a1-b10-funcA  todo
      a1-b10-funcB  todo
      a1-b11-draw   todo
      a1-b11-funcA  todo
      a1-b11-funcB  todo
[...]
```

Another method is using the `job_id` keyword argument to `context.comp()` :

using_compmake3.py

```
from mycomputations import funcA, funcB, draw

if __name__ == '__main__':
    from compmake import Context
    context = Context()

    for param_a in [1, 2, 3]:
        for param_b in [10, 11, 12]:
            prefix = 'a%s-b%s' % (param_a, param_b)
            context.comp_prefix(prefix)

            # use job_id to override default naming
            res1 = context.comp(funcA, param_a,
                                job_id='preparing')
            res2 = context.comp(funcB, res1, param_b,
                                job_id='computing')
            context.comp(draw, res2,
                         job_id='drawing')

    context.compmake_console()
```

Now the `ls` command gives:

```
@: ls
      a1-b10-computing  todo
      a1-b10-drawing    todo
      a1-b10-preparing  todo
      a1-b11-computing  todo
      a1-b11-drawing    todo
      a1-b11-preparing  todo
[...]
```

F. Tolerance to job failure

If a some of the jobs fail (e.g., they throw an exception), Compmake will go forward with the rest of the jobs.

To try this behavior, see the example example_fail.py. In this example some jobs will launch an exception.

When Compmake runs this application, it will tell which jobs failed:

```
@: make
Job 'a2-b11-computing' failed:
| Exception raised for b = 11.
Job 'a3-b11-computing' failed:
| Exception raised for b = 11.
Job 'a1-b11-computing' failed:
| Exception raised for b = 11.
Make failed (3 failed, 3 blocked)
```

The console displays the exception for the job that failed. To see further details about the errors, including the backtrace, use the command `details`.

Some jobs will have a status of `failed`. The jobs that depend on them will have status of `blocked`:

```
@: ls a1-*
       a1-b10-computing     done
       a1-b10-drawing       done
       a1-b10-preparing     done
       a1-b11-computing   failed
       a1-b11-drawing    blocked
       a1-b11-preparing     done
       a1-b12-computing     done
       a1-b12-drawing       done
```

If you run `make` again, Compmake will try again to run only the jobs that failed previously.

G. Cleaning and remaking

Now that you know how to give names to your jobs, you can use them for referring to them. For example

```
@: make a1-b11-drawing
```

You can use the “ `*` ” wildcard. This is very useful to refer only to part of the jobs. In the example, you can write

```
@: remake *-b11-*
```

to re-do only the subset of computations with a certain value of the parameters. Or, you can remake the last stage of the computation:

```
@: remake *-drawing
```

H. Single-host multiprocessing

To use single-host multiprocessing, instead of using `make`, simply use `parmake`:

```
@: parmake
```

Optionally, you can specify the number of processes to spawn:

```
@: parmake n=11
```

If you don’t specify a number, Compmake will use the number of detected processors. If your jobs are IO-bound rather than CPU-bound, you should specify a larger number.

What’s happening under the hood is that Compmake spawns n workers processes using the *multiprocessing* module. So be aware that each job will run in a different process.

Another backend supported is SGE, described later in Section IX.

I. The `compmake` executable

Compmake comes with a command-line program called, unsurprisingly, `compmake`. This program can be used to start a session with a pre-existing job database and to run commands in batch mode. The syntax is:

```
$ copmpmake <job_db> [-c <command>]
```

For example, suppose the script `example.py` was executed like this:

```
$ python example.py
```

By default the jobs DB is created in the directory `out-<script>`. In this case, the jobs database is in `out-example`:

```
$ ls out-example
ls out-example/
cm-args-draw-2.pickle   cm-args-funcA-4.pickle
cm-args-funcB-6.pickle  cm-job-draw-8.pickle
cm-job-funcA.pickle     cm-args-draw-3.pickle
[...]
```

Now by using `compmake` one can start a session just by doing:

```
$ copmpmake out-example
```

This will load the existing jobs DB:

```
Loading existing jobs DB 'out-example1'.
Compmake 3.3 (27 jobs loaded)
@:
```

By using the `-c` switch one can run commands in batch mode. For example, this command cleans the previous computation and runs it again:

```
$ copmpmake out-example -c "clean; parmake; ls"
```

V. In detail: defining the jobs graph

Compmake provides much flexibility about the definition of jobs. Jobs can depend on other jobs, they can create other jobs, and they can "redirect" to other jobs.

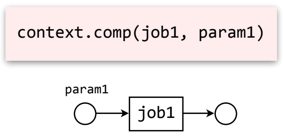
A. The basic job definition

Fig. 3 illustrates the graphical convention used to describe the job graph. One job is created using the invocation

```
context.comp(job1, param1)
```

Here `job1()` is a function, or any callable *and* pickable object, and `param1` is any (pickable) parameter.

The resulting job graph is illustrated below. It has one node, $\boxed{\texttt{job1}}$ indicating the job, and two other nodes, pictured with circles, indicating the parameter and the result of the job.



```
context.comp(job1, param1)
```

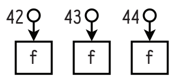
Figure 3. Graphic language for describing jobs and jobs dependencies.

The listing in Fig. 4 shows a complete Compmake program. This programs defines three jobs, each being an application of the function `f` with a different parameter. Thus these three jobs can be executed in parallel.

compmake_1.py

```python
def f(x):
    print('processing %s' % x)

if __name__ == '__main__':
    from compmake import Context
    c = Context()
    for p in [42, 43, 44]:
        c.comp(f, x=p)
    c.batch_command('clean;parmake')
```

(a) Source code



(b) Resulting job graph

Figure 4. Python/Compmake program that creates 3 independent jobs and executes them in parallel. The inset shows the *jobs graph*, using boxes to represent jobs, and circles for parameters.

B. Jobs with dependencies

A job can depend on another, in the sense that the result of the second job becomes a parameter of the first. The basic case is shown in Fig. 5.

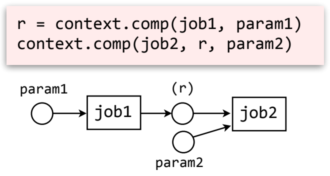
The first job is created as follows:

```
r =  context.comp(job1, param1)
```

The value `r` is a placeholder, a "promise", that represents the result of the job. This value can be used as a parameter to another job definition. For example:

```
context.comp(job2, r, param2)
```

The second job now depends on the first job. Graphically, this is represented by making the output node of the first job be the input node of the second job (Fig. 5).



```
r = context.comp(job1, param1)
context.comp(job2, r, param2)
```

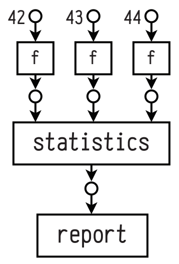
Figure 5. Graphic language for describing jobs and jobs dependencies.

The listing in Fig. 6 shows a typical program that creates jobs with dependencies. The `report` function depends on the output of `statistics`, which depends on three calls of the function `f`.

compmake_jobs_deps.py

```python
def f(x):
    print('f(x=%r)' % x)
    return x * 2

def statistics(res):
    print('statistics(res=%s)' % res.__repr__())
    return sum(res)

def report(val):
    print('The sum is: %r' % val)

if __name__ == '__main__':
    from compmake import Context
    c = Context()
    params = [42, 43, 44]
    jobs = [c.comp(f, x=p) for p in params]
    summary = c.comp(statistics, jobs)
    c.comp(report, summary)
    c.batch_command('clean;parmake echo=1')
```

(a) Source code



(b) Jobs graph

Figure 6. The typical scientific data application has three kinds of jobs: 1) the jobs that perform the "meat" of the computation (like the function `f` in this example); 2) Jobs that compute statistics from the computation (like the function `statistics`); and 3) Jobs that visualize the results (like the function `report`). The job graph is a tree structure. In the inset, the dependence between jobs is represented by the little circles representing both the output of a job and the input of another.

C. “Dynamic” jobs defining other jobs

Compmake supports design patterns in which jobs can define other jobs recursively. A job can be marked as “dynamic” if it is created using “ `context.comp_dynamic` ” rather than “ `context.comp` ”. For example:

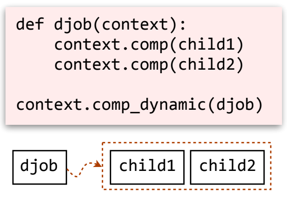
```
context.comp_dynamic(djob)
```

The function `djob()` must take as first argument a `context` , which is a reference that can be used to define further jobs. For example:

```
def djob(context):
    assert isinstance(context, compmake.Context)
    context.comp(child1)
    context.comp(child2)
```

When the job is executed two new jobs are created. If the job is cleaned and recomputed, the same jobs are overwritten. In general, Compmake is smart about keeping track of what job generated what.

The graphical representation of this is shown in Fig. 7. A dashed brown arrow indicates that the job generated the others in the dashed rectangle.



```
def djob(context):
    context.comp(child1)
    context.comp(child2)

context.comp_dynamic(djob)
```

Figure 7. Graphic language for describing jobs and jobs dependencies.

A complete example is shown in Fig. 8. The parameter `recurse=1` to `parmake` instructs Compmake to schedule the current jobs as well as any other jobs that might be created. Without that option, the three jobs are defined but not executed.

D. Jobs redirecting to other jobs

So far we have seen two possible relations between jobs:

1) A job *depends* on another job
2) A job *defines* another job.

There is another relation between jobs: when a job *redirects* its output to be the output of another. This is one of those cases where the difference is very little from the point of view of the user, but the implementation became quite complicated.

For example, consider the code

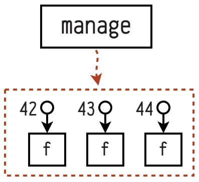
```
def djob(context):
    return context.comp(child)
```

The function `djob` is a dynamic job that defines another job `child` . In addition, the return value of the job itself is the return value of the child. This means that a job that depends on `djob` will be having as input the output `child` , and Compmake will take care of everything in the background for this to happen smoothly. This is a complete example:

compmake_jobs_dynamic.py

```
def f(x):
    print('f(x=%r)' % x)
    return x * 2

def schedule(context, params):
    print('schedule(context, params=%s)' % params.__repr__())
    for p in [42, 43, 44]:
        context.comp(f, x=p)

if __name__ == '__main__':
    from compmake import Context
    c = Context()
    c.comp_dynamic(schedule, params=[42, 43, 44])
    c.batch_command('clean;parmake echo=1 recurse=1')
```

(a) Source code



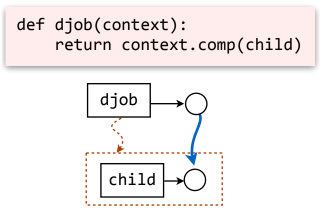
(b) Jobs graph

Figure 8. Jobs can be marked as “dynamic” and are then passed a Context object that can be used to define other jobs recursively. This relation between jobs is represented using the dashed line in the inset.

```
def child():
    return "output-of-child"
def djob(context):
    return context.comp(child)
def another(res):
    print res
if __name__ == '__main__':
    res = context.comp_dynamic(djob)
    context.comp(another, res)
    context.batch_command('make')
```

The output of this will be `"output-of-child"` . Note that here the job `another` becomes dependent on `child` , so that if you remake `child` also `another` will be re-done.

Graphically, this relation between jobs is represented by a black arrow from the output of `djob` to the output of `child` (Fig. 9).



```
def djob(context):
    return context.comp(child)
```

Figure 9. A job that defines a child and redirects to its result.

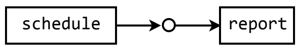
A complete example is reported in Fig. 10. Here, at definition time, the job graph looks as in Fig. 10b: the job `report` depends only on the job `schedule` . However, when the job `schedule` is executed, it creates three `f` jobs and the job `statistics` whose promise is returned as the result.

Therefore, after the execution of `schedule` the job graph looks as in Fig. 10c. Now `report` depends on all the other jobs. If one of the `f` jobs fails, then `report` will have a state of `blocked` at the end of execution.

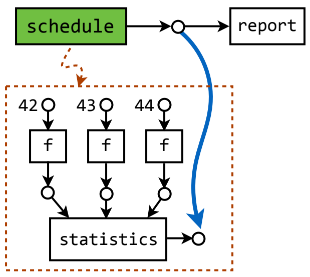
compmake_jobs_returning.py

```python
def f(x):
    print('f(x=%r)' % x)
    return x * 2

def statistics(res):
    print('statistics(res=%s)' % res.__repr__())
    return sum(res)

def schedule(context, params):
    print('schedule(context, params=%s)' % params.__repr__())
    jobs = [context.comp(f, x=p) for p in params]
    summary = context.comp(statistics, jobs)
    # returns a job "promise", not a value!
    return summary

def report(summary):
    print('report(summary=%r)' % summary)

if __name__ == '__main__':
    from compmake import Context
    c = Context()
    summary = c.comp_dynamic(schedule, [42, 43, 44])
    c.comp(report, summary)
    c.batch_command('clean;parmake echo=1 recurse=1')
```

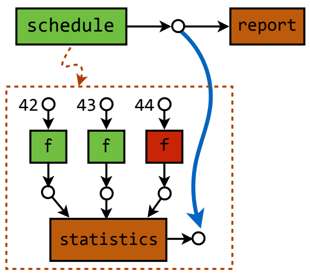
(a) Source code



(b) Jobs graph before executing `schedule`



(c) Jobs graph after executing `schedule`



(d) State of the jobs graph assuming one of the `f` fails.

Figure 10. Returning the value of another job

VI. Console Commands Reference

A. Job aliases

All commands that take as argument a list of jobs understand wildcards, a few predetermined *aliases* and some logical operators to describe the list of jobs on which they need to operate. The list of aliases is shown in Table II.

1) By job ID : The console supports the use of the wildcard "*". For example, this matches all jobs that have "drawing" in the job ID:

```
@: ls *drawing*
```

2) By function name: Compmake also keeps track of the function name, which is different from the job ID. You refer to the function name using the syntax " `funcname()` ".

For example:

```
def funcA():
    pass

context.comp(funcA, job_id='preparation')
```

The resulting job will have the id "`preparation`" but the name of the function "`funcA`" will be associated to it as well.

So it is possible to refer to that job using:

```
@: make preparation
```

as well as using

```
@: make funcA()
```

3) By job status: There are several aliases that refer to the status of the job: `all` (all jobs), `failed` , `blocked` , `done` , `todo` .

The alias `uptodate` refers to the jobs that are `done` and for which all dependencies (recursively) are `done` as well.

4) By definition depth: The alias `root` refers to all jobs that are defined in the main context. The alias `level1` refers to the jobs defined by `root` jobs. The alias `level2` refers to the jobs defined by those in `level1` and so forth.

5) By type: The alias `dynamic` refers to the jobs that are marked as dynamic—those that were defined using `context.comp_dynamic` and that take a `context` argument.

6) By dependencies relations: The alias `bottom` refers to jobs that have no dependencies.

The alias `top` refers to all those jobs that are the "top" of the graph, in the sense that no other jobs depends on them.

B. Logical operations on jobs lists

The console also supports some logical operations on jobs lists: `and` , `except` , `not` . If two lists are specified next to each other, "or" is implied.

1) Implied or: For example, this lists all jobs matching "drawing" or "computing":

```
@: ls *drawing* *computing*
```

2) And: This lists all failed jobs that match "drawing":

```
@: ls failed and *drawing*
```

3) Except: This lists all failed jobs *except* those matching "drawing":

```
@: ls failed except *drawing*
```

4) Not: The conjunction "not *list*" is equivalent to "all except *list*". For example this:

```
@: ls not *drawing*
```

is equivalent to

```
@: ls all except *drawing*
```

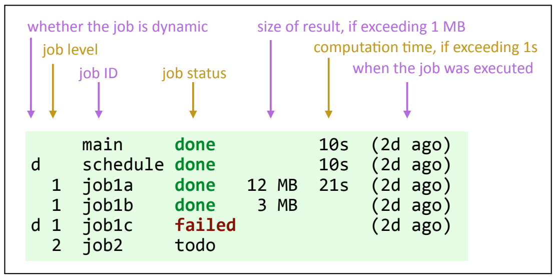
Table II
COMPMAKE CONSOLE JOB ALIASES

	by name
*name**	Any job whose ID matches the regexp.
`funcname()`	Any job whose function name matches the given name. (Note that the function name is different than the ID.)
	by job status
`all` or `*`	All jobs.
`failed`	Evaluates to list of failed jobs.
`done`	Evaluates to list of done jobs.
`todo`	Evaluates to list of todo jobs.
`blocked`	Evaluates to list of blocked jobs.
`uptodate`	Jobs that are done and whose dependencies are done.
	by definition depth
`root`	All jobs defined in the main context.
`level` *d*	Jobs at depth d.
	by type and dependencies relations
`dynamic`	All jobs that are dynamic.
`bottom`	All jobs that have no dependencies.
`top`	All jobs that are not dependencies of any other job.

C. The command `ls`

We have already seen the command `ls` [<jobs>]. It lists the jobs or lists of jobs given on the command line. Apart from the ID, it also gives much more information.

A possible output for `ls` for an advanced example is shown in Fig. 11.


whether the job is dynamic
job level
job ID
job status
size of result, if exceeding 1 MB
computation time, if exceeding 1s
when the job was executed

```
     main     done          10s  (2d ago)
d    schedule done          10s  (2d ago)
  1  job1a    done    12 MB 21s  (2d ago)
  1  job1b    done     3 MB      (2d ago)
d 1  job1c    failed             (2d ago)
  2  job2     todo
```

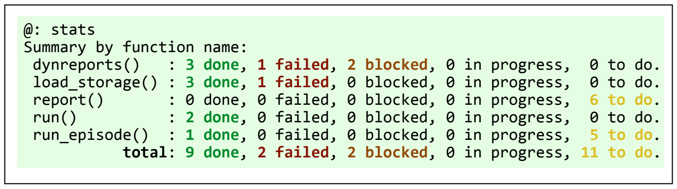
Figure 11. Example output for command `ls`.

From left to right, the fields that are displayed are:

- A flag “d” if this is a dynamic job.
- The level if greater than 0.
- The job ID.
- The job status.
- The size of the job result, if exceeding 1 MB. This is useful to keep the disk usage in check.
- The length of the computation, if exceeding 1 s.
- When the job was executed.

D. The command `stats`

The command `stats` groups functions by their name.



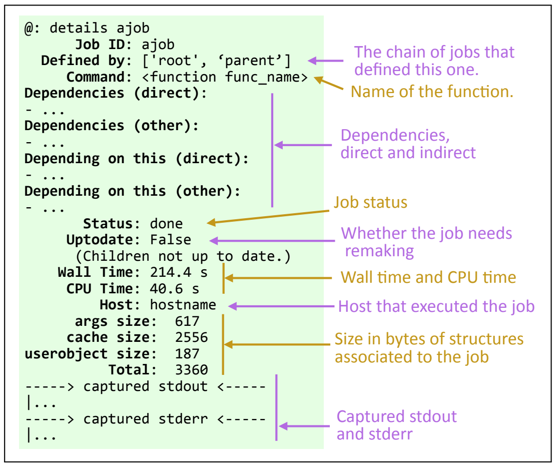
```
@: stats
Summary by function name:
 dynreports()   : 3 done, 1 failed, 2 blocked, 0 in progress,  0 to do.
 load_storage() : 3 done, 1 failed, 0 blocked, 0 in progress,  0 to do.
 report()       : 0 done, 0 failed, 0 blocked, 0 in progress,  6 to do.
 run()          : 2 done, 0 failed, 0 blocked, 0 in progress,  0 to do.
 run_episode()  : 1 done, 0 failed, 0 blocked, 0 in progress,  5 to do.
          total: 9 done, 2 failed, 2 blocked, 0 in progress, 11 to do.
```

Figure 12. Example output for command `stats`.

E. The command `details`

The command `details` shows much more information about the job, including the dependencies relations, as well as the stdout and stderr recorded during the execution.

A typical example of the output is shown in Fig. 13.


The chain of jobs that defined this one.
Name of the function.
Dependencies, direct and indirect
Job status
Whether the job needs remaking
Wall time and CPU time
Host that executed the job
Size in bytes of structures associated to the job
Captured stdout and stderr

```
@: details ajob
      Job ID: ajob
  Defined by: ['root', 'parent']
     Command: <function func_name>
Dependencies (direct):
- ...
Dependencies (other):
- ...
Depending on this (direct):
- ...
Depending on this (other):
- ...
        Status: done
      Uptodate: False
     (Children not up to date.)
     Wall Time: 214.4 s
      CPU Time: 40.6 s
          Host: hostname
     args size:  617
    cache size:  2556
userobject size:  187
         Total:  3360
-----> captured stdout <-----
|...
-----> captured stderr <-----
|...
```

Figure 13. Example output for command `details`.

The information displayed is the following:

Job ID

“Defined by” This is the chain of jobs that defined this one. For a job defined in the main context this is just “ `['root']` ”.

Command This is the name of the function/callable associated to the job, as reported by the method `__str__()`.

Dependencies (direct)/(other): These two fields list the job’s dependencies, both the direct ones, and all dependencies of those recursively.

Depending on this (direct)/(other): Similarly, these two fields show the jobs that depend on this, both directly and recursively.

Status One of those reported in Table I.

Uptodate A job can be `done` but still need to be remade because its dependencies have been updated. This field clarifies this situation.

Wall/CPU time This is the wall time and CPU time associated to the job. Because of the nature of parallel computations, the wall time is not reliable at all.

Host This is the name of the host that processed this job.

Args/cache/userobject size This is the size in bytes of the data structures in Compmake’s DB associated to this job. The size “args” is the size of the pickled command and its arguments. The size “cache” is mainly the size of captured stdout/stderr plus other fixed fields. The size “userobject” is the size of the pickled return value.

Captured stdout/stderr These are the captured stdout and stderr during the execution of the job.

F. Commands for making: `make`, `parmake`, `sgemake`

The commands `make`, `parmake`, `sgemake` start the job processing, each on a different backend.

1) The option `recurse`: The option `recurse=1` instructs any of the `*make` commands that if a target job defines other jobs, those jobs should be executed as well.

For example, suppose the job graph is defined as follows:

```
def f():
    pass
def djob(context):
^^Icontext.comp(f)
...
context.comp_dynamic(djob)
```

In this case, using just `make` will execute `djob` but not the newly created job `f`:

```
@: ls
   djob  todo
@: make djob
@: ls
   djob  done
   f     todo
```

Using the `recurse=1` option will have both jobs done:

```
@: ls
   djob  todo
@: make recurse=1 djob
@: ls
   djob  done
   f     done
```

2) The option `new_process`: `make` and `parmake` also have an option `new_process=1` that makes them start an additional process from scratch. So in total there are 5 different backends:

`make` Uses serial processing.

`make new_process=1` Uses serial processing, but each job is run in a separate Python interpreter by calling the `compmake` executable.

`parmake` Uses parallel processing. In particular this is achieved by using one new Python Process per job, which is forked from the original process.

`parmake new_process=1` runs each parallel job in a separate Python interpreter

`sgemake` Uses SGE for cluster processing. See Section IX for details.

The `new_process` switch is very useful as a workaround instead of “reloading” the code—see Section VIII-B for details.

3) The option `n`: The option `n` gives the number of parallel processes for the commands `make` and `parmake`:

```
@: parmake n=8   # 8 concurrent jobs
```

If it is not specified it defaults to the value of the config `max_parallel_jobs`, which is default the number of CPUs in the system.

4) The option `echo`: Usually the stdout/stderr from the jobs is suppressed. The commands `make` and `parmake` have an option `echo=1` to display the output as it is produced. This option is not compatible with `new_process=1`—see Section VIII-C for details.

G. Commands for cleaning and remaking: `clean`, `remake`, `parremake`

The command `clean` is used to clean the result of the computation. Any job is returned to the state of `todo`:

```
@: ls
    job1  failed
    job2  done
@: clean job1 job2; ls
    job1  todo
    job2  todo
```

The commands `remake` and `parremake` are just shortcuts for `clean; make` and `clean; parmake`, respectively.

H. Other useful commands

1) `exit`: Terminates the console session.

2) `help`: Use `help <command>` to see a brief help about the command.

3) `config` : The command `config` is used for setting configuration variables. It is discussed later in Section VII-A.

I. Other advanced commands used for debugging

There are a few other commands that are useful for the advanced user or developer.

1) `dump` : Usage:

```
@: dump directory=<directory> <jobs>
```

Dumps the result of jobs as pickle files in the given directory..

2) `dump_stdout` : Usage:

```
@: dump_stdout directory=<directory> <jobs>
```

Dumps the result of jobs on the stdout using `print` .

3) `delete` : Completely deletes a job from the DB. Use with caution, as it might compromise the job consistency.

To reset everything use:

```
@: delete not root; clean
```

4) `graph` : Creates and render a GraphViz graph of the given targets and dependencies using the `gvgen` module.

5) `reload` : Reloads a module. See Section VIII-B for a discussion on the limitations of this command.

6) `check_consistency` : Checks the consistency of the DB.

7) `debug_priority` : Shows the computed priority of the jobs.

8) `make_single` : Used internally for SGE backend.

9) `commands_html` : Writes an HTML output describing the commands.

10) `config_config` : Writes an HTML output describing the configuration.

VII. Configuration reference

Compmake has many configuration options. They can be set with the command `config` (Section VII-A) or by reading an initialization file `.compmake.rc` (Section VII-B) or with the command line (Section VII-C).

A. Setting configurations using the command `config`

The command `config` is used to get/set the configuration options.

To display the current configuration use

```
@: config
```

To set a configuration option, use:

```
@: config <option> <value>
```

For example, use

```
@: config colorize False
```

B. Using an initialization file

When the executable `compmake` starts it looks for an initialization file in various locations. These are, in order:

```
~/.compmake/compmake.rc
~/.config/compmake.rc
~/compmake.rc
~/.compmake.rc
compmake.rc
.compmake.rc
```

The contents of each file is interpreted as a console command. In particular you can write `config` commands:

```
$ cat compmake.rc
config colorize False
```

C. Setting configurations using the command line

The executable `compmake` takes all options as switches. For example:

```
@: compmake --colorize False <directory>
```

Is equivalent to

```
@: config colorize False
```

D. Configuration options for processing

1) `recurse` (default False): Default value for the `recurse` option to the `*make` commands. See Section VI-F1.

2) `new_process` (default False): Default value for the `new_process` option to the `*make` commands. See Section VI-F2.

3) `max_parallel_jobs` (default = number of CPUs): This option gives the default value for the `n` option to `sgemake` and `parmake`. See Section VI-F3.

E. Configuration options for visualization

1) `echo` (default False) : Default value for the `echo` option to the `*make` commands. See Section VI-F4.

2) `echo_stderr` (default True): If `echo` is True, stderr can be suppressed by setting `echo_stderr` to False.

3) `echo_stdout` (default True): If `echo` is True, stdout can be suppressed by setting `echo_stdout` to False.

4) `status_line_enabled` (default True): If False, suppress the animation showing the state of the computation.

5) `colorize` (default True): If False, suppress colorization of the output.

6) `readline` (default True): If True, Compmake tries to use the `readline` or `pyreadline` libraries.

7) `set_proc_title` (default True): If True, Compmake changes the process title to reflect the job currently executing.

8) `verbose_definition` (default True): If True, Compmake is verbose in displaying the names of the jobs being defined.

VIII. Limitations of Compmake

Compmake has a series of limitations that need to be taken into account. Some of these are intrinsic limitations of Python. Some other are design choices to keep the design simple. Some other might be implemented in the future.

A. All functions and parameters need to be pickable

All callables and their parameters need to be pickable. In general, Python's pickle system is quite flexible, but there are a few well-known limitations.

1) Cannot use lambda functions: It's not possible to use lambda functions in jobs definitions. For example, this will not work:

```
f = lambda x: x * 2
context.comp(f, 3)
```

This will throw an exception.

The workaround is often to define a class that can be pickled. For example this works:

```
class F():
   def __call__(self, x):
       return x*2
context.comp(F(), 3)
```

Of course, the class `F` must be defined in the module and must be itself pickable.

Also look at the module `functools` [10] which provides many related facilities such as partial function application ("currying") which creates objects that can be pickled.

2) Using functions defined directly in `__main__` might prevent some functionality: Some of the examples throughout have used functions defined directly in the `__main__` module. For example:

```
def func():
     pass
if __name__ == '__main__':
     context = Context()
     context.comp(func)
     context.compmake_console()
```

This works fine for basic cases, but it fails in more complex case, such as using the `new_process=1` option:

```
context.batch_command('make new_process=1')
```

This will fail citing a pickling error. This behavior was extremely tricky to debug. In short, this is a known bug of Python. For more information see [11] and the relevant bug report [12].

The workaround is to always define functions in another module:

```
from othermodule import func

if __name__ == '__main__':
     context = Context()
     context.comp(func)
     context.compmake_console()
```

B. Reloading modules

A functionality that is always requested is the ability to reload the code of a module, so that when a job fail, the user can edit the code, and immediately the job executed the updated code.

Python does have the ability to "reload" a module, and actually Compmake has a command `reload` but in practice its use is not advised because it never does what one expects. There are two main problems:

1) It is difficult for the user to keep track of which modules need to be reloaded. For example, one might be editing many files at once.
2) Reloading a module out of order might have very weird results regarding the initialization of data structures.

The workaround is to use the option `new_process=1` to the commands `make` and `parmake` :

```
@: make new_process=1 failed
```

In this way, the failed jobs are executed in a new process, different than the one that is displaying the console. The consequence is that the code that the user is editing is immediately reloaded.

C. No stdout/stderr visualization when using `new_process`

There is an option `echo=1` for `make` and `parmake` that displays the output of the jobs as they are executed. This functionality is not implemented when also the option `new_process=1` is specified. Compmake will warn about this and ignore the `echo` option.

It was preferred not to implement inter-process communication for things that are not strictly necessary, like visualizing the output of a process. The reason is that if a job is very verbose it might saturate a queue or the bandwidth of the user's terminal. So at that point there should be some logic to discard data to maintain responsiveness of the manager.

Note that you can examine the output of a process using the command `details <job>` after the execution.

D. Some libraries are just picky

Some libraries just don't like to run in child processes and so will fail when using `parmake` . Sometimes the errors mention the function `exec()` . For example:

```
The process has forked and you cannot use this Core
Foundation functionality safely. You MUST exec().
```

The workaround is to use `parmake` for most jobs and then use `make` for the picky ones. For example:

```
@: parmake most*; make picky; parmake *
```

E. Jobs cannot communicate with each other

Jobs cannot communicate with each other. Think of them as little units of computation that can be executed each on a different computer.

IX. The SGE Backend

Compmake uses SGE (Sun Grid Engine) to run jobs on a cluster. Zero configuration is needed on the part of Compmake once SGE is configured, but setting up SGE can take up a few minutes.

(See also the screencast at `purl.org/censi/compmake-sge`)

A. What is SGE?

The Sun Grid Engine became the “Oracle Grid Engine” when Sun was acquired by Oracle. Last year Oracle pulled out of the market, but the code has been open source for years. Currently there are several forks, free and commercial. The Open Grid Scheduler [2] is the main one and the one that is available in Linux distributions. The company *Univa* provides a commercial fork that runs on OS X as well [13].

B. Using SGE from Compmake

Once SGE is configured the user experience is very easy. Instead of using `make` or `parmake`, just use the command `sgemake` to run the computation using SGE:

```
@: sgemake
```

The command takes the usual parameters. In particular the option `n` gives the number of concurrent jobs that are submitted to the queue:

```
@: sgemake n=100
```

C. Setting up SGE on a local machine with Ubuntu

There are several guides for this. See for example [14].

1) Setting up DNS: An important note: the reason why SGE installation might fail incomprehensibly is because DNS is not set up correctly. Before installing SGE, make sure that the server has a fully-qualified hostname. To check this, type

```
$ hostname
```

The result must be a fully-qualified hostname which can be pinged from other hosts in the network. So `mycomputer` does not work, but `mycomputer.mycompany.com` works. An address such as `mycomputer.local` works.

On Ubuntu 14.04, a permanent change can be done by editing `/etc/hosts` and `/etc/hostname`. It is advised to reboot to check that the change is permanent. Reboot before installing SGE with the commands below so that the automatic configuration script will pick up the correct address.

2) Installation using `apt-get`: These are the packages needed in Ubuntu 14.04:

```
$ sudo apt-get install gridengine-master gridengine-client
  gridengine-common gridengine-qmon gridengine-exec
```

Make sure you give correct information for the configuration dialogs pop up.

It is needed to install some fonts for the QMon GUI to work. Just install all xfonts:

```
$ sudo apt-get install xfonts-\*
```

3) Configuration : The following steps are setting up a queue and give yourself permissions to submit to it. These steps can be done using the `qmon` GUI or with the command-line program `qconf`.

To add an admin user `<user>`:

```
$ sudo qconf -ao <user>
$ sudo qconf -am <user>
```

Next, add a submit host:

```
$ sudo qconf -as <mycomputer>
```

Here `<mycomputer>` must be a fully-qualified hostname as discussed above. Finally, add a queue, using

```
$ sudo qconf -aq queue1
```

By default each queue executes one job at a time. On Ubuntu the command above starts an editor; change `slots` to the number of CPUs in your system. If you want to have multiple jobs executed concurrently, you can either add more queues, or change the capacity of this queue using the `qmon` interface.

The next two steps need to be done using the GUI `qmon`:

- In the “User Configuration” tab, add your user to one of the user groups.
- In the “Job Control” tab, add that user group to the queue.

4) Testing SGE: Here’s a simple script `hello.sh` to try:

```
#!/bin/bash
echo "Hello" > /tmp/hello.txt
```

To submit this job, use:

```
$ qsub hello.sh
```

If everything is set up correctly after a few seconds the file `/tmp/hello.txt` will be created.

If you get a message like:

```
Unable to run job: warning: \
<user> your job is not allowed to run in any queue
```

It means that the last two steps were not executed correctly.

D. Useful SGE commands

1) Monitoring the queue: The command `qstat` can be used to monitor the status of the queues:

```
$ watch qstat
```

2) Deleting jobs: If Compmake receives a `KeyboardInterrupt` exception (CTRL-C) then it will delete the current jobs from the SGE queues. However if it is interrupted again then some jobs might be remaining in the queue. To delete all current jobs in the queue, use the command

```
$ qdel -u <user>
```

E. Using Starcluster to set up a cluster in the cloud

This guide only looked at setting up SGE on a single machine. For setting up a cluster in the cloud, one possibility is using the software developed by the *StarCluster* project [15]. Using StarCluster it is very very easy to run a full-fledged cluster on the Amazon Elastic Compute Cloud [16].

Please refer to the StarCluster documentation for setting up your AWS account and authentication.

1) Starcluster configuration of a Compmake-compatible cluster: You probably want to modify the configuration file in /.starcluster/config to define your cluster type with the appropriate dependencies for your project.

The following is the basic definition of a cluster "class" `c`ompmakecluster to use Compmake with:

```
[cluster compmakecluster]
KEYNAME = mykey
CLUSTER_SIZE = 4
CLUSTER_USER = sgeadmin
CLUSTER_SHELL = bash
NODE_INSTANCE_TYPE = cc1.4xlarge
NODE_IMAGE_ID = ami-52a0c53b
# use a plugin to install Compmake on the cluster
PLUGINS = compmake-installer
```

The `c`ompmake-installer plugin simply installs the Compmake python package:

```
[plugin compmake-installer]
setup_class = starcluster.plugins.pypkginstaller.PyPkgInstaller
packages = compmake
```

F. Limitations for SGE backend

1) SGE workers need to share a filesystem: So far there is only one storage backend implemented which stores the data on disk. Therefore all SGE workers need to be able to see the storage directory under the same name.

A backend for Compmake is just a key-value store. In the past I experimented with a Redis [17] backend. Other backends such as MongoDB [18] could be implemented easily.

X. The Multyvac backend (experimental)

Compmake has a Multyvac [19] backend. This backend is currently experimental.

(See also the screencast at purl.org/censi/compmake-multyvac)

A. What is Multyvac?

Multyvac is the successor of PiCloud after PiCloud has been bought by Dropbox in November 2013. It allows to schedule remote execution of Python functions, taking care of all code serialization.

B. Using Multyvac from Compmake

Once Multyvac is configured, instead of using `make` or `parmake`, just use the command `cloudmake` to run your computation using Multyvac. For example, this command runs the computation using 50 cloud workers:

```
@: cloudmake n=50
```

Sometimes there is some latency in the cloud job execution. To check the status of your jobs, login to your Multyvac account and use the interface at

https://www.multyvac.com/account/jobs/

C. Configuration

1) Sign up for an account: First, you need to sign up for a Multyvac account at the URL:

https://www.multyvac.com/account/register/

2) Install Multyvac: To install Multyvac, you can use `pip`:

```
$ pip install multyvac
```

3) Set up the API key: To create an API key, use:

```
$ python -m multyvac.setup
```

4) Optional: creating "layers": Multyvac will serialize your Python code automatically. However some libraries need to be installed on the workers.

Multyvac calls "layer" a configuration of the system. Suppose your code needs to use Numpy and PIL. These libraries have a C implementation that must be compiled, so they cannot be simply serialized like pure Python code.

Proceeds as follow. First, open a Python console:

```
$ python
```

In Python, use the following commands to create a layer called "*myconfiguration*":

```
>>> multyvac.layer.create('myconfiguration')
>>> layer = multyvac.layer.get('myconfiguration')
>>> modify_job = layer.modify()
>>> modify_job.open_ssh_console()
```

The last command will give you a SSH shell on Multyvac's servers, which currently run Ubuntu 12.04. On that shell you can install any software. For example, to install Numpy, Scipy, and PIL, use

```
$ sudo apt-get install python-numpy python-imaging python-scipy
$ exit
```

Once you exit the SSH shell, you are still in Python. Use this command to save the configuration:

```
>>> modify_job.snapshot()
```

At this point, you have available a layer called "*myconfiguration*" that has Numpy and PIL installed. To tell Compmake to use this layer, set the config `multyvac_layer`:

```
@: config multyvac_layer myconfiguration
```

It is probably useful to create a configuration file `/.compmake/compmake.rc` containing this command.

D. Configuration reference for Multyvac backend

These are the configuration option used by the backend.

1) `multyvac_debug`: If set to True, the logging output of the `multyvac` module is written on the screen. Otherwise the logging in that module is disabled.

2) `multyvac_layer`: This option allows to specify which Multyvac "layer" to use (Section X-C4).

3) `multyvac_sync_up`: Directories to be synchronized up (e.g. containing datasets).

4) `multyvac_sync_down`: Directories to be synchronized up (e.g. containing output data).

5) `multyvac_max_jobs`: Default number of cloud jobs to be instantiated. This can be overridden using the `n` parameter to `cloudmake`.

E. Commands reference for Multyvac backend

These are the configuration option used by the backend.

1) `cloudclean`: Deletes all the content of the remote directories that were specified with `multyvac_sync_down`.

2) `cloud_sync_down`: Synchronizes the data down, for the directories specified by `multyvac_sync_down`.

3) `cloud_sync_up`: Synchronizes the data up, for the directories specified by `multyvac_sync_up`.

F. Limitations of the Multyvac backend

1) "Dynamic" jobs are not run remotely: For now, the main limitation of the Multyvac backend compared with the others is that "dynamic" jobs, which are those created with `comp_dynamic` rather than `comp` (V-C). If these jobs are encountered, they will be run locally rather than on the cloud.

XI. Troubleshooting

A. Installation of the `readline` library fails

Compmake uses the `readline` [20] library to provide advanced command line functionality like command history and completion. In recent versions if `readline` is not installed then Compmake tries to import the substitute `pyreadline` [21].

1) Installation on Ubuntu 14: If this library is not already installed, `pip` or `easy_install` will try to install it but fail. On Ubuntu 14, the following steps should be enough.

First install the dependencies:

```
$ sudo apt-get install build-essential libreadline-\*
  lib\*curses\*
```

And then use `pip` or `easy_install` install the package:

```
$ sudo easy_install readline
```

Before trying to install Compmake again, check that this command succeeds:

```
$ python -c "import readline"
```

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