

Running tasks in sequence: SequentialTaskCollection and StagedTaskCollection

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Basic use of SequentialTaskCollection

```
from gc3libs.workflow \
  import SequentialTaskCollection

class MySequence (SequentialTaskCollection):
  # ...
  def __init__(self, ...):
    app1 = FirstApp(...)
    app2 = SecondApp(...)
    SequentialTaskCollection.__init__(
    self, [app1, app2])
```

A SequentialTaskCollection runs a list of tasks one at a time, in the order given.

Basic use of SequentialTaskCollection

```
from gc3libs.workflow \
  import SequentialTaskCollection

class MySequence(SequentialTaskCollection):
  # ...
  def __init__(self, ...):
    app1 = FirstApp(...)
    app2 = SecondApp(...)
    SequentialTaskCollection.__init__(
    self, [app1, app2])
```

Initialize a SequentialTaskCollection with a list of tasks to run.

Running tasks in sequence

```
class MyScript(SessionBasedScript):
    # ...
    def new_tasks(self, extra):
        tasks_to_run = [
            MySequence(...)
        ]
    return tasks_to_run
```

You can then run the entire sequence by returning it from new tasks().

Exercise 8.A:

Write a priceplot.py script that performs the following two steps:

- 1. Run the simAsset.R script (from Exercise 6.D) with the parameters given on the command line, and
- 2. Feed the results.csv file it outputs into the saplot.py script and retrieve the produced saplot.pdf file.

Run it like simAsset.R, for example:

\$ python priceplot.py 50 0.04 0.1 0.27 10 40

Running jobs in sequence

StagedTaskCollection provides a simple interface for constructing sequences of tasks, but only when the number and content of steps is *known and fixed* at programming time.

(By contrast, the most general

SequentialTaskCollection can alter the sequence on the fly, insert new stages while running and loop back. But the code is also harder to write.)

```
class Pipeline (StagedTaskCollection) :
  def __init__(self, image):
                                                    Example:
    super(Pipeline).__init__(self)
                                                subclassing a
    self.source = image
                                      StagedTaskCollection
  def stage0(self):
    # ...
  def stage1(self):
    # ...
  def stageX(self):
    # ...
```

```
class Pipeline(StagedTaskCollection):
  def __init__(self, image):
    super(Pipeline).__init__(self)
    self.source = image
  def stage0(self):
  def stage1(self):
  # ...
  def stageX(self) :
    # ...
```

Stages are numbered starting from 0.

You can have as many stages as you want.

```
class Pipeline(StagedTaskCollection):
  # ...
  def stage0(self):
    # run 1st step
    return Application (
      ['convert', self.source,
       '-colorspace', 'gray',
       'grayscale_' + self.source],
      inputs = [self.source],
      ...)
```

Each stage X method can return a Task instance, that will run as the X-th step in the sequence.

```
class Pipeline(StagedTaskCollection):
  # . . .
  def stage1(self):
    if self.tasks[0].execution.exitcode != 0:
      # bail out.
                                           In later stages you
      return (0, 1)
    else:
                                           can check the exit.
      # run 2nd step
                                         code of earlier ones.
      return Application (...)
                                         and decide whether
                                              to continue the
                                          sequence or abort.
  def stageX(self):
    # . . .
```

```
class Pipeline(StagedTaskCollection):
  # ...
  def stage1(self):
    if ...:
      # bail out
       return (0, 1)
    else:
      # run 2nd step
      return Application (...)
  def stageX(self):
    # . . .
```

To abort the sequence, return an integer (termination status) or a pair (signal, exit code), instead of a Task instance.

This sets the collections' own signal and exit code, and also sets the state as TERMINATED.

Detour: BLAST, again

Another use of the BLAST tool is to search for given "query" proteins in a data base. Large curated DBs are available, but one may want to build a custom DB.

Building a DB from a set of FASTA-format files p1.faa p2.faa and p3.faa, and querying it is a 3-step process:

```
cat p1.faa p2.faa p3.faa > db.faa
formatdb -i db.faa
blastpgp -i q.faa -d db.faa -e ...
```

The formatdb step produces output files db.faa.phr, db.faa.pin, and db.faa.psq; all these files are inputs to the blastpqp program.

Exercise 8.B: Write a blastdb.py script to build a BLAST DB and query it.

The blastdb.py script shall be invoked like this:

\$ python blastdb.py query.faa p1.faa [p2.faa ...]

where arguments new.faa, p1.faa, etc. are FASTA-format files.

The script should build a BLAST DB out of the files pN.faa. Then, it should query this database for occurrences of the proteins in query. faa using blastpgp.

Exercise 8.C: Find out by running the blastdb.py script of Ex. 8.B:

- 1. What happens if an intermediate step fails and does not produce complete output?
- 2. After the whole sequence turns to TERMINATED state, what is the value of its signal and exitcode?

Exercise 8.D: Implement (in blastdb.py) a "cleanup" feature that removes intermediate results (e.g., the ".phr" files) and only keeps the output from blastpgp if the whole sequence was successfully executed