University of Zurich^UZH

S3IT

GC3Pie basics

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S3IT: Services and Support for Science IT

University of Zurich

September 12–13, 2016

Concepts and glossary

Parts of GC3Pie

GC3Pie consists of three main components:

GC3Libs:
Python library for controlling the life-cycle of computational job collections.

GC3Utils:
This is a small set of low-level utilities exposing the main functionality provided by GC3Libs.

GC3Apps:
A collection of driver scripts to run large job campaigns.

GC3Pie glossary: Application

GC3Pie runs user applications
on clusters and IaaS cloud resources

An `Application` is just a command to execute.

GC3Pie glossary: Application

GC3Pie runs user applications
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An `Application` is just a command to execute.

If you can run it in the terminal,
you can run it in GC3Pie.

GC3Pie glossary: Application

GC3Pie runs user applications
on clusters and IaaS cloud resources

An `Application` is just a command to execute.

A single execution of an `Application`
is indeed called a `Run`.

(Other systems might call this a “job”.)

GC3Pie glossary: Task

GC3Pie runs user applications
on clusters and IaaS cloud resources

More generally, GC3Pie runs `Task`s.

`Task`s are a superset of applications,
in that they include workflows.

GC3Pie glossary: Resources

GC3Pie runs user applications
on clusters and IaaS cloud resources

`Resource`s are the computing infrastructures where GC3Pie executes applications.

Resources include: your laptop, the “Hydra” cluster, the Science Cloud, Amazon AWS.

Workflow scaffolding

Let's start coding!

```python
from gc3libs.cmdline \
  import SessionBasedScript

if __name__ == '__main__':
  import ex2a
  ex2a.AScript().run()

class AScript(SessionBasedScript):
  """
  Minimal workflow scaffolding.
  """
  def __init__(self):
    super(AScript, self).__init__(
        version='1.0')
  def new_tasks(self, extra):
    return []
```

Exercise 2.A:

You can find the `ex2a.py` in the 'download' folder on your training instance.

1. Run the following command:

   ```
   $ python ex2a.py --help
   ```

   Where does the program description in the help text come from? Is there anything weird in other parts of the help text?

2. Run the following command:

   ```
   $ python ex2a.py
   ```

   What happens?

```
from gc3libs.cmdline \
  import SessionBasedScript

if __name__ == '__main__':
  import ex2a
  ex2a.AScript().run()

class AScript(SessionBasedScript):
  """
  Minimal workflow scaffolding.
  """
  def __init__(self):
    super(AScript, self).__init__(
        version='1.0')
  def new_tasks(self, extra):
    return []
```

These lines are needed in every session-based script.

See issue 95 for details.

```
from gc3libs.cmdline \
  import SessionBasedScript

if __name__ == '__main__':
  import ex2a
  ex2a.AScript().run()

class AScript(SessionBasedScript):
  """
  Minimal workflow scaffolding.
  """
  def __init__(self):
    super(AScript, self).__init__(
        version='1.0')
  def new_tasks(self, extra):
    return []
```

For this to work, it is **needed** that this is the actual file name.

```
from gc3libs.cmdline \
  import SessionBasedScript

if __name__ == '__main__':
  import ex2a
  ex2a.AScript().run()

class AScript(SessionBasedScript):
  """
  Minimal workflow scaffolding.
  """
  def __init__(self):
    super(AScript, self).__init__(
        version='1.0')
  def new_tasks(self, extra):
    return []
```

This is the program's help text!

```python
from gc3libs.cmdline \
  import SessionBasedScript

if __name__ == '__main__':
  import ex2a
  ex2a.AScript().run()

class AScript(SessionBasedScript):
  """
  Minimal workflow scaffolding.
  """
  def __init__(self):
    super(AScript, self).__init__(
      version='1.0' )
  def new_tasks(self, extra):
    return []
```

A version number is **mandatory**.

```
from gc3libs.cmdline \
  import SessionBasedScript

if __name__ == '__main__':
  import ex2a
  ex2a.AScript().run()

class AScript(SessionBasedScript):
  """
  Minimal workflow scaffolding.
  """
  def __init__(self):
    super(AScript, self).__init__(
        version='1.0')
  def new_tasks(self, extra):
    return []
```

This is the core of the script.

Return a list of `Application` objects, that GC3Pie will execute.

The `Application` object

Specifying commands to run, I

You need to “describe” an application to GC3Pie, in order for GC3Pie to use it.

This “description” is a blueprint from which many actual command instances can be created.

(A few such “descriptions” are already part of the core library.)

GC3Pie application model

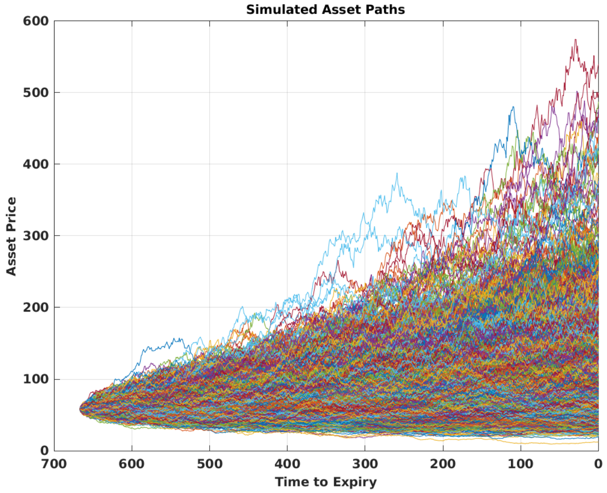
In GC3Pie, an application “description” is an object of the `gc3libs.Application` class (or subclasses thereof).

At a minimum: provide application-specific command-line invocation.

Advanced users can customize pre- and post-processing, react on state transitions, set computational requirements based on input files, influence scheduling. (This is standard OOP: subclass and override a method.)

A basic example: gasset

```
$ matlab -r 'simAsset 58 0.043 0.13 0.02 667 3000 1'
```



Here is how you would run that command in GC3Pie.

```
from gc3libs import Application

class GassetApp(Application):
  """Run Asset cost evolution function."""
  def __init__(self, params, mscript):
      args = ""
      for param in params:
         args += " %s " % param
      mfunct = os.path.basename(mscript).split('.')[0]
      Application.__init__(
         self,
         arguments="matlab -r '"+mfunct+" "+args+"'"
         inputs=[mscript],
         outputs=['./results/'],
         output_dir="gasset.d"
         stdout="stdout.txt",
         stderr="stderr.txt",
         requested_memory=1*GB,
         requested_walltime=8*hours
      )
```

Always inherit from Application

Your application class must inherit from class `gc3libs.Application`

```
from gc3libs import Application
```

```
class GassetApp(Application):
  """Run Asset cost evolution function."""
  def __init__(self, params, mscript):
      args = ""
      for param in params:
          args += " %s " % param
      mfunct = os.path.basename(mscript).split('.')[0]
      Application.__init__(
        self,
        arguments="matlab -r '"+mfunct+" "+args+"'"
        ...
```

The `arguments` parameter

The `arguments=` parameter is the actual command-line to be invoked.

```
from gc3libs import Application

class GassetApp(Application):
  """Run Asset cost evolution function."""
  def __init__(self, params, mscript):
      args = ""
      for param in params:
          args += " %s " % param
      mfunct = os.path.basename(mscript).split('.')[0]
      Application.__init__(
        self,
        arguments="matlab -r '"+mfunct+" "+args+"'"
        ...
```

The `inputs` parameter, I

The `inputs` parameter holds a list of files that you want to *copy* to the location where the command is executed.
Remember: this might be a remote computer!

```
class GassetApp(Application):
  """Run Asset cost evolution function."""
  def __init__(self, params, mscript):
      ...
      mfunct = os.path.basename(mscript).split('.')[0]
      Application.__init__(
        self,
        arguments="matlab -r '"+mfunct+" "+args+"'"
        inputs=[mscript],
        outputs=['./results/'],
        output_dir="gasset.d",
        stdout="stdout.txt",
        ...
```

The `inputs` parameter, II

Input files retain their name during the copy, but not the entire path.

For example:

```
    inputs = [
      '/data/values.dat',
      '/data/stats.csv',
    ]
```

will make files *values.dat* and *stats.csv* available in the command execution directory.

The `inputs` parameter, III

You need to pass the full path name into the `inputs` list, but use only the “base name” in the command invocation.

```
class GassetApp(Application):
  """Run Asset cost evolution function."""
  def __init__(self, params, mscript):
      ...
      mfunct = os.path.basename(mscript).split('.')[0]
      Application.__init__(
        self,
        arguments="matlab -r '"+ mfunct +" "+args+"'"
        inputs=[mscript],
        outputs=['./results/'],
        output_dir="gasset.d",
        stdout="stdout.txt",
        ...
```

The `outputs` parameter, I

The `outputs` argument list files that should be copied from the command execution directory back to your computer.

```
class GassetApp(Application):
  """Run Asset cost evolution function."""
  def __init__(self, params, mscript):
      ...
      mfunct = os.path.basename(mscript).split('.')[0]
      Application.__init__(
        self,
        arguments="matlab -r '"+mfunct+" "+args+"'"
        inputs=[mscript],
        outputs=['./results/'],
        output_dir="gasset.d",
        stdout="stdout.txt",
        ...
```

The `outputs` parameter, II

Output file names are *relative to the execution directory*. For example:

```
    outputs = ['result.dat', 'program.log']
```

(Contrast with input files, which must be specified by *absolute path*, e.g., `/data/values.dat`)

Any file with the given name that is found in the execution directory will be copied back. (*Where?* See next slides!)

If an output file is *not* found, this is *not* an error. In other words, **output files are optional**.

The `output_dir` parameter, I

The `output_dir` parameter specifies where output filess will be downloaded.

```
class GassetApp(Application):
  """Run Asset cost evolution function."""
  def __init__(self, params, mscript):
      ...
      mfunct = os.path.basename(mscript).split('.')[0]
      Application.__init__(
        self,
        arguments="matlab -r '"+mfunct+" "+args+"'"
        inputs=[mscript],
        outputs=['./results/'],
        output_dir="gasset.d"
        stdout="stdout.txt",
        ...
```

The *output_dir* parameter, II

By default, GC3Pie does not overwrite an existing output directory: it will move the existing one to a backup name.

So, if `gasset.d` already exists, GC3Pie will:

1. rename it to `gasset.d.~1~`
2. create a new directory `gasset.d`
3. download output files into the new directory

The `stdout` parameter

This specifies that the command's *standard output* should be saved into a file named `stdout.txt` and retrieved along with the other output files.

```
class GassetApp(Application):
  """Run Asset cost evolution function."""
  def __init__(self, params, mscript):
      ...
      mfunct = os.path.basename(mscript).split('.')[0]
      Application.__init__(
        self,
        arguments="matlab -r '"+mfunct+" "+args+"'"
        inputs=[mscript],
        outputs=['./results/'],
        output_dir="gasset.d",
        stdout="stdout.txt",
        stderr="stderr.txt",
        ...
```

(The `stderr` parameter)

There's a corresponding `stderr` option for the command's *standard error* stream.

```
class GassetApp(Application):
  """Run Asset cost evolution function."""
  def __init__(self, params, mscript):
      ...
      mfunct = os.path.basename(mscript).split('.')[0]
      Application.__init__(
        self,
        arguments="matlab -r '"+mfunct+" "+args+"'"
        inputs=[mscript],
        outputs=['./results/'],
        output_dir="gasset.d",
        stdout="stdout.txt",
        stderr="stderr.txt" )
        ...
```

Mixing `stdout` and `stderr` capture

You can specify **either one** of the `stdout` and `stderr` parameters, **or both**.

If you give both, and they have the same value, then `stdout` and `stderr` will be intermixed just as they are in normal screen output.

Let's run!

In order for a session-based script to execute something, its `new_tasks()` method must return a list of `Application` objects to run.

```
class Ascript(SessionBasedScript):
  # ...
  def new_tasks(self, extra):
    # 'self.param.args' is the list
    # of command-line arguments
    input_params = parse(self.params.args[0])[0]
    matalb_script = abspath(self.params.args[1])
    app = GassetApp(input_params,matlab_script)
    return [app]
```

Exercise 2.B:
Edit the `ex2a.py` file: insert the code to define the `GassetApp` application, and modify the `new_tasks()` method to return one instance of it (as in the previous slide).

Run the script and display the generated plot.

You can find the code for `GassetApp` and the `paramers.csv` file in the 'download' folder on your training instance.

Exercise 2.C:
Edit the script from Exercise 2.B above and run the `GassetApp` for each input parametes in the `paramers.csv` input file: for each input parametes, an instance of `GassetApp` should be run.

Resource definition

The gservers command

The gservers command is used to see configured and available resources.

```
$ gservers
+----------------------+--------------------------+-----------+
|                      | localhost                |           |
+----------------------+--------------------------+-----------+
|             frontend | ( Frontend host name )   | localhost |
|                 type | ( Access mode )          | shellcmd  |
|              updated | ( Accessible? )          | True      |
|               queued | ( Total queued jobs )    | 0         |
|          user_queued | ( Own queued jobs )      | 0         |
|             user_run | ( Own running jobs )     | 6         |
|     max_cores_per_job | ( Max cores per job )    | 4         |
|  max_memory_per_core | ( Max memory per core )  | 8GiB      |
|          max_walltime | ( Max walltime per job ) | 8hour     |
+----------------------+--------------------------+-----------+
```

Resources are defined in file `$HOME/.gc3/gc3pie.conf`

The gservers command

The gservers command is used to see configured and available resources.

```
$ gservers
+----------------------+---------------------------+-----------+
|                      | localhost                 |           |
+----------------------+---------------------------+-----------+
|             frontend | ( Frontend host name )    | localhost |
|                 type | ( Access mode )           | shellcmd  |
|              updated | ( Accessible? )           | True      |
|               queued | ( Total queued jobs )     | 0         |
|          user_queued | ( Own queued jobs )       | 0         |
|             user_run | ( Own running jobs )      | 6         |
|    max_cores_per_job | ( Max cores per job )     | 4         |
|  max_memory_per_core | ( Max memory per core )   | 8GiB      |
|         max_walltime | ( Max walltime per job )  | 8hour     |
+----------------------+---------------------------+-----------+
```

Resources are defined in file `$HOME/.gc3/gc3pie.conf`

Example execution resources: local host

Allow GC3Pie to run tasks on the local computer.

This is the default installed by GC3Pie into

`$HOME/.gc3/gc3pie.conf`

```
[resource/localhost]
enabled = yes
type = shellcmd
frontend = localhost
transport = local
max_cores_per_job = 2
max_memory_per_core = 2GiB
max_walltime = 8 hours
max_cores = 2
architecture = x86_64
auth = none
override = no
```

Example execution resources: SLURM

Allow submission of jobs to the “Hydra” cluster.

```
[resource/hydra]
enabled = no
type = slurm
frontend = login.s3it.uzh.ch
transport = ssh
auth = ssh_user_rmurri
max_walltime = 1 day
max_cores = 96
max_cores_per_job = 64
max_memory_per_core = 1 TiB
architecture = x86_64
prologue_content =
  module load cluster/largemem

[auth/ssh_user_rmurri]
type=ssh
username=rmurri
```

Example execution resources: OpenStack

```
[resource/sciencecloud]
enabled=no
type=openstack+shellcmd
auth=openstack

vm_pool_max_size = 32
security_group_name=default
security_group_rules=
  tcp:22:22:0.0.0.0/0,
  icmp:-1:-1:0.0.0.0/0
network_ids=
  c86b320c-9542-4032-a951-c8a068894cc2

# definition of a single execution VM
instance_type=1cpu-4ram-hpc
image_id=f42b1c84-c9f6-4621-aa48-0ad84c78ff2d

max_cores_per_job = 8
max_memory_per_core = 4 GiB
max_walltime = 90 days
max_cores = 32
architecture = x86_64

# how to connect
vm_auth=ssh_user_ubuntu
keypair_name=rmurri
public_key=~/.ssh/id_dsa.pub
```

```
[auth/ssh_user_ubuntu]
# default user on Ubuntu VM images
type=ssh
username=ubuntu


[auth/openstack]
# only need to set the 'type' here;
# any other value will be taken from
# the 'OS_*' environment variables
type = openstack
```

Allow running tasks on the “ScienceCloud” VM infrastructure.

Exercise 2.D: Change the configuration file `~/.gc3/gc3pie.conf` to enable the `sciencecloud` resource. Verify with the `gservers` command that it works.

Exercise 2.E: Run the script from Exercise 2.C on Science Cloud. Do you need to change anything in the code?