An Introduction to GC3Pie
Session-based scripts

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What is GC3Pie?

GC3Pie is . . .

1. An *opinionated* Python framework for defining and running computational workflows;
2. A *rapid development toolkit* for running user applications on clusters and IaaS cloud resources;
3. The worst name ever given to a middleware piece. . .

As *users*, you're mostly interested in this part.

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Who am I?

Systems administrator and programmer.

At UZH since 2010, first at GC3 then at S3IT.

Developer of GC3Pie since 2010.

and what about you?

About this training, 1

1. Concepts and glossary
2. Usage of a session-based script
3. Command-line tools mainly useful for debugging

About this training, 2

We'd like the training to be
as interactive and informal as possible.

If you have a question, just ask – don't wait.

Concepts and glossary

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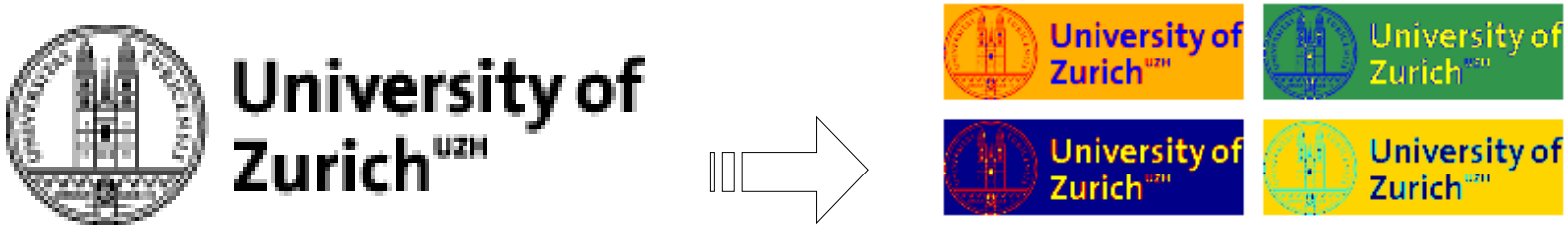
However, you need to understand the basic concepts ;-)

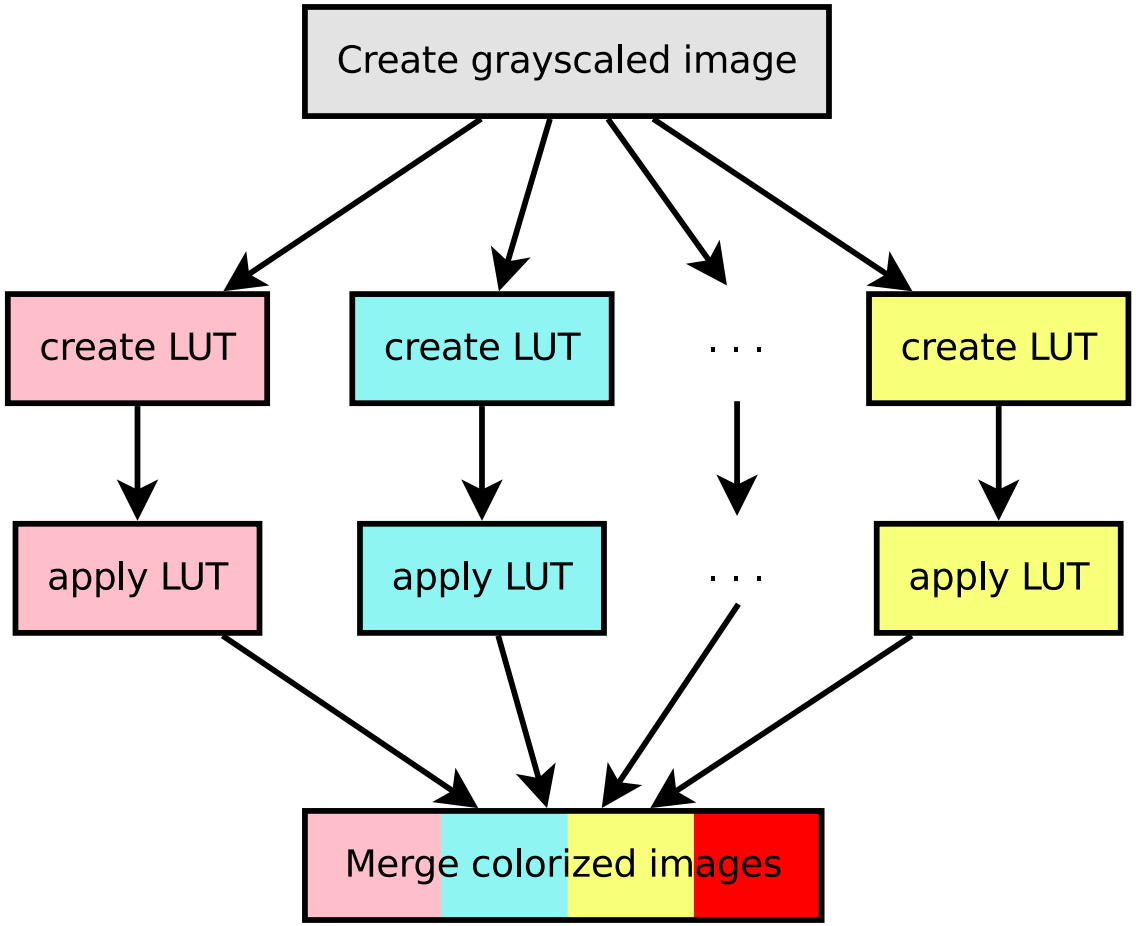
A typical GC3Pie script?

```
> ./warholize.py uzh-logo.png --watch 1
```



How does “Warholize” work?

It is a GC3Pie *workflow*: each box is a distinct application instance that is run.



What GC3Pie handles for you

1. Resource allocation (e.g. starting new instances on ScienceCloud)
2. Selection of resources for each application in the session
3. Data transfer (e.g. copying input files in the new instances)
4. Remote execution of the application
5. Retrieval of results (e.g. copying output files from the running instance)
6. De-allocation of resources

GC3Pie glossary: Application

GC3Pie runs user applications
on clusters and IaaS cloud resources

An `Application` is just a command to execute.

GC3Pie glossary: Application

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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.

▸ More on this later!

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.

Hands-on time!

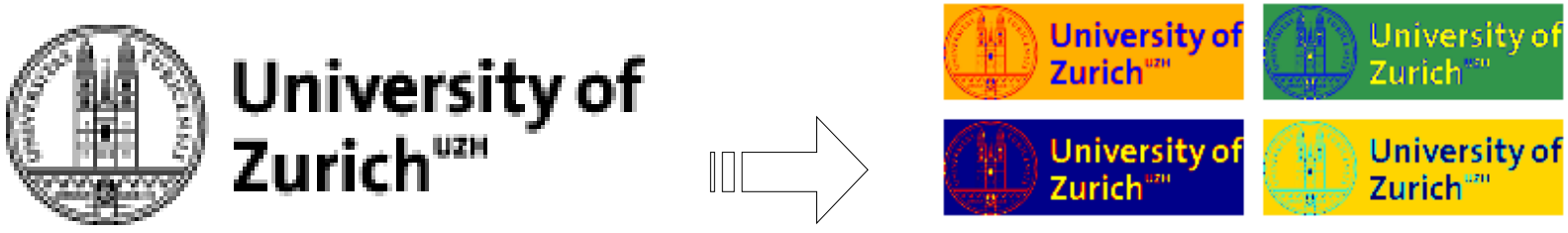
Start a VM on Science Cloud, using the "GC3Pie Tools Training" snapshot.

Exercise A:

1. Run the `./warholize.py` script to get a new "warholized" version of the UZH logo.
2. What command-line option lets you run the whole workflow in one go?
3. How can you warholize multiple images at once?

Warholize!

```
> ./warholize.py uzh-logo.png -C 1
```



Session-based scripts

`warholize.py` is a typical *session-based script*.

A *session* is just a named collection of jobs.

A *session-based script* creates a session and runs all the jobs in it until completion.

The output directory

If you don't specify an output directory for your job,
a session-based script collects output
in the current working directory
(but this can change from script to script).

If an output directory already exists,
it will be *renamed* and never overwritten.

If you pass the option `-o DIRECTORY` to the script,
all the output dirs will be saved inside that directory.

Create a session

A session-based script creates a session
and runs all the jobs in it until completion.

Create session `logo`:

```
> ./warholize.py uzh-logo.png -s logo
```

Run a session until done

A session-based script creates a session
and runs all the jobs in it until completion.

Run jobs in session `logo`, polling for updates every 5 seconds:

```
> ./warholize.py uzh-logo.png -s logo --watch
5
```

You can stop a GC3Pie script by pressing *Ctrl*+*C*. Run it again to resume activity from where it stopped.

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5
```

You can stop a GC3Pie script by pressing *Ctrl*+*C*. Run it again to resume activity from where it stopped.

Alternate display of session contents, I

Display top-level tasks in session `logo`:

```
> gsession list logo
```

Exercise B: Now try it yourself.

WTF??

```
> gsession list logo
gc3.gc3libs: WARNING: Failed loading file '/home/ubuntu/logo/jobs/WarholizeWorkflow.108': In
  ...
LoadError: Failed retrieving object from file '/home/ubuntu/logo/jobs/WarholizeWorkflow.108
gc3.gc3libs: WARNING: Ignoring error from loading 'ParallelTaskCollection.107': Failed retr
+-------+----------+-------+------+
| JobID | Job name | State | Info |
+-------+----------+-------+------+
+-------+----------+-------+------+
```

In order to work, all GC3Pie utilities need to access the Python script that generated the tasks and session.

To fix: set the `PYTHONPATH` variable to the directory containing your script:

```
> export PYTHONPATH=$PWD
```

WTF??

```
> gsession list logo
gc3.gc3libs: WARNING: Failed loading file '/home/ubuntu/logo/jobs/WarholizeWorkflow.108': In
  ...
LoadError: Failed retrieving object from file '/home/ubuntu/logo/jobs/WarholizeWorkflow.108
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+-------+----------+-------+------+
| JobID | Job name | State | Info |
+-------+----------+-------+------+
+-------+----------+-------+------+
```

In order to work, all GC3Pie utilities need to access the Python script that generated the tasks and session.

To fix: set the `PYTHONPATH` variable to the directory containing your script:

```
> export PYTHONPATH=$PWD
```

Alternate display of session contents, II

Display *all* tasks in session `logo`:

```
> gsession list --recursive logo
```

▸ Workflows and task hierarchy

Alternate display of session contents, III

Display summary of tasks in session `logo`:

```
> gstat -n -b -s logo
```

Display session history

Show log of activity on tasks in session `logo`:

```
> gsession log logo
```

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

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| 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 = yes
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=2b227d15-8f6a-42b0-b744-ede52ebe59f7

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.

Hands-on time!

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

Select execution resource

Select where applications will be run with option `-r`:

```
> ./warholize.py -s logo -r localhost
```

The resource name must exists in the configuration file (i.e., check `gservers`' output).

Stopping a script and re-starting it with a different resource will likely result in an error: old tasks can no longer be found.

Passing requirements to the application

Some options are used to specify some requirements of *all* applications in a session:

-c NUM Set the number of CPU cores required for each job.

-m GB Set the amount of memory required per execution core

-w DURATION Set the time limit for each job; default is script-dependent.

These options have proven not to be much useful except for debugging/experimentation,
so they might be removed in a future release!

Cloud backend management

Hands-on time!

Exercise D: Run the "Warholize" workflow on the ScienceCloud.

See what VMs are in use

Use the `gcloud` command to show cloud usage:

```
> gcloud list
```

Limit concurrently-running jobs

Limit the maximum number of concurrently-running tasks with option `-J`:

```
> ./warholize.py -s logo -J 1
```

In large computational campaigns, it is important not to flood the execution resources with too many tasks.

Hands-on time!

Exercise E:

1. Run the "Warholize" workflow on the ScienceCloud. Stop the script while it's running. Now start it again. What happens?
2. Run the "Warholize" workflow on the ScienceCloud. Stop the script while it's running; list the jobs in the session and note down the IDs. Now run the script again, **adding the "`-N`" option**. When the script terminates, inspect the session again and note the IDs. What has happened? Why?

Use `-N` with caution!

From the session-based script's `--help` output:

```
-N, --new-session
  Discard any information saved in the session dir
  (see '--session' option) and start a new session
  afresh.  Any information about previous jobs is lost.
```

Cleanup unused VMs

Use the `gcloud` command again:

- To stop *all* unused VMs:

  ```
  > gcloud cleanup
  ```

  Exercise F: Do it. Now.

- To stop a specific VM:

  ```
  > gcloud terminate f031d6ad-bd6c-439e-9a98-4d64
  ```

Session management

Aborting a single task

To stop and abort a single task, use the `gkill` command:

```
> gkill -s logo MyApplication.123
```

Exercise : What happens if you try to abort a task collection?

Aborting a single task

To stop and abort a single task, use the `gkill` command:

```
> gkill -s logo MyApplication.123
```

Exercise : What happens if you try to abort a task collection?

Aborting a whole session

Kill all the running tasks in a session again using the `gkill` command:

```
> gkill -s logo -A
```

Alternatively you can use `gsession abort`:

```
> gsession abort logo
```

Selecting tasks from a session, I

The `gselect` command is the go-to tool for selective listing of tasks in a session. For example, to list finished tasks:

```
> gselect -s logo --state TERMINATED
```

The output of `gselect` is a list of task, IDs, to be fed into another GC3Pie command. For example, to kill all queued tasks:

```
> gselect -s logo --state SUBMITTED | xargs gkill -s logo
```

Selecting tasks from a session, II

The `gselect` command has many different options to select tasks:

```
> gselect --help
usage: gselect [-h] [-V] [-v] [--config-files CONFIG_FILES] -s SESSION
               [--error-message REGEXP] [--input-file FILENAME]
               [--jobname REGEXP] [--jobid REGEXP] [-l STATES]
               [--output-file FILENAME] [--output-message REGEXP]
               [--successful] [--submitted-after DATE]
               [--submitted-before DATE] [--unsuccessful]
```

Exercise : Use `gselect` to print the IDs of the "TricolorizeImage" tasks in the last "Warholize" session.

Thank you!

Any questions?

GC3Pie manual: http://gc3pie.readthedocs.io/

Mailing-list: gc3pie@googlegroups.com
or read online at
http://dir.gmane.org/gmane.comp.python.gc3pie

Workflows

The "Warholize" workflow

How do we "warholize" an arbitrary image?

1. Convert the original image to grayscale.
2. Colorize the grayscale image using three different colors for each tile.
3. Arrange all the colorized images into an $N \times N$ frame.

Reference: http://gc3pie.readthedocs.org/en/master/programmers/tutorials/warholize/warholize.html

GC3Pie glossary: Task Collections

The basic unit of work in a GC3Pie workflow is called a `Task`.

The `Application` class that you already know is a kind of `Task` (in programming speak, it's a derived class).

A set of `Task`s is itself a `Task`, and is called a `TaskCollection`.

Running tasks in sequence

To run tasks in an ordered sequence, one after the other, GC3Pie provides a `SequentialTaskCollection` class.

It is created with a list of tasks, and runs all of them in the order given. The sequence is dynamic, in that you can add new tasks on the fly, re-run existing ones, or remove future tasks.

A `SequentialTaskCollection` is itself a task.

Running tasks in parallel

To run tasks in parallel (i.e., they have no inter-dependency), GC3Pie provides a `ParallelTaskCollection` class.

It is created with a list of tasks, and runs all of them in parallel (compatibly with the computational resource limits).

A `ParallelTaskCollection` is itself a task.

Putting it all together

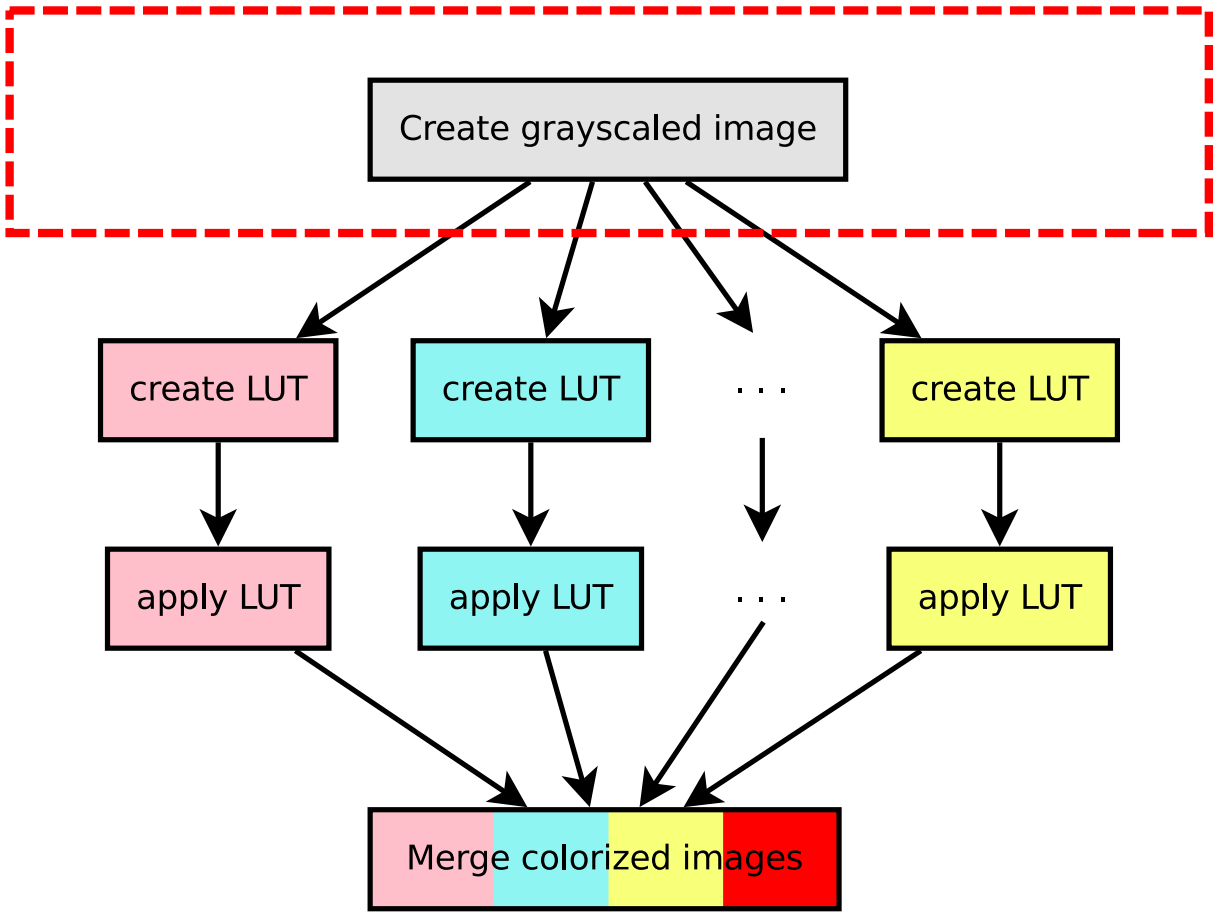
So tasks can be:

- `Application` instances,
- `SequentialTaskCollection`s,
- `ParallelTaskCollection`s.

So you can nest them, and create parallelly-running sequences, or sequences of "job explosions" (many jobs in parallel), or any combination of this.

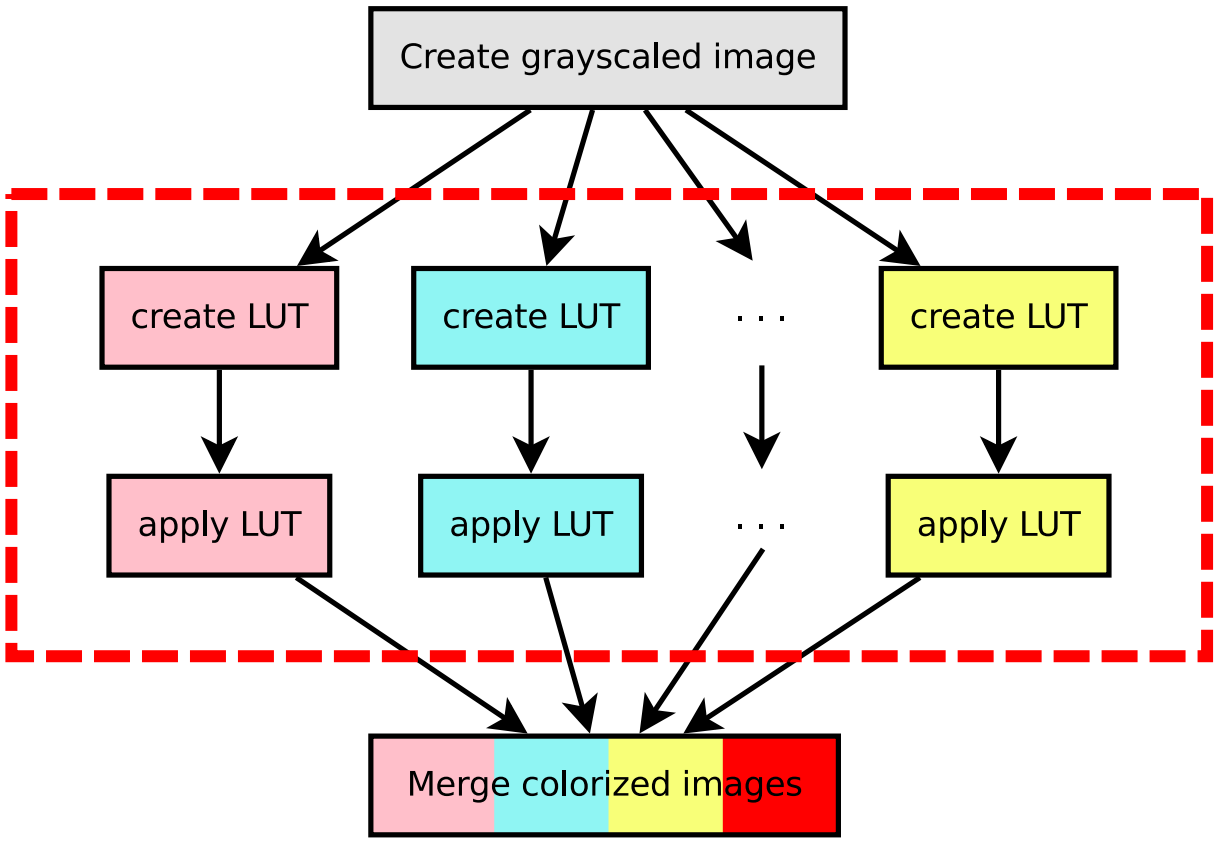
The Warholize workflow, I

1. Convert the original image to grayscale.



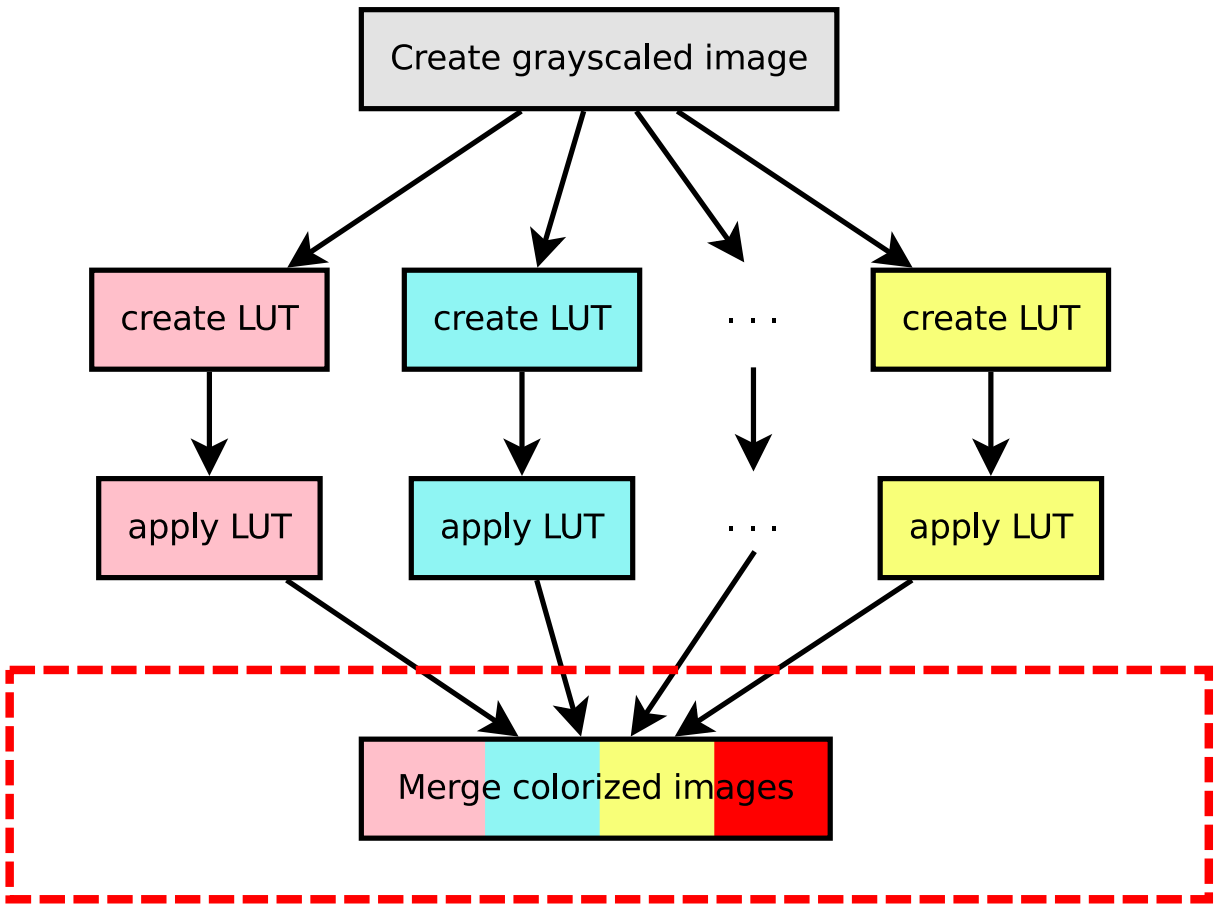
The Warholize workflow, II

2. Colorize the grayscale image using three different colors for each tile.



The Warholize workflow, III

3. Arrange all the colorized images into an $N \times N$ frame.

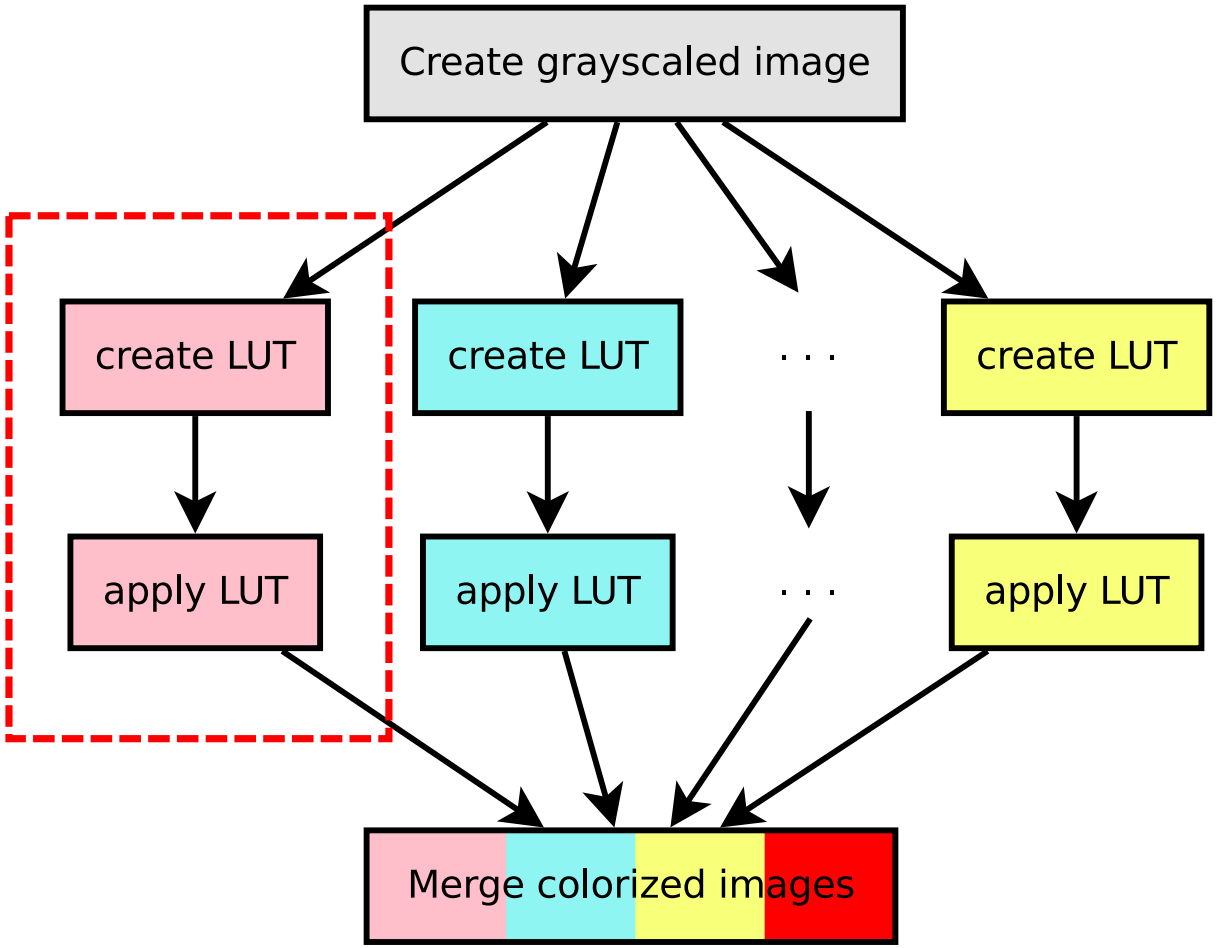


The Warholize workflow, IV

Step 2 actually entails two sub-steps:

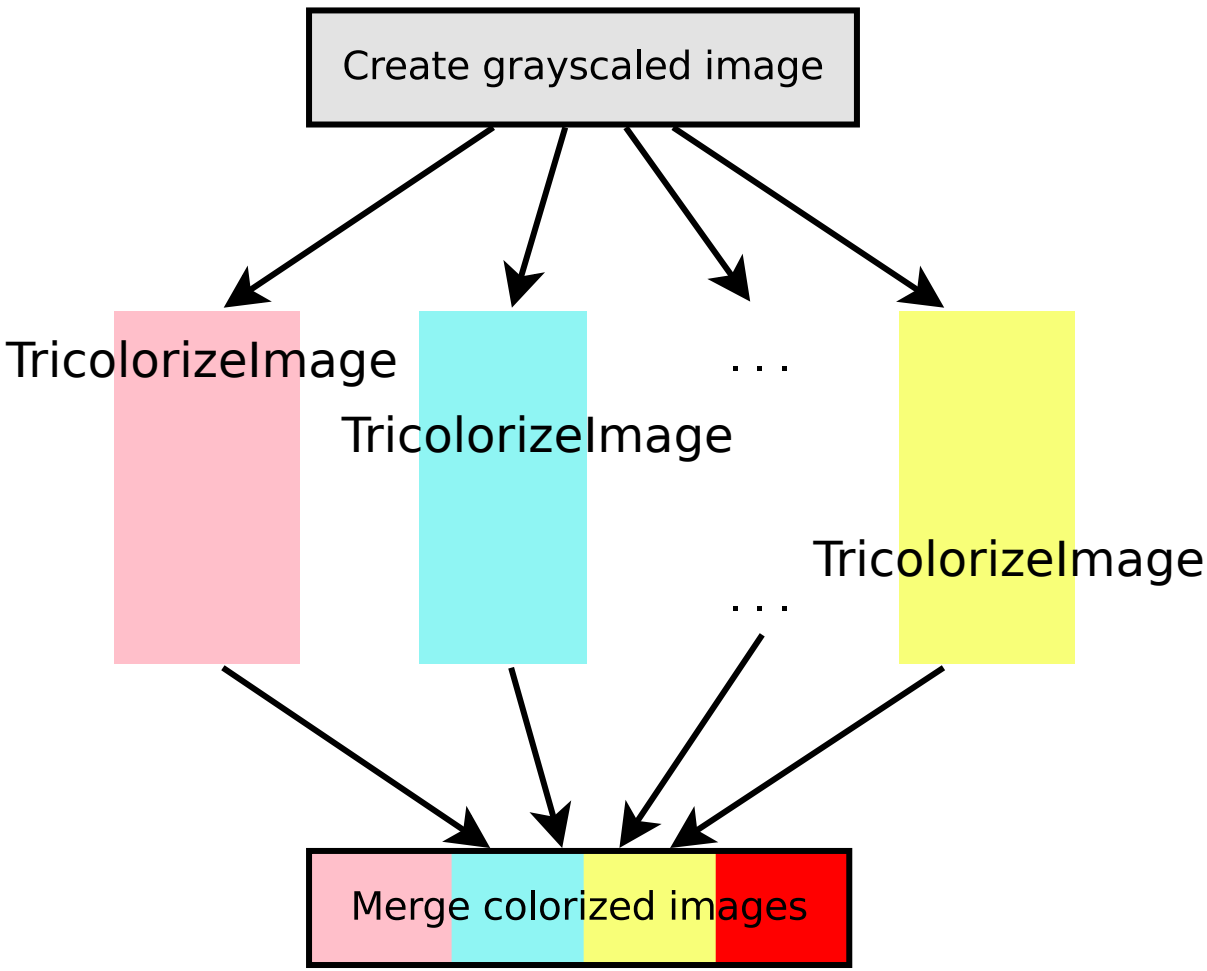
a) mapping greyscale levels to random colors,

b) applying this mapping to produce new images



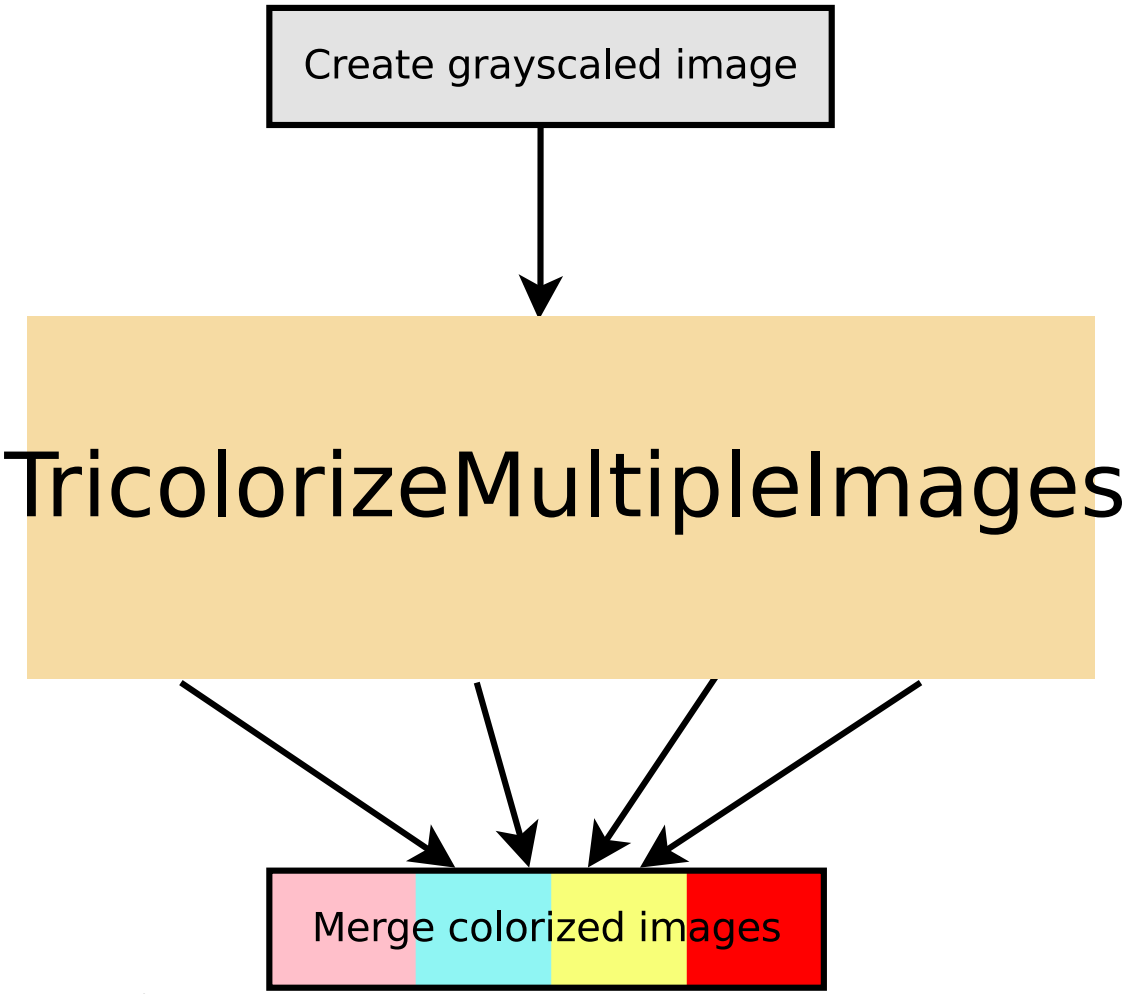
The Warholize workflow, V

So, Step 2 is a `SequentialTaskCollection`-type task. Let's call this two-pass sequence `TricolorizeImage`.



The Warholize workflow, VI

All the `TricolorizeImage` instances run in parallel. Collect them into a `ParallelTaskCollection`-type task, called `TricolorizeMultipleImages`.



The Warholize workflow, VII

Now we are left with a three-step sequence: greyscale, `TricolorizeMultipleImages`, montage. This can be defined again as a `SequentialTaskCollection`-type task, the `WarholizeWorkflow`.