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IRB
BARCELONA

The `PanPipe` Workflow Manager

Daniel Ortiz

Genome Data Science Group

Institute for Research in Biomedicine

Table of Contents

1. Introduction
2. Package Overview
3. Main Tools and File Formats
4. Toy Pipeline Example

Introduction

Introduction

- Pipeline execution is a complex task
    - Pipeline composed of very heterogeneous tasks/steps
    - Steps may present dependencies with other ones
    - Often necessary to add or remove pipeline steps
    - Need to allocate computational resources
    - Independent steps should be executed concurrently
    - Hard to maintain and reuse code
    - ...
- `PanPipe` has been created as a highly portable, configurable and extensible solution

Package Overview

Package Dependencies

- Shell Bash
- Python
- Slurm Workload Manager (optional)

Package Installation

- Obtain the package using git:

```
git clone https://github.com/daormar/panpipe.git
```

- Change to the directory with the package's source code and type:

```
./reconf
./configure
make
make install
```

NOTE: use `--prefix` option of `configure` to install the package in a custom directory

Functionality

- PanPipe is an engine to execute general pipelines
- Executes only those pipeline steps that are pending
- Handles computational resources for each step
- Executes job arrays

Execution Model

- PanPipe follows the *flow-based programming* paradigm
  - Network of *black box* processes
  - Relations between processes are defined by the data they exchange
  - Component oriented
- PanPipe follows a simple execution model based on a file enumerating a list of pipeline steps to be executed
- Steps are executed simultaneously unless dependencies are specified
- Step implementation is given in module files

Main Tools and File Formats

Main Tools

- `pipe_exec`
- `pipe_exec_batch`
- `pipe_check`
- `pipe_status`

`pipe_exec`

- Automates execution of general pipelines
- Main input parameters:
  - `--pfile <string>`: file with pipeline steps to be performed
  - `--outdir <string>`: output directory
  - `--sched <string>`: scheduler used for pipeline execution
  - `--showopts`: show pipeline options
  - `--checkopts`: check pipeline options
  - `--debug`: do everything except launching pipeline steps

pipe_exec: Output

- Content of output directory:
  - scripts: directory containing the scripts used for each pipeline step
  - <pipeline_step_name>: directory containing the results of the pipeline step of the same name
- Additional directories may be created depending on the pipeline

pipe_exec: Available Schedulers

- **Built-in Scheduler**
    - Allows to execute pipelines locally
    - Incorporates a basic resource allocation mechanism
- **Slurm Scheduler**
    - Allows to exploit large computational resources
    - Usage transparent to the user
    - Slurm behavior influenced by pipeline description

pipe_exec_batch

- Automates execution of pipeline batches
- Main input parameters:
  - `-f <string>`: file with a set of `pipe_exec` commands
  - `-m <string>`: Maximum number of concurrently executed pipelines
  - `-o <string>`: Output directory to move output of each pipeline

pipe_check

- Checks correctness of pipelines and converts them to other formats
- Main input parameters:
  - `-p <string>`: pipeline file
  - `-g`: print pipeline in `graphviz` format

pipe_status

- Checks execution status of a given pipeline
- Main input parameters:
  - `-d <string>`: directory where the pipeline steps are stored
  - `-s <string>`: step name whose status should be determined (optional)

The `panpipe_lib.sh` Library

- Shell library with functions used by the previously described tools
- Functions can be classified as follows:
  - Implementation of the package execution model
  - Automated creation of scripts executing pipeline steps
  - Helper functions to implement pipeline steps

File Formats

- **Pipeline file**: file enumerating all of the pipeline steps to be carried out when processing a normal-tumor sample
- **Module file**: file defining the code of the pipeline steps
- **Pipeline automation script**: file with a sequence of `pipe_exec` commands automating the analysis of a dataset

Pipeline File

- **Module import** (module names separated by commas)
- **Entry format** (one entry per line)

  Step name, Slurm account, Slurm partition, CPUs, Memory limit, Time limit, Dependencies, ...
- **Dependency types**: `none`, `after`, `afterok`, `afternotok`, `afterany`

```
#import pipe_software_test
#
step_a  cpus=1 mem=32 time=00:01:00 stepdeps=none
step_b  cpus=1 mem=32 time=00:01:00 stepdeps=afterok:step_a
step_c  cpus=1 mem=32 time=00:01:00 throttle=2 stepdeps=afterok:step_a
```

Module File

- Contains the definition of the different steps
- Written in `bash`
- Three `bash` functions should be defined for each step:
    - `stepname_explain_cmdline_opts()`
    - `stepname_define_opts()`
    - `stepname()`

Module File: `stepname_explain_cmdline_opts()`

- This function documents the command line options that the step needs to work
- The aggregated documentation for the different steps is shown when executing `pipe_exec --showopts`
- Whenever two steps share the same option, it is important to give it the same name

Module File: `stepname_explain_cmdline_opts()`

```
step_a_explain_cmdline_opts()
{
    # -a option
    description="Sleep time in seconds for step_a (required)"
    explain_cmdline_opt "-a" "<int>" "$description"
}
```

Module File: `stepname_define_opts()`

- This function should create a string containing the options that are specific to the step
- The main idea is to map command line options to step options
- The package provides multiple built-in functions to make the implementation of this function easier

Module File: stepname_define_opts()

```
stepname_define_opts()
{
    # Initialize variables
    local cmdline=$1
    local jobspec=$2
    local optlist=""

    # Use built-in functions to add options to optlist variable
    ...

    # Save option list
    save_opt_list optlist
}
```

Module File: stepname_define_opts()

```
step_a_define_opts()
{
    # Initialize variables
    local cmdline=$1
    local jobspec=$2
    local optlist=""

    # -a option
    define_cmdline_opt "$cmdline" "-a" optlist || exit 1

    # Save option list
    save_opt_list optlist
}
```

Module File: `stepname()`

- Implements the step
- The function should incorporate code at the beginning to read the options defined by `stepname_define_opts()`

Module File: `stepname()`

```
step_a()
{
    # Initialize variables
    local sleep_time=`read_opt_value_from_line "$*" "-a"`

    # Sleep some time
    sleep ${sleep_time}
}
```

Pipeline Automation Script

- Automates the analysis of a whole dataset
- At each entry (one per line), `pipe_exec` tool is used to execute a whole pipeline
- Can be used as input for `pipe_exec_batch`
- Entry example:

```
pipe_exec --pfile example.ppl --outdir outdir1 --sched SLURM -opt1 <opt1_val> -opt2 <opt2_val> ...
pipe_exec --pfile example.ppl --outdir outdir2 --sched SLURM -opt1 <opt1_val> -opt2 <opt2_val> ...
pipe_exec --pfile example.ppl --outdir outdir3 --sched SLURM -opt1 <opt1_val> -opt2 <opt2_val> ...
...
pipe_exec --pfile example.ppl --outdir outdirn --sched SLURM -opt1 <opt1_val> -opt2 <opt2_val> ...
```

Extending Modules

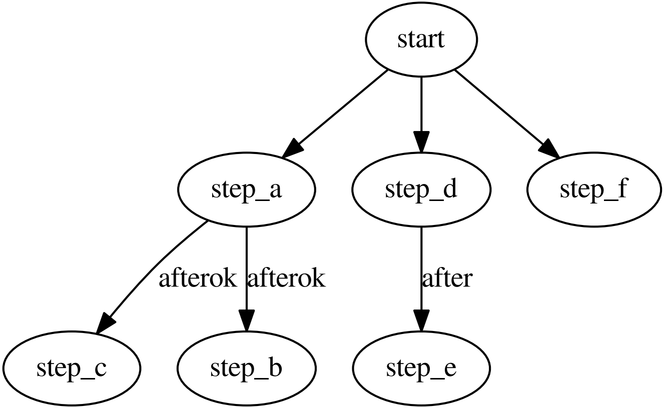
- Since multiple imports are permitted, a new module may contain step definitions missing in another one
- The order in which modules are imported is relevant
  - if two modules define the same function, the definition in the module imported last will prevail
  - the previous property can be used to modify a specific step without repeating the code of the whole module

Toy Pipeline Example

Pipeline File

```
#import pipe_software_test
#
step_a cpus=1 mem=32 time=00:01:00 stepdeps=none
step_b cpus=1 mem=32 time=00:01:00 stepdeps=afterok:step_a
step_c cpus=1 mem=32 time=00:01:00 throttle=2 stepdeps=afterok:step_a
step_d cpus=1 mem=32 time=00:01:00 stepdeps=none
step_e cpus=1 mem=32 time=00:01:00 stepdeps=after:step_d
step_f cpus=1 mem=32 time=00:01:00 stepdeps=none
```

Pipeline Representation


start
step_a
step_d
step_f
afterok
afterok
after
step_c
step_b
step_e