Organizing your Workflow

Keeping your workspace organized

Motivation: Reproducibility and Traceability

- Can I **reproduce** my workflow
  - Tomorrow?
  - 1 month from now?
  - 1 year from now?
- Give a set of analysed results – can I **trace back** my workflow all the way to the beginning?

Your environment and .bashrc

- Tip: try to keep your login environment clean (don’t pollute your .bashrc)

Your environment and .bashrc

- Tip: try to define your environment based on what you are currently working on.
  - Use (carefully) python environments
  - source a script that defines the environment for your current work

```
#  OpenIFS configuration
#  Sets correct user environment
#
#  source this file to correctly set environment
#   e.g.   source ./oifs-config.sh
#  If your site uses modules, then load the correct
#  module environment first.
module purge
module load buildenv-intel/2018.u1-bare
module load grib_api/1.24.0-nsc1-intel-2018a-eb

#  OpenIFS version: IFS CYCLE and RELEASE
#  Must be upper case. Used to set directories.
export OIFS_CYCLE=CY40R1
echo "Environment for OpenIFS: $OIFS_CYCLE"

#  OpenIFS home. Set this to the directory
#  containing this file (and 'src', 'bin' etc)
export OIFS_HOME=${PWD}
echo "OpenIFS home directory: $OIFS_HOME"

#  OpenIFS data directory.
#  Parent directory of the climatology files, vtables, rtables etc.
export OIFS_DATA_DIR=${OIFS_HOME}/ifsdata
echo "OpenIFS top-level data directory: $OIFS_DATA_DIR"

#  Location of grib-api (or eccodes) directory (may be set by module)
export OIFS_GRIB_API_DIR=${GRIB_API_DIR}
echo "OpenIFS GRIB_API directory: $OIFS_GRIB_API_DIR"

#  OpenIFS compilation environment
export OIFS_COMP=intel_mkl_impi    # gnu, intel or ccb (see make/cfg)
export OIFS_BUILD=opt     # opt, noopt, or nansC (see make/cfg)

#  PATH.
#  Add OpenIFS supplied FCM and grib-api to user path
export PATH=$PATH:$OIFS_HOME/fcm/bin:$OIFS_GRIB_API_DIR/bin
echo "Added OpenIFS FCM and GRIB_API to user path"

#  Create some useful aliases
echo "Creating command aliases for OpenIFS..."
alias omake="fcm make -v -j4 -f $OIFS_HOME/make/oifs.cfg"
alias omakenew="fcm make --new -v -j4 -f $OIFS_HOME/make/oifs.cfg"
alias oenv='env|grep OIFS_'
```

Load modules

Set environment variables

Append PATH

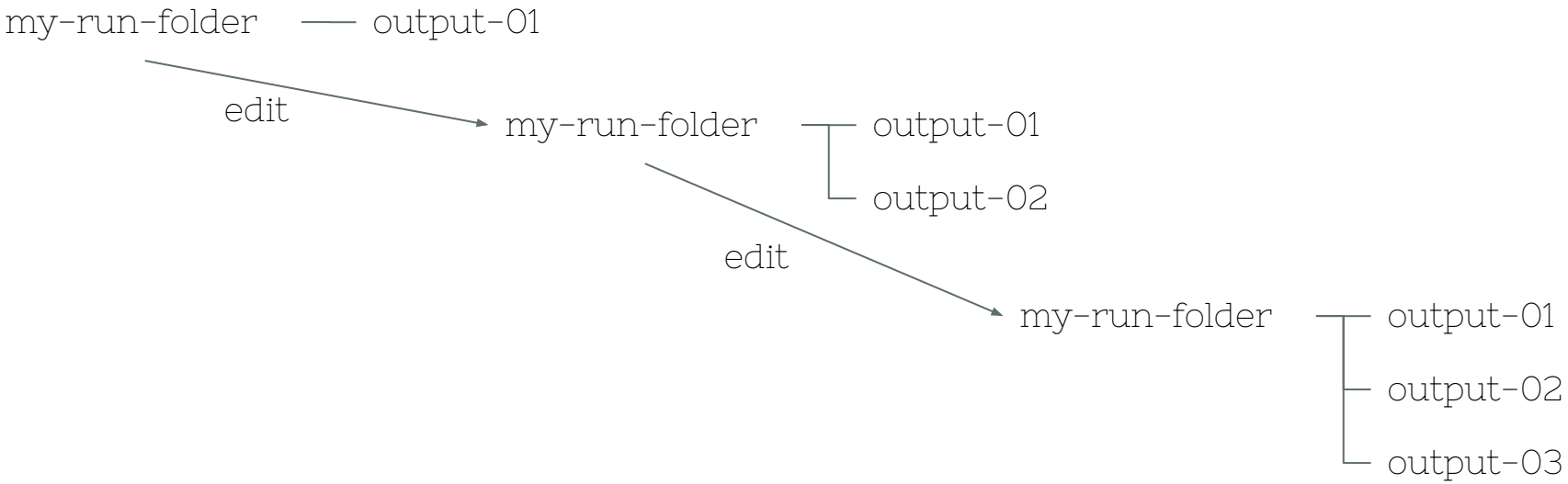
Set aliases

File, folder organization and annotation

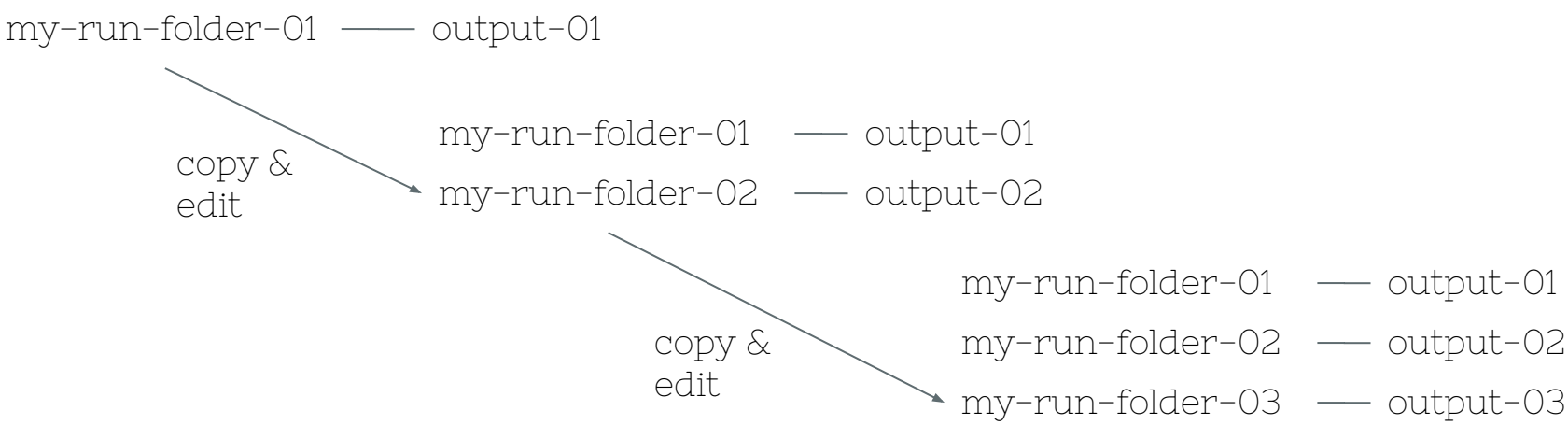
- Remember tab completion
  - Tab completion means it is practical (recommended) to use descriptive names for files and folders
  - Tips for file naming
  - What not to do (file naming)
  - Tips for folder structures

File, folder organization and annotation

- Tip: Try to avoid reusing run folders



File, folder organization and annotation



File, folder organization and annotation

- Tip: Don’t worry about deep folder structures
  - You can always use symbolic links or aliases to help navigate efficiently

File, folder organization and annotation

- Tip: It's never too late
  - mv (rename) within a file system is an efficient, atomic operation

File, folder organization and annotation

- Tip: get into the habit of annotating everything – be kind to the future you
  - Comment your code
  - Comment your scripts (incl. run scripts)
  - Add README files in your folders
  - …

File, folder organization and annotation

- Version control tools can be helpful, especially in shared workspaces
  - If you don't have any particular preferences, consider git
  - If you are not familiar with git check out Software Carpentry (or Code Refinery in the Nordics)

Workflow management

Workflow management

- If you follow a sequence of steps when working you have a **workflow**
- If you repeatedly follow the same steps (workflow) it can pay to manage your workflow.
  - repeatability
  - convenience
  - sharing

Workflow management: Tools

- A notebook
  - paper
  - electronic
- shell script
- Jupyter notebook

Workflow management: Tools

- Kepler (fusion research)
- Pegasus
- Galaxy (life sciences)
- Cylc, Autosubmit, ecFlow (Earth sciences)
- Taverna, COMPSs (Astrophysics)