

Formative assessment week 9: Snakemake, Conda, HPC

You have so far:

- Generated the code that performs your analysis
- Developed a reproducible environment for your project
- Integrated the environment and code into a Snakemake pipeline
- Version controlled the code, pipelining and environments using git and GitHub

We will now:

- Migrate the code, data and environments to HPC
- Update the Snakemake configuration to run on HPC
- Document these changes for ease of future reproducibility

1. Setting up on HPC

A. Getting our codebase on HPC

Your project should all be under version control on GitHub. This makes it extremely easy to create a clone of your code on another machine (such as HPC).

1. Login to bluecrystal4
2. Create a directory where you would like to keep your projects. A good option is to create a directory called `$WORK/projects/`
3. Navigate to `$WORK/projects` and clone your GitHub repository there.
 - Add the git module in bluecrystal4
 - Get the git repository's HTTPS URL from GitHub
 - Use `git clone` to clone the repository

If your code is not on github you can use WinSCP or something similar to copy your code into the relevant directory.

B. Getting our data on HPC

Use WinSCP or similar to copy your original data into `$WORK/projects/<formative>/data/original`. You can see how the data was setup originally on your computer in the `directory-setup-commands.sh` script.

C. Setup your conda environment

You should have conda ready to run on HPC from the practical sessions. Create the environment needed for your formative assessment.

Remember you will need to add the slurm plugin (<https://snakemake.github.io/snakemake-plugin-catalog/plugins/executor/slurm.html>).

D. Check that your scripts work as expected

- Ideally you would only run analysis on HPC by submitting your scripts to the worker nodes. However it is prudent to check that trivial errors are not present such as incorrect directory names etc. You can check this by starting to run your analysis scripts and seeing if it works.

2. Create a submission script

Using examples from the week 9 `practical_1` example, create a job submission script that will run your pipeline on HPC by submitting a single job that runs all the steps.

3. Use Snakemake to submit the analysis to HPC

A. Snakemake dry-run

Try a dry-run of the whole pipeline *without* submitting it to HPC (e.g. just run it interactively as if you were running it on your local computer). Check for any issues and fix.

B. Snakemake execution

You have setup a `slurm_profile` that can specify how the Snakemake pipeline can be executed on the HPC worker nodes. Using the examples in the week 9 `practical_2` session, try submitting the whole pipeline to HPC.

Note that it may be prudent to run this within a `tmux` session (why?)

4. Update your project repository

Given the changes that you have made, what should you do to finalise and record these processes?