Huygens Professional and Core on HPC Bunya Guide

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July 8, 2025

Abstract

A brief guide on how to use Huygens Professional and Core on HPC Bunya, including running Huygens Core by submitting a job to the Simple Linux Utility for Resource Management (SLURM) scheduler.

Preamble

This is HPC Bunya:
`https://rcc.uq.edu.au/systems/high-performance-computing/bunya`.

If you haven't done so already, apply for a Bunya account here:
`https://services.qriscloud.org.au/services/request/new/ee6def64259741a095c1fed20743e3fb`.
Copy questions 2) - 8) into the "Request details" box on the form and provide details for each item. Incomplete applications will be rejected and applicants will be required to fill in a new form.

Bunya training is available here:
`https://rcc.uq.edu.au/training-support/training-courses`.
Register via email to `rcc-support@uq.edu.au` to attend UQ-only training sessions.

Read the Bunya user guide here:
`https://github.com/UQ-RCC/hpc-docs/blob/main/guides/Bunya-User-Guide.md`
and the Bunya OnDemand guide here:
`https://github.com/UQ-RCC/hpc-docs/blob/main/guides/OnDemand-Guide.md`.

You can then request access to Huygens Professional and Core on HPC Bunya using this link:
`https://services.qriscloud.org.au/access/6211d1e3482544b2b73fc85156446e2c/member`.

Running Huygens Professional and Core via OnDemand

1. Go to the OnDemand site:
   https://bunya-ondemand.rcc.uq.edu.au/

2. Navigate to Interactive Apps > GPU-Accelerated Desktop. Give the job a name, choose your Bunya account group, and specify the number of GPUs, CPU cores per task, number of tasks, and maximum running time. Click "Launch."

3. OnDemand will prompt: "Please be patient as your job currently sits in queue. The wait time depends on the number of cores as well as time requested."
   Click "Launch GPU-Accelerated Desktop" when the desktop is running (Fig. 1).

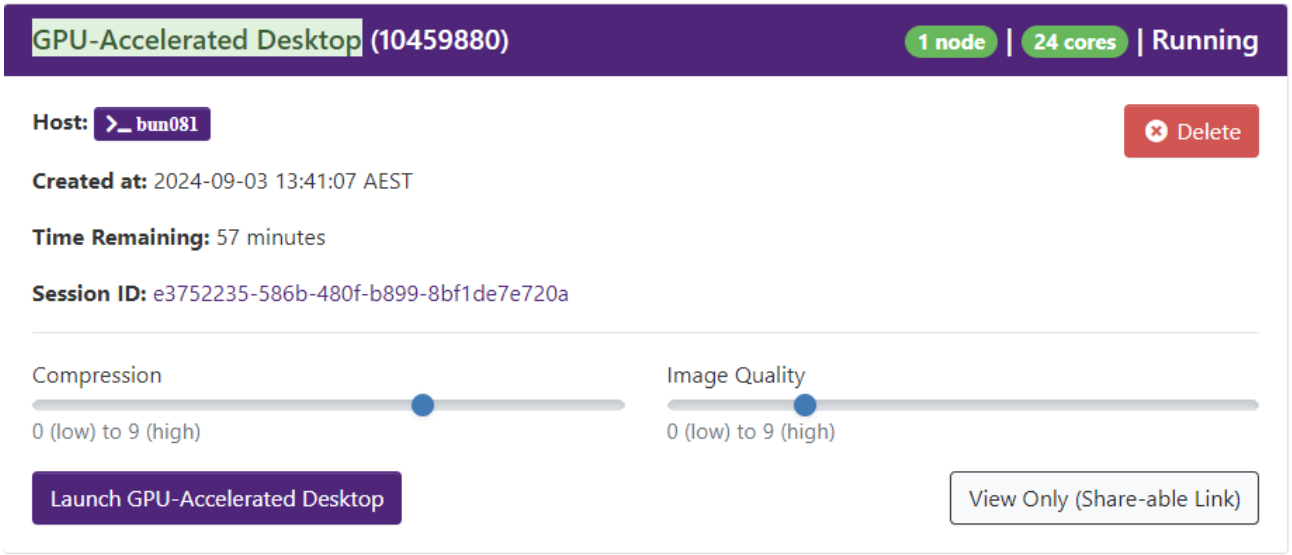

Figure 1: HPC Bunya OnDemand GPU-accelerated desktop running.

4. On the visualisation desktop, open a MATE terminal by navigating to Applications > System Tools > MATE Terminal and type:
   `module load huygens`
   `huygenspro`
   (Fig. 2).

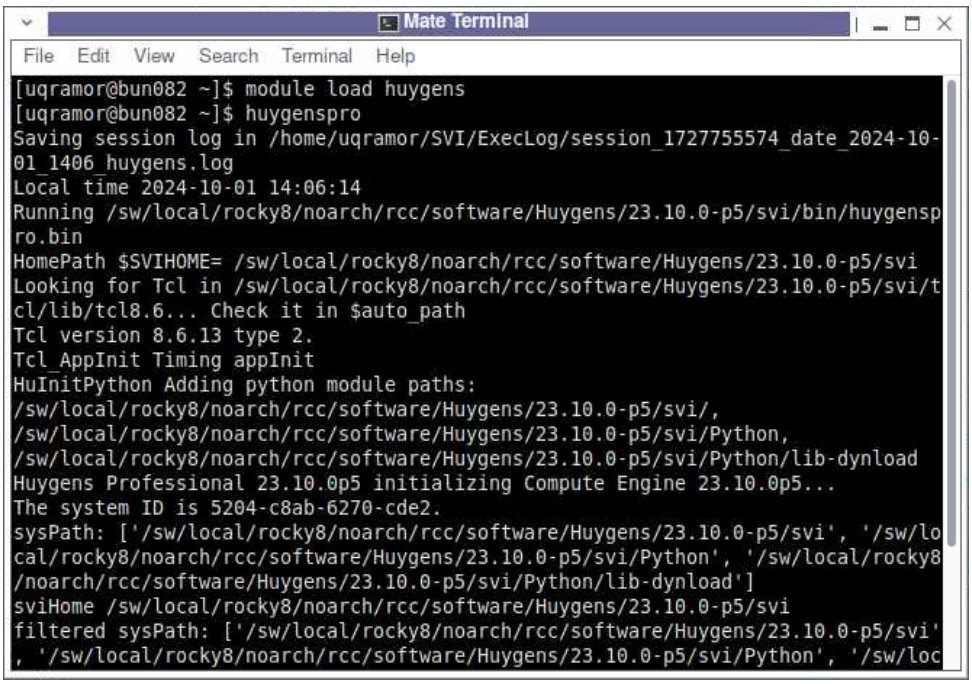

Figure 2: Running Huygens Professional via the MATE terminal.

5. This launches the Huygens Professional graphical user interface (GUI, Fig. 3).

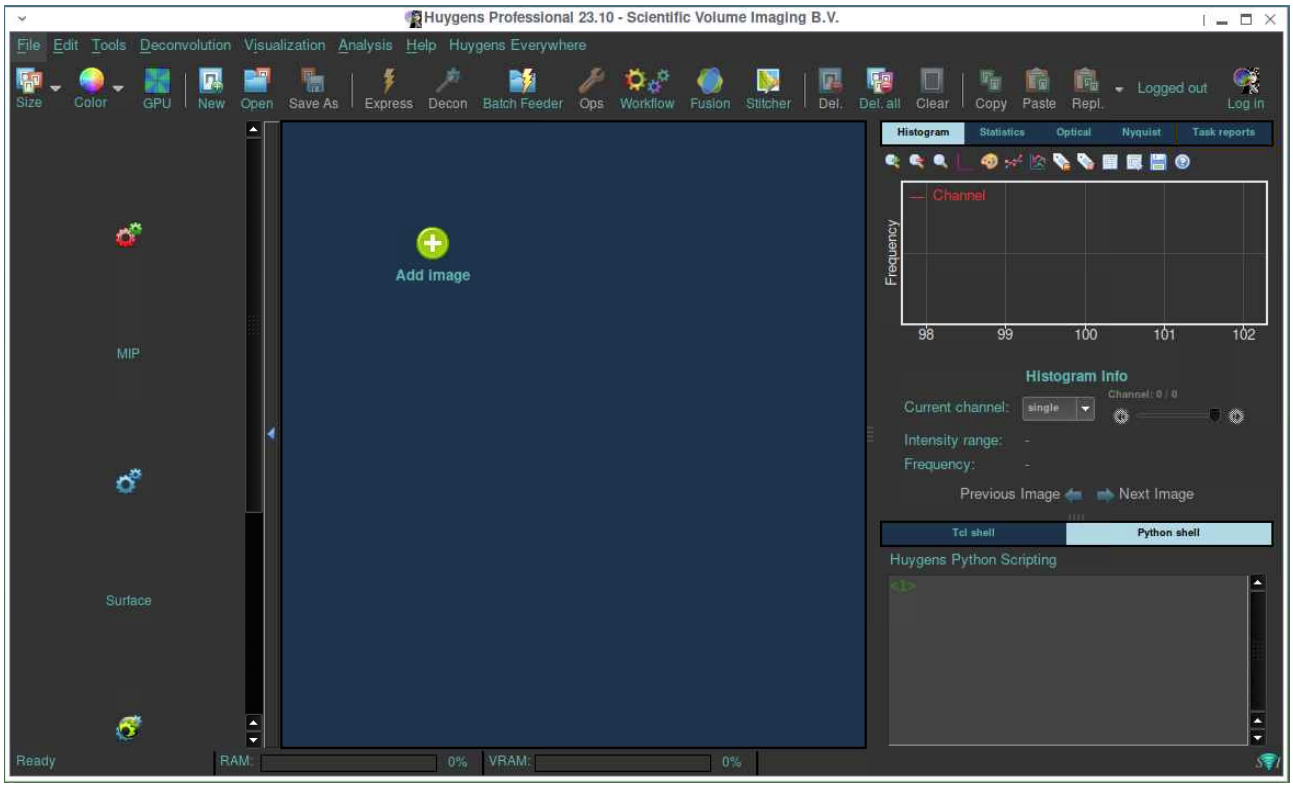

Figure 3: The Huygens Professional GUI.

6. Open an image and create a microscope template as normal (Fig. 4).

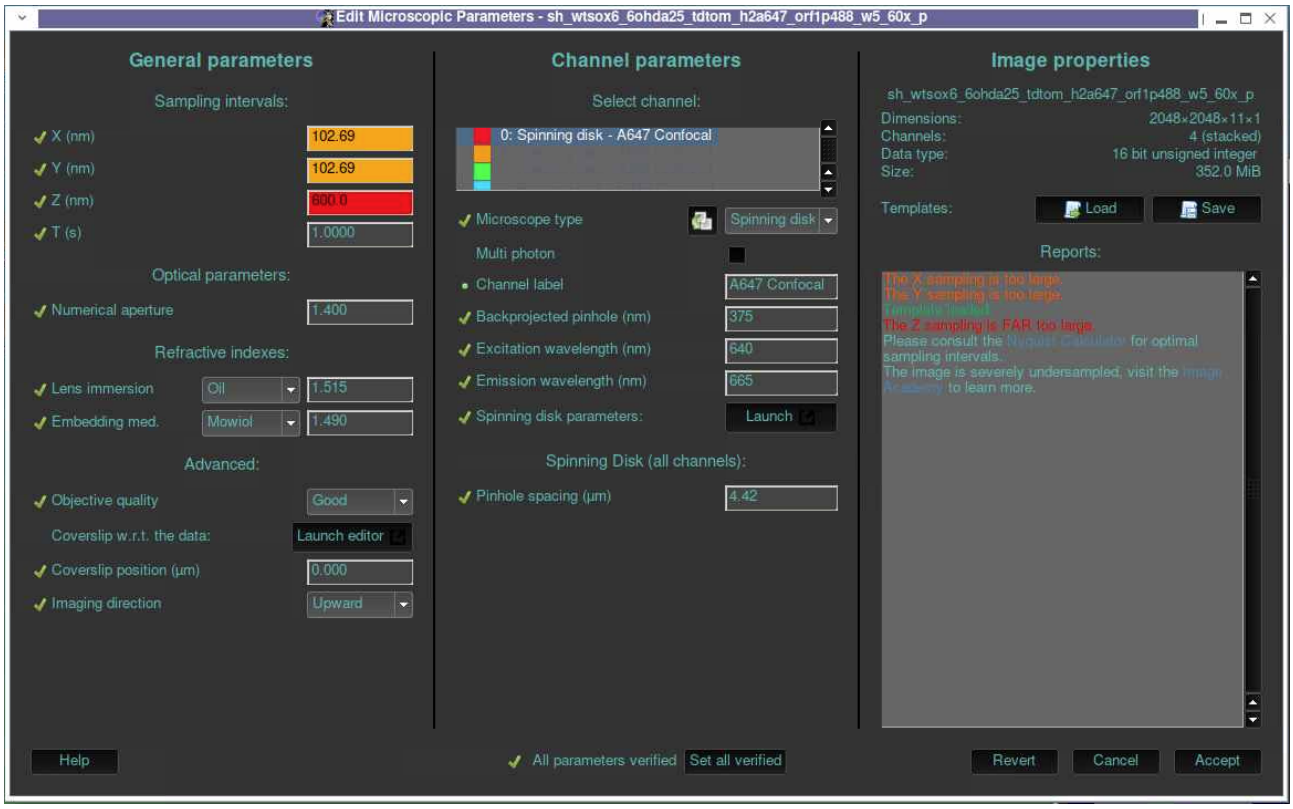

Figure 4: Creating a microscope template.

7. Do a deconvolution run using the wizard and save the deconvolution template as normal (Fig. 5).

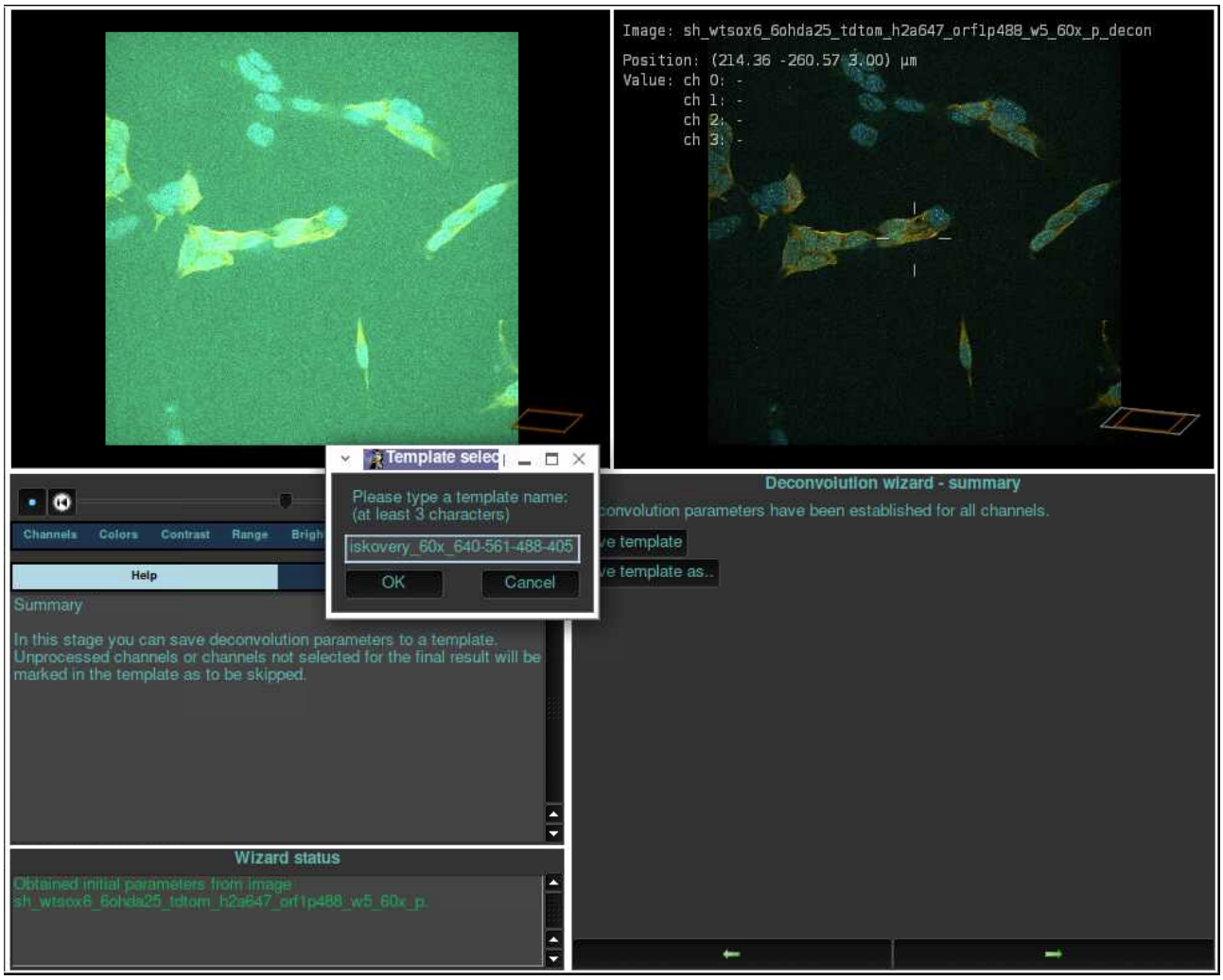

Figure 5: Saving a deconvolution template.

8. Open the Workflow Processor and create a batch job, specifying the input images or folder, the microscope template, deconvolution template, and output file format and directory (Fig. 6).

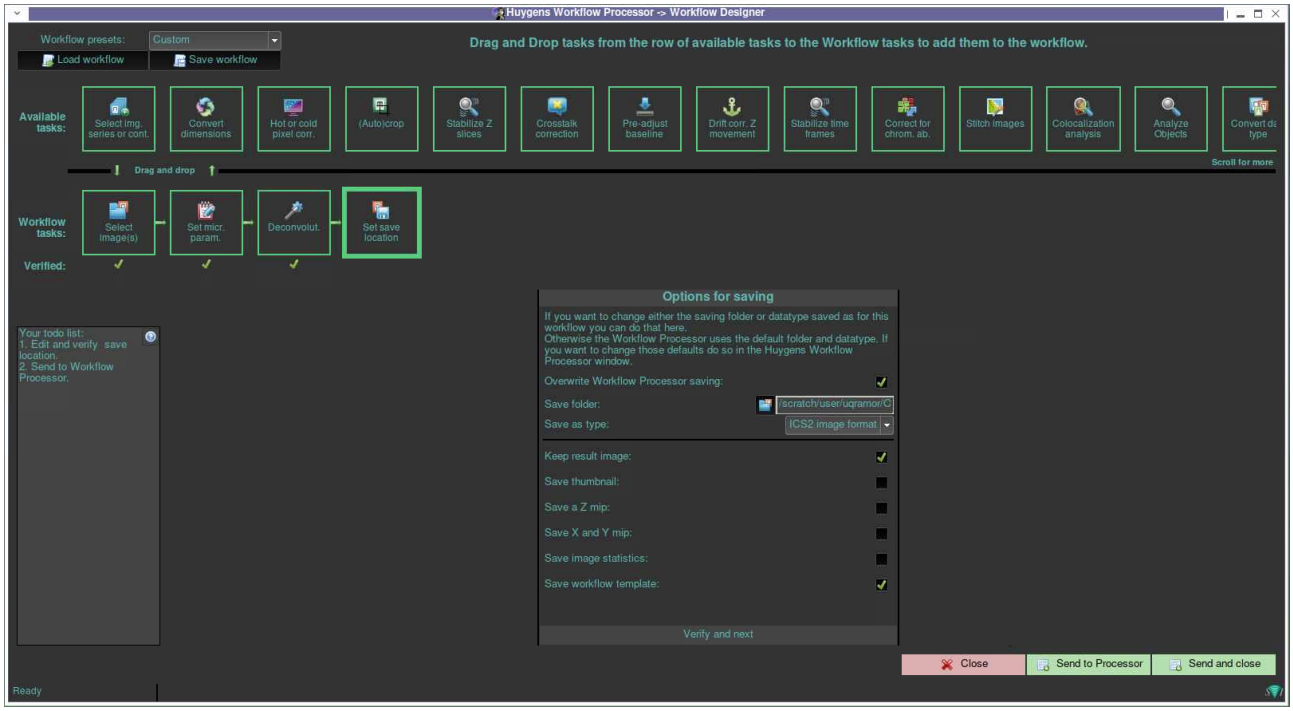

Figure 6: Creating a batch job on the Workflow Processor.

9. Save the batch template (`.hgsb` file, Fig. 7). You will use this template file to run batch jobs with Huygens Core, on the visualisation desktop and on SLURM.

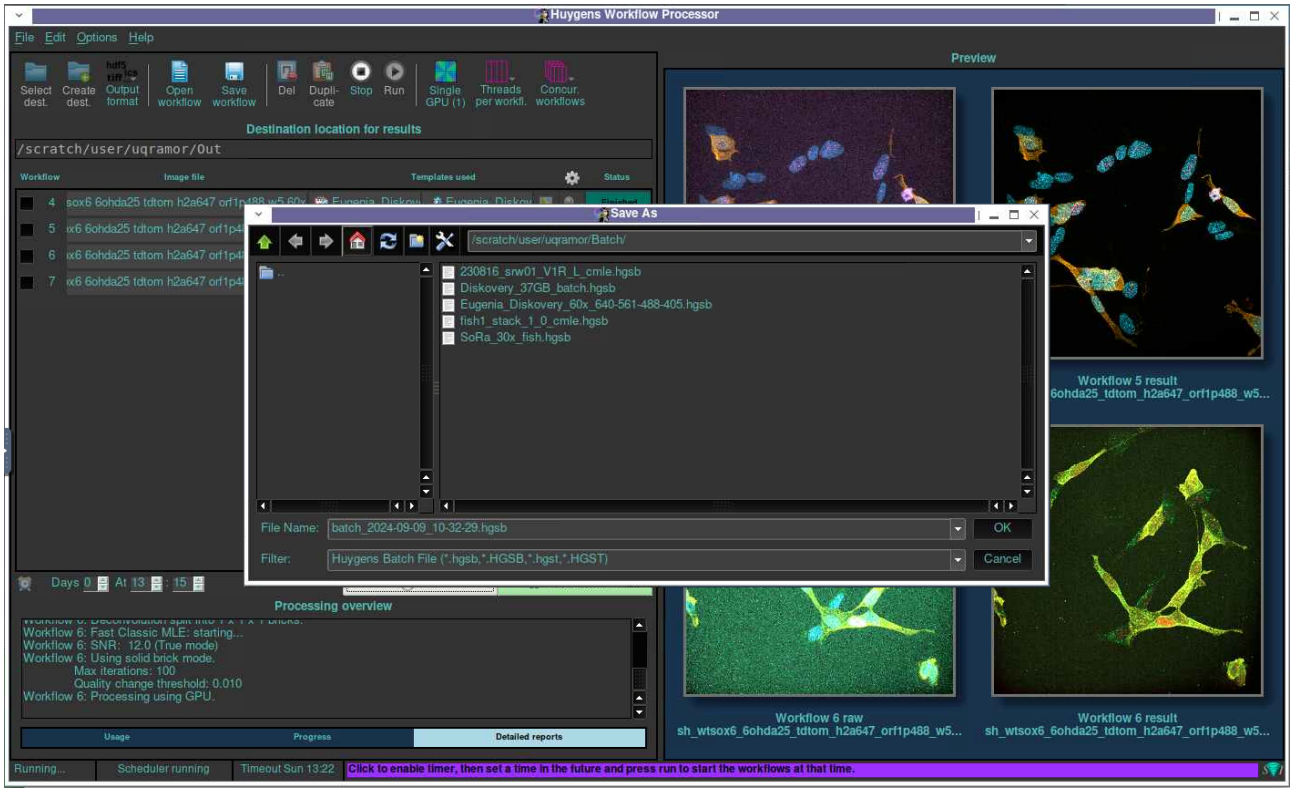

Figure 7: Saving a batch template.

10. Run Huygens Core by opening a new terminal and typing:
    `module load huygens`
    `hucore -template ‘‘batch_template_location’’`

    for example,

    `hucore -template ‘‘/scratch/user/uqramor/Batch/Eugenia_Diskovery_60x_640-561-488-405.hgsb’’` (Fig. 8).

    Huygens Core will then run the batch job and save the outputs in the directory specified on the batch template.

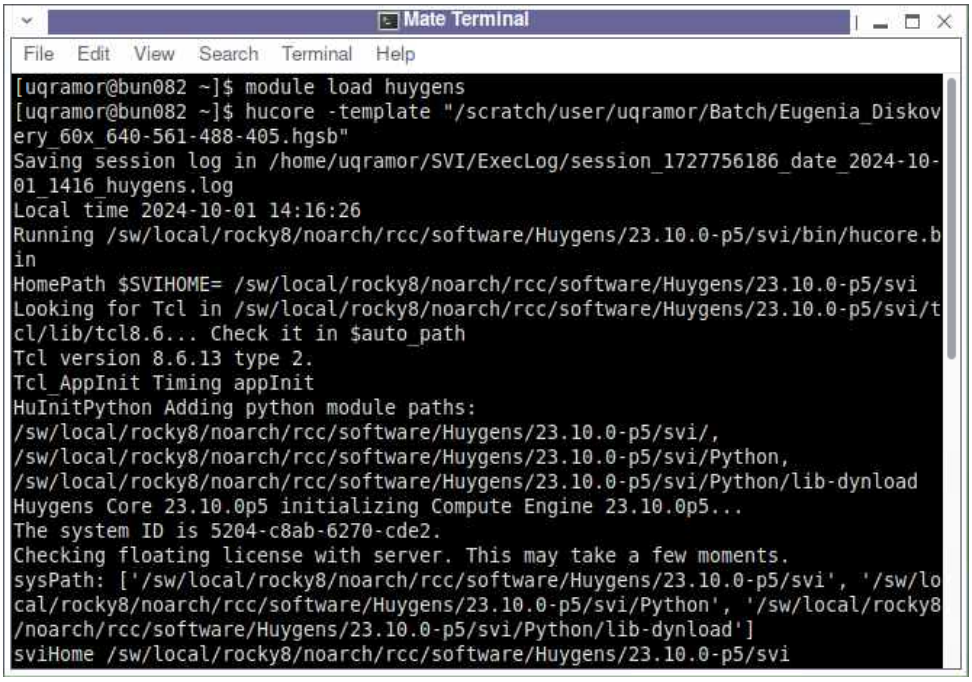

Figure 8: Running Huygens Core via OnDemand.

Huygens SLURM on Bunya

1. On your machine, open a terminal window. Log on to Bunya by typing:
   `ssh USERID@bunya.rcc.uq.edu.au`

   Enter your UQ password. Go through the Duo authentication prompts. You will then be logged on to Bunya (Fig. 9).

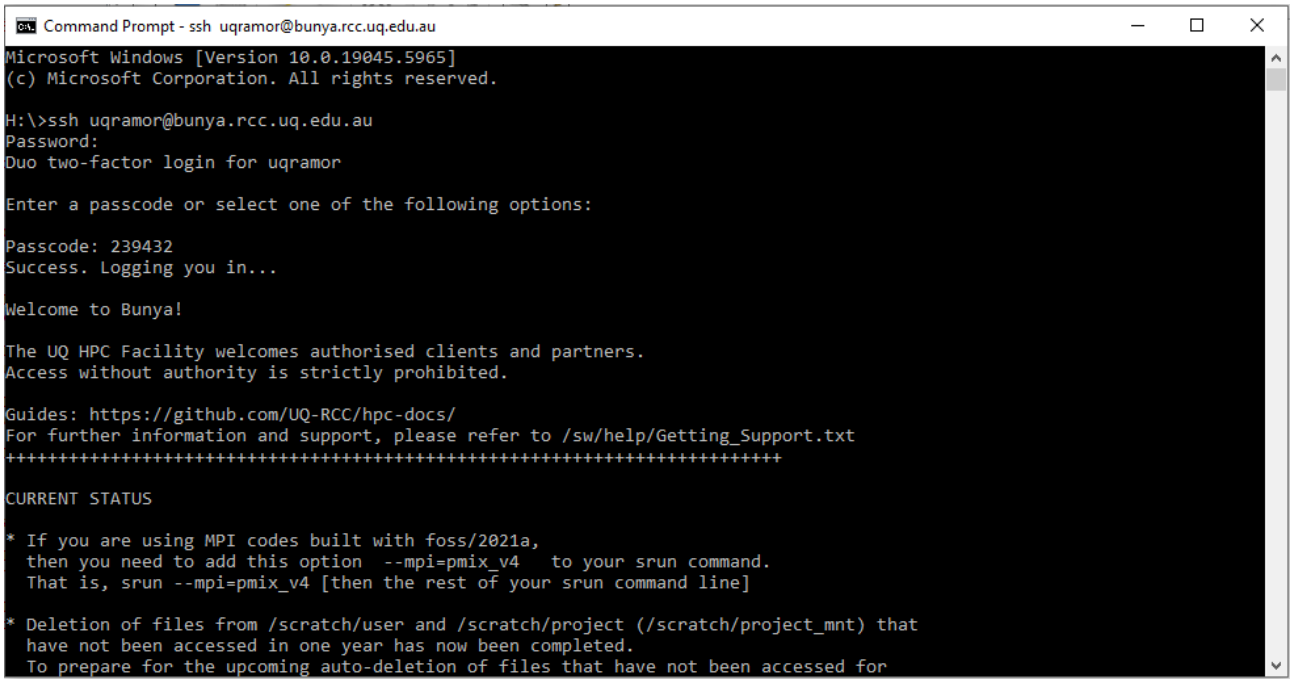

Figure 9: Connecting to Bunya via ssh on a terminal window.

2. By default, you will be on the /home directory. Print the current working directory:
   `$ pwd`

   (Note: "$" indicates a command line and is not part of the command.)

   UQ RCC requires that all jobs are called from the /scratch directory. Change to your /scratch directory:
   `$ cd /scratch/user/USERID`
   (Fig. 10).

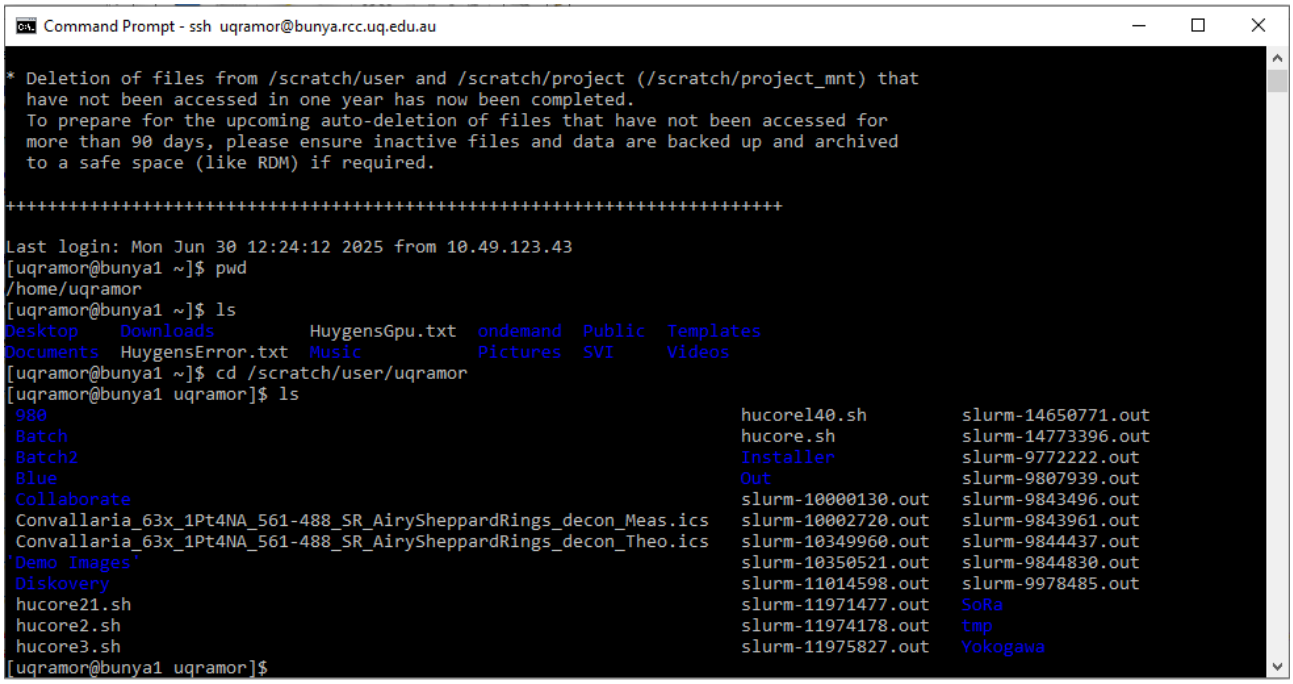

Figure 10: Printing the current working directory and changing to the scratch directory.

3. Create a script to submit your job to the SLURM scheduler. Use vi, or a similar editor. Give the script a name, and use .sh as the extension (Fig. 11).

   Watch QCIF's quick overview of vi here:
   `https://www.youtube.com/watch?v=TuR9d9Z_Fis`

Figure 11: An example script to submit a Huygens Core job to SLURM.

A short description of the lines on the script follows. The Bunya User Guide has more information.

`#!/bin/bash -l`
→ We are using BASH (the Bourne Again SHell), a shell program and command language for Linux. The `-l` command makes the shell a login shell.

The `SBATCH` commands are for allocating resources:
`#SBATCH --nodes=1` → number of nodes

`#SBATCH --ntasks-per-node=1` → 1 for single- and multi-thread jobs

`#SBATCH --cpus-per-task=24` → number of threads

`#SBATCH --mem=16G` → RAM per job in MB, GB, TB; see the Bunya guide

`#SBATCH --job-name=HUCORE` → the name you give your job

`#SBATCH --time=01:00:00` → time the job needs to complete; max=168 hrs for gpu_cuda, =24hrs for gpu_viz

`#SBATCH --qos=gpu` → the Quality of Service name; see the QoS guide

`#SBATCH --partition=gpu_cuda` → you are using the GPU partition; you can also use the gpu_viz partition

`#SBATCH --gres=gpu:1` → GPU number

`#SBATCH --gres=gpu:l40:1` → using the L40 GPU; or use gres=gpu:nvidia_a100_80gb_pcie_1g.10gb:1, or gres=gpu:a16:1 if using gpu_viz

`#SBATCH --account=a_qbi_microscopy` → your accounting group

The next two lines launch Huygens Core for batch runs:
`module load huygens` → launches the Huygens module

`hucore -template ''.hgsb batch file''` → launches Huygens Core and runs the batch job as specified in the template

4. Submit the job to SLURM:
   `$ sbatch SCRIPT_FILENAME`

```
[uqramor@bunya2 uqramor]$ sbatch hucore2.sh
Submitted batch job 14773396
[uqramor@bunya2 uqramor]$
```

Figure 12: Submitting the job to SLURM.

5. Check the status in the job queue:
   `$ squeue --me`

```
[uqramor@bunya2 uqramor]$ squeue --me
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
          14773396  gpu_cuda   HUCORE  uqramor  R       0:36      1 bun080
[uqramor@bunya2 uqramor]$
```

Figure 13: Checking the status in the queue.

6. Monitor the job by using the `tail` command.
   `$ tail -f slurm-JOBID.out`

   To exit the `tail` command, press Ctrl + C.

```
Command Prompt - ssh uqramor@bunya.rcc.uq.edu.au
[uqramor@bunya2 uqramor]$ tail -f slurm-14773396.out

                Bleaching correction for task cmle:3:
z dim: 1.000
t dim: 1.000
Doing task imgSave...
Scaling mode while saving: -cmode scale
Scaling mode while saving: -cmode scale
Saving image using command: sh_wtsox6_6ohda25_tdtom_h2a647_orf1p488_w5_60x_p001_cmle__14_ save {/scratch/user/uqramor/Ou
t/sh_wtsox6_6ohda25_tdtom_h2a647_orf1p488_w5_60x_p001_cmle_(14).ics} -type ics2  -cmode scale
Successfully saved results to: {/scratch/user/uqramor/Out/sh_wtsox6_6ohda25_tdtom_h2a647_orf1p488_w5_60x_p001_cmle_(14).
ics}
Launching workflow 6 for client 0, ID: 2 on cpu group 0
Setting export option type to hdf5
Setting export option multidir to 0
Setting export option cmode to scale
Setting export option compr to 0
Setting export option subResolutions to 0
Setting export option subSamplingFactor to 2
Complete envArr:
key gpuDevice ; val 0
key useMultiGpu ; val 0
key OMP_DYNAMIC ; val 0
key retainProcess ; val false
key inputConversion ; val int
key resultDir ; val /scratch/user/uqramor/Out
key attemptGpu ; val 1
key exportFormat ; val type hdf5 multidir 0 cmode scale
key timeOut ; val 172800
key concurrentJobCnt ; val 1
```

Figure 14: Monitoring the job.

7. When the job is done, use scp (**s**ecure **cop**y) to transfer individual files to your RDM collection:
   `$ scp FILENAME USERID@bunya.rcc.uq.edu.au:/RDM_FILE_PATH`

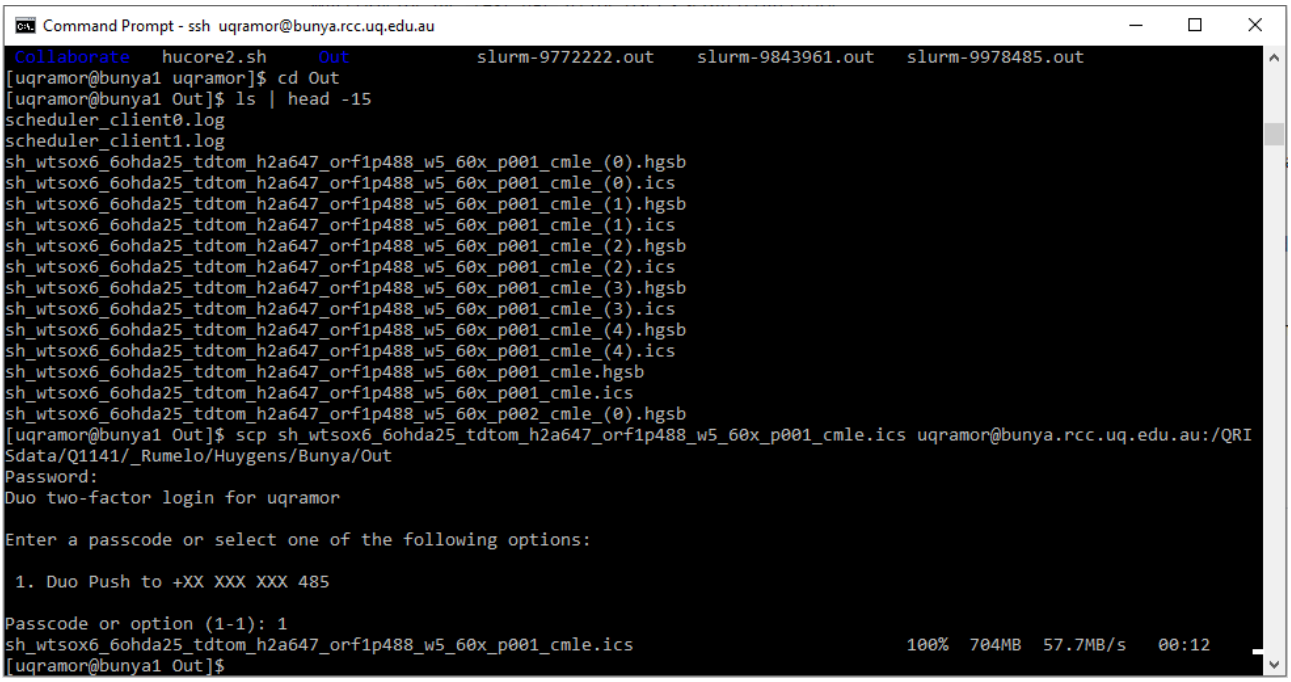

Figure 15: Transferring a file using scp.

or copy the whole output directory:

```
$ scp -r OUTPUT_DIRECTORY USERID@bunya.rcc.uq.edu.au:/RDM_FILE_PATH
```

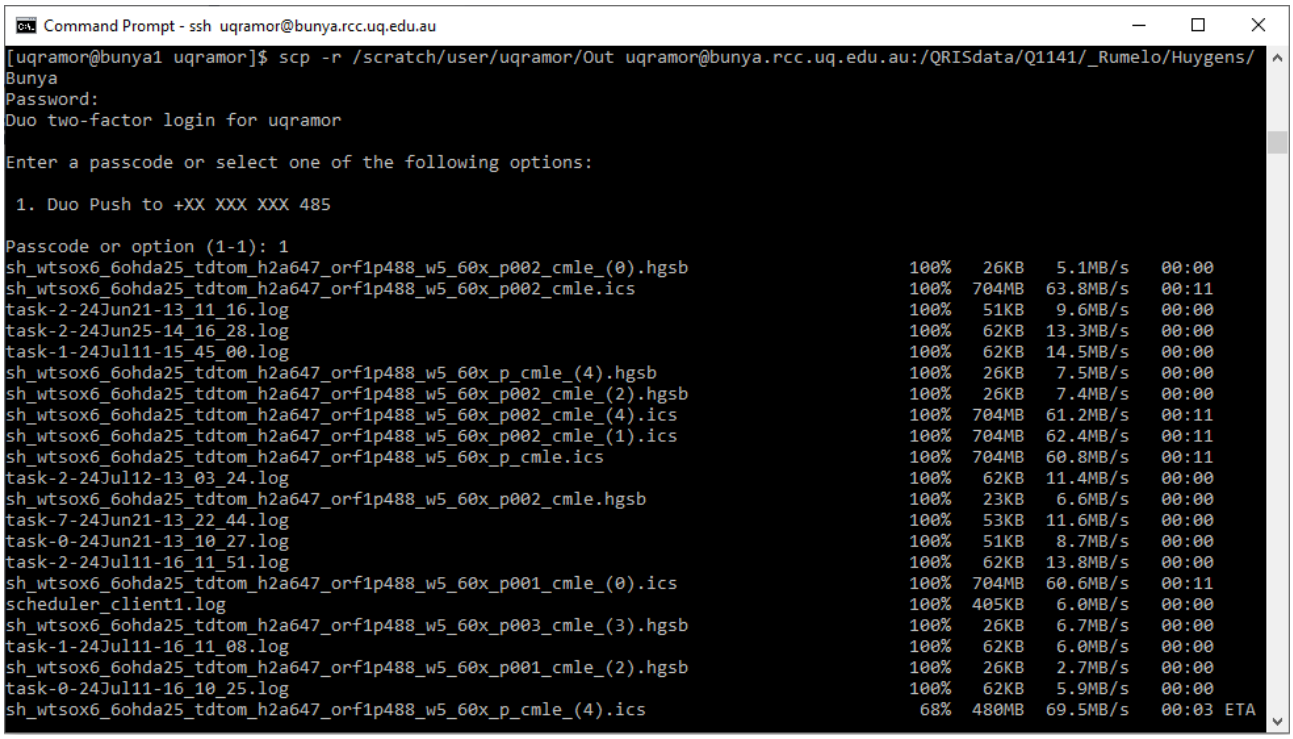

Figure 16: Transferring the output directory using scp.

Acknowledgments

We thank Jake Carroll, Sarah Walters, Marlies Hankel, Edan Scriven, and Owen Powell of UQ RCC and Vincent Schoonderwoert of SVI for making Huygens Professional and Core happen on Bunya OnDemand and SLURM and Eugenia Ferreiro of the QBI Faulkner Lab for the use of her image data for testing.

We are grateful to Jacqui Romero, whose document, "Bunya SPINS guide," portions of the text here were adapted from.