

Run ProxiPal on WEHI compute

1. Visit: <https://rap.wehi.edu.au/global-protect/portal/portal.esp>
2. Choose: OnDemand
3. Choose: Jupyter Notebook
4. Request a Notebook Server as below.

Copy this: `--notebook-dir=/stornext/Sysbio/data/Projects/CFHAC_ProxiPal`

Jupyter Notebook

This app will launch a Jupyter Notebook server on one or more nodes.

Partition

Partition to submit the job to

Extra Jupyter arguments (optional)

Job Name (optional)

Optional name for the job

Additional modules (optional)

Space separated list of additional modules to load (i.e. R singularity/3.6.2)

#CPUs

Max: interactive 16, regular 56, gpuq 24

Memory (GB)

Max: interactive 64GB, regular 500GB, gpuq 124GB

Runtime hours (max: 24)

Slurm time limit

Launch

* The Jupyter Notebook session data for this session can be accessed under the [data root directory](#).

5. Click “Connect to Jupyter”, then choose *ProxiPal > Python > ProxiPal_Report_v1_4.ipynb*
NB. If you haven’t set up your WEHI compute profile then follow the steps in the appendix

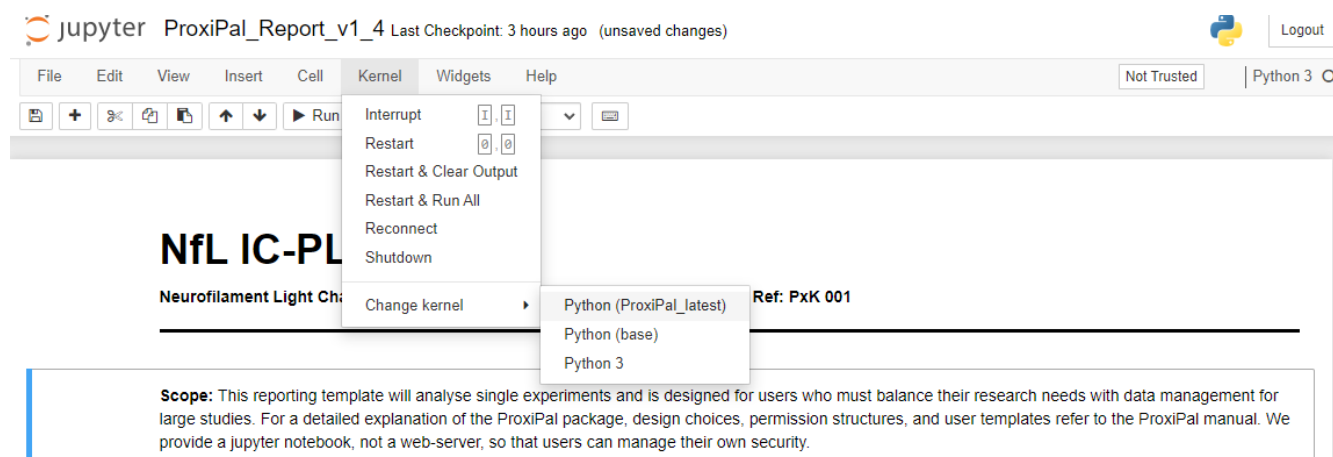


Files Running Clusters

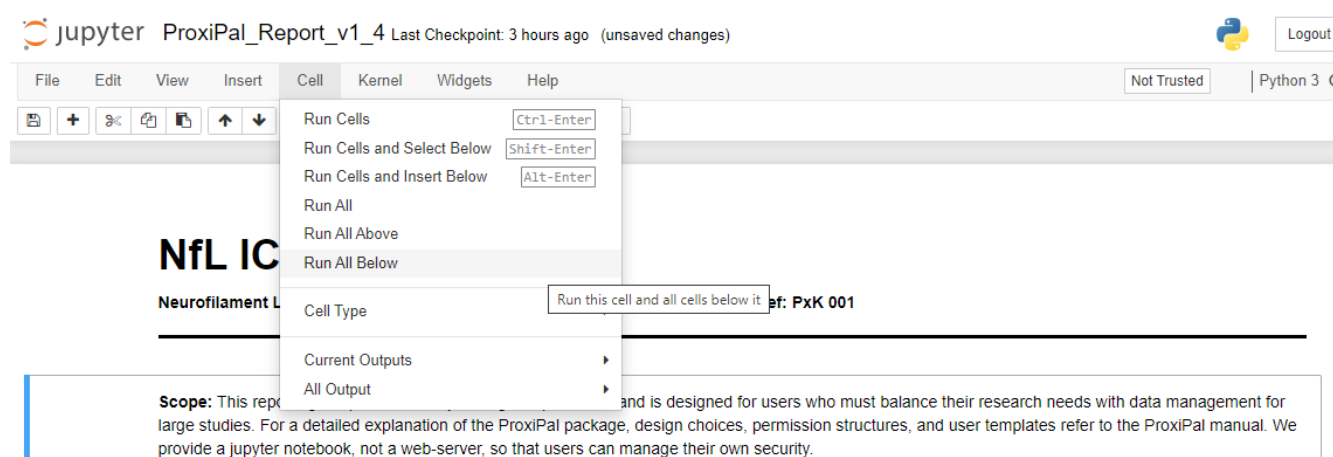
Select items to perform actions on them.

	0	1	2	3	4	5	6	7	8	9	+
<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
/ ProxiPal / python											
..											
<input type="checkbox"/>	ProxiPal_Docs_v1_0.ipynb										
<input type="checkbox"/>	ProxiPal_Report_v1_4.ipynb										
<input type="checkbox"/>	Logo_Large.JPG										
<input type="checkbox"/>	Logo_Small.JPG										
<input type="checkbox"/>	proxipal-logo.png										
<input type="checkbox"/>	ProxiPal.py										
<input type="checkbox"/>	ProxiPal_v0.py										

6. Switch the kernel to “ProxiPal”



7. Then, initialise the report by running all cells below the red text.



8. Once initialised you can use the “Toggle Code Cells” button to close all the code cells. Use the buttons to navigate the report.

NB: Because WEHI Jupyter Notebook Servers don't have nbconvert installed you won't be able to use Qgrid, or export to html/pdf.

If you want to save an html or pdf report I recommend you install a chrome add-on like “Save Page WE”

<https://chrome.google.com/webstore/detail/save-page-we/dhhpefjklgkmgaeafimnjhojgjamof>

Appendix: Set up your WEHI compute profile for ProxiPal

A. After getting your Notebook server, click on the hashkey next to “Session ID”

Interactive Apps

Desktops

GPU Desktop

Milton Desktop

Seqmonk

Servers

Code Server

Jupyter Notebook (12511054) 1 node | 4 cores | Running

Host: sml-n06.hpc.wehi.edu.au Delete

Created at: 2023-06-21 16:05:22 AEST

Time Remaining: 23 hours and 59 minutes

Session ID: c5a65daa-c733-4348-86e5-2472afb82315

Connect to Jupyter

B. Then “Open Terminal”

Open in Terminal Refresh New File New Directory Upload Download Copy/Move Delete

/ home / users / allstaff / smith.j / ondemand / data / sys / dashboard / batch_connect / sys / Jupyter / output /
c5a65daa-c733-4348-86e5-2472afb82315 / Change directory Copy path

☐ Show Owner/Mode ☐ Show Dotfiles Filter:

Showing 9 rows - 0 rows selected

Type	Name	Size	Modified at
<input type="checkbox"/>	after.sh	492 Bytes	4/7/2023 11:32:42 PM
<input type="checkbox"/>	before.sh	2.1 KB	6/21/2023 4:05:22 PM
<input type="checkbox"/>	config.py	404 Bytes	6/21/2023 4:05:24 PM
<input type="checkbox"/>	connection.yml	81 Bytes	6/21/2023 4:05:28 PM
<input type="checkbox"/>	job_script_content.sh	4.36 KB	6/21/2023 4:05:22 PM
<input type="checkbox"/>	job_script_options.json	523 Bytes	6/21/2023 4:05:22 PM
<input type="checkbox"/>	output.log	1.15 KB	6/21/2023 4:05:28 PM
<input type="checkbox"/>	script.sh	453 Bytes	6/21/2023 4:05:22 PM
<input type="checkbox"/>	user_defined_context.json	239 Bytes	6/21/2023 4:05:22 PM

C. You'll get a Linux Bash terminal.

```
ondemand.hpc.wehi.edu.au/pun/sys/shell/ssh/default/home/users/allstaff/smith.j/ondemand/data/...  
Host: slurm-login.hpc.wehi.edu.au Initial directory: /home/users/allstaff/smith.j/ondemand/data/sys/dashboard/batch_connect/sys/Jupyter/output/c5a65daa-c733-4348-86e5-2472afb82315  
smith.j@slurm-login.hpc.wehi.edu.au's password:  
Linux slurm-login02.hpc.wehi.edu.au 3.10.0-1160.88.1.el7.x86_64 #1 SMP Tue Mar 7 15:41:52 UTC 2023 x86_64 x86_64 x86_64 GNU/Linux  
16:21:29 up 74 days, 22:40, 17 users, load average: 1.08, 1.05, 1.05  
(base) slurm-login02 344 %
```

D. now substitute “smith.j” for your username and enter one line at a time as below:

```
module load anaconda3/latest  
conda init  
conda activate base  
python -m ipykernel install --user --name base --display-name "Python (base)"  
conda create -p /home/users/allstaff/smith.j/myenvs/ProxiPal_latest  
conda activate /home/users/allstaff/smith.j/myenvs/ProxiPal_latest  
python -m ipykernel install --user --name ProxiPal --display-name "Python (ProxiPal)"  
conda install -c conda-forge qgrid  
conda install -c anaconda scikit-learn  
conda install -c plotly plotly  
conda deactivate  
conda activate /home/users/allstaff/smith.j/myenvs/ProxiPal_latest
```

E. You can return to step 5.