

Interactive Session Jupiter to launch openfold environment gui example

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Jupyter

This app will launch a Jupyter server using Python.

Jupyter interface

Lab

This defines the interface of Jupyter you want to start (Notebook or Lab).

Jupyter Python

Custom(Specify below)

This defines the Python distribution of Jupyter you want to start.

Custom Python Environment

```
module load anaconda/miniconda3_4.8.3-jupyter
source /common/software/install/manual/miniforge3/24.3/etc/profile.d/conda.sh
conda activate openfold-env
echo "CONDA_PREFIX=$CONDA_PREFIX"
echo "PATH=$PATH"
```

Enter commands (module load, source activate, etc) to create your desired Jupyter environment; jupyter MUST be on your path and either notebook or jupyterlab installed in your Python environment.

Notebook Root

/scratch.global/rayma017/Workspace/FinalProject/

The root notebook folder to use. If empty, defaults to your home directory.

Account

ee4940

Select Slurm account to charge, will also set Jupyter's GID to this group.

Resources

Interactive GPU-16 cores,60 GB, 100 GB local scratch,1 A40

Time Limit

24 hours

Shorter times will probably start faster ☐ I would like to receive an email when the session starts

For the Gui examples two notebooks were create to run on the MSI:
The openfold-env has been already created.

Run once:

```
conda activate openfold-env
```

```
python -m ipykernel install --name openfold-env --display-name "Python openfold-env"
```

launch a jupyter session with the setup from prior page.

- example_notebook.ipynb
- example_py3dmol.ipynb