Using Jupyter

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Jupyter is not an HPC application and no support beyond this documentation will be provided by SCITAS.

The Jupyter documentation can be found at http://jupyter.org/documentation

Why not IPython?

IPython is the interactive python kernel used by Jupyter: https://ipython.org

Using IPython without Jupyter greatly simplifies the launch process and is much more suitable for use on a HPC cluster.

Installing IPython and Jupyter

The key to successfully installing the tools is using python virtual environments. Please note that you will need to install for each architecture (the $SYS_TYPE variable used below).

Load a compiler and python using modules

```
$ module load gcc
$ module load python
```

or

```
$ module load intel
$ module load python
```

Create a virtual environment

Shown here for GCC but the same applies for the Intel compiler.

```
$ virtualenv --system-site-packages opt/$SYS_TYPE/venv-gcc
```

Using base prefix '/ssoft/spack/cornalin/v1/opt/spack/linux-rhel7-x86_E5v4_Mellanox/gcc-5.4.0/python-3.6.1-moc7d7wihugzp5f14ew7zsa5muzwvrn6'

New python executable in /home/user/opt/x86_E5v4_Mellanox/venv-gcc/bin/python3.6
Also creating executable in /home/user/opt/x86_E5v4_Mellanox/venv-gcc/bin/python
Installing setuptools, pip, wheel...done.

Activate the virtual environment

```
$ source opt/$SYS_TYPE/venv-gcc/bin/activate
```

(venv-gcc) [user@fidis ~]$


Install Jupyter and ipyparallel

```bash
(venv-gcc) [user@fidis ~]$ pip install jupyter ipyparallel
Collecting jupyter
```

MPI4PY

At this point you may wish to install MPI4PY - see the documentation for how to do this.

Running IPython

The easiest way to use IPython is via the Sinteract tool which gives interactive access to a compute node:

```bash
[user@fidis ~]$ /usr/bin/Sinteract -p debug -n 1 -c 28 -t 01:00:00 -m 120G
```

You now have all the power of IPython on a dedicated compute node.

Running Jupyter

Running Jupyter is a lot more complicated as we need to launch the server on the login node but ensure that the computational tasks are executed on a compute node. This is why we installed ipyparallel alongside Jupyter.

Here we show how to launch multiple tasks in parallel - it is an HPC cluster after all!

After loading the virtual environment we use ipcluster to start worker engines on the node(s)

```bash
ipcluster start --init --profile=default --ip="*" -n=<ntasks> --engines=Slurm --SlurmEngineSetLauncher. timelimit=<timelimit> --SlurmEngineSetLauncher.queue=<partition> --SlurmEngineSetLauncher.account=<account>
```

Note:
To find your account, type the following command:
Make sure that you choose meaningful values for ntasks, timelimit, partition and account

Behind the scenes ipcluster submits a batch job to SLURM so the usual caveats about batch jobs apply. The Job ID is given when you launch so the normal squeue/scontrol commands can be used to see what's going on.

We now launch jupyter on the login node:

jupyter notebook --ip="$(hostname -s).epfl.ch"

Create a notebook on your local machine by opening the URL and try:

import ipyparallel as ipp

c = ipp.Client(profile="default")

This will connect to the engines on the node(s). It may fail if the engines are not spawned yet.

%%px

import os
import platform

print("{} on 

The %%px magic expresses that the full cell in the notebook should be run in parallel.
Once you have finished don’t forget to stop the ipcluster server!

```
(venv-gcc) [user@fidis ~]$ ipcluster stop
```

Now you have a working parallel setup it's possible to make it a bit more user friendly

The file `~/.ipython/profile_default/ipcluster_config.py` that contains most of the configurations was created - you can edit it and add the options passed to the ipcluster command.

```bash
jupyter nbextension enable --user --py ipyparallel
```

If you rerun jupyter you should see a IPython Clusters tab and in there a line with your default profile. You can choose the number of cores to use

**Customize sbatch options**

If you need to add options to sbatch like memory constraints, you can create a sbatch template that you provide to the ipcluster command.

Create a `sbatch_jupyter.sh` file with additionaln `#SBATCH --arguments`

```bash
#!/bin/sh
#SBATCH --job-name=ipy-controller-{cluster_id}
#SBATCH --ntasks=1
#SBATCH --mem 8G
%s --profile-dir="{profile_dir}" --cluster-id="{cluster_id}"
```

Run the ipcluster command with the `--SlurmEngineSetLauncher.batch_template_file` argument
ipcluster start --init --profile=default --ip="*" -n=<ntasks> \\
--engines=Slurm \\
--SlurmEngineSetLauncher.timelimit=<timelimit> \\
--SlurmEngineSetLauncher.queue=<partition> \\
--SlurmEngineSetLauncher.account=<account> \\
--SlurmEngineSetLauncher.batch_template_file=./sbatch_jupyter.sh