

# Day 1 Recap & Using Python at NERSC



New User Training  
September 8, 2023

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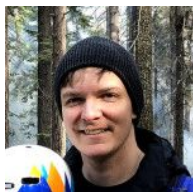
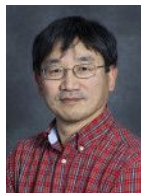
National Energy Research Scientific Computing Center

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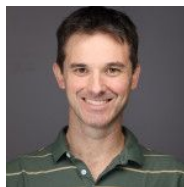
# Interacting with NERSC

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# Day 1 Recap

## Programming Environments and Compilation Best Practices:

- Use `module spider`
- Use compiler wrappers `–CC`, `cc`, and `ftn–` with `PrgEnv` modules
- Verify CMake builds with `ccmake`
- man files are the source of truth, i.e. `man intro_mpi`
- See examples builds at <https://github.com/NERSC/community-software>
- More questions? Need help? ... **<http://help.nersc.gov/>**

# Day 1 Recap

## Running Jobs (Scheduling) Best Practices/Tips:

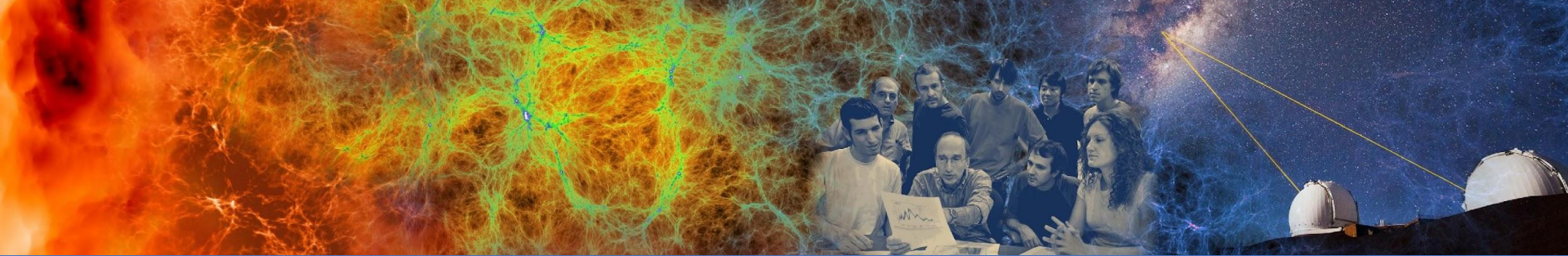
- One job with a large allocation
  - Per node priority ageing is the highest
  - Can get scheduled first
- Shorter time length jobs
  - Easier to schedule as backfill
  - Use a workflow manager
- Choose the right time from Slurm
  - Balance between enough runtime
  - Waiting in the queue for a long job
- Utilize Workflow tools
  - GNU Parallel, Parsl, Fireworks, etc.
- Make Use of Job Script Generator
  - Provides sample option for slurm batch scripts

# Python users, welcome to NERSC!

What we'll cover in this intro to Python at NERSC:

- Using Python at NERSC
  - python/conda modules
  - creating environments/installing packages
  - tips for parallel python
- Getting started with Python on GPUs!
  - high-level overview





# Using Python at NERSC



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# How can I use Python at NERSC?

- To get started, load the python module:

```
> module load python/3.11
```

```
(nersc-python)> python
```

```
Python 3.11.7 | packaged by conda-forge | (main, Dec 23 2023,  
14:43:09) [GCC 12.3.0] on linux  
Type "help", "copyright", "credits" or "license" for more  
information.
```

```
>>> print("Welcome to NERSC New User Training Feb 2024!!!")
```

```
Welcome to NERSC New User Training Feb 2024!!!
```

<https://docs.nersc.gov/development/languages/python/>



# The NERSC Python Module

The NERSC python module provides python via a conda environment. It's convenient for simple use cases that only need relatively common Python packages in the scientific computing.

```
> module load python/3.11
(nersc-python)> conda list
# packages in environment at /global/common/software/.../nersc-python:
#
# Name                                Version                                Build      Channel
...
matplotlib                            3.8.2                                py311h38be061_0    conda-forge
...
numpy                                  1.26.3                               py311h64a7726_0    conda-forge
...
scipy                                  1.11.4                               py311h64a7726_0    conda-forge
...
```

# Other options for using Python at NERSC

## Create a custom conda environment:

```
> module load conda
> conda create -n myenv python=3.11 numpy scipy
> conda activate myenv
```

```
(myenv)> python
```

```
Python 3.11.7 (main, Dec 23 2023, 14:43:09) [GCC 12.3.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>>
```

## Use Python from a container:

```
> shifter --image=docker:library/python:latest python
```

```
Python 3.11.4 (main, Aug 16 2023, 19:58:34) [GCC 12.2.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
```

```
>>>
```

```
perlmutter> which python
/usr/bin/python
```

~~This is not the Python  
you're looking for!~~

# The NERSC Conda Module

conda is an environment and package management tool that is very popular in the scientific python community.

conda environments are great for creating isolated and reproducible software environments for your projects. The conda package manager is great for installing and resolving package dependencies for your projects.

Loading the conda module initializes conda. There is no need to run “conda init” or initialize conda in your ~/.bashrc (or similar shell startup file).

# Package installation tips:

- Most packages installed via conda or pip should work at NERSC
  - packages installed via conda can come from different “channels”. Channels are specified with “`-c defaults`” or “`-c conda-forge`”.
  - In many cases it’s fine to mix packages from different channels and/or pip but this can sometimes lead to version conflicts. Check the packages installed in your environment with “`conda list`”
- Some python packages should be compiled with the “compiler wrappers” available on the system. For example, mpi4py (see next slide) and potentially h5py (if you’re using parallel IO features).
- cudatoolkit: module vs conda package:
  - Some GPU-enabled packages installed from conda-forge will install cudatoolkit into your conda environment. This may conflict with the cudatoolkit module that is loaded by default.

# Building and using mpi4py

- mpi4py provides a Python interface to MPI
- mpi4py is available via `module load python`
- This mpi4py is with CUDA support in cray-mpich
- To install mpi4py with CUDA support in cray-mpich, follow this recipe:

```
> module load PrgEnv-gnu cudatoolkit craype-accel-nvidia80 conda
> conda create -n mpi4py-gpu python=3.9 -y
> conda activate mpi4py-gpu
> MPICC="cc -shared" pip install --force-reinstall --no-cache-dir
--no-binary=mpi4py mpi4py
```

- Be aware that with any CUDA-aware mpi4py, you must have `cudatoolkit` loaded, even for code that does not use the GPU

# Use pip with caution

- Be careful with pip!!! pip maintains a local package cache which , but sometimes you don't want this.
- Packages installed with `--user` are not confined to a particular environment
  - If you use `pip install --user <package>`, it will install packages to the location specified by `PYTHONUSERBASE`, which may be set to something like `$HOME/.local/perlmutter/python-3.11`
- Best practices for pip:
  - Install packages inside of a conda environment, not outside (don't use `pip install --user <package>`)
  - Use `pip install --no-cache-dir --force-reinstall <package>` (Did you notice this in our mpi4py recipe?)

# Running Python at scale at NERSC

Python startup/module imports can put significant load on shared global filesystems, especially when running in parallel.

To avoid this we recommend:

- Use a container (run with shifter or podman)
- Use `/global/common/software/<project>`
  - use the `-p/--prefix` option when creating conda environments:

```
> conda create -p /global/common/software/<project>/envs/myenv python=3.11
```

```
> conda activate /global/common/software/<project>/envs/myenv
```
- Avoid `$HOME`
- Avoid `$CFS`

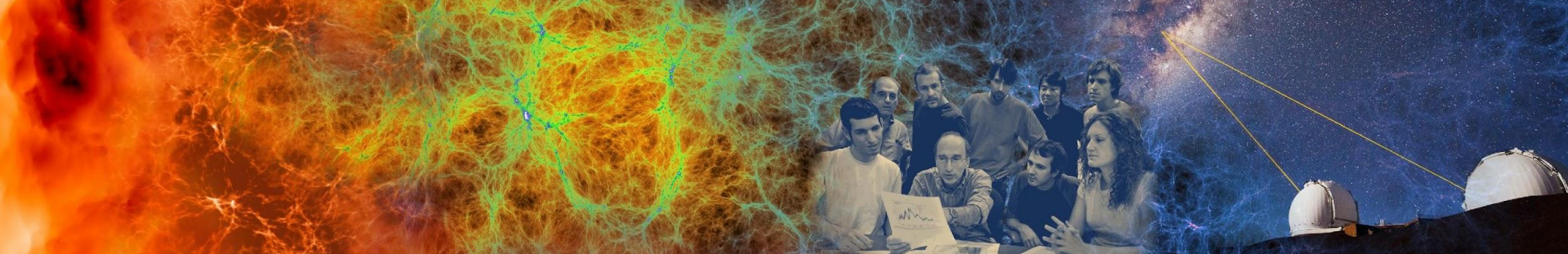
# Other common parallel Python pitfalls

- Unexpected oversubscription due to indirect parallelism.
  - numpy uses OpenMP threading under the hood.
    - When using multiple processes, make sure `num_processes_per_node x OMP_NUM_THREADS` does not exceed the number of physical CPU cores per node.
  - Default worker pool size in multiprocessing.
    - It's common for Python applications to use the value of ``os.cpu_count()`` to set a default value for the number of processes / workers. This does not account for cpu-binding.
    - For nested parallel applications, you should specify the number of workers to use and not trust the default.



# Using Python at NERSC Summary

- Use conda environments (or containers!) for customizable Python sandboxes.
- Use the `/global/common/software/<project>` filesystem (or containers!) for better performance when running in parallel.
- Use the compiler wrappers to build packages such as mpi4py.
- Avoid running “`conda init`” which will hardcode conda initialization in your shell startup file (`$HOME/.bashrc`)
- Be careful using pip.
- Avoid using the system python from `/usr/bin` !
- Watch out for defaults which may unexpectedly lead to oversubscription of resources.



# Using Python on GPUs



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# Getting started with GPUs in Python

- NumPy and SciPy do not utilize GPUs out of the box
- There are many Python GPU frameworks out there:
  - “drop in” replacements for numpy, scipy, pandas, scikit-learn, etc
    - **CuPy**, **RAPIDS**
  - “machine learning” libraries that also support general GPU computing
    - **PyTorch**, **TensorFlow**, **JAX**
  - “I want to write my own GPU kernels”
    - **Numba**, **CUDA Python**
  - multi-gpu / multi-node / distributed memory:
    - **mpi4py+X**, **dask**, **cuNumeric**
- Many of these GPU libraries have adopted the [CUDA Array Interface](#) which makes it easier to pass array-like objects stored in GPU memory between the libraries
- There is also effort in the community to standardize around a common [Python array API](#)



```
numpy:      mean(a, axis=None, dtype=None, out=None, keepdims=<no value>)
dask.array: mean(a, axis=None, dtype=None, out=None, keepdims=<no value>)
cupy:      mean(a, axis=None, dtype=None, out=None, keepdims=False)
jax.numpy: mean(a, axis=None, dtype=None, out=None, keepdims=False)
mxnet.np:  mean(a, axis=None, dtype=None, out=None, keepdims=False)
sparse:    s.mean(axis=None, keepdims=False, dtype=None, out=None)
torch:     mean(input, dim, keepdim=False, out=None)
tensorflow: reduce_mean(input_tensor, axis=None, keepdims=None, name=None,
                        reduction_indices=None, keep_dims=None)
```

# cuda toolkit dependency via module

```
> module load conda
```

Note: cuda toolkit module is loaded by default  
Current default version is cuda toolkit/11.7

```
> conda create --name cupy-demo python=3.11 numpy scipy
```

```
> conda activate cupy-demo
```

```
> pip install cupy-cuda11X
```

Check your package documentation to see  
cuda toolkit compatibility requirements

```
> python
```

```
>>> import cupy as cp
```

```
>>> print(cp.array([1, 2, 3]))
```

```
[1 2 3]
```

See documentation at <https://docs.nersc.gov/development/languages/python/using-python-perlmutter/>

# cuda toolkit dependency via conda

```
> module load conda
> module unload cudatoolkit
> conda create --name cupy-demo python=3.11 numpy scipy
> conda activate cupy-demo
> conda install -c conda-forge cupy
> python
>>> import cupy as cp
>>> print(cp.array([1, 2, 3]))
[1 2 3]
```

cupy conda-forge package will pull cudatoolkit dependencies into conda env

cupy conda-forge package will pull cudatoolkit dependencies into conda env

See documentation at <https://docs.nersc.gov/development/languages/python/using-python-perlmutter/>

# Is my code a good fit for a GPU?

CPU → low latency  
GPU → high throughput

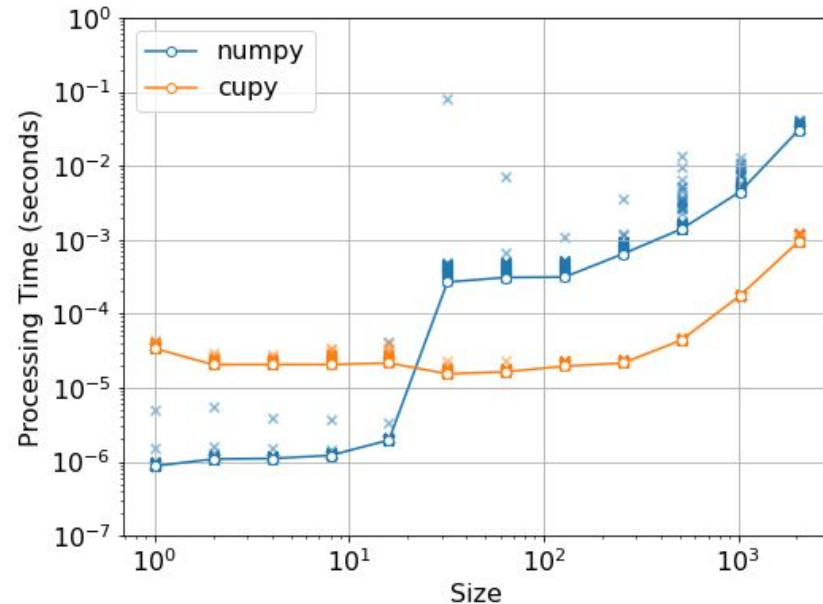
GPUs are likely a good fit if the following are true for your application:

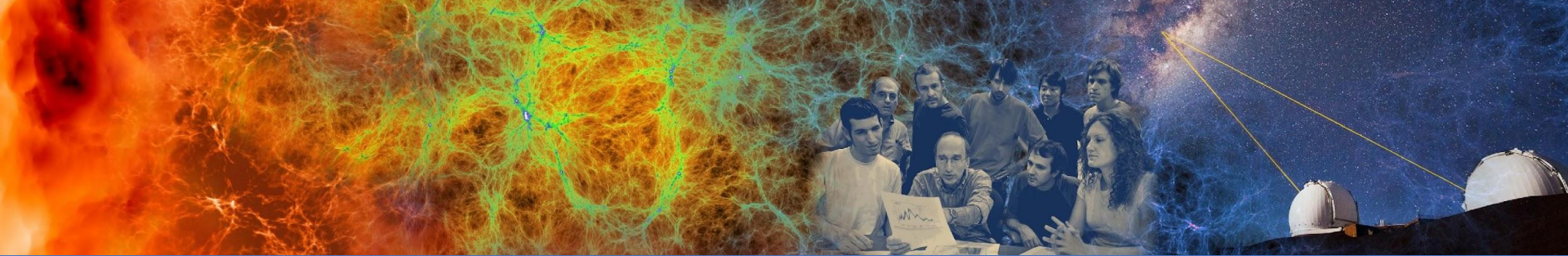
- Performs computation using large arrays, matrices, or images
- Dataset can fit in GPU memory
  - (40GB for Perlmutter's A100 GPUs)
- IO is not a bottleneck

For more help choosing a GPU-accelerated Python framework:

<https://docs.nersc.gov/development/languages/python/perlmutter-prep/>

```
a = xp.random.rand(size, size)
b = xp.random.rand(size, size)
def f(a, b):
    return xp.dot(a, b)
```





# Wrap Up



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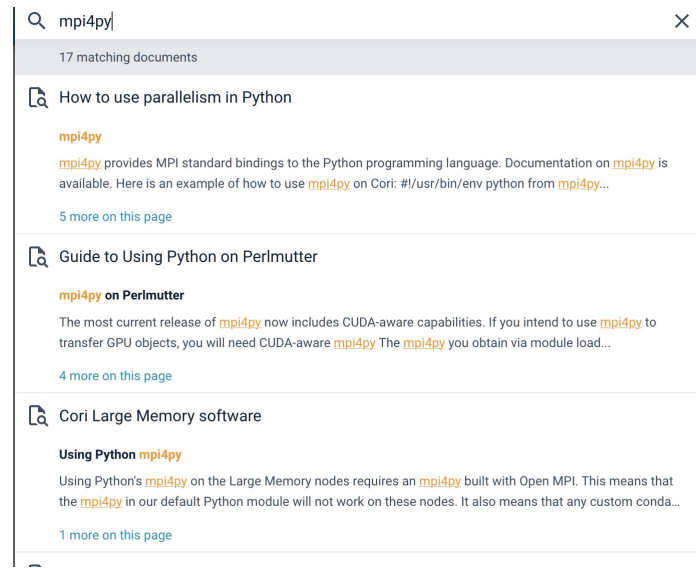


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# Best Practices & Where to get Python information

- Utilize Conda
- 
- Check out Python in NERSC docs:
  - [Python at NERSC](#)
  - [Python on Perlmutter](#)
  - [Jupyter at NERSC](#)
  - Try the search bar at [docs.nersc.gov](https://docs.nersc.gov), it's pretty good!
- Can't find the answer? Submit a ticket at [help.nersc.gov](https://help.nersc.gov)





# Summary

- Welcome to NERSC!
- We are here to help you use Python productively on Perlmutter
- If you have questions, please check our [docs.nersc.gov](https://docs.nersc.gov) or file a ticket at [help.nersc.gov](https://help.nersc.gov)



Thank You and  
Welcome to  
NERSC!

