

Introduction to practical sessions, and logistics



Practical sessions are scheduled from 1:30pm to 4:00pm

1:30 pm - 2:45 pm - Practical session

2:45 pm - 3:00 pm - Break

3:00 pm - 4:00 pm - Practical session

During the practical sessions, you can work through the exercises at your own pace

Instructors will be in the practical sessions in case you have questions or would like to discuss anything covered in the lectures

The practical sessions of this tutorial will be run on Derecho



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323,712 processor cores	3rd Gen AMD EPYC™ 7763 Milan processors
2,488 CPU-only computation nodes	Dual-socket nodes, 64 cores per socket 256 GB DDR4 memory per node
82 GPU nodes	Single-socket nodes, 64 cores per socket 512 GB DDR4 memory per node 4 NVIDIA 1.41 GHz A100 Tensor Core GPUs per node 600 GB/s NVIDIA NVLink GPU interconnect
328 total A100 GPUs	40GB HBM2 memory per GPU 600 GB/s NVIDIA NVLink GPU interconnect



Don't forget to enable X11 forwarding when connecting!

```
ssh -X <username>@derecho.hpc.ucar.edu
```

On macOS systems you might try `-Y` rather than `-X`

```
ssh -Y <username>@derecho.hpc.ucar.edu
```

During scheduled practice sessions we will have 40 nodes reserved for this tutorial

- Submit jobs to the `s6200749` queue
- This is the default in the job scripts that we provide

Since we have 35 participants and 40 nodes, please try to only have one job queued¹ via `qsub` at a time

Feel free to work on exercises outside of scheduled practice sessions

- However, submit jobs to the `main` queue instead
- All that you need to do is to uncomment one line and comment another in your job script

¹In the `s6200749` queue

Job scripts

```
#!/bin/bash

#PBS -A UMMM0008
#PBS -N jobname
#PBS -q S6200749
##PBS -q main
#PBS -l walltime=00:30:00
#PBS -l select=1:ncpus=128:mpiprocs=128

mpiexec ./atmosphere_model
```

Job scripts are
submitted to the
queuing system
with `qsub`

Checking on queued jobs

The `qstat` command is used on Derecho to check the status of queued jobs

- `qstat` with no arguments shows all jobs on the system, which is usually not useful
- `qstat -u $USER` shows only your jobs

But...

The information shown by `qstat` is only refreshed every 30 seconds or so. Therefore, after submitting a job, it may take a bit before you see your job with `qstat`. If you think your job may have already finished, try `qstat -xu $USER` to see running and completed jobs.

Running with qcmd

For some parts of practical exercises, we will run programs on a batch node without a job script via `qcmd`

```
qcmd -A UMMM0008 -- ./init_atmosphere_model
```

By default, jobs run with `qcmd` go through the `main` queue

Any options that you can provide in a job script can be given to `qcmd`, e.g.,

```
qcmd -A UMMM0008 -q S6200749 -- \  
./init_atmosphere_model
```

Resource allocations

All of our computing will be under the UMMM0008 project

We have 50,000 core-hours

- Divided evenly between 35 participants -> everyone has about 1400 core-hours
- One Derecho node for one wallclock hour = 128 core-hours
- You can continue to work with MPAS-Atmosphere on your own time

The UMMM0008 project is available until the end of October

Use the UMMM0008 project *only for MPAS-Atmosphere* tutorial work, and please don't hesitate to contact one of the tutorial organizers if you have any questions at all!

Practical exercises

We have a web page to guide you through some exercises:

<https://www2.mmm.ucar.edu/projects/mpas/tutorial/Howard2024/>



Welcome to the MPAS tutorial practice guide

This web page is intended to serve as a guide through the practice exercises of this tutorial. Exercises are split into seven main sections, each of which focuses on a particular aspect of using the MPAS-Atmosphere model.

While going through this practice guide, you may find it helpful to have a copy of the MPAS-Atmosphere Users' Guide available in another window. Click [here](#) to open the Users' Guide in a new window.

In case you would like to refer to any of the recorded lectures or lecture slides, you can open the [Tutorial Agenda](#), which contains links to the lectures, in another window.

You can proceed through the sections of this practical guide at your own pace. It is highly recommended to go through the exercises in order, since later exercises may require the output of earlier ones. Clicking the grey headers will expand each section or subsection.

0. Prerequisites and environment setup

1. Compiling MPAS, and creating static files and idealized ICs

2. Creating real-data ICs and running a simulation

Practical exercises

We have a web page to guide you through some exercises:

<https://www2.mmm.ucar.edu/projects/mpas/tutorial/Howard2024/>

If you're logged in to Derecho, you can get this URL with:

```
cat ~duda/url
```

Practical exercises

Blocks of shell commands can be selected all at once

Before going through any of the exercises in subsequent slides, we need to prepare our environment. Firstly, we will purge all loaded modules (with no modules loaded); then, we will load several modules, including as well as an MPI implementation:

```
$ module --force purge  
$ module load ncarenv/23.09  
$ module load craype/2.7.23  
$ module load gcc/13.2.0  
$ module load ncarcompilers/1.0.0  
$ module load cray-mpich/8.1.27
```

Practical exercises

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```

Environment setup

As noted in the practice guide, you should **set up your environment every time you log in:**

If you've logged out of Derecho and would like a quick list of commands to set up your environment again after logging back in, you can copy and paste the following commands into your terminal:

```
module --force purge
module load ncarenv/23.09
module load craype/2.7.23
module load gcc/13.2.0
module load ncarcompilers/1.0.0
module load cray-mpich/8.1.27
module load parallel-netcdf/1.12.3
module load netcdf/4.9.2
module load conda
conda activate npl
export PYTHONPATH=/glade/campaign/mmm/wmr/mpas_tutorial/python_scripts
module load ncview
export PATH=/glade/campaign/mmm/wmr/mpas_tutorial/metis/bin:${PATH}
module reload gcc/13.2.0
```

Asking questions

After the conclusion of the tutorial, if you encounter issues or have any questions, the forum might be a good place to discuss those:

<https://forum.mmm.ucar.edu/>