Introduction to practical sessions, and logistics







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

1:30 pm - 2:45 pm - Practical session with instructors2:45 pm - 3:00 pm - Practical session - break for instructors3:00 pm - 4:00 pm - Practical session with instructors

Instructors will monitor main room on Zoom for questions

- If you have a question, "raise your hand" or type your question in the chat
- An instructor will invite you to a breakout room to discuss
- Feel free to come and go as you need



Cheyenne

The practical sessions of this tutorial will be run on Cheyenne



145,152 processor cores	2.3-GHz Intel Xeon E5-2697V4 (Broadwell) processors 16 flops per clock
4,032 computation nodes	Dual-socket nodes, 18 cores per socket
6 login nodes	Dual-socket nodes, 18 cores per socket 256 GB memory/node
313 TB total system memory	64 GB/node on 3,168 nodes, DDR4-2400 128 GB/node on 864 nodes, DDR4-2400
Mellanox EDR InfiniBand high-speed interconnect	Partial 9D Enhanced Hypercube single-plane interconnect topology Bandwidth: 25 GBps bidirectional per link Latency: MPI ping-pong < 1 μ s; hardware link 130 ns
3 times Yellowstone computational capacity	Comparison based on the relative performance of the CISL High Performance Computing Benchmarks run on each system.
> 3.5 times Yellowstone peak performance	5.34 peak petaflops (vs. 1.504)



Cheyenne

The practical sessions of this tutorial will be run on Cheyenne



Don't forget to enable X11 forwarding when connecting!

ssh -X <username>@cheyenne.ucar.edu

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

ssh -Y <username>@cheyenne.ucar.edu



Queues

During scheduled practice sessions (1:30 pm – 4:00 pm MDT) we have 50 nodes reserved for this tutorial

- Submit jobs to the S9905760 queue
- This is the default in the job scripts that we provide

Since we have 42 participants and only 50 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 regular queue instead
- All that you need to do is to uncomment one line and comment another in your job script



```
#!/usr/bin/env bash
                                Job scripts are
                                submitted to the
#PBS -N 120km
                                queuing system
#PBS -A UMMM0002
                                with qsub
#PBS -1 walltime=01:00:00
#PBS -q S9905760
##PBS -q regular
#PBS −j oe
#PBS -k eod
#PBS -l select=1:ncpus=36:mpiprocs=36
export MPI TYPE DEPTH=16
mpiexec mpt ./atmosphere model
```



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

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

But...

The information shown by qstat (without options that shall not be mentioned) 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 SUSER to see running and completed jobs.



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

qcmd -A UMMM0002 -- ./init_atmosphere_model

By default, jobs run with qcmd go through the regular queue

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

qcmd -A UMMM0002 -q S9905760 -- \
 ./init_atmosphere_model



All of our computing will be under the UMMM0002 project

We have 50,000 core-hours

- Divided evenly between 42 participants -> everyone has about 1,200 core-hours
- One Cheyenne node for one wallclock hour = 36 core-hours
- You can continue to work with MPAS-Atmosphere on your own time

The UMMM0002 project is available until 31 May

Use the UMMM0002 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!



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

https://www2.mmm.ucar.edu/projects/mpas/tutorial/Virtual2023/



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 <u>here</u> 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 <u>Tutorial</u> <u>Agenda</u>, 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



If you have questions or encounter issues during this tutorial, we can answer those on Zoom during our scheduled practical sessions.

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/