Introduction to practical sessions, and logistics

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MPAS
Model for Prediction Across Scales

Generalities

We have a total of about 7 hours of scheduled practical sessions for the MPAS-A part of this course

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

Derecho

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

Derecho

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
```

Job scripts

```
#!/bin/bash

#PBS -A UMMM0012
#PBS -N jobname
#PBS -q main
#PBS -l job_priority=premium
#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`

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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.

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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 UMMM0012 -- ./init_atmosphere_model
```

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

```
qcmd -A UMMM0012 -l job_priority=premium -- \
                    ./init_atmosphere_model
```

Resource allocations

All of our computing will be under the `UMMM0012` project

We have 50,000 core-hours

- Divided evenly between 25 participants -> everyone has about 2000 core-hours
- One Derecho node for one wallclock hour = 128 core-hours
- You can continue to work with MPAS-Atmosphere on your own time

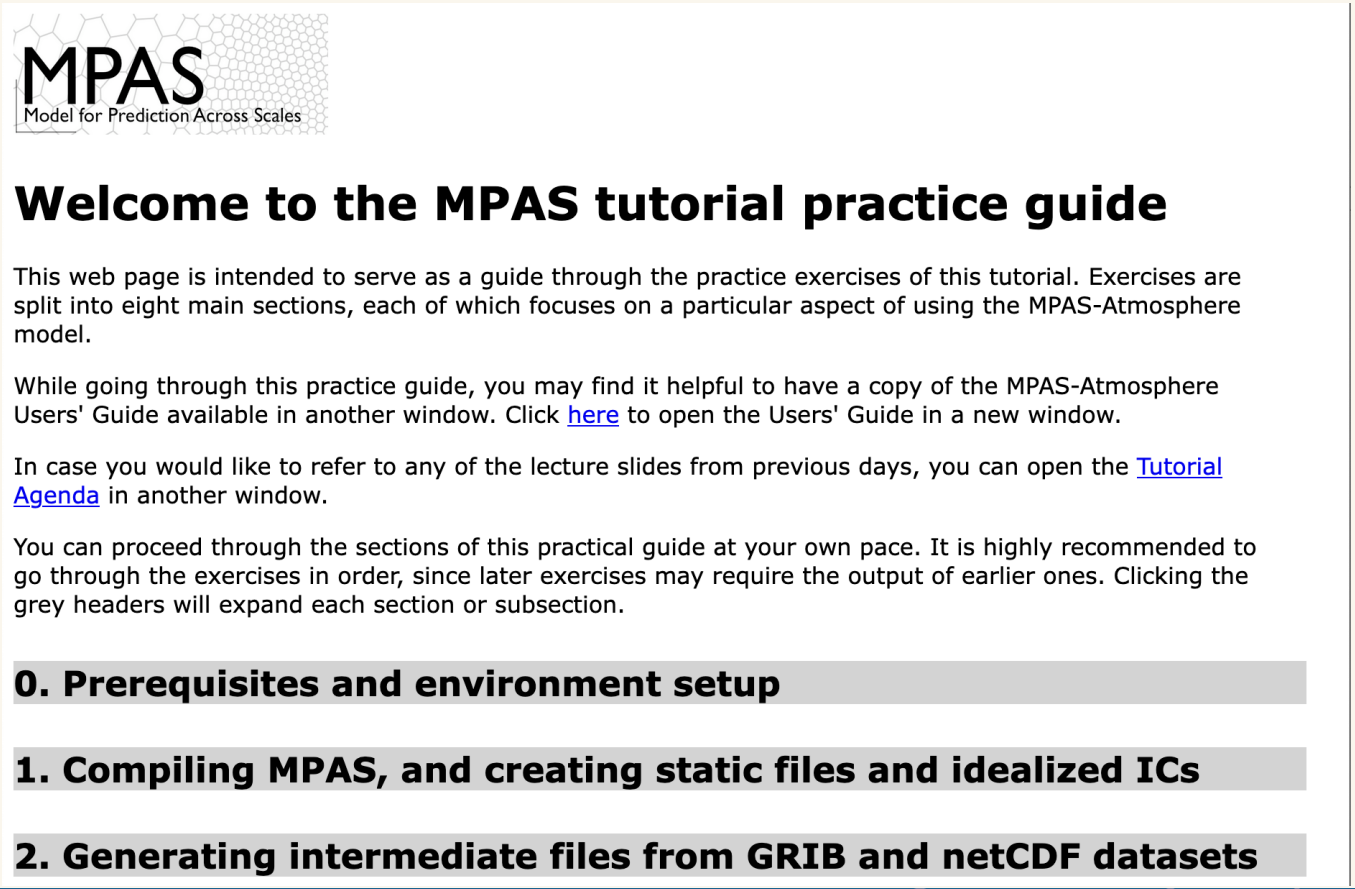
The `UMMM0012` project is available until the end of June

Use the UMMM0012 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/StAndrews2025/



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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 eight 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 lecture slides from previous days, you can open the Tutorial Agenda 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. Generating intermediate files from GRIB and netCDF datasets

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Practical exercises

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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 subsequer
to prepare our environment. Firstly, we will purge all lo
point (with no modules loaded); then, we will load seve
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
```

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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/