MPAS-A System Requirements and Installation

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Motivation

Can I run MPAS-A on my computer?



Left: A Cray-1 supercomputer.

(Trivia: In 1977, the National Center for Atmospheric Research acquired a Cray-1, serial number 3.)

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If so, how do I install MPAS-A on it?





Motivation

MPAS-Atmosphere is distributed as source code

No pre-compiled model or binary distribution!



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

Compiling MPAS, and creating static files and idealized ICs

- 2. Generating intermediate files from GRIB and netCDF datasets
- 3. Creating real-data ICs and running a simulation
- 4. Running MPAS with variable resolution, and basic visualization
- 5. Running limited-area simulations

The first practical exercise will involve compiling your own copy of MPAS-A on Derecho.

Compiling MPAS-A is probably also the first step on your own machine!



System Requirements

What system attributes need to be considered?

<u>Hardware</u>

Processor(s)

Memory (RAM)

<u>Software</u>

Operating system

Compilers

Libraries

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MPAS-A itself does not require any particular kind of processors

Consider this (not actual MPAS-A) Fortran code:

```
! Compute temperature in K from temperature in deg. C
do i = 1, n
   tk(i) = tc(i) + 273.15
end do
```

Nothing here is processor-specific!

Any of the following processor architectures should be fine:

• ARM

- POWER
- Various GPU architectures!

- x86_64
- RISC-V



If you are patient enough, a single processor is all that you need.



In practice, using multiple processors is critical for achieving useful simulation rates





The memory requirement is a function of:

- 1. The number of grid columns in the mesh (simulation domain)
- 2. Choice of physics schemes / suite
- 3. The number of MPI tasks
- 4. The number of I/O tasks
- A reasonable starting point:
 - 0.4 MB / grid column

(for the default MPAS-A configuration with 55 layers, 'mesoscale_reference' physics suite, single precision).





Generally, a UNIX-like OS is needed

- *E.g.*, Linux, *BSD, macOS, AIX
- Also need make, grep, awk, sed, cat, ranlib/libtool, git, etc.

Fortran 2008, C, and C++ compilers

• E.g., GCC, Intel oneAPI, NVIDIA NVHPC, Cray, NAG

Libraries

- MPI (OpenMPI, MPICH, etc.)
- Parallel-NetCDF





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Example systems that run MPAS-A





Working under the assumption that we have a system that meets the basic requirements, we can then ask:

How do I get a copy of the source code?

If you are working on a machine with the <u>git</u> command-line tools and internet access, this can be done in <u>under 10 seconds</u>!



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The MPAS-Atmosphere code is developed on and distributed through a GitHub repository: https://github.com/MPAS-Dev/MPAS-Model

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From the command-line, the following should be sufficient:

git clone https://github.com/MPAS-Dev/MPAS-Model.git

Cloning the repository should take about 10 seconds or less...

• (I timed this at home, and it took 5.65 s)

```
$ git clone https://github.com/MPAS-Dev/MPAS-Model.git
Cloning into 'MPAS-Model'...
remote: Enumerating objects: 71, done.
remote: Counting objects: 100% (71/71), done.
remote: Compressing objects: 100% (47/47), done.
remote: Total 46608 (delta 38), reused 42 (delta 23), pack-reused
46537
Receiving objects: 100% (46608/46608), 19.65 MiB | 2.57 MiB/s,
done.
Resolving deltas: 100% (35848/35848), done.
```



As a new user, you may like to:

- Register this is completely optional, but helpful for us to gauge how widely used MPAS-A is, justify development and support resources, etc.
- Join the mpas-atmosphere-users mailing list Very low traffic, mostly announcements of tutorials, workshops, and code releases

Links for the above are available from the MPAS-A website: https://www2.mmm.ucar.edu/projects/mpas/site/





Optional: Registration and Mailing Lists







Cloning the MPAS-Model repository provides all MPAS models, not just MPAS-Atmosphere

- All models share a common set of infrastructure modules
- Each MPAS model is implemented as a "core" that lives in its own sub-directory
- The MPAS models are not coupled in this repository!
- You must select which "core" to compile





Model Organization



- The init_atmosphere core is responsible for
 - Interpolating static fields to the mesh
 - Generating a vertical grid
 - Horizontally and vertically interpolating meteorological data to the 3-d grid
- The **atmosphere** core is the model itself; integrates forward in time from initial state







There is no "configuration" step for MPAS

• All build flags are either set in the top-level Makefile or on the command-line

General MPAS build command:

\$ make target CORE=core <options>

target can be either clean or gnu intel nvhpc llvm ... plus a few others...

For MPAS-Atmosphere, core may be

atmosphere init_atmosphere

<options> can be any of

DEBUG=true AUTOCLEAN=true PRECISION=double OPENMP=true OPENACC=true





Historically, building both the init_atmosphere and atmosphere cores involved:

make gnu CORE=init_atmosphere (build init_atmosphere_model)

make gnu CORE=atmosphere (build atmosphere model)

By default, MPAS cores are built with single-precisi

Beginning with MPAS v8.2.0, an intermediate "clean" step is no longer needed!

MPAS-Atmosphere can be built in double precision

- Add PRECISION=double to build commands for double-precisoin executables
- Execution time is slower compared with single-precision
- Output files approximately twice as large



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Typical build of both the init_atmosphere and atmosphere cores involves:

make -j8 gnu CORE=init_atmosphere (build init_atmosphere_model)

make -j8 gnu CORE=atmosphere (build atmosphere model)

The -j8 option causes make to use up to 8 jobs (simultaneous commands) to compile the code and can reduce build times; values other than 8 can be used.

By default, MPAS cores are built with single-precision floating-point variables

MPAS-Atmosphere can be built in double precision

- Add PRECISION=double to build commands for double-precisoin executables
- Execution time is slower compared with single-precision
- Output files approximately twice as large



- Ensure that you have a system running a UNIX-like operating system with the usual commands: make, awk, sed, grep, *git*, etc.
 - Available memory dictates maximum number of grid cells
- Ensure that you have modern Fortran, C, and C++ compilers
- Install supporting libraries (MPI, Parallel-NetCDF)
- Obtain the MPAS-Model source code with *git clone*
- Compile the *init_atmosphere* and *atmosphere* cores

