User Guide for using the Model for Prediction Across Scales (MPAS) with the Community Multiscale Air Quality (CMAQ) model.

USEPA

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WARNING: The version of CMAQ described in this document is for preliminary testing and evaluation and is not intended for regulatory use. Familiarity with CMAQ and either WRF or MPAS is strongly recommended

This user guide is a living document and will be updated as needed. Ensure that you are viewing the latest version of this user guide when attempting to use MPAS-CMAQ.

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1 Overview

The Model for Prediction Across Scales (MPAS) is a global model that can be used be used for simulations on global and regional domains, from coarse to convective-resolving resolutions. The Community Multiscale Air Quality (CMAQ) model is an air quality model that has long been used for simulations on limited area domains. The two models have been coupled to create a new system that can be used for global air quality simulations with resolution refinement over regions of interest.

A description and evaluation of the MPAS-CMAQ system using the CB6r5m chemical mechanism is available in Wong et al. (2024).

2 Downloading and Compiling

2.0.1 CMAQ

The CMAQ code that supports copuling with MPAS is available from the USEPA's GitHub repository. To get started, clone the repository.

```
git clone -b MPAS_CMAQ https://github.com/USEPA/CMAQ.git CMAQ_REPO
cd CMAQ_REPO
```

Note that the clone command specifies the MPAS_CMAQ branch of the CMAQ repository. Check the README.md for recent updates to this branch. In bldit_project.csh, modify the variable $CMAQ_HOME to identify the folder that you would like to build CMAQ in. For example:

```
set CMAQ_HOME = [your_install_path]/CMAQ_5.5
```

Now execute the script and navigate to the scripts directory.

```
./bldit_project.csh
cd [your_install_path]/CMAQ_v5.5/CCTM/scripts
```

The bldit_cctm.csh script has already been modified to uncomment the line:

```
setenv build_mpas_cmaq
```

This option is new for the BLDMAKE program, and will aggregate the required CMAQ code into a build directory. It will also prepare the Makefile. CMAQ compiliation occurs later when compiling the MPAS code.

A compiler is required for the bldmake program. This is set in config_cmaq.csh as myFC. Make sure that there is a value for mpiifort (intel) or mpifort (pgi/gcc). For example, you can check the location for intel with:

```
which mpiifort
```

With this variable set you can run the build script.

```
./bldit_cctm.csh [compiler]
```

Successful execution of this script creates a BLD* directory with CMAQ code and a Makefile. The CMAQ code is now ready to be compiled as part of the MPAS model.

2.0.2 MPAS

We are providing a modified version of MPAS based on the MPAS 7.0 release. The modifications are described by Gilliam et al. (2021) and include Four-Dimensional Data Assimilation (FDDA, (Bullock Jr. et al., 2018)), ACM2 boundary layer physics, PX land surface model, and more.

To download the modified MPAS code, clone the repository from the following link:

```
git clone -b MPAS7.0 git@github.com:USEPA/CMAQ.git MPAS
cd MPAS
```

Notice that this checks out a branch called MPAS7.0. We are working to make CMAQ stable with the current release of MPAS, which is version 8.2.2 at the time of writing. Version 8.2.2 of MPAS does not require PIO to be compiled, which will eventually simplify its use with CMAQ. This document will be updated when support for MPAS version 8.2.2 is available.

Follow the steps to build the MPAS code described in Chapter 3 of the MPAS user guide. This involves installing the prerequisite NetCDF, parallel-NetCDF, and PIO2 libraries.

The CMAQ build directory from the previous section needs to be copied to the MPAS src/core_atmosphere directory and named "cmaq."

```
cp -r [.../scripts/BLD_xxx] [.../MPAS/src/core_atmosphere/cmaq]
```

In addition to EPA physics and FDDA changes, this repository includes MPAS files that have been modified to support CMAQ coupling. These include:

```
core_atmosphere/Makefile
core_atmosphere/dynamics/Makefile
core_atmosphere/dynamics/mpas_atm_time_integration.F
core_atmosphere/Registry.xml
```

The MPAS code is now ready to be compiled with the CMAQ code.

```
make [compiler] CORE=atmosphere USE_PIO2=true
```

This will create an executable called atmosphere_model that runs both MPAS and CMAQ. We are providing MPAS inputs for the configuration described in the Domains and Inputs section. Users are not required to compile init_atmosphere or create initial conditions and static files for MPAS.

2.0.3 Input Data

Emissions, meteorological inputs, and other CMAQ files are available in an Amazon Web Services (AWS) S3 bucket. The bucket includes MPAS and CMAQ input files needed to simulate the year 2017. MPAS and CMAQ inputs are summarized by a Dataverse entry can be downloaded using the AWS command line interface (CLI). For MPAS inputs:

```
aws s3 --no-sign-request cp --recursive
        s3://mpas-cmaq/120_uniform/mpas_inputs/ .
```

These MPAS files are required for the provided test cases on the 120 km mesh. They include the following:

```
x1.40962.fdda.2017.nc          - FDDA targets for u,v,T, and q
restart.2017-01-01_00.00.00.nc - Restart file with spin up from
                                 simulation described in Wong et al. (2024)
x1.40962.init.20170101.nc      - Initial condition for optional
                                 fresh initialization
x1.40962.soilndg.2017.nc       - Soil nudging targets for PX LSM
x1.40962.sfc_update.2017.nc    - Surface fields for MPAS
x1.40962.ozone.2017.nc         - Stratospheric ozone from CAMS reanalysis
```

The largest file is the full year of 3-D FDDA targets, at 112 Gb. CMAQ inputs for the supplied test case can be downloaded using the command:

```
aws s3 --no-sign-request cp --recursive
  s3://mpas-cmaq/120_uniform/cmaq_inputs/other/ .
```

The files downloaded with this command include:

```
megan_input.nc             - Input for MEGAN BVOC emissioins
                             and BDSNP soil NO
omi_cmaq_2017.dat          - OMI input data for photolysis
ocean_file_120_[month].nc  - Ocean file describing areas of OPEN and SURF
```

For emissions, a one-day benchmark and a full year are available as the bzip2 files one_day.tar.bz2 and 2017_full_year.tar.bz2. To download a single day of emissions data, use the command:

```
aws s3 --no-sign-request
   cp s3://mpas-cmaq/120_uniform/cmaq_inputs/emissions/one_day.tar.bz2 .
```

or for the full year:

```
aws s3 --no-sign-request cp
  s3://mpas-cmaq/120_uniform/cmaq_inputs/emissions/2017_120km.tar.bz2 .
```

The full year of emissions is 2.5 Tb when uncompressed and will take an extended time to unzip.

It may be helpful aggregate all input files into a common directory by linking to their full paths.

```
mkdir links
cd links
ln -s [full/path/to/mpas_inputs/*] .
ln -s [full/path/to/cmaq_inputs/emissions/one_day/*] .
ln -s [full/path/to//cmaq_inputs/other/*] .
```

This will simplify the run script.

3 Configuring and Running

3.1 Domains and Inputs

For the initial release of MPAS-CMAQ we are providing MPAS and CMAQ inputs on a uniform 120 km resolution mesh for the year 2017. We may make other inputs available depending on user interest. Other meshes that we have developed include a 92-25 km mesh, a 60-12 km mesh, and 60-12-4 km multistage refinement meshes. EPA is developing software that can be used to create customized emissions, CMAQ inputs, and meshes. This document will be updated as those software packages become publicly available.

3.2 Model Configuration

Not all CMAQ model options are available at this time. For example, there is no support for the Integrated Source Apportionment Method (ISAM) or the Decoupled Direct Method (DDM). The Process Analysis (PA) and budget tools are not disabled at this time. ELMO may not work as in the standard CMAQ model.

The benchmark configuration is set up with the recommended physics and chemistry options used by Wong et al. (2024). This includes inline emissions from the Model for Emissions of Gases and Aersols from Nature (MEGAN), windblown

dust, and sea spray. The Community Regional Atmospheric Chemistry Multiphase Mechanism (CRACMM version 2) does not yet include a representation of marine halogen chemistry. The lack of halogen chemisry results in higher ozone concentrations relative to CB6r5m, especially over the ocean. See the supplied run script for a full accounting of pre-configured CMAQ and MPAS options.

3.3 Models I/O (MIO)

The version of CMAQ that can be coupled with MPAS uses a new I/O system called MIO. This I/O code is in the CCTM/src/mio directory and is compiled along with MPAS and CMAQ. There is no need to compile a separate I/O API library for this CMAQ configuration.

MPAS-CMAQ outputs instantaneous concentrations of CMAQ's chemical species to the MPAS history file (history.YYYY-MM-DD.nc). The history file also contains all MPAS output. All other CMAQ output, including from the Detailed Emissions Scaling, Isolation, and Diagnostic (DESID) module, is handled by Models I/O (MIO).

Changing the input or output files requires modifying the mio_file_info text file. Two text files are located in the MPAS/run directory:

```
file_input_c2_bdsnp.txt
```

and

```
file_input_c2_bdsnp_no_soilinp.txt
```

The first file is for model restarts where MEGAN's restart files (SOILINP and BDSNPINP) from the previous day are available. The seccond text file is for when these files are not available. The strucutre of the mio_file_info files is:

```
in [number of input files] out [number of output files]
[list of input files]
[output file name]
[output file variable description]
[output file variable description]
[output file variable description]
```

In order to exclude an emission file from a simulation, then, the user must modify the mio_file_info text file to update the [number of input files] and remove the emission file from the list of input files.
We are releasing MIO version 1.0 with CMAQ 5.5 for use with MPAS. Future versions of MIO are likely to eliminate the requirement that users modify this text file in order to describe CMAQ input and output.

Further information about MIO can be found in Wong et al. (2024).

3.4 Run Script

An example run script for the prescribed configuration is located in the MPAS directory at MPAS/run/run.csh. Users will need to modify the header information in this run script as described by the commments within the script. The header of run.csh is set up for a high performance computing system using the Slurm Workload Manager. This section will need to be modified if on a system that is using an alternative job manager (e.g., Sun Grid or PBS). The input_path and MPAS_path_output variables will also need to be updated to direct the script to your input and output directories, respectively.

When executed, the run script will create the MPAS_path_output directory and copy or link the required inputs to the directory. Log files include the CTM_LOG_XXX files that describe CMAQ output, and the log.atmosphere.0000 file that contains MPAS output. Errors may also be reported in the job log (for Slurm, run_%J.log) located in the run directory. At the end of a simulation day the MPAS and CMAQ log files will be moved to the directory:

```
$MPAS_path_output/YYYYMMDD
```

The benchmark configuration will create the following output files for the first day:

```
CCTM_SOILOUT_20170101.nc   - MEGANv3.2 restart
CCTM_BDSNPOUT_20170101.nc  - MEGANv3.2 restart
CCTM_BDSNPDIAG_20170101.nc - MEGANv3.2 diagnostic
history.2017-01-01.nc      - Hourly MPAS output and
                             CMAQ concentrations
CCTM_EMIS_DIAG_20170101.nc - Combined emissions
CCTM_OUT20170101.nc        - Wet/dry deposition and
                             some phot diag variables
```

Modify the START_DATE and END_DATE to continue the simulation beyond January 1st. This requires the full year of emissions described in the Input Data section.

4 Post processing

For the release of CMAQ version 5.5 the post processing utilities COMBINE and SITECMP do not support MPAS-style output. Support for this workflow will be added to the MPAS_CMAQ branch of the CMAQ repository as soon as possible. Future MPAS-CMAQ workflows may be less dependent on the COMBINE program, as the Explicit and Lumped Model Output (ELMO) module is able to carry out the species lumping necessary for most post processing.

The popular tool for quickly viewing the content of NetCDF files, "ncview," does support MPAS-style output. Software packages that readily support MPAS-style output include ncvis, developed by Paul A. Ullrich, and the Visual Environment for Rich Data Interpretation (VERDI), developed by EPA. Packages in common languages, such as python, NCL, and R can also be useful for plotting MPAS and MPAS-CMAQ output. Tools such as convert_mpas can be used to quickly remap output from the unstructured MPAS mesh to a structured grid, and may be useful for analysis or visualization. Note that some information may be lost when remapping.

5 Revision History

2 October 2024

Initial Version

References

Bullock Jr., O. R., Foroutan, H., Gilliam, R. C., and Herwehe, J. A.: Adding four-dimensional data assimilation by analysis nudging to the Model for Prediction Across Scales – Atmosphere (version 4.0), Geoscientific Model Development, 11, 2897–2922, https://doi.org/10.5194/gmd-11-2897-2018, 2018.

Gilliam, R. C., Herwehe, J. A., Bullock Jr, O. R., Pleim, J. E., Ran, L., Campbell, P. C., and Foroutan, H.: Establishing the Suitability of the Model for Prediction Across Scales for Global Retrospective Air Quality Modeling, Journal of Geophysical Research: Atmospheres, 126, e2020JD033 588, https://doi.org/https://doi.org/10.1029/2020JD033588, e2020JD033588 2020JD033588, 2021.

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