

# **MDTF Getting Started Guide**

Release 3.0 beta 2

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**CHAPTER** 

**ONE** 

## **GETTING STARTED**

## 1.1 Overview

Welcome! In this section we'll describe what the Model Diagnostics Task Force (MDTF) framework is, how it works, and how you can contribute your own diagnostic scripts.

## 1.1.1 Purpose

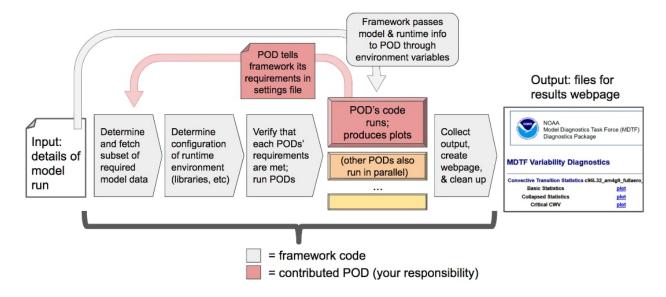
The scientific motivation and content behind the framework was described in E. D. Maloney et al. (2019): Process-Oriented Evaluation of Climate and Weather Forecasting Models. BAMS, 100 (9), 1665–1686, doi:10.1175/BAMS-D-18-0042.1<sup>1</sup>.

Also see the section of this site devoted to documentation of individual diagnostics.

<sup>&</sup>lt;sup>1</sup> https://doi.org/10.1175/BAMS-D-18-0042.1

#### 1.1.2 Framework operation

The design goal of the MDTF framework is to provide a portable and adaptable means to run processoriented diagnostic scripts, abbreviated as PODs below. By "portability," we mean the ideal of "run once, run anywhere": the purpose of the framework is to automate retrieval of model data from different local or remote sources, and transform that data into a layout (field names, variable units, etc.) your script expects. This will empower your analysis to be run by a wider range of researchers on a wider range of models.



As shown in the figure above, the MDTF framework itself performs common data management and support tasks (gray boxes) before and after the individual POD scripts are run. The PODs (colored boxes) are developed by different research groups and run independently of one another. Each POD takes as input

- 1. requested variables from the model run, along with
- 2. any required observational or supporting data, performs an analysis, and produces
- 3. a set of figures which are presented to the user in a series of .html files.

We do not include or require a mechanism for publishing these webpages on the internet; html is merely used as a convenient way to present a multimedia report to the user.

#### 1.1.3 Getting started for users

The rest of the documentation in this section describes next steps for end users of the framework:

- We provide instructions on how to download and install (page 3) the framework and run it on sample model data.
- We describe the most common configuration options (page 9) for running the framework on your own model data. Also see the full list of command-line options.
- If you encounter a bug, check the GitHub issue tracker<sup>2</sup>.

 $<sup>^2\</sup> https://github.com/NOAA-GFDL/MDTF-diagnostics/issues$ 

## 1.1.4 Getting started for POD developers

Information for researchers wishing to contribute a POD to the framework is provided in the Developer section; consult the quickstart guide for an overview and the checklist of items needed for submitting your POD.

The framework is designed to require minimal changes to existing analysis scripts. We recommend that developers of new PODs start independently of the framework and adapt it for the framework's use once it's fully debugged. As summarized in the figure above, the changes needed to convert an existing analysis script for use in the framework are:

- Provide a settings file which tells the framework what it needs to do: what languages and libraries your code need to run, and what model data your code takes as input.
- Adapt your code to load data files from locations set in unix shell environment variables (we use this as a language-independent way for the framework to communicate information to the POD).
- Provide a template web page which links to, and briefly describes, the plots generated by the script.

## 1.2 Quickstart installation instructions

This section provides basic directions for downloading, installing and running a test of the Model Diagnostics Task Force (MDTF) Process-Oriented Diagnostics package using sample model data. The current MDTF package has been tested on UNIX/LINUX, Mac OS, and Windows Subsystem for Linux.

Throughout this document, % indicates the UNIX/LINUX command line prompt and is followed by commands to be executed in a terminal in fixed-width font, and \$ indicates strings to be substituted, e.g., the string \$CODE\_ROOT below should be substituted by the actual path to the MDTF-diagnostics directory. While the package contains quite a few scripts, the most relevant for present purposes are:

- conda\_env\_setup.sh: automated script for installing necessary Conda environments.
- default\_tests.jsonc: configuration file for running the framework.

#### 1.2.1 Summary of steps for running the package

You will need to download a) the source code, b) digested observational data, and c) two sets of sample model data (Section 1.2.2). Afterwards, we describe how to install necessary Conda environments and languages (Section 1.2.3) and run the framework on the default test case (Section 1.2.5 and Section 1.2.5).

Summary of steps for installing the framework

You will need to download the source code, digested observational data, and sample model data (Section 1.2.2). Afterwards, we describe how to install software dependencies using the conda<sup>3</sup> package manager (Section 1.2.3, Section 1.2.5) and run the framework on sample model data (Section 1.2.5 and Section 1.2.5).

<sup>3</sup> https://docs.conda.io/en/latest/

#### 1.2.2 Obtaining the code

The official repo for the MDTF code is hosted at the GFDL GitHub account<sup>4</sup>. We recommend that end users download and test the latest official release<sup>5</sup>.

To install the MDTF framework, create a directory named mdtf and unzip the code downloaded from the release page<sup>6</sup> there. This will create a directory titled MDTF-diagnostics-3.0-beta.2 containing the files listed on the GitHub page. Below we refer to this MDTF-diagnostics directory as \$CODE\_ROOT. It contains the following subdirectories:

- diagnostics/: directory containing source code and documentation of individual PODs.
- doc/: directory containing documentation (a local mirror of the documentation site).
- src/: source code of the framework itself.
- tests/: unit tests for the framework.

For advanced users interested in keeping more up-to-date on project development and contributing feedback, the main branch contains features that haven't yet been incorporated into an official release, which are less stable or thoroughly tested.

For POD developers, the develop branch is the "beta test" version of the framework. POD developers should begin by locally cloning the repo and checking out this branch, as described in ref-dev-git-intro.

#### 1.2.3 Obtaining supporting data

Supporting observational data and sample model data are available via anonymous FTP at ftp://ftp.cgd.ucar. edu/archive/mdtf. The observational data is required for the PODs' operation, while the sample model data is provided for default test/demonstration purposes. The files most relevant for package installation and default tests are:

- Digested observational data (159 Mb): MDTF\_v2.1.a.obs\_data.tar<sup>7</sup>.
- NCAR-CESM-CAM sample data (12.3 Gb): model.QBOi.EXP1.AMIP.001.tar<sup>8</sup>.
- NOAA-GFDL-CM4 sample data (4.8 Gb): model.GFDL.CM4.c96L32.am4g10r8.tar<sup>9</sup>.

Note that the above paths are symlinks to the most recent versions of the data and will be reported as zero bytes in an FTP client.

Download these three files and extract the contents in the following hierarchy under the mdtf directory:

```
mdtf
   MDTF-diagnostics
   inputdata
   model ( = $MODEL_DATA_ROOT)
```

(continues on next page)

<sup>&</sup>lt;sup>4</sup> https://github.com/NOAA-GFDL/MDTF-diagnostics

<sup>&</sup>lt;sup>5</sup> https://github.com/NOAA-GFDL/MDTF-diagnostics/releases/tag/v3.0-beta.1

<sup>&</sup>lt;sup>6</sup> https://github.com/NOAA-GFDL/MDTF-diagnostics/releases/tag/v3.0-beta.2

<sup>&</sup>lt;sup>7</sup> ftp://ftp.cgd.ucar.edu/archive/mdtf/MDTF\_v2.1.a.obs\_data.tar

<sup>8</sup> ftp://ftp.cgd.ucar.edu/archive/mdtf/model.QBOi.EXP1.AMIP.001.tar

<sup>&</sup>lt;sup>9</sup> ftp://ftp.cgd.ucar.edu/archive/mdtf/model.GFDL.CM4.c96L32.am4g10r8.tar

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```
GFDL.CM4.c96L32.am4g10r8
       day
           GFDL.CM4.c96L32.am4g10r8.precip.day.nc
           (... other .nc files )
   QBOi.EXP1.AMIP.001
       1hr
           QBOi.EXP1.AMIP.001.PRECT.1hr.nc
           (... other .nc files )
       3hr
           QBOi.EXP1.AMIP.001.PRECT.3hr.nc
       day
           QBOi.EXP1.AMIP.001.FLUT.day.nc
           (... other .nc files )
       mon
           QBOi.EXP1.AMIP.001.PS.mon.nc
            (... other .nc files )
obs data ( = $OBS DATA ROOT)
    (... supporting data for individual PODs )
```

The default test case uses the QBOi.EXP1.AMIP.001 sample. The GFDL.CM4.c96L32.am4g10r8 sample is only for testing the MJO Propagation and Amplitude POD. Note that mdtf now contains both MDTF-diagnostics and inputdata directories.

You can put the observational data and model output in different locations (e.g., for space reasons) by changing the values of OBS\_DATA\_ROOT and MODEL\_DATA\_ROOT as described below in Section 1.2.5.

#### Install the conda package manager, if needed

For users unfamiliar with Conda, :numref:`ref-conda-install` can be skipped if Conda has been installed, but :numref:`ref-conda-env-install` CANNOT be skipped regardless.

The MDTF framework code is written in Python 2.7, but supports running PODs written in a variety of scripting languages and combinations of libraries. We use Conda<sup>10</sup>, a free, open-source package manager to install and manage these dependencies. Conda is one component of the Miniconda<sup>11</sup> and Anaconda<sup>12</sup> python distribution, so having Miniconda/Anaconda is sufficient but not necessary.

For maximum portability and ease of installation, we recommend that all users manage dependencies through Conda using the provided script src/conda/conda\_env\_setup.sh, even if they have independent installations of the required languages. A complete installation of all dependencies will take roughly 5 Gb, less if you've already installed some of the dependencies through Conda. The location of this installation can be changed with the \$CONDA ENV DIR setting described below.

If these space requirements are prohibitive, we provide an alternate method of operation which makes no use of conda and relies on the user to install external dependencies, at the expense of portability. This is documented in a separate section.

<sup>10</sup> https://docs.conda.io/en/latest/

<sup>11</sup> https://docs.conda.io/en/latest/miniconda.html

<sup>12</sup> https://www.anaconda.com/

#### 1.2.4 Conda installation

Here we are checking that the Conda command is available on your system. We recommend doing this via Miniconda or Anaconda installation. You can proceed directly to section 2.2 if Conda is already installed.

- To determine if conda is installed, run % conda --version as the user who will be using the framework. The framework has been tested against versions of conda >= 4.7.5.
- If the command doesn't return anything, i.e., you do not have a pre-existing Conda on your system, we recommend using the Miniconda installer available here<sup>13</sup>. Any version of Miniconda/Anaconda (2 or 3) released after June 2019 will work. Installation instructions here<sup>14</sup>.
- Toward the end of the installation process, enter "yes" at "Do you wish the installer to initialize Miniconda2 by running conda init?" (or similar) prompt. This will allow the installer to add the Conda path to the user's shell login script (e.g., ~/.bashrc or ~/.cshrc).
- Restart the terminal to reload the updated shell login script.

The framework's environments will co-exist with an existing Miniconda/Anaconda installation. Do not reinstall Miniconda/Anaconda if it's already installed for the user who will be running the framework: the installer will break the existing installation (if it's not managed with, e.g., environment modules.)

#### 1.2.5 Framework-specific environment installation

Here we set up the necessary environments needed for running the framework and individual PODs via the provided script. These are sometimes referred to as "Conda environments" conventionally.

After making sure that Conda is available, run % conda info --base as the user who will be using the framework to determine the location of your Conda installation. This path will be referred to as \$CONDA\_ROOT below.

• If this path points to /usr/ or a subdirectory therein, we recommend having a separate Miniconda/Anaconda installation of your own following Conda installation (page 6).

Next, run

```
% cd $CODE_ROOT
% ./src/conda/conda_env_setup.sh --all --conda_root $CONDA_ROOT --env_dir $CONDA_ENV_DIR
```

to install all necessary environments (and create an executable; Location of the MDTF executable (page 8)), which takes ~10 min. The names of all framework-created environments begin with "\_MDTF", so as not to conflict with any other environments.

- Substitute the actual paths for \$CODE\_ROOT, \$CONDA\_ROOT, and \$CONDA\_ENV\_DIR.
- The --env\_dir flag allows you to put the program files in a designated location \$CONDA\_ENV\_DIR (for space reasons, or if you don't have write access). You can omit this flag, and the environments will be installed within \$CONDA\_ROOT/envs/ by default.

<sup>13</sup> https://docs.conda.io/en/latest/miniconda.html

<sup>14</sup> https://docs.conda.io/projects/conda/en/latest/user-guide/install/linux.html

- The --all flag makes the script install all environments prescribed by the YAML (.yml) files under src/conda/ (one YAML for one environment). You can install the environments selectively by using the --env flag instead. For instance, % ./src/conda/conda\_env\_setup.sh --env base --conda\_root \$CONDA\_ROOT --env\_dir \$CONDA\_ENV\_DIR will install the "\_MDTF\_base" environment prescribed by env\_base.yml, and so on. With --env, the current script can install one environment at a time. Repeat the command for multiple environments.
- Note that \_MDTF\_base is mandatory for the framework's operation, and the other environments are optional, see Framework interaction with Conda environments (page 8).

After installing the framework-specific Conda environments, you shouldn't manually alter them (i.e., never run conda update on them). To update the environments after updating the framework code, re-run the above commands. These environments can be uninstalled by simply deleting "\_MDTF" directories under \$CONDA\_ENV\_DIR (or \$CONDA\_ROOT/envs/ for default setting).

#### Configure framework paths

The MDTF framework supports setting configuration options in a file as well as on the command line. An example of the configuration file format is provided at src/default\_tests.jsonc<sup>15</sup>. We recommend configuring the following settings by editing a copy of this file:

src/default\_tests.jsonc is a template/example for configuration options that will be passed to the executable as an input. Open it in an editor (we recommend working on a copy). The following adjustments
are necessary before running the framework:

- If you've saved the supporting data in the directory structure described in Obtaining supporting data (page 4), the default values for OBS\_DATA\_ROOT and MODEL\_DATA\_ROOT pointing to mdtf/inputdata/obs\_data/ and mdtf/inputdata/model/ will be correct. If you put the data in a different location, these values should be changed accordingly.
- OUTPUT\_DIR should be set to the location you want the output files to be written to (default: mdtf/wkdir/; will be created by the framework). The output of each run of the framework will be saved in a different subdirectory in this location.
- conda\_root should be set to the value of \$CONDA\_ROOT used above in Framework-specific environment installation (page 6).
- If you specified a custom environment location with \$CONDA\_ENV\_DIR, set conda\_env\_root to that value; otherwise, leave it blank.

We recommend using absolute paths in default\_tests.jsonc, but relative paths are also allowed and should be relative to \$CODE\_ROOT.

<sup>&</sup>lt;sup>15</sup> https://github.com/NOAA-GFDL/MDTF-diagnostics/blob/main/src/default\_tests.jsonc

#### Run the MDTF framework on sample data

#### 1.2.6 Location of the MDTF executable

The setup script (Framework-specific environment installation (page 6)) will have created an executable at \$CODE\_ROOT/mdtf which sets the correct Conda environments before running the framework and individual PODs. To test the installation, % \$CODE\_ROOT/mdtf --help will print help text on the command-line options. Note that, if your current working directory is \$CODE\_ROOT, you will need to run % ./mdtf --help.

For interested users, the mdtf executable is also a script, which calls src/conda/conda\_init.sh and src/mdtf.py.

## 1.2.7 Run the framework on sample data

If you've installed the Conda environments using the --all flag (Framework-specific environment installation (page 6)), you can now run the framework on the CESM sample model data:

```
% cd $CODE_ROOT
% ./mdtf -f src/default_tests.jsonc
```

Run time may be 10-20 minutes, depending on your system.

- If you edited/renamed default\_tests.jsonc, pass that file instead.
- The output files for this test case will be written to \$OUTPUT\_DIR/QBOi.EXP1.AMIP. 001\_1977\_1981. When the framework is finished, open \$OUTPUT\_DIR/QBOi.EXP1.AMIP. 001\_1977\_1981/index.html in a web browser to view the output report.
- The above command will execute PODs included in pod\_list of default\_tests.jsonc. Skip-ping/adding certain PODs by uncommenting/commenting out the POD names (i.e., deleting/adding //). Note that entries in the list must be separated by ,. Check for missing or surplus , if you encounter an error (e.g., "ValueError: No closing quotation").
- Currently the framework only analyzes data from one model run at a time. To run the MJO\_prop\_amp POD on the GFDL.CM4.c96L32.am4g10r8 sample data, delete or comment out the section for QBOi.EXP1.AMIP.001 in "caselist" of default\_tests.jsonc, and uncomment the section for GFDL.CM4.c96L32.am4g10r8.

#### 1.2.8 Framework interaction with Conda environments

As just described in Run the framework on sample data (page 8), when you run the mdtf executable, among other things, it reads pod\_list in the configuration file and executes POD codes accordingly. For a POD included in the list (referred to as \$POD\_NAME):

1. The framework will first try to determine whether there is a Conda environment named \_MDTF\_\$POD\_NAME under \$CONDA\_ENV\_DIR. If yes, the framework will switch to this environment and run the POD.

- 2. If not, the framework will then look into the POD's settings.jsonc file in \$CODE\_ROOT/diagnostics/\$POD\_NAME.runtime\_requirements in the settings file specifies the programming language(s) adopted by the POD:
  - a). If purely Python, the framework will switch to MDTF python base and run the POD.
  - b). If NCL is used, then \_MDTF\_NCL\_base.

If you choose to selectively install Conda environments using the --env flag (Framework-specific environment installation (page 6)), remember to install all the environments needed for the PODs you're interested in, and that \_MDTF\_base is mandatory for the framework's operation.

- For instance, the minimal installation for running the EOF\_500hPa and convective\_transition\_diag PODs requres \_MDTF\_base (mandatory), \_MDTF\_NCL\_base (because of b), and \_MDTF\_convective\_transition\_diag (because of 1). These can be installed by passing base, NCL\_base, and convective\_transition\_diag to the --env flag one at a time (Framework-specific environment installation (page 6)).
- The framework defaults to running all available PODs, which is overridden by the pod\_list option in the src/default\_tests.jsonc configuration file. Individual PODs can be specified as a commadelimited list of POD names.

Consult the next section (page 9) for how to run the framework on your own data and configure general settings.

## 1.3 Framework configuration for user model data

In this section we describe how to run the framework with your own model data, and more configuration options than the test case described in Quickstart installation instructions (page 3).

The complete set of configuration options is described in ref\_cli, or by running % ./mdtf --help. All options can be specified as a command-line flag (e.g., --OUTPUT\_DIR) or as a JSON configuration input file of the form provided in src/default\_tests.jsonc<sup>16</sup>. We recommend using this file as a template, making copies and customizing it as needed.

Options given on the command line always take precedence over the input file. This is so you can store options that don't frequently change in the file (e.g., the input/output data paths) and use command-line flags to set only those options you want to change from run to run (e.g., the analysis period start and end years). In all cases, the complete set of option values used in each run of the framework will be included in the log file as part of the output, for reproducibility and provenance.

Summary of steps for running the framework on user data

- 1. Save or link model data files following the framework's filename convention.
- 2. Select the variable name convention used by the model.
- 3. Edit the configuration input file accordingly, then
- 4. Run the framework.

<sup>&</sup>lt;sup>16</sup> https://github.com/NOAA-GFDL/MDTF-diagnostics/blob/develop/src/default\_tests.jsonc

## 1.3.1 Adding your model data

Currently the framework is only able to run on model data in the form of NetCDF files on a locally mounted disk following a specific directory hierarchy and filename convention, with one variable per file. We hope to offer more flexibility in this area in the near future.

The directory/filename convention we use is

\$MODEL\_DATA\_ROOT/\$CASENAME/\$frequency/\$CASENAME.\$variable.\$frequency.nc,

where

- \$CASENAME is any string used to identify the model run (experiment) that generated the data,
- \$frequency is the frequency at which the data is sampled: one of 1hr, 3hr, 6hr, day, mon or year.
- \$variable is the name of the variable in your model's convention.

As an example, here's how the sample model data is organized:

```
inputdata
  model ( = $MODEL DATA ROOT)
      GFDL.CM4.c96L32.am4g10r8
          day
              GFDL.CM4.c96L32.am4g10r8.precip.day.nc
              (... other .nc files )
      QBOi.EXP1.AMIP.001
          1hr
              QBOi.EXP1.AMIP.001.PRECT.1hr.nc
              (... other .nc files )
          3hr
              QBOi.EXP1.AMIP.001.PRECT.3hr.nc
          day
              QBOi.EXP1.AMIP.001.FLUT.day.nc
              (... other .nc files )
              QBOi.EXP1.AMIP.001.PS.mon.nc
              (... other .nc files )
  obs_data ( = $OBS_DATA_ROOT)
       (... supporting data for individual PODs )
```

If your model data is available on a locally mounted disk, we recommend creating symlinks<sup>17</sup> that have the needed filenames and point to the data, rather than making copies of the files. For example,

will create a link to the file in the first argument that can be accessed normally:

<sup>&</sup>lt;sup>17</sup> https://en.wikipedia.org/wiki/Symbolic\_link

(continued from previous page)

```
GFDL.CM4.c96L32.am4g10r8
QB0i.EXP1.AMIP.001
my_new_experiment
   day
        my_new_experiment.pr.day.nc
```

#### 1.3.2 Select the model's variable name convention

The framework requires specifying a convention for variable names used in the model data. Currently recognized conventions are

- CMIP, for CF-compliant output produced as part of CMIP6;
- CESM, for the NCAR community earth system model<sup>18</sup>;
- AM4, for the NOAA-GFDL atmosphere model<sup>19</sup>;
- SPEAR, for the NOAA-GFDL seasonal model<sup>20</sup>.

We hope to offer support for the variable naming conventions of a wider range of models in the future. For the time being, please process output of models not on this list with CMOR<sup>21</sup> to make them CF-compliant.

Alternatively, the framework will load any lookup tables of the form src/fieldlist\_\$convention. jsonc and use them for variable name conversion. Users can add new files in this format to specify new conventions. For example, in src/fieldlist\_CESM.jsonc the line "pr\_var": "PRECT" means that the CESM name for the precipitation rate is PRECT (case sensitive). In addition, "pr\_conversion\_factor": 1000 specifies the conversion factor to CF standard units for this variable.

#### 1.3.3 Running the code on your data

After adding your model data to the directory hierarchy as described above, you can run the framework on that data using the following options. These can either be set in the caselist section of the configuration input file (see src/default\_tests.jsonc<sup>22</sup> for an example/template), or individually as command-line flags (e.g., --CASENAME my\_new\_experiment). Required settings are:

- CASENAME should be the same string used to label your model run.
- convention describes the variable naming convention your model uses, determined in the previous section.
- FIRSTYR and LASTYR specify the analysis period.
- model and experiment are recorded if given, but not currently used.

<sup>18</sup> http://www.cesm.ucar.edu/

<sup>19</sup> https://www.gfdl.noaa.gov/am4/

<sup>&</sup>lt;sup>20</sup> https://www.gfdl.noaa.gov/research\_highlight/spear-the-next-generation-gfdl-modeling-system-for-seasonal-to-multidecadal-prediction-and-

<sup>21</sup> https://cmor.llnl.gov/

<sup>&</sup>lt;sup>22</sup> https://github.com/NOAA-GFDL/MDTF-diagnostics/blob/develop/src/default\_tests.jsonc

When the framework is run, it determines whether the data each POD needs to run is present in the model data being provided. Specifically, the model must provide all variables needed by a POD at the required frequency. Consult the documentation for a POD to determine the data it requires.

If the framework can't find data requested by a POD, an error message will be logged in place of that POD's output that should help you diagnose the problem. We hope to add the ability to transform data (eg, to average daily data to monthly frequency) in order to simplify this process.

#### 1.3.4 Other framework settings

The paths to input and output data (described in Configure framework paths (page 7)) only need to be modified if the corresponding data is moved, or if you'd like to send output to a new location. Note that the framework doesn't retain default values for paths, so if you don't specify a configuration file, all required paths will need to be given explicitly on the command line.

Other relevant flags controlling the framework's output are:

- save\_ps: set to true to retain the vector .eps figures generated by PODs, in addition to the bitmap images linked to from the webpage.
- save\_nc: set to true to retain netcdf files of any data output at intermediate steps by PODs for further analysis.
- make\_variab\_tar: set to true to save the entire output directory as a .tar file, for archival or file transfer purposes.
- overwrite: set to true to overwrite previous framework output in \$0UTPUT\_DIR. By default, output with the same CASENAME and date range is assigned a unique name to ensure preexisting results are never overwritten.

These can be set as command-line flags each time the framework is run (e.g.,. --save\_ps), or as true/false values in the input file ("save\_ps": true). Note that true and false in JSON must be written all lower-case, with no quotes.

#### 1.3.5 Modifying POD settings

Individual PODs may provide user-configurable options in the "pod\_env\_vars" section of their settings. jsonc file, which is located in each POD's source code directory under /diagnostics. These only need to be changed in rare or specific cases. Consult the POD's documentation for details.

**CHAPTER** 

**TWO** 

#### SITE-SPECIFIC INFORMATION

## 2.1 GFDL-specific information

This page contains information specific to the site installation at the Geophysical Fluid Dynamics Laboratory<sup>23</sup>.

#### 2.1.1 Site installation

The DET team maintains a site-wide installation of the framework and all supporting data at /home/mdteam/DET/analysis/mdtf/MDTF-diagnostics. This is kept up-to-date and is accessible from both workstations and PPAN. Please contact us if your use case can't be accommodated by this installation.

#### 2.1.2 FRE-centric modes of operation

In addition to the standard, interactive method of running MDTF diagnostics as described in the rest of the documentation, the site installation provides alternative ways to run the diagnostics within GFDL's existing workflow.

- 1. Within FRE XMLs. This is done by calling the mdtf\_gfdl.csh<sup>24</sup> wrapper script from an <analysis> tag in the XML. Currently, FRE requires that each analysis script be associated with a single model <component>. This poses difficulties for diagnostics which use data generated by multiple components. We provide two ways to address this issue:
  - A. If it's known ahead of time that a given <component> will dominate the run time and finish last, one can call mdtf\_gfdl.csh from an <analysis> tag in that component only. In this case, the framework will search all data present in the /pp/ output directory when it's called. The <component> being used doesn't need to generate data analyzed by the diagnostics; in this case it's only used to schedule the diagnostics' execution.
  - B. If one doesn't know which <component> will finish last, a more robust solution is to call mdtf\_gfdl.csh --component\_only from each <component> generating data to be analyzed. When the --component\_only flag is set, every time the framework is called it will only run the diagnostics for which all the input data is available and which haven't run already (which haven't written their output to \$OUTPUT\_DIR.

<sup>&</sup>lt;sup>23</sup> https://www.gfdl.noaa.gov/

 $<sup>^{24}\</sup> https://github.com/NOAA-GFDL/MDTF-diagnostics/blob/feature/gfdl-data/src/mdtf\_gfdl.csh$ 

- 2. As a batch job on PPAN, managed via slurm. This is handled via the mdtf\_gfdl\_interactive.csh<sup>25</sup> wrapper script.
- 3. Called from an interactive shell on PPAN or workstations.

## 2.1.3 Data retrieval options

The framework is currently configured to search data from two types of directory hierarchies. The framework will determine what's intended based on its input, but this choice can be overridden by passing the following options with the --data\_manager flag:

- The /pp/ hierarchy used by FRE (--data\_manager Gfdl\_PP). In this case CASE\_ROOT\_DIR should be set to the root of the directory hierarchy (ie, ending in /pp).
- The CMIP6 DRS for published data on the Unified Data Archive (--data\_manager Gfdl\_UDA\_CMIP6). In this case CASE\_ROOT\_DIR should not be set, but the --model and --experiment settings should be populated.
- The CMIP6 DRS for unpublished data on /data\_cmip6. This option must be requested explicitly with --data\_manager Gfdl\_data\_cmip6. In this case CASE\_ROOT\_DIR should not be set, but the --model and --experiment settings should be populated.

## 2.1.4 GFDL-specific options

In addition to the framework's normal command-line options, the following site-specific options are recognized:

- --GFDL-PPAN-TEMP, --GFDL\_PPAN\_TEMP <DIR>: If running on the GFDL PPAN cluster, set the \$MDTF\_GFDL\_TMPDIR environment variable to this location and create temp files here. Note: must be accessible via gcp. Defaults to \$TMPDIR.
- --GFDL-WS-TEMP, --GFDL\_WS\_TEMP <DIR>: If running on a GFDL workstation, set the \$MDTF\_GFDL\_TMPDIR environment variable to this location and create temp files here. The directory will be created if it doesn't exist. Note: must be accessible via gcp. Defaults to /net2/\$USER/tmp.
- --frepp: Normally this is set by the mdtf\_gfdl.csh<sup>26</sup> wrapper script, and not directly by the user. Set flag to run framework in "online" mode (1a. or 1b. above), processing data as part of the FRE pipeline.
- --ignore-component, --ignore\_component: Normally this is set by the mdtf\_gfdl.csh<sup>27</sup> wrapper script, and not directly by the user. If set, this flag tells the framework to search the entire /pp/ directory for model data (1a. above); default is to restrict to model component passed by FRE. Ignored if --frepp is not set.

<sup>&</sup>lt;sup>25</sup> https://github.com/NOAA-GFDL/MDTF-diagnostics/blob/feature/gfdl-data/src/mdtf\_gfdl\_interactive.csh

<sup>&</sup>lt;sup>26</sup> https://github.com/NOAA-GFDL/MDTF-diagnostics/blob/feature/gfdl-data/src/mdtf\_gfdl.csh

<sup>&</sup>lt;sup>27</sup> https://github.com/NOAA-GFDL/MDTF-diagnostics/blob/feature/gfdl-data/src/mdtf\_gfdl.csh

## 2.1.5 GFDL-specific defaults

The following paths are set to more useful default values:

- --OBS-DATA-REMOTE, --OBS\_DATA\_REMOTE <DIR>: Site-specific installation of observational data used by individual PODs at /home/Oar.Gfdl.Mdteam/DET/analysis/mdtf/obs\_data. If running on PPAN, this data will be GCP'ed to the current node.
- --OBS-DATA-ROOT, --OBS\_DATA\_ROOT <DIR>: Local directory for observational data. Defaults to \$MDTF\_GFDL\_TMPDIR/inputdata/obs\_data, where the environment variable \$MDTF\_GFDL\_TMPDIR is defined as described above.
- --MODEL-DATA-ROOT, --MODEL\_DATA\_ROOT <DIR>: Local directory for model data. Defaults to \$MDTF\_GFDL\_TMPDIR/inputdata/model, where the environment variable \$MDTF\_GFDL\_TMPDIR is defined as described above.
- --WORKING-DIR, --WORKING\_DIR <DIR>: Working directory. Defaults to \$MDTF\_GFDL\_TMPDIR/wkdir, where the environment variable \$MDTF\_GFDL\_TMPDIR is defined as described above.
- --OUTPUT-DIR, --OUTPUT\_DIR, -o <DIR>: Destination for output files. Defaults to \$HOME/mdtf\_out, which will be created if it doesn't exist.

**CHAPTER** 

**THREE** 

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## 3.1 Disclaimer

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<sup>28</sup> https://www.noaa.gov/

<sup>&</sup>lt;sup>29</sup> https://cpo.noaa.gov/Meet-the-Divisions/Earth-System-Science-and-Modeling/MAPP

<sup>30</sup> https://www.ucla.edu/

<sup>31</sup> https://www.gfdl.noaa.gov/

<sup>32</sup> https://ncar.ucar.edu/

<sup>33</sup> https://www.colostate.edu/

<sup>34</sup> https://www.llnl.gov/

<sup>35</sup> https://www.energy.gov/

<sup>&</sup>lt;sup>36</sup> https://cpo.noaa.gov/Meet-the-Divisions/Earth-System-Science-and-Modeling/MAPP/MAPP-Task-Forces/Model-Diagnostics-Task-Force