

MDTF Developer's Walkthrough

Release 3.0 beta 2

Yi-Hung Kuo^a Dani Coleman^b Chih-Chieh (Jack) Chen^b J. David Neelin^a Eric Maloney^d Thomas Jackson^c Andrew Gettelman^b John Krasting^c

(a: UCLA; b: NCAR; c: GFDL; d:CSU)

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CHAPTER

ONE

DEVELOPER INFORMATION

1.1 Introduction for POD developers

This walkthrough contains information for developers wanting to contribute a process-oriented diagnostic (POD) module to the MDTF framework. There are two tracks through the material: one for developers who have an existing analysis script they want to adapt for use in the framework, and one for developers who are writing a POD from scratch.

Section 1.4 provides instructions for setting up POD development, in particular managing language and library dependencies through conda. For developers already familiar with version 2.0 of the framework, Section 1.2 summarizes changes from v2.0 to facilitate migration to v3.0. New developers can skip this section, as the rest of this walkthrough is self-contained.

Section 1.3 Provides a list of instructions for submitting a POD for inclusion in the framework. We require developers to submit PODs through GitHub¹. See Section 1.9 for how to manage code through the GitHub website.

Section 1.5 provides overall guidelines for POD development. Section 1.6 is a reference for the POD's settings file format. In Section 1.7, we walk the developers through the workflow of the framework, focusing on aspects that are relevant for the operation of individual PODs, and using the Example Diagnostic POD² as a concrete example to illustrate how a POD works under the framework Section 1.8 provides coding best practices to address common issues encountered in submitted PODs..

1.1.1 Scope of a process-oriented diagnostic

The MDTF framework imposes requirements on the types of data your POD outputs and takes as input. In addition to the scientific scope of process-oriented diagnostics, the analysis that you intend to do needs to fit the following model:

Your POD should accept model data as input and express the results of its analysis in a series of figures, which are presented to the user in a web page. Input model data will be in the form of one NetCDF file (with accompanying dimension information) per variable, as requested in your POD's settings file (page 14). Because your POD may be run on the output of any model, you should be careful about the assumptions your code makes about the layout of these files (eg, the range of longitude or the positive³ convention for vertical

¹ https://github.com/NOAA-GFDL/MDTF-diagnostics

² https://github.com/NOAA-GFDL/MDTF-diagnostics/tree/main/diagnostics/example

³ http://cfconventions.org/faq.html#vertical_coords_positive_attribute

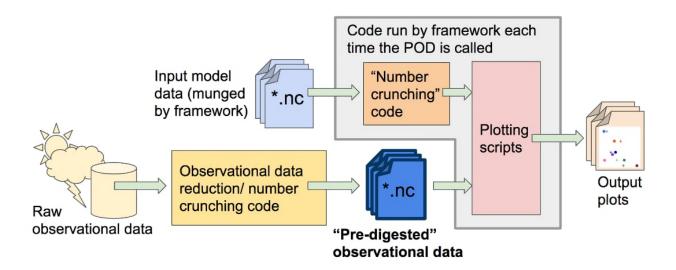
coordinates). Supporting data may be in any format and will not be modified by the framework (see next section).

The above data sources are your POD's only input: your POD should not access the internet or other networked resources. You may provide options in the settings file for the user to configure when the POD is installed, but these cannot be changed each time the POD is run.

To achieve portability, the MDTF cannot accept PODs written in closed-source languages (eg, MATLAB or IDL). We also cannot accept PODs written in compiled languages (eg, C or Fortran): installation would rapidly become impractical if users had to check compilation options for each POD.

The output of your POD should be a series of figures in vector format (.eps or .ps). Optionally, we encourage POD developers to also save relevant output data (e.g., the output data being plotted) as netcdf files, to give users the ability to take the POD's output and perform further analysis on it.

1.1.2 POD code organization and supporting data



In order to make your code run faster for the users, we request that you separate any calculations that don't depend on the model data (e.g., pre-processing of observational data), and instead save the end result of these calculations in data files for your POD to read when it is run. We refer to this as "digested observational data," but it refers to any quantities that are independent of the model being analyzed. For purposes of data provenance, reproducibility, and code maintenance, we request that you include all the pre-processing/data reduction scripts used to create the digested data in your POD's code base, along with references to the sources of raw data these scripts take as input (yellow box in the figure).

Digested data should be in the form of numerical data, not figures, even if the only thing the POD does with the data is produce an unchanging reference plot. We encourage developers to separate their "number-crunching code" and plotting code in order to give end users the ability to customize output plots if needed. In order to keep the amount of supporting data needed by the framework manageable, we request that you limit the total amount of digested data you supply to no more than a few gigabytes.

In collaboration with PCMDI, a framework is being advanced that can help systematize the provenance of observational data used for POD development. This section will be updated when this data source is ready

for public use.

1.2 Migration from framework v2.0

In this section we describe the major changes made from v2.0 to v3.0 of the framework that are relevant for POD developers. The scope of the framework has expanded in version 3.0, which required changes in the way the PODs and framework interact. New developers can skip this section, as the rest of this documentation is self-contained.

1.2.1 Getting Started and Developer's Walkthrough

A main source of documentation for v2.0 of the framework were the "Getting Started" and "Developer's Walkthrough" documents. Updated versions of these documents are:

- Getting Started v3.0 (PDF)⁴
- Developer's Walkthrough v3.0 (PDF)⁵

Note: These documents contain a subset of information available on this website, rather than new material: the text is reorganized to be placed in the same order as the v2.0 documents, for ease of comparison.

1.2.2 Checklist for migrating a POD from v2.0

Here we list the broad set of tasks needed to update a POD written for v2.0 of the framework to v3.0.

- Update settings and varlist files: In v3.0 these have been combined into a single settings.jsonc file. See the settings file guide (page 14), reference (page 32), and example for descriptions of the new format.
- Update references to framework environment variables: See the table below for an overview, and the reference (page 42) for complete information on what environment variables the framework sets. Note that your POD should not use any hard-coded paths or variable names, but should read this information in from the framework's environment variables.
- Resubmit digested observational data: To minimize the size of supporting data users need to download, we ask that you only supply observational data specifically needed for plotting (preferably size within MB range), as well as any code used to perform that data reduction from raw sources.
- Remove HTML templating code: Version 2.0 of the framework required that your POD's top-level driver script take particular steps to assemble its HTML file. In v3.0 these tasks are done by the framework: all that your POD needs to do is generate figures of the appropriate formats and names in the specified folders, and the framework will convert and link them appropriately.

 $^{^4\} https://mdtf-diagnostics.readthedocs.io/en/latest/_static/MDTF_getting_started.pdf$

⁵ https://mdtf-diagnostics.readthedocs.io/en/latest/_static/MDTF_walkthrough.pdf

⁶ https://github.com/NOAA-GFDL/MDTF-diagnostics/tree/main/diagnostics/example/settings.jsonc

1.2.3 Conversion from v2.0 environment variables

In v3.0, the paths referred to by the framework's environment variables have been changed to be specific to your POD. The variables themselves have been renamed to avoid possible confusion. Here's a table of the appropriate substitutions to make:

Path Description	v2.0 environment variable expression	Equivalent v3.0 variable
Top-level code repository	\$DIAG_HOME	No variable set: PODs should not access
		files outside of their own source code direc-
		tory within \$POD_HOME
POD's source code	\$VARCODE/ <pod name=""></pod>	\$POD_HOME
POD's observa-	\$VARDATA/ <pod name=""></pod>	\$OBS_DATA
tional/supporting data		
POD's working directory	<pre>\$variab_dir/<pod name=""></pod></pre>	\$WK_DIR
Path to requested NetCDF	Currently unchanged:	
data file for <variable< td=""><td>\$DATADIR/<freq>/\$CASENAM</freq></td><td>E.<variable< td=""></variable<></td></variable<>	\$DATADIR/ <freq>/\$CASENAM</freq>	E. <variable< td=""></variable<>
name> at date frequency	name>. <freq>.nc</freq>	
<freq></freq>		
Other v2.0 paths	\$DATA_IN, \$DIAG_ROOT,	No equivalent variable set. PODs shouldn't
	\$WKDIR	access files outside of their own directories;
		instead use one of the quantities above.

Table 1: Environment variable name conversion

1.3 POD development checklist

This section lists all the steps that need to be taken in order to submit a POD for inclusion in the MDTF framework.

1.3.1 Code and documentation submission

The material in this section must be submitted though a pull request⁷ to the NOAA-GFDL GitHub repo⁸. This is described in Git-based development workflow (page 28).

The example POD⁹ should be used as a reference for how each component of the submission should be structured.

⁷ https://docs.github.com/en/github/collaborating-with-issues-and-pull-requests/about-pull-requests

⁸ https://github.com/NOAA-GFDL/MDTF-diagnostics

⁹ https://github.com/NOAA-GFDL/MDTF-diagnostics/tree/main/diagnostics/example

POD source code

All scripts should be placed in a subdirectory of diagnostics/. Among the scripts, there should be 1) a main driver script, 2) a template html, and 3) a settings.jsonc file. The POD directory and html template should be named after your POD's short name.

- For instance, diagnostics/convective_transition_diag/ contains its driver script convective_transition_diag.py, convective_transition_diag.html, and settings. jsonc, etc.
- The framework will call the driver script, which calls the other scripts in the same POD directory.
- If you need a new Conda environment, add a new .yml file to src/conda/, and install the environment using the conda_env_setup.sh script as described in the Getting Started.

POD settings file

The format of this file is described in POD settings file summary (page 14) and in more detail in Diagnostic settings file format (page 32).

POD html template for output

• The html template will be copied by the framework into the output directory to display the figures generated by the POD. You should be able to create a new html template by simply copying and modifying the example templates from existing PODs even without prior knowledge about html syntax.

Preprocessing scripts for digested data

The "digested" supporting data policy is described in Section 1.1.2.

For maintainability and provenance purposes, we request that you include the code used to generate your POD's "digested" data from raw data sources (any source of data that's permanently hosted). This code will not be called by the framework and will not be used by end users, so the restrictions and guidelines concerning the POD code don't apply.

POD documentation

- The documentation for the framework is automatically generated using sphinx¹⁰, which works with files in reStructured text¹¹ (reST, .rst) format. In order to include documentation for your POD, we require that it be in this format.
 - Use the example POD documentation¹² as a template for the information required for your POD, by modifying its .rst source code¹³. This should include a one-paragraph synopsis of the POD,

¹⁰ https://www.sphinx-doc.org/en/master/index.html

¹¹ https://docutils.sourceforge.io/rst.html

¹² https://mdtf-diagnostics.readthedocs.io/en/latest/sphinx_pods/example.html

¹³ https://raw.githubusercontent.com/NOAA-GFDL/MDTF-diagnostics/main/diagnostics/example/doc/example.rst

developers' contact information, required programming language and libraries, and model output variables, a brief summary of the presented diagnostics as well as references in which more indepth discussions can be found.

- The .rst files and all linked figures should be placed in a doc subdirectory under your POD directory (e.g., diagnostics/convective_transition_diag/doc/) and put the .rst file and figures inside.
- The most convenient way to write and debug reST documentation is with an online editor. We recommend https://livesphinx.herokuapp.com/ because it recognizes sphinx-specific commands as well.
- For reference, see the reStructured text introduction¹⁴, quick reference¹⁵ and in-depth guide¹⁶.
- Also see a reST syntax comparison¹⁷ to other text formats you may be familiar with.
- For maintainability, all scripts should be self-documenting by including in-line comments. The main driver script (e.g., convective_transition_diag.py) should contain a comprehensive header providing information that contains the same items as in the POD documentation, except for the "More about this diagnostic" section.
- The one-paragraph POD synopsis (in the POD documentation) as well as a link to the full documentation should be placed at the top of the html template (e.g., convective_transition_diag.html).

Preprocessing script documentation

The "digested" supporting data policy is described in Section 1.1.2.

For maintainability purposes, include all information needed for a third party to reproduce your POD's digested data from its raw sources in the doc directory. This information is not published on the documentation website and can be in any format. In particular, please document the raw data sources used (DOIs/versioned references preferred) and the dependencies/build instructions (eg. conda environment) for your preprocessing script.

1.3.2 Sample and supporting data submission

Data hosting for the MDTF framework is currently managed manually. The data is currently hosted via anonymous FTP on UCAR's servers. Please contact the MDTF team leads via email to arrange a data transfer.

¹⁴ http://docutils.sourceforge.net/docs/user/rst/quickstart.html

http://docutils.sourceforge.net/docs/user/rst/quickref.html

¹⁶ http://docutils.sourceforge.net/docs/ref/rst/restructuredtext.html

¹⁷ http://hyperpolyglot.org/lightweight-markup

Digested observational or supporting data

The "digested" supporting data policy is described in Section 1.1.2.

Create a directory under inputdata/obs_data/ named after the short name, and put all your digested observation data in (or more generally, any quantities that are independent of the model being analyzed).

- Digested data should be in the form of numerical data, not figures.
- The data files should be small (preferably a few MB) and just enough for producing figures for model comparison.
- If you really cannot reduce the data size or require GB of space, consult with the lead team.

Sample model data

For PODs dealing with atmospheric phenomena, we recommend that you use sample data from the following sources, if applicable:

- A timeslice run of NCAR CAM5¹⁸
- A timeslice run of GFDL AM4¹⁹ (contact the leads for password).

1.4 Developer quickstart guide

This section contains instructions for beginning to

1.4.1 Developer installation instructions

To download and install the framework for development, follow the instructions for end users given in start_install, with the following developer-specific modifications:

Obtaining the source code

POD developers should work from the develop branch²⁰ of the framework code. This is the "beta test" version, used for testing changes before releasing them to end users.

Developers may download the code from GitHub as described in ref-download, but we strongly recommend that you clone the repo in order to keep up with changes in the develop branch, and to simplify submitting pull requests with your POD's code. Instructions for how to do this are given in Git-based development workflow (page 28).

¹⁸ https://www.earthsystemgrid.org/dataset/ucar.cgd.ccsm4.NOAA-MDTF.html

¹⁹ http://data1.gfdl.noaa.gov/MDTF/

²⁰ https://github.com/NOAA-GFDL/MDTF-diagnostics/tree/develop

Installing dependencies via conda

Regardless of development language, we strongly recommend that developers use conda to manage their language and library versions. Note that Conda is not Python-specific, but allows coexisting versioned environments of most scripting languages, including, R²¹, NCL²², Ruby²³, PyFerret²⁴, and more.

We recommend that new PODs be written in Python 3. We provide a developer version of the python3_base environment (described below) that includes Jupyter and other developer-specific tools. This is not installed by default, and must be requested by passing the -all-dev flag to the conda setup script:

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

1.4.2 POD development using existing Conda environments

To prevent the proliferation of dependencies, we suggest that new POD development use existing Conda environments whenever possible, e.g., python3_base²⁵, NCL_base²⁶, and R_base²⁷ for Python, NCL, and R, respectively.

In case you need any exotic third-party libraries, e.g., a storm tracker, consult with the lead team and create your own Conda environment following instructions (page 9) below.

Python

The framework provides the _MDTF_python3_base²⁸ Conda environment (recall the _MDTF prefix for framework-specific environment) as the generic Python environment, which you can install following the instructions. You can then activate this environment by running in a terminal:

```
% source activate $CONDA_ENV_DIR/_MDTF_python3_base
```

where \$CONDA_ENV_DIR is the path you used to install the Conda environments. After you've finished working under this environment, run % conda deactivate or simply close the terminal.

²¹ https://anaconda.org/conda-forge/r-base

²² https://anaconda.org/conda-forge/ncl

²³ https://anaconda.org/conda-forge/ruby

²⁴ https://anaconda.org/conda-forge/pyferret

 $^{^{25}\} https://github.com/NOAA-GFDL/MDTF-diagnostics/blob/develop/src/conda/env_python3_base.yml$

²⁶ https://github.com/NOAA-GFDL/MDTF-diagnostics/blob/develop/src/conda/env_NCL_base.yml

²⁷ https://github.com/NOAA-GFDL/MDTF-diagnostics/blob/develop/src/conda/env_R_base.yml

²⁸ https://github.com/NOAA-GFDL/MDTF-diagnostics/blob/develop/src/conda/env_pythone3_base.yml

Other languages

The framework also provides the $_MDTF_NCL_base^{29}$ and $_MDTF_R_base^{30}$ Conda environments as the generic NCL and R environments.

1.4.3 POD development using a new Conda environment

If your POD requires languages that aren't available in an existing environment or third-party libraries unavailable through the common conda-forge³¹ and anaconda³² channels, we ask that you notify us (since this situation may be relevant to other developers) and submit a YAML (.yml) file³³ that creates the environment needed for your POD.

- The new YAML file should be added to src/conda/, where you can find templates for existing environments from which you can create your own.
- The YAML filename should be env_\$your_POD_short_name.yml.
- The first entry of the YAML file, name of the environment, should be MDTF \$your POD short name.
- We recommend listing conda-forge as the first channel to search, as it's entirely open source and has the largest range of packages. Note that combining packages from different channels (in particular, conda-forge and anaconda channels) may create incompatibilities.
- We recommend constructing the list of packages manually, by simply searching your POD's code for import statements referencing third-party libraries. Please do not exporting your development environment with % conda env export, which gives platform-specific version information and will not be fully portable in all cases; it also does so for every package in the environment, not just the "top-level" ones you directly requested.
- We recommend specifying versions as little as possible, out of consideration for end-users: if each POD specifies exact versions of all its dependencies, conda will need to install multiple versions of the same libraries. In general, specifying a version should only be needed in cases where backward compatibility was broken (e.g., Python 2 vs. 3) or a bug affecting your POD was fixed (e.g., postscript font rendering on Mac OS with older NCL). Conda installs the latest version of each package that's consistent with all other dependencies.

²⁹ https://github.com/NOAA-GFDL/MDTF-diagnostics/blob/develop/src/conda/env_NCL_base.yml

 $^{^{30}\} https://github.com/NOAA-GFDL/MDTF-diagnostics/blob/develop/src/conda/env_R_base.yml$

³¹ https://conda-forge.org/feedstocks/

³² https://docs.anaconda.com/anaconda/packages/pkg-docs/

³³ https://docs.conda.io/projects/conda/en/latest/user-guide/tasks/manage-environments.html#creating-an-environment-file-manually

Framework interaction with conda environments

As described in ref-execute, when you run the mdtf executable, among other things, it reads pod_list in default_tests.jsonc and executes POD codes accordingly. For a POD included in the list (referred to as \$POD_NAME):

- 1. The framework will first try to look for the YAML file src/conda/env_\$POD_NAME.yml. If it exists, the framework will assume that the corresponding conda environment _MDTF_\$POD_NAME has been installed under \$CONDA_ENV_DIR, and 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/. The runtime_requirements section in settings.jsonc specifies the programming language(s) adopted by the POD:
 - a). If purely Python 3, the framework will look for src/conda/env_python3_base.yml and check its content to determine whether the POD's requirements are met, and then switch to _MDTF_python3_base and run the POD.
 - b). Similarly, if NCL or R is used, then NCL_base or R_base.

Note that for the 6 existing PODs depending on NCL (EOF_500hPa, MJO_prop_amp, MJO_suite, MJO_teleconnection, precip_diurnal_cycle, and Wheeler_Kiladis), Python is also used but merely as a wrapper. Thus the framework will switch to $\underline{\texttt{MDTF}}\underline{\texttt{NCL}}$ base when seeing both NCL and Python in settings. jsonc.

The framework verifies PODs' requirements via looking for the YAML files and their contents. Thus if you choose to selectively install conda environments using the --env flag (ref-conda-env-install), 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 (ref-conda-env-install).

Testing with a new Conda environment

If you've updated an existing environment or created a new environment (with corresponding changes to the YAML file), verify that your POD works.

Recall how the framework finds a proper Conda environment for a POD. First, it searches for an environment matching the POD's short name. If this fails, it then looks into the POD's settings.jsonc and prepares a generic environment depending on the language(s). Therefore, no additional steps are needed to specify the environment if your new YAML file follows the naming conventions above (in case of a new environment) or your settings.jsonc correctly lists the language(s) (in case of updating an existing environment).

- For an updated environment, first, uninstall it by deleting the corresponding directory under \$CONDA_ENV_DIR.
- Re-install the environment using the conda_env_setup.sh script as described in the installation instructions, or create the new environment for you POD:

```
% cd $CODE_ROOT
% ./src/conda/conda_env_setup.sh --env $your_POD_short_name --conda_root

$CONDA_ROOT --env_dir $CONDA_ENV_DIR
```

- Have the framework run your POD on suitable test data.
 - 1. Add your POD's short name to the pod_list section of the configuration input file (template: src/default_tests.jsonc).
 - 2. Prepare the test data as described in start_config.

1.5 POD development guidelines

1.5.1 Admissible languages

The framework itself is written in Python, and can call PODs written in any scripting language. However, Python support by the lead team will be "first among equals" in terms of priority for allocating developer resources, etc.

- To achieve portability, the MDTF cannot accept PODs written in closed-source languages (e.g., MAT-LAB and IDL; try Octave³⁴ and GDL³⁵ if possible). We also cannot accept PODs written in compiled languages (e.g., C or Fortran): installation would rapidly become impractical if users had to check compilation options for each POD.
- Python is strongly encouraged for new PODs; PODs funded through the CPO grant are requested to be developed in Python. Python version >= 3.6 is required. Official support for Python 2 was discontinued as of January 2020.
- If your POD was previously developed in NCL or R (and development is not funded through a CPO grant), you do not need to re-write existing scripts in Python 3 if doing so is likely to introduce new bugs into stable code, especially if you're unfamiliar with Python.
- If scripts were written in closed-source languages, translation to Python 3.6 or above is required.

1.5.2 Preparation for POD implementation

We assume that, at this point, you have a set of scripts, written in languages consistent with the framework's open source policy, that a) read in model data, b) perform analysis, and c) output figures. Here are 3 steps to prepare your scripts for POD implementation.

We recommend running the framework on the sample model data again with both save_ps and save_nc in the configuration input src/default_tests.jsonc set to true. This will preserve directories and files created by individual PODs in the output directory, which could come in handy when you go through the instructions below, and help understand how a POD is expected to write output.

• Give your POD an official name (e.g., Convective Transition; referred to as long_name) and a short name (e.g., convective_transition_diag). The latter will be used consistently to name the directories

³⁴ https://www.gnu.org/software/octave/

³⁵ https://github.com/gnudatalanguage/gdl

and files associated with your POD, so it should (1) loosely resemble the long_name, (2) avoid space bar and special characters (!@#\$%^&*), and (3) not repeat existing PODs' name (i.e., the directory names under diagnostics/). Try to make your POD's name specific enough that it will be distinct from PODs contributed now or in the future by other groups working on similar phenomena.

- If you have multiple scripts, organize them so that there is a main driver script calling the other scripts, i.e., a user only needs to execute the driver script to perform all read-in data, analysis, and plotting tasks. This driver script should be named after the POD's short name (e.g., convective transition diag.py).
- You should have no problem getting scripts working as long as you have (1) the location and filenames of model data, (2) the model variable naming convention, and (3) where to output files/figures. The framework will provide these as environment variables that you can access (e.g., using os.environ in Python, or getenv in NCL). DO NOT hard code these paths/filenames/variable naming convention, etc., into your scripts. See the complete list of environment variables supplied by the framework.
- Your scripts should not access the internet or other networked resources.

1.5.3 An example of using framework-provided environment variables

The framework provides a collection of environment variables, mostly in the format of strings but also some numbers, so that you can and MUST use in your code to make your POD portable and reusable.

For instance, using 3 of the environment variables provided by the framework, CASENAME, DATADIR, and pr_var, the full path to the hourly precipitation file can be expressed as

```
MODEL_OUTPUT_DIR = os.environ["DATADIR"]+"/1hr/"
pr_filename = os.environ["CASENAME"]+"."+os.environ["pr_var"]+".1hr.nc"
pr_filepath = MODEL_OUTPUT_DIR + pr_filename
```

You can then use pr_filepath in your code to load the precipitation data.

Note that in Linux shell or NCL, the values of environment variables are accessed via a \$ sign, e.g., os. environ["CASENAME"] in Python is equivalent to \$CASENAME in Linux shell/NCL.

1.5.4 Relevant environment variables

The environment variables most relevant for a POD's operation are:

- POD_HOME: Path to directory containing POD's scripts, e.g., diagnostics/convective_transition_diag/.
- OBS_DATA: Path to directory containing POD's supporting/digested observation data, e.g., inputdata/obs_data/convective_transition_diag/.
- DATADIR: Path to directory containing model data files for one case/experiment, e.g., inputdata/model/QBOi.EXP1.AMIP.001/.
- WK_DIR: Path to directory for POD to output files. Note that this is the only directory a POD is allowed to write its output. E.g., wkdir/MDTF_QBOi.EXP1.AMIP.001_1977_1981/convective_transition_diag/.

- 1. Output figures to \$WK_DIR/obs/ and \$WK_DIR/model/ respectively.
- \$WK_DIR/obs/PS/ and \$WK_DIR/model/PS/: If a POD chooses to save vector-format figures, save them as EPS under these two directories. Files in these locations will be converted by the framework to PNG for HTML output. Caution: avoid using PS because of potential bugs in recent matplotlib and converting to PNG.
- 3. \$WK_DIR/obs/netCDF/ and \$WK_DIR/model/netCDF/: If a POD chooses to save digested data for later analysis/plotting, save them in these two directories in NetCDF.

Note that (1) values of POD_HOME, OBS_DATA, and WK_DIR change when the framework executes different PODs; (2) the WK_DIR directory and subdirectories therein are automatically created by the framework. Each POD should output files as described here so that the framework knows where to find what, and also for the ease of code maintenance.

More environment variables for specifying model variable naming convention can be found in the src/filedlist_\$convention.jsonc files. Also see the list of environment variables supplied by the framework.

1.5.5 Guidelines for testing your POD

Test before distribution. Find people (eg, nearby postdocs/grads and members from other POD-developing groups) who are not involved in your POD's implementation and are willing to help. Give the tar files and point your GitHub repo to them. Ask them to try running the framework with your POD following the Getting Started instructions. Ask for comments on whether they can understand the documentation.

Test how the POD fails. Does it stop with clear errors if it doesn't find the files it needs? How about if the dates requested are not presented in the model data? Can developers run it on data from another model? Here are some simple tests you should try:

- Move the inputdata directory around. Your POD should still work by simply updating the values of OBS_DATA_ROOT and MODEL_DATA_ROOT in the configuration input file.
- Try to run your POD with a different set of model data.
- If you have problems getting another set of data, try changing the files' CASENAME and variable naming convention. The POD should work by updating CASENAME and convention in the configuration input.
- Try your POD on a different machine. Check that your POD can work with reasonable machine configuration and computation power, e.g., can run on a machine with 32 GB memory, and can finish computation in 10 min. Will memory and run time become a problem if one tries your POD on model output of high spatial resolution and temporal frequency (e.g., avoid memory problem by reading in data in segments)? Does it depend on a particular version of a certain library? Consult the lead team if there's any unsolvable problems.

1.5.6 Other tips on implementation

- 1. Structure of the code package: Implementing the constituent PODs in accordance with the structure described in earlier sections makes it easy to pass the package (or just part of it) to other groups.
- 2. Robustness to model file/variable names: Each POD should be robust to modest changes in the file/variable names of the model output; see Getting Started regarding the model data filename structure, An example of using framework-provided environment variables (page 12) and POD development checklist (page 4) regarding using the environment variables and robustness tests. Also, it would be easier to apply the code package to a broader range of model output.
- 3. Save digested data after analysis: Can be used, e.g., to save time when there is a substantial computation that can be re-used when re-running or re-plotting diagnostics. See Step 5: Output and cleanup (page 22) regarding where to save the output.
- 4. Self-documenting: For maintenance and adaptation, to provide references on the scientific underpinnings, and for the code package to work out of the box without support. See POD development checklist (page 4).
- 5. Handle large model data: The spatial resolution and temporal frequency of climate model output have increased in recent years. As such, developers should take into account the size of model data compared with the available memory. For instance, the example POD precip_diurnal_cycle and Wheeler_Kiladis only analyze part of the available model output for a period specified by the environment variables FIRSTYR and LASTYR, and the convective transition diag module reads in data in segments.
- 6. Basic vs. advanced diagnostics (within a POD): Separate parts of diagnostics, e.g, those might need adjustment when model performance out of obs range.
- 7. Avoid special characters (!@#\$\/^&*) in file/script names.

See ref-execute and :doc: framework operation walkthrough <dev_walkthrough> for details on how the package is called. See the command line reference for documentation on command line options (or run mdtf --help).

Avoid making assumptions about the machine on which the framework will run beyond what's listed here; a development priority is to interface the framework with cluster and cloud job schedulers to enable individual PODs to run in a concurrent, distributed manner.

1.6 POD settings file summary

This page gives a quick introduction to how to write the settings file for your POD. See the full documentation (page 32) on this file format for a complete list of all the options you can specify.

1.6.1 Overview

The MDTF framework can be viewed as a "wrapper" for your code that handles data fetching and munging. Your code communicates with this wrapper in two ways:

- The settings file is where your code talks to the framework: when you write your code, you document what model data your code uses and what format it expects it in. When the framework is run, it will fulfill the requests you make here (or tell the user what went wrong).
- When your code is run, the framework talks to it by setting environment variables (page 42) containing paths to the data files and other information specific to the run.

In the settings file, you specify what model data your diagnostic uses in a vocabulary you're already familiar with:

- The CF conventions³⁶ for standardized variable names and units.
- The netCDF4 (classic) data model, in particular the notions of variables³⁷ and dimensions³⁸ as they're used in a netCDF file.

1.6.2 Example

```
// Any text to the right of a '//' is a comment
{
  "settings" : {
    "long_name": "My example diagnostic",
    "driver": "example diagnostic.py",
    "realm": "atmos",
    "runtime_requirements": {
      "python": ["numpy", "matplotlib", "netCDF4"]
    }
  },
  "data" : {
    "frequency": "day"
  },
  "dimensions": {
    "lat": {
      "standard name": "latitude"
    },
    "lon": {
      "standard_name": "longitude"
    },
    "plev": {
      "standard name": "air pressure",
      "units": "hPa",
      "positive": "down"
    },
    "time": {
```

(continues on next page)

³⁶ http://cfconventions.org/

³⁷ https://www.unidata.ucar.edu/software/netcdf/workshops/2010/datamodels/NcVars.html

³⁸ https://www.unidata.ucar.edu/software/netcdf/workshops/2010/datamodels/NcDims.html

(continued from previous page)

```
"standard_name": "time",
    "units": "day"
  }
},
"varlist" : {
  "my precip data": {
    "standard_name": "precipitation_flux",
    "path_variable": "PATH_TO_PR_FILE",
    "units": "kg m-2 s-1",
    "dimensions" : ["time", "lat", "lon"]
  },
  "my 3d u data": {
    "standard name": "eastward wind",
    "path variable": "PATH TO UA FILE",
    "units": "m s-1",
    "dimensions" : ["time", "plev", "lat", "lon"]
  }
}
```

1.6.3 Settings section

This is where you describe your diagnostic and list the programs it needs to run.

long_name: Display name of your diagnostic, used to describe your diagnostic on the top-level index.html page. Can contain spaces.

driver: Filename of the driver script the framework should call to run your diagnostic.

realm: One or more of the eight CMIP6 modeling realms (aerosol, atmos, atmosChem, land, landIce, ocean, ocnBgchem, seaIce) describing what data your diagnostic uses. This is give the user an easy way to, eg, run only ocean diagnostics on data from an ocean model.

runtime_requirements: This is a list of key-value pairs describing the programs your diagnostic needs to run, and any third-party libraries used by those programs.

- The key is program's name, eg. languages such as "python³⁹" or "ncl⁴⁰" etc. but also any utilities such as "ncks⁴¹", "cdo⁴²", etc.
- The value for each program is a list of third-party libraries in that language that your diagnostic needs. You do not need to list built-in libraries: eg, in python, you should to list numpy⁴³ but not math⁴⁴. If no third-party libraries are needed, the value should be an empty list.

³⁹ https://www.python.org/

⁴⁰ https://www.ncl.ucar.edu/

⁴¹ http://nco.sourceforge.net/

⁴² https://code.mpimet.mpg.de/projects/cdo

⁴³ https://numpy.org/

⁴⁴ https://docs.python.org/3/library/math.html

1.6.4 Data section

This section contains settings that apply to all the data your diagnostic uses. Most of them are optional.

frequency: The time frequency the model data should be provided at, eg. "1hr", "6hr", "day", "mon", ...

1.6.5 Dimensions section

This section is where you list the dimensions (coordinate axes) your variables are provided on. Each entry should be a key-value pair, where the key is the name your diagnostic uses for that dimension internally, and the value is a list of settings describing that dimension. In order to be unambiguous, all dimensions must specify at least:

standard_name: The CF standard name⁴⁵ for that coordinate.

units: The units the diagnostic expects that coordinate to be in (using the syntax of the UDUnits library⁴⁶). This is optional: if not given, the framework will assume you want CF convention canonical units⁴⁷.

In addition, any vertical (Z axis) dimension must specify:

positive: Either "up" or "down", according to the CF conventions⁴⁸. A pressure axis is always "down" (increasing values are closer to the center of the earth).

1.6.6 Varlist section

This section is where you list the variables your diagnostic uses. Each entry should be a key-value pair, where the key is the name your diagnostic uses for that variable internally, and the value is a list of settings describing that variable. Most settings here are optional, but the main ones are:

standard_name: The CF standard name⁴⁹ for that variable.

path_variable: Name of the shell environment variable the framework will use to pass the location of the file containing this variable to your diagnostic when it's run. See the environment variable documentation (page 42) for details.

units: The units the diagnostic expects the variable to be in (using the syntax of the UDUnits library⁵⁰). This is optional: if not given, the framework will assume you want CF convention canonical units⁵¹.

dimensions: List of names of dimensions specified in the "dimensions" section, to specify the coordinate dependence of each variable.

⁴⁵ http://cfconventions.org/Data/cf-standard-names/72/build/cf-standard-name-table.html

⁴⁶ https://www.unidata.ucar.edu/software/udunits/udunits-2.0.4/udunits2lib.html#Syntax

⁴⁷ http://cfconventions.org/Data/cf-standard-names/current/build/cf-standard-name-table.html

⁴⁸ http://cfconventions.org/faq.html#vertical_coords_positive_attribute

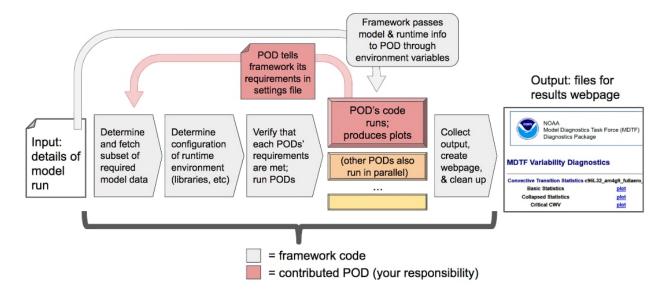
⁴⁹ http://cfconventions.org/Data/cf-standard-names/72/build/cf-standard-name-table.html

⁵⁰ https://www.unidata.ucar.edu/software/udunits/udunits-2.0.4/udunits2lib.html#Syntax

⁵¹ http://cfconventions.org/Data/cf-standard-names/current/build/cf-standard-name-table.html

1.7 Walkthrough of framework operation

In this section, we describe the actions that are taken when the framework is run, focusing on aspects that are relevant for the operation of individual PODs. The Example Diagnostic POD⁵² (short name: example) is used as a concrete example here to illustrate how a POD is implemented and integrated into the framework.



We begin with a reminder that there are 2 essential files for the operation of the framework and POD:

- src/default_tests.jsonc: configuration input for the framework.
- diagnostics/example/settings.jsonc: settings file for the example POD.

1.7.1 Step 1: Framework invocation

The user runs the framework by executing the framework's main driver script \$CODE_ROOT/mdtf, rather than executing the PODs directly. This is where the user specifies the model run to be analyzed, and chooses which PODs to run via the pod_list section in default_tests.jsonc.

• Some of the configuration options can be input through command line, see the command line reference or run % \$CODE_ROOT/mdtf --help.

At this stage, the framework also creates the directory \$OUTPUT_DIR/ (default: mdtf/wkdir/) and all sub-directories therein for hosting the output files by the framework and PODs from each run.

• If you've run the framework with both save_ps and save_nc in default_tests.jsonc set to true, check the output directory structure and files therein.

Note that when running, the framework will keep collecting the messages relevant to individual PODs, including (1) the status of required data and environment, and (2) texts printed out by PODs during execution, and will save them as log files under each POD's output directory. These log files can be viewed via the

 $^{^{52}\} https://github.com/NOAA-GFDL/MDTF-diagnostics/tree/main/diagnostics/example$

top-level results page index.html and, together with messages printed in the terminal, are useful for debugging.

Example diagnostic

Run the framework using the NCAR-CAM5.timeslice case. After successful execution, open the index. html under the output directory in a web browser. The plots links to the webpage produced by the example POD with figures, and log to example.log including all example-related messages collected by the framework. The messages displayed in the terminal are not identical to those in the log files, but also provide a status update on the framework-POD operation.

1.7.2 Step 2: Data request

Each POD describes the model data it requires as input in the varlist section of its settings.jsonc, with each entry in varlist corresponding to one model data file used by the POD. The framework goes through all the PODs to be run in pod_list and assembles a list of required model data from their varlist. It then queries the source of the model data (\$DATADIR/) for the presence of each requested variable with the requested characteristics (e.g., frequency, units, etc.).

- The most important features of settings.jsonc are described in the settings documentation (page 14) and full detail on the reference page (page 32).
- Variables are specified in varlist following CF convention⁵³ wherever possible. If your POD requires derived quantities that are not part of the standard model output (e.g., column weighted averages), incorporate necessary preprocessing for computing these from standard output variables into your code. PODs are allowed to request variables outside of the CF conventions (by requiring an exact match on the variable name), but this will severely limit the POD's application.
- Some of the requested variables may be unavailable or without the requested characteristics (e.g., frequency). You can specify a backup plan for this situation by designating sets of variables as alternates if feasible: when the framework is unable to obtain a variable that has the alternates attribute in varlist, it will then (and only then) query the model data source for the variables named as alternates.
- If no alternates are defined or the alternate variables are also unavailable, the framework will skip executing your POD, and an error log will be presented in index.html.

Once the framework has determined which PODs are able to run given the model data, it prepares the necessary environment variables, including directory paths and the requested variable names (as defined in src/filedlist_\$convention.jsonc) for PODs' operation.

 At this step, the framework also checks the PODs' observational/supporting data under inputdata/ obs_data/. If the directory of any of the PODs in pod_list is missing, the framework would terminate with error messages showing on the terminal. Note that the framework only checks the presence of the directory, but not the files therein.

⁵³ http://cfconventions.org/

Example diagnostic

The example POD uses only one model variable in its varlist⁵⁴: surface air temperature, recorded at monthly frequency.

- In the beginning of example.log, the framework reports finding the requested model data file under Found files.
- If the framework could not locate the file, the log would instead record Skipping execution with the reason being missing data.

1.7.3 Step 3: Runtime environment configuration

The framework reads the other parts of your POD's settings.jsonc, e.g., pod_env_vars, and generates additional environment variables accordingly (on top of those being defined through default_tests.jsonc).

Furthermore, in the runtime_requirements section of settings.jsonc, we request that you provide a list of languages and third-party libraries your POD uses. The framework will check that all these requirements are met by one of the Conda environments under \$CONDA_ENV_DIR/.

- The requirements should be satisfied by one of the existing generic Conda environments (updated by you if necessary), or a new environment you created specifically for your POD.
- If there isn't a suitable environment, the POD will be skipped.

Note that the framework's information about the Conda environments all comes from the YMAL (.yml) files under src/conda/ (and their contents) by assuming that the corresponding Conda environments have been installed using (thus are consistent with) the YAML files.

- The framework doesn't directly check files under \$CONDA_ENV_DIR/, where the Conda environments locate.
- Therefore, it's imperative that you keep the Conda environments and the YAML files consistent at all time so the framework can properly function.

Example diagnostic

In its settings.jsonc, the example POD lists its requirements⁵⁵: Python 3, and the matplotlib, xarray and netCDF4 third-party libraries for Python. In this case, the framework assigns the POD to run in the generic python3_base⁵⁶ environment provided by the framework.

• In example.log, under Env vars: is a comprehensive list of environment variables prepared for the POD by the framework. A great part of them are defined as in src/fieldlist_CMIP.jsonc⁵⁷ via setting convention in default_tests.jsonc to CMIP. Some of the environment variables are POD-specific as defined under pod_env_vars⁵⁸ in the POD's settings.jsonc, e.g., EXAMPLE_FAV_COLOR.

⁵⁴ https://github.com/NOAA-GFDL/MDTF-diagnostics/blob/main/diagnostics/example/settings.jsonc#L46

⁵⁵ https://github.com/NOAA-GFDL/MDTF-diagnostics/blob/main/diagnostics/example/settings.jsonc#L38

⁵⁶ https://github.com/NOAA-GFDL/MDTF-diagnostics/blob/main/src/conda/env_python3_base.yml

 $^{^{57}\} https://github.com/NOAA-GFDL/MDTF-diagnostics/blob/main/src/fieldlist_CMIP.jsonc$

⁵⁸ https://github.com/NOAA-GFDL/MDTF-diagnostics/blob/main/diagnostics/example/settings.jsonc#L29

• In example.log, after --- MDTF.py calling POD example, the framework verifies the Condarelated paths, and makes sure that the runtime_requirements in settings.jsonc are met by the python3_base environment via checking env_python3_base.yml⁵⁹.

1.7.4 Step 4: POD execution

At this point, your POD's requirements have been met, and the environment variables are set. The framework then activates the right Conda environment, and begins execution of your POD's code by calling the top-level driver script listed in its settings.jsonc.

- See Relevant environment variables (page 12) for most relevant environment variables, and how your POD is expected to output results.
- All information passed from the framework to your POD is in the form of Unix/Linux shell environment variables; see reference for a complete list of environment variables (another good source is the log files for individual PODs).
- For debugging, we encourage that your POD print out messages of its progress as it runs. All text written to stdout or stderr (i.e., displayed in a terminal) will be captured by the framework and added to a log file available to the users via index.html.
- Properly structure your code/scripts and include error and exception handling mechanisms so that simple issues will not completely shut down the POD's operation. Here are a few suggestions:
 - A. Separate basic and advanced diagnostics. Certain computations (e.g., fitting) may need adjustment or are more likely to fail when model performance out of observed range. Organize your POD scripts so that the basic part can produce results even when the advanced part fails.
 - B. If some of the observational data files are missing by accident, the POD should still be able to run analysis and produce figures for model data regardless.
 - C. Say a POD reads in multiple variable files and computes statistics for individual variables. If some of the files are missing or corrupted, the POD should still produce results for the rest (note that the framework would skip this POD due to missing data, but PODs should have this robustness property for ease of workarounds or running outside the framework).
- The framework contains additional exception handling so that if a POD experiences a fatal or unrecoverable error, the rest of the tasks and POD-calls by the framework can continue. The error messages, if any, will be included in the POD's log file.

In case your POD requires derived quantities that are not part of the standard model output, and you've incorporated necessary preprocessing into your code (e.g., compute column average temperature from a vertically-resolved temperature field), one might be interested in saving these derived quantities as intermediate output for later use, and you may include this functionality in your code.

- Here we are referring to derived quantities gridded in a similar way to model output, instead of highlydigested data that is just enough for making figures.
- Save these as NetCDF files to the same directory containing the original model files. One file for one variable, following the filename convention spelled out in Getting Started.

⁵⁹ https://github.com/NOAA-GFDL/MDTF-diagnostics/blob/main/src/conda/env_python3_base.yml

You must provide an option so that users can choose not to save the files (e.g., because of write permission, disk space, or files are accessed via soft links). Include this option through pod_env_vars in your POD's settings.jsonc, with "not to save" as default. You can remind users about this option by printing out messages in the terminal during runtime, or include a reminder in your POD documentation.

Example diagnostic

The framework activates the _MDTF_python3_base Conda environment, and calls the driver script example-diag.py⁶⁰ listed in settings.jsonc. Take a look at the script and the comments therein.

example-diag.py performs tasks roughly in the following order:

- 1) It reads the model surface air temperature data at input_path,
- 2) computes the model time average,
- 3) saves the model time averages to \$WK_DIR/model/netCDF/temp_means.nc for later use,
- 4) plots model figure \$WK DIR/model/PS/example model plot.eps,
- 5) reads the digested data in time-averaged form at \$OBS_DATA/example_tas_means.nc, and plots the figure to \$WK_DIR/obs/PS/example_obs_plot.eps.

Note that these tasks correspond to the code blocks 1) through 5) in the script.

- When the script is called and running, it prints out messages which are saved in example.log. These are helpful to determine when and how the POD execution is interrupted if there's a problem.
- The script is organized to deal with model data first, and then to process digested observations. Thus if something goes wrong with the digested data, the script is still able to produce the html page with model figures. This won't happen if code block 5) is moved before 4), i.e., well-organized code is more robust and may be able to produce partial results even when it encounters problems.

In code block 7) of example-diag.py, we include an example of exception handling by trying to access a non-existent file (the final block is just to confirm that the error would not interrupt the script's execution because of exception-handling).

• The last few lines of example.log demonstrate the script is able to finish execution despite an error having occurred. Exception handling makes code robust.

1.7.5 Step 5: Output and cleanup

At this point, your POD has successfully finished running, and all remaining tasks are handled by the framework. The framework converts the postscript plots to bitmaps according to the following rule:

- \$WK_DIR/model/PS/filename.eps → \$WK_DIR/model/filename.png
- \$WK_DIR/obs/PS/filename.eps → \$WK_DIR/obs/filename.png

The html template for each POD is then copied to \$WK DIR by the framework.

 $^{^{60}\} https://github.com/NOAA-GFDL/MDTF-diagnostics/blob/main/diagnostics/example/example_diag.py$

- In writing the template file all plots should be referenced as relative links to this location, e.g., "". See templates from existing PODs.
- Values of all environment variables referenced in the html template are substituted by the framework, allowing you to show the run's CASENAME, date range, etc. Text you'd like to change at runtime must be changed through environment variables (the v3 framework doesn't allow other ways to alter the text of your POD's output webpage at runtime).
- If save_ps and save_nc are set to false, the .eps and .nc files will be deleted.

Finally, the framework links your POD's html page to the top-level index.html, and copies all files to the specified output location (OUTPUT_DIR in default_tests.jsonc; same as WK_DIR by default).

• If make_variab_tar in default_tests.jsonc is set to true, the framework will create a tar file for the output directory, in case you're working on a server, and have to move the file to a local machine before viewing it.

Example diagnostic

Open the html template diagnostics/example/example.html and the output \$WK_DIR/example.html in a text editor, and compare. All the environment variables in the template have been substituted, e.g., {EXAMPLE_FAV_COLOR} becomes blue (defined in pod_env_vars in settings.jsonc).

1.8 POD coding best practices

In this section we describe issues we've seen in POD code that have caused problems in the form of bugs, inefficiencies, or unintended consequences.

1.8.1 All languages

• PS vs. EPS figures: Save vector plots as .eps (Encapsulated PostScript), not .ps (regular PostScript).

Why: Postscript (.ps) is perhaps the most common vector graphics format, and almost all plotting packages are able to output postscript files. Encapsulated Postscript⁶¹ (.eps) includes bounding box information that describes the physical extent of the plot's contents. This is used by the framework to generate bitmap versions of the plots correctly: the framework calls ghostscript⁶² for the conversion, and if not provided with a bounding box ghostscript assumes the graphics use an entire sheet of (letter or A4) paper. This can cause plots to be cut off if they extend outside of this region.

Note that many plotting libraries will set the format of the output file automatically from the filename extension. The framework will process both *.ps and *.eps files.

⁶¹ https://en.wikipedia.org/wiki/Encapsulated_PostScript

⁶² https://www.ghostscript.com/

1.8.2 Python: General

• Whitespace: Indent python code with four spaces per indent level.

Why: Python uses indentation to delineate nesting and scope within a program, and indentation that's not done consistently is a syntax error. Using four spaces is not required, but is the generally accepted standard.

Indentation can be configured in most text editors, or fixed with scripts such as reindent.py described here⁶³. We recommend using a linter⁶⁴ such as pylint to find common bugs and syntax errors.

Beyond this, we don't impose requirements on how your code is formatted, but voluntarily following standard best practices (such as described in PEP8⁶⁵ or the Google style guide⁶⁶) will make it easier for you and others to understand your code, find bugs, etc.

• Filesystem commands: Use commands in the os⁶⁷ and shutil⁶⁸ modules to interact with the filesystem, instead of running unix commands using os.system(), commands (which is deprecated), or subprocess.

Why: Hard-coding unix commands makes code less portable. Calling out to a subprocess introduces overhead and makes error handling and logging more difficult. The main reason, however, is that Python already provides these tools in a portable way. Please see the documentation for the os⁶⁹ and shutil⁷⁰ modules, summarized in this table:

Table 2: Recommended python functions for filesystem interaction

Task	Recommended function
Construct a path from dir1, dir2,, filename	os.path.join ⁷¹ (dir1, dir2,, filename)
Split a path into directory and filename	os.path.split ⁷² (path) and related functions in
	os.path ⁷³
List files in directory dir	os.scandir ⁷⁴ (dir)
Move or rename a file or directory from old_path to	shutil.move ⁷⁵ (old_path, new_path)
new_path	
Create a directory or sequence of directories dir	os.makedirs ⁷⁶ (dir)
Copy a file from path to new_path	shutil.copy2 ⁷⁷ (path, new_path)
Copy a directory dir, and everything inside it, to	shutil.copytree ⁷⁸ (dir, new_dir)
new_dir	
Delete a single file at path	os.remove ⁷⁹ (path)
Delete a directory dir and everything inside it	shutil.rmtree ⁸⁰ (dir)

⁶³ https://stackoverflow.com/q/1024435

⁶⁴ https://books.agiliq.com/projects/essential-python-tools/en/latest/linters.html

⁶⁵ https://www.python.org/dev/peps/pep-0008/

⁶⁶ https://github.com/google/styleguide/blob/gh-pages/pyguide.md

⁶⁷ https://docs.python.org/3.7/library/os.html

⁶⁸ https://docs.python.org/3.7/library/shutil.html

⁶⁹ https://docs.python.org/3.7/library/os.html

⁷⁰ https://docs.python.org/3.7/library/shutil.html

In particular, using os.path.join 81 is more verbose than joining strings but eliminates bugs arising from missing or redundant directory separators.

1.8.3 Python: Arrays

To obtain acceptable performance for numerical computation, people use Python interfaces to optimized, compiled code. NumPy⁸² is the standard module for manipulating numerical arrays in Python. xarray⁸³ sits on top of NumPy and provides a higher-level interface to its functionality; any advice about NumPy applies to it as well.

NumPy and xarray both have extensive documentation and many tutorials, such as:

- NumPy's own basic⁸⁴ and intermediate⁸⁵ tutorials; xarray's overview⁸⁶ and climate and weather examples⁸⁷;
- A demonstration⁸⁸ of the features of xarray using earth science data;
- The 2020 SciPy conference has open-source, interactive tutorials⁸⁹ you can work through on your own machine or fully online using Binder⁹⁰. In particular, there are tutorials for NumPy⁹¹ and xarray⁹².
- Eliminate explicit for loops: Use NumPy/xarray functions instead of writing for loops in Python that loop over the indices of your data array. In particular, nested for loops on multidimensional data should never need to be used.

Why: For loops in Python are very slow compared to C or Fortran, because Python is an interpreted language. You can think of the NumPy functions as someone writing those for-loops for you in C, and giving you a way to call it as a Python function.

It's beyond the scope of this document to cover all possible situations, since this is the main use case for NumPy. We refer to the tutorials above for instructions, and to the following blog posts that discuss this specific issue:

⁷¹ https://docs.python.org/3.7/library/os.path.html?highlight=os%20path#os.path.join

⁷² https://docs.python.org/3.7/library/os.path.html?highlight=os%20path#os.path.split

⁷³ https://docs.python.org/3.7/library/os.path.html?highlight=os%20path

⁷⁴ https://docs.python.org/3.7/library/os.html#os.scandir

⁷⁵ https://docs.python.org/3.7/library/shutil.html#shutil.move

⁷⁶ https://docs.python.org/3.7/library/os.html#os.makedirs

⁷⁷ https://docs.python.org/3.7/library/shutil.html#shutil.copy2

⁷⁸ https://docs.python.org/3.7/library/shutil.html#shutil.copytree

⁷⁹ https://docs.python.org/3.7/library/os.html#os.remove

⁸⁰ https://docs.python.org/3.7/library/shutil.html#shutil.rmtree

⁸¹ https://docs.python.org/3.7/library/os.path.html?highlight=os%20path#os.path.join

⁸² https://numpy.org/doc/stable/index.html

⁸³ http://xarray.pydata.org/en/stable/index.html

⁸⁴ https://numpy.org/doc/stable/user/absolute beginners.html

⁸⁵ https://numpy.org/doc/stable/user/quickstart.html

⁸⁶ http://xarray.pydata.org/en/stable/quick-overview.html

⁸⁷ http://xarray.pydata.org/en/stable/examples.html

⁸⁸ https://rabernat.github.io/research_computing/xarray.html

⁸⁹ https://www.scipy2020.scipy.org/tutorial-information

⁹⁰ https://mybinder.org/

⁹¹ https://github.com/enthought/Numpy-Tutorial-SciPyConf-2020

⁹² https://xarray-contrib.github.io/xarray-tutorial/index.html

- "Look Ma, no for-loops⁹³," by Brad Solomon;
- "Turn your conditional loops to Numpy vectors⁹⁴," by Tirthajyoti Sarkar;
- "Vectorized' Operations: Optimized Computations on NumPy Arrays⁹⁵", part of "Python like you mean it⁹⁶," a free resource by Ryan Soklaski.
- Use xarray with netCDF data:

Why: This is xarray's use case. You can think of NumPy as implementing multidimensional matrices in the fully general, mathematical sense, and xarray providing the specialization to the case where the matrix contains data on a lat-lon-time-(etc.) grid.

xarray lets you refer to your data with human-readable labels such as 'latitude,' rather than having to remember that that's the second dimension of your array. This bookkeeping is essential when writing code for the MDTF framework, when your POD will be run on data from models you haven't been able to test on.

In particular, xarray provides seamless support for time axes⁹⁷, with support⁹⁸ for all CF convention calendars through the cftime library. You can, eg, subset a range of data between two dates without having to manually convert those dates to array indices.

See the xarray tutorials linked above for more examples of xarray's features.

• Memory use and views vs. copies: Use scalar indexing and slices⁹⁹ (index specifications of the form start_index:stop_index:stride) to get subsets of arrays whenever possible, and only use advanced indexing to features (indexing arrays with other arrays) when necessary.

Why: When advanced indexing is used, NumPy will need to create a new copy of the array in memory, which can hurt performance if the array contains a large amount of data. By contrast, slicing or basic indexing is done in-place, without allocating a new array: the NumPy documentation calls this a "view."

Note that array slices are native Python objects¹⁰¹, so you can define a slice in a different place from the array you intend to use it on. Both NumPy and xarray arrays recognize slice objects.

This is easier to understand if you think about NumPy as a wrapper around C-like functions: array indexing in C is implemented with pointer arithmetic, since the array is implemented as a contiguous block of memory. An array slice is just a pointer to the same block of memory, but with different offsets. More complex indexing isn't guaranteed to follow a regular pattern, so NumPy needs to copy the requested data in that case.

See the following references for more information:

- The NumPy documentation¹⁰² on indexing;

⁹³ https://realpython.com/numpy-array-programming/

⁹⁴ https://towardsdatascience.com/data-science-with-python-turn-your-conditional-loops-to-numpy-vectors-9484ff9c622e

⁹⁵ https://www.pythonlikeyoumeanit.com/Module3_IntroducingNumpy/VectorizedOperations.html

⁹⁶ https://www.pythonlikeyoumeanit.com/

⁹⁷ http://xarray.pydata.org/en/stable/time-series.html

⁹⁸ http://xarray.pydata.org/en/stable/weather-climate.html

⁹⁹ https://numpy.org/doc/stable/reference/arrays.indexing.html#basic-slicing-and-indexing

¹⁰⁰ https://numpy.org/doc/stable/reference/arrays.indexing.html#advanced-indexing

¹⁰¹ https://docs.python.org/3.7/library/functions.html?highlight=slice#slice

¹⁰² https://numpy.org/doc/stable/reference/arrays.indexing.html

- "Numpy Views vs Copies: Avoiding Costly Mistakes¹⁰³," by Jessica Yung;
- "How can I tell if NumPy creates a view or a copy? 104" on stackoverflow.
- MaskedArrays instead of NaNs or sentinel values: Use NumPy's MaskedArrays¹⁰⁵ for data that may contain missing or invalid values, instead of setting those entries to NaN or a sentinel value.

Why: One sometimes encounters code which sets array entries to fixed "sentinel values" (such as 1.0e+20 or NaN^{106}) to indicate missing or invalid data. This is a dangerous and error-prone practice, since it's frequently not possible to detect if the invalid entries are being used by mistake. For example, computing the variance of a timeseries with missing elements set to 1e+20 will either result in a floating-point overflow, or return zero.

NumPy provides a better solution in the form of MaskedArrays¹⁰⁷, which behave identically to regular arrays but carry an extra boolean mask to indicate valid/invalid status. All the NumPy mathematical functions will automatically use this mask for error propagation. For example¹⁰⁸, trying to divide an array element by zero or taking the square root of a negative element will mask it off, indicating that the value is invalid: you don't need to remember to do these sorts of checks explicitly.

1.8.4 Python: Plotting

• Use the 'Agg' backend when testing your POD: For reproducibility, set the shell environment variable MPLBACKEND to Agg when testing your POD outside of the framework.

Why: Matplotlib can use a variety of backends¹⁰⁹: interfaces to low-level graphics libraries. Some of these are platform-dependent, or require additional libraries that the MDTF framework doesn't install. In order to achieve cross-platform portability and reproducibility, the framework specifies the 'Agg' non-interactive (ie, writing files only) backend for all PODs, by setting the MPLBACKEND environment variable.

When developing your POD, you'll want an interactive backend – for example, this is automatically set up for you in a Jupyter notebook. When it comes to testing your POD outside of the framework, however, you should be aware of this backend difference.

1.8.5 NCL

• Deprecated calendar functions: Check the function reference¹¹⁰ to verify that the functions you use are not deprecated in the current version of NCL¹¹¹. This is especially necessary for date/calendar functions¹¹².

¹⁰³ https://www.jessicayung.com/numpy-views-vs-copies-avoiding-costly-mistakes/

¹⁰⁴ https://stackoverflow.com/questions/11524664/how-can-i-tell-if-numpy-creates-a-view-or-a-copy

¹⁰⁵ https://numpy.org/doc/stable/reference/maskedarray.generic.html

¹⁰⁶ https://en.wikipedia.org/wiki/NaN

¹⁰⁷ https://numpy.org/doc/stable/reference/maskedarray.html

¹⁰⁸ https://numpy.org/doc/stable/reference/maskedarray.generic.html#numerical-operations

¹⁰⁹ https://matplotlib.org/tutorials/introductory/usage.html#backends

¹¹⁰ https://www.ncl.ucar.edu/Document/Functions/index.shtml

¹¹¹ https://www.ncl.ucar.edu/

¹¹² https://www.ncl.ucar.edu/Document/Functions/date.shtml

Why: The framework uses a current version of NCL^{113} (6.6.x), to avoid plotting bugs that were present in earlier versions. This is especially relevant for calendar functions: the ut_* set of functions have been deprecated in favor of counterparts beginning with cd_ that take identical arguments (so code can be updated using find/replace). For example, use cd_calendar¹¹⁴ instead of the deprecated ut calendar¹¹⁵.

This change is necessary because only the cd_* functions support all calendars defined in the CF conventions, which is needed to process data from some models (eg, weather or seasonal models are typically run with a Julian calendar.)

1.9 Git-based development workflow

We recommend developers to manage the MDTF package using the GitHub webpage interface:

- If you have no prior experience with GitHub¹¹⁶, create an account first.
- Create a fork of the project by clicking the Fork button in the upper-right corner of NOAA's MDTF GitHub page¹¹⁷. This will create a copy (also known as repository, or simply repo) in your own GitHub account which you have full control over.
- Before you start working on the code, remember to switch to the develop branch (instead of main) as expected from a POD developer.

It should be easy to figure out how to add/edit files through your repo webpage interface.

- After updating the code in your repo, submit a Pull request so that the changes you have made can be incorporated into the official NOAA's repo.
- Your changes will not affect the official NOAA's repo until the pull request is accepted by the lead-team programmer.

Note that if any buttons are missing, try CRTL + + or CRTL + - to adjust the webpage font size so the missing buttons may magically appear.

Managing through the webpage interface as described above is quick and easy. Another approach, unfortunately with a steeper learning curve, is to create a local repo on your machine and manage the code using the git command in a terminal. In the interests of making things self-contained, the rest of this section gives brief step-by-step instructions on git for interested developers.

Before following the instructions below, make sure that a) you've created a fork of the project, and b) the git command is available on your machine (installation instructions 118).

¹¹³ https://www.ncl.ucar.edu/

¹¹⁴ https://www.ncl.ucar.edu/Document/Functions/Built-in/cd_calendar.shtml

¹¹⁵ https://www.ncl.ucar.edu/Document/Functions/Built-in/ut_calendar.shtml

¹¹⁶ https://github.com/

¹¹⁷ https://github.com/NOAA-GFDL/MDTF-diagnostics

¹¹⁸ https://git-scm.com/download/

1.9.1 Some online git resources

If you are new to git and unfamiliar with many of the terminologies, Dangit, Git?!¹¹⁹ provides solutions in plain English to many common mistakes people have made.

There are many comprehensive online git tutorials, such as:

- The official git tutorial ¹²⁰.
- A more verbose introduction 121 to the ideas behind git and version control.
- A still more detailed walkthrough 122, assuming no prior knowledge.

1.9.2 Set up SSH with GitHub

- You have to generate an SSH key¹²³ and add it¹²⁴ to your GitHub account. This will save you from having to re-enter your GitHub username and password every time you interact with their servers.
- When generating the SSH key, you'll be asked to pick a passphrase (i.e., password).
- The following instructions assume you've generated an SSH key. If you're using manual authentication instead, replace the "git@github.com:" addresses in what follows with "https://github.com/".

1.9.3 Clone a local repository onto your machine

- Clone your fork onto your computer: git clone git@github.com:<your_github_account>/ MDTF-diagnostics.git. This not only downloads the files, but due to the magic of git also gives you the full commit history of all branches.
- Enter the project directory: cd MDTF-diagnostics.
- Clone additional dependencies of the code: git submodule update --recursive --init.
- Git knows about your fork, but you need to tell it about NOAA's repo if you wish to contribute changes back to the code base. To do this, type git remote add upstream git@github.com:NOAA-GFDL/MDTF-diagnostics.git. Now you have two remote repos: origin, your GitHub fork which you can read and write to, and upstream, NOAA's code base which you can only read from.

¹¹⁹ https://dangitgit.com/

¹²⁰ https://git-scm.com/docs/gittutorial

¹²¹ https://www.atlassian.com/git/tutorials/what-is-version-control

¹²² http://swcarpentry.github.io/git-novice/

¹²³ https://help.github.com/en/articles/generating-a-new-ssh-key-and-adding-it-to-the-ssh-agent

¹²⁴ https://help.github.com/en/articles/adding-a-new-ssh-key-to-your-github-account

1.9.4 Start coding

- Switch to the develop branch: git checkout develop.
- If it's been a while since you created your fork, other people may have updated NOAA's develop branch. To make sure you're up-to-date, get these changes with git pull upstream develop and git submodule update --recursive --remote.
- That command updates the working copy on your computer, but you also need to tell your fork on GitHub about the changes: git push origin develop.
- Now you're up-to-date and ready to start working on a new feature. git checkout -b feature/ <my_feature_name> will create a new branch (-b flag) off of develop and switch you to working on that branch.
 - If you are unfamiliar with git and want to practice with the commands listed here, we recommend
 you to create an additional feature branch just for this. Remember: your changes will not affect
 NOAA's repo until you've submitted a pull request through the GitHub webpage and accepted by
 the lead-team programmer.
 - If you encounter problems during practice, you can first try looking for plain English instructions to unmess the situation at Dangit, Git?!¹²⁵.
- Write your code! A useful command is git status to remind you what branch you're on and changes you've made (but have not committed yet). git branch -a lists all branches with * indicating the branch you're on.
- If you've added new files, git add --all before commit the changes.
- Commit changes with git commit -a. This creates a snapshot of the code into the history in your local repo.
 - The snapshot will exist until you intentionally delete it (after confirming a warning message).
 You can always revert to a previous snapshot.
 - Don't commit code that you know is buggy or non-functional!
 - You'll be asked to enter a commit message. Good commit messages are key to making the project's history useful.
 - Write in present tense describing what the commit, when applied, does to the code not what you did to the code.
 - Messages should start with a brief, one-line summary, less than 80 characters. If this is too short, you may want to consider entering your changes as multiple commits.
- When finish updating your feature, merge it back into develop: first git checkout develop then git merge --no-ff feature/<my_feature_name>. The '-no-ff' flag is important: it tells git not to compress ("fast-forward") your commit history onto the develop branch.
- git push origin so that the changes to your local repo is incorporated to the your GitHub fork (displayed on the webpage).
 - Enter the SSH key passphrase when asked for password.

¹²⁵ https://dangitgit.com/

- If you haven't finished working on your feature, you can checkout and update the local feature branch again by repeating the above commands.
- When your feature is ready, submit a pull request by going to the GitHub page of your fork and clicking on the Pull request button. This is your proposal to the maintainers to incorporate your feature into NOAA's repo.
- When the feature branch is no longer needed, delete the branch locally with git branch -d feature/<my_feature_name>. If you pushed it to your fork, you can delete it remotely with git push --delete origin feature/<my_feature_name>.
 - Remember that branches in git are just pointers to a particular commit, so by deleting a branch you don't lose any history.
- If you want to let others work on your feature, push its branch to your GitHub fork with git push -u origin feature/<my_feature_name>. The -u flag is for creating a new branch remotely and only needs to be used the first time.

CHAPTER

TWO

FRAMEWORK REFERENCE

2.1 Diagnostic settings file format

The settings file is how your diagnostic tells the framework what it needs to run, in terms of software and model data.

Each diagnostic must contain a text file named settings.jsonc in the JSON¹²⁶ format, with the addition that any text to the right of // is treated as a comment and ignored (sometimes called the "JSONC" format).

2.1.1 Brief summary of JSON

We'll briefly summarize subset of JSON syntax used in this configuration file. The file's JSON expressions are built up out of items, which may be either

- 1. a boolean, taking one of the values true or false (lower-case, with no quotes).
- 2. a number (integer or floating-point).
- 3. a case-sensitive string, which must be delimited by double quotes.

In addition, for the purposes of the configuration file we define

4. a "unit-ful quantity": this is a string containing a number followed by a unit, eg. "6hr". In addition, the string "any" may be used to signify that any value is acceptable.

Items are combined in compound expressions of two types:

- 5. arrays, which are one-dimensional ordered lists delimited with square brackets. Entries can be of any type, eg [true, 1, "two"].
- 6. objects, which are un-ordered lists of key:value pairs separated by colons and delimited with curly brackets. Keys must be strings and must all be unique within the object, while values may be any expression, eg. {"red": 0, "green": false, "blue": "bagels"}.

Compound expressions may be nested within each other to an arbitrary depth.

¹²⁶ https://en.wikipedia.org/wiki/JSON#Data_types_and_syntax

2.1.2 File organization

```
{
  "settings" : {
    <...properties describing the diagnostic..>
  },
  "data" : {
   <...properties for all requested model data...>
  },
  "dimensions" : {
    "my_first_dimension": {
      <...properties describing this dimension...>
   },
    "my_second_dimension": {
      <...properties describing this dimension...>
   },
  },
  "varlist" : {
   "my_first_variable": {
      <...properties describing this variable...>
   },
   "my_second_variable": {
      <...properties describing this variable...>
   },
 }
}
```

At the top level, the settings file is an object (page 32) containing four required entries, described in detail below.

- settings (page 34): properties that label the diagnostic and describe its runtime requirements.
- data (page 35): properties that apply to all the data your diagnostic is requesting.
- dimensions (page 37): properties that apply to the dimensions (in netCDF¹²⁷ terminology) of the model data. Each distinct dimension (coordinate axis) of the data being requested should be listed as a separate entry here.
- varlist (page 39): properties that describe the individual variables your diagnostic operates on. Each variable should be listed as a separate entry here.

¹²⁷ https://www.unidata.ucar.edu/software/netcdf/workshops/2010/datamodels/NcDims.html

2.1.3 Settings section

This section is an object (page 32) containing properties that label the diagnostic and describe its runtime requirements.

Example

```
"settings" : {
   "long_name" : "Effect of X on Y diagnostic",
   "driver" : "my_script.py",
   "realm" : ["atmos", "ocean"],
   "runtime_requirements": {
        "python": ["numpy", "matplotlib", "netCDF4", "cartopy"],
        "ncl": ["contributed", "gsn_code", "gsn_csm"]
   },
   "pod_env_vars" : {
        // RES: Spatial Resolution (degree) for Obs Data (0.25, 0.50, 1.00).
        "RES": "1.00"
   }
}
```

Diagnostic description

long_name: String, required. Human-readable display name of your diagnostic. This is the text used to describe your diagnostic on the top-level index.html page. It should be in sentence case (capitalize first word and proper nouns only) and omit any punctuation at the end.

driver: String, required. Filename of the top-level driver script the framework should call to run your diagnostic's analysis.

realm: String or array (page 32) (list) of strings, required. One of the eight CMIP6 modeling realms (aerosol, atmos, atmosChem, land, landIce, ocean, ocnBgchem, seaIce) describing what data your diagnostic uses. If your diagnostic uses data from multiple realms, list them in an array (eg. ["atmos", "ocean"]). This information doesn't affect how the framework fetches model data for your diagnostic: it's provided to give the user a shortcut to say, eg., "run all the atmos diagnostics on this output."

Diagnostic runtime

runtime_requirements: object (page 32), required. Programs your diagnostic needs to run (for example, scripting language interpreters) and any third-party libraries needed in those languages. Each executable should be listed in a separate key-value pair:

• The key is the name of the required executable, eg. languages such as "python¹²⁸" or "ncl¹²⁹" etc. but also any utilities such as "ncks¹³⁰", "cdo¹³¹", etc.

¹²⁸ https://www.python.org/

¹²⁹ https://www.ncl.ucar.edu/

¹³⁰ http://nco.sourceforge.net/

¹³¹ https://code.mpimet.mpg.de/projects/cdo

• The value corresponding to each key is an array (page 32) (list) of strings, which are names of third-party libraries in that language that your diagnostic needs. You do not need to list standard libraries or scripts that are provided in a standard installation of your language: eg, in python, you need to list numpy 132 but not math 133. If no third-party libraries are needed, the value should be an empty list.

In the future we plan to offer the capability to request specific versions¹³⁴. For now, please communicate your diagnostic's version requirements to the MDTF organizers.

pod_env_vars: object (page 32), optional. Names and values of shell environment variables used by your diagnostic, in addition to those supplied by the framework. The user can't change these at runtime, but this can be used to set site-specific installation settings for your diagnostic (eg, switching between low-and high-resolution observational data depending on what the user has chosen to download). Note that environment variable values must be provided as strings.

2.1.4 Data section

This section is an object (page 32) containing properties that apply to all the data your diagnostic is requesting.

Example

```
"data": {
    "format": "netcdf4_classic",
    "rename_dimensions": false,
    "rename_variables": false,
    "multi_file_ok": true,
    "frequency": "3hr",
    "min_frequency": "1hr",
    "max_frequency": "6hr",
    "min_duration": "5yr",
    "max_duration": "any"
}
```

Example

format: String. Optional: assumed "any_netcdf_classic" if not specified. Specifies the format(s) of model data your diagnostic is able to read. As of this writing, the framework only supports retrieval of netCDF formats, so only the following values are allowed:

```
• "any_netcdf" includes all of:
```

```
- "any_netcdf3" includes all of:
    * "netcdf3_classic" (CDF-1, files restricted to < 2 Gb)
    * "netcdf3_64bit_offset" (CDF-2)</pre>
```

¹³² https://numpy.org/

 $^{^{133}\} https://docs.python.org/3/library/math.html$

¹³⁴ https://docs.conda.io/projects/conda/en/latest/user-guide/concepts/pkg-specs.html#package-match-specifications

```
* "netcdf3_64bit_data" (CDF-5)
- "any_netcdf4" includes all of:
    * "netcdf4_classic"
    * "netcdf4"
```

• "any_netcdf_classic" includes all the above except "netcdf4" (classic data model only).

See the netCDF FAQ¹³⁵ (under "Formats, Data Models, and Software Releases") for information on the distinctions. Any recent version of a supported language for diagnostics with netCDF support will be able to read all of these. However, the extended features of the "netcdf4" data model are not commonly used in practice and currently only supported at a beta level in NCL, which is why we've chosen "any_netcdf_classic" as the default.

- rename_dimensions: Boolean. Optional: assumed false if not specified. If set to true, the framework will change the name of all dimensions (page 37) in the model data from the model's native value to the string specified in the name property for that dimension. If set to false, the diagnostic is responsible for reading dimension names from the environment variable. See the environment variable documentation (page 42) for details on how these names are provided.
- rename_variables: Boolean. Optional: assumed false if not specified. If set to true, the framework will change the name of all variables (page 39) in the model data from the model's native value to the string specified in the name property for that variable. If set to false, the diagnostic is responsible for reading dimension names from the environment variable. See the environment variable documentation (page 42) for details on how these names are provided.
- multi_file_ok: Boolean. Optional: assumed false if not specified. If set to true, the diagnostic can handle datasets for a single variable spread across multiple files, eg xarray¹³⁶.
- min_duration, max_duration: Unit-ful quantities (page 32). Optional: assumed "any" if not specified. Set minimum and maximum length of the analysis period for which the diagnostic should be run: this overrides any choices the user makes at runtime. Some example uses of this setting are:
 - If your diagnostic uses low-frequency (eg seasonal) data, you may want to set min_duration to ensure the sample size will be large enough for your results to be statistically meaningful.
 - On the other hand, if your diagnostic uses high-frequency (eg hourly) data, you may want to set max_duration to prevent the framework from attempting to download a large volume of data for your diagnostic if the framework is called with a multi-decadal analysis period.

The following properties can optionally be set individually for each variable in the varlist section (page 39). If so, they will override the global settings given here.

- dimensions_ordered: Boolean. Optional: assumed false if not specified. If set to true, the framework will ensure that the dimensions of each variable's array are given in the same order as listed in dimensions. If set to false, your diagnostic is responsible for handling arbitrary dimension orders: eg. it should not assume that 3D data will be presented as (time, lat, lon).
- frequency, min_frequency, max_frequency: Unit-ful quantities (page 32). Time frequency at which the data is provided. Either frequency or the min/max pair, or both, is required:

¹³⁵ https://www.unidata.ucar.edu/software/netcdf/docs/faq.html

¹³⁶ http://xarray.pydata.org/en/stable/generated/xarray.open_mfdataset.html

- If only frequency is provided, the framework will attempt to obtain data at that frequency. If that's not available from the data source, your diagnostic will not run.
- If the min/max pair is provided, the diagnostic must be capable of using data at any frequency within that range (inclusive). The diagnostic is responsible for determining the frequency if this option is used.
- If all three properties are set, the framework will first attempt to find data at frequency. If that's not available, it will try data within the min/max range, so your code must be able to handle this possibility.

2.1.5 Dimensions section

This section is an object (page 32) contains properties that apply to the dimensions of model data. "Dimensions" are meant in the sense of the netCDF data model¹³⁷: informally, they are "coordinate axes" holding the values of independent variables that the dependent variable is sampled at.

All dimensions (page 41) and scalar coordinates (page 41) referenced by variables in the variest section must have an entry in this section. If two variables reference the same dimension, they will be sampled on the same set of values.

Note that the framework only supports the (simplest and most common) "independent axes" case of the CF conventions 138. In particular, the framework only deals with data on lat-lon grids.

Example

```
"dimensions": {
 "lat": {
     "standard_name": "latitude",
     "units": "degrees_N",
     "range": [-90, 90],
     "need bounds": false
 },
 "lon": {
     "standard name": "longitude",
     "units": "degrees E",
     "range": [-180, 180],
     "need bounds": false
 },
 "plev": {
     "standard_name": "air_pressure",
     "units": "hPa",
     "positive": "down",
     "need_bounds": false
 },
 "time": {
```

(continues on next page)

¹³⁷ https://www.unidata.ucar.edu/software/netcdf/workshops/2010/datamodels/NcDims.html

 $^{^{138}\} http://cfconventions.org/Data/cf-conventions/cf-conventions-1.8/cf-conventions.html \#_independent_latitude_longitude_vertical_and_time_axes$

(continued from previous page)

```
"standard_name": "time",
    "units": "days",
    "calendar": "noleap",
    "need_bounds": false
}
```

Latitude and Longitude

standard_name: Required, string. Must be "latitude" and "longitude", respectively.

- units: Optional. String, following syntax of the UDUnits library¹³⁹. Units the diagnostic expects the dimension to be in. Currently the framework only supports decimal degrees_north and degrees_east, respectively.
- range: Array (page 32) (list) of two numbers. Optional. If given, specifies the range of values the diagnostic expects this dimension to take. For example, "range": [-180, 180] for longitude will have the first entry of the longitude variable in each data file be near -180 degrees (not exactly -180, because dimension values are cell midpoints), and the last entry near +180 degrees.
- need_bounds: Boolean. Optional: assumed false if not specified. If true, the framework will ensure that bounds are supplied for this dimension, in addition to its midpoint values, following the CF conventions¹⁴⁰: the bounds attribute of this dimension will be set to the name of another netCDF variable containing the bounds information.

Time

standard_name: Required. Must be "time".

- units: String. Optional, defaults to "day". Units the diagnostic expects the dimension to be in. Currently the diagnostic only supports time axes of the form "<units> since <reference data>", and the value given here is interpreted in this sense (eg. settings this to "day" would accommodate a dimension of the form "[decimal] days since 1850-01-01".)
- calendar: String, Optional. One of the CF convention calendars or the string "any". Defaults to "any" if not given. Calendar convention used by your diagnostic. Only affects the number of days per month.
- need_bounds: Boolean. Optional: assumed false if not specified. If true, the framework will ensure that bounds are supplied for this dimension, in addition to its midpoint values, following the CF conventions¹⁴²: the bounds attribute of this dimension will be set to the name of another netCDF variable containing the bounds information.

¹³⁹ https://www.unidata.ucar.edu/software/udunits/udunits-2.0.4/udunits2lib.html#Syntax

¹⁴⁰ http://cfconventions.org/Data/cf-conventions/cf-conventions-1.8/cf-conventions.html#cell-boundaries

¹⁴¹ http://cfconventions.org/Data/cf-conventions/cf-conventions-1.8/cf-conventions.html#calendar

¹⁴² http://cfconventions.org/Data/cf-conventions/cf-conventions-1.8/cf-conventions.html#cell-boundaries

Z axis (height/depth, pressure, ...)

- standard_name: Required, string. Standard name¹⁴³ of the variable as defined by the CF conventions¹⁴⁴, or a commonly used synonym as employed in the CMIP6 MIP tables.
- units: Optional. String, following syntax of the UDUnits library¹⁴⁵. Units the diagnostic expects the dimension to be in. If not provided, the framework will assume CF convention canonical units¹⁴⁶.
- positive: String, required. Must be "up" or "down", according to the CF conventions 147. A pressure axis is always "down" (increasing values are closer to the center of the earth), but this is not set automatically.
- need_bounds: Boolean. Optional: assumed false if not specified. If true, the framework will ensure that bounds are supplied for this dimension, in addition to its midpoint values, following the CF conventions 148: the bounds attribute of this dimension will be set to the name of another netCDF variable containing the bounds information.

Other dimensions (wavelength, ...)

- standard_name: Required, string. Standard name¹⁴⁹ of the variable as defined by the CF conventions¹⁵⁰, or a commonly used synonym as employed in the CMIP6 MIP tables.
- units: Optional. String, following syntax of the UDUnits library¹⁵¹. Units the diagnostic expects the dimension to be in. If not provided, the framework will assume CF convention canonical units¹⁵².
- need_bounds: Boolean. Optional: assumed false if not specified. If true, the framework will ensure that bounds are supplied for this dimension, in addition to its midpoint values, following the CF conventions¹⁵³: the bounds attribute of this dimension will be set to the name of another netCDF variable containing the bounds information.

2.1.6 Varlist section

This section is an object (page 32) contains properties that apply to the model variables your diagnostic needs for its analysis. "Dimensions" are meant in the sense of the netCDF data model¹⁵⁴: informally, they are the "independent variables" whose values are being computed as a function of the values stored in the dimensions.

¹⁴³ http://cfconventions.org/Data/cf-standard-names/72/build/cf-standard-name-table.html

¹⁴⁴ http://cfconventions.org/

¹⁴⁵ https://www.unidata.ucar.edu/software/udunits/udunits-2.0.4/udunits2lib.html#Syntax

¹⁴⁶ http://cfconventions.org/Data/cf-standard-names/current/build/cf-standard-name-table.html

¹⁴⁷ http://cfconventions.org/faq.html#vertical_coords_positive_attribute

¹⁴⁸ http://cfconventions.org/Data/cf-conventions/cf-conventions-1.8/cf-conventions.html#cell-boundaries

¹⁴⁹ http://cfconventions.org/Data/cf-standard-names/72/build/cf-standard-name-table.html

¹⁵⁰ http://cfconventions.org/

¹⁵¹ https://www.unidata.ucar.edu/software/udunits/udunits-2.0.4/udunits2lib.html#Syntax

¹⁵² http://cfconventions.org/Data/cf-standard-names/current/build/cf-standard-name-table.html

¹⁵³ http://cfconventions.org/Data/cf-conventions/cf-conventions-1.8/cf-conventions.html#cell-boundaries

¹⁵⁴ https://www.unidata.ucar.edu/software/netcdf/workshops/2010/datamodels/NcVars.html

Each entry corresponds to a distinct data file (or set of files, if multi_file_ok is true) downloaded by the framework. If your framework needs the same physical quantity sampled with different properties (eg. slices of a variable at multiple pressure levels), specify them as multiple entries.

Varlist entry example

```
"u500": {
    "standard_name": "eastward_wind",
    "path_variable": "U500_FILE",
    "units": "m s-1",
    "dimensions" : ["time", "lat", "lon"],
    "dimensions_ordered": true,
    "scalar_coordinates": {"pressure": 500},
    "requirement": "optional",
    "alternates": ["another_variable_name", "a_third_variable_name"]
}
```

Varlist entry properties

The key in a varlist key-value pair is the name your diagnostic uses to refer to this variable (and must be unique). The value of the key-value pair is an object (page 32) containing properties specific to that variable:

standard_name: String, required. Standard name¹⁵⁵ of the variable as defined by the CF conventions¹⁵⁶, or a commonly used synonym as employed in the CMIP6 MIP tables (eg. "ua" instead of "eastward wind").

path_variable: String, required. Name of the shell environment variable the framework will set with the location of this data. See the environment variable documentation (page 42) for details.

- If multi_file_ok is false, <path_variable> will be set to the absolute path to the netcdf file containing this variable's data.
- If multi_file_ok is true, <path_variable> will be a single path or a colon-separated list of paths to the files containing this data. Files will be listed in chronological order.
- If the variable is listed as "optional" or "alternate" or has alternate variables listed, <path_variable> will be defined but set to the empty string if the framework couldn't obtain this data from the data source. Your diagnostic should test for this possibility.

use_exact_name: Boolean. Optional: assumed false if not specified. If true, the framework will ignore the model's naming conventions and only look for a variable with a name matching the key of this entry, regardless of what model or data source the framework is using. The only use case for this setting is to give diagnostics the ability to request data that falls outside the CF conventions: in general, you should rely on the framework to translate CF standard names to the native field names of the model being analyzed.

¹⁵⁵ http://cfconventions.org/Data/cf-standard-names/72/build/cf-standard-name-table.html

¹⁵⁶ http://cfconventions.org/

- units: Optional. String, following syntax of the UDUnits library¹⁵⁷. Units the diagnostic expects the variable to be in. If not provided, the framework will assume CF convention canonical units¹⁵⁸.
- dimensions: Required. List of strings, which must be selected the keys of entries in the dimensions (page 37) section. Dimensions of the array containing the variable's data. Note that the framework will not reorder dimensions (transpose) unless dimensions ordered is additionally set to true.
- dimensions_ordered: Boolean. Optional: assumed false if not specified. If true, the framework will ensure that the dimensions of this variable's array are given in the same order as listed in dimensions. If set to false, your diagnostic is responsible for handling arbitrary dimension orders: eg. it should not assume that 3D data will be presented as (time, lat, lon). If given here, overrides the values set globally in the data section (see description (page 36) there).
- scalar_coordinates: object (page 32), optional. This implements what the CF conventions refer to as "scalar coordinates¹⁵⁹", with the use case here being the ability to request slices of higher-dimensional data. For example, the snippet at the beginning of this section shows how to request the u component of wind velocity on a 500 mb pressure level.
 - keys are the key (name) of an entry in the dimensions (page 37) section.
 - values are a single number (integer or floating-point) corresponding to the value of the slice to extract. Units of this number are taken to be the units property of the dimension named as the key.

In order to request multiple slices (eg. wind velocity on multiple pressure levels, with each level saved to a different file), create one varlist entry per slice.

frequency, min_frequency, max_frequency: Unit-ful quantities (page 32). Optional. Time frequency at which the variable's data is provided. If given here, overrides the values set globally in the data section (see description (page 36) there).

requirement: String. Optional: assumed "required" if not specified. One of three values:

- "required": variable is necessary for the diagnostic's calculations. If the data source doesn't provide the variable (at the requested frequency, etc., for the user-specified analysis period) the framework will not run the diagnostic, but will instead log an error message explaining that the lack of this data was at fault.
- "optional": variable will be supplied to the diagnostic if provided by the data source. If not available, the diagnostic will still run, and the path_variable for this variable will be set to the empty string. The diagnostic is responsible for testing the environment variable for the existence of all optional variables.
- "alternate": variable is specified as an alternate source of data for some other variable (see next property). The framework will only query the data source for this variable if it's unable to obtain one of the other variables that list it as an alternate.
- alternates: Array (page 32) (list) of strings, which must be keys (names) of other variables. Optional: if provided, specifies an alternative method for obtaining needed data if this variable isn't provided by the data source.

¹⁵⁷ https://www.unidata.ucar.edu/software/udunits/udunits-2.0.4/udunits2lib.html#Syntax

¹⁵⁸ http://cfconventions.org/Data/cf-standard-names/current/build/cf-standard-name-table.html

 $^{^{159}\} http://cf conventions.org/Data/cf-conventions/cf-conventions-1.8/cf-conventions.html \# scalar-coordinate-variables$

- If the data source provides this variable (at the requested frequency, etc., for the user-specified analysis period), this property is ignored.
- If this variable isn't available as requested, the framework will query the data source for all of the variables listed in this property. If all of the alternate variables are available, the diagnostic will be run; if any are missing it will be skipped. Note that, as currently implemented, only one set of alternates may be given (no "plan B", "plan C", etc.)

2.2 MDTF Environment variables

This page describes the environment variables that the framework will set for your diagnostic when it's run.

2.2.1 Overview

The MDTF framework can be viewed as a "wrapper" for your code that handles data fetching and munging. Your code communicates with this wrapper in two ways:

- The settings file (page 14) is where your code talks to the framework: when you write your code, you document what model data your code uses (not covered on this page, follow the link for details).
- When your code is run, the framework talks to it by setting shell environment variables ¹⁶⁰ containing paths to the data files and other information specific to the run. The framework communicates all runtime information this way: this is in order to 1) pass information in a language-independent way, and 2) to make writing diagnostics easier (you don't need to parse command-line settings).

Note that environment variables are always strings. Your script will need to cast non-text data to the appropriate type (eg. the bounds of the analysis time period, FIRSTYR, LASTYR, will need to be converted to integers.)

Also note that names of environment variables are case-sensitive.

2.2.2 Paths

- OBS_DATA: Path to the top-level directory containing any observational or reference data you've provided as the author of your diagnostic. Any data your diagnostic uses that doesn't come from the model being analyzed should go here (ie, you supply it to the framework maintainers, they host it, and the user downloads it when they install the framework). The framework will ensure this is copied to a local filesystem when your diagnostic is run, but this directory should be treated as read-only.
- POD_HOME: Path to the top-level directory containing your diagnostic's source code. This will be of the form .../MDTF-diagnostics/diagnostics/<your POD's name>. This can be used to call sub-scripts from your diagnostic's driver script. This directory should be treated as read-only.
- WK_DIR: Path to your diagnostic's working directory, which is where all output data should be written (as well as any temporary files).

The framework creates the following subdirectories within this directory:

¹⁶⁰ https://en.wikipedia.org/wiki/Environment_variable

- \$WK_DIR/obs/PS and \$WK_DIR/model/PS: All output plots produced by your diagnostic should be written to one of these two directories. Only files in these locations will be converted to bitmaps for HTML output.
- \$WK_DIR/obs/netCDF and \$WK_DIR/model/netCDF: Any output data files your diagnostic wants to make available to the user should be saved to one of these two directories.

2.2.3 Model run information

CASENAME: User-provided label describing the run of model data being analyzed.

FIRSTYR, LASTYR: Four-digit years describing the analysis period.

2.2.4 Locations of model data files

These are set depending on the data your diagnostic requests in its settings file (page 14). Refer to the examples below if you're unfamiliar with how that file is organized.

Each variable listed in the varlist section of the settings file must specify a path_variable property. The value you enter there will be used as the name of an environment variable, and the framework will set the value of that environment variable to the absolute path to the file containing data for that variable.

From a diagnostic writer's point of view, this means all you need to do here is replace paths to input data that are hard-coded or passed from the command line with calls to read the value of the corresponding environment variable.

- If the framework was not able to obtain the variable from the data source (at the requested frequency, etc., for the user-specified analysis period), this variable will be set equal to the empty string. Your diagnostic is responsible for testing for this possibility for all variables that are listed as optional or have alternates listed (if a required variable without alternates isn't found, your diagnostic won't be run.)
- If multi_file_ok is set to true in the settings file, this environment variable may be a list of paths to multiple files in chronological order, separated by colons. For example, /dir/precip_1980_1989. nc:/dir/precip_1990_1999.nc:/dir/precip_2000_2009.nc for an analysis period of 1980-2009.

2.2.5 Names of variables and dimensions

These are set depending on the data your diagnostic requests in its settings file (page 14). Refer to the examples below if you're unfamiliar with how that file is organized.

For each dimension: If <key> is the name of the key labeling the key:value entry for this dimension, the framework will set an environment variable named <key>_dim equal to the name that dimension has in the data files it's providing.

• If rename_dimensions is set to true in the settings file, this will always be equal to <key>. If If rename_dimensions is false, this will be whatever the model or data source's native name for this dimension is, and your diagnostic should read the name from this variable. Your diagnostic

should only use hard-coded names for dimensions if rename_dimensions is set to true in its settings file (page 32).

For each variable: If <key> be the name of the key labeling the key:value entry for this variable in the variist section, the framework will set an environment variable named <key>_var equal to the name that variable has in the data files it's providing.

• If rename_variables is set to true in the settings file, this will always be equal to <key>. If If rename_variables is false, this will be whatever the model or data source's native name for this variable is, and your diagnostic should read the name from this variable. Your diagnostic should only use hard-coded names for dimensions if rename_dimensions is set to true in its settings file (page 32).

2.2.6 Simple example

We only give the relevant parts of the settings file (page 32) below.

```
"data": {
 "rename_dimensions": false,
  "rename variables": false,
  "multi_file_ok": false,
},
"dimensions": {
  "lat": {
    "standard_name": "latitude",
 },
  "lon": {
    "standard name": "longitude",
   . . .
 },
  "time": {
    "standard_name": "time",
 }
},
"varlist": {
  "pr": {
    "standard_name": "precipitation_flux",
    "path_variable": "PR_FILE"
  }
}
```

The framework will set the following environment variables:

- 1. lat_dim: Name of the latitude dimension in the model's native format (because rename_dimensions is false).
- 2. lon_dim: Name of the longitude dimension in the model's native format (because rename_dimensions is false).

- 3. time_dim: Name of the time dimension in the model's native format (because rename_dimensions is false).
- 4. pr_var: Name of the precipitation variable in the model's native format (because rename_variables is false).
- 5. PR_FILE: Absolute path to the file containing pr data, eg. /dir/precip.nc.

2.2.7 More complex example

Let's elaborate on the previous example, and assume that the diagnostic is being called on model that provides precipitation_flux but not convective_precipitation_flux.

```
"data": {
 "rename_dimensions": true,
  "rename_variables": false,
  "multi_file_ok": true,
},
"dimensions": {
  "lat": {
    "standard_name": "latitude",
  },
  "lon": {
   "standard name": "longitude",
  },
  "time": {
    "standard_name": "time",
  }
},
"varlist": {
  "prc": {
    "standard_name": "convective_precipitation_flux",
    "path_variable": "PRC_FILE",
    "alternates": ["pr"]
  },
  "pr": {
    "standard_name": "precipitation_flux",
    "path variable": "PR FILE"
  }
}
```

Comparing this with the previous example:

- lat_dim, lon_dim and time_dim will be set to "lat", "lon" and "time", respectively, because rename_dimensions is true. The framework will have renamed these dimensions to have these names in all data files provided to the diagnostic.
- prc_var and pr_var will be set to the model's native names for these variables. Names for all variables are always set, regardless of which variables are available from the data source.

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- In this example, PRC_FILE will be set to '', the empty string, because it wasn't found.
- PR_FILE will be set to /dir/precip_1980_1989.nc:/dir/precip_1990_1999.nc:/dir/precip_2000_2009.nc, because multi_file_ok was set to true.

CHAPTER

THREE

ACKNOWLEDGEMENTS

Development of this code framework for process-oriented diagnostics was supported by the National Oceanic and Atmospheric Administration¹⁶¹ (NOAA) Climate Program Office Modeling, Analysis, Predictions and Projections¹⁶² (MAPP) Program (grant # NA18OAR4310280). Additional support was provided by University of California Los Angeles¹⁶³, the Geophysical Fluid Dynamics Laboratory¹⁶⁴, the National Center for Atmospheric Research¹⁶⁵, Colorado State University¹⁶⁶, Lawrence Livermore National Laboratory¹⁶⁷ and the US Department of Energy¹⁶⁸.

Many of the process-oriented diagnostics modules (PODs) were contributed by members of the NOAA Model Diagnostics Task Force¹⁶⁹ under MAPP support. Statements, findings or recommendations in these documents do not necessarily reflect the views of NOAA or the US Department of Commerce.

3.1 Disclaimer

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¹⁶¹ https://www.noaa.gov/

¹⁶² https://cpo.noaa.gov/Meet-the-Divisions/Earth-System-Science-and-Modeling/MAPP

¹⁶³ https://www.ucla.edu/

¹⁶⁴ https://www.gfdl.noaa.gov/

¹⁶⁵ https://ncar.ucar.edu/

¹⁶⁶ https://www.colostate.edu/

¹⁶⁷ https://www.llnl.gov/

¹⁶⁸ https://www.energy.gov/

¹⁶⁹ https://cpo.noaa.gov/Meet-the-Divisions/Earth-System-Science-and-Modeling/MAPP/MAPP-Task-Forces/Model-Diagnostics-Task-Force