
pymake

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CONTENTS

1	Getting Started	3
1.1	Command Line Usage	3
1.2	From Python	5
1.3	Notes	5
2	pymake Installation	7
3	Building Applications	9
4	API-docs	11
4.1	pymake.pymake module	11
4.2	pymake.pymake_build_apps module	13
4.3	pymake.pymake_base module	14
4.4	pymake.pymake_parser module	16
4.5	pymake.plot package	17
4.6	pymake.autotest package	18
4.7	pymake.utils package	25
4.8	pymake package	31
5	Indices and tables	45
	Python Module Index	47
	Index	49

This is a python package for compiling MODFLOW-based and other Fortran, C, and C++ programs. The package determines the build order using a directed acyclic graph and then compiles the source files using GNU compilers (`gcc`, `g++`, `gfortran`) or Intel compilers (`ifort`, `icc`).

pymake can be run from the command line or it can be called from within python. By default, pymake sets the optimization level, Fortran flags, C/C++ flags, and linker flags that are consistent with those used to compile MODFLOW-based programs released by the USGS.

pymake includes example scripts for building MODFLOW 6, MODFLOW-2005, MODFLOW-NWT, MODFLOW-USG, MODFLOW-LGR, MODFLOW-2000, MODPATH 6, MODPATH 7, GSFLOW, VS2DT, MT3DMS, MT3D-USGS, SEAWAT, and SUTRA. Example scripts for creating the utility programs CRT, Triangle, and GRIDGEN are also included. The scripts download the distribution file from the USGS (and other organizations) and compile the source into a binary executable.

The main documentation for the site is organized into the following sections:

GETTING STARTED

Pymake can be used directly from the command line and within a python script. Examples of both use cases are given below.

1.1 Command Line Usage

pymake can be used to compile MODFLOW 6 directly from the command line using the Intel Fortran compiler `ifort` from a subdirectory at the same level as the `src` subdirectory by specifying:

```
python -m pymake ../src/ ../bin/mf6 -mc --subdirs -fc ifort
```

To see help for running from command line, use the following statement.

```
python -m pymake -h
```

The help message identifies required positional arguments and optional arguments that can be provided to override default values.

```
usage: __main__.py [-h] [-fc {ifort,mpiifort,gfortran,ftn,none}] [-cc {gcc,clang,clang++,  
→icc,icl,mpiicc,g++,cl,none}] [-ar {ia32,ia32_intel64,intel64}] [-mc] [-dbl] [-dbg] [-  
→e] [-dr] [-sd] [-ff FFLAGS] [-cf CFLAGS] [-sl {-lc,-lm}] [-mf] [-md] [-cs COMMONSRC] [-  
→ef EXTRAFILES] [-exf EXCLUDEFILES] [-so]  
→[ad APPDIR] [-v] [--keep] [--zip ZIP] [--inplace] [--networkx] [--  
→mb] [-mbd]  
srcdir target
```

This **is** the pymake program **for** compiling fortran, c, **and** c++ source files, such **as** the
→source files that come **with** MODFLOW. The program works by building a directed acyclic
→graph of the module dependencies **and** then compiling the source files **in** the proper
→order.

positional arguments:

srcdir	Path source directory.
target	Name of target to create. (can include path)

optional arguments:

-h, --help	show this help message and exit
-fc {ifort,mpiifort,gfortran,ftn,none}	Fortran compiler to use. (default is gfortran)
-cc {gcc,clang,clang++,icc,icl,mpiicc,g++,cl,none}	

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```

C/C++ compiler to use. (default is gcc)
-ar {ia32,ia32_intel64,intel64}, --arch {ia32,ia32_intel64,intel64}
    Architecture to use for Intel and Microsoft compilers on Windows.
↳ (default is intel64)
-mc, --makeclean    Clean temporary object, module, and source files when done.
↳ (default is False)
-dbl, --double      Force double precision. (default is False)
-dbg, --debug       Create debug version. (default is False)
-e, --expedite      Only compile out of date source files. Clean must not have been
↳ used on previous build. (default is False)
-dr, --dryrun       Do not actually compile. Files will be deleted, if --makeclean
↳ is used. Does not work yet for ifort. (default is False)
-sd, --subdirs      Include source files in srcdir subdirectories. (default is None)
-ff FFLAGS, --fflags FFLAGS
    Additional Fortran compiler flags. Fortran compiler flags should
↳ be enclosed in quotes and start with a blank space or separated from the name (-ff or -
↳ fflags) with a equal sign (-ff='-O3'). (default is None)
-cf CFLAGS, --cflags CFLAGS
    Additional C/C++ compiler flags. C/C++ compiler flags should be
↳ enclosed in quotes and start with a blank space or separated from the name (-cf or --
↳ cflags) with a equal sign (-cf='-O3'). (default is None)
-sl {-lc,-lm}, --syslibs {-lc,-lm}
    Linker system libraries. Linker libraries should be enclosed in
↳ quotes and start with a blank space or separated from the name (-sl or --syslibs) with
↳ a equal sign (-sl='-libgcc'). (default is None)
-mf, --makefile      Create a GNU make makefile. (default is False)
-md, --makefile-dir  GNU make makefile directory. (default is '.')
-cs COMMONSRC, --commonsrc COMMONSRC
    Additional directory with common source files. (default is None)
-ef EXTRAFILES, --extrafiles EXTRAFILES
    List of extra source files to include in the compilation.
↳ extrafiles can be either a list of files or the name of a text file that contains a
↳ list of files. (default is None)
-exf EXCLUDEFILES, --excludefiles EXCLUDEFILES
    List of extra source files to exclude from the compilation.
↳ excludefiles can be either a list of files or the name of a text file that contains a
↳ list of files. (default is None)
-so, --sharedobject  Create shared object or dll on Windows. (default is False)
-ad APPDIR, --appdir APPDIR
    Target path that overrides path defined target path (default is
↳ None)
-v, --verbose       Verbose output to terminal. (default is False)
--keep             Keep existing executable. (default is False)
--zip ZIP          Zip built executable. (default is False)
--inplace          Source files in srcdir are used directly. (default is False)
--networkx         Use networkx package to build Directed Acyclic Graph use to
↳ determine the order source files are compiled in. (default is False)
--mb, --meson-build Use meson to build executable. (default is False)
-mbd, --mesonbuild-dir
    meson directory. (default is '.')

```

Note that the source directory should not contain any bad or duplicate source files as all source files in the source directory, the common source file directory (srcdir2) and the extra files (extrafiles) will be built and linked. Files can be excluded by using the excludefiles command line switch.

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Note that command line arguments for Fortran flags, C/C++ flags, and syslib libraries should be enclosed in quotes and start with a space prior to the first value (`-ff ' -03 '`) or use an equal sign separating the command line argument and the values (`-ff='-03'`). The command line argument to use an `-03` optimization level when compiling MODFLOW 6 with the `ifort` compiler would be:

```
python -m pymake ../src/ ../bin/mf6 -mc --subdirs -fc ifort -ff='-03'
```

1.2 From Python

1.2.1 Script to compile MODFLOW 6

When using the `pymake` object (`Pymake()`) only the positional arguments (`srcdir`, `target`) need to be specified in the script.

```
import pymake
pm = pymake.Pymake()
pm.srcdir = '../src'
pm.target = 'mf6'
pm.include_subdirs = True
pm.build()
```

It is suggested that optional variables required for successful compiling and linking be manually specified in the script to minimize the potential for unsuccessful builds. For MODFLOW 6, subdirectories in the `src` subdirectory need to be included and `'pm.include_subdirs = True'` has been specified in the script. Custom optimization levels and compiler flags could be specified to get consistent builds.

Non-default values for the optional arguments can be specified as command line arguments. For example, MODFLOW 6 could be compiled using Intel compilers instead of the default GNU compilers with the script listed above by specifying:

```
python mymf6script.py -fc ifort -cc icc
```

1.3 Notes

If `gfortran` is used to compile MODFLOW-based codes, the `openspec.f` and `FILESPEC.inc` (MT3DMS) files will automatically be changed to the following so that binary files are created properly using standard Fortran:

```
c -- created by pymake.py
CHARACTER*20 ACCESS,FORM,ACTION(2)
DATA ACCESS/'STREAM'/
DATA FORM/'UNFORMATTED'/
DATA (ACTION(I),I=1,2)/'READ','READWRITE'/
c -- end of include file
```

Use of `STREAM` access does not delete an existing unformatted file before opening it for writing. As a result, data from previous runs may exist in the file if the model is run for a shorter period of time. This does not apply to MODFLOW 6 simulations.

PYMAKE INSTALLATION

To install a stable version from PyPI:

```
pip install mfpymake
```

To install pymake directly from the git repository type:

```
pip install https://github.com/modflowpy/pymake/zipball/master
```

To update your version of pymake with the latest from the git repository type:

```
pip install https://github.com/modflowpy/pymake/zipball/master --upgrade
```


BUILDING APPLICATIONS

The following scripts can be run directly from the command line to build MODFLOW 6, MODFLOW-2005, MODFLOW-NWT, MODFLOW-USG, MODFLOW-LGR, MODFLOW-2000, MODPATH 6, MODPATH 7, MT3DMS, MT3D-USGS, and SEAWAT binaries on Linux, Mac, and Windows. The scripts will download the distribution file from the USGS (requires internet connection), unzip the file, and compile the source. MT3DMS will be downloaded from the University of Alabama and Triangle will be downloaded from netlib.org. The scripts use the `pymake.build_apps()` method which download and unzip the distribution files and set all of the pymake settings required to build the program. Available example scripts include:

1. `make_modflow6.py`
2. `make_mf2005.py`
3. `make_mfnwt.py`
4. `make_mfusg.py`
5. `make_mflgr.py`
6. `make_mf2000.py`
7. `make_modpath6.py`
8. `make_modpath7.py`
9. `make_gsflow.py`
10. `make_vs2dt.py`
11. `make_mt3d.py`
12. `make_mt3dusgs.py`
13. `make_swtv4.py`
14. `make_crt.py`
15. `make_gridgen.py`
16. `make_triangle.py`

Optional command line arguments can be used to customize the build (`-fc`, `-cc`, `--fflags`, etc.). MODFLOW 6 could be built using intel compilers and an O3 optimization level by specifying:

```
python make_mf6.py -fc=ifort --fflags='-O3'
```


This section contains the Documentation of the Application Programming Interface (API) of pymake. The information in this section is automatically created from the documentation strings in original Python code. In the left-hand menu you will find the different categories of the API documentation.

4.1 pymake.pymake module

`Pymake()` class to make a binary executable for a FORTRAN, C, or C++ program, such as MODFLOW 6.

An example of how to build MODFLOW-2005 from source files in the official release downloaded from the USGS using Intel compilers is:

```
import pymake

# create an instance of the Pymake object
pm = pymake.Pymake(verbose=True)

# reset select pymake settings
pm.target = "mf2005"
pm.appdir = "../bin"
pm.fc = "ifort"
pm.cc = "icc"
pm.fflags = "-O3 -fbacktrace"
pm.cflags = "-O3"

# download the target
pm.download_target(pm.target, download_path="temp")

# build the target
pm.build()

# clean up downloaded files
pm.finalize()
```

All other settings not specified in the script would be based on command line arguments or default values. The same `Pymake()` object could be used to compile MODFLOW 6 by appending the following code to the previous code block:

```
# reset the target
pm.target = "mf6"
```

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```
# download the target
pm.download_target(pm.target, download_path="temp")

# build the target
pm.build()

# clean up downloaded files
pm.finalize()
```

The Intel compilers and fortran flags defined previously would be used when MODFLOW 6 was built.

class Pymake(*name='pymake', verbose=None*)

Bases: object

Pymake class for interacting with pymake functionality. This is essentially a wrapper for all of the pymake functions needed to download and build a target.

argv_reset_settings(*args*)

Reset settings using command line arguments

Parameters *args* (*Namespace object*) – reset self.variables using command line arguments

build(*target=None, srcdir=None, modify_exe_name=False*)

Build the target

Parameters

- **target** (*str*) – target name. If target is None self.target is used. (default is None)
- **srcdir** (*str*) – path to directory with source files. (default is None)
- **modify_exe_name** (*bool*) – boolean that determines if the target name can be modified to include precision (dbl) and debugging (d) indicators.

compress_targets()

Compress targets in build_targets list.

download_setup(*target, url=None, download_path='.', verify=True, timeout=30*)

Setup download

Parameters

- **target** (*str*) – target name
- **url** (*str*) – url of asset
- **download_path** (*str*) – path where the asset will be saved
- **verify** (*bool*) – boolean defining ssl verification
- **timeout** (*int*) – download timeout in seconds (default is 30)

download_target(*target, url=None, download_path='.', verify=True, timeout=30*)

Setup and download url

Parameters

- **target** (*str*) – target name
- **url** (*str*) – url of asset
- **download_path** (*str*) – path where the asset will be saved
- **verify** (*bool*) – boolean defining ssl verification

- **timeout** (*int*) – download timeout in seconds (default is 30)

Returns **success** – boolean flag indicating download success

Return type `bool`

download_url()

Download files from the url

Returns **success** – boolean flag indicating download success

Return type `bool`

finalize()

Finalize Pymake class

reset(target)

Reset PyMake object variables for a target

Parameters **target** (*str*) – target name

set_build_target_bool(target=None)

Evaluate if the executable exists and if so and the command line argument `--keep` is specified then the executable is not built.

Parameters **target** (*str*) – target name. If target is None self.target will be used. (default is None)

Returns **build** – boolean indicating if the executable should be built

Return type `bool`

update_build_targets()

Add target to build_targets list if it is not in the list

update_target(target, modify_target=False)

Update target name with executable extension on Windows and based on pymake settings.

Parameters

- **target** (*str*) – target name
- **modify_target** (*bool*) – boolean indicating if the target name can be modified based on pymake double and debug settings (default is False)

Returns **target** – updated target name

Return type `str`

4.2 pymake.pymake_build_apps module

Function to build MODFLOW-based models and other utility software based on targets defined in the usgsprograms database (usgsprograms.txt). The usgsprograms database can be queried using functions in the usgsprograms module. An example of using `pymake.build_apps()` to build MODFLOW 6 is:

```
import pymake
pymake.build_apps(["mf6",])
```

which will download the latest MODFLOW 6 software release, compile the code, and delete the downloaded files after successfully building the application. Multiple applications can be built by adding additional targets to the tuple in `pymake.build_apps()`. For example, MODFLOW 6 and MODFLOW-2005 could be built by specifying:

```
import pymake
pymake.build_apps(["mf6", "mf2005"])]])
```

Applications are built in the order they are listed in the list. All valid USGS applications are built if no list is passed to `pymake.build_apps()`.

build_apps(*targets=None, pymake_object=None, download_dir=None, appdir=None, verbose=None, release_precision=True, meson=False, mesondir='.', clean=True*)

Build all of the current targets or a subset of targets.

Parameters

- **targets** (*str or list of str*) – targets to build. If targets is None, all current targets will be build. Default is None
- **pymake_object** (`Pymake()`) – Pymake object created outside of build_apps
- **download_dir** (*str*) – download directory path
- **appdir** (*str*) – target path
- **release_precision** (*bool*) – boolean indicating if only the release precision version should be build. If release_precision is False, then the release precision version will be compiled along with a double precision version of the program for programs where the standard_switch and double_switch in usgsprograms.txt is True. default is True.
- **meson** (*bool*) – boolean indicating that the executable should be built using the meson build system. (default is False)
- **mesondir** (*str*) – Main meson.build file path
- **clean** (*bool*) – boolean determining if final download should be removed

Returns **returncode** – integer value indicating successful completion (0) or failure (>0)

Return type int

4.3 pymake.pymake_base module

Main pymake function, `pymake.main()`, that is called when pymake is run from the command line. `pymake.main()` can also be called directly from a script in combination with `pymake.parser()`.

```
import pymake
args = pymake.parser()
pymake.main(
    args.srcdir,
    args.target,
    fc=args.fc,
    cc=args.cc,
    makeclean=args.makeclean,
    expedite=args.expedite,
    dryrun=args.dryrun,
    double=args.double,
    debug=args.debug,
    include_subdirs=args.subdirs,
    fflags=args.fflags,
    cflags=args.cflags,
```

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```

arch=args.arch,
syslibs=args.syslibs,
makefile=args.makefile,
srcdir2=args.commonsrc,
extrafiles=args.extrafiles,
excludefiles=args.excludefiles,
sharedobject=args.sharedobject,
appdir=args.appdir,
verbose=args.verbose,
inplace=args.inplace,
)

```

The script could be run from the command line using:

```
python myscript.py ../src myapp -fc=ifort -cc=icc
```

get_temporary_directories(*appdir=None*)

Get paths to temporary object, module, and source files

Parameters **appdir** (*str*) – path for executable

Returns

- **obj_temp** (*str*) – path to temporary object files
- **mod_temp** (*str*) – path to temporary module files
- **src_temp** (*str*) – path to temporary source files

main(*srcdir=None, target=None, fc='gfortran', cc='gcc', makeclean=True, expedite=False, dryrun=False, double=False, debug=False, include_subdirs=False, fflags=None, cflags=None, syslibs=None, arch='intel64', makefile=False, makefiledir='.', srcdir2=None, extrafiles=None, excludefiles=None, sharedobject=False, appdir=None, verbose=False, inplace=False, networkx=False, meson=False, mesondir='.')*

Main pymake function.

Parameters

- **srcdir** (*str*) – path for directory containing source files
- **target** (*str*) – executable name or path for executable to create
- **fc** (*str*) – fortran compiler
- **cc** (*str*) – c or cpp compiler
- **makeclean** (*bool*) – boolean indicating if intermediate files should be cleaned up after successful build
- **expedite** (*bool*) – boolean indicating if only out of date source files will be compiled. Clean must not have been used on previous build.
- **dryrun** (*bool*) – boolean indicating if source files should be compiled. Files will be deleted, if makeclean is True.
- **double** (*bool*) – boolean indicating a compiler switch will be used to create an executable with double precision real variables.
- **debug** (*bool*) – boolean indicating is a debug executable will be built
- **include_subdirs** (*bool*) – boolean indicating source files in srcdir subdirectories should be included in the build

- **fflags** (*list*) – user provided list of fortran compiler flags
- **cflags** (*list*) – user provided list of c or cpp compiler flags
- **syslibs** (*list*) – user provided syslibs
- **arch** (*str*) – Architecture to use for Intel Compilers on Windows (default is intel64)
- **makefile** (*bool*) – boolean indicating if a GNU make makefile should be created
- **makefiledir** (*str*) – GNU make makefile path
- **srcdir2** (*str*) – additional directory with common source files.
- **extrafiles** (*str*) – path for extrafiles file that contains paths to additional source files to include
- **excludefiles** (*str*) – path for excludefiles file that contains filename of source files to exclude from the build
- **sharedobject** (*bool*) – boolean indicating a shared object will be built
- **appdir** (*str*) – path for executable
- **verbose** (*bool*) – boolean indicating if output will be printed to the terminal
- **inplace** (*bool*) – boolean indicating that the source files in srcdir, srcdir2, and defined in extrafiles will be used directly. If inplace is False, source files will be copied to a directory named srcdir_temp. (default is False)
- **networkx** (*bool*) – boolean indicating that the NetworkX python package will be used to create the Directed Acyclic Graph (DAG) used to determine the order source files are compiled in. The NetworkX package tends to result in a unique DAG more often than the standard algorithm used in pymake. (default is False)
- **meson** (*bool*) – boolean indicating that the executable should be built using the meson build system. (default is False)
- **mesondir** (*str*) – Main meson.build file path

Returns `returncode` – return code

Return type `int`

4.4 pymake.pymake_parser module

Parser used to process command line arguments when running pymake directly from the command line or in a script. The standard argparse module is used to parse command line arguments. Available command line arguments are programmatically developed by a protected dictionary. The parser can be accessed using:

```
import pymake
args = pymake.parser()
```

parser()

Construct the parser and return argument values.

Returns `args` – Namespace with command line arguments

Return type Namespace object

4.5 pymake.plot package

4.5.1 Submodules

pymake.plot.dependency_graphs module

Dependency graphs for applications can be created using:

```
import os
import pymake

srcpth = os.path.join("../", "src")
deppth = "dependencies"
if not os.path.exists(deppth):
    os.makedirs(deppth)

pymake.visualize.make_plots(srcpth, deppth, include_subdir=True)
```

make_plots(*srcdir*, *outdir*, *include_subdir=False*, *level=3*, *extension='.png'*, *verbose=False*, *networkx=False*)
Create plots of module dependencies.

Parameters

- **srcdir** (*str*) – path for source files
- **outdir** (*str*) – path for output images
- **include_subdir** (*bool*) – boolean indicating if subdirectories in the source file directory should be included
- **level** (*int*) – dependency level (1 is the minimum)
- **extension** (*str*) – output extension (default is .png)
- **verbose** (*bool*) – boolean indicating if output will be printed to the terminal
- **networkx** (*bool*) – boolean indicating that the NetworkX python package will be used to create the Directed Acyclic Graph (DAG) used to determine the order source files are compiled in. The NetworkX package tends to result in a unique DAG more often than the standard algorithm used in pymake. (default is False)

to_pydot(*dag*, *filename='mygraph.png'*)
Create a png file of a Directed Acyclic Graph

Parameters

- **dag** (*object*) – directed acyclic graph
- **filename** (*str*) – path of the graph png

4.5.2 Module contents

Functions to plot source code dependencies determined using a directed acyclic graph (DAG). pydotplus is used to plot the DAG.

4.6 pymake.autotest package

4.6.1 Submodules

pymake.autotest.autotest module

A typical example of using the autotest functionality for MODFLOW-2005 and comparing the MODFLOW-2005 results to MODFLOW-2000 results is:

```
import pymake

# Setup
testpth = "../test/mytest"
nam1 = "model1.nam"
pymake.setup(nam1, testpth)

# run test models
success, buff = flopy.run_model(
    "mf2005", nam1, model_ws=testpth, silent=True
)
if success:
    testpth_reg = os.path.join(testpth, "mf2000")
    nam2 = "model2.name"
    pymake.setup(nam2, testpth_reg)
    success_reg, buff = flopy.run_model(
        "mf2000", nam2, model_ws=testpth_reg, silent=True
    )

# compare results
if success and success_reg:
    fpth = os.path.split(os.path.join(testpth, nam1))[0]
    outfile1 = os.path.join(fpth, "bud.cmp")
    fpth = os.path.split(os.path.join(testpth, nam2))[0]
    outfile2 = os.path.join(fpth, "hds.cmp")
    success_reg = pymake.compare(
        os.path.join(testpth, nam1),
        os.path.join(testpth_reg, nam2),
        max_cumpd=0.01,
        max_incpd=0.01,
        htol=0.001,
        outfile1=outfile1,
        outfile2=outfile2,
    )

# Clean things up
```

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```

if success_reg:
    pymake.teardown(testpth)

```

Note: autotest functionality will likely be removed from pymake in the future to a dedicated GitHub repository.

compare(*namefile1*, *namefile2*, *precision*='auto', *max_cumpd*=0.01, *max_incpd*=0.01, *htol*=0.001, *outfile1*=None, *outfile2*=None, *files1*=None, *files2*=None)

Compare the budget and head results for two MODFLOW-based model simulations.

Parameters

- **namefile1** (*str*) – namefile path for base model
- **namefile2** (*str*) – namefile path for comparison model
- **precision** (*str*) – precision for binary head file (“auto”, “single”, or “double”) default is “auto”
- **max_cumpd** (*float*) – maximum percent discrepancy allowed for cumulative budget terms (default is 0.01)
- **max_incpd** (*float*) – maximum percent discrepancy allowed for incremental budget terms (default is 0.01)
- **htol** (*float*) – maximum allowed head difference (default is 0.001)
- **outfile1** (*str*) – budget comparison output file name. If outfile1 is None, no budget comparison output is saved. (default is None)
- **outfile2** (*str*) – head comparison output file name. If outfile2 is None, no head comparison output is saved. (default is None)
- **files1** (*str*) – base model output file. If files1 is not None, results will be extracted from files1 and namefile1 will not be used. (default is None)
- **files2** (*str*) – comparison model output file. If files2 is not None, results will be extracted from files2 and namefile2 will not be used. (default is None)

Returns **success** – boolean indicating if the budget and head differences are less than *max_cumpd*, *max_incpd*, and *htol*.

Return type bool

compare_budget(*namefile1*, *namefile2*, *max_cumpd*=0.01, *max_incpd*=0.01, *outfile*=None, *files1*=None, *files2*=None)

Compare the budget results from two simulations.

Parameters

- **namefile1** (*str*) – namefile path for base model
- **namefile2** (*str*) – namefile path for comparison model
- **max_cumpd** (*float*) – maximum percent discrepancy allowed for cumulative budget terms (default is 0.01)
- **max_incpd** (*float*) – maximum percent discrepancy allowed for incremental budget terms (default is 0.01)
- **outfile** (*str*) – budget comparison output file name. If outfile is None, no comparison output is saved. (default is None)
- **files1** (*str*) – base model output file. If files1 is not None, results will be extracted from files1 and namefile1 will not be used. (default is None)

- **files2** (*str*) – comparison model output file. If files2 is not None, results will be extracted from files2 and namefile2 will not be used. (default is None)

Returns **success** – boolean indicating if the difference between budgets are less than max_cumpd and max_incpd

Return type bool

compare_concs(*namefile1*, *namefile2*, *precision*='auto', *ctol*=0.001, *outfile*=None, *files1*=None, *files2*=None, *difftol*=False, *verbose*=False)

Compare the mt3dms and mt3dusgs concentration results from two simulations.

Parameters

- **namefile1** (*str*) – namefile path for base model
- **namefile2** (*str*) – namefile path for comparison model
- **precision** (*str*) – precision for binary head file (“auto”, “single”, or “double”) default is “auto”
- **ctol** (*float*) – maximum allowed concentration difference (default is 0.001)
- **outfile** (*str*) – concentration comparison output file name. If outfile is None, no comparison output is saved. (default is None)
- **files1** (*str*) – base model output file. If files1 is not None, results will be extracted from files1 and namefile1 will not be used. (default is None)
- **files2** (*str*) – comparison model output file. If files2 is not None, results will be extracted from files2 and namefile2 will not be used. (default is None)
- **difftol** (*bool*) – boolean determining if the absolute value of the concentration difference greater than ctol should be evaluated (default is False)
- **verbose** (*bool*) – boolean indicating if verbose output should be written to the terminal (default is False)

Returns **success** – boolean indicating if the concentration differences are less than ctol.

Return type bool

compare_heads(*namefile1*, *namefile2*, *precision*='auto', *text*='head', *text2*=None, *htol*=0.001, *outfile*=None, *files1*=None, *files2*=None, *difftol*=False, *verbose*=False, *exfile*=None, *exarr*=None, *maxerr*=None)

Compare the head results from two simulations.

Parameters

- **namefile1** (*str*) – namefile path for base model
- **namefile2** (*str*) – namefile path for comparison model
- **precision** (*str*) – precision for binary head file (“auto”, “single”, or “double”) default is “auto”
- **htol** (*float*) – maximum allowed head difference (default is 0.001)
- **outfile** (*str*) – head comparison output file name. If outfile is None, no comparison output is saved. (default is None)
- **files1** (*str*) – base model output file. If files1 is not None, results will be extracted from files1 and namefile1 will not be used. (default is None)
- **files2** (*str*) – comparison model output file. If files2 is not None, results will be extracted from files2 and namefile2 will not be used. (default is None)

- **diff_tol** (*bool*) – boolean determining if the absolute value of the head difference greater than *htol* should be evaluated (default is *False*)
- **verbose** (*bool*) – boolean indicating if verbose output should be written to the terminal (default is *False*)
- **exfile** (*str*) – path to a file with exclusion array data. Head differences will not be evaluated where exclusion array values are greater than zero. (default is *None*)
- **exarr** (*numpy.ndarray*) – exclusion array. Head differences will not be evaluated where exclusion array values are greater than zero. (default is *None*).
- **maxerr** (*int*) – maximum number of head difference greater than *htol* that should be reported. If *maxerr* is *None*, all head difference greater than *htol* will be reported. (default is *None*)

Returns *success* – boolean indicating if the head differences are less than *htol*.

Return type *bool*

compare_stages (*namefile1=None, namefile2=None, files1=None, files2=None, htol=0.001, outfile=None, diff_tol=False, verbose=False*)

Compare SWR process stage results from two simulations.

Parameters

- **namefile1** (*str*) – namefile path for base model
- **namefile2** (*str*) – namefile path for comparison model
- **precision** (*str*) – precision for binary head file (“auto”, “single”, or “double”) default is “auto”
- **htol** (*float*) – maximum allowed stage difference (default is 0.001)
- **outfile** (*str*) – head comparison output file name. If *outfile* is *None*, no comparison output is saved. (default is *None*)
- **files1** (*str*) – base model output file. If *files1* is not *None*, results will be extracted from *files1* and *namefile1* will not be used. (default is *None*)
- **files2** (*str*) – comparison model output file. If *files2* is not *None*, results will be extracted from *files2* and *namefile2* will not be used. (default is *None*)
- **diff_tol** (*bool*) – boolean determining if the absolute value of the stage difference greater than *htol* should be evaluated (default is *False*)
- **verbose** (*bool*) – boolean indicating if verbose output should be written to the terminal (default is *False*)

Returns *success* – boolean indicating if the stage differences are less than *htol*.

Return type *bool*

compare_swrbudget (*namefile1, namefile2, max_cumpd=0.01, max_incpd=0.01, outfile=None, files1=None, files2=None*)

Compare the SWR budget results from two simulations.

Parameters

- **namefile1** (*str*) – namefile path for base model
- **namefile2** (*str*) – namefile path for comparison model
- **max_cumpd** (*float*) – maximum percent discrepancy allowed for cumulative budget terms (default is 0.01)

- **max_incpd** (*float*) – maximum percent discrepancy allowed for incremental budget terms (default is 0.01)
- **outfile** (*str*) – budget comparison output file name. If outfile is None, no comparison output is saved. (default is None)
- **files1** (*str*) – base model output file. If files1 is not None, results will be extracted from files1 and namefile1 will not be used. (default is None)
- **files2** (*str*) – comparison model output file. If files2 is not None, results will be extracted from files2 and namefile2 will not be used. (default is None)

Returns **success** – boolean indicating if the difference between budgets are less than max_cumpd and max_incpd

Return type bool

get_entries_from_namefile(*namefile*, *ftype=None*, *unit=None*, *extension=None*)

Get entries from a namefile. Can select using FTYPE, UNIT, or file extension.

Parameters

- **namefile** (*str*) – path to a MODFLOW-based model name file
- **ftype** (*str*) – package type
- **unit** (*int*) – file unit number
- **extension** (*str*) – file extension

Returns **entries** – list of tuples containing FTYPE, UNIT, FNAME, STATUS for each namefile entry that meets a user-specified value.

Return type list of tuples

get_input_files(*namefile*)

Return a list of all the input files in this model.

Parameters **namefile** (*str*) – path to a MODFLOW-based model name file

Returns **filelist** – list of MODFLOW-based model input files

Return type list

get_mf6_blockdata(*f*, *blockstr*)

Return list with all non comments between start and end of block specified by blockstr.

Parameters

- **f** (*file object*) – open file object
- **blockstr** (*str*) – name of block to search

Returns **data** – list of data in specified block

Return type list

get_mf6_comparison(*src*)

Determine comparison type for MODFLOW 6 simulation.

Parameters **src** (*str*) – directory path to search for comparison types

Returns **action** – comparison type

Return type str

get_mf6_files(*mfnamefile*)

Return a list of all the MODFLOW 6 input and output files in this model.

Parameters **mfnamefile** (*str*) – path to the MODFLOW 6 simulation name file

Returns

- **filelist** (*list*) – list of MODFLOW 6 input files in a simulation
- **outplist** (*list*) – list of MODFLOW 6 output files in a simulation

get_mf6_ftypes(*namefile, ftypekeys*)

Return a list of FTYPEs that are in the name file and in ftypekeys.

Parameters

- **namefile** (*str*) – path to a MODFLOW 6 name file
- **ftypekeys** (*list*) – list of desired FTYPEs

Returns **ftypes** – list of FTYPEs that match ftypekeys in namefile

Return type *list*

get_mf6_mshape(*disfile*)

Return the shape of the MODFLOW 6 model.

Parameters **disfile** (*str*) – path to a MODFLOW 6 discretization file

Returns **mshape** – tuple with the shape of the MODFLOW 6 model.

Return type *tuple*

get_mf6_nper(*tdisfile*)

Return the number of stress periods in the MODFLOW 6 model.

Parameters **tdisfile** (*str*) – path to the TDIS file

Returns **nper** – number of stress periods in the simulation

Return type *int*

get_namefiles(*pth, exclude=None*)

Search through a path (pth) for all .nam files.

Parameters

- **pth** (*str*) – path to model files
- **exclude** (*str or list*) – File or list of files to exclude from the search (default is None)

Returns **namefiles** – List of namefiles with paths

Return type *list*

get_sim_name(*namefiles, rootpth=None*)

Get simulation name.

Parameters

- **namefiles** (*str or list of strings*) – path(s) to MODFLOW-based model name files
- **rootpth** (*str*) – optional root directory path (default is None)

Returns **simname** – list of namefiles without the file extension

Return type *list*

setup(*namefile, dst, remove_existing=True, extrafiles=None*)

Setup MODFLOW-based model files for autotests.

Parameters

- **namefile** (*str*) – MODFLOW-based model name file.
- **dst** (*str*) – destination path for comparison model or file(s)
- **remove_existing** (*bool*) – boolean indicating if an existing comparison model or file(s) should be replaced (default is True)
- **extrafiles** (*str or list of str*) – list of extra files to include in the comparison

setup_comparison(*namefile, dst, remove_existing=True*)

Setup a comparison model or comparison file(s) for a MODFLOW-based model.

Parameters

- **namefile** (*str*) – MODFLOW-based model name file.
- **dst** (*str*) – destination path for comparison model or file(s)
- **remove_existing** (*bool*) – boolean indicating if an existing comparison model or file(s) should be replaced (default is True)

setup_mf6(*src, dst, mfnamefile='mfsim.nam', extrafiles=None, remove_existing=True*)

Copy all of the MODFLOW 6 input files from the src directory to the dst directory.

Parameters

- **src** (*src*) – directory path with original MODFLOW 6 input files
- **dst** (*str*) – directory path that original MODFLOW 6 input files will be copied to
- **mfnamefile** (*str*) – optional MODFLOW 6 simulation name file (default is mfsim.nam)
- **extrafiles** (*bool*) – boolean indicating if extra files should be included (default is None)
- **remove_existing** (*bool*) – boolean indicating if existing file in dst should be removed (default is True)

Returns

- **mf6inp** (*list*) – list of MODFLOW 6 input files
- **mf6outp** (*list*) – list of MODFLOW 6 output files

setup_mf6_comparison(*src, dst, remove_existing=True*)

Setup comparison for MODFLOW 6 simulation.

Parameters

- **src** (*src*) – directory path with original MODFLOW 6 input files
- **dst** (*str*) – directory path that original MODFLOW 6 input files will be copied to
- **remove_existing** (*bool*) – boolean indicating if existing file in dst should be removed (default is True)

Returns *action* – comparison type

Return type *str*

teardown(*src*)

Teardown a autotest directory.

Parameters **src** (*str*) – autotest directory to teardown

4.6.2 Module contents

Autotest functionality for MODFLOW-based models. Includes functionality for copying existing model and comparison files, comparing results, and tearing down test and comparison models.

4.7 pymake.utils package

4.7.1 Submodules

pymake.utils.download module

Utility functions to:

1. download and unzip software releases from the USGS and other organizations (triangle, MT3DMS).
2. download the latest MODFLOW-based applications and utilities for MacOS, Linux, and Windows from <https://github.com/MODFLOW-USGS/executables>
3. determine the latest version (GitHub tag) of a GitHub repository and a dictionary containing the file name and the link to a asset on contained in a github repository
4. compress all files in a list, files in a list of directories

download_and_unzip(*url*, *pth*='.', *delete_zip*=True, *verify*=True, *timeout*=30, *max_requests*=10, *chunk_size*=2048000, *verbose*=False)

Download and unzip a zip file from a url.

Parameters

- **url** (*str*) – url address for the zip file
- **pth** (*str*) – path where the zip file will be saved (default is the current path)
- **delete_zip** (*bool*) – boolean indicating if the zip file should be deleted after it is unzipped (default is True)
- **verify** (*bool*) – boolean indicating if the url request should be verified
- **timeout** (*int*) – url request time out length (default is 30 seconds)
- **max_requests** (*int*) – number of url download request attempts (default is 10)
- **chunk_size** (*int*) – maximum url download request chunk size (default is 2048000 bytes)
- **verbose** (*bool*) – boolean indicating if output will be printed to the terminal

get_repo_assets(*github_repo*=None, *version*=None, *error_return*=False, *verify*=True)

Return a dictionary containing the file name and the link to the asset contained in a github repository.

Parameters

- **github_repo** (*str*) – Repository name, such as MODFLOW-USGS/modflow6. If github_repo is None set to 'MODFLOW-USGS/executables'
- **version** (*str*) – github repository release tag
- **error_return** (*bool*) – boolean indicating if None will be returned if there are GitHub API issues
- **verify** (*bool*) – boolean indicating if the url request should be verified

Returns **result_dict** – dictionary of file names and links

Return type dict

getmfexes(*pth='.', version=None, platform=None, exes=None, verbose=False, verify=True*)

Get the latest MODFLOW binary executables from a github site (<https://github.com/MODFLOW-USGS/executables>) for the specified operating system and put them in the specified path.

Parameters

- **pth** (*str*) – Location to put the executables (default is current working directory)
- **version** (*str*) – Version of the MODFLOW-USGS/executables release to use. If version is None the github repo will be queried for the version number.
- **platform** (*str*) – Platform that will run the executables. Valid values include mac, linux, win32 and win64. If platform is None, then routine will download the latest asset from the github repository.
- **exes** (*str or list of strings*) – executable or list of executables to retain
- **verbose** (*bool*) – boolean indicating if output will be printed to the terminal
- **verify** (*bool*) – boolean indicating if the url request should be verified

getmfnightly(*pth='.', platform=None, exes=None, verbose=False, verify=True*)

Get the latest MODFLOW 6 binary nightly-build executables from github (<https://github.com/MODFLOW-USGS/modflow6-nightly-build/>) for the specified operating system and put them in the specified path.

Parameters

- **pth** (*str*) – Location to put the executables (default is current working directory)
- **platform** (*str*) – Platform that will run the executables. Valid values include mac, linux, win32 and win64. If platform is None, then routine will download the latest asset from the github repository.
- **exes** (*str or list of strings*) – executable or list of executables to retain
- **verbose** (*bool*) – boolean indicating if output will be printed to the terminal
- **verify** (*bool*) – boolean indicating if the url request should be verified

class pymakeZipFile(*file, mode='r', compression=0, allowZip64=True, compresslevel=None*)

Bases: zipfile.ZipFile

ZipFile file attributes are not being preserved. This class preserves file attributes as described on StackOverflow at <https://stackoverflow.com/questions/39296101/python-zipfile-removes-execute-permissions-from-binaries>

static compressall(*path, file_pths=None, dir_pths=None, patterns=None*)

Compress selected files or files in selected directories.

Parameters

- **path** (*str*) – output zip file path
- **file_pths** (*str or list of str*) – file paths to include in the output zip file (default is None)
- **dir_pths** (*str or list of str*) – directory paths to include in the output zip file (default is None)
- **patterns** (*str or list of str*) – file patterns to include in the output zip file (default is None)

Returns **success** – boolean indicating if the output zip file was created

Return type bool

extract(*member*, *path*=None, *pwd*=None)

Parameters

- **member** (*str*) – individual file to extract. If member does not exist, all files are extracted.
- **path** (*str*) – directory path to extract file in a zip file (default is None, which results in files being extracted in the current directory)
- **pwd** (*str*) – zip file password (default is None)

Returns **ret_val** – return value indicating status of file extraction

Return type int

extractall(*path*=None, *members*=None, *pwd*=None)

Extract all files in the zipfile.

Parameters

- **path** (*str*) – directory path to extract files in a zip file (default is None, which results in files being extracted in the current directory)
- **members** (*str*) – individual files to extract (default is None, which extracts all members)
- **pwd** (*str*) – zip file password (default is None)

repo_latest_version(*github_repo*=None, *verify*=True)

Return a string of the latest version number (tag) contained in a github repository release.

Parameters **github_repo** (*str*) – Repository name, such as MODFLOW-USGS/modflow6. If github_repo is None set to 'MODFLOW-USGS/executables'

Returns **version** – string with the latest version/tag number

Return type str

zip_all(*path*, *file_pths*=None, *dir_pths*=None, *patterns*=None)

Compress all files in the user-provided list of file paths and directory paths that match the provided file patterns.

Parameters

- **path** (*str*) – path of the zip file that will be created
- **file_pths** (*str or list*) – file path or list of file paths to be compressed
- **dir_pths** (*str or list*) – directory path or list of directory paths to search for files that will be compressed
- **patterns** (*str or list*) – file pattern or list of file patterns s to match to when creating a list of files that will be compressed

pymake.utils.usgsprograms module

Utility functions to extract information for a target from the USGS application database. Available functionality includes:

1. Get a list of available targets
2. Get data for a specific target
3. Get a dictionary with the data for all targets
4. Get the current version of a target
5. Get a list indicating if single and double precision versions of the target application should be built
6. Functions to load, update, and export a USGS-style “code.json” json file containing information in the USGS application database

A table listing the available pymake targets is included below:

Table 1: Available pymake targets

target	version	current	url	dirname	srcdir	standard_switch	double_switch	shared_object
mf6	6.3.0	True	https://github.com/MODFLOW-USGS/modflow6/releases/download/6.3.0/mf6.3.0_linux.zip	mf6.3.0_linux	src	True	False	False
zbud6	6.3.0	True	https://github.com/MODFLOW-USGS/modflow6/releases/download/6.3.0/mf6.3.0_linux.zip	mf6.3.0_linux	utils/zonebudget/src	True	False	False
libmf6	6.3.0	True	https://github.com/MODFLOW-USGS/modflow6/releases/download/6.3.0/mf6.3.0_linux.zip	mf6.3.0_linux	src/bmi	True	False	True
mp7	7.2.001	True	https://water.usgs.gov/water-resources/software/MODPATH/modpath_7_2_001.zip	mod-path_7_2_001	source	True	False	False
mt3dms	5.3.0	True	https://hydro.geo.ua.edu/mt3d/mt3dms_530.exe	mt3dms5.3.0	src/true-binary	True	False	False
mt3dusgs	1.1.0	True	https://water.usgs.gov/water-resources/software/MT3D-USGS/mt3dusgs1.1.0.zip	mt3dusgs1.1.0	src	True	False	False
vs2dt	3.3	True	https://water.usgs.gov/water-resources/software/VS2DI/vs2dt3_3.zip	vs2dt3_3	include	True	False	False
triangle	1.6	True	https://www.netlib.org/voronoi/triangle.zip	triangle1.6	src	True	False	False
gridgen	1.0.02	True	https://water.usgs.gov/water-resources/software/GRIDGEN/gridgen.1.0.02.zip	grid-gen.1.0.02	src	True	False	False
crt	1.3.1	True	https://water.usgs.gov/ogw/CRT/CRT_1.3.1.zip	CRT_1.3.1	SOURCE	True	False	False
gsflow	2.2.0	True	https://water.usgs.gov/water-resources/software/gflow/gflow_2.2.0_linux.zip	gs-flow_2.2.0_linux	src	True	False	False
4.7. pymake.utils package								29
sutra	3.0	True	https://water.usgs.gov/	Sutra-Suite	SU-TRA_3.0/source	True	False	False

class dotdict

Bases: dict

dot.notation access to dictionary attributes.

class usgs_program_data

Bases: object

USGS program database class.

static export_json(*fpth*='code.json', *prog_data*=None, *current*=False, *update*=True, *write_markdown*=False, *verbose*=False)

Export USGS program data as a json file.

Parameters

- **fpth** (*str*) – Path for the json file to be created. Default is “code.json”
- **prog_data** (*dict*) – User-specified program database. If *prog_data* is None, it will be created from the USGS program database
- **current** (*bool*) – If False, all USGS program targets are listed. If True, only USGS program targets that are defined as current are listed. Default is False.
- **update** (*bool*) – If True, existing targets in the user-specified program database with values in the USGS program database. If False, existing targets in the user-specified program database will not be updated. Default is True.
- **write_markdown** (*bool*) – If True, write markdown file that includes the target name, version, and the last-modified date of the download asset (url). Default is False.
- **verbose** (*bool*) – boolean for verbose output to terminal

static get_keys(*current*=False)

Get target keys from the USGS program database.

Parameters **current** (*bool*) – If False, all USGS program targets are listed. If True, only USGS program targets that are defined as current are listed. Default is False.

Returns **keys** – list of USGS program targets

Return type list

static get_precision(*key*)

Get the dictionary for a specified target.

Parameters **key** (*str*) – Target USGS program

Returns **precision** – List

Return type list

static get_program_dict()

Get the complete USGS program database.

Returns **program_dict** – Dictionary with USGS program attributes for all targets

Return type dict

static get_target(*key*)

Get the dictionary for a specified target.

Parameters **key** (*str*) – Target USGS program that may have a path and an extension

Returns **program_dict** – Dictionary with USGS program attributes for the specified key

Return type dict

static get_version(*key*)

Get the current version of the specified target.

Parameters **key** (*str*) – Target USGS program

Returns **version** – current version of the specified target

Return type *str*

static list_json(*fpth*='code.json')

List an existing code json file.

Parameters **fpth** (*str*) – Path for the json file to be listed. Default is “code.json”

static list_targets(*current*=False)

Print a list of the available USGS program targets.

Parameters **current** (*bool*) – If False, all USGS program targets are listed. If True, only USGS program targets that are defined as current are listed. Default is False.

static load_json(*fpth*='code.json')

Load an existing code json file. Basic error checking is done to make sure the file contains the correct keys.

Parameters **fpth** (*str*) – Path for the json file to be created. Default is “code.json”

Returns **json_dict** – Valid USGS program database

Return type *dict*

static update_json(*fpth*='code.json', *temp_dict*=None)

UPDATE an existing code json file.

Parameters

- **fpth** (*str*) – Path for the json file to be listed. Default is “code.json”
- **temp_dict** (*dict*) – Dictionary with USGS program data for a target

4.7.2 Module contents

Utility functions to 1) download and uncompress software releases containing source code or executables, 2) zip files, 3) query a USGS software and utility program database for information on current software releases.

4.8 pymake package

4.8.1 Subpackages

4.8.2 Submodules

pymake.config module

4.8.3 Module contents

pymake is a python package for compiling MODFLOW-based and other Fortran, C, and C++ programs. The package determines the build order using a directed acyclic graph and then compiles the source files using GNU compilers (gcc, g++, gfortran) or Intel compilers (ifort, icc).

class Pymake(*name='pymake', verbose=None*)

Bases: object

Pymake class for interacting with pymake functionality. This is essentially a wrapper for all of the pymake functions needed to download and build a target.

argv_reset_settings(*args*)

Reset settings using command line arguments

Parameters *args* (*Namespace object*) – reset self.variables using command line arguments

build(*target=None, srcdir=None, modify_exe_name=False*)

Build the target

Parameters

- **target** (*str*) – target name. If target is None self.target is used. (default is None)
- **srcdir** (*str*) – path to directory with source files. (default is None)
- **modify_exe_name** (*bool*) – boolean that determines if the target name can be modified to include precision (dbl) and debugging (d) indicators.

compress_targets()

Compress targets in build_targets list.

download_setup(*target, url=None, download_path='.', verify=True, timeout=30*)

Setup download

Parameters

- **target** (*str*) – target name
- **url** (*str*) – url of asset
- **download_path** (*str*) – path where the asset will be saved
- **verify** (*bool*) – boolean defining ssl verification
- **timeout** (*int*) – download timeout in seconds (default is 30)

download_target(*target, url=None, download_path='.', verify=True, timeout=30*)

Setup and download url

Parameters

- **target** (*str*) – target name
- **url** (*str*) – url of asset
- **download_path** (*str*) – path where the asset will be saved
- **verify** (*bool*) – boolean defining ssl verification
- **timeout** (*int*) – download timeout in seconds (default is 30)

Returns *success* – boolean flag indicating download success

Return type bool

download_url()

Download files from the url

Returns *success* – boolean flag indicating download success

Return type bool

finalize()

Finalize Pymake class

reset(*target*)

Reset PyMake object variables for a target

Parameters **target** (*str*) – target name

set_build_target_bool(*target=None*)

Evaluate if the executable exists and if so and the command line argument `--keep` is specified then the executable is not built.

Parameters **target** (*str*) – target name. If target is None self.target will be used. (default is None)

Returns **build** – boolean indicating if the executable should be built

Return type bool

update_build_targets()

Add target to build_targets list if it is not in the list

update_target(*target*, *modify_target=False*)

Update target name with executable extension on Windows and based on pymake settings.

Parameters

- **target** (*str*) – target name
- **modify_target** (*bool*) – boolean indicating if the target name can be modified based on pymake double and debug settings (default is False)

Returns **target** – updated target name

Return type str

build_apps(*targets=None*, *pymake_object=None*, *download_dir=None*, *appdir=None*, *verbose=None*, *release_precision=True*, *meson=False*, *mesondir='.'*, *clean=True*)

Build all of the current targets or a subset of targets.

Parameters

- **targets** (*str or list of str*) – targets to build. If targets is None, all current targets will be build. Default is None
- **pymake_object** ([Pymake](#) ()) – Pymake object created outside of build_apps
- **download_dir** (*str*) – download directory path
- **appdir** (*str*) – target path
- **release_precision** (*bool*) – boolean indicating if only the release precision version should be build. If release_precision is False, then the release precision version will be compiled along with a double precision version of the program for programs where the standard_switch and double_switch in usgsprograms.txt is True. default is True.
- **meson** (*bool*) – boolean indicating that the executable should be built using the meson build system. (default is False)
- **mesondir** (*str*) – Main meson.build file path
- **clean** (*bool*) – boolean determining if final download should be removed

Returns **returncode** – integer value indicating successful completion (0) or failure (>0)

Return type int

compare(*namefile1*, *namefile2*, *precision*='auto', *max_cumpd*=0.01, *max_incpd*=0.01, *htol*=0.001, *outfile1*=None, *outfile2*=None, *files1*=None, *files2*=None)

Compare the budget and head results for two MODFLOW-based model simulations.

Parameters

- **namefile1** (*str*) – namefile path for base model
- **namefile2** (*str*) – namefile path for comparison model
- **precision** (*str*) – precision for binary head file (“auto”, “single”, or “double”) default is “auto”
- **max_cumpd** (*float*) – maximum percent discrepancy allowed for cumulative budget terms (default is 0.01)
- **max_incpd** (*float*) – maximum percent discrepancy allowed for incremental budget terms (default is 0.01)
- **htol** (*float*) – maximum allowed head difference (default is 0.001)
- **outfile1** (*str*) – budget comparison output file name. If outfile1 is None, no budget comparison output is saved. (default is None)
- **outfile2** (*str*) – head comparison output file name. If outfile2 is None, no head comparison output is saved. (default is None)
- **files1** (*str*) – base model output file. If files1 is not None, results will be extracted from files1 and namefile1 will not be used. (default is None)
- **files2** (*str*) – comparison model output file. If files2 is not None, results will be extracted from files2 and namefile2 will not be used. (default is None)

Returns **success** – boolean indicating if the budget and head differences are less than max_cumpd, max_incpd, and htol.

Return type bool

compare_budget(*namefile1*, *namefile2*, *max_cumpd*=0.01, *max_incpd*=0.01, *outfile*=None, *files1*=None, *files2*=None)

Compare the budget results from two simulations.

Parameters

- **namefile1** (*str*) – namefile path for base model
- **namefile2** (*str*) – namefile path for comparison model
- **max_cumpd** (*float*) – maximum percent discrepancy allowed for cumulative budget terms (default is 0.01)
- **max_incpd** (*float*) – maximum percent discrepancy allowed for incremental budget terms (default is 0.01)
- **outfile** (*str*) – budget comparison output file name. If outfile is None, no comparison output is saved. (default is None)
- **files1** (*str*) – base model output file. If files1 is not None, results will be extracted from files1 and namefile1 will not be used. (default is None)
- **files2** (*str*) – comparison model output file. If files2 is not None, results will be extracted from files2 and namefile2 will not be used. (default is None)

Returns **success** – boolean indicating if the difference between budgets are less than max_cumpd and max_incpd

Return type bool

compare_concs(*namefile1*, *namefile2*, *precision*='auto', *ctol*=0.001, *outfile*=None, *files1*=None, *files2*=None, *diff_tol*=False, *verbose*=False)

Compare the mt3dms and mt3dusgs concentration results from two simulations.

Parameters

- **namefile1** (*str*) – namefile path for base model
- **namefile2** (*str*) – namefile path for comparison model
- **precision** (*str*) – precision for binary head file (“auto”, “single”, or “double”) default is “auto”
- **ctol** (*float*) – maximum allowed concentration difference (default is 0.001)
- **outfile** (*str*) – concentration comparison output file name. If outfile is None, no comparison output is saved. (default is None)
- **files1** (*str*) – base model output file. If files1 is not None, results will be extracted from files1 and namefile1 will not be used. (default is None)
- **files2** (*str*) – comparison model output file. If files2 is not None, results will be extracted from files2 and namefile2 will not be used. (default is None)
- **diff_tol** (*bool*) – boolean determining if the absolute value of the concentration difference greater than ctol should be evaluated (default is False)
- **verbose** (*bool*) – boolean indicating if verbose output should be written to the terminal (default is False)

Returns **success** – boolean indicating if the concentration differences are less than ctol.

Return type bool

compare_heads(*namefile1*, *namefile2*, *precision*='auto', *text*='head', *text2*=None, *htol*=0.001, *outfile*=None, *files1*=None, *files2*=None, *diff_tol*=False, *verbose*=False, *exfile*=None, *exarr*=None, *maxerr*=None)

Compare the head results from two simulations.

Parameters

- **namefile1** (*str*) – namefile path for base model
- **namefile2** (*str*) – namefile path for comparison model
- **precision** (*str*) – precision for binary head file (“auto”, “single”, or “double”) default is “auto”
- **htol** (*float*) – maximum allowed head difference (default is 0.001)
- **outfile** (*str*) – head comparison output file name. If outfile is None, no comparison output is saved. (default is None)
- **files1** (*str*) – base model output file. If files1 is not None, results will be extracted from files1 and namefile1 will not be used. (default is None)
- **files2** (*str*) – comparison model output file. If files2 is not None, results will be extracted from files2 and namefile2 will not be used. (default is None)
- **diff_tol** (*bool*) – boolean determining if the absolute value of the head difference greater than htol should be evaluated (default is False)
- **verbose** (*bool*) – boolean indicating if verbose output should be written to the terminal (default is False)

- **exfile** (*str*) – path to a file with exclusion array data. Head differences will not be evaluated where exclusion array values are greater than zero. (default is None)
- **exarr** (*numpy.ndarray*) – exclusion array. Head differences will not be evaluated where exclusion array values are greater than zero. (default is None).
- **maxerr** (*int*) – maximum number of head difference greater than htol that should be reported. If maxerr is None, all head difference greater than htol will be reported. (default is None)

Returns **success** – boolean indicating if the head differences are less than htol.

Return type bool

compare_stages (*namefile1=None, namefile2=None, files1=None, files2=None, htol=0.001, outfile=None, diff_tol=False, verbose=False*)

Compare SWR process stage results from two simulations.

Parameters

- **namefile1** (*str*) – namefile path for base model
- **namefile2** (*str*) – namefile path for comparison model
- **precision** (*str*) – precision for binary head file (“auto”, “single”, or “double”) default is “auto”
- **htol** (*float*) – maximum allowed stage difference (default is 0.001)
- **outfile** (*str*) – head comparison output file name. If outfile is None, no comparison output is saved. (default is None)
- **files1** (*str*) – base model output file. If files1 is not None, results will be extracted from files1 and namefile1 will not be used. (default is None)
- **files2** (*str*) – comparison model output file. If files2 is not None, results will be extracted from files2 and namefile2 will not be used. (default is None)
- **diff_tol** (*bool*) – boolean determining if the absolute value of the stage difference greater than htol should be evaluated (default is False)
- **verbose** (*bool*) – boolean indicating if verbose output should be written to the terminal (default is False)

Returns **success** – boolean indicating if the stage differences are less than htol.

Return type bool

compare_swrbudget (*namefile1, namefile2, max_cumpd=0.01, max_incpd=0.01, outfile=None, files1=None, files2=None*)

Compare the SWR budget results from two simulations.

Parameters

- **namefile1** (*str*) – namefile path for base model
- **namefile2** (*str*) – namefile path for comparison model
- **max_cumpd** (*float*) – maximum percent discrepancy allowed for cumulative budget terms (default is 0.01)
- **max_incpd** (*float*) – maximum percent discrepancy allowed for incremental budget terms (default is 0.01)
- **outfile** (*str*) – budget comparison output file name. If outfile is None, no comparison output is saved. (default is None)

- **files1** (*str*) – base model output file. If files1 is not None, results will be extracted from files1 and namefile1 will not be used. (default is None)
- **files2** (*str*) – comparison model output file. If files2 is not None, results will be extracted from files2 and namefile2 will not be used. (default is None)

Returns **success** – boolean indicating if the difference between budgets are less than max_cumpd and max_incpd

Return type bool

download_and_unzip(*url*, *pth*='./', *delete_zip*=True, *verify*=True, *timeout*=30, *max_requests*=10, *chunk_size*=2048000, *verbose*=False)

Download and unzip a zip file from a url.

Parameters

- **url** (*str*) – url address for the zip file
- **pth** (*str*) – path where the zip file will be saved (default is the current path)
- **delete_zip** (*bool*) – boolean indicating if the zip file should be deleted after it is unzipped (default is True)
- **verify** (*bool*) – boolean indicating if the url request should be verified
- **timeout** (*int*) – url request time out length (default is 30 seconds)
- **max_requests** (*int*) – number of url download request attempts (default is 10)
- **chunk_size** (*int*) – maximum url download request chunk size (default is 2048000 bytes)
- **verbose** (*bool*) – boolean indicating if output will be printed to the terminal

get_entries_from_namefile(*namefile*, *ftype*=None, *unit*=None, *extension*=None)

Get entries from a namefile. Can select using FTYPE, UNIT, or file extension.

Parameters

- **namefile** (*str*) – path to a MODFLOW-based model name file
- **ftype** (*str*) – package type
- **unit** (*int*) – file unit number
- **extension** (*str*) – file extension

Returns **entries** – list of tuples containing FTYPE, UNIT, FNAME, STATUS for each namefile entry that meets a user-specified value.

Return type list of tuples

get_input_files(*namefile*)

Return a list of all the input files in this model.

Parameters **namefile** (*str*) – path to a MODFLOW-based model name file

Returns **filelist** – list of MODFLOW-based model input files

Return type list

get_mf6_blockdata(*f*, *blockstr*)

Return list with all non comments between start and end of block specified by blockstr.

Parameters

- **f** (*file object*) – open file object

- **blockstr** (*str*) – name of block to search

Returns **data** – list of data in specified block

Return type list

get_mf6_comparison(*src*)

Determine comparison type for MODFLOW 6 simulation.

Parameters **src** (*str*) – directory path to search for comparison types

Returns **action** – comparison type

Return type str

get_mf6_files(*mfnamefile*)

Return a list of all the MODFLOW 6 input and output files in this model.

Parameters **mfnamefile** (*str*) – path to the MODFLOW 6 simulation name file

Returns

- **filelist** (*list*) – list of MODFLOW 6 input files in a simulation
- **outplist** (*list*) – list of MODFLOW 6 output files in a simulation

get_mf6_ftypes(*namefile, ftypekeys*)

Return a list of FTYPES that are in the name file and in ftypekeys.

Parameters

- **namefile** (*str*) – path to a MODFLOW 6 name file
- **ftypekeys** (*list*) – list of desired FTYPES

Returns **ftypes** – list of FTYPES that match ftypekeys in namefile

Return type list

get_mf6_mshape(*disfile*)

Return the shape of the MODFLOW 6 model.

Parameters **disfile** (*str*) – path to a MODFLOW 6 discretization file

Returns **mshape** – tuple with the shape of the MODFLOW 6 model.

Return type tuple

get_mf6_nper(*tdisfile*)

Return the number of stress periods in the MODFLOW 6 model.

Parameters **tdisfile** (*str*) – path to the TDIS file

Returns **nper** – number of stress periods in the simulation

Return type int

get_namefiles(*pth, exclude=None*)

Search through a path (pth) for all .nam files.

Parameters

- **pth** (*str*) – path to model files
- **exclude** (*str* or *list*) – File or list of files to exclude from the search (default is None)

Returns **namefiles** – List of namefiles with paths

Return type list

get_repo_assets(*github_repo=None, version=None, error_return=False, verify=True*)

Return a dictionary containing the file name and the link to the asset contained in a github repository.

Parameters

- **github_repo** (*str*) – Repository name, such as MODFLOW-USGS/modflow6. If github_repo is None set to 'MODFLOW-USGS/executables'
- **version** (*str*) – github repository release tag
- **error_return** (*bool*) – boolean indicating if None will be returned if there are GitHub API issues
- **verify** (*bool*) – boolean indicating if the url request should be verified

Returns **result_dict** – dictionary of file names and links

Return type dict

get_sim_name(*namefiles, rootpth=None*)

Get simulation name.

Parameters

- **namefiles** (*str or list of strings*) – path(s) to MODFLOW-based model name files
- **rootpth** (*str*) – optional root directory path (default is None)

Returns **simname** – list of namefiles without the file extension

Return type list

getmfexes(*pth='.', version=None, platform=None, exes=None, verbose=False, verify=True*)

Get the latest MODFLOW binary executables from a github site (<https://github.com/MODFLOW-USGS/executables>) for the specified operating system and put them in the specified path.

Parameters

- **pth** (*str*) – Location to put the executables (default is current working directory)
- **version** (*str*) – Version of the MODFLOW-USGS/executables release to use. If version is None the github repo will be queried for the version number.
- **platform** (*str*) – Platform that will run the executables. Valid values include mac, linux, win32 and win64. If platform is None, then routine will download the latest asset from the github repository.
- **exes** (*str or list of strings*) – executable or list of executables to retain
- **verbose** (*bool*) – boolean indicating if output will be printed to the terminal
- **verify** (*bool*) – boolean indicating if the url request should be verified

main(*srcdir=None, target=None, fc='gfortran', cc='gcc', makeclean=True, expedite=False, dryrun=False, double=False, debug=False, include_subdirs=False, fflags=None, cflags=None, syslibs=None, arch='intel64', makefile=False, makefiledir='.', srcdir2=None, extrafiles=None, excludefiles=None, sharedobject=False, appdir=None, verbose=False, inplace=False, networkx=False, meson=False, mesondir='.')*

Main pymake function.

Parameters

- **srcdir** (*str*) – path for directory containing source files
- **target** (*str*) – executable name or path for executable to create
- **fc** (*str*) – fortran compiler

- **cc** (*str*) – c or cpp compiler
- **makeclean** (*bool*) – boolean indicating if intermediate files should be cleaned up after successful build
- **expedite** (*bool*) – boolean indicating if only out of date source files will be compiled. Clean must not have been used on previous build.
- **dryrun** (*bool*) – boolean indicating if source files should be compiled. Files will be deleted, if makeclean is True.
- **double** (*bool*) – boolean indicating a compiler switch will be used to create an executable with double precision real variables.
- **debug** (*bool*) – boolean indicating is a debug executable will be built
- **include_subdirs** (*bool*) – boolean indicating source files in srcdir subdirectories should be included in the build
- **fflags** (*list*) – user provided list of fortran compiler flags
- **cflags** (*list*) – user provided list of c or cpp compiler flags
- **syslibs** (*list*) – user provided syslibs
- **arch** (*str*) – Architecture to use for Intel Compilers on Windows (default is intel64)
- **makefile** (*bool*) – boolean indicating if a GNU make makefile should be created
- **makefiledir** (*str*) – GNU make makefile path
- **srcdir2** (*str*) – additional directory with common source files.
- **extrafiles** (*str*) – path for extrafiles file that contains paths to additional source files to include
- **excludefiles** (*str*) – path for excludefiles file that contains filename of source files to exclude from the build
- **sharedobject** (*bool*) – boolean indicating a shared object will be built
- **appdir** (*str*) – path for executable
- **verbose** (*bool*) – boolean indicating if output will be printed to the terminal
- **inplace** (*bool*) – boolean indicating that the source files in srcdir, srcdir2, and defined in extrafiles will be used directly. If inplace is False, source files will be copied to a directory named srcdir_temp. (default is False)
- **networkx** (*bool*) – boolean indicating that the NetworkX python package will be used to create the Directed Acyclic Graph (DAG) used to determine the order source files are compiled in. The NetworkX package tends to result in a unique DAG more often than the standard algorithm used in pymake. (default is False)
- **meson** (*bool*) – boolean indicating that the executable should be built using the meson build system. (default is False)
- **mesondir** (*str*) – Main meson.build file path

Returns **returncode** – return code

Return type **int**

make_plots(*srcdir*, *outdir*, *include_subdir=False*, *level=3*, *extension='.png'*, *verbose=False*, *networkx=False*)
Create plots of module dependencies.

Parameters

- **srcdir** (*str*) – path for source files
- **outdir** (*str*) – path for output images
- **include_subdir** (*bool*) – boolean indicating if subdirectories in the source file directory should be included
- **level** (*int*) – dependency level (1 is the minimum)
- **extension** (*str*) – output extension (default is .png)
- **verbose** (*bool*) – boolean indicating if output will be printed to the terminal
- **networkx** (*bool*) – boolean indicating that the NetworkX python package will be used to create the Directed Acyclic Graph (DAG) used to determine the order source files are compiled in. The NetworkX package tends to result in a unique DAG more often than the standard algorithm used in pymake. (default is False)

parser()

Construct the parser and return argument values.

Returns **args** – Namespace with command line arguments

Return type Namespace object

repo_latest_version(github_repo=None, verify=True)

Return a string of the latest version number (tag) contained in a github repository release.

Parameters **github_repo** (*str*) – Repository name, such as MODFLOW-USGS/modflow6. If github_repo is None set to 'MODFLOW-USGS/executables'

Returns **version** – string with the latest version/tag number

Return type str

setup(namefile, dst, remove_existing=True, extrafiles=None)

Setup MODFLOW-based model files for autotests.

Parameters

- **namefile** (*str*) – MODFLOW-based model name file.
- **dst** (*str*) – destination path for comparison model or file(s)
- **remove_existing** (*bool*) – boolean indicating if an existing comparison model or file(s) should be replaced (default is True)
- **extrafiles** (*str or list of str*) – list of extra files to include in the comparison

setup_comparison(namefile, dst, remove_existing=True)

Setup a comparison model or comparison file(s) for a MODFLOW-based model.

Parameters

- **namefile** (*str*) – MODFLOW-based model name file.
- **dst** (*str*) – destination path for comparison model or file(s)
- **remove_existing** (*bool*) – boolean indicating if an existing comparison model or file(s) should be replaced (default is True)

setup_mf6(src, dst, mfnamefile='mfsim.nam', extrafiles=None, remove_existing=True)

Copy all of the MODFLOW 6 input files from the src directory to the dst directory.

Parameters

- **src** (*src*) – directory path with original MODFLOW 6 input files

- **dst** (*str*) – directory path that original MODFLOW 6 input files will be copied to
- **mfnamefile** (*str*) – optional MODFLOW 6 simulation name file (default is mfsim.nam)
- **extrafiles** (*bool*) – boolean indicating if extra files should be included (default is None)
- **remove_existing** (*bool*) – boolean indicating if existing file in dst should be removed (default is True)

Returns

- **mf6inp** (*list*) – list of MODFLOW 6 input files
- **mf6outp** (*list*) – list of MODFLOW 6 output files

setup_mf6_comparison(*src*, *dst*, *remove_existing=True*)

Setup comparison for MODFLOW 6 simulation.

Parameters

- **src** (*src*) – directory path with original MODFLOW 6 input files
- **dst** (*str*) – directory path that original MODFLOW 6 input files will be copied to
- **remove_existing** (*bool*) – boolean indicating if existing file in dst should be removed (default is True)

Returns *action* – comparison type

Return type *str*

teardown(*src*)

Teardown a autotest directory.

Parameters **src** (*str*) – autotest directory to teardown

to_pydot(*dag*, *filename='mygraph.png'*)

Create a png file of a Directed Acyclic Graph

Parameters

- **dag** (*object*) – directed acyclic graph
- **filename** (*str*) – path of the graph png

class usgs_program_data

Bases: *object*

USGS program database class.

static export_json(*fpth='code.json'*, *prog_data=None*, *current=False*, *update=True*,
write_markdown=False, *verbose=False*)

Export USGS program data as a json file.

Parameters

- **fpth** (*str*) – Path for the json file to be created. Default is “code.json”
- **prog_data** (*dict*) – User-specified program database. If *prog_data* is None, it will be created from the USGS program database
- **current** (*bool*) – If False, all USGS program targets are listed. If True, only USGS program targets that are defined as current are listed. Default is False.
- **update** (*bool*) – If True, existing targets in the user-specified program database with values in the USGS program database. If False, existing targets in the user-specified program database will not be updated. Default is True.

- **write_markdown** (*bool*) – If True, write markdown file that includes the target name, version, and the last-modified date of the download asset (url). Default is False.
- **verbose** (*bool*) – boolean for verbose output to terminal

static get_keys(*current=False*)

Get target keys from the USGS program database.

Parameters **current** (*bool*) – If False, all USGS program targets are listed. If True, only USGS program targets that are defined as current are listed. Default is False.

Returns **keys** – list of USGS program targets

Return type list

static get_precision(*key*)

Get the dictionary for a specified target.

Parameters **key** (*str*) – Target USGS program

Returns **precision** – List

Return type list

static get_program_dict()

Get the complete USGS program database.

Returns **program_dict** – Dictionary with USGS program attributes for all targets

Return type dict

static get_target(*key*)

Get the dictionary for a specified target.

Parameters **key** (*str*) – Target USGS program that may have a path and an extension

Returns **program_dict** – Dictionary with USGS program attributes for the specified key

Return type dict

static get_version(*key*)

Get the current version of the specified target.

Parameters **key** (*str*) – Target USGS program

Returns **version** – current version of the specified target

Return type str

static list_json(*fpth='code.json'*)

List an existing code json file.

Parameters **fpth** (*str*) – Path for the json file to be listed. Default is “code.json”

static list_targets(*current=False*)

Print a list of the available USGS program targets.

Parameters **current** (*bool*) – If False, all USGS program targets are listed. If True, only USGS program targets that are defined as current are listed. Default is False.

static load_json(*fpth='code.json'*)

Load an existing code json file. Basic error checking is done to make sure the file contains the correct keys.

Parameters **fpth** (*str*) – Path for the json file to be created. Default is “code.json”

Returns **json_dict** – Valid USGS program database

Return type dict

static update_json(*fpth*='code.json', *temp_dict*=None)

UPDATE an existing code json file.

Parameters

- **fpth** (*str*) – Path for the json file to be listed. Default is “code.json”
- **temp_dict** (*dict*) – Dictionary with USGS program data for a target

zip_all(*path*, *file_pths*=None, *dir_pths*=None, *patterns*=None)

Compress all files in the user-provided list of file paths and directory paths that match the provided file patterns.

Parameters

- **path** (*str*) – path of the zip file that will be created
- **file_pths** (*str or list*) – file path or list of file paths to be compressed
- **dir_pths** (*str or list*) – directory path or list of directory paths to search for files that will be compressed
- **patterns** (*str or list*) – file pattern or list of file patterns s to match to when creating a list of files that will be compressed

INDICES AND TABLES

- genindex
- modindex
- search

PYTHON MODULE INDEX

p

- `pymake`, 31
- `pymake.autotest`, 25
- `pymake.autotest.autotest`, 18
- `pymake.config`, 31
- `pymake.plot`, 18
- `pymake.plot.dependency_graphs`, 17
- `pymake.pymake`, 11
- `pymake.pymake_base`, 14
- `pymake.pymake_build_apps`, 13
- `pymake.pymake_parser`, 16
- `pymake.utils`, 31
- `pymake.utils.download`, 25
- `pymake.utils.usgsprograms`, 28

A

`argv_reset_settings()` (*Pymake method*), 12, 32

B

`build()` (*Pymake method*), 12, 32

`build_apps()` (*in module pymake*), 33

`build_apps()` (*in module pymake.pymake_build_apps*), 14

C

`compare()` (*in module pymake*), 33

`compare()` (*in module pymake.autotest.autotest*), 19

`compare_budget()` (*in module pymake*), 34

`compare_budget()` (*in module pymake.autotest.autotest*), 19

`compare_concs()` (*in module pymake*), 35

`compare_concs()` (*in module pymake.autotest.autotest*), 20

`compare_heads()` (*in module pymake*), 35

`compare_heads()` (*in module pymake.autotest.autotest*), 20

`compare_stages()` (*in module pymake*), 36

`compare_stages()` (*in module pymake.autotest.autotest*), 21

`compare_swrbudget()` (*in module pymake*), 36

`compare_swrbudget()` (*in module pymake.autotest.autotest*), 21

`compress_targets()` (*Pymake method*), 12, 32

`compressall()` (*pymakeZipFile static method*), 26

D

`dotdict` (*class in pymake.utils.usgsprograms*), 30

`download_and_unzip()` (*in module pymake*), 37

`download_and_unzip()` (*in module pymake.utils.download*), 25

`download_setup()` (*Pymake method*), 12, 32

`download_target()` (*Pymake method*), 12, 32

`download_url()` (*Pymake method*), 13, 32

E

`export_json()` (*usgs_program_data static method*), 30, 42

`extract()` (*pymakeZipFile method*), 27

`extractall()` (*pymakeZipFile method*), 27

F

`finalize()` (*Pymake method*), 13, 32

G

`get_entries_from_namefile()` (*in module pymake*), 37

`get_entries_from_namefile()` (*in module pymake.autotest.autotest*), 22

`get_input_files()` (*in module pymake*), 37

`get_input_files()` (*in module pymake.autotest.autotest*), 22

`get_keys()` (*usgs_program_data static method*), 30, 43

`get_mf6_blockdata()` (*in module pymake*), 37

`get_mf6_blockdata()` (*in module pymake.autotest.autotest*), 22

`get_mf6_comparison()` (*in module pymake*), 38

`get_mf6_comparison()` (*in module pymake.autotest.autotest*), 22

`get_mf6_files()` (*in module pymake*), 38

`get_mf6_files()` (*in module pymake.autotest.autotest*), 22

`get_mf6_ftypes()` (*in module pymake*), 38

`get_mf6_ftypes()` (*in module pymake.autotest.autotest*), 23

`get_mf6_mshape()` (*in module pymake*), 38

`get_mf6_mshape()` (*in module pymake.autotest.autotest*), 23

`get_mf6_nper()` (*in module pymake*), 38

`get_mf6_nper()` (*in module pymake.autotest.autotest*), 23

`get_namefiles()` (*in module pymake*), 38

`get_namefiles()` (*in module pymake.autotest.autotest*), 23

`get_precision()` (*usgs_program_data static method*), 30, 43

`get_program_dict()` (*usgs_program_data static method*), 30, 43

`get_repo_assets()` (*in module pymake*), 38

- get_repo_assets() (in module *py-*
make.utils.download), 25
- get_sim_name() (in module *pymake*), 39
- get_sim_name() (in module *pymake.autotest.autotest*),
23
- get_target() (*usgs_program_data* static method), 30,
43
- get_temporary_directories() (in module *py-*
make.pymake_base), 15
- get_version() (*usgs_program_data* static method), 30,
43
- getmfexes() (in module *pymake*), 39
- getmfexes() (in module *pymake.utils.download*), 26
- getmfnightly() (in module *pymake.utils.download*), 26
- L**
- list_json() (*usgs_program_data* static method), 31, 43
- list_targets() (*usgs_program_data* static method),
31, 43
- load_json() (*usgs_program_data* static method), 31, 43
- M**
- main() (in module *pymake*), 39
- main() (in module *pymake.pymake_base*), 15
- make_plots() (in module *pymake*), 40
- make_plots() (in module *py-*
make.plot.dependency_graphs), 17
- module
 - pymake*, 31
 - pymake.autotest*, 25
 - pymake.autotest.autotest*, 18
 - pymake.config*, 31
 - pymake.plot*, 18
 - pymake.plot.dependency_graphs*, 17
 - pymake.pymake*, 11
 - pymake.pymake_base*, 14
 - pymake.pymake_build_apps*, 13
 - pymake.pymake_parser*, 16
 - pymake.utils*, 31
 - pymake.utils.download*, 25
 - pymake.utils.usgsprograms*, 28
- P**
- parser() (in module *pymake*), 41
- parser() (in module *pymake.pymake_parser*), 16
- pymake*
 - module, 31
- Pymake* (class in *pymake*), 31
- Pymake* (class in *pymake.pymake*), 12
- pymake.autotest*
 - module, 25
- pymake.autotest.autotest*
 - module, 18
- pymake.config*
- module*, 31
- pymake.plot*
 - module, 18
- pymake.plot.dependency_graphs*
 - module, 17
- pymake.pymake*
 - module, 11
- pymake.pymake_base*
 - module, 14
- pymake.pymake_build_apps*
 - module, 13
- pymake.pymake_parser*
 - module, 16
- pymake.utils*
 - module, 31
- pymake.utils.download*
 - module, 25
- pymake.utils.usgsprograms*
 - module, 28
- pymakeZipFile* (class in *pymake.utils.download*), 26
- R**
- repo_latest_version() (in module *pymake*), 41
- repo_latest_version() (in module *py-*
make.utils.download), 27
- reset() (*Pymake* method), 13, 33
- S**
- set_build_target_bool() (*Pymake* method), 13, 33
- setup() (in module *pymake*), 41
- setup() (in module *pymake.autotest.autotest*), 23
- setup_comparison() (in module *pymake*), 41
- setup_comparison() (in module *py-*
make.autotest.autotest), 24
- setup_mf6() (in module *pymake*), 41
- setup_mf6() (in module *pymake.autotest.autotest*), 24
- setup_mf6_comparison() (in module *pymake*), 42
- setup_mf6_comparison() (in module *py-*
make.autotest.autotest), 24
- T**
- teardown() (in module *pymake*), 42
- teardown() (in module *pymake.autotest.autotest*), 24
- to_pydot() (in module *pymake*), 42
- to_pydot() (in module *py-*
make.plot.dependency_graphs), 17
- U**
- update_build_targets() (*Pymake* method), 13, 33
- update_json() (*usgs_program_data* static method), 31,
43
- update_target() (*Pymake* method), 13, 33
- usgs_program_data* (class in *pymake*), 42

`usgs_program_data` (class in `pymake.utils.usgsprograms`), 30

Z

`zip_all()` (in module `pymake`), 44

`zip_all()` (in module `pymake.utils.download`), 27