MODFLOW 6 Release Notes

Version mf6.2.0—October 22, 2020

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Introduction

This document describes MODFLOW 6 Version mf6.2.0. This distribution is packaged for personal computers using the Microsoft Windows 7 and 10 operating systems, although it may run on other versions of Windows. The executable file was compiled for 64-bit Windows operating systems and should run on most personal computers.

Version numbers for MODFLOW 6 will follow a major.minor.revision format. The major number will be increased when there are substantial new changes that may break backward compatibility. The minor number will be increased when important, but relatively minor new functionality is added. The revision number will be added when errors are corrected in either the program or input files.

MODFLOW 6 is tested with a large number of example problems, and new capabilities are thoroughly tested as they are integrated into the program. Additional testing can sometimes reveal errors in the program. These errors are fixed as soon as possible and made available in a subsequent release. Every effort is made to maintain backward compatibility of the format for MODFLOW 6 input files; however, this goal is not always possible, especially for newer packages and models. Changes to the program to add new functionality, correct errors, or alter the format for an input file are summarized in this release notes document.

History

This section describes changes introduced into MODFLOW 6 for the current release. Changes introduced in previous releases are in Appendix A. These changes may substantially affect users.

- Version mf6.2.0–October 16, 2020

  NEW FUNCTIONALITY

  - A new Buoyancy (BUY) Package for the Groundwater Flow (GWF) Model is introduced in this release as a way to represent variable-density groundwater flow. The BUY Package is based on the hydraulic head formulation described by Langevin and others (2020). Extensive testing of the BUY Package has been performed but changes to the code and input may be required in response to user needs and testing.

  - A new Groundwater Transport (GWT) Model is introduced in this release as a way to simulate the fate and transport of a dissolved solute. Extensive testing of the GWT Model has been performed but changes to the code and input may be required in response to user needs and testing.

  - The Basic Model Interface (BMI) capabilities were first released in version 6.1.1. Extensive testing of the BMI capabilities has been performed but changes to the code and calling procedures be required in response to user needs and testing.

  EXAMPLES

  - The format for the examples included in the distribution has changed. The examples are now described in the modflow6-examples.pdf file in the doc folder. The examples have been renamed, and they are no longer numbered. Most of the examples are the same as those distributed with the previous release; however some have been modified, updated, combined or eliminated based on standardization of example construction, testing, and documentation.

  BUG FIXES AND OTHER CHANGES TO EXISTING FUNCTIONALITY
  BASIC FUNCTIONALITY

- The observation routines were improved to handle very large numbers of observations written to the same comma-separated-value (CSV) file. Non-advancing input-output is now used to write the CSV header instead of constructing a header string. This change should substantially improve memory and runtime problems with models containing thousands of observations.

- If the CONTINUE option is specified in mfsim.nam, do not force models to write budget tables when the solver does not converge. Instead, always use Output Control options to determine when budget tables are written if CONTINUE option is specified and the solver does not converge. Also, if the CONTINUE option is specified, calculate and write observations even if the model does not converge. Observations were being written as zero if the model did not converge, but the CONTINUE flag was set.

- Allow the program to read input files with very long lines. Previously, the program was limited to a maximum line length of 50,000 characters. The program now uses dynamic memory allocation, when necessary, to read any sized line in an input file.

- Fixed an error in the implementation of the Newton-Raphson correction for XT3D. The error in the code would have only affected simulations that used the NEWTON option together with the XT3D RHS option.

ADVANCED STRESS PACKAGES

- Fix error in calculated Newton-Raphson MAW-GWF connection terms for the MAW Package. This correction should improve model convergence and may change existing model results. This correction does not affect simulations that use the FLOW_CORRECTION option introduced in version 6.1.1.

- The program will now terminate with an error message if the skin radius for a GWF connection in the MAW Package is less than or equal to the well radius. Warning messages are also issued when the well bottom, screen top for a GWF connection, or screen bottom for a GWF connection are reset by the program for one or more MAW Package wells.

- An SFR reach can have zero specified connections. In this case, an entry is still required in the CONNECTIONDATA block for that reach. The error check for this required entry was not implemented and so the program would continue with unexpected results. The program now verifies that an entry is present in CONNECTIONDATA for every reach, even those with zero connections.

- If a GWF "NONE" connection was specified for SFR then the program would terminate with an error or proceed with unexpected results if GWF or SFR flow terms were written to binary output files. The program was fixed so that GWF "NONE" connections for SFR are not written to the binary budget files.

- Increase the length of boundname to its intended size of 40 characters. Boundnames were being truncated after 16 characters for the LAK, MAW, and SFR Packages.

SOLUTION

- A fix was implemented in the biconjugate gradient stabilized linear solver routine so that the maximum change in the dependent value is calculated and stored correctly.

- Corrected the SIMPLE and COOLEY under-relaxation schemes in the Iterative Model Solution (IMS). The methods were not applying the correct under-relaxation factor. The SIMPLE scheme now uses the user-specified value for gamma as the factor. The COOLEY scheme updates the factor based on solver history.

Known Issues

This section describes known issues with this release of MODFLOW 6.

1. The AUXMULTNAME option can be used to scale input values, such as riverbed conductance, using values in an auxiliary column. When this AUXMULTNAME option is used, the multiplier value in the AUXMULTNAME column should not be represented with a time series unless the value to scale is also represented with a time series.

2. The capability to use Unsaturated Zone Flow (UZF) routing beneath lakes and streams has not been implemented.

Distribution File

The following distribution file is for use on personal computers: `mf6.2.0.zip`. The distribution file is a compressed zip file. The following directory structure is incorporated in the zip file:

```
mf6.2.0/
    bin/
    doc/
    examples/
        ex-gwf-advtidal/
        ex-gwf-bcf2ss-p01a/
        ex-gwf-bcf2ss-p02a/
        ex-gwf-bump-p01a/
        ex-gwf-bump-p01b/
        ex-gwf-bump-p01c/
        ex-gwf-csub-p01/
        ex-gwf-csub-p02a/
        ex-gwf-csub-p02b/
        ex-gwf-csub-p03a/
        ex-gwf-csub-p03b/
        ex-gwf-csub-p04/
        ex-gwf-disvmesh/
        ex-gwf-drn-p01a/
        ex-gwf-drn-p01b/
        ex-gwf-fhb/
        ex-gwf-hanic/
        ex-gwf-hanir/
        ex-gwf-hanix/
        ex-gwf-lak-p01/
        ex-gwf-lak-p02/
        ex-gwf-lgr/
        ex-gwf-lgrv-gc/
        ex-gwf-lgrv-gr/
        ex-gwf-lgrv-lgr/
        ex-gwf-maw-p01a/
        ex-gwf-maw-p01b/
```

```
ex-gwf-maw-p02/
ex-gwf-maw-p03a/
ex-gwf-nwt-p02a/
ex-gwf-nwt-p02b/
ex-gwf-nwt-p03a/
ex-gwf-nwt-p03b/
ex-gwf-sagehen/
ex-gwf-sfr-p01/
ex-gwf-sfr-p01b/
ex-gwf-spbc/
ex-gwf-twri01/
    mf2005/
ex-gwf-u1disv/
ex-gwf-u1disv-x/
ex-gwf-whirl/
ex-gwf-zaidel/
ex-gwt-henry-a/
ex-gwt-henry-b/
ex-gwt-keating/
    mf6gwf/
    mf6gwt/
ex-gwt-moc3d-p01a/
    mf6gwf/
    mf6gwt/
ex-gwt-moc3d-p01b/
    mf6gwf/
    mf6gwt/
ex-gwt-moc3d-p01c/
    mf6gwf/
    mf6gwt/
ex-gwt-moc3d-p01d/
    mf6gwf/
    mf6gwt/
ex-gwt-moc3d-p02/
    mf6gwf/
    mf6gwt/
ex-gwt-moc3d-p02tg/
    mf6gwf/
    mf6gwt/
ex-gwt-mt3dms-p01a/
    mt3d/
ex-gwt-mt3dms-p01b/
    mt3d/
ex-gwt-mt3dms-p01c/
    mt3d/
ex-gwt-mt3dms-p01d/
    mt3d/
ex-gwt-mt3dms-p03/
```

```
        mt3d/
    ex-gwt-mt3dms-p04a/
        mt3d/
    ex-gwt-mt3dms-p04b/
        mt3d/
    ex-gwt-mt3dms-p04c/
        mt3d/
    ex-gwt-mt3dms-p05/
        mt3d/
    ex-gwt-mt3dms-p06/
        mt3d/
    ex-gwt-mt3dms-p07/
        mt3d/
    ex-gwt-mt3dms-p08/
        mt3d/
    ex-gwt-mt3dms-p09/
        mt3d/
    ex-gwt-mt3dms-p10/
        mt3d/
    ex-gwt-mt3dsupp631/
        mf2005/
        mf6gwf/
        mf6gwt/
        mt3d/
    ex-gwt-mt3dsupp632a/
        mf2005/
        mf6gwf/
        mf6gwt/
        mt3d/
    ex-gwt-mt3dsupp632b/
        mf2005/
        mf6gwf/
        mf6gwt/
        mt3d/
    ex-gwt-mt3dsupp632c/
        mf2005/
        mf6gwf/
        mf6gwt/
        mt3d/
    ex-gwt-mt3dsupp82/
        mf2005/
        mf6gwf/
        mf6gwt/
        mt3d/
    ex-gwt-prudic2004t2/
        mf6gwf/
        mf6gwt/
make/
```

```
msvs/
src/
     Exchange/
     Model/
          Geometry/
          GroundWaterFlow/
          GroundWaterTransport/
          ModelUtilities/
     Solution/
          SparseMatrixSolver/
     Timing/
     Utilities/
          Memory/
          Observation/
          OutputControl/
          TimeSeries/
srcbmi/
utils/
     mf5to6/
          make/
          msvs/
          src/
               LGR/
               MF2005/
               NWT/
               Preproc/
     zonebudget/
          make/
          msvs/
          src/
```

It is recommended that no user files are kept in the mf6.2.0 directory structure. If you do plan to put your own files in the mf6.2.0 directory structure, do so only by creating additional subdirectories.

Installation and Execution

There is no installation of MODFLOW 6 other than the requirement that `mf6.2.0.zip` must be unzipped into a location where it can be accessed.

To make the executable versions of MODFLOW 6 accessible from any directory, the directory containing the executables should be included in the PATH environment variable. Also, if a prior release of MODFLOW 6 is installed on your system, the directory containing the executables for the prior release should be removed from the PATH environment variable.

As an alternative, the executable file, "`mf6.exe`", in the mf6.2.0/bin directory can be copied into a directory already included in the PATH environment variable.

To run MODFLOW 6, simply type `mf6` in a terminal window. The current working directory must be set to a location where the model input files are located. Upon execution, MODFLOW 6 will immediately look for file with the name `mfsim.nam` in the current working directory, and will terminate with an error if it does

not find this file.

Compiling MODFLOW 6

MODFLOW 6 has been compiled using Intel Visual Fortran and gfortran on the Windows and Mac/OS operating systems. Because the program uses relatively new Fortran extensions, newer versions of the compilers may be required for successful compilation. For example, to use gfortran to compile MODFLOW 6, gfortran version 4.9 or newer must be used. If you have gfortran installed on your computer, you can tell which version it is by entering "`gfortran --version`" at a terminal window.

This distribution contains the Microsoft Visual Studio solution and project files for compiling MODFLOW 6 on Windows using the Intel Fortran Compiler. The files have been used successfully with Microsoft Visual Studio Community 2019 and Intel(R) Visual Fortran Compiler 2020.0.166. To compile MODFLOW 6, open the mf6.sln file in the msvs folder and click Build > Build Solution. A separate Visual Studio solution file is also included for building the BMI dynamically linked library version of MODFLOW 6.

This distribution also comes with a makefile for compiling MODFLOW 6 with `gfortran`. The makefile is contained in the `make` folder.

For those familiar with Python, the pymake package can also be used to compile MODFLOW 6. Additional information on the Python pymake utility can be found at: https://github.com/modflowpy/pymake.

System Requirements

MODFLOW 6 is written in Fortran. It uses features from the 95, 2003, and 2008 language. The code has been used on UNIX-based computers and personal computers running various forms of the Microsoft Windows operating system.

Testing

The examples distributed with MODFLOW 6 can be run by navigating to the examples folder and executing the "`run.bat`" batch files within each example folder. Alternatively, there is a "`runall.bat`" batch file under the examples folder that will run all of the test problems.

MODFLOW 6 Documentation

Details on the numerical methods and the underlying theory for MODFLOW 6 are described in the following reports:

- Hughes, J.D., Langevin, C.D., and Banta, E.R., 2017, Documentation for the MODFLOW 6 framework: U.S. Geological Survey Techniques and Methods, book 6, chap. A57, 36 p., accessed August 4, 2017, at https://doi.org/10.3133/tm6A57

- Langevin, C.D., Hughes, J.D., Provost, A.M., Banta, E.R., Niswonger, R.G., and Panday, Sorab, 2017, Documentation for the MODFLOW 6 Groundwater Flow (GWF) Model: U.S. Geological Survey Techniques and Methods, book 6, chap. A55, 197 p., accessed August 4, 2017, at https://doi.org/10.3133/tm6A55

- Provost, A.M., Langevin, C.D., and Hughes, J.D., 2017, Documentation for the "XT3D" Option in the Node Property Flow (NPF) Package of MODFLOW 6: U.S. Geological Survey Techniques and Methods, book 6, chap. A56, 46 p., accessed August 4, 2017, at https://doi.org/10.3133/tm6A56

Description of the MODFLOW 6 input and output is included in this distribution in the "doc" folder as mf6io.pdf.

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References Cited

Hoffmann, Jörn, Leake, S.A., Galloway, D.L., and Wilson, A.M., 2003, MODFLOW-2000 Ground-Water Model—User Guide to the Subsidence and Aquifer-System Compaction (SUB) Package: U.S. Geological Survey Open-File Report 03–233, 44 p., accessed June 27, 2017, at https://pubs.usgs.gov/of/2003/ofr03-233/.

Hughes, J.D., Langevin, C.D., and Banta, E.R., 2017, Documentation for the MODFLOW 6 framework: U.S. Geological Survey Techniques and Methods, book 6, chap. A57, 36 p., accessed August 4, 2017, at https://doi.org/10.3133/tm6A57.

Langevin, C.D., Hughes, J.D., Provost, A.M., Banta, E.R., Niswonger, R.G., and Panday, Sorab, 2017, Documentation for the MODFLOW 6 Groundwater Flow (GWF) Model: U.S. Geological Survey Techniques and Methods, book 6, chap. A55, 197 p., accessed August 4, 2017, at https://doi.org/10.3133/tm6A55.

Langevin, C.D., Panday, Sorab, and Provost, A.M., 2020, Hydraulic-head formulation for density-dependent flow and transport: Groundwater, v. 58, no. 3, p. 349–362.

Leake, S.A., and Galloway, D.L., 2007, MODFLOW Ground-water model—User guide to the Subsidence and Aquifer-System Compaction Package (SUB-WT) for Water-Table Aquifers: U.S. Geological Survey Techniques and Methods, book 6, chap. A23, 42 p., accessed June 27, 2017, at https://pubs.er.usgs.gov/publication/tm6A23.

Panday, Sorab, Langevin, C.D., Niswonger, R.G., Ibaraki, Motomu, and Hughes, J.D., 2013, MODFLOW-USG version 1—An unstructured grid version of MODFLOW for simulating groundwater flow and tightly coupled processes using a control volume finite-difference formulation: U.S. Geological Survey Techniques and Methods, book 6, chap. A45, 66 p., accessed June 27, 2017, at https://pubs.usgs.gov/tm/06/a45/.

Peckham, S.D., Hutton, E.W., and Norris, Boyana, 2013, A component-based approach to integrated modeling in the geosciences: The design of CSDMS: Computers & Geosciences, v. 53, p. 3 – 12, accessed March 24, 2020, at https://doi.org/https://doi.org/10.1016/j.cageo.2012.04.002.

Provost, A.M., Langevin, C.D., and Hughes, J.D., 2017, Documentation for the "XT3D" Option in the Node Property Flow (NPF) Package of MODFLOW 6: U.S. Geological Survey Techniques and Methods, book 6, chap. A56, 46 p., accessed August 4, 2017, at https://doi.org/10.3133/tm6A56.

Appendix A. Changes Introduced in Previous Versions

This appendix describes changes introduced into MODFLOW 6 in previous releases. These changes may substantially affect users.

- Version mf6.1.1–June 12, 2019

  <u>NEW FUNCTIONALITY</u>

  – Refactor the source code to support the Basic Model Interface (BMI) developed by the Community Surface Dynamics Modeling System (CSDMS) group. BMI is a set of standard control and query functions that, when added to a model code, make that model both easier to learn and easier to couple with other software elements (Peckham and others, 2013). Furthermore, the BMI makes it possible to control MODFLOW 6 execution from scripting languages using bindings for the BMI (for example, python bindings for the BMI available through pymt). The BMI in this version is considered preliminary (alpha release). Limited testing of the BMI has been performed but significant changes are expected in future releases. User support for the MODFLOW 6 BMI may be provided in the future.

  – Add silent command line switch (`-s` or `--silent`) that sends all screen output (STDOUT) to a text file (with the name "mfsim.stdout").

  – Add screen output command line switch (`-l <str>` or `--level <str>`) that controls output to the screen (STDOUT). If `<str>` is summary, stress period and time step data are not written to STDOUT. If `<str>` is debug, normal and debug output are written to STDOUT.

  – Add simulation mode command line switch (`-m <str>` or `--mode <str>`) that controls the solution mode. If `<str>` is validate, model input will be read and checked for errors, but the coefficient matrix or matrices will not be assembled or solved and solution output will not be written.

  – Add SAVE_SATURATION option to the Node Property Flow Package. When invoked, cell saturation is written to the binary budget file as an auxiliary column for a record with the name "DATA-SAT". The cell saturation can be used by post-processors to determine how much of the cell is saturated without having to know the value for ICELLTYPE or the value for head. If a cell is marked as confined (ICELLTYPE=0) then saturation is always one. If ICELLTYPE is one, then saturation ranges between zero and one.

  – Add option for saving package convergence for the CSUB Package to a comma-separated values (CSV) file. Package convergence is enabled by specifying PACKAGE_CONVERGENCE FILEOUT <package_convergence_filename> in the options block for the package.

  – Add option for saving package convergence for the LAK, SFR, and UZF Packages to comma-separated values (CSV) files. Package convergence for the LAK, SFR, and UZF Packages is enabled by specifying PACKAGE_CONVERGENCE FILEOUT <package_convergence_filename> in the options block for the package.

  – Add CSV_OUTER_OUTPUT output option to save outer iteration information to a comma-separated values (CSV) file. The maximum of the model or package dependent-variable change for the outer iteration is written to the CSV file at the end of each outer iteration.

  – Add CSV_INNER_OUTPUT output option to save inner iteration information to a comma-separated values (CSV) file. The CSV output also the includes maximum dependent-variable change and maximum residual convergence information for the solution and each model (if the solution includes more than one model) and linear acceleration information for each inner iteration. The inner iteration CSV output, which contains a separate line for each inner iteration, is written to the CSV file all at once at the end of each outer iteration.

- Add OUTER_DVCLOSE and INNER_DVCLOSE variables to replace OUTER_HCLOSE and INNER_HCLOSE variables in the IMS Package input file. "DV" is used now instead to more generally refer to dependent variable. Warning messages will be issued if OUTER_HCLOSE and/or INNER_HCLOSE variables are specified. OUTER_HCLOSE and INNER_HCLOSE variables will eventually be deprecated.

- Add option to scale drain conductance as a function of simulated head over a user-defined range (drainage depth). Linear-conductance scaling is used with the Standard Formulation. Cubic-conductance scaling is used with the Newton-Raphson Formulation. The additional drainage depth variable is specified as an auxiliary variable and AUXDEPTHNAME is used to identify the auxiliary variable defining the drainage depth. The cubic-conductance scaling can be used as a replacement for the groundwater seepage option in the UZF Package. The scaled drainage conductance option can also be used to represent vertical seepage faces and improve model convergence in cells where simulated heads fluctuate around the elevation where the drain begins to discharge groundwater.

- Add timeseries support for the reach upstream fraction variable in the SFR package.

- Add Picard iterations for the SFR package to minimize differences in SFR package results between subsequent GWF Picard (non-linear) iterations as a result of non-optimal reach numbering. The number of SFR package Picard iterations can be controlled by specifying the maximum number of Picard iteration to be used in the OPTIONS block (MAXIMUM_PICARD_ITERATIONS). If reaches are numbered in order, from upstream to downstream, MAXIMUM_PICARD_ITERATIONS can be set to 1 to reduce model run time. Specifying MAXIMUM_PICARD_ITERATIONS to 1 will result in identical SFR package performance to previous versions of MODFLOW 6.

- Add flow correction option for the MAW package that corrects the MAW-GWF exchange in cases where the head in a multi-aquifer well is below the bottom of the screen for a connection or the head in a convertible cell connected to a multi-aquifer well is below the cell bottom. When flow corrections are activated, unit head gradients are used to calculate the flow between a multi-aquifer well and a connected GWF cell. This option is identical to the MODFLOW-USG "flow-to-dry-cell" option for flow between a CLN cell and a GWF cell if the cell is convertible (Panday and others, 2013). Flow corrections are enabled by specifying FLOW_CORRECTION in the OPTIONS block. By default, flow corrections are not made. *Prior to this release (version 6.1.1), flow corrections were made anytime the head in a multi-aquifer well was below the bottom of the screen for a connection–this may result in different results for existing models that can be resolved by using the FLOW_CORRECTION option.*

- Add new document, "MODFLOW 6 – Supplemental Technical Information," to the doc folder. This document contains information that was in the mf6io.pdf appendices. This technical information document may expand with future versions as new features are added.

BUG FIXES AND OTHER CHANGES TO EXISTING FUNCTIONALITY
BASIC FUNCTIONALITY

- Correct an error in how the discretization package (for regular MODFLOW grids) calculates the distance between two cells when one or both of the cells are unconfined. The error in the code would have only affected XT3D simulations with a regular grid, unconfined conditions, and specification of ANGLE2 in the NPF Package.

- Correct an error in the use of the AUXMULTNAME option for boundary packages when time series are used. A problem remains when time series are used for AUXMULTNAME but not for the column that is scaled by AUXMULTNAME. This situation should be avoided.

STRESS PACKAGES

– Fix a bug in binary budget file header for CSUB Package budget data written using IMETH=6 (CSUB-ELASTIC and CSUB-INELASTIC) .

– Add information on the CSUB Package budget terms and compaction data written the the Input/Output document in the 'Description of Groundwater Flow (GWF) Model Binary Output Files' section.

– Prior to this release, calculated flows between a standard stress package (WEL, DRN, RIV, GHB, RCH, and EVT) and the connected model cell were based on the RHS and HCOF terms from the previous iteration. This was not consistent with previous MODFLOW versions. These packages were modified so that the flows are recalculated using the final converged head solution. As a result of this change, simulated groundwater flows for these packages may be slightly different (compared to previous releases) if the package HCOF and RHS values depend on the simulated groundwater head.

ADVANCED STRESS PACKAGES

– The code for saving the budget terms for the advanced packages was refactored to use common routines. These changes should have no affect on simulation results.

– In previous releases, the LAK Package would accept negative user-input values for RAINFALL, EVAPORATION, RUNOFF, INFLOW, and WITHDRAWAL even though the user guide mentioned that negative values are not allowed for these flow terms. Error checks were added to ensure these values are specified as positive.

– Add a storage term to the SFR Package binary output file. This term is always zero with the present implementation. An auxiliary variable, called VOLUME, is also written with the storage budget term. This term contains the calculated water volume in the reach.

– Refactor the SFR Package to remove use of RectangularChGeometry objects and added required functionality as private methods in the SFR module.

– Improve error trapping in the MAW Package to catch divide by zero errors when calculating the saturated conductance for wells using the SKIN CONDEQN in connections where the cell transmissivity (the product of geometric mean of the horizontal hydraulic conductivity and cell thickness) and well transmissivity (the product of HK_SKIN and screen thickness) is equal to one. Also add error trapping for well connections using the 1) SKIN CONDEQN where the contrast between the cell and well transmissivities are less than one and 2) SKIN and MEAN CONDEQN where the calculated connection saturated conductance is less than zero.

– For the Lake Package, the outlet number was written as ID1 and ID2 for the TO-MVR record in the binary budget file. This has been changed so that the lake number of the connected outlet is written to ID1 and ID2. This change was implemented so that lake budgets can be calculated using the information in the lake budget file.

– The Lake, Streamflow Routing, and Multi-Aquifer Well Packages were modified to save the user-specified stage or head to the binary output file for lakes, reaches, or wells that are specified as being CONSTANT. Prior to this change, a no-flow value was written to the package binary output files for constant stage lakes and streams and constant head multi-aquifer wells. The no-flow value is still written for those lakes, streams, or wells that are specified by the user as being inactive. This change should make it easier to post-process the results from these packages.

SOLUTION

- Fix a bug in the linear solver when using the STRICT RCLOSE_OPTION that prevented termination of inner iterations when the INNER_DVCLOSE and INNER_RCLOSE criteria were met but the inner iteration count was greater than one. The inner iterations are now terminated when the INNER_DVCLOSE and INNER_RCLOSE criteria are met but the linear solver is considered non-converged if the inner iteration count is greater than one.

- Deprecate the CSV_OUTPUT output option in the OPTIONS BLOCK because the output to the comma-separated values (CSV) file was based on the PRINT_OPTION option. If CSV_OUTPUT is specified, it is used to define the file name for the CSV_OUTER_OUTPUT output option.

- Modify the outer iteration information written to the simulation listing file when PRINT_OPTION is not NONE to improve the ability of users to evaluate model convergence. Added Package convergence data, eliminated dependent variable changes adjusted by under-relaxation, and flags to indicate when an outer iterations step is considered converged. Information is also provided if PTC causes non-convergence for a outer iteration (even if the model is converged) and if NEWTON UNDER_RELAXATION resets outer iteration convergence from FALSE to TRUE. Dependent-variable changes for the under-relaxation step in an outer iteration are no longer reported because under-relaxation is only applied if the model or package outer iteration steps do not converge and by definition reduce dependent-variable changes and are not used to evaluate outer iteration convergence.

- Deprecate the OUTER_RCLOSEBND optional variable in the NONLINEAR BLOCK because OUTER_DVCLOSE is used for all terms used to evaluate package convergence. An warning will be issued if OUTER_RCLOSEBND is specified.

- Deprecate the CSV_OUTPUT output option. A warning will be issued if the CSV_OUTPUT option is specified and outer iteration information will be saved to the specified FILEOUT comma-separated values (CSV) file.

- Version mf6.1.0

NEW FUNCTIONALITY

- Added the Skeletal Storage, Compaction, and Subsidence (CSUB) Package. The one-dimensional effective-stress based compaction theory implemented in the CSUB Package is documented in Leake and Galloway (2007). The numerical approach used for delay interbeds in the CSUB package is documented in Hoffmann and others (2003) and uses the same one-dimensional effective-stress based compaction theory as coarse-grained and fine-grained no-delay interbed sediments. A number of example problems that use the CSUB Package are documented in the "MODFLOW 6 CSUB Package Example Problems" pdf document included in this and subsequent releases.

BASIC FUNCTIONALITY

- Added an error check to the DISU Package that ensures that an underlying cell has a top elevation that is less than or equal to the bottom of an overlying cell. An underlying cell is one in which the IHC value for the connection is zero and the connecting node number is greater than the cell node number.

- Added restricted IDOMAIN support for DISU grids. Users can specify an optional IDOMAIN in the DISU Package input file. IDOMAIN values must be zero or one. Vertical pass-through cells (specified with an IDOMAIN value of -1 in the DIS or DISV Package input files) are not supported for DISU.

- NPF Package will now write a message to the GWF Model list file to indicate when the SAVE_SPECIFIC_DISCHARGE option is invoked.

- Added two new options to the NPF Package. The K22OVERK option allows the user to enter the anisotropy ratio for K22. If activated, the K22 values entered by the user in the NPF input file will be multiplied by the K values entered in the NPF input file. The K33OVERK option allows the user to enter the anisotropy ratio for K33. If activated, the K33 values entered by the user in the NPF input file will be multiplied by the K values entered in the NPF input file. With this K33OVERK option, for example, the user can specify a value of 0.1 for K33 and have all K33 values be one tenth of the values specified for K. The program will terminate with an error if these options are invoked, but arrays for K22 and/or K33 are not provided in the NPF input file.

- Added new MAXERRORS option to mfsim.nam. If specified, the maximum number of errors stored and printed will be limited to this number. This can prevent a situation where memory will run out when there are an excessive number of errors.

- Refactored many parts of the code to remove unused variables, conform to stricter FORTRAN standard checks, and allow for new development efforts to be included in the code base.

STRESS PACKAGES

- There was an error in the calculation of the segmented evapotranspiration rate for the case where the rate did not decrease with depth. There was another error in which PETM0 was being used as the evapotranspiration rate at the surface instead of the proportion of the evapotranspiration rate at the surface.

ADVANCED STRESS PACKAGES

- Corrected the way auxiliary variables are handled for the advanced packages. In some cases, values for auxiliary variables were not being correctly written to the GWF Model budget file or to the advanced package budget file. A consistent approach for updating and saving auxiliary variables was implemented for the MAW, SFR, LAK, and UZF Packages.

- The user guide was updated to include a missing laksetting that was omitted from the PERIOD block. The laksetting description now includes an INFLOW option; a description for INFLOW is also now included.

- The LAK package was incorrectly making an error check against NOUTLETS instead of NLAKES.

- For the advanced stress packages, values assigned to the auxiliary variables were not written correctly to the GWF Model budget file, but the values were correct in the advanced package budget file. Program was modified so that auxiliary variables are correctly written to the GWF Model budget file.

- Corrected several error messages issued by the SFR Package that were not formatted correctly.

- Fixed a bug in which the lake stage stable would sometimes result in touching numbers. This only occurred for negative lake stages.

- The UZF Package was built on the UZFKinematicType, which used an array of structures. A large array like this, can cause memory problems. The UZFKinematicType was replaced with a new Uzf-CellGroupType, which is a structure of arrays and is much more memory efficient. The underlying UZF algorithm did not change.

SOLUTION

- Add ALL and FIRST options to optional NO_PTC optional keyword in OPTIONS block. If NO_PTC option is FIRST, PTC is disabled for the first stress period but is applied in all subsequent steady-state stress periods. If NO_PTC option is ALL, PTC is disabled for all steady-state stress

periods. If the NO_PTC options is not defined, PTC is disabled for all steady-state stress periods (this is consistent with the behaviour of the NO_PTC option in previous versions).

- Version mf6.0.4–Feb. 27, 2019

BASIC FUNCTIONALITY

- Addressed issue with pointing contiguous pointer vectors/arrays to non-contiguous pointer vectors/arrays that caused code compilation failure with gfortran-8. A consequence of addressing this issue is that all pointer vectors/arrays that are allocated or pointed to using the memory manager must be defined to be contiguous.

- Corrected a problem with the reading of grid data from a binary file, in which the program was reading a binary header for each row of data.

- Added a new error check for very small time steps. If the value of the starting time is equal to the ending time (starting time plus the time step length), then the time step is too small to be differentiated by the program based on the precision of floating point numbers. The program will terminate with an error in this case. The program will also terminate if the storage package with a transient stress period has a time step length of zero.

- The observation package was modified to use non-advancing output instead of fixed length strings when writing ascii output. The previous use of fixed length strings resulted in truncation of ascii observation output when the product of user-specified `digits + 7` and the number of observations exceeded 5000.

- Corrected an error in the GWF-GWF Exchange module that caused the specific discharge values in the child model to be calculated incorrectly. The calculation was incorrect because the face normal for the child model was pointing toward the center of the cell instead of outward.

- Minor refactoring to improve code clarity.

STRESS PACKAGES

- Minor refactoring to improve code clarity.

ADVANCED STRESS PACKAGES

- Modified the Multi-Aquifer Well (MAW) Package so that the HEAD_LIMIT and RATE_SCALING options work for injection wells. Prior to this change, these options only worked for extraction wells. These options can be used to reduce or even shut off well injection as the head in the well rises above user-specified levels.

- Added stage and residual convergence checks to the SFR package to make sure that stage and upstream flow changes between successive outer iterations are less than OUTER_HCLOSE and OUTER_RCLOSEBND, respectively. This addition is expected to be useful for steady-state simulations with complicated networks and simple reaches.

- Modified the final convergence check for the LAK package to use OUTER_HCLOSE when evaluating lake stage changes between successive outer iterations.

- Modified the final convergence check for the UZF package to use OUTER_RCLOSEBND when evaluating rejected infiltration, groundwater recharge, and groundwater seepage changes between successive outer iterations.

- Minor refactoring to improve code clarity.

SOLUTION

– Modified pseudo-transient continuation (PTC) approach to use PTC for steady-state stress period for models using the Newton-Raphson formulation for problems with and without the storage (STO) package. Previously, PTC was only used with problems that did not include the STO package (this was not the intended behavior of PTC).

– Added NO_PTC option to disable PTC for problems where PTC degrades/prevents model convergence. Option only applies to steady-state stress periods for models using the Newton-Raphson formulation. For many problems, PTC can significantly improve convergence behavior for steady-state simulations, and for this reason it is active by default. In some cases, however, PTC can worsen the convergence behavior, especially when the initial conditions are similar to the solution. When the initial conditions are similar to, or exactly the same as, the solution and convergence is slow, then this NO_PTC option should be used to deactivate PTC. This NO_PTC option should also be used in order to compare convergence behavior with other MODFLOW versions, as PTC is only available in MODFLOW 6.

– Small improvements to PTC to reduce the initial PTCDEL value loaded on the diagonal. This reduces the number of iterations required to achieve convergence for steady-state stress periods for most problems.

– Added OUTER_RCLOSEBND variable that is used when performing final convergence checks on model packages that solve a separate equation not solved by the IMS linear solver. This value represents the maximum allowable residual at any single model package element between successive outer iterations. An example of a model package that would use OUTER_RCLOSEBND to evaluate convergence is the SFR package which solves a continuity equation for each reach.

– Minor refactoring to improve code clarity.

- Version mf6.0.3–Aug. 9, 2018

  BASIC FUNCTIONALITY

  – Fixed issues with observations specified using boundnames that are enclosed in quotes. Previously, the closing quote was retained on a boundname enclosed in quotes and resulted in an error (the erroneous observation boundname could not be found in the package).

  STRESS PACKAGES

  – If the AUXMULTNAME keyword was used in combination with time series, then the multiplier was erroneously applied to all time series, and not just the time series in the column to be scaled.

  – For the array-based recharge and evapotranspiration packages, the IRCH and IEVT variables (if specified) must be specified as the first variable listed in the PERIOD block. A check was added so that the program will terminate with an error if IRCH or IEVT is not the first variable listed in the PERIOD block.

  – For the standard boundary packages, the "to mover" term (such as DRN-TO-MVR) written to the GWF Model budget was incorrect. The budget terms were incorrect because the accumulator variables were not initialized to zero.

  – For regular MODFLOW grids, the recharge and evapotranspiration arrays of size (NCOL, NROW) were being echoed to the listing file (if requested by the user) of size (NCOL * NROW).

  ADVANCED STRESS PACKAGES

  – Fixed spelling of the THIEM keyword in the source code and in the input instructions of the MAW Package.

– Fixed an issue with the SFR package when the specified evaporation exceeds the sum of specified and calculated reach inflows, rainfall, and specified runoff. In this case, evaporation is set equal to the sum of specified and calculated reach inflows, rainfall, and specified runoff. Also if a negative runoff is specified and this value exceeds specified and calculated reach inflows, and rainfall then runoff is set to the sum of reach inflows and evaporation is set to zero.

– Fixed an issue in the MAW package budget information written to the listing file and MAW cell-by-cell budget file when a previously active well is inactivated. The ratesim variable was not being reset to zero for these wells and the simulated rate from the last stress period when the well was active was being reported.

– Program now terminates with an error if the OUTLETS block is present in the LAK package file and NOUTLETS is not specified or specified to be zero in the DIMENSIONS block. Previously, this did not cause an error condition in the LAK package but would result in a segmentation fault error in the MVR package if LAK package OUTLETS are specified as providers.

– Program now terminates with an error when a DIVERSION block is present in a SFR package file but no diversions (all ndiv values are 0) are specified in the PACKAGEDATA block.

SOLUTION

– Fixed bug related to not allocating the preconditioner work array if a non-zero drop tolerance is specified but the number of levels is not specified or specified to be zero. In the case where the number of levels is not specified or specified to be zero the preconditioner work array is dimensioned to the product of the number of cells (NEQ) and the maximum number of connections for any cell.

– Updated linear solver output so number of levels and drop tolerance are output if either are specified to be greater than zero.

- Version mf6.0.2–Feb 23, 2018

BASIC FUNCTIONALITY

– Added a new option, called SAVE_SPECIFIC_DISCHARGE to the Node Property Flow Package. When invoked, x, y, and z specific discharge components are calculated for the center of each model cell and written to the binary budget file.

– For binary input of grid data, such as initial heads, the array reading utility was not reading a header record consisting of KSTP, KPER, PERTIM, TOTIM, TEXT, NLAY, NROW, NCOL. This meant that a binary head file written by MODFLOW could not be used as input for a subsequent simulation. For binary input, the array reading utility now reads a header record before reading the array values.

– The NOGRB option in the discretization packages was not working. This option will now prevent the binary grid file from being written.

– Removed the PRIVATE attribute for two methods of the discretization packages so that the program works as intended with the latest Intel Fortran release.

– Switched to using a long integer for the memory manager so that memory usage is calculated correctly for large models.

STRESS PACKAGES

– If a steady-state stress period followed a transient stress period, the storage terms written to the budget file were not being reset to zero. The program now initializes these budget values to zero for steady-state periods before they are written.

ADVANCED STRESS PACKAGES

– The STATUS INACTIVE option was not working correctly for the MAW Package.

– Modified the MAW connection conductance calculation so that a linear relation between the water level in a cell and saturation is used for the standard formulation. In the previous version, the same quadratic saturation function was being used for the standard and Newton-Raphson formulation to calculate the MAW connection conductance.

– Modified the MAW Package so that the top and bottom of the screen for a connection are reset to the top and bottom of the cell, respectively, for SPECIFIED, THEIM, SKIN, and CUMULATIVE conductance equations (CONDEQN). Also, the program will now terminate with an error if a MAW well using SPECIFIED, THEIM, SKIN, or CUMULATIVE conductance equations has more than one connection to a single GWF cell.

– Modified the MAW package so that the well bottom (BOTTOM) is reset to the cell bottom in the lowermost GWF cell connection in cases where the specified well bottom is above the bottom of this GWF cell.

SOLUTION

– Prior to applying pseudo transient continuation terms, the Iterative Model Solution confirms that the L2-norm exceeds the previous L2-norm. If it doesn't then pseudo transient continuation is turned off. This fixes a rare situation in which convergence could not be achieved for consecutive steady state solutions with the same or similar answers.

- Version mf6.0.1–Sep 28, 2017

BASIC FUNCTIONALITY

– There is no requirement that FTYPE entries in the GWF name file should be upper case; however, an upper case convention was being enforced. FTYPE entries can now be specified using any case.

– Tab characters within model input files were not being skipped correctly. This has been fixed.

– The program was updated to use the "approved for release" disclaimer. The previous version was still using a "preliminary software" disclaimer.

– The source code for time series and time array series was refactored. Included in the refactoring was a correction to time array series to allow the time array to change from one stress period to the next. The source file TimeSeriesGroupList.f90 was renamed to TimeSeriesFileList.f90.

STRESS PACKAGES

– Fixed inconsistency with CHD package observation name in code (`chd-flow`) and name in the input-output document (`chd`). Using name defined in input-output document (`chd`).

– The cell area was not being used in the calculation of recharge and evapotranspiration when list input was used with time series.

– The AUXMULTNAME option was not being applied for recharge and evapotranspiration when the READASARRAYS option was used.

– The program was not terminating with an error if a PERIOD block was encountered with an iper value equal to the previous iper value. Program now terminates with an error.

ADVANCED STRESS PACKAGES

- Fixed incorrect sign for SFR package exchange with GWF model (`sfr`).

- Added option to specify `none` as the `bedleak` for a lake-GWF connection in lake (LAK) package. This option makes the lake-GWF connection conductance solely a function of aquifer properties in the connected GWF cell and lakebed sediments are assumed to be absent for this connection.

- Fixed bug in lake (LAK) and multi-aquifer well (MAW) packages that only reset steady-state flag if lake and/or multi-aquifer data are read for a stress period (in the pak_rp() routines). Using pointer to GWF iss variable in the LAK package and resetting the MAW steady state flag in maw_rp() routine every stress period, regardless of whether MAW data are specified for a stress period.

- Added a convergence check routine to the GWF Mover Package that requires at least two outer iterations if there are any active movers. Because mover rates are lagged by one outer iteration, at least two outer iterations are required for some problems.

- Changed the behavior of the LAK Package so that recharge and evapotranspiration are applied to a vertically connected GWF model cell if the lake status is INACTIVE. Prior to this change, recharge and evapotranspiration were only applied to an underlying GWF model cell if the lake was dry.

SOLUTION

- Fixed bug in IMS that allowed convergence when outer iteration HCLOSE value was satisfied but the model did not converge during the inner iterations.

- Added STRICT rclose_option that uses a infinity-Norm RCLOSE criteria but requires HCLOSE and RCLOSE be satisfied on the first inner iteration of an outer iteration. The STRICT option is identical to the closure criteria approach use in the PCG Package in MODFLOW-2005.

EXCHANGES

- Use of an OPEN/CLOSE file was not being allowed for the OPTIONS and DIMENSIONS blocks of the GWF6-GWF6 exchange input file. OPEN/CLOSE input is now allowed for both of these blocks.

- Version mf6.0.0—August 10, 2017

BASIC FUNCTIONALITY

- Removed support for the SINGLE observation type. All observations must be CONTINUOUS, which means observation values are written for every time step.

- Added support for a no-data value (3.0E30), which can be used as a placeholder in a time-series file containing multiple time series. Use of the no-data value facilitates combining separate time series into a single file when the time series contain records for differing simulation times.

- Model names specified in the simulation name file cannot have spaces in them. A check was implemented to terminate with an error if the model name contains spaces. Model names cannot exceed 16 characters. Trailing spaces are allowed.

- The name and version of the compiler used to make the run file is now written to the terminal and to the simulation list file.

- Many of the Fortran source files were modified and reformatted. Unused variables were removed.

ADVANCED STRESS PACKAGES

- Updated MAW package so that well connection conductance calculations correctly account for THICKSTRT in the NPF package for layers that use THICKSTRT (and are confined).

- Added CUMULATIVE coneqn (conductance) option to MAW package.
- Fixed bug in LAK package weir lake outlet calculation.
- Fixed bug in LAK package when internal outlets were specified and combined with the MVR package that was also moving water internally in the same LAK package.
- Updated the table created when PRINT_FLOWS is specified in the LAK package OPTIONS block to include internal flow terms if NOUTLETS is greater than 0.
- Renamed Lake Tables DIMENSIONS block NENTRIES to NROW and added NCOL to DIMENSIONS block.
- Eliminated MAXIMUM_OUTLET_DEPTH = 10 [L] as default behavior for MANNING and WEIR LAK package lake outlet types. The maximum depth threshold was used in MODFLOW-2005 lake package because a table was used to calculate lake outflows to SFR. Can still use maximum depth threshold in develop versions of MODFLOW 6 by specifying MAXIMUM_OUTLET_DEPTH in the options block with a value.
- Removed MULTILAYER option for UZF package—this option didn't actually do anything.
- Added the requirement that the UZF number be specified as the first value on each line in the PACKAGEDATA block.
- Renamed MAXBOUND in the DIMENSIONS block of the SFR Package to be NREACHES.
- Implemented a check in the SFR Package to make sure that information is specified in the PACKAGEDATA block for every reach. Program terminates with an error if information for a reach is not found.

- Version mf6beta0.9.03—June 23, 2017

  BASIC FUNCTIONALITY

  - Renamed all FTYPE keywords to version 6. They were named with an 8. So, for example, the GHB Package is now activated in the GWF name file using "GHB6" instead of "GHB8".
  - Keywords in the simulation name file must now be specified as TDIS6, GWF6, and GWF6-GWF6 to be consistent.
  - The DIS Package had grid offsets (XOFFSET and YOFFSET) that could be specified as options. These offsets were relative to the upper-left corner of the model grid. The default value for YOFFSET was set to the sum of DELR so that (0, 0) would correspond to the lower-left corner of the model grid. These options have been removed and replaced with XORIGIN and YORIGIN, which is the coordinate of the lower-left corner of the model grid. The default value is zero for XORIGIN and YORIGIN.
  - Can now specify XORIGIN, YORIGIN, and ANGROT as options for the DISV and DISU packages. These values are written to the binary grid file, which can be used by post-processors to locate the model grid in space. These options have no affect on the simulation results. The default value is 0.0 if not specified.
  - Added a new option to the TDIS input file called START_DATE_TIME. This is a 30 character string that represents the simulation starting date and time, preferably in the format described at https://www.w3.org/TR/NOTE-datetime. The value provided by the user has no affect on the simulation, but if it is provided, the value is written to the simulation list file.
  - Changed default behavior for how memory usage is written to the end of the simulation list file. Added new MEMORY_PRINT_OPTION to simulation options to control how memory usage is written.

– Corrections were made to the memory manager to ensure that all memory is deallocated at the end of a simulation.

INTERNAL FLOW PACKAGES

– Changed the way hydraulic conductivity is specified in the NPF Package. Users no longer specify HK, VK, and HANI. Hydraulic conductivity is now specified as "K". If hydraulic conductivity is isotropic, then this is all that needs to be specified. For anisotropic cases, the user can specify an optional "K22" array and an optional "K33" array. For an unrotated conductivity ellipsoid "K22" corresponds to hydraulic conductivity in the y direction and "K33" corresponds to hydraulic conductivity in the z direction, respectively.

ADVANCED STRESS PACKAGES

– Modified the MAW Package to include the effects of aquifer anisotropy in the calculation of conductance.

– Simplified the SFR Package connectivity to reflect feedback from beta users. There is no longer a requirement to connect reaches that do not have flow between them. Program will now terminate with an error if this condition is encountered.

– Added simple routing option to SFR package. This is the equivalent of the specified depth option (icalc=0) in previous versions of MODFLOW. If water is available in the reach, then there can be leakage from the SFR reach into the aquifer. If no water is available, then no leakage is applied. STAGE keyword also added and only applies to reaches that use the simple routing option. If the STAGE keyword is not specified for reaches that use the simple routing option the specified stage is set to the top of the reach (depth = 0).

– Added functionality to pass SFR leakage to the aquifer to the highest active layer.

– Converted SFR Manning's to a time-varying, time series aware variable.

– Updated LAK package so that conductance calculations correctly account for THICKSTRT in the NPF package for layers that use THICKSTRT (and are confined). Also updated EMBEDDEDH and EMBEDDEDV so that the conductance for these connection types are constant for confined layers.

– Converted UZF stress period data to time series aware data.

– Added time-series aware AUXILIARY variables to UZF package.

– Implemented AUXMULTNAME in options block for UZF package (AUXILIARY variables have to be specified). AUXMULTNAME is applied to the GWF cell area and is used to simulated more than one UZF cell per GWF cell. This could be used to simulate different land use classifications (i.e., agricultural and natural land use types) in the same GWF cell.

SOLUTION

– Reworked IMS convergence information so that model specific convergence information is also printed to each model listing file when PRINT_OPTION ALL is specified in the IMS OPTIONS block.

– Added csv output option for IMS convergence information. Solution convergence information and model specific convergence information (if the solution includes more than one model) is written to a comma separated value file. If PRINT_OPTION is NONE or SUMMARY, csv output includes maximum head change convergence information at the end of each outer iteration for each time step. If PRINT_OPTION is ALL, csv output includes maximum head change and maximum residual convergence information for the solution and each model (if the solution includes more than one model) and linear acceleration information for each inner iteration.

- Version mf6beta0.9.02—May 19, 2017

    – Renamed gwf3.f90 to be lower case.

    – Added the missing "divrate" variable to the "sfrsetting" description in mf6io.pdf.

    – Added additional error trapping to the array reading utilities.

    – There was a problem with the binary budget file when a GWF Exchange was used to connect a GWF Model with itself. This has been fixed.

    – Standardized 'to-mvr' cell-by-cell item in standard stress packages and UZF package.

    – Fixed incorrect 'UZF-EVT' budget accumulator used in GWF listing budget.

    – Standardized justification of cell-by-cell 'text' strings.

    – Standardized use of AUXILIARY keyword.

- Version mf6beta0.9.01—May 11, 2017

    – Added a copy of the third MODFLOW 6 report.

    – Made several minor corrections to doc/mf6io.pdf.

    – If vertices were specified for DISU, then the last header line was not written to the binary grid file. This has been corrected.

- Version mf6beta0.9.00—May 10, 2017

    – First public release of MODFLOW 6 in beta form.