the U.S. Geological Survey Water Availability and Use Science Program

MODFLOW 6 Release Notes

Version mf6.5.0—May 23, 2024

U.S. Department of the Interior
U.S. Geological Survey

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Introduction

This document describes MODFLOW 6 Version mf6.5.0. This distribution is packaged for personal computers using modern versions of the Microsoft Windows, Macintosh, and Linux operating systems, although the programs included in the distribution may run on older operating system versions. The binary executable files in the distribution should run on most personal computers.

Version numbers for MODFLOW 6 follow a major.minor.revision format. The major number is increased when there are substantial new changes that may break backward compatibility. The minor number is increased when important, but relatively minor new functionality is added. The revision number is incremented 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.

Release History

A list of all MODFLOW 6 releases is shown in table 1. Changes introduced in previous releases are described in Appendix A.

Table 1. List of MODFLOW 6 Releases.

MODFLOW Version	Date	Digital Object Identifier
6.0.0	August 11, 2017	https://doi.org/10.5066/F76Q1VQV
6.0.1	September 28, 2017	same as above
6.0.2	February 23, 2018	same as above
6.0.3	August 9, 2018	same as above
6.0.4	March 7, 2019	same as above
6.1.0	December 12, 2019	same as above
6.1.1	June 12, 2020	same as above
6.2.0	October 20, 2020	same as above
6.2.1	February 18, 2021	same as above
6.2.2	July 30, 2021	same as above
6.3.0	March 4, 2022	https://doi.org/10.5066/P97FFF9M
6.4.0	November 30, 2022	https://doi.org/10.5066/P9FL1JCC
6.4.1	December 9, 2022	https://doi.org/10.5066/P9FL1JCC
6.4.2	June 28, 2023	https://doi.org/10.5066/P9FL1JCC
6.4.3	February 7, 2024	https://doi.org/10.5066/P9FL1JCC
6.4.4	February 13, 2024	https://doi.org/10.5066/P9FL1JCC
6.5.0	May 23, 2024	https://doi.org/10.5066/P13COJJM

Changes Introduced in this Release

This section describes changes introduced into MODFLOW 6 for the current release. These changes may substantially affect users.

- Version mf6.5.0—May 23, 2024

  <u>NEW FUNCTIONALITY</u>

    – A new Groundwater Energy (GWE) transport model was added to simulate heat transport in the subsurface. GWE Models can be coupled together using a new GWE-GWE Exchange. Additional information for activating the GWE model type within a MODFLOW 6 simulation is available within the mf6io.pdf document. Technical details about the GWE Model are given in the supplemental technical information document (mf6suptechinfo) provided with the release. New example problems have been developed for testing and demonstrating GWE capabilities (in addition to other internal tests that help verify the accuracy of GWE); however, additional changes to the code and input may be necessary in response to user needs and further testing.

    – A new Particle Tracking (PRT) Model was added to simulate forward tracking of particles for Groundwater Flow (GWF) Models. Additional information for activating the PRT model type within a MODFLOW 6 simulation is available within the mf6io.pdf document. Technical details about the PRT Model are given in the supplemental technical information document (mf6suptechinfo) provided with the release. New example problems have been developed for testing and demonstrating PRT capabilities (in addition to other internal tests that help verify the accuracy of PRT); however, additional changes to the code and input may be necessary in response to user needs and further testing.

    – A new capability has been introduced to optionally write user-provided input arrays to external ASCII files. In some cases, such as when the user provides binary files as input, it can be useful to inspect the text representation of that input. Exporting to external ASCII files can be turned on for supported packages by specifying the EXPORT_ARRAY_ASCII option. When activated supported variables will be written to files that are named based on the model, package, variable, and layer. Only those arrays specified for the model grid can be exported.

    – Added capability to vary the hydraulic conductivity of the reach streambed (RHK) by stress period in the Streamflow Routing (SFR) package. RHK can be modified by stress period using the BEDK SFRSETTING. RHK can also be defined using a timeseries string in the PACKAGEDATA or PERIOD blocks.

    – Extend binary input support to all list style input blocks that have a regular shape and don't contain string fields (e.g. BOUNDNAME).

    – A special extended version of MODFLOW can be compiled to simulate multiple models in parallel. This extended version of MODFLOW 6 is based on the Message Passing Interface (MPI) and the Portable, Extensible Toolkit for Scientific Computation (PETSc) libraries. Testing of the extended version has been performed on laptops, desktops, and supercomputers. Information on the extended version of MODFLOW 6 is available through a dedicated page on the MODFLOW 6 repository. There are several recent improvements to parallel capabilities. A new optional High Performance Computing (HPC) input file can be activated in the OPTION block in the simulation NAM file to configure the load balance for parallel simulations. The CSV convergence report in parallel mode has been improved by adding individual model data similar to those produced for serial simulations. A modified ILU preconditioner is now available in parallel simulations and can be configured

through IMS parameters. Settings configured in the IMS input file are now used for parallel simulations. Simulations with multiple GWE Models can be parallelized.

<u>EXAMPLES</u>

– Examples were added to demonstrate the new Groundwater Energy (GWE) Model. These examples include: danckwerts, geotherm, gwe-prt, and gwe-radial.

– Examples were added to demonstrate the new Particle Tracking (PRT) Model. These examples include two of the test problems used to demonstrate MODPATH Version 7.

BUG FIXES AND OTHER CHANGES TO EXISTING FUNCTIONALITY
<u>BASIC FUNCTIONALITY</u>

– When the Adaptive Time Step (ATS) Package was activated, and failed time steps were rerun successfully using a shorter time step, the cumulative budgets reported in the listing files were incorrect. Cumulative budgets included contributions from the failed time steps. The program was fixed so that cumulative budgets are not tallied until the time step is finalized.

– For multi-model groundwater flow simulations that use the Buoyancy (BUY) Package, variable-density terms were not included, in all cases, along the interface between two GWF models. The program was corrected so that flows between two GWF models include the variable-density terms when the BUY Package is active.

<u>STRESS PACKAGES</u>

– Floating point overflow errors would occur when negative conductance (COND) or auxiliary multiplier (AUXMULT) values were specified in the Drain, River, and General Head stress packages. This bug was fixed by checking if COND and AUXMULT values are greater than or equal to zero. The program will terminate with and error if negative COND or AUXMULT values are found.

<u>ADVANCED STRESS PACKAGES</u>

– A divide by zero error would occur in the Streamflow Routing package when reaches were deactivated during a simulation. This bug was fixed by checking if the downstream reach is inactive before calculating the flow to the downstream reach.

– When using the mover transport (MVT) package with UZF and UZT, rejected infiltration was paired with the calculated concentration of the UZF object rather than the user-specified concentration assigned to the infiltration. This bug was fixed by instead pairing the rejected infiltration transferred by the MVR and MVT packages with the user-specified concentration assigned in UZTSETTING with the keyword "INFILTRATION." With this change, MODFLOW 6 simulations that use UZF with the "SIMULATE_GWSEEP" option will not transfer this particular source of water with the correct concentration. Instead, the DRN package should be used to simulate groundwater discharge to land surface. By simulating groundwater discharge to land surface with the DRN package and rejected infiltration with the UZF package, the correct concentrations will be assigned to the water transferred by the MVR package.

– The SIMULATE_GWSEEP variable in the UZF package OPTIONS block will eventually be deprecated. The same functionality may be achieved using an option available within the DRN package called AUXDEPTHNAME. The details of the drainage option are given in the supplemental technical information document (mf6suptechinfo) provided with the release. Deprecation of the SIMULATE_GWSEEP option is motivated by the potential for errors noted above.

– The capability to deactivate lakes (using the STATUS INACTIVE setting) did not work properly for the GWF Lake Package. The Lake Package was fixed so that inactive lakes have a zero flow value with connected GWF model cells and that the lake stage is assigned the inactive value (1.E30). The listing, budget, and observation files were modified to accurately report inactive lakes.

– The Streamflow Routing package would not calculate groundwater discharge to a reach in cases where the groundwater head is above the top of the reach and the inflow to the reach from upstream reaches, specified inflows, rainfall, and runoff is zero. This bug has been fixed by eliminating the requirement that the conductance calculated based on the initial calculated stage is greater than zero in order to solve for groundwater. As a result, differences in groundwater and surface-water exchange and groundwater heads in existing models may occur.

– The Streamflow Routing package stage tables written to the model listing file have been modified so that inactive reaches are identified to be INACTIVE and dry reaches are identified to be DRY.

– The Streamflow Routing package would not correctly report reach flow terms for unconnected reaches even though reach flows were correctly calculated. This bug has been fixed by modifying the budget routine so that it correctly reports unconnected reach flows in the model listing file and cell-by-cell budget files. Simulated groundwater flow results should not change but differences may be observed in post-processed results and transport simulations that rely on binary cell-by-cell data.

EXCHANGES

– In some cases, concentration instabilities appeared at the interface between two transport models. The artifacts were present for rare configurations connecting more than 2 transport models with identical grids in series. The problem was identified in the GWT-GWT Exchange and corrected.

PARALLEL

– Several issues were fixed for parallel simulations that used the Buoyancy Package for the GWF model. When a simulation was run with the Buoyancy Package, irrelevant messages could be written to the screen. In some cases, the Buoyancy Package produced strange results at the interface between two models. These issues have been corrected.

– For parallel simulations, calculation of the residual norm used for pseudo-transient continuation (PTC) and backtracking was incorrect. The program was fixed to calculate the correct residual norm.

– Enabling XT3D on exchanges in a parallel simulation caused the program to hang for certain configurations. This issue has been corrected.

– GNC is not supported on flow exchanges when running in parallel or when the XT3D option is enabled on the exchange. The program terminates with an error if the user attempts to use GNC in these cases.

Known Issues and Incompatibilities

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

1. The READARRAY utility is used by some packages to read arrays of numeric values provided by the user. The READARRAY utility has an IPRN option (as described in the MODFLOW 6 Description of Input and Output), which will cause the array to be written to the model listing file. Support for the IPRN option has been removed for some packages and will ultimately be removed for all packages. A new

option, called "EXPORT_ARRAY_ASCII" has been implemented for some packages to support writing of gridded data to external text files. This option has been implemented to replace the IPRN functionality.

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

3. For the Groundwater Transport (GWT) Model, the decay and sorption processes do not apply to the LKT, SFT, MWT and UZT Packages.

4. The GWT Model does not work with the CSUB Package of the GWF Model.

5. The GWT-GWT Exchange requires that both GWF Models are run concurrently in the same simulation. There is not an option to read GWF-GWF flows from a previous simulation.

6. The Buoyancy (BUY) Package of the GWF Model cannot be used when the XT3D option is activated for the Node Property Flow (NPF) Package.

7. If a GWF-GWF Exchange is activated with the XT3D option, then the two connected GWF Models cannot have BUY Packages active.

8. The Time-Variable Hydraulic Conductivity (TVK) Package is incompatible with the Horizontal Flow Barrier (HFB) Package if the TVK Package is used to change hydraulic properties of cells near horizontal flow barriers.

9. If a GWF-GWF Exchange is active, then neither of the connected GWF Models can have an active Viscosity (VSC) Package.

10. If a GWT-GWT Exchange is active, then constant concentration conditions cannot be assigned on the interface between the two connected models.

In addition to the issues shown here, a comprehensive and up-to-date list is available under the issues tab at https://github.com/MODFLOW-USGS/modflow6.

Distribution File

The MODFLOW 6 distribution is provided in the form of a compressed zip file. Distributions are available for several different operating systems, including Windows, Mac, and Linux. Distributions are marked with an operating system tag, called "ostag". Values for "ostag" include "win64", "mac", and "linux", for example. Distribution files for the current release are labeled as `mf6.5.0_[ostag].zip`. Thus, the distribution file for Windows for the current release is `mf6.5.0_win64.zip`.

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

Installation and Execution

There is no installation of MODFLOW 6 other than the requirement that `mf6.5.0_[ostag].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 (named "`mf6.exe`" on Windows or "`mf6`" on Mac and Linux) in the mf6.5.0_[ostag]/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 a 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 Fortran and GNU Fortran on Windows, macOS, and several Linux operating systems. All MODFLOW 6 distributions are currently compiled with Intel Fortran. Because the program uses relatively new Fortran functionality, recent versions of the compilers may be required for successful compilation. MODFLOW 6 has been successfully compiled with the latest versions of the Intel toolchain.

MODFLOW 6 is currently tested with gfortran 11-13 on Linux, macOS, and Windows. The gfortran version can be queried with "`gfortran --version`". Intel Fortran Compiler Classic version 2022.3.0 is currently tested on all three platforms. Some 2021 versions have also been reported compatible. MODFLOW 6 is also compatible with the next-generation Intel Fortran Compiler 'ifx'; however, additional testing is underway.

Instructions for compiling the parallel version of MODFLOW 6 are available through a dedicated page on the MODFLOW 6 repository.

There are several options for building MODFLOW, as described below.

- Meson is the recommended build tool for MODFLOW 6. Refer to the detailed compilation instructions for more information.

- The distribution includes Microsoft Visual Studio solution and project files for compiling MODFLOW 6 on Windows using the Intel Fortran Compiler Classic. The files have been used successfully with recent versions of Microsoft Visual Studio Community 2019 and the Intel Fortran Compiler Classic.

- This distribution also includes 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.

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 on Windows 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. For Linux and Mac distributions, equivalent shell scripts (`run.sh` and `runall.sh`) are included.

MODFLOW 6 Documentation

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

- 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., https://doi.org/10.3133/tm6A57

- Langevin, C.D., Hughes, J.D., Provost, A.M., Banta, E.R., Niswonger, R.G., and Panday, S., 2017, Documentation for the MODFLOW 6 Groundwater Flow (GWF) Model: U.S. Geological Survey Techniques and Methods, book 6, chap. A55, 197 p., 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., https://doi.org/10.3133/tm6A56

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

- Morway, E.D., Langevin, C.D., and Hughes, J.D., 2021, Use of the MODFLOW 6 water mover package to represent natural and managed hydrologic connections: Groundwater, v. 59, no. 6, p. 913–924, https://doi.org/10.1111/gwat.13117

- Hughes, J.D., Russcher, M.J., Langevin, C.D., Morway, E.D., and McDonald, R.R., 2022a, The MODFLOW Application Programming Interface for simulation control and software interoperability: Environmental Modelling & Software, v. 148, article 105257, https://doi.org/10.1016/j.envsoft.2021.105257

- Langevin, C.D., Provost, A.M., Panday, S., and Hughes, J.D., 2022, Documentation for the MODFLOW 6 Groundwater Transport (GWT) Model: U.S. Geological Survey Techniques and Methods, book 6, chap. A61, 56 p., https://doi.org/10.3133/tm6A61

- Hughes, J.D., Leake, S.A., Galloway, D.L., and White, J.T., 2022b, Documentation for the Skeletal Storage, Compaction, and Subsidence (CSUB) Package of MODFLOW 6: U.S. Geological Survey Techniques and Methods, book 6, chap. A62, 57 p., https://doi.org/10.3133/tm6A62

- Langevin, C.D., Hughes, J.D., Provost, A.M., Russcher, M.J., and Panday, S., 2024, MODFLOW as a configurable multi-model hydrologic simulator: Groundwater, v. 62, no. 1, p. 111–123, https://doi.org/10.1111/gwat.13351

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

Deprecations

Deprecated/removed options in the current version of MODFLOW 6. Deprecated options are not suggested for use and may (but need not) be removed in a future version of MODFLOW 6. Removed options are no longer available in the current version of MODFLOW 6.

Table 2.   List of deprecations and removals.

Model–Package	Option	Deprecated	Removed
sln-ims	csv_output_filerecord	6.1.1	
sln-ims	csv_output	6.1.1	
sln-ims	csvfile	6.1.1	
sln-ims	outer_hclose	6.1.1	
sln-ims	outer_rclosebnd	6.1.1	
sln-ims	inner_hclose	6.1.1	
gwf-sfr	unit_conversion	6.4.2	
sln-pts	csv_output_filerecord	6.1.1	
sln-pts	csv_output	6.1.1	
sln-pts	csvfile	6.1.1	
gwf-uzf	simulate_gwseep	6.5.0	

Run-Time Comparison

Comparison of run times of the current version of MODFLOW 6 to the previous version. The distribution example models are used to compare run times. Simulations that fail are indicated by '–'. The percent difference, where calculated, is relative to the simulation run time for the previous version. Percent differences for example problems with short run times (less than 30 seconds) may not be significant.

Table 3.   List of run time comparsons.

Example Problem	Current Version	Previous Version	Percent difference
ex-gwt-uzt-2d-a	10.577 Seconds	10.241 Seconds	3.28%
ex-gwt-moc3d-p01c/mf6gwf	0.007 Seconds	0.006 Seconds	16.67%
ex-gwt-moc3d-p01c/mf6gwt	0.053 Seconds	–	–
ex-gwf-csub-p01	0.138 Seconds	0.139 Seconds	-0.72%
ex-gwf-u1disv	0.008 Seconds	0.008 Seconds	0.00%
ex-gwf-sfr-p01	0.234 Seconds	0.234 Seconds	0.00%
ex-gwt-mt3dms-p04c	6.616 Seconds	6.666 Seconds	-0.75%
ex-gwf-nwt-p03b	2.137 Seconds	2.147 Seconds	-0.47%
ex-gwt-uzt-2d-b	10.262 Seconds	10.230 Seconds	0.31%
ex-gwf-u1gwfgwf-s1	0.016 Seconds	0.016 Seconds	0.00%
ex-gwt-keating/mf6gwf	5.414 Seconds	5.714 Seconds	-5.25%
ex-gwt-keating/mf6gwt	41.110 Seconds	–	–

Example Problem	Current Version	Previous Version	Percent difference
ex-gwt-moc3d-p01d/mf6gwf	0.007 Seconds	0.007 Seconds	0.00%
ex-gwt-moc3d-p01d/mf6gwt	0.051 Seconds	–	–
ex-gwt-mt3dms-p10	53.793 Seconds	59.368 Seconds	-9.39%
ex-gwt-prudic2004t2/mf6gwf	1.725 Seconds	1.742 Seconds	-0.98%
ex-gwt-prudic2004t2/mf6gwt	21.390 Seconds	–	–
ex-gwf-capture	0.019 Seconds	0.019 Seconds	0.00%
ex-gwf-sfr-p01b	7.384 Seconds	7.452 Seconds	-0.91%
ex-gwt-mt3dsupp632c/mf6gwf	0.007 Seconds	0.007 Seconds	0.00%
ex-gwt-mt3dsupp632c/mf6gwt	0.036 Seconds	–	–
ex-gwf-nwt-p02a	7.206 Seconds	7.165 Seconds	0.57%
ex-gwt-mt3dms-p02b/mf6gwf	0.341 Seconds	0.342 Seconds	-0.29%
ex-gwt-mt3dms-p02b/mf6gwt	0.489 Seconds	–	–
ex-gwt-mt3dms-p02c/mf6gwf	0.345 Seconds	0.337 Seconds	2.37%
ex-gwt-mt3dms-p02c/mf6gwt	0.399 Seconds	–	–
ex-gwf-lgrv-gr	29.702 Seconds	29.654 Seconds	0.16%
ex-gwt-mt3dms-p01b	0.054 Seconds	0.055 Seconds	-1.82%
ex-gwt-henry-b	6.998 Seconds	6.993 Seconds	0.07%
ex-gwf-hanix	0.035 Seconds	0.035 Seconds	0.00%
ex-gwt-gwtgwt-p10	1 Minutes, 9.687 Seconds	1 Minutes, 11.447 Seconds	-2.46%
ex-gwf-bump-p01c	0.069 Seconds	0.069 Seconds	0.00%
ex-gwt-saltlake	15.677 Seconds	15.546 Seconds	0.84%
ex-gwf-hanir	0.017 Seconds	0.016 Seconds	6.25%
ex-gwt-mt3dms-p09	1.622 Seconds	1.614 Seconds	0.50%
ex-gwf-maw-p03b	0.088 Seconds	0.087 Seconds	1.15%
ex-gwt-mt3dsupp632a/mf6gwf	0.008 Seconds	0.008 Seconds	0.00%
ex-gwt-mt3dsupp632a/mf6gwt	0.047 Seconds	–	–
ex-gwt-mt3dms-p05	0.197 Seconds	0.196 Seconds	0.51%
ex-gwf-lgr	0.096 Seconds	0.097 Seconds	-1.03%
ex-gwf-maw-p01b	0.905 Seconds	0.914 Seconds	-0.98%
ex-gwt-mt3dms-p02a/mf6gwf	0.342 Seconds	0.341 Seconds	0.29%
ex-gwt-mt3dms-p02a/mf6gwt	0.511 Seconds	–	–
ex-gwf-zaidel	0.008 Seconds	0.008 Seconds	0.00%
ex-gwt-mt3dms-p02e/mf6gwf	0.345 Seconds	0.342 Seconds	0.88%
ex-gwt-mt3dms-p02e/mf6gwt	0.446 Seconds	–	–
ex-gwt-hecht-mendez-b/mf6gwf	1.560 Seconds	1.578 Seconds	-1.14%
ex-gwt-hecht-mendez-b/mf6gwt	1 Minutes, 0.922 Seconds	–	–
ex-gwf-bcf2ss-p02a	0.012 Seconds	0.012 Seconds	0.00%
ex-gwf-lak-p02	7.469 Seconds	7.557 Seconds	-1.16%
ex-gwf-twri01	0.024 Seconds	0.024 Seconds	0.00%
ex-gwf-bump-p01a	0.413 Seconds	0.413 Seconds	0.00%
ex-gwe-danckwerts	1.553 Seconds	–	–

Example Problem	Current Version	Previous Version	Percent difference
ex-gwe-geotherm/mf6gwf	0.963 Seconds	0.957 Seconds	0.63%
mf6gwe	21.274 Seconds	–	–
ex-gwt-moc3d-p02/mf6gwf	0.100 Seconds	0.100 Seconds	0.00%
ex-gwt-moc3d-p02/mf6gwt	8.721 Seconds	–	–
ex-gwf-nwt-p02b	4.046 Seconds	3.969 Seconds	1.94%
ex-gwf-rad-disu	0.057 Seconds	0.055 Seconds	3.64%
ex-gwf-drn-p01b	2.320 Seconds	2.310 Seconds	0.43%
ex-gwf-csub-p02a	0.042 Seconds	0.042 Seconds	0.00%
ex-gwt-mt3dms-p08	16.176 Seconds	16.368 Seconds	-1.17%
ex-gwf-hanic	0.016 Seconds	0.016 Seconds	0.00%
ex-gwt-rotate	3 Minutes, 27.824 Seconds	3 Minutes, 28.504 Seconds	-0.33%
ex-gwf-bcf2ss-p01a	0.015 Seconds	0.015 Seconds	0.00%
ex-gwf-fhb	0.011 Seconds	0.011 Seconds	0.00%
ex-gwf-drn-p01a	1.667 Seconds	1.681 Seconds	-0.83%
ex-gwt-mt3dms-p03	1.730 Seconds	1.745 Seconds	-0.86%
ex-gwf-disvmesh	0.182 Seconds	0.181 Seconds	0.55%
ex-gwt-mt3dms-p01d	0.056 Seconds	0.056 Seconds	0.00%
ex-gwt-mt3dms-p01c	0.054 Seconds	0.055 Seconds	-1.82%
ex-gwt-mt3dms-p02d/mf6gwf	0.342 Seconds	0.337 Seconds	1.48%
ex-gwt-mt3dms-p02d/mf6gwt	0.455 Seconds	–	–
ex-gwf-csub-p03a	13.015 Seconds	12.876 Seconds	1.08%
ex-gwf-lgrv-gc	0.280 Seconds	0.278 Seconds	0.72%
hb-010	0.551 Seconds	0.549 Seconds	0.36%
es-005	0.581 Seconds	0.581 Seconds	0.00%
es-100	0.582 Seconds	0.582 Seconds	0.00%
hb-001	0.553 Seconds	0.546 Seconds	1.28%
es-010	0.581 Seconds	0.581 Seconds	0.00%
hb-020	0.550 Seconds	0.546 Seconds	0.73%
hb-002	0.551 Seconds	0.546 Seconds	0.92%
es-001	0.579 Seconds	0.584 Seconds	-0.86%
hb-100	0.585 Seconds	0.585 Seconds	0.00%
es-002	0.581 Seconds	0.578 Seconds	0.52%
hb-050	0.546 Seconds	0.546 Seconds	0.00%
es-020	0.583 Seconds	0.580 Seconds	0.52%
hb-005	0.551 Seconds	0.550 Seconds	0.18%
es-050	0.579 Seconds	0.584 Seconds	-0.86%
ex-gwe-radial-slow/mf6gwf	0.754 Seconds	0.744 Seconds	1.34%
mf6gwe-b	29.618 Seconds	–	–
ex-gwf-u1disv-x	0.009 Seconds	0.009 Seconds	0.00%
gwf	0.069 Seconds	0.069 Seconds	0.00%
prt	0.090 Seconds	–	–
gwe	29.366 Seconds	–	–

Example Problem	Current Version	Previous Version	Percent difference
ex-gwf-lgrv-lgr	6.565 Seconds	7.306 Seconds	-10.14%
ex-gwf-curve-90	0.012 Seconds	0.011 Seconds	9.09%
gwf	0.052 Seconds	0.051 Seconds	1.96%
prt	0.169 Seconds	–	–
ex-gwf-advtidal	0.586 Seconds	0.582 Seconds	0.69%
ex-gwt-mt3dsupp631/mf6gwf	0.008 Seconds	0.010 Seconds	-20.00%
ex-gwt-mt3dsupp631/mf6gwt	0.019 Seconds	–	–
ex-gwt-hecht-mendez-c/mf6gwf	1.744 Seconds	1.746 Seconds	-0.11%
ex-gwt-hecht-mendez-c/mf6gwt	1 Minutes, 13.314 Seconds	–	–
ex-gwt-mt3dms-p04a	6.571 Seconds	6.671 Seconds	-1.50%
ex-gwt-mt3dsupp632b/mf6gwf	0.007 Seconds	0.007 Seconds	0.00%
ex-gwt-mt3dsupp632b/mf6gwt	0.047 Seconds	–	–
gwf	0.020 Seconds	0.020 Seconds	0.00%
prt	0.509 Seconds	–	–
ex-gwt-stallman	10.580 Seconds	10.692 Seconds	-1.05%
ex-gwt-synthetic-valley/mf6gwf	3.246 Seconds	3.253 Seconds	-0.22%
ex-gwt-synthetic-valley/mf6gwt	28.435 Seconds	–	–
ex-gwt-mt3dms-p06	3.776 Seconds	3.792 Seconds	-0.42%
ex-gwt-mt3dms-p04b	9.783 Seconds	9.931 Seconds	-1.49%
ex-gwt-mt3dms-p07	0.390 Seconds	0.390 Seconds	0.00%
ex-gwt-moc3d-p02tg/mf6gwf	0.591 Seconds	0.591 Seconds	0.00%
ex-gwt-moc3d-p02tg/mf6gwt	18.474 Seconds	–	–
ex-gwf-maw-p03c	0.092 Seconds	0.093 Seconds	-1.08%
ex-gwt-mt3dms-p02f/mf6gwf	0.344 Seconds	0.339 Seconds	1.47%
ex-gwt-mt3dms-p02f/mf6gwt	0.463 Seconds	–	–
ex-gwf-sagehen	2 Minutes, 11.189 Seconds	2 Minutes, 13.535 Seconds	-1.76%
ex-gwf-maw-p01a	0.895 Seconds	0.900 Seconds	-0.56%
ex-gwt-henry-a	6.802 Seconds	6.812 Seconds	-0.15%
ex-gwf-maw-p02	2.258 Seconds	2.257 Seconds	0.04%
ex-gwt-mt3dms-p01a	0.052 Seconds	0.051 Seconds	1.96%
ex-gwf-csub-p04	1.977 Seconds	2.032 Seconds	-2.71%
ex-gwf-curvilin	0.021 Seconds	0.019 Seconds	10.53%
ex-gwf-bump-p01b	0.101 Seconds	0.104 Seconds	-2.88%
ex-gwt-mt3dsupp82/mf6gwf	0.015 Seconds	0.014 Seconds	7.14%
ex-gwt-mt3dsupp82/mf6gwt	0.141 Seconds	–	–
ex-gwf-u1gwfgwf-s2	0.016 Seconds	0.016 Seconds	0.00%
ex-gwf-nwt-p03a	0.209 Seconds	0.209 Seconds	0.00%
ex-gwf-spbc	0.129 Seconds	0.133 Seconds	-3.01%
ex-gwf-u1gwfgwf-s4	0.025 Seconds	0.024 Seconds	4.17%
ex-gwf-whirl	0.090 Seconds	0.089 Seconds	1.12%
ex-gwf-lak-p01	7.603 Seconds	7.566 Seconds	0.49%

Example Problem	Current Version	Previous Version	Percent difference
ex-gwt-moc3d-p01a/mf6gwf	0.006 Seconds	0.006 Seconds	0.00%
ex-gwt-moc3d-p01a/mf6gwt	0.044 Seconds	–	–
ex-gwf-maw-p03a	0.091 Seconds	0.091 Seconds	0.00%
ex-gwf-csub-p03b	12.987 Seconds	12.955 Seconds	0.25%
ex-gwf-csub-p02b	0.045 Seconds	0.043 Seconds	4.65%
ex-gwt-moc3d-p01b/mf6gwf	0.007 Seconds	0.006 Seconds	16.67%
ex-gwt-moc3d-p01b/mf6gwt	0.044 Seconds	–	–
ex-gwf-u1gwfgwf-s3	0.027 Seconds	0.026 Seconds	3.85%
Total simulation time	11 Minutes, 48.157 Seconds	11 Minutes, 59.535 Seconds	-1.58%

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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 mf6.4.4–February 13, 2024

ADVANCED STRESS PACKAGES

- Refactoring of the Water Mover package in version 6.4.3 introduced a reduction in performance for GWF models with a large number of movers. The program was corrected so that performance is similar to previous versions.

- Deprecation warnings in the Lake and Streamflow Routing Packages, which can be issued by MODFLOW 6 at run time, incorrectly listed the version number as 6.5.0. The warning was modified to show 6.4.3 as the version number for the deprecation.

PARALLEL

- A memory leak was identified in the way MPI messages were constructed and cached. The memory leak caused problems for large models with many time steps. The message construction and caching was fixed and tests confirm that the memory leak is no longer present.

Version mf6.4.3–February 7, 2024

NEW FUNCTIONALITY

- The Input Data Processor (IDP), first released in version 6.4.2, is a general utility for reading user-provided input files. Package-specific routines for reading input files continue to be replaced by the IDP approach. For packages that use IDP for input, logging information is written to the simulation list file (mfsim.lst). Additional information on the IDP and the list of supported packages is contained in the MODFLOW 6 Description of Input and Output (mf6io.pdf) under a section titled "Processing of Program Input."

- The source code was refactored to support compilation of a parallel version of MODFLOW 6 based on the Message Passing Interface (MPI) and the Portable, Extensible Toolkit for Scientific Computation (PETSc) libraries. The parallel version of MODFLOW is considered preliminary. Limited testing of the parallel version has been performed on laptops, desktops, and supercomputers, but significant changes are expected in future releases. User support for the parallel version of MODFLOW 6 may be provided in the future.

EXAMPLES

- A new exampled called ex-gwf-rad-disu was added. This new example uses a DISU grid to represent radial groundwater flow to a pumping well.

- A new exampled called ex-gwf-curv-90 was added. This new example demonstrates use of a DISV grid to represent a curvilinear spatial discretization. For this example, the curvilinear grid is applied to one quarter of a radial groundwater flow system.

- A new exampled called ex-gwf-curvilin was added. This new example uses a curvilinear grid, represented with the DISV Package, to simulate groundwater flow through a multi-region aquifer with bends in the domain boundaries.

BUG FIXES AND OTHER CHANGES TO EXISTING FUNCTIONALITY
BASIC FUNCTIONALITY

- Improve error message if the size of data read from a binary array file is inconsistent with READARRAY control line and variable description keywords.

- The area calculation for cells in the DISV package was inaccurate for some cases with very large cell vertex coordinates. The area calculation was improved by using transformed cell vertex coordinates prior to making the area calculation.

- Auxiliary variables in RCH and EVT Array-Based input packages are now reset to zero when otherwise not specified in period input data and the auxiliary parameter is not controlled by a time-series.

INTERNAL FLOW PACKAGES

- The data header in the binary output file written by the viscosity (VSC) package was printing " VIS-COSI" instead of " VISCOSITY". The viscosity package now prints the full " VISCOSITY" header in the binary output file.

- The CSUB Package did not support output of z-displacement arrays for models using the DISU package. The CSUB package was updated to support calculation of z-displacement arrays for DISU model grids.

STRESS PACKAGES

- This release contains a fix for a longstanding issue related to the use of AUXMULTNAME and time series. Previous release notes included the following description of a known issue: *"The AUXMULT-NAME 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."* With this release, the Input Data Processor (IDP) is now used to read stress package input files, and the limitation with AUXMULTNAME and time series no longer applies.

ADVANCED STRESS PACKAGES

- Added functionality to support zero values for each grid dimension when specifying the CELLID for SFR reaches that are not connected to an underlying groundwater grid cell. For example, for a DIS grid a CELLID of 0 0 0 should be specified for reaches with no connection to a groundwater cell. Warning messages will be issued if NONE is specified for the CELLID of an unconnected reach. Specifying a CELLID of NONE will eventually be deprecated and will cause MODFLOW 6 to terminate with an error.

- Added functionality to support specification of a DNODATA (3.0E+30) BEDLEAK value for LAK package connections. This DNODATA value is used to identify lake-GWF connections where conductance is solely a function of aquifer properties in the connected GWF cell. In this case, the lakebed sediments are assumed to be absent and all resistance to flow is assumed to be within the GWF cell. Warning messages are now issued if NONE is specified for LAK package connections. Specifying a BEDLEAK value equal to NONE will eventually be deprecated and will cause MODFLOW 6 to terminate with an error.

- SFR diversion would not be updated if the outflow of its upstream reach is zero. If diversion was not zero in the previous stress period, it would report mass balance error in the SFR budget. This bug was fixed by always updating the diversion.

EXCHANGES

- A model budget error would occur when a constant-head (CHD) cell in one model had a direct connection to an active cell in another model. For the model budget to be calculated correctly a new term called "FLOW-JA-FACE-CHD" was added to the GWF model budget. This term is only included in the budget table when the GWF Model is connected to another GWF Model using a GWF-GWF Exchange. Additionally, the CHD budget calculation for a very specific (and rare) configuration was also incorrect. The incorrect budget calculation occurred when the following conditions were met: (1) a GWF model was connected to another GWF model with a GWF-GWF Exchange; (2) the model as well as the Exchange had the XT3D option enabled, and (3) the model was configured with a CHD cell that is either an Exchange cell, i.e. a cell that is part of the EXCHANGEDATA block, or a cell directly connected to such an Exchange cell. The size of the error depends on the degree of anisotropy around the particular CHD cell and shows up as a discrepancy in the volume budget table reported in the GWF list file. The program has been updated with the correct budget calculation.

Version mf6.4.2–June 28, 2023

<u>NEW FUNCTIONALITY</u>

- The source code was refactored to support compilation of a parallel version of MODFLOW 6 based on the Message Passing Interface (MPI) and the Portable, Extensible Toolkit for Scientific Computation (PETSc) libraries. The parallel version of MODFLOW is considered preliminary (alpha release). Limited testing of the parallel version has been performed on laptops, desktops, and supercomputers, but significant changes are expected in future releases. User support for the parallel version of MODFLOW 6 may be provided in the future.

- The Groundwater Transport (GWT) model was modified for simulations involving a mobile domain and one or more immobile domains. The modifications do not affect GWT Models without the Immobile Storage and Transfer (IST) Package. The original IST Package formulation described by Langevin and others (2022) was based on a limiting assumption about how the mobile and immobile domains are apportioned within a model cell. The changes introduced here require the user to explicitly specify in the IST Package the volume fraction of each cell that is immobile. This change also redefines the meaning of several input parameters. As described in a new chapter (Chapter 9) in the Supplemental Technical Information document, porosity and bulk density values must now be entered per domain volume rather than per cell volume. Consequently, for simulations that include one or more IST Packages, these changes are not backward compatible, and will require updates to IST and MST input. Suggestions for updating existing parameter values is included in Chapter 9 of the Supplemental Technical Information document, which is included with the distribution.

- Add LENGTH_CONVERSION and TIME_CONVERSION variables to replace the UNIT_CONVERSION variable in the SFR Package input file. The LENGTH_CONVERSION and TIME_CONVERSION variables are used to convert user-specified Manning's roughness coefficients from SI units (sec/m$^{1/3}$) to model length and time units. LENGTH_CONVERSION does not need to be specified if LENGTH_UNITS are meters. TIME_CONVERSION does not need to be specified if TIME_UNITS are seconds. Warning messages will be issued if UNIT_CONVERSION variable is specified. The model will terminate with an error if UNIT_CONVERSION and LENGTH_CONVERSION and TIME_CONVERSION variables are specified. The UNIT_CONVERSION variable in the SFR Package input file will eventually be deprecated.

- Add MAXIMUM_ITERATIONS and MAXIMUM_STAGE_CHANGE variables in the LAK Package input file. The MAXIMUM_ITERATIONS variable is used to change the maximum number of iterations and would only need to be increased from the default value if one or more lakes in a simulation has

a large water budget error. The MAXIMUM_STAGE_CHANGE variable defines the stage closure tolerance for each lake. The MAXIMUM_STAGE_CHANGE variable would only need to be increased or decreased from the default value if the water budget error for one or more lakes is too small or too large.

- The Input Data Processor (IDP) is introduced in this release to read user-provided input files and store user-provided input data in memory for subsequent use by simulation, model, and package components. Components that have been integrated with IDP no longer handle input files directly but rather retrieve all input data from named locations, called memory paths, allocated in managed memory. The collection of all simulation input data in managed memory is called the input context. IDP uses existing descriptions of input variables, called variable definitions, to interpret and store input. The program variable definition set and its representation in the input context is described as the Input Data Model (IDM). Input variables can be recognized in a memory dump (e.g., with the MEMORY_PRINT_OPTION activated in the options block of mfsim.nam) by their memory path prefix string "__INPUT__". Components that later access input typically copy data from the input context to their own memory space; therefore, the present implementation of the IDP results in an increased memory footprint for the program. Among its advantages include the consolidation of all input processing early in program runtime, and outside of any particular component, enabling the support of alternative types of input data sources. Input file types that are currently processed by IDP include DIS6, DISU6, DIV6, NPF6, DSP6, and Name File inputs for the Simulation (mfsim.nam) and GWF and GWT models.

EXAMPLES

- A new example called ex-gwt-synthetic-valley was added. This new problem simulates groundwater flow and solute transport using a Voronoi model grid. Additional details for this example problem are described by Hughes and others (2024).

BUG FIXES AND OTHER CHANGES TO EXISTING FUNCTIONALITY
BASIC FUNCTIONALITY

- The input for some stress packages is read in a list format consisting of a cellid, the form of which depends on the type of discretization package, and stress information on each line. The cellid is checked upon reading to ensure that the cell is within the model grid. If the cell is outside the model grid, the program issues an error message and terminates. This cellid check was not implemented when the list was provided from an OPEN/CLOSE binary input file. The program was modified to include this check for both text and binary input.

- In some cases, unrecognized keywords and invalid auxiliary input did not terminate with a useful error message. The program was corrected to provide error handling for these cases.

- The SSM Package for the GWT Model did not work properly with Stress Package Concentration (SPC) input with the READARRAY option for transient models. Under these conditions, the program would prematurely terminate looking for the next BEGIN PERIOD block. The program was corrected so that SPC input can be read for transient conditions.

- For some Linux systems, observations were not being correctly written to formatted observation output files when the source code was compiled with the Intel IFORT 19.1.0.166 20191121 compiler. This issue has been addressed by adding a flush statement to ObsUtilityModule::write_unfmtd_obs after writing each observation for a time step. This change will not affect simulated observations and should not affect simulation run times.

- The wetted area written to the binary LAK package output was modified to be zero when the lake stage is below the bottom of a connected groundwater cell. The code uses the lak_calculate_conn_warea() function to determine the wetted area, which makes sense for calculating the flow conductance.

- Fix issue with reading boundary package stress period data from binary files when auxiliary data is included.

INTERNAL FLOW PACKAGES

- The ICELLTYPE input variable in the Node Property Flow (NPF) Package behaves differently depending on whether or not the THICKSTRT option is specified by the user. In some cases, the program would give unexpected results if a negative value was specified for ICELLTYPE and the THICKSTRT option was not active. For example, the Horizontal Flow Barrier (HFB) Package did not work properly when negative values for ICELLTYPE were specified by the user, but the THICKSTRT option was not activated. The program was modified so that negative ICELLTYPE values provided by the user are automatically reassigned a value of one when the user does not activate the THICKSTRT option. This is the intended behavior and is consistent with the input and output guide.

ADVANCED STRESS PACKAGES

- Added additional convergence checks to the Streamflow Routing (SFR), Lake (LAK) and Unsaturated Zone Flow (UZF) Packages to ensure that flows from the Water Mover (MVR) Package meet solver tolerance. Mover flows are converted into depths using the time step length and area, and the depths are compared to the Iterative Model Solution (IMS) DVCLOSE input parameter. If a depth is greater than DVCLOSE, then the iteration is marked as not converged. The maximum depth change between iterations and the advanced package feature number is written for each outer iteration to a comma-separated value file, provided the PACKAGE_CONVERGENCE option is specified in the options block.

- Added an additional convergence check to the Lake (LAK) Package to ensure that the lake residual meets solver tolerance. In previous versions, it was possible for a time step to converge even if there was a relatively large lake residual. The lake residual is converted to a depth, using the time step length and lake surface area. This depth is compared to the Iterative Model Solution (IMS) DVCLOSE input parameter. If the residual depth is greater than DVCLOSE, then the iteration is marked as not converged. The maximum residual depth and the advanced package feature number (lake number) is written for each outer iteration to a comma-separated value file, provided the PACKAGE_CONVERGENCE option is specified in the options block. This fix may increase the number of iterations required to reach convergence for existing models that use the LAK Package.

- The secant method used in the LAK Package when Newton-Raphson iterations result in lake stages below the lake bottom or when Newton-Raphson iterations stall has been updated. The updates to the secant method improve convergence under drying and wetting conditions in a lake.

- Based on the LAK package input-output instructions (mf6io.pdf), the variable "connlen must be greater than zero for a HORIZONTAL, EMBEDDEDH, or EMBEDDEDV lake-GWF connection." However, a value of zero could be specified and the model would run with no LAK-groundwater exchange. A minor fix was made to enforce connlen to be strictly greater than zero per the input instructions. The error message issued when connlen is specified as zero was augmented with additional information for assisting the user.

- When n-point cross-sections are active in SFR, the evaporation calculation uses the variable rwid (see mf6io.pdf) to calculate the total amount of evaporation even though the wetted topwidth is less than

rwid. For example, using a trapezoidal cross-section geometry with an rwid of 10, an rlen of 100, and prescribed evaporation rate of 0.1, the calculated evaporative losses would equal 100 even when the wetted top width was only 5.0 units wide. With this bug fix, the evaporation in this example results in only 50 units of evaporation loss. It is also worth mentioning that the precipitation calculation currently uses rwid. Since the precipitation falling outside the margins of the wetted top width but within rwid would likely be accumulated in a channel, it makes sense to leave this calculation as is.

- An SFR channel defined with the n-point cross-section option was calculating the wetted cross-sectional area incorrectly for rectangular cross sections and for some other cross-section configurations. The cross sectional area of a triangular section was being calculated as one-half multiplied by the depth of the channel, as opposed to one-half multiplied by the base width multiplied by the height. As a result, the units in the Manning's equation were not correct owing to the missing dimension in the area calculation. The change in the area calculation will slightly alter the solution found using Manning's equation since the cross-sectional area term appears in it. As a result, existing models may reflect slightly different answers in groundwater and surface-water exchange amounts owing to slight differences in the calculated stream stage. In addition to the fix, some clarifying text, including a new figure, was added to mf6io.pdf.

SOLUTION

- Fixed the residual calculation used to calculate the pseudo-transient time-step length used when psuedo-transient continuation is used for steady-state stress periods in models using the Newton-Raphson method. This fix may change the number of iterations required to achieve convergence for existing models that use psuedo-transient continuation.

Version mf6.4.1–December 9, 2022

BUG FIXES AND OTHER CHANGES TO EXISTING FUNCTIONALITY
INTERNAL FLOW PACKAGES

- The Viscosity (VSC) Package introduced in version 6.4.0 would report an error for certain types of stress packages if the IDOMAIN capability was activated by the user. In some cases, the error message would indicate that a boundary was not assigned to a valid cell. This invalid error would prevent the simulation from proceeding. The error was corrected by removing the invalid check so that the program can proceed normally.

Version mf6.4.0–November 30, 2022

NEW FUNCTIONALITY

- A new Viscosity (VSC) package for the Groundwater Flow (GWF) Model is introduced in this release. The effects of viscosity are accounted for by updates to intercell conductance, as well as the conductance between the aquifer and head-dependent boundaries, based on simulated concentrations andor temperatures. The VSC Package is activated by specifying "VSC6" as the file type in a GWF name file. Changes to the code and input may be required in the future in response to user needs and testing. Implementation details for the VSC Package are described in the Supplemental Technical Information guide, which is included with the MODFLOW 6 distribution. For this first implementation, the VSC Package cannot be used for a GWF Model that is connected to another GWF Model with a GWF-GWF Exchange.

EXAMPLES

- A new example called ex-gwt-stallman was added. This new problem uses the GWT Model as a surrogate for simulating heat flow. The example represents one-dimensional heat convection and conduction in the subsurface in response to a periodic temperature boundary condition imposed at land surface. Results from the MODFLOW 6 simulation are in good agreement with an analytical solution.

BUG FIXES AND OTHER CHANGES TO EXISTING FUNCTIONALITY
BASIC FUNCTIONALITY

- Corrected programming error in XT3D functionality that could affect coupled flow models or coupled transport models. The XT3D code would result in a memory access error when a child model with a much larger level of refinement was coupled to a coarser parent model. The XT3D code was generalized to handle this situation.

- Corrected a programming error in which the final message would be written twice to the screen and twice to mfsim.lst when the simulation terminated prematurely.

- Terminate with error if METHOD or METHODS not specified in time series input files. Prior to this change, the program would continue without an interpolated value for one or more time series records.

- When a GWF Model and a corresponding GWT model are solved in the same simulation, the GWF Model must be solved before the corresponding GWT model. The GWF Model must also be solved by a different IMS than the GWT Model. There was not a check for this in previous versions and if these conditions were not met, the solution would often not converge or it would give erroneous results.

- The DISV Package would not raise an error if a model cell was defined as a line. The program was modified to check for the case where the calculated cell area is equal to zero. If the calculated cell area is equal to zero, the program terminates with an error.

- When searching for a required block in an input file, the program would not terminate with a sensible error message if the end of file was found instead of the required block. Program now indicates that the required block was not found.

- This release contains a first step toward implementation of generic input routines to read input files. The new input routines were implemented for the DIS, DISV, and DISU Packages of the GWF and GWT Models, for the NPF Package of the GWF Model, and the DSP Package of the GWT Model. Output summaries written to the GWF and GWT Model listing files are different from summaries written using previous versions of MODFLOW 6. For packages that use the new input data model, the IPRN capability of the READARRAY utility (described in mf6io.pdf) is no longer supported as a way to write input arrays to the model listing file. The IPRN capability may not be supported in future versions as the new generic input routines are implemented for other packages.

- Corrected an error in ZONEBUDGET for MODFLOW 6 that prevented the program from running properly in workspaces that contain one or more spaces in the path.

INTERNAL FLOW PACKAGES

- Corrected programming error in the Time-Variable Hydraulic Conductivity (TVK) Package in which the vertical hydraulic conductivity was not reset properly if the K33OVERK option was invoked in the Node Property Flow (NPF) Package.

- The Node Property Flow (NPF) Package had an error in how the saturated thickness at the interface between two cells was calculated for a DISU connection that is marked as vertically staggered (IHC = 2). The calculation was corrected so that the thickness for two confined cells is based on the overlap of the cells rather than the average thickness of the two cells.

STRESS PACKAGES

- The Evapotranspiration (EVT) Package was modified to include a new error check if the segmented evapotranspiration capability is active. If the number of ET segments is greater than 1, then the user must specify values for PXDP (as well as PETM). For a cell, PXDP is a one-dimensional array of size NSEG - 1. Values in this array must be greater than zero and less than one. Furthermore, the values in PXDP must increase monotonically. The program now checks for these conditions and terminates with an error if these conditions are not met. The segmented ET capability can be used for list-based EVT Package input. Provided that the PXDP conditions are met, this new error check should have no effect on simulation results.

- The Evapotranspiration (EVT) Package would throw an index error when SURF_RATE_SPECIFIED was specified in the OPTIONS block and NSEG was set equal to 1. The code now supports this combination of input options.

ADVANCED STRESS PACKAGES

- When the LAK Package was used with a combination of outlets that routed water to another lake and outlets that did not, then the budget information stored for the LAK Package had uninitialized records for LAK to LAK flows. These uninitialized records were used by the LKT Package and possibly other programs. The LAK to LAK budget information was modified to include only valid records.

- When a WITHDRAWAL value was specified for lakes, only the withdrawal value for the last lake would be reported in budget files, lake budget tables, and in lake withdrawal observations. This error would also be propagated to the GWT Lake Transport (LKT) Package, if active. This error would only show up for models with more than one lake and if the lake withdrawal term was included.

- When lakes were assigned with the STATUS CONSTANT setting to prescribe the lake stage, the CONSTANT term used in the lake budget table was tabulated using an incorrect sign for aquifer leakage. This error would result in inaccurate budget tables. The program modified to use the correct leakage values for calculating the CONSTANT term.

- There were several problems in the observation utility for the Streamflow Transport (SFT), Lake Transport (LKT), Multi-Aquifer Well Transport (MWT), and Unsaturated Zone Transport (UZT) Packages. These issues were corrected as well as the descriptions for the observations in the user input and output guide.

- The BUDGETCSV option for the advanced stress packages would intermittently cause an error due to a variable not being set properly. The BUDGETCSV option did not work at all for the GWT advanced packages. The BUDGETCSV option was fixed to work properly.

- For multi-layer GWF Models, the UZF Package should generally have UZF cells assigned to each GWF cell that can be dry or partially saturated. If a UZF cell was assigned to an upper layer of a GWF Model, but not to underlying GWF layers, then outflow from the upper UZF cell would not always flow to the water table. The program was modified so that outflow from UZF cells is transferred into the GWF Model when there are no underlying UZF cells. This routing of water to GWF may not work properly unless the Newton-Raphson formulation is active.

EXCHANGES

- The GWT-GWT Exchange did not work when the XT3D_OFF option was specified. The program was fixed so that the XT3D dispersion terms can be shut off for a GWT-GWT Exchange. GWT-GWT Exchange keywords were renamed from ADVSCHEME, XT3D_OFF, and XT3D_RHS to ADV_SCHEME, DSP_XT3D_OFF, and DSP_XT3D_RHS, respectively, to more clearly indicate how the keywords relate to the underlying processes.

Version mf6.3.0–March 4, 2022

NEW FUNCTIONALITY

- New publications describing MODFLOW 6 were released, including Hughes and others (2022a), Langevin and others (2022), and Hughes and others (2022b).

- The GWF-GWF Exchange was updated to support XT3D flow calculations along the edges of connected GWF Models. The XT3D flow calculation is an alternative to the ghost-node correction and has been shown to provide accurate flow calculations for cell connections that do not meet the control-volume finite-difference requirements. This new capability allows the GWF-GWF Exchange to tightly couple a wide variety of parent and child grid configurations. The new XT3D option for the GWF-GWF Exchange can be activated by specifying XT3D in the options block of the GWF-GWF Exchange input file. The XT3D implementation for GWF-GWF is based on a new generalized coupling method that is described in the Supplemental Technical Information document distributed with this release.

- A new capability was added to support tight coupling of GWT Models through a new GWT-GWT Exchange. The new GWT-GWT Exchange can be used to connect any two GWT Models in a manner similar to the GWF-GWF Exchange. This allows transport to be represented from one GWT Model to another. The GWT-GWT Exchange calculates advective and dispersive fluxes and also supports the Mover Transport (MVT) Package. This first release of the GWT-GWT Exchange is limited to simulations in which the corresponding GWF Models and GWF-GWF Exchanges are run concurrently within the same simulation; the new capability does not support simulation of transport using groundwater flows saved from a previous simulation; however, this may be supported in the future. The new GWT-GWT functionality is activated by creating a GWT-GWT input file and specifying a GWT6-GWT6 exchange in the EXCHANGEDATA block of the simulation name file (mfsim.nam). The GWT-GWT Exchange is based on a new generalized coupling method that is described in the Supplemental Technical Information document distributed with this release.

- This release introduces the Time-Varying hydraulic conductivity (TVK) and the Time-Varying Storage (TVS) options for the Node Property Flow (NPF) and Storage (STO) Packages, respectively, of the GWF Model. The TVK option is activated by specifying the TVK6 keyword in the OPTIONS block of the NPF Package and by providing a TVK6 input file. The TVS option is activated by specifying the TVS6 keyword in the OPTIONS block of the STO Package, and by providing a TVS6 input file. The TVK6 and TVS6 input files are described in input and output guide (mf6io.pdf). Technical information about the TVK and TVS options is provided in the Supplemental Technical Information report that is provided with the distribution.

- The option already existed to provide binary budget and head file information from a GWF simulation for only the first time step of a given stress period, in which case that information will be used for all time steps in that stress period in a GWT simulation that reads from those files. The behavior of this option has been extended such that if the binary budget and head file information provided for the final stress period of the GWF simulation is for only one time step, that information will be used for any subsequent time steps and stress periods in the GWT simulation. This extended behavior includes as a special case the use

of binary budget and head file information from only one time step in only one stress period (for example, a single steady-state GWF stress period) for all time steps in all stress periods in a GWT simulation.

- Added new file-based input capability for the GWT Source and Sink Mixing (SSM) Package. The SSM Package previously required that all source and sink concentrations be provided as auxiliary variables for corresponding GWF stress packages. The SSM Package now supports an optional new FILEINPUT block, which can be provided with package names and file names. Files referenced in the FILEINPUT block can be used to provide time-varying source and sink concentrations. Descriptions for this new capability are described in the input and output guide (mf6io.pdf) under the GWT SSM Package, and the GWT Stress Package Concentrations (SPC) for list-based input and array-based input. If used, a single SPC6 input file can be provided for a corresponding GWF stress package. Either an SPC6 input file or the auxiliary variable approach can be used to supply concentrations for a single GWF stress package, but not both.

- Added BUDGETCSV option to GWF and GWT model output control and to advanced packages (SFR, LAK, MAW, UZF, MVR, SFT, LKT, MWT, UZT, and MVT) that produce summary tables of budget information. If activated, this option will cause a comma-separated value (CSV) file of the model budget terms to be written to a user-specified output file. These output CSV files can be easily read into a spreadsheet or scripting language for plotting of budget terms.

- Added option to use irregular cross sections to define the reach geometry for individual reaches in the SFR Package. Cross-section data for irregular cross-sections are defined in a separate Cross-Section Table Input File. The station-elevation data for an irregular cross section are specified as xfraction and height data, which is converted to station position using the specified reach width (RWID) and elevation using the specified bottom elevation of the reach (RTP). Manning's roughness coefficient fractions can optionally be specified with the xfraction-height data for a irregular cross section to represent roughness coefficient variations in a channel (for example, different channel and overbank Manning's roughness coefficients). SFR Package irregular cross sections and the method used to solve for streamflow in a reach with non-uniform Manning's roughness coefficients is a generalization of the methods used for 8-point cross-sections in the SFR Package for previous versions of MODFLOW (Prudic and others, 2004).

EXAMPLES

- A new example, ex-gwtgwt-mt3dms-p10, was added to demonstrate the new GWT-GWT Exchange.

BUG FIXES AND OTHER CHANGES TO EXISTING FUNCTIONALITY
BASIC FUNCTIONALITY

- Fixed a bug that caused the last binary budget and head file information provided by a GWF simulation in a given stress period to be used for all subsequent GWT simulation time steps in that stress period, even if binary budget and head file information was provided for more than one time step in that stress period. In that situation, the GWF time steps must match the GWT time steps one-for-one.

- Boundary packages, such as WEL, DRN and GHB, for example, read lists of data using a general list reader. For text input, the list of data would not be read correctly if it was longer than 300 characters wide. Most lists would normally be less than 300 characters unless a large number of auxiliary variables were specified. In this case, information beyond 300 characters would not be read. The list reader was modified to use an unlimited character length so that any number of auxiliary variables can be specified.

- The Observation (OBS) functionality can optionally write simulated values to a comma-separated value (CSV) output file. The OBS input file contains a DIGITS option, which controls the number of digits

written to the CSV output file. In some cases the "E" character was not written, making it difficult to read the CSV output file with other programs. New functionality was programmed to write observations using the maximum number of digits stored internally by the program using the G0 Fortran specifier. The default value for DIGITS was five, but this has been changed to this maximum number of digits. This maximum number of digits can also be activated by specifying a zero for DIGITS. For most applications, observations should be written with the default number of digits so that no precision is lost in the output.

- Added a check to the Flow Model Interface (FMI) Package of the GWT Model that will cause the program to terminate with an error if flow and budget files needed from a flow model cannot be located.

- The Output Control Package did not correctly determine if the end of a stress period was reached if the Adaptive Time Stepping (ATS) option was active. Output Control works correctly now with ATS.

- Budget information for individual boundary package entries can be written to the model list file in a table form. The table no longer includes boundaries that are in cells that are dry.

- When the simulated concentration in a cell is negative, which can occur due to the numerical methods used to solve the transport equation, then any sinks present in the cell should not add or remove mass. The program was modified so that transport through sinks is deactivated if the simulated concentration in a cell is negative.

- Parsing of observation input was corrected so that observation names can have spaces if the observation name is enclosed in quotations.

- The GWF Node Property Flow (NPF) Package can optionally calculate the three components of specific discharge. The program calculates these components using an interpolation method based on the XT3D method, the simulated flows across each cell face, and distances from the center of the cell to each cell face. This release contains a fix for a coding error in the calculation of the distance from the center of the cell to the cell face. The fix will affect the calculated specific discharge for model grids that have variable cell sizes. Because specific discharge is used in the calculation of the dispersion coefficients for GWT Models, simulated concentrations with this release may be different from simulated concentrations from previous releases; however, these concentration differences are expected to be minor.

STRESS PACKAGES

- Fixed a bug in the Recharge (RCH) and Evapotranspiration (EVT) Packages that would occur with array-based input (READASARRAYS) combined with the Time-Array Series (TAS) functionality. Because the TAS functionality only works for DIS and DISV models, this fix does not have any effect on models that use DISU discretization. The bug would occur when one or more cells in the upper layer were removed using the IDOMAIN capability. In this special case, the time-array series values did not carry over to the correct locations in the RCH and EVT arrays. This error would be difficult to identify for complex models, because the model would run to completion without any errors. The RCH and EVT Packages were modified to maintain direct correspondence between the `nodelist` and `bound` arrays with the arrays provided to the TAS utility. A small and intended consequence of this fix is that the ID2 value written to the binary budget file for array-based RCH and EVT Packages will correspond to the consecutive cell number in the top layer.

- Recharge and evapotranspiration flows that are written to the GWF Model binary budget file are marked with the text headers "RCH" and "EVT", respectively. In order to support the array-based input for SSM concentrations, these text headers are marked as "RCHA" and "EVTA", respectively, if the READASAR-RAYS option is specified for the package. This change will have no effect on simulation results; however, post processing capabilities may need to be adjusted to account for this minor renaming convention.

- When the PRINT_FLOWS option was used with the Source and Sink Mixing (SSM) Package, the cell ID numbers written to the listing file were incorrect. The SSM Package was fixed to output the correct cell ID.

- Add new AUTO_FLOW_REDUCE_CSV option for the Well Package. If activated, then this option will result in information being written to a comma-separated value file for each well and for each time step in which the extraction rate is reduced. Well extraction rates can be reduced for some groundwater conditions if the AUTO_FLOW_REDUCE option is activated. Information is not written for wells in which the extraction rate is equal to the user-specified extraction rate.

ADVANCED STRESS PACKAGES

- The Streamflow Routing (SFR) Package would terminate with a floating point error when calculating the stream depth as a function of flow rate, if the flow rate was slightly negative. Added a conditional check to ensure that the stream depth is calculated as zero if the calculated flow rate is zero or less.

SOLUTION

- The way in which constant head and constant concentration boundary conditions are handled when the conjugate gradient method is used for the linear solve was modified. In previous versions, constant head and concentration conditions would result in an asymmetric coefficient matrix. The program has been modified so that if the conjugate gradient method is selected for the linear solution, then matrix symmetry is preserved by adding adding flows into and out of constant head and concentration cells to the right-hand side of connected cells.

Version mf6.2.2–July 30, 2021

NEW FUNCTIONALITY

- A new Adaptive Time Step (ATS) utility was added. The ATS utility allows any stress period to be over-ridden with an alternative time stepping approach. The ATS utility implements two main capabilities (1) the capability to retry failed time steps with a shorter time step repeatedly until convergence is achieved, and (2) the capability to shorten and lengthen time steps based on simulation behavior. These capabilities are described in the user input and output guide in a new section on the ATS utility.

- A new option for printing water contents to a dedicated output file has been added to UZF. To activate, the keyword WATER_CONTENT is added to the OPTIONS block of UZF, followed by FILEOUT, followed by the user-specified output file name, for example "water-content.uzf.bin". The approach is analogous to the STAGE option within the SFR options block. Contents of the new file will be written in binary and can be read using flopy's binaryfile utility.

- The residual balance error for groundwater flow and solute transport is now written to the diagonal position of the flowja array, which is marked with the text description "FLOW-JA-FACE". The flowja array is optionally written to the binary model budget file according to user settings in the output control file and other package input files.

- A new option for simulating specific storage changes only when a cell is fully saturated has been added to the storage (STO) package. To activate, the SS_CONFINED_ONLY keyword is added to the OPTIONS block in the STO Package. This option is identical to the approach used to calculate storage changes under confined conditions in MODFLOW-2005.

- A new observation type called "wel-reduction" was added for the Well Package. This observation type reports the reduction in the well discharge that can occur when the `AUTO_FLOW_REDUCE` option is specified.

  EXAMPLES

- Added the following new examples:

  – ex-gwt-hecht-mendez

  – ex-gwf-capture (This example is described in mf6examples.pdf to demonstrate functionality of the Application Programming Interface; it is not included in the examples folder of this distribution as it requires python and several python packages)

- Added new citation to this document. The Morway and others (2021) paper describes the use of the Water Mover Package in MODFLOW 6 to represent natural and managed hydrologic connections.

BUG FIXES AND OTHER CHANGES TO EXISTING FUNCTIONALITY
BASIC FUNCTIONALITY

- The specific storage formulation in the storage (STO) package has been modified to eliminate the dependency of the original formulation on the vertical datum. The original specific storage formulation also overestimated storage changes for cells that resaturated or desaturated in successive time steps. Furthermore, the sign of the specific storage change was incorrect in cells with negative heads and resaturated or desaturated in successive time steps. The revised specific storage formulation resolves all of the deficiencies of the original formulation and accurately simulates specific storage changes under water table conditions but will change the results for existing models. Testing indicates that the differences between models run with the original and revised specific storage formulation are generally small but tend to increase in models with large specific storage values or have cells that repeatedly resaturated or desaturated in successive time steps.

- The convergence failure message message written to GWF and GWT listing files (FAILED TO MEET SOLVER CONVERGENCE CRITERIA) is now written after the budget summary tables. In previous releases this convergence failure message was written prior to printing heads and concentrations, which often resulted in this message being unnoticed by users.

- The order of output written to the GWF and GWT listing files for a time step was reorganized in a consistent manner with model and package flows coming first, followed by dependent variables, and then concluding with budget summary tables.

- The DISU Package checks to make sure that the top of a cell is not higher than the bottom of an overlying cell. A new option was added to the DISU Package to allow the user to specify the vertical offset tolerance used in this check. This new optional input variable is VERTICAL_OFFSET_TOLERANCE.

- Add DISU Package check to ensure that JA(IA(n)) is equal to n and that no values in JA are less than zero or greater than nodes.

- When IDOMAIN is used with the DISU Package and any IDOMAIN value is zero, then the program was expecting all JA values to be positive. The program is supposed to allow a negative JA value to be specified for the corresponding cell (in the diagonal position), but this was not working. A fix was implemented to allow a negative cell number to be specified in the diagonal position of the JA array when the IDOMAIN capability is active.

- A new check was added to the Horizontal Flow Barrier (HFB) Package to ensure that barriers are between cells that are horizontally connected. The program would previously continue running if a barrier was between vertically connected cells.

- There was no check to prevent the zero-order decay functionality of the Mobile Storage and Transfer (MST) and Immobile Storage and Transfer (IST) Packages in the GWT Model from producing negative concentrations. The program now reduces the zero-order decay rate for the aqueous and sorbed phases (for the mobile and immobile domains) to ensure that decay does not consume more mass than is available. These changes do not affect zero-order growth.

- If a binary budget file from a GWF Model was larger than about 2 Gigabytes, then it could not be used as input for a subsequent GWT Model. The program was modified to use a long integer to store the byte position.

- The program was terminating with a non-zero return code if the simulation did not converge. This is the intended behavior, unless the CONTINUE option is specified in the simulation name file. The program now terminates with a return code of zero if the simulation does not converge, but the CONTINUE option is set and the program reaches the end of the simulation.

ADVANCED STRESS PACKAGES

- The UZF water-content observation by depth was giving an error, because a check was using the wrong index to retrieve the cell top and bottom elevations for the requested observation. The program was modified to use the correct index, and the output is now as expected. Note that this bug is not related to the new WC keyword in the OPTIONS block, but rather is related to OBS6 output option.

- Amend surfdep error check with landflag. Deep cells (non-land surface cells) should not require surfdep > 0

- In the LAK observation package, users can specify "lak" to get a summary of lake-groundwater exchange. Users could specify a lake number without specifying a specific connection number (variable "iconn"). Code will now stop if lake number is provided without a matching connection number. Code will still provide a summary of total lake-groundwater exchange when BOUNDNAME is entered for the variable ID. This also will fix a similar issue for the observation types "wetted-area" and "conductance", since both require ID2 when ID is an integer corresponding to a lake number.

- In the MAW observation package, users can specify "maw" to get a summary of well-groundwater exchange. The code was allowing users to specify a well number without requiring specification of a connection number (variable "icon"). Code will now stop if well number is provided without a matching connection number. Code will still provide a summary of total well-groundwater exchange when BOUNDNAME is entered for the variable ID. This also will fix a similar issue for the observation type "conductance", since both require ID2 when ID is an integer corresponding to a well number.

SOLUTION

- An optional new input variable called ATS_OUTER_MAXIMUM_FRACTION can now be entered for the IMS Package. This variable has no effect unless the new ATS capability is active.

Version mf6.2.1–February 18, 2021

NEW FUNCTIONALITY

- The Source and Sink Mixing (SSM) Package for the Groundwater Transport Model was modified to include an alternative option for the concentration value assigned to sinks. A new AUXMIXED option was added to represent evaporation-like sinks where the solute or a portion of the solute may be left behind. The AUXMIXED option provides an alternative method for determining the groundwater sink concentration. If the cell concentration is larger than the user-specified sink concentration, then the concentration of the sink will be assigned as the specified concentration. Alternatively, if the specified concentration is larger than the cell concentration, then water will be withdrawn at the cell concentration. Thus, the AUXMIXED option is designed to work with the Evapotranspiration and Recharge packages where water may be withdrawn at a concentration that is less than the cell concentration.

- Add support for the Freundlich and Langmuir isotherms to the Mass Storage and Transfer (MST) Package of the Groundwater Transport Model.

  EXAMPLES

- Added the following new examples:

    – ex-gwt-mt3dms-p02
    – ex-gwt-rotate
    – ex-gwt-saltlake
    – ex-gwt-uzt-2d

BUG FIXES AND OTHER CHANGES TO EXISTING FUNCTIONALITY
BASIC FUNCTIONALITY

- The way in which the dispersion coefficients are calculated with the simple option (XT3D_OFF) for the Dispersion Package was modified. When the velocity within a cell is not aligned with a principal grid direction, the dispersion coefficients are calculated using a simple arithmetic weighting, rather than harmonic weighting as is done for the simple option for anisotropic flow in the NPF Package. The arithmetic weighting option eliminates a possible discontinuity when a principal flow-aligned dispersion component is zero.

- The mass flow between two cells is calculated and optionally written to the GWT budget file. There was an error in this calculation of mass flow when the TVD scheme was specified in the Advection (ADV) Package. Consequently, the mass flows written to the budget file were not correct in this situation. Because these mass flows are also used in the budget calculations for the Constant Concentration (CNC) Package, reported CNC mass flows were also not correct. This could result in large budget discrepancies in the GWT budget table. Simulated concentrations were not affected by this error. A small correction was made to the routine that adds the advective mass flow for the TVD scheme.

- Several packages had input blocks that could not be specified using the OPEN/CLOSE keyword. The program was modified so that OPEN/CLOSE is supported for all intended blocks.

- The Immobile domain Storage and Transfer (IST) Package for the GWT Model is based on a conceptual model in which the immobile domain is always fully saturated, and so the saturation of the immobile domain does not depend on head in a cell. The program was modified so that none of the immobile domain terms include saturation, except for the mass transfer equation itself, in which the transfer of solute between the mobile and immobile domain is multiplied by the cell saturation.

- Budget terms for the Immobile domain Storage and Transfer (IST) Package were not being written to the binary budget file for the GWT Model. The package was modified to write these rate terms to the GWT binary budget file using the settings specified in the GWT Output Control file.

- Bulk density does not need to be specified for the Immobile domain Storage and Transfer (IST) Package if sorption is not active; however the program was trying to access bulk density even though it is not needed, which resulted in an access violation. Program was fixed so that bulk density does not need to be specified by the user unless sorption is active for the IST Package.

- Budget tables printed to the listing file had numeric values that were missing the 'E' character if the exponent had three digits (e.g. 1.e-100 or 1.e100). Writing of the budget table was modified to include the 'E' character in this case. This change should make it easier for programs written in other languages to parse these tables.

- In the Mass Transfer and Storage (MST) and the Immobile Storage and Transfer (IST) Packages, the keyword to activate sorption was changed from SORBTION to SORPTION. The program will still accept SORBTION, but this keyword will be deprecated in the future.

- Revised several of the text strings written to the headers within the GWT binary budget file. A table of possible text strings for the GWT binary budget file are now included in the mf6io.pdf document.

ADVANCED STRESS PACKAGES

- The CONSTANT term used to report the rate of mass provided by a constant-concentration condition in the LKT, SFT, MWT, and UZT did not include the contribution to adjacent package features. For example, if a stream reach was marked as constant-concentration boundary and it had flow into a downstream reach, then that flow was not included in the budget calculations. Consequently, reported budgets in the listing file would show discrepancies that were larger than what was actually simulated by the model. The program code was modified to include these mass flows to adjacent features.

- The ET formulation in UZF was not reducing the residual pET passed to deeper UZF objects when the extinction depth spanned multiple UZF objects (layers). As a result, too much water was removed when the water table was shallow. Or, in some cases, water was removed from dry cells that were above the water table but within the extinction depth interval. The ET code within the UZF package was modified to remove only eligible water from the unsaturated and saturated zones.

- The UZF package should exit with an appropriate error message when SURFDEP > cell thickness. When this condition is not enforced, bad mass balances may result.

- The FLOW_IMBALANCE_CORRECTION implemented in the GWT FMI Package did not work properly with the GWF UZF Package. The issue was fixed by ensuring that the FMI Package could accurately calculate the flow residual for cells that had a UZF entry.

- The SFR package should exit with an appropriate error message when a diversion has a cprior type of FRACTION but the divflow value is outside the range 0.0 to 1.0 as stated in the documentation.

Version mf6.2.0–October 20, 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.

Version mf6.1.1–June 12, 2020

NEW FUNCTIONALITY

- 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, EVAPO-RATION, 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–December 12, 2019

  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 UzfCellGroup-Type, 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 SPEC-IFIED, 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 low-ermost 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 THICK-STRT 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 PACKAGE-DATA 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 PACKAGE-DATA 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 EMBED-DEDV 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.