Updates for GSFLOW version 1.1.5
January 2012

Version 1.1.5 includes a number of enhancements, modifications, and bug fixes that are summarized in this document. The initial release of GSFLOW (version 1.0) is documented in Markstrom and others (2008). Additional updates are described in the "release.txt" file and in PDF files located in the GSFLOW documentation directory.

The major enhancements for this release are:

Addition of Newton Formulation for MODFLOW: One of the major enhancements made for GSFLOW version 1.1.5 was addition of MODFLOW-NWT, a Newton Formulation of MODFLOW-2005 (Niswonger and others, 2011). Thus, GSFLOW is now the integration of PRMS and MODFLOW-NWT (which is based on MODFLOW-2005 and can be used in MODFLOW-2005 mode as well). The Newton method is an alternative to the Picard method that is used by MODFLOW-2005 for linearizing the groundwater-flow equation. The Newton formulation extends the applicability of MODFLOW, especially to those problems representing unconfined aquifers and surface-water/groundwater interaction; such are the conditions in most GSFLOW models. MODFLOW-NWT solves the three-dimensional groundwater-flow equation in the same manner as MODFLOW-2005, except linearization is done using the Newton method. MODFLOW-NWT uses unstructured, asymmetric matrix solvers to calculate groundwater head. MODFLOW-NWT was designed to work with a new internal flow package called the Upstream-Weighting (UPW) Package to solve complex unconfined groundwater-flow simulations including those characterized by drying and rewetting of cells. The UPW Package computes the horizontal-conductance terms for the unconfined groundwater-flow equation in a different manner than do the BCF, LPF, and HUF internal flow packages of MODFLOW-2005, and is a replacement to these three packages for calculating conductance and storage terms in MODFLOW-NWT. Accordingly, MODFLOW-NWT requires two new input files that are not used by MODFLOW-2005. These new input files are (1) the UPW Package input file that contains input required for the internal-flow calculations, and (2) the NWT input file that contains input values required by the Newton and matrix solver methods.

In order to accommodate the Newton formulation, changes were made to some of the existing MODFLOW stress packages supported by GSFLOW to calculate the stress derivative with respect to head and add them appropriately to the Jacobian matrix that is solved by MODFLOW-NWT. The WEL Package, the Streamflow-Routing Package, and the Unsaturated-Zone Flow Package are solved using the Newton method, and the derivative of groundwater inflow or outflow as a function of groundwater head are calculated in the Formulate subroutines of these packages. Thus, new versions of these packages accompany the other MODFLOW-NWT source files. In addition to these new source files, other packages that rely on hydraulic conductance values calculated by the optional internal flow packages were modified to include conductance values calculated by the UPW Package. These packages include the Multi-Node Well (MNW1 and MNW2) Packages, the Horizontal-Flow Barrier Package, and the Lake Package. Refer to table 1 of Niswonger and others (2011) for a list of packages supported by MODFLOW-NWT, input instructions for the NWT solver input file and UPW Package input file, and further descriptions of the code. [The report by Niswonger and others (2011) is located in the MODFLOW documentation subdirectory (file 'tm6a37_NWT.pdf'); also see http://water.usgs.gov/nrp/gwsoftware/modflow_nwt/ModflowNwt.html. Example input files for a GSFLOW simulation using MODFLOW-NWT are provided for the Sagehen example problem, in the data subdirectory of this release; see file “Readme.sagehen.txt” in that directory.]

Addition of the PRMS Map Results and Climate by HRU Distribution modules: Two new PRMS modules have been added. The first, Map Results module, replaces the Grid Report module that was initially released with GSFLOW version 1.1.3. The Map Results module is more general than the Grid Report module in that it can be used to output any variable from a hydrologic response unit (HRU) to a target map, such as a MODFLOW grid-cell map. The original Grid Report module was restricted to output of potential recharge computed by PRMS to the MODFLOW grid-cell map. Models that used the Grid Report module will need to be updated by replacing parameters in the Control and Parameter Files related to the Grid Report module with those used by the Map Results module, although some of the parameters used by the Map Results module are equivalent to those used for the Grid Report module. The module, which can only be used for PRMS-only simulations, is described in detail in the file “Map_results.pdf.”

The second new module, Climate by HRU Distribution Module (**climate_hru**), provides an alternative approach to the Data File for input of time-series climate data sets, pre-distributed to each HRU. Thus, it is possible to use any method to pre-process and distribute climate data to HRUs outside of a PRMS-only or GSFLOW simulation. Because climate data are pre-processed before a simulation, use of climate_hru may reduce the run time of a simulation. The module can be specified for Control File parameters `temp_module`, `precip_module`, `solrad_module`, and `et_module`. A new simulation mode also was added to allow generation of climate-by-HRU (CBH) files for use with the **climate_hru** module. Module **climate_hru** and the WRITE_CLIMATE simulation mode are described in detail in the file “Climate_hru.pdf.”

Examples of the use of the Map Results and Climate by HRU Distribution Modules are provided with the Sagehen example problem.

Additional enhancements and changes for version 1.1.5 are described below. It should be noted that the changes made to the code resulted in decreased simulation run times for the Sagehen sample problem compared to previous releases; moreover, the MODFLOW-NWT version of the sample problem (simulation condition 2) has lower water-budget errors than the PCG version (simulation condition 1), partly because of different convergence criteria used for the MODFLOW-NWT version. Updates to input parameters also are identified in the file “Appendix1_Tables_v1.1.5.pdf.’

Recommendations for Model Convergence Criteria:

Background: GSFLOW is based on an iterative-solution method in which convergence for each time step is dependent on whether or not changes in groundwater heads and flow rates meet closure criteria specified in the MODFLOW solver packages. If the MODFLOW convergence criteria are met, then GSFLOW continues to the next time step; if the convergence criteria are not met but the maximum number of MODFLOW iterations per time step is exceeded (as specified using one of the variables MAXITEROUT, MXITER or ITMX, depending on which of the MODFLOW solver packages is used), then GSFLOW will print a warning message and continue to the next time step. Note that this differs from MODFLOW, in which MODFLOW stops if MAXITEROUT, MXITER or ITMX are exceeded.

Convergence of groundwater heads and flow rates is dependent in part on the amount of gravity drainage that drains from the soil zone to the underlying unsaturated and saturated zones. The amount of gravity drainage is dependent on the potential gravity drainage computed by the Soil Zone Module and the vertical hydraulic conductivity and heads within the MODFLOW finite-difference cells. In many cases, heads and groundwater flow rates may converge faster if the amount of gravity drainage from the soil zone is no longer changing, which means that the MODFLOW computations will no longer be dependent on feedback from the Soil Zone Module.

Three GSFLOW input parameters are provided to allow the user to stop the soil-zone computations prior to convergence of MODFLOW. These parameters, which are specified in the Parameters File, are (1) `szconverge`, which is the maximum allowed change in gravity drainage from the soil zone for all HRUs between iterations required before the soil-zone iterations cease; (2) `mnsziter`, which is the minimum number of iterations per time step that are computed by the Soil Zone Module; and (3) `mxsziter`, which is the maximum number of iterations per time step that are computed by the Soil Zone Module. Parameters `szconverge` and `mxsziter` have been available since the initial release of GSFLOW and parameter `mnsziter` was introduced with version 1.1.1 (see Table A1-28 in the Appendix1_Tables document). Computations within the soil zone cease under three conditions listed in order of precedence: (1) the MODFLOW closure criteria are met or MAXITEROUT, MXITER, or ITMX is reached; (2) the maximum number of soil-zone iterations is reached, as specified by parameter `mxsziter`; or (3) the maximum change in gravity drainage from the soil zone for all HRUs between iterations is less than the value specified for parameter `szconverge`. When conditions 2 or 3 are met, all computations done by the Soil Zone Module are held constant for the remainder of the current time step until MODFLOW-related convergence criteria are met (or MAXITEROUT, MXITER, or ITMX is exceeded). In addition, the amount of interflow and surface runoff to streams and lakes are held constant when soil-zone computations cease within a time step.

Recommendations: Limiting the number soil-zone iterations can be useful for speeding up GSFLOW simulation times; however, this option can also lead to mass-balance errors and erroneous results. Errors in GSFLOW can occur if soil-zone computations stop within a time step before the MODFLOW solution reaches a stable value; this may cause groundwater gravity drainage or discharge from some finite-difference cells in subsequent iterations to be significantly different than that computed at the iteration in which the soil-zone computations ceased. Thus, it is recommended that models be run with the requirement that soil-zone computations iterate until MODFLOW converges. This can be done by setting the PRMS parameters `mnsziter` and `mxsziter` equal to the maximum number of outer iterations specified for MODFLOW (that is, `mnsziter` = `mxsziter` = MAXITEROUT, for the NWT solver, or MXITER or ITMX for MODFLOW-2005 solvers). Additionally, `mnsziter` = `mxsziter` = MAXITEROUT (or MXITER or ITMX) is the default condition for GSFLOW, and if `mnsziter` or `mxsziter` are either unspecified or specified as 0 in the PRMS parameter file, then the default condition will be used.

General Changes and Critical Issues for GSFLOW and PRMS modules:

(1) Caution: A significant bug was corrected in the PRMS Soil Zone module that allowed the gravity and preferential-flow reservoirs to exceed the maximum storage capacity prior to computing the following flows: gravity drainage, Dunnian surface runoff, slow interflow, and fast interflow. The code now checks for maximum storage capacity in the gravity and preferential-flow reservoirs and moves excess water to the appropriate place (either the preferential flow reservoir or Dunnian surface runoff) prior to flow computations. The bug fix may produce significant changes in model results in the soil zone, which changes the storage and flows within the unsaturated and saturated zones, that may require re-calibration of a PRMS-only or GSFLOW simulation. The primary change in simulations is the possibility that the proportion of Dunnian surface runoff increases as flow cascades to the stream network. The greater the number of HRUs in a cascading flow path, the greater this increase can propagate. This can result in water cascading significantly more rapidly into the stream segments, which increases the flashiness of streamflow. The increased Dunnian surface runoff is the result of gravity reservoirs within the soil zone filling to saturation further from the stream network. Some of the input parameters that might be used to recalibrate the model are: slowcoef_lin, slowcoef_sq, fastcoef_lin, fastcoef_sq, sat_threshold, ssr2gw_rate, and ssr2gw_exp. Models may be particularly sensitive to values specified for parameter slowcoef_sq.

(2) Variables in GSFLOW and PRMS modules that are used in computations of large values, or used in many computations within a single time step and thus more susceptible to round-off issues, are declared using the Fortran DOUBLE PRECISION language element. This practice was partially implemented in earlier releases of GSFLOW and may not be complete in this release; for example, this practice has not been implemented for the PRMS parameter hru_area. The definition of large is not exact. In general, a large value for these modules is considered to be a variable requiring eight significant digits, such as needed for volume-, basin-, and area-weighted averages, and areal computations, as well as computations involving the possibility of long distances between points, such as between climate stations. Reducing the effects of round-off issues within computations involving large values becomes increasingly important as modeled areas increase in size, such as in a regional model. This change may produce very slight changes in results from previous GSFLOW releases.

(3) The minimum fraction of pervious area was reduced from 1 percent to 0.1 percent to allow HRUs to be specified with a greater fraction of impervious area to allow slightly more direct surface runoff from impervious surfaces; if the parameter `hru_percent_imperv` is specified with a value greater than 0.999 a warning message is printed and the value is set to 0.999. This change might be helpful for small HRUs.

(4) Added additional value for the optional control parameter `print_debug`; the new value -1 minimizes screen output.

(5) Added control parameters `cascade_flag`, `cascadegw_flag`, and `subbasin_flag` to the Control File to allow users to turn on or off computations of HRU and/or GWR (groundwater reservoir) cascades and subbasins, respectively, without requiring the removal of the associated cascade and subbasin parameters and dimensions in the Parameter File. Setting any of these

parameters to the value 0 disables computation of the corresponding process: `cascade_flag`=0 turns off computation of cascading HRU flow, which means all HRU generated flows are sent to the basin outlet and not to individual stream segments; `cascadegw_flag`=0 turns off computation of GWR cascading flow in PRMS-only mode, which means all GWR generated flows are sent to the basin outlet and not to individual stream segments; and `subbasin_flag`=0 turns off use of the Subbasin module.

Modifications to GSFLOW and PRMS Modules and MODFLOW Packages

Several minor modifications and bug fixes were made to some of the GSFLOW and PRMS modules and MODFLOW Packages, which are described below. Many of these modifications do not affect GSFLOW computations and are therefore transparent to GSFLOW users.

(a) GSFLOW Modules

Computational-Sequence Control Module for PRMS and GSFLOW (gsflow_prms)

Default values for dimensions `nrain` and `ntemp` are changed from 1 to 0. This was necessary with the addition of the **climate_hru** module because this allows users to not specify at least one column of measured precipitation, one column of minimum air temperature, and one column of maximum air temperature, which are optional for the **climate_hru** module. For all other precipitation and air temperature distribution modules, the requirement that at least one column and in some cases two columns of measured precipitation and minimum and maximum air temperature values must be included in the PRMS Data File remains.

Added a simulation mode to allow generation of climate-by-HRU files for use with the **climate_hru** module based on the selected climate modules (air temperature, precipitation, solar radiation, and potential evaporation). To activate this mode, set the value of the control parameter `model_mode` to WRITE_CLIMATE. For full simulations, be sure to set `model_mode` to GSFLOW, PRMS, or MODFLOW. See file “Climate_hru.pdf” for more details.

Computational-Sequence Control for MODFLOW Module (gsflow_modflow)

Merged with the NWT version of MODFLOW with addition of PCGN, UPW, and NWT. (Note that GSFLOW has not been tested with the PCGN solver.)

Unit-Conversions Module (gsflow_setconv)

Several variables changed from double to single precision having to do with checking of percentage differences between HRU, GVR and MODFLOW cell areas. This change may produce very slight changes in results and also reduces memory requirements.

It is no longer necessary to input parameter `gvr_cell_pct` if dimensions `nhru` and `nhrucell` are equal. This parameter defaults to 1.0, which is the required value when `nhru` equals `nhrucell`. This change reduces memory requirements and the size of the Parameter File.

PRMS to MODFLOW Integration Module (gsflow_prms2mf)

Added check for inactive HRUs when any associated MODFLOW cell is active; if this condition is found, an error message is printed to the user's screen and the simulation halts.

Watershed-Budget Summary Module (gsflow_budget)

All variables changed from single to double precision, which produces slightly improved water budgets; this change may produce slight changes in results from previous versions of the code.

Flow-Components Summary Module (gsflow_sum)

Most variables changed from single to double precision, which produces slightly improved water budgets; this change may produce slight changes in results from previous versions of the code.

Only output summary report lines for wells when wells are included in the model.

Bug fix of initial water balance: the storage within the soil zone is now computed based on initial values as specified in the PRMS Parameter File, providing an accurate water balance between initiation of an execution and the end of the first time step; this change may produce slight changes in initial water balance from previous versions of the code.

Bug fix to eliminate possible double accounting for water added to the preferential-flow reservoir after an infiltration or snowmelt event; this change may produce slight changes in results from previous versions of the code.

(b) PRMS Modules

General change:

Suffixes in the names of most PRMS modules were removed. This change does not require modification to existing GSFLOW Control Files (that is, users can continue to use the original module names); however, it is suggested that the new module names be used in new GSFLOW Control Files. The old and new module names are:

Module	Old name	New name
Basin	basin_prms	basin
Cascading-Flow	cascade_prms	cascade
Observed-Data	obs_prms	obs
Potential Solar-Radiation	soltab_hru_prms	soltab
One-Station Temperature-Distribution	temp_1sta_prms	temp_1sta
Lapse-Station Temperature-Distribution	temp_laps_prms	temp_laps
Inverse-Distance Temperature-Distribution	temp_dist2_prms	temp_dist2
One-Station Precipitation-Distribution	precip_prms	precip_1sta
Lapse-Station Precipitation-Distribution	precip_laps_prms	precip_laps
Inverse-Distance Precipitation-Distribution	precip_dist2_prms	precip_dist2
Degree-Day Solar-Radiation Distribution	ddsolrad_hru_prms	ddsolrad
Cloud-Cover Solar-Radiation Distribution	ccsolrad_hru_prms	ccsolrad
Jensen-Haise Potential-Evapotranspiration	potet_jh_prms	potet_jh
Hamon Potential-Evapotranspiration	potet_hamon_hru_prms	potet_hamon
Pan-Evaporation Potential-Evapotranspiration	potet_pan_prms	potet_pan

Active Transpiration Period	transp_tindex_prms	transp_tindex
Precipitation-Interception	intcp_prms	intcp
Snow	snowcomp_prms	snowcomp
Nonlinear Source Area Surface-Runoff and Infiltration	srunoff_smidx_casc	srunoff_smidx
Linear Source Area Surface-Runoff and Infiltration	srunoff_carea_casc	srunoff_carea
Soil-Zone	soilzone_prms	soilzone
Groundwater Reservoir	gwflow_casc_prms	gwflow
Subbasin	subbasin_prms	subbasin
Streamflow	strmflow_prms	strmflow
HRUs Flow-Summary	hru_sum_prms	hru_sum
Watershed Flow-Summary	basin_sum_prms	basin_sum

Basin Module (basin)

Changed value used to check if single-precision values from computations or comparison of two values are within a round-off tolerance of 0.0. The value used for this check was changed from 1.0E-08 to 1.0E-07; this change may produce very slight changes in results.

Climate-Flow Module (climateflow)

New module that is used to allocate, declare, and initialize common states and fluxes that are shared among PRMS modules. The set of functions and FORTRAN module allow for decreased storage requirements and unnecessary duplication of code.

Observed-Data Module (obs) and Adjusted Observed Data Module (obs_adjust_prms)

Changed some variables related to conversion factors from single to double precision; this change may produce very slight changes in results

Bug fix: the checks made for missing values were done incorrectly for the **temp_dist2** module; these checks were supposed to be performed only for temp modules **temp_1sta** and **temp_laps**. This fix allowed for the deletion of the **obs_adjust_prms** module.

The variable `form_data`, which can be input in the PRMS Data File, is ignored if included. Data for this variable are unavailable in general and as implemented in the code was applied to set the form of precipitation on all HRUs, which, in general, is a poor assumption.

Cascading-Flow Module (cascade_prms)

Changed input inconsistency check between cascade parameters and the `hru_type` parameter from an error to a warning. If cascade parameters are specified such that any HRU is determined to be a swale, that is, the HRU does not cascade to another HRU or stream segment and the value of hru_type for such an HRU was not set to 3 (swale), a warning message is printed and the value of `hru_type` for such an HRU is set to 3.

Degree-Day and Cloud-Cover Solar-Radiation Distribution Modules (ddsolrad and ccsolrad)

Measured solar-radiation values input in a PRMS Data File with a value of zero previously were considered to be missing values when used by the ccsolrad or ddsolrad modules, which allows

HRUs to be assigned measured values instead of computing estimated solar-radiation values. If a measured solar-radiation value is input in the PRMS Data File with a negative value or a value greater than 1,000 it is ignored. Whether or not a valid measured value is used to assign a solar-radiation value to an HRU is based on (1) whether measured solar radiation values are included in the PRMS Data File and (2) the value of parameter hru_solsta indicates a measured value is to be used for any HRU. The parameter hru_solsta is specified in the PRMS Parameter File.

Bug fix: In previous versions of the code, it was possible in very rare circumstances, that a solar-radiation value might have been set higher than the maximum value specified by the parameter `radmax`. Previously, a radiation-adjustment factor was computed, compared with parameter `radmax` to be sure it did not exceed `radmax`, and then precipitation adjustment was applied. It was possible that after applying the precipitation adjustment, the computed value would be greater than `radmax`. Now the precipitation factor is applied before the comparison to the parameter `radmax`.

Temperature-Distribution Modules (temp_1sta, temp_laps, and temp_dist2)

Checks were added to be sure that the maximum and minimum temperatures used in solar-radiation computations (modules **ccsolrad** and **ddsolrad**) are valid. These temperature values are based on measured values for the temperature station defined by parameter `basin_tsta`. If either of these values are invalid (<-89 or >150), they are set to the last valid value.

Inverse-Distance-Squared, Weighted Precipitation-Distribution Module (precip_dist2)

Check all values of psta_mon to be sure they are > 0 to avoid divide by zero; if a value is specified as 0.0 it is set to 0.00001.

Check to be sure that the distance between each HRU and temperature station is not 0; if it is, set the distance to 1.0

Note: previous versions of the module expected required measured temperature and temperature-related parameter values to be specified in units of degrees Fahrenheit, and required measured precipitation and precipitation-related parameter values to be specified in inches; this was changed to allow determination of input units of measured climate values and associated parameters to be based on parameters `temp_units` and `precip_units`.

Changed check of measured precipitation values to be between 0 and <= the value of parameter maxday_prec, instead of between –1.0E-07 and < maxday_prec as was done in the original module. This is only an issue if a precipitation value computed using the dist2 method was between -1.0E-7 and 0. The check was changed to be sure all computed precipitation values are >=0.0. This condition would be extremely rare.

Precipitation-Interception Module (intcp_prms)

If the net precipitation is < 0.0000001 inches, leave all precipitation in the canopy; this avoids unnecessary computations to be performed in subsequent modules. This condition would be extremely rare.

Snow Module (snowcomp)

Bug fix: added check to be sure output variable `snowevap` is not greater than `potet-hru_intcpevap`; previously it was possible, but unlikely, that the sum of the computed snow evaporation plus evaporation from the canopy would exceed the potential evapotranspiration for an HRU.

Linear and Nonlinear Source Area Surface-Runoff and Infiltration Modules (srunoff_carea and srunoff_smidx)

Bug fix: added check to be sure output variable `hru_impervevap` cannot be greater than unsatisfied potential evapotranspiration (ET). In previous versions of the modules, it was possible, but unlikely, that evaporation from impervious surfaces on an HRU could have been set to a value greater than the value of the potential ET – canopy ET – snow ET.

Soil-Zone Module (soilzone)

Fixed bug that could have double counted inflow to preferential-flow reservoirs (see description above).

Groundwater Reservoir Module (gwflow)

Added parameter gwstor_min (documented in Mastin and Vacarro, 2002), which allows the assignment of a minimum storage in any groundwater reservoir (GWR). Thus, for a GWR with a positive value specified for gwstor_min, the base-flow contribution to the stream network will have a minimum value. This change affects PRMS-only simulations. The default condition is that all GWRs can have 0 storage. This parameter might be useful for areas in a PRMS model where the source of storage in a GWR comes from a source other than gravity drainage from the associated HRU or cascading groundwater flow from upslope GWRs. Such areas might be in Karst terrain or with injection wells from another basin.

Watershed Flow-Summary Module (basin_sum)

Bug fix: For PRMS-only simulations with previous versions of the code, the basin summary table used a minimum and maximum temperature value that may not have been the best representative value for the average temperatures; the maximum and minimum temperatures printed in the table are now the basin, area-weighted average temperatures of the modeled area.

(c) MODFLOW Packages

In addition to the inclusion of the Newton Solver and Upstream-Weighting Packages for this release of GSFLOW, modifications also were made to the Streamflow-Routing, Lake, and Unsaturated-Zone Flow Packages. These modifications are described below. Also, the PCGN solver (Preconditioned Conjugate Gradient Solver with Improved Nonlinear Control Package) was added to GSFLOW; the PCGN solver is described in Naff and Banta (2008; see http://wwwbrr.cr.usgs.gov/projects/GW_stoch/pcgn/index.shtml)

Streamflow-Routing Package (gwf2sfr7_NWT.f and gwfsfrmodule.f)

Modifications were made to the SFR2 Package (Niswonger and Prudic, 2005) for use with MODFLOW-NWT. These changes include additional calculations of derivatives for seepage calculations. See Niswonger and others (2011) for further details. The SFR2 input instructions have been updated slightly for the MODFLOW-NWT functionality; see file "SFR2_for_GSFLOW_v1.1.5.pdf."

Modifications were made to correct the effects of lakes inundating stream cells. Seepage in inundated stream cells was not being set to zero in the budget routine. This change could affect mass-balance errors for models that include lakes that grow and inundate stream cells.

Modifications were made to correct a bug that occurred when the specific yield specified in the Block-Centered Flow (BCF7) Package was used for calculating the residual water content for the unsaturated zone beneath streams. Changes were made such that the code searches through model layers to find the corresponding layer that stores the specific yield for the case when the BCF7 input variable LAYCON is 2 or 3.

Modifications were made to add a smoothing function for the calculation of wetted channel area when the SFR2 input variable ICALC is set to 1 (constant stream width). In previous versions of the package, a discontinuity could form if the stream channel became dry during the outer iteration of a time step, because stream width would oscillate between the specified value and a value of zero. To avoid such conditions, a smoothing function was used to smooth the transition between the constant (specified) stream width and a zero stream width over the interval between zero depth and 1.0x10-5 (units defined on the basis of the DIS file input variable LENUNI). Smoothing is applied automatically if ICALC=1 and the stream depth is between zero and 1.0×10^{-5}; users should refer to the calculated stream depths to determine if smoothing was applied to a particular reach in a simulation. SFR2 smoothes the constant-to-zero-width transition using the same smoothing function that is used for the WEL Package to decrease specified pumping rates to zero when unconfined cells are dry (see Niswonger and others, 2011, p. 14).

Unsaturated-Zone Flow Package (gwf2uzf1_NWT.f and gwfuzfmodule.f)

Three new options were added to this package to allow specification of the residual water content (`THTR`), to provide the option of specifying initial water content (`THTI`) for simulations that begin with a steady-state recharge period, and to turn off calculation of surface leakage. These changes were made for the following reasons.

`THTR` originally was calculated internally by the UZF Package on the basis of the difference between the saturated water content (`THTS`) and the specific yield (`SY`) of the aquifer receiving recharge (Niswonger and others, 2006). However, the ability to specify `THTR` can be useful for some applications in which the maximum storage in the unsaturated zone (`THTS-THTR`) is different than the instantaneous drainage from the aquifer (`SY`). For these cases, specifying `THTR` based on external calculations provides greater flexibility for parameterizing the unsaturated zone. The option to specify `THTR` is activated using the key word ***SPECIFYTHTR***. This key word is input on line 1a of the revised UZF1 input file (see revised input instructions below). Values for `THTR` are input following variable `THTS` (see below).

Originally, `THTI` was not specified for simulations that included both a steady-state and one or more transient stress periods. For this case, `THTI` was calculated internally by the code on the basis of the steady-state infiltration rate and the unsaturated-zone hydraulic properties (`FINF`, `FKS`, `EPS`, `THTS`, and `THTR`). However, in well-drained soils, the steady-state recharge rate corresponds to an initial water content that is too large for coarse sediments. Consequently, drainage from the unsaturated zone during the first transient stress period could result in an unrealistically large recharge rate. Additionally, the head dependency on recharge that does not occur during steady-state stress periods but that can occur during transient stress periods can cause a sudden increase in recharge during the transition between these stress periods. For these circumstances, it is more realistic to specify the initial water content for the first transient stress period that follows a steady-state stress period. The option to specify `THTI` in simulations that include both steady-state and one or more transient stress periods is activated using the key word ***SPECIFYTHTI***. This key word is input on line 1a of the UZF1 input file, and follows the key word ***SPECIFYTHTR*** if ***SPECIFYTHTR*** is specified. Values for `THTI` are input following variable `THTR` (if it is input) or variable `THTS` (see below).

UZF1 simulates surface leakage from cells that are connected to the gravity reservoir of the PRMS soilzone if the groundwater head is greater than the altitude of the cell top that is connected to the soilzone. For MODFLOW-only simulations, surface leakage occurs in the uppermost active cell if groundwater head is greater than the top of this cell. Surface leakage is a nonlinear boundary condition that can slow model convergence, and in some cases it is beneficial to inactive this boundary condition. Surface leakage is inactivated by the key word ***NOSURFLEAK*** that is specified on line 1a of the UZF1 input file. This key word is specified following the key word ***SPECIFYTHTI*** (if ***SPECIFYTHTI*** is specified). If the key word ***NOSURFLEAK*** is specified, water will not be removed from the uppermost active cell when groundwater head rises above the top of this cell for either a GSFLOW or MODFLOW-only simulation.

In addition to these new input options, the default value for `SURFDEP` was changed. In prior versions of UZF1, if the value for `SURFDEP` was specified as 0, it was reset internally to 1.0. In this new version of UZF1, `SURFDEP` is reset to 1.0×10^{-6}. This change could affect simulated results if the value of `SURFDEP` was specified as 0 in the input file.

Finally, changes were made to the UZF1 Package for use with MODFLOW-NWT. These changes include additional calculations of derivatives for all head-dependent fluxes that are applied to groundwater cells in the UZF1 package, including the calculation of infiltration and surface leakage during shallow groundwater conditions, and head-dependent evapotranspiration from the water table. See Niswonger and others (2011) for further details. These changes will not affect model results, but they may speed the convergence rate or increase model stability.

Modified input instructions for the UZF1 input file for specifying optional key words:

0. Data: `{#Text}` (As in previous versions of the code)

The revised input structure for Item 1 is as follows:

1a. Data: {***SPECIFYTHTR***} {***SPECIFYTHTI***} {***NOSURFLEAK***}

SPECIFYTHTR	key word for specifying optional input variable THTR
SPECIFYTHTI	key word for specifying optional input variable THTI
NOSURFLEAK	key word for inactivating calculation of surface leakage

Note that the keywords must be entered in the order shown. For example, if keywords ***SPECIFYTHTR*** and ***NOSURFLEAK*** are specified, then ***SPECIFYTHTR*** must precede ***NOSURFLEAK***. Alternatively, if only ***SPECIFYTHTI*** is specified, then the other two keywords should not be specified.

1b. Data: `NUZTOP IUZFOPT IRUNFLG IETFLG IUZFCB1 IUZFCB2 NTRAIL2 NSETS2 NUZGAG SURFDEP NUZTOP` (As in previous versions of the code)

Items 2-5: As in previous versions of the code.

6a. Data: `THTS(NCOL,NROW)` –U2DREL

Refer to UZF1 documentation report (Niswonger and others, 2006) for definition of THTS.

6b. Data: `{THTR(NCOL,NROW)}` –U2DREL

`THTR` An array of positive real values used to define the residual water content for each vertical column of cells in units of volume of water to total volume (L^3L^{-3}). `THTR` is the irreducible water content and the unsaturated water content cannot drain to water contents less than `THTR`. This variable is not included unless the key word ***SPECIFYTHTR*** is specified.

7. Data: `{THTI(NCOL,NROW)}` –U2DREL

Refer to UZF1 documentation report (Niswonger and others, 2006) for definition of `THTI`. This variable is not included for simulations with a steady-state stress period unless the key word ***SPECIFYTHTI*** is specified.

Items 8-16: As in previous versions of the code.

Lake Package (gwf2lak7_NWT.f)

A major change was made to the Lake Package to add the option for the user to specify the lake bathymetry information directly through external text files. If the optional key word ***TABLEINPUT*** is specified on the first line of the Lake Package input file, then the program reads values of lake stage, volume, and area from external lake-bathymetry text files. The unit number of the external text file for each lake is read from the end of item 3, following the variable `STAGES` or the optional variables `SSMN` and `SSMX`, if they are specified. Additionally, the file type, unit number, and file name must be specified in the MODFLOW Name file if ***TABLEINPUT*** is specified. See revised input instructions below for more details. Each external lake-bathymetry input file must contain 151 lines, with values of lake stage and the corresponding lake volume and area in each line; 151 lines are required to ensure a smooth relationship between lake stage, volume, and area. Values are read as free format, either as space or comma delimited. See example input file excerpt below. Seepage between lakes and groundwater is calculated on a cell-by-cell basis using the area of cells inundated by the lake, and not the lake surface area specified with the external lake bathymetry file.

Modified input instructions for the Lake Package input file for specifying the optional key word ***TABLEINPUT*** follow:

0. Data: `{#Text}` (As in previous versions of the code)

1a. Data: {***TABLEINPUT***}

TABLEINPUT optional key word for specifying lake-bathymetry information using external files

1b. Data: `NLAKES ILKCB` (As in previous versions of the code)

Item 2: As in previous versions of the code.

3. Data: `STAGES {SSMN} {SSMX} {IUNITLAKTAB}`

This data set should consist of 1 line for each lake, where line 1 includes data for lake 1 and line `NLAKES` includes data for lake `NLAKES`. See Merritt and Konikow (2000) for more information about variables `STAGES`, `SSMN`, and `SSMX`. A lake-bathymetry file must be specified for each lake if the key word ***TABLEINPUT*** is specified in item 1a (that is, if ***TABLEINPUT*** is specified, then all lakes must have their bathymetry specified through external text files).

Items 4-9: As in previous versions of the code.

Example input file using ***TABLEINPUT*** option:

```
# Example input for specifying lake bathymetry information using external
# text files using key word option TABLEINPUT
TABLEINPUT                       Item 1a: KEY WORD
   1         0                   Item 1b: NLAKES,ILKCB
   0.00      50      0.001       Item 2:  THETA,NSSITER,SSCNCR
 110.0     100.0     170.0   22  Item 3:  STAGES,SSMN,SSMX,IUNITLAKTAB
```

The rest of the file is unchanged from the original version.

The lake-bathymetry input file has been assigned `IUNIT` 22 and `Fname` ‘lak1b_bath.txt’ in the Name File:

```
data     22  lak1b_bath.txt
```

File ‘lak1b_bath.txt’ must have exactly 151 lines of data, and each line contains the stage, volume, and surface area, respectively. Comment lines are not supported. The first five are:

```
      9.70000E+01   0.00000E+00   2.25000E+06
      9.96867E+01   6.04500E+06   2.25000E+06
      1.02373E+02   1.20900E+07   2.25000E+06
      1.05060E+02   1.81350E+07   2.25000E+06
      1.07747E+02   3.49267E+07   6.25000E+06
```

The lake stage, volume, and surface area are echoed to the MODFLOW-2005 LIST file.

An additional smaller change also was made to the Lake Package in which a format statement was modified to allow proper printout of the number of dry lake cells to the main Listing file. This change does not affect simulation results.

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