SUTRA Version 4.0.0 Release Notes

These release notes provide basic information about the release of SUTRA Version 4.0.0, which was developed from the previous public release, Version 3.0.0. These notes will be updated as new releases are issued.

Revision history

<u>Version 4.0.0</u>

Major new capabilities and changes relative to Version 3.0.0:

- Added the capability to simulate groundwater freezing and thawing simulations under saturated and unsaturated conditions.
- Added preprogrammed, user-selectable functions for total-water saturation as function of pressure, relative permeability as a function of liquid-water saturation, and liquid-water saturation as a function of temperature under saturated conditions. Previous versions of SUTRA offered only one function for the (total-water) saturation and one function for the relative permeability, and the function parameters could be changed only by reprogramming, and not through user input. The liquid-water saturation function was not offered previously because it is needed only for freezing simulations. SUTRA 4.0.0 offers several options for each of the three functions, and function parameters are set through user input. The code and input have been structured to facilitate addition of user-programmed functions, as well.
- Added a nonlinear density function (liquid-water density as a function of temperature) for energy-transport simulations as an alternative to the linear density function available in this and previous versions of SUTRA.
- Added geometric-mean and harmonic-mean bulk thermal conductivity functions as alternatives to the arithmetic-mean function available in this and previous versions of SUTRA.
- Many input parameters that previously were assigned a single value for the entire model can now vary spatially throughout the model. Input for such parameters is either nodewise (value for each node), elementwise (value for each element), or regionwise (value for each user-defined region of nodes and elements).
- Output has been enhanced to provide more detailed budget information and to report Darcy velocities.

Other changes and bug fixes:

- Added reporting of total water and solute/energy exchange between groundwater and lakes to the budget in the LST (main output) output file. This information was, and remains, also available in the LKBU (lakes budget) output file.

- Velocities at element centroids were previously based on the flow solution entering a time step and are now based on the final flow solution at the end of the time step. Centroid velocities are now more representative of the flow solution for a given time step, and the reported values may differ slightly from values reported by previous versions of SUTRA.
- Output values of saturations were based on the latest flow solution in the LST (main output) file and on the previous iteration in the NOD (nodewise output) and OBS/OBC (observation output) files. All output values of saturations are now based on the latest flow solution, and values reported in the NOD and OBS/OBC files may differ slightly from values reported by previous versions of SUTRA.
- The way the limiting time TIMEL influences the formulation of TIME CYCLE schedules was restored to the way it was prior to SUTRA Version 3.0.0. In Version 3.0.0, the final time in the cycle is less than TIMEL. In all other versions of SUTRA to date, including Version 4.0.0, the final time in the cycle can be equal to TIMEL.
- The van Genuchten total-water saturation and relative permeability functions, which have been available in all versions of SUTRA to date, now use exclusively double-precision calculations, which may have a slight effect on model results compared with results from previous versions of SUTRA.
- Various changes to input and output formats to accommodate the new capabilities.
- Added a missing declaration of variable KTYPE to some subroutines. No known effect of the bug other than possible compiler warnings/errors.
- Added a missing declaration of variable LAKUP to subroutine SLAKE. The bug could have affected updating of lake information during a simulation.
- Fixed bugs in do loops in subroutines LBCSOP and LBCSOU that could have affected calculations of exchanges between lakes and fluid source/sink and solute/energy source/sink boundary conditions and could have caused the code to crash in some cases.
- Fixed an erroneous subscript in subroutine BUDPBG that could have affected calculations of exchanges between lakes and generalized-flow boundary conditions acting analogously to fluid sources/sinks and could have caused the code to crash in some cases.
- Fixed the setting of lake-related flags in subroutine BUDGET. The bug could have affected output of lake-related budget information.
- Removed an extraneous line involving an undeclared variable, LAKELG, from subroutine BUDUBG. No known effect of the bug other than possible compiler warnings/errors.
- Fixed a bug in setting the maximum number of time steps, ITMAX, in subroutine INDAT0. The bug could have affected time stepping and could have caused the code to crash in some cases.

- Fixed erroneous subscripts in subroutine INDAT2 that could have affected initialization of time-dependent generalized-flow boundary conditions and could have caused the code to crash in some cases.
- Fixed a bug in the output of the temperature label to the OBC (observation output file) header for energy-transport simulations.
- Fixed a bug in the formatting of output of the lakes-related flag LPBGSP to the RST (restart) file, which could have affected restarting of simulations with lakes.
- Fixed a bug in subroutine SUTRA that could have affected scheduling of observation output and could have caused the code to crash in some cases.
- Addressed incomplete and incorrect explanatory comments in subroutine BCTIME.
- Fixed an erroneous subscript in subroutine BCG that could have affected proper application of generalized-flow boundary conditions.
- Fixed a bug that involved trying to read the numbers of time-dependent generalized boundary conditions when the input is in v2.2 format.
- Fixed erroneous wording in two SUTERR error messages.
- Fixed a bug that affected proper formulation of specified U boundary conditions in cases where matrix UMAT was not being recalculated, such as during steady flow and transient transport.
- Fixed a file close issue that showed up in code recompiled using gfortran on linux

<u>Version 3.0.0</u>

Major new capabilities and changes relative to Version 2.2:

- Support for "generalized" boundary conditions, a modified implementation of specified pressures and concentrations or temperatures, and lakes. Two new types of "generalized" boundary conditions facilitate simulation of a wide range of hydrologic processes that interact with the groundwater model, such as rivers, drains, and evapotranspiration.
- The way in which two of the original types of SUTRA boundary conditions—specified-pressure and specified-concentration or temperature—are formulated numerically within SUTRA has been modified such that user-specified, conductance-like factors (known as GNUP and GNUU in previous versions of SUTRA) are no longer required.
- A lake capability, which works with all types of SUTRA boundary conditions, including the new generalized boundary conditions, enables simulation of the interaction of groundwater flow and transport with lake water "ponded" on the surface of a three-dimensional model. Coalescence and splitting of lakes is tracked as lake stages increase or decrease, respectively.

Other changes and bug fixes:

- Fixed bugs that affected printing of observations to the OBS and OBC output files on the last time step.

- The second velocity angle (VANG2) was left unset in the case of a two-dimensional (2D) simulation, which could result in meaningless values. That angle is now explicitly set to zero in that case.
- Time-dependent boundary condition flag arrays BCSFL and BCSTR were uninitialized, which could cause anomalous solution cycling. They are now initialized to "FALSE".
- The BCS identifier array was uninitialized, which could result in meaningless values. It is now initialized to "" (blank).
- The BCS identifier counter NCID was being reset to zero on every call to subroutine BCSTEP, which could cause improper accounting of BCS identifiers. NCID is now set to zero only one the first call to BCSTEP.
- Fixed a bug in the file-opening routine FOPEN that could result in misidentification of error condition "FIL-4" when checking BCS filenames.
- Fixed a bug that caused observation output to occur before steady-state transport had been solved for.
- Fixed a bug that could cause SUTRA to incorrectly report in the LST output file that time-dependent solute sources/sinks will be set in subroutine BCTIME.
- To avoid the number of observations written per line, NOBLIN, from exceeding the total number of observations, NOBS, which could cause output problems, NOBLIN is now limited to a maximum possible value of NOBS.
- Local array ELAPSD was not being deallocated. It is now deallocated when no longer needed.
- For more appropriate evaluation of the solution error, particularly when specified-pressure of specified-concentration or temperature boundary conditions are used, scaled residuals and right-hand-sides (instead of unscaled residuals and right-hand sides) are now used in evaluating convergence of iterative solutions.
- Setting the maximum number of time step cycles allowed in a schedule, NSMAX in INP dataset 6, to a very large number could result in a very long delay at the start of the run. This issue was resolved by changing from linked-list-based to array-based storage of schedules internally within the code. Input parameters for schedules remain the same, but schedule "TIME_STEPS" must now be defined before any other schedules are defined, and time-step numbers and times must now be listed in ascending order within each 'STEP LIST' or 'TIME LIST' schedule.
- Refactoring of various sections of code to improve program structure and modularity.

Known issues

- Changes in the time/iteration levels of output values of centroid velocities and saturations, as well as the use of exclusively double-precision calculations in the unsaturated functions, in SUTRA Version 4.0.0 (see above) can result in slight changes in output values compared with previous versions of SUTRA.

- The way the limiting time TIMEL influences the execution of TIME CYCLE schedules was changed in SUTRA Version 3.0.0 relative to previous versions of SUTRA. In SUTRA Version 4.0.0, the behavior related to TIMEL was restored to the way it was prior to Version 3.0.0. Thus, the final time in TIME CYCLE schedules may be different in simulations run using Version 3.0.0. In Version 3.0.0, the final time in the cycle is less than TIMEL. In all other version of SUTRA, the final time in the cycle can be equal to TIMEL.
- Starting with SUTRA Version 3.0.0, specified-pressure and specified-concentration or temperature boundary conditions are now incorporated into the matrix equations for pressure and concentration or temperature using a different numerical paradigm that no longer depends on user-input values of GNUP and GNUU. Therefore, SUTRA Versions 3.0.0 and later will typically give slightly different numerical results than previous versions of SUTRA for problems that involve specified-pressure and specified-concentration or temperature boundary conditions. The differences should be minor if GNUP and GNUU were chosen appropriately and the numerical solutions were well converged in the original model runs. This is not a bug; it simply reflects an algorithmic change in the code.
- Because specified-pressure and specified-concentration or temperature boundary conditions are implemented using a new method starting with SUTRA Version 3.0.0, and because scaled residuals and right-hand-sides (instead of unscaled residuals and right-hand sides) are now used in evaluating convergence of iterative solutions, users will notice different convergence behavior when rerunning old SUTRA simulations using Versions 3.0.0 and later. Typically, if the convergence criteria for the iterative solvers (TOLP and TOLU in INP datasets 7B and 7C) are not changed, simulations rerun with Versions 3.0.0 and later will result in more iterations than with previous versions, but the accuracy of the solution – as measured by the budget errors – will be significantly better (much smaller budget errors) with Versions 3.0.0 and later. Test runs to date suggest that relaxing the convergence criteria (using larger values of TOLP and TOLU) to achieve budget errors comparable to those obtained with previous versions results in a roughly comparable number of solver iterations on average. In other words, convergence criteria used with previous versions of SUTRA are often more stringent than necessary for SUTRA Versions 3.0.0 and later if a comparable solution accuracy is desired.

Distribution file, installation, and compilation

The SUTRA Version 4.0.0 release is contained in two distribution files, which are available for download at https://doi.org/10.5066/P9OL5IYX. The first file, “SUTRA_4_0_0.zip”, contains executable code, documentation, and source code in the following directory structure, which parallels the directory structure of recent SUTRA releases:

```
SutraSuite/
     SUTRA_4_0/
          bin/
          documentation/
          source/
```

These release notes (“ReleaseNotes_SUTRA_4_0_0.pdf”) are contained in the SUTRA_4_0 subdirectory. The second file, “SUTRA_4_0_Examples.zip”, contains examples created to test and demonstrate the new features in SUTRA Version 4.0. The directory structure of the second file is

```
SutraSuite/
     SUTRA_4_0/
          Examples/
               2D/
                    FrozenWall/
               3D/
                    UnsatFreezeThaw/
```

To install SUTRA Version 4.0.0, simply unzip the distribution files. The “SutraSuite/” directory structure may already exist on your computer from previous installations of SUTRA. To install SUTRA Version 4.0.0 within the existing directory structure, unzip each of the distribution files to the directory that contains the top-level “SutraSuite/” directory (typically “C:/”).

The SUTRA executable code provided in the “bin/” subdirectory is compiled for 64-bit Windows® using the Intel® Visual Fortran Compiler 19.0.0052.12. SUTRA Version 4.0.0 can be recompiled using any compiler that supports standard Fortran 90 source code.

Documentation

The “documentation/” subdirectory contains the SUTRA documentation for Versions 2.2, 3.0.0, and 4.0.0:

Version 2.2:
Voss, C.I., and Provost, A.M., 2002 (Version of September 22, 2010), SUTRA, A model for saturated-unsaturated variable-density ground-water flow with solute or energy transport: U.S. Geological Survey Water-Resources Investigations Report 02–4231, 291 p., http://pubs.er.usgs.gov/publication/wri024231.

Version 3.0.0:
Provost, A.M., and Voss, C.I., 2019, SUTRA, a model for saturated-unsaturated, variable-density groundwater flow with solute or energy transport—Documentation of generalized boundary conditions, a modified implementation of specified pressures and concentrations or temperatures, and the lake capability: U.S. Geological Survey Techniques and Methods, book 6, chap. A52, 62 p., https://doi.org/10.3133/tm6A52.

Version 4.0.0:
Voss, C.I., Provost, A.M., McKenzie, J.M. and Kurylyk, B.L., 2024, SUTRA—A code for simulation of saturated-unsaturated, variable-density groundwater flow with solute or energy transport—Documentation of the version 4.0 enhancements—freeze-thaw capability, saturation and relative-permeability relations, spatially varying properties, and enhanced budget and velocity outputs: U.S. Geological Survey Techniques and Methods, book 6, chap. A63, 91 p., https://doi.org/10.3133/tm6A63.

The Appendix of the SUTRA Version 4.0.0 documentation describes modifications and additions to the input instructions introduced in Version 4.0.0. A complete, up-to-date description of all SUTRA input datasets is included in the “documentation/” subdirectory of this release (https://doi.org/10.5066/P9OL5IYX).

Execution

To perform a SUTRA simulation, first prepare the requisite input files according to the input instructions in the SUTRA documentation. Required input files include “SUTRA.FIL”, which points to the remaining input files. To run the simulation, run the SUTRA executable in the directory that contains “SUTRA.FIL.” The example problems included in the distribution each come with the requisite input files and a batch file, “RUNSUTRA.BAT”, that calls the SUTRA executable. To run SUTRA on an example problem, double-click on “RUNSUTRA.BAT” or open a command window, navigate to the example directory, and enter “RUNSUTRA.BAT” on the command line.

Example problems

Two example problems demonstrate the new features in SUTRA Version 4.0. Both examples are documented in detail in the SUTRA Version 4.0.0 documentation.

The first example, which is in the “FrozenWall/” subdirectory and is summarized in “FrozenWall-readme.pdf”, is a two-dimensional (2D), saturated problem that simulates creation of a low-permeability “wall” of frozen groundwater to shield a portion of an aquifer from regional groundwater flow to avoid the spread of contaminants to a larger area.

The second example, which is in the “UnsatFreezeThaw/” subdirectory and is summarized in “UnsatFreezeThaw-readme.pdf”, simulates freezing and thawing of water in a hypothetical laboratory experiment conducted on a column of partially saturated soil. Part A simulates freezing due to a temperature decrease imposed at the top of the column. Part B simulates subsequent thawing of frozen water due to inflow of warmer water at the bottom of the column.

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