

# Release Notes for SUTRA Version 2.1

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## Summary of release

These Release Notes describe a revision to the U.S. Geological Survey (USGS) **SUTRA** code (Voss, 1984; Voss & Provost, 2002, Version of June 21, 2003). This revision (*Version 2.1*) adds the ability to use irregular 3D meshes, conveniently incorporate input data from separate files, define schedules to control time stepping and observation output, interpolate observations in time and space, and output observations in an alternative format. Utility codes for pre- and post-processing in 2D and 3D are provided with this new version of **SUTRA**. These codes are briefly mentioned herein and are described in more detail in the respective Release Notes for each code. Together, all of these utility codes and **SUTRA** are called **SutraSuite**.

The new code includes changes in the input and output formats. The new input structure is not compatible with previous versions of **SUTRA**. However, **SUTRA Version 2.1** can read input files created for use with *Version 2.0 (2D3D.1)*.

At present, information on **SUTRA Version 2.1** includes these Release Notes and the revised **SUTRA** documentation (Voss and Provost, 2002, Version of June 2, 2008), which may be downloaded from a US Geological Survey web site (<http://water.usgs.gov/nrp/gwsoftware/sutra.html>).

The distribution package for **SUTRA Version 2.1** contains Fortran-90 source code and a Windows™ executable; this informational file; three example 2D simulations that are described in the documentation; and input and output files for three 3D simulation examples, one of which is described in the documentation. The examples also include setup files for the **SutraSuite** pre- and post-processors.

In this release, **SUTRA** is distributed as an executable code (compiled with Digital® Fortran Version 6.0.A) that runs under Microsoft Windows® XP, 2000, NT, or 95/98 operating systems.

## Software Release Notice

**SUTRA** and related utility codes are public-domain software and are released to you cost-free by USGS for any purposes you choose. This is a general public release.

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*USGS much appreciates your support in reporting any problems that may occur so that the codes can be improved.*

## Utility codes

**SUTRA** is included with a number of utility codes for both pre- and post-processing (see table below) in a package called **SutraSuite**. The utility codes are described in detail in separate Release Notes that accompany each code.

**SutraGUI** (Winston and Voss, 2003, a revision of Voss and others, 1997) is a pre-processor that is applicable to both 2D and 3D problems. **SutraPrep** (Provost, 2002) is a text-based preprocessor that creates 3D input datasets for **SUTRA Version 2.0 (2D3D.1)**, which can also be read by **SUTRA Version 2.1**.

There are three post-processors for 2D problems: **SutraPlot** (Souza, 1999); **ModelViewer** (Hsieh and Winston, 2002); and **SutraGUI**. There are two post-processors for 3D problems: **SutraPlot** creates rotatable 3D plots of the mesh, 2D contours of results, and plots of velocity vectors; **ModelViewer** creates rotatable 3D color visualizations of results and plots of velocity vectors.

**NOTE:** A version of **SutraPlot** that is compatible with **SUTRA** Version 2.1 is currently under development. Please check the web site

<http://water.usgs.gov/nrp/gwsoftware/sutraplot/sutraplot.html> for updates.

Two additional post-processing tools for both 2D and 3D simulations are available. **GW\_Chart** can graphically display **SUTRA** fluid, solute and energy budgets, as well as hydrographs for **SUTRA** observation node output, showing pressure, concentration, and temperature as a function of time (Winston, 2000). The utility **CheckMatchBC** aids in setting boundary condition conductances for a **SUTRA** simulation; it checks the match of specified and simulated pressures, concentrations and temperatures and reports the number of matching digits. **GW\_Chart** and **CheckMatchBC** are distributed with the installation files for **SutraGUI**.

Examples in 2D and/or 3D for pre-processing and post-processing accompany the utility codes.

All of these codes are available free of charge; however, use of **SutraGUI** requires purchase of a commercial product, ArgusONE™ (<http://www.argusint.com>).

# SutraSuite utilities

Utility code	Pre-processor	Post-processor	Description
<b>SutraPrep</b>	<i>3D</i>		Generates 3D, regular <b>SUTRA</b> meshes and creates input data files for <b>SUTRA Version 2.0 [2D3D.1]</b> , which can be read by <b>SUTRA Version 2.1</b> . <i>Instructions for using <b>SutraPrep</b> can be found in the documentation that accompanies the code.</i>
<b>SutraGUI</b>	<i>2D and 3D</i>	<i>2D</i>	Graphical environment for setting up and executing 2D and 3D <b>SUTRA</b> runs, and for visualizing results from 2D <b>SUTRA</b> runs. <i>Instructions for using <b>SutraGUI</b> can be found in the documentation that accompanies the code.</i>
<b>SutraPlot</b>		<i>2D and 3D</i>	Creates 2D and rotatable 3D plots from 2D and 3D <b>SUTRA</b> output data. <i>Instructions for using <b>SutraPlot</b> can be found in the documentation that accompanies the code.</i>  <b>NOTE:</b> A version of <b>SutraPlot</b> that is compatible with <b>SUTRA Version 2.1</b> is currently under development. Please check the web site <a href="http://water.usgs.gov/nrp/gwsoftware/sutraplot/sutraplot.html">http://water.usgs.gov/nrp/gwsoftware/sutraplot/sutraplot.html</a> for updates.
<b>Model Viewer</b>		<i>2D (fishnet meshes only) and 3D</i>	Creates rotatable 3D color visualizations and animations from 2D and 3D <b>SUTRA</b> output data. <i>Instructions for using <b>Model Viewer</b> can be displayed by accessing the Help menu.</i>
<b>GW_Chart</b>		<i>2D and 3D</i>	Graphical display of fluid, solute and energy budgets and observation node output, showing pressure, concentration, and temperature as a function of time (hydrographs). <i>Instructions for using <b>GW_Chart</b> can be displayed by accessing the Help menu.</i>
<b>CheckMatchBC</b>		<i>2D and 3D</i>	Checks match of specified and simulated pressures, concentrations and temperatures and reports number of matching digits. This aids in setting boundary condition conductances.

## General Instructions

Except where stated otherwise, the following instructions assume that **SUTRA** has been installed into the default directory recommended during the installation process, c:\SutraSuite\SUTRA\_2\_1. If a directory other than the default directory was selected, \SutraSuite will not be located directly under c:\, but the directory structure below \SutraSuite will remain as described below.

Instructions that involve mouse clicks refer to clicking on file names or icons displayed under the Windows Explorer file manager. For example, to "double-click on *file.txt*", use Windows Explorer to display the contents of the directory (folder) that contains the file *file.txt*, then click twice (in rapid succession) on the file name *file.txt* or its corresponding icon using the left mouse button. To "right-click", click once using the right mouse button.

## Installation

After the **SUTRA** code (*Version 2.1*) is unzipped, most of the associated files will be in a new directory, c:\SutraSuite\SUTRA\_2\_1. This directory contains four subdirectories: \source, which contains the Fortran source files; \examples, which contains example datasets; \documentation, which contains this *ReleaseNotes.doc* file; and \bin, which contains the **SUTRA** executable file, *sutra\_2\_1.exe*, and a shortcut to this executable file. Please note that the \examples subdirectory will be empty until the large zipped example files are separately downloaded and installed.

In c:\SutraSuite\SUTRA\_2\_1, there is a file called *RunSUTRA.bat*, which is used to run the SUTRA code. *RunSUTRA.bat* contains the line

```
c:\SutraSuite\SUTRA_2_1\bin\sutra_2_1.exe
```

which provides the path for the **SUTRA** executable file, *sutra\_2\_1.exe*. If **SUTRA** was installed into a directory other than the default directory, please make certain that this line contains the correct pathname to where *SUTRA\_2\_1.exe* is located. Use a text editor to change the line if necessary.

## Running SUTRA

To run **SUTRA** manually, create the file SUTRA filename assignments file, *SUTRA.FIL*, in the desired working directory. There are two ways to run **SUTRA**. 1- Double-click on the *RunSUTRA.bat* in the same directory. 2- Create a *Windows shortcut* to the *sutra\_2\_1.exe* file in the directory in which you will work, and then double click the shortcut to run **SUTRA**. For both methods, a window will appear indicating that the **SUTRA** code is running.

**SUTRA** may also be run directly from the **SutraGUI** preprocessing utility and directions for doing this may be found in the **SutraGUI** documentation (Winston and Voss, 2003) and in some example simulations, including step-by-step instructions (see Rocky and Henry examples) provided in the directory \SUTRA\_2\_1\examples.

## New in SUTRA Version 2.1

A brief description of the main changes in *Version 2.1* follows:

### ***IRREGULAR 3D MESHES***

\* In the previous version of **SUTRA** (*Version 2.0 [2D3D.1]*), meshes for 3D simulations were restricted to being logically rectangular (REGULAR or BLOCKWISE). In *Version 2.1*, this restriction has been removed; 3D meshes can have irregular structure.

\* A new type of mesh structure has been added to dataset 2B of the main (INP) input file: LAYERED. A LAYERED mesh is a 3D mesh that can be thought of as being formed from a vertical stack of 2D meshes. Each 2D mesh in the stack has the same connectivity, though that 2D connectivity can be irregular.

\* The designation of mesh type (REGULAR, BLOCKWISE, LAYERED, or IRREGULAR) has no effect on the calculations performed by **SUTRA** *Version 2.1* to solve the flow and transport equations. **SUTRA** writes mesh-type information to the headers of output files, where it can be read by post-processing software.

### ***FILE INSERTION***

\* **SUTRA** input files can be quite large, particularly for 3D simulations. To facilitate management of SUTRA input datasets, *Version 2.1* offers the ability to “insert” input data from separate files into the main (INP) and initial conditions (ICS) input files. Thus, SUTRA input data can be distributed conveniently among various files, and the INP and ICS files can consist (partially or wholly) of “insert” statements that tell **SUTRA** which file contains the next line(s) of input data.

### ***SCHEDULES***

\* **SUTRA** *Version 2.1* offers users significantly more flexibility in specifying time stepping and the timing of observation output. Both are now controlled using user-defined “schedules,” which are sequences of simulation times or time steps.

\* A special schedule named “TIME\_STEPS” gives users complete control over the times at which the simulation time steps end.

\* Schedules can be used to produce observation output at any time during the simulated period, not only at the ends of time steps. For output times that fall within a time step, SUTRA interpolates results between the beginning and end of the time step.

### ***OBSERVATIONS***

\* Observations can be output at any time during the simulated period. (See “SCHEDULES” above.)

\* Observations can be made at any point in the model domain, not only at nodes. **SUTRA** interpolates nodewise results in space using the finite-element basis functions.

\* Observation results can be written in either the traditional OBS format, or in a new OBC format. Both formats present the same information, but they are organized differently. In an OBS output file, all results computed at a given time are listed across the page on one line, unless a line wrapping option is invoked to avoid generating extremely long lines of output. The organization of an OBC output file is analogous to that of an NOD or ELE output file: results computed at a given time are preceded by a header and are listed one observation point per line.

## Documentation

These Release Notes and the **SUTRA** manual (Voss and Provost, 2002, Version of June 2, 2008) are the primary documentation of the code. The **SUTRA** manual is available, free of charge, in electronic (*pdf*) format from the USGS website <http://water.usgs.gov/nrp/gwsoftware/sutra.html>.

## 2D examples provided

Three example 2D simulations are provided in sub-directories of the directory SutraSuite\SUTRA\_2\_1\examples. All input and output files for each problem are included there. (The examples may be run manually [see 'RUNNING SUTRA', above] or may be recreated using the pre-processor described in the *ReadMe* file that accompanies each example and run through the pre-processor.) It is recommended that the utility and input files be copied to a new working directory for testing runs, so that the user's new **SUTRA** output does not overwrite the existing output files that were downloaded. The 2D examples include the Rocky Mountain Arsenal contaminant plume problem (\Rocky), and the Henry seawater intrusion problem (\Henry). The input files were created with the utility **SutraGUI**. Information on the setup of the 2D examples may be found in the **SUTRA** documentation (Voss and Provost, 2002, Version of June 2, 2008) and in the respective *ReadMe* files that accompany each example. Users are also encouraged to download, install, and try using **Model Viewer** to view results of these runs. Creation of the input files and post-processing using **SutraGUI** is described in the **SutraGUI** Release Notes. Also provided is the Island2D example, in which the mesh has been modified since the previous release to facilitate comparison with the updated 3D version described just below.

## 3D examples provided

Three example 3D simulations are provided in sub-directories of the directory, SutraSuite\Sutra\_2\_1\examples. These may be found in sub-directories \Bf, \Pond, and \Island3D. All input and output files for each problem are included there. (The examples may be run manually [see 'RUNNING SUTRA', above] or may be recreated using the pre-processor described in the *ReadMe* file that accompanies each example and run through the pre-processor). The island problem is described in the SUTRA documentation (Voss and Provost, 2002, Version of June 2, 2008), and the other two problems are described in the *ReadMe* file that accompanies each example. The Island3D problem has been modified since the previous release to feature an irregular 3D mesh. It is recommended that the utility and input files be copied to a new working directory for testing runs so that the user's new **SUTRA** output does not overwrite the existing output files that were downloaded. Users are encouraged to download, install, and try using **Model Viewer** to view results of these runs. (This tool also comes with examples.)

## References

- Burnett, R.D., and Frind, E.O., 1987, Simulation of contaminant transport in three dimensions 2. dimensionality effects, *Water Resources Research*, 23(4), 695-705.
- Hsieh, P.A., and Winston, R.B., 2002, User's guide to **Model Viewer**, a program for three-dimensional visualization of ground-water model results: U.S. Geological Survey Open-File Report 02-106, 18 p. <http://water.usgs.gov/nrp/gwsoftware/modelviewer/ModelViewer.html>
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- Souza, W.R., 1999, **SutraPlot**, a graphical post-processor for SUTRA, a model for ground-water flow with solute or energy transport: U.S. Geological Survey Open-File Report 99-220, 30 p. <http://water.usgs.gov/nrp/gwsoftware/sutra.html>
- Voss, C. I., 1984, **SUTRA**, A finite-element simulation model for saturated-unsaturated fluid density-dependent ground-water flow with energy transport or chemically-reactive single-species solute transport, U.S. Geological Survey Water-Resources Investigations Report 84-4369, 409 p.
- Voss, C. I., and Provost, A.M., 2002 (Version of June 21, 2003), **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, 250 p.
- Voss, C. I., and Provost, A.M., 2002 (Version of June 2, 2008), **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, 270 p. <http://water.usgs.gov/nrp/gwsoftware/sutra.html>
- Voss, Clifford I., Boldt, David, and Shapiro, Allen, 1997, **SUTRA-GUI**, A graphical-user interface for the U.S. Geological Survey's SUTRA code using ArgusONE, U.S. Geological Survey Open-File Report 97-421, 106p.
- Winston, R.B., 2000, Graphical User Interface for MODFLOW, Version 4: U.S. Geological Survey Open-File Report 00-315, 27 p. <http://water.usgs.gov/nrp/gwsoftware/modflow.html>
- Winston, R.B. and Voss, C.I., 2003, **SutraGUI**, a graphical-user interface for SUTRA, a model for ground-water flow with solute or energy transport: U.S. Geological Survey Open-File Report 03-285, 114 p. <http://water.usgs.gov/nrp/gwsoftware/sutra.html>

## File types for SUTRA *Version 2.1* and associated codes

Code	<i>File types for current SUTRA version (2.1) and Version 2.0 (2D3D.1)</i>	<i>Content</i>
<b>SUTRA</b> <i>input</i>	SUTRA.FIL .inp .ics	file assignments main input initial conditions
<i>output</i>	.smy (defaults to SUTRA.SMY) .lst .rst .nod .ele .obs .obc ( <i>Version 2.1 only</i> )	simulation summary or file assignment errors main results listing restart file nodewise results elementwise results observation results observation results
<b>SutraPrep*</b> <i>input</i>	.prp .inp .prl	main input existing SUTRA .inp file SutraPrep log
<i>output</i>	.inp .ics .wrl	3D blocks or mesh in VRML
<b>SutraGUI</b> <i>input</i>	.nod .ele	
<i>output</i>	.inp .ics	
<b>SutraPlot**</b> <i>input</i>	.inp .nod .ele	
<i>output</i>	.gr2 .gr3 .spl	2D grid of results 3D grid of results plot layout
<b>Model Viewer</b> <i>input</i>	.inp .nod .ele	
<i>output</i>	.mvb .wrl .bmp	Binary version of .nod & .ele 3D view of image bitmap of image
<b>GW_Chart</b> <i>input</i>	.obs .lst	For hydrographs For budget charts
<i>output</i>	.wmf	Saved image
<b>CheckMatchBC</b> <i>input</i>	.inp .nod	
<i>output</i>		

(Uppercase names are not user selectable.)

\***SutraPrep** creates input for **SUTRA** *Version 2.0 (2D3D.1)*, which can be read by **SUTRA** *Version 2.1*.

\*\*A version of **SutraPlot** that is compatible with **SUTRA** *Version 2.1* is currently under development. Please check the web site <http://water.usgs.gov/nrp/gwsoftware/sutraplot/sutraplot.html> for updates.