

Advances in Modeling Groundwater Flow and Transport with MODFLOW

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EPA CLU-IN Webinar, February 3, 2021



BACKGROUND







MODFLOW Philosophy





MODFLOW Support Environment













WHAT'S NEW?

Active Development

MODFLOW 6

- Groundwater Flow (GWF) Model (released Aug 2017)
- Compaction and Subsidence (CSUB) Package (released Dec 2019)
- Groundwater Transport (GWT) Model (released Oct 2020)
- Coupled Variable-Density Flow and Transport (released Oct 2020)
- MODFLOW API (released Jun 2020)
- Related Programs
 - FloPy
 - MODPATH
 - MT3D-USGS





Regular or Unstructured Grids

3 Discretization Approaches Regular MODFLOW grid (DIS)

- Discretization by Vertices (DISV)
- Generalized Unstructured (DISU)



Pahute Mesa - Oasis Valley Example

- Nevada National Security Site
- Navarro Research and Engineering Inc. funded by DOE
- Develop a groundwater flow model for scenario testing





Hydrostratigraphic Framework Model

- 77 hydrostratigraphic units
- 98 faults and structural features
- Convert Earthvision hydrostratigraphic model into a MODFLOW 6 GWF model





MODFLOW 6 Model

 Python and the FloPy Package used to convert Earthvision hydrostratigraphic model into MODFLOW 6 model





Multi-Model Coupling

- Any number of models can be included in a simulation
- Models coupled at matrix level
- Flexibility supports coupling of parent, child, grandchild models, stacked models or adjacent models





Nested Grids





Water Mover

- Generalized package for transferring water from one MODFLOW package to another
- Water can be transferred from a "provider" to a "receiver" subject to simplified rules
- All transfers are tracked in a water budget



MODFLOW 6 GWF + MT3D-USGS

- MT3D-USGS developed and maintained in cooperation with S.S. Papadopulos & Associates Inc.
- Works with standard head and budget files produced by MODFLOW 6
- Regular MODFLOW grids





MODFLOW 6 Groundwater Transport Model

- First released October 2020
- New model type in MODFLOW 6
- Developed in collaboration with Sorab Panday, GSI Environmental Inc.



Patterned after MT3D, USG-Transport, MODFLOW-GWT, SUTRA

$$\frac{\partial \left(S_w \theta C\right)}{\partial t} = -\nabla \cdot \left(qC\right) + \nabla \cdot \left(S_w \theta D \nabla C\right) + q'_s C_s + M_s - \lambda_1 \theta S_w C - \gamma_1 \theta S_w$$
$$-f_m \rho_b \frac{\partial \left(S_w \overline{C}\right)}{\partial t} - \lambda_2 f_m \rho_b S_w \overline{C} - \gamma_2 f_m \rho_b S_w - \sum_{im=1}^{nim} \zeta_{im} S_w \left(C - C_{im}\right)$$





























Support for advanced flow packages

Immobile

Domain

- Simulate concentration in individual features (stream reaches, lakes, wells, unsaturated zone)
- Simulate mass transfer between flow packages
- Alternative to SSM
















MODFLOW 6 GWF and GWT Approach (Option 1: Separate Simulations)





Can use different time-step lengths for GWT Model

MODFLOW 6 GWF and GWT Approach (Option 2: Coupled Simulation)





Must use same time-step lengths for both models

Groundwater Transport Model Status

- Available now in MODFLOW 6
- Fully supported in FloPy
- Theory report is in review
- Limitations:
 - Represents a single species, BUT, can have any number of GWT Models
 - No transport across grids (yet)





In review





Newton Formulation for Water Table Aquifers

Minimizes wetting and drying complications





Transport Solution for Perched Aquifers

Instantaneous solute routing through the unsaturated zone





Advanced Packages and Water Mover







Surface and Groundwater Flow and Transport





Comparison between MODFLOW 6 (solid lines) and GWT (dashed lines)



Coupled Variable-Density Flow and Transport

- Run GWF and GWT in same simulation
- Turn on Buoyancy Package in GWF Model
- Represent salt as a chemical species









Coupled Flow and Transport Capabilities





Does MODFLOW 6 work with PEST?



Does MODFLOW 6 work with PEST?

Of course!



Optimal Plume Management

- Example from Jeremy White, INTERA Inc.
- Simple synthetic problem
- 50 m cells
- 10 km x 5 km x 1 layer
- 20 years of treatment







Optimal Plume Management

 Standard 5-spot injector/extractor configuration



Extractor



Optimal Plume Management

Extractor

- 20 years of treatment
- Configuration works, but could it be better?





pestpp-mou (beta)

- **Constrained multi-objective** optimization under uncertainty within the PEST interface
 - Template files, instruction files, control files
- Treat "risk" (probability of success) as an objective
- Uses first-order second-moment or "stack"-based "chances"
 - Plays nicely with other PEST and PEST++ tools
- Fault-tolerant, model-independent, parallel run management

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PEST++, a Software Suite for Parameter Estimation, Uncertainty Analysis, Management Optimization and Sensitivity Analysis

Release Date: AUGUST 13, 2020

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PEST++ provides environmental modeling practitioners access to tools to support decision making with environmental models, including tools for global sensitivity analysis (PESTPP-SEN); least-squares parameter estimation with integrated first-order, second-moment parameter and forecast uncertainty estimation (PESTPP-GLM); an iterative, localized ensemble smoother (PESTPP-IES); and a tool for management optimization under uncertainty (PESTPP-OPT). Additionally, all PEST++ tools have a built-in fault-tolerant, multithreaded parallel run manager and are model independent, using the same protocol as the widely used PEST software suite.

domain.)

phi progres

The PEST++ software suite is object-oriented universal computer code written in C++ that expands on and extends the algorithms included in PEST, a widely used narameter estimation onde written in Fortran. PEST++ is designed to lower the barriers of entry for users and developers while providing efficient algorithms that can accommodate large highly parameterized problems. This effort has focused on: (1) implementing and extending the most popular features of PEST in a way that is easy for novice or experienced modelers to use: and (2) creating a software design that is easy to extend with future advances.

Information and Downloads

Documentation for the code may be viewed here:

White, J.T., Hunt, R.J., Fienen, M.N., and Doherty, J.E., 2020, Approaches to Highly Parameterized Inversion: PEST++ Version 5, a Software Suite for Parameter Estimation, Uncertainty Analysis, Management Optimization and Sensitivity Analysis: U.S. Geological Survey Techniques and Methods 7C26, 51 p., https://doi.org/10.3133/tm7C26.

Supported Computing Platforms and Source **Code Compilation**

The PEST++ Version 5 software suite can be compiled for Microsoft Windows®1 and Unix-based operating systems such as Apple[®] and Linux⁸⁰; the source code is available with a Microsoft Visual Studio⁸⁴ 2019 solution; and CMake support for all three operating system is also provided

Compiled PEST++ Executables



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Explore More Science

PEST Uncertainty analysis Model calibration Data, Tools, and Technology Water



≈USGS

initial parameter values

Wy all stores

The left axis is a visualization of an ensemble of

solutions (crosses and dashed lines) iteratively moving

down gradient on an objective function surface (color

flood) in 2-D parameters space, with the associated

prior (grav) and posterior (blue) parameter marginal

(Credit: USGS, Texas Water Science Center, Public

distributions shown on the two right stacked axes.



Mapping Tradeoff Between Objectives

- Decision Variables
 - Injector location
 - Extractor location
 - Extraction rate
 - Injector apportioning
- Objectives
 - Mass treated
 - Total cost (drilling + operation)
 - Final maximum concentration

Constraints

- Concentration at compliance point < 5-spot
- Mass flux to downstream boundary < 5-spot







MODFLOW API

MODFLOW API

API = Application Programming Interface



API for MODFLOW 6

- Developed in collaboration with Martijn Russcher, Deltares
- Full control of MODFLOW while it's running
- Access to MODFLOW internal variables (as a copy or pointer)
- Three different levels of control
 - Between time steps
 - Within a time step
 - Within an iteration
- Well-defined interfaces based on Basic Model Interface (BMI) standard
- Uses identical code base as executable version





MODFLOW API – Between Time Steps





MODFLOW API – Between Time Steps





MODFLOW API – Between Time Steps



```
mf6 = XmiWrapper('libmf6.dll')
mf6.initialize('mfsim.nam')
current_time = 0.
end_time = mf6.get_end_time()
```

```
while current_time < end_time:
    mf6.update()
    current_time = mf6.get_current_time()
```

mf6.finalize()



MODFLOW API – Within a Time Step





MODFLOW API – Within a Time Step





MODFLOW API – Within a Time Step



```
mf6 = XmiWrapper('libmf6.dll')
mf6.initialize('mfsim.nam')
current_time = 0.
end_time = mf6.get_end_time()
```

while current_time < end_time:</pre>

dt = mf6.get_time_step()
mf6.prepare_time_step(dt)
mf6.do_time_step()
mf6.finalize_time_step()

current time = mf6.get current time()

update

mf6.finalize()



MODFLOW API – Within an Iteration





MODFLOW API – Within an Iteration





MODFLOW API – Within an Iteration



```
mf6.initialize('mfsim.nam')
current time = 0.
end time = mf6.get end time()
while current time < end time:
  dt = mf6.get time step()
  mf6.prepare_time_step(dt)
```

```
kiter = 0
mf6.prepare solve(1)
while kiter < max iter:</pre>
  has converged = mf6.solve(1)
  if has converged:
    break
mf6.finalize solve(1)
```

do time step

mf6.finalize_time_step() current time = mf6.get current time()

```
mf6.finalize()
```

Why We're Excited about the API!

- Tight integration with other models
- Callable from other languages, such as Python; access to 3rd party tools
- Sensitivity analysis, adjoint state, parameter estimation, optimization, uncertainty analysis
- Alternative solvers (PETSc, …)
- Alternative data input (netCDF, database access, online services, ...)
- MODFLOW can be customized by our users





ONLINE RESOURCES



MODFLOW Distribution

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Water Resources

MODFLOW and Related Programs

Overview Publications Software

MODFLOW is the USGS's modular hydrologic model. MODFLOW is considered an international standard for simulating and predicting groundwater conditions and groundwater/surface-water interactions. MODFLOW 6 is presently the core MODFLOW version distributed by the USGS. The previous core version, MODFLOW-2005, is actively maintained and supported as well.

Originally developed and released solely as a groundwater-flow simulation code when first published in 1984, MOCPLOWS modular structure has provided a robust framework for integration of additional simulation capabilities that build on and enhance its original scope. The family of MOCPLOW-related programs now includes capabilities to simulate coupled groundwater/surface-water systems, solute transport, variable-density flow (including saltwater, auglier-system compaction and land subsidence, parameter estimation, and groundwater management.

MODFLOW Development Plans, July 20, 2020

The USGS Water Mission Area actively develops and supports the MODFLOW suite of programs. Ongoing efforts include providing maintenance and support for existing versions of MODFLOW such as

MODFLOW 6, MODFLOW-2005, MODFLOW-NWT, MODFLOW-USG, MODPATH, MT3D-USGS, and related and supporting programs such as FIOPy and PEST++. Current development efforts are focused on adding new capabilities to MODFLOW 6. These development efforts include:

Core Versions

- MODFLOW 6: current core version
- MODFLOW-2005: previous core version

MODFLOW Variants: Newer, specialized, or advanced versions of MODFLOW for use by experienced modelers

- MODFLOW-NWT: MODFLOW-NWT uses a Newton-Raphson formulation to improve solution of unconfined groundwater-flow problems.
- MODFLOW-USG: MODFLOW-USG uses an unstructured-grid approach to simulate groundwater flow and tightly coupled processes using a control volume finite-difference formulation.
- GSFLOW: GSFLOW is a coupled groundwater and surface-water flow model based on the USGS Precipitation-Runoff Modeling System (PRMS), MODFLOW-2005, and MODFLOW-NWT.
- GWM: The Groundwater Management (GWM) Process for MODFLOW-2000 and MODFLOW-2005 is used to simulate groundwater management



Status - Active

-



MODFLOW 6: USGS Modular Hydrologic Model

SCIENCE

Topics center

Release Date: OCTOBER 22, 2020

For over 30 years, the MODFLOW program has been widely used by academics, private consultants, and government scientists to accurately, reliably, and efficiently simulate groundwater flow, with time, growing interest in surface and groundwater interactions, local refinement with nested and unstructured grids, karst groundwater flow, solute transport, and saltwater intrusion, has led to the development of numerous MODFLOW versions. Although these MODFLOW versions are often based on the core MODFLOW version (previously MODFLOW: 2005), there are often incompatibilities that restrict their use with other MODFLOW versions. In many cases, development of these alternative MODFLOW versions has been challenging due to the underlying program structure, which was designed for the simulation of a single groundwater flow model using a regular MODFLOW did consisting of layers, rows, and columns.

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Overview of MODFLOW 6

MODFLOW 6 is an object-oriented program and framework developed to provide a platform for supporting multiple models and multiple types of models within the same simulation. This version of MODFLOW is labeled with a "6" because it is the sixth core version of MODFLOW to be released by the USGS (previous core versions were released in 1984, 1988, 1996, 2000, and 2005). In the new design, any number of models can be included in a simulation. These models can be independent of one another with no interaction, they can exchange information with one another, or they can be tightly coupled at the matrix level by adding them to the same numerical solution. Transfer of information between models is isolated to exchange objects, which allow models to be developed and used independently of one another. Within this new framework, a regional-scale groundwater model may be coupled with multiple local-scale groundwater models. Or, a surface-water flow model could be coupled to multiple groundwater flow models. The framework naturally allows for future extensions to include the simulation of solute transport.

Groundwater Flow (GWF) and Groundwater Transport (GWT) Models

MODFLOW 6 presently contains two types of hydrologic models, the Groundwater Flow (GWF) Model and the Groundwater Transport (GWT) Model. The GWF Model for MODFLOW 6 is based on a generalized control-

Contacts

USGS MODFLOW Team Email: modflow@usgs.gov

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This figure shows a triangular grid in which the size of the triangular cells is reduced in areas with relatively large hydraulic gradients, such as around the shoreline of a lake, near pumping wells, and along a stream. This type of layered grid can be represented using the Discretization by Vertices (DISV) Package in MODFLOW 6.

Additional Online Resources

Main Repository

MODFLOW 6: USGS Modular Hydrologic Model

This is the development repository for the USOS MODFLOW 6 Hydrologic Model. The official USOS distribution is available at USOS Release Page.

Version 6.2.1 release candidate

C HODFLOW 6 CI with latest plutture present

() HODELOW & HIGHLY SUM

Branches

This repository contains branches of ongoing MODFLOW 6 development. The two main branches in this repository are:

- · master -- the state of the MODFLOW 6 repository corresponding to the last official USGS release
- develop -- the current development version of the MODFLOW 6 program

The sevelop branch is under active and frequent updates by the MODFLOW development team and other interested contributors. We follow a fork and pull request workflow and require that pull requests pass our test suite before they are considered a possible candidate for emerge into develop.

This repository may contain other branches with various levels of development code; however, these branches may be merged into develop or deleted without notice.



E sauth linder

Introduction

Fiely includes support for MODFLOW 6, MODFLOW-2005, MODFLOW-WWT, MODFLOW-USG, and MODFLOW-2000. Other supported MODFLOW-based models include MODPATH (version 6 and 7), MT3DMS, MT3D-USGS, and SEXWAT.

For general modeling issues, please consult a modeling forum, such as the MODFLOW Users Group. Other MODFLOW resources are listed in the MODFLOW Resources section.

Pymake

pymake

Python package for compiling MODFLOW-based programs.

Version 1.2

🔿 pymake continuous integration 📷 👘 codecov 👀 🗘 code quality 👗 docs 🌆 🖬

This is a python package for compiling MODFLOW-based and other Fortran, C, and C++ programs. The package determines the build order using a directed acyclic graph and then compiles the source files using GNU compilers (acc. g++, gfortran) or Intel compilers (ifort, icc.).

pymake can be run from the command line or it can be called from within python. By default, pymake sets the optimization tevel, Fortran flags, C/C++ flags, and linker flags that are consistent with those used to compile MODFL/W-based programs released by the USSS.

pymake includes example scripts for building MODFLOW 4, MODFLOW-2005, MODFLOW-WT, MODFLOW-USA MODFLOW-LOR, MODFLOW-2000, MODPATH 6, MODPATH 7, OSFLOW, VS20T, MT3DMS, MT3D-USGS, ESAWAT, and SOTRA. Example scripts for creating the utility programs CRT, Triangle, and CRIDGEN are also included. The scripts download the distribution file from the USDS (and other organizations) and compile the source into a binary exercutable.

Nightly Build

MODFLOW 6 development version of binary executables

The develop branch of the MODFLOW 6 repository contains bug files and new functionality that may be incorporated into the next approved MODFLOW 5 reliases. Each night, at 2 AM UTC, Fortran source code from the development branch is compiled for Windows, MacOS, and Uburtu 18.04.4 ITC using glottan. The binary executables released here represent release candidates for the next approved version of MODFLOW 6 but are considered perlimitary or provisioni.

The compiled codes for the latest nightly build are available as operating specific release assets (vin64.zip , mac.zip , and linux.zip). Each operating specific release asset includes:

- 1. mf6 (MODFLOW 6)
- 2. mf5to6 (the MODFLOW 5 to 6 converter)
- 3. zbud6 (the zone budget utility for MODFLOW 6)
- 4. libmf6.dll or libmf6.so (a dynamic-linked library or shared object version of MODFLOW 6)

Each release also includes a copy of the 'MODFLOW 6 - Description of input and Output' document (nf610.pdf) for the latest MODFLOW 6 release candidate.

Release tags are based on the date (YYYYMMDD) the MODFLOW 6 codes were compiled and the release was made. Previous nightly build releases are retained for 30 days in the event that there are issues with the latest release candidate.



MODFLOW EXECUTABLES

win64.zip				
• win32.r/p				
 mac.zip 				
 Inus.zip 			mpß	6.0.1
The programs and version numbers for the present release are			mp7	7.2.001
	ogram Version		mflgr	2.0.0
Program			mt3dms	5.3.0
m/2000	1.19.05		mt3dungs	110
m/2005	1.12.00		vs2m	33
tweline	1.2.0		stangle	1.6
mfung	1.5		aridgen	10.02
peribudung	1.5		Ebudron	3.01
m#6	6.2.0			
ibrol6	620		6/1	1.3.1
			gsflow	2.1.0
zbudē	6.2.0		si,tra	3.0



O Edit on GitHub

247. D.889.

MODFLOW 6 Example Problems



MODFLOW 6 – Example problems

Docs + MODFLOW 6 Example Problems

MODFLOW 6 Examples - Jupyter Notebooks

Revision dc5c8128.

Built with Sphinx using a theme provided by Read the Docs.

CONCLUDING REMARKS



Summary

MODFLOW 6 is presently the "core" MODFLOW

- GWF Model
- GWT Model
- Coupled flow and transport
- New MODFLOW API
- Ongoing and planned efforts
 - Parallelization
 - Particle tracking
 - Time-variable properties (mining applications)
 - Adaptive time stepping, Richard's equation, heat transport, …



Any Questions?



Or feel free to email me at langevin@usgs.gov

Final Poll



We value your input! Please consider sending comments and recommendations.