Groundwater

MODFLOW as a Configurable Multi-Model Hydrologic Simulator

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Abstract

MODFLOW 6 is the latest in a line of six "core" versions of MODFLOW released by the U.S. Geological Survey. The MODFLOW 6 architecture supports incorporation of additional hydrologic processes, in addition to groundwater flow, and allows interaction between processes. The architecture supports multiple model instances and multiple types of models within a single simulation, a flexible approach to formulating and solving the equations that represent hydrologic processes, and recent advances in interoperability, which allow MODFLOW to be accessed and controlled by external programs. The present version of MODFLOW 6 consolidates popular capabilities available in MODFLOW variants, such as the unstructured grid support in MODFLOW-USG, the Newton-Raphson formulation in MODFLOW-NWT, and the support for partitioned stress boundaries in MODFLOW-CDSS. The flexible multi-model capability allows users to configure MODFLOW 6 simulations to represent the local-grid refinement (LGR) capabilities available in MODFLOW-LGR, the multi-species transport capabilities in MT3DMS, and the coupled variable-density capabilities available in SEAWAT. This paper provides a new, holistic and integrated overview of simulation capabilities made possible by the MODFLOW 6 architecture, and describes how ongoing and future development can take advantage of the program architecture to integrate new capabilities in a way that is minimally invasive and automatically compatible with the existing MODFLOW 6 code.

Introduction

MODFLOW was first released in the early 1980s by the U.S. Geological Survey (USGS). It was designed as a generalized groundwater flow simulator to address a proliferation of custom groundwater modeling codes at the USGS that were being developed for specific projects (McDonald and Harbaugh 2003; Barlow and Harbaugh 2006). The popularity of MODFLOW is attributed to its thorough documentation, portability, institutional support, unrestrictive license, and its intuitive modular design, which allows users and developers to focus on individual aspects of the program. MODFLOW is used worldwide by academics, government agencies, and consultants to simulate a wide range of groundwater problems. MODFLOW is developed and maintained by the USGS with numerous contributions from the broader hydrologic modeling community.

Since its inception, MODFLOW has been based on a design philosophy that emphasizes modularity in code construction and organization of model input and output. Hydrologic components and boundary conditions are organized into program units to systematize the representation of interactions between hydrologic processes and the addition of new processes as much as possible. MODFLOW 6, the latest core MODFLOW version released by the USGS, adheres to the same general design philosophy, although the program architecture has evolved considerably to take advantage of modern programming paradigms and practices. The MODFLOW 6 program architecture allows closer and more adaptable coupling between hydrologic process models and the systematic incorporation of more complex and sophisticated capabilities than ever before. As a result, MODFLOW 6 offers many new capabilities that would have been difficult or impossible to implement in previous versions

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and provides a platform for closely integrating a wide range of hydrologic process models, including processes simulated using codes external to MODFLOW.

While there are numerous MODFLOW 6 publications, they are typically focused on narrow aspects of specific simulation capabilities. Users and developers would benefit from additional high-level information on how these individual simulation capabilities are related to one another and how they can be combined and configured to solve complex problems. The intent of this paper is to provide a new, holistic, and integrated overview of simulation capabilities made possible by the MODFLOW 6 architecture. The paper summarizes the underlying modular structure in MODFLOW 6, presents current simulation capabilities made possible by these structural improvements, and describes future directions for program enhancement. The remainder of the paper begins by describing the MODFLOW design approach and the role that "core" versions and variants of MODFLOW play in advancing capabilities while maintaining program modularity. The paper then describes the revisions in program architecture in MODFLOW 6, the cornerstones of which are object-oriented program design, a flexible approach to formulating and solving the equations that represent hydrologic processes, and recent advances in interoperability, which allow MODFLOW to be accessed and controlled by external programs. After that, the paper describes new capabilities that were made possible or were facilitated by the revised program architecture and are now available to users. Finally, the paper discusses ongoing efforts to further enhance modeling capabilities and performance of MODFLOW as a generalized hydrologic simulator.

This paper is intended to serve MODFLOW users as well as those interested in developing new modeling capabilities for MODFLOW. The next section is of general interest and provides the historical context for how MODFLOW development at the USGS has resulted in core versions and customized MODFLOW variants. The succeeding overview of the MODFLOW 6 architecture includes a description of the simulation components and how they can be configured and combined by the user to perform single model or complex multi-model simulations. The architecture overview also includes design details for developers and those interested in understanding how these new capabilities are organized and made possible in MODFLOW 6. The concluding discussion highlights for users the core capabilities presently available and points to future directions in MODFLOW development.

Design Approach and Strategies for Maintaining Modularity

Modularity remains a fundamental design principle for the continued maintenance and development of MODFLOW. This section summarizes the USGS modular design approach and strategy for preserving modularity by releasing core updates and customized MODFLOW variants.

Design Approach

The documentation for the first public release of MODFLOW articulated an approach to program design based on modularity and flexibility (McDonald and Harbaugh 1984):

> "The modular structure consists of a Main Program and a series of highly independent subroutines called 'modules.' The modules are grouped into 'packages.' Each package deals with a specific feature of the hydrologic system which is to be simulated, such as flow from rivers or flow into drains, or with a specific method of solving linear equations which describe the flow system ... The division of the program into modules permits the user to examine specific hydrologic features of the model independently. This also facilitates development of additional capabilities because new modules or packages can be added to the program without modifying the existing modules or packages. The input and output systems of the computer program are also designed to permit maximum flexibility."

The program was also designed around a standardized set of internal steps or operations, called "procedures," that were followed in carrying out a simulation, and which dealt with various aspects of model input, problem formulation, problem solution, and model output. Thus, each module performed a specific, well-defined procedure in the simulation sequence for a specific package that dealt with a particular process or component within the groundwater simulation. The same overall design approach has continued to guide the development of MODFLOW as it has evolved from a single-model groundwater flow simulator to a multi-model simulator designed to integrate a wide variety of hydrologic processes.

One of the guiding principles of the MODFLOW design approach is to enable users to easily add or remove components when constructing a simulation (McDonald and Harbaugh 1988). Underlying this principle is the definition of simulation components that are independent in terms of their input requirements. The concept of "packages" is still used and retains its original meaning (parts of the model code that handle a specific hydrologic component or simulation aspect), but the multi-model framework of MODFLOW 6 called for the introduction of higher-level simulation components (Hughes et al. 2017). The concept of a "model" has been formalized to distinguish it from the simulation as a whole. A model implements a hydrologic process using a collection of packages. A model "instance" is an application of the model to a specific geographic area. The concept of an "exchange" has also been introduced; an exchange is used to encapsulate the information needed to couple models together. Coupled models are grouped and solved together in a "solution," and a simulation can include multiple solutions. This modularization at all levels helps with conceptualizing the interrelated parts of a complex hydrologic simulation and facilitates the mechanics of organizing, assembling, and modifying the user input and interpreting the output.

The other guiding principle is to enable developers to systematically add new capabilities as easily as possible and with minimal disruption of existing code. In MODFLOW 6, this is accomplished using object-oriented programming (Hughes et al. 2017). Simulation components are programmed such that, in addition to maintaining independent input requirements, the components are highly independent in terms of the information they store and the calculations and other operations they perform. The program units that encapsulate various simulation components are, by design, unaware of the inner workings of other program units. Exchange of information between components is handled as systematically and generically as possible to avoid the proliferation of invasive, highly customized dependencies between program units that would make subsequent code enhancements complicated and error-prone. Object-oriented class inheritance is used to create variants of simulation components, such as different types of Numerical Models, that share a significant amount of higher-level functionality but differ in their particular implementations. Programming of each simulation component continues to be structured around a sequence of standardized procedures. The procedures have been modified and expanded but still serve their original purpose of systematizing the main operations performed by simulation components.

The result is a MODFLOW 6 program with highly structured input, output, and program architecture. Simulation components that represent various hydrologic processes can be flexibly coupled within a simulation while maintaining a high degree of modularity for the user and within the program itself. Although a less structured approach might be expedient for some aspects of code development in the short term, the added complexity associated with the new program architecture serves to minimize the overall complexity of the code in the long run. This makes the code easier to understand and expand, more maintainable and reliable, and ultimately easier to use, particularly in applications that involve complex interaction between various hydrologic processes.

MODFLOW Core Versions and Customized Variants

MODFLOW 6 (Hughes et al. 2017) is the latest in a line of six "core" versions of MODFLOW released by the USGS, beginning with MODFLOW-84 (McDonald and Harbaugh 1984) (Table 1). Core versions embody major updates to MODFLOW that synthesize recent advances, support new capabilities, remove outdated functionality, take advantage of new programming features and patterns, and provide a new baseline for further development.

Core MODFLOW versions are designed to be reliable, stable, and general. Therefore, new capabilities are incorporated into the core version only after careful consideration of the benefits. Advances in computing and modeling technology influence the capabilities that are added to, or, infrequently, removed from, the core version. For example, in MODFLOW-2005 the approach for managing memory was redesigned using Fortran allocatable arrays, which replaced the less flexible, static allocation of arrays used in previous MODFLOW versions. On the other hand, the parameter estimation and sensitivity analysis capabilities implemented in MODFLOW-2000 (Hill et al. 2000) were not included in MODFLOW-2005 because those capabilities became available through external programs such as PEST (Doherty 2010).

Table 1
Core MODFLOW Versions Released by the U.S. Geological Survey

Name	Citation
MODFLOW-84	McDonald and Harbaugh (1984)
MODFLOW-88	McDonald and Harbaugh (1988)
MODFLOW-96	Harbaugh and McDonald (1996)
MODFLOW-2000	Harbaugh et al. (2000); Hill et al. (2000)
MODFLOW-2005	Harbaugh (2005)
MODFLOW 6	Hughes et al. (2017)

To promote new ideas and advance modeling capabilities, the USGS has encouraged the development and release of customized MODFLOW variants, such as those shown in Table 2. These MODFLOW variants are full-fledged, and in some cases widely used, versions of MODFLOW. However, they also support the development of core versions by offering a way to implement and test new capabilities, assess the utility of new capabilities to the hydrologic modeling community, and refine existing capabilities in response to user feedback. Popular and generally useful capabilities from MODFLOW variants are brought into a future core version whenever possible, and if necessary, the architecture of the core version is redesigned to preserve modularity and cleanly accommodate the new capability. Integration of popular capabilities into the core version also provides an opportunity to revisit their input and output requirements, underlying structure, and documentation, and revise as necessary to maintain consistency with other core features.

The program architecture of the MODFLOW 6 core version is designed to accommodate future advances whose specific implementations are difficult to anticipate. The initial motivation for redesigning the architecture, however, was to facilitate incorporating popular and advanced capabilities from MODFLOW variants. Most of the capabilities that debuted in MODFLOW variants (Table 2) require simulation of additional hydrologic processes (such as solute transport, watershed components, conduit flow, surface water routing, and farm demands, for example) in addition to groundwater flow. Another common thread between the MODFLOW variants listed in Table 2 is that many of their capabilities require solving a more general system of equations than is required for traditional MODFLOW groundwater flow formulations. The numerical solver packages available in the traditional MODFLOW versions, for example, the Strongly Implicit Procedure and the Pre-Conditioned Conjugate Gradient Packages (Hill 1990), were designed for regular grids with a fixed stencil and cannot be used to solve more general linear equations with unstructured connectivity patterns and asymmetric coefficient matrices.

Table 2
Description of Capabilities Implemented in Selected MODFLOW Variants

Variant Name	Description
MOC3D/MODFLOW-GWT	Coupled version of MODFLOW with the Groundwater Transport process for simulation of coupled groundwater flow and solute transport (Konikow et al. 1996; Winston et al. 2018)
SEAWAT	Coupled version of MODFLOW and MT3DMS for simulation of variable-density groundwater flow and multi-species solute transport (Guo and Langevin 2002; Langevin et al. 2003, 2008)
MODFLOW-GWM	Groundwater management optimization (Ahlfeld et al. 2005, 2009)
MODFLOW-VSF	Variably-saturated groundwater flow (Thoms et al. 2006)
MODFLOW-FMP/MODFLOW-OWHM	Coupled version of MODFLOW and the Farm process (Schmid et al. 2006; Schmid and Hanson 2009; Hanson et al. 2014; Boyce et al. 2020)
MODFLOW-LGR	Local Grid Refinement version of MODFLOW for simulating coupled parent and child grid configurations (Mehl and Hill 2007, 2013)
GSFLOW	Coupled version of MODFLOW and PRMS for integrated watershed and groundwater simulation (Markstrom et al. 2008)
MODFLOW-CFP	Conduit flow process, a coupled version of MODFLOW and a pipe-network model (Shoemaker et al. 2008)
MODFLOW-CDSS	Colorado decision support system version of MODFLOW for partitioning stress boundary packages (Banta 2011)
MODFLOW-NWT	MODFLOW Newton formulation for representing nonlinear water table problems (Niswonger et al. 2011)
MODFLOW-SWR	Coupled version of MODFLOW and the Surface Water Routing process (Hughes et al. 2012)
MODFLOW-USG	Unstructured grid version of MODFLOW, includes Newton formulation for nonlinear water table problems and the Connected Linear Network (CLN) for simulating flow through conduits (Panday et al. 2013); the USG-Transport successor also simulates variable-density groundwater flow and multi-species solute transport (Panday 2020)
MODSIM-MODFLOW	Coupled version of MODSIM with MODFLOW (Morway et al. 2016)
MODSIM-GSFLOW	Coupled version of MODSIM with GSFLOW (Kitlasten et al. 2021)

Several of the variants in Table 2 (MODFLOW-GWM, MODSIM-MODFLOW, and MODSIM-GSFLOW) require interaction with another type of model, such as an optimization model. The need to efficiently accommodate the types of advanced capabilities found in the MODFLOW variants set many of the requirements for the MODFLOW 6 architecture.

Overview of MODFLOW 6 Architecture

To address the design requirements motivated by the MODFLOW variants and to support a wide range of new capabilities, MODFLOW 6 was written using an object-oriented programming design (Hughes et al. 2017). The object-oriented design offers significant advantages over the procedural programming design used in previous MODFLOW versions. Simulation components are written as classes, which encapsulate the data and methods associated with a component, and multiple instances of a class can be created within a single simulation. The concept of abstraction is used to manage and hide complexity and make it possible for others to add complex new hydrologic process models without interfering with other contributors. Class inheritance is also used within the program as a way to efficiently implement base functionality that can be used, overridden, or extended by child classes. Because much of the essential functionality and interconnectedness between simulation components is programmed at a high level within MODFLOW 6, new components and features can be added systematically and efficiently. For MODFLOW users this results in powerful new capabilities, such as support for multiple models and multiple types of models within the same simulation. A multi-model LGR example (a coarse parent model with two child models and a grandchild model) is shown in Figure 1. The ability to have multiple objects of the same class is also used within models to support multiple packages, including the capability to create multiple stress packages of the same type.

This remainder of this section begins by describing the overall design and major simulation components of MODFLOW 6. It then explains how simulations can be configured by connecting models using exchanges, and how systems of equations for hydrologic processes are constructed and solved. Finally, this section describes how interoperability with other programs is supported by MODFLOW 6.

Simulation Components: Models, Exchanges, Solutions, and Timing

The user input and internal organization of the MODFLOW 6 program are based on four major simulation components: models, exchanges, solutions, and a timing module (Hughes et al. 2017). A model contains the equations that represent a hydrologic process. An exchange facilitates the communication between two models. A solution solves one or more models that may be connected to one another through one or more exchanges. The timing module controls the lengths of time steps

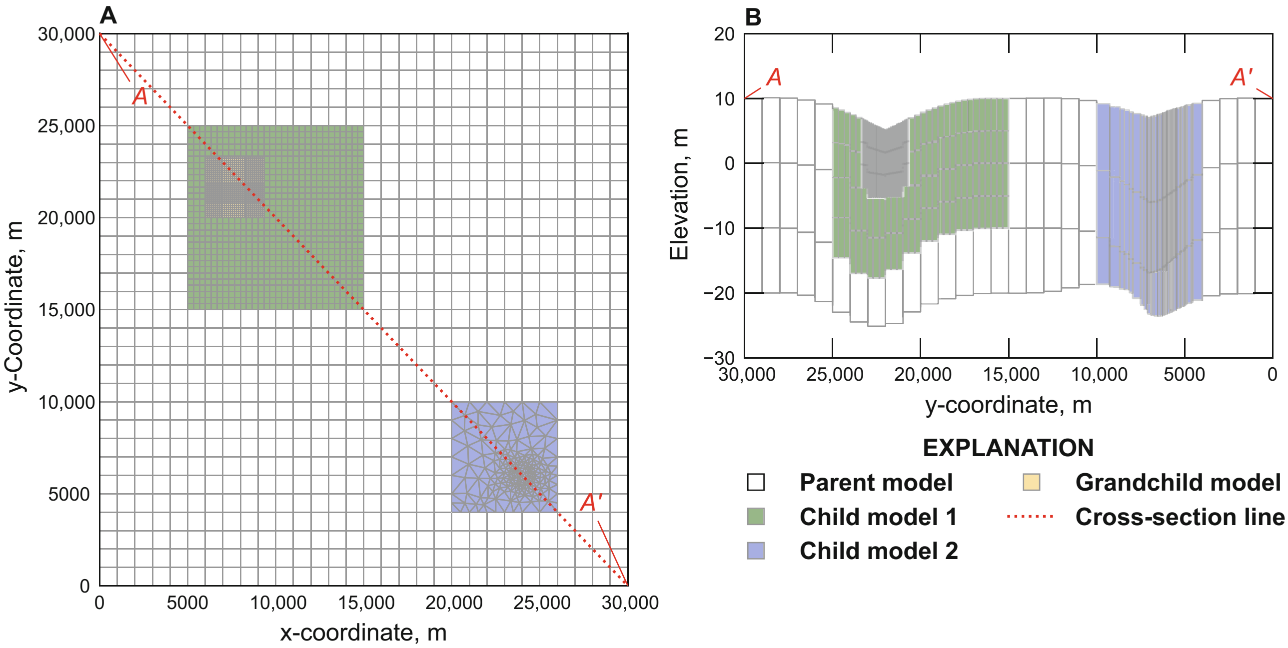

Figure 1. Example of multiple models coupled together in a single simulation. (A) Map view of a parent model with two embedded, more finely discretized child models and one further discretized grandchild model embedded in child model 1. (B) Cross-section through the composite model domain showing the vertical discretization of the parent, child, and grandchild models. Child model 1 is discretized into four model layers and is connected horizontally to layers 1 and 2 and vertically to layer 3 of the parent model. The grandchild model is discretized into three layers and is connected horizontally to layers 1 and 2 and vertically to layer 3 of child model 1. Each of the three layers of child model 2 is connected to the corresponding layer of the parent model. The figure highlights the flexibility to couple groundwater models with different types of spatial discretization.

and determines when the end of the simulation has been reached. It is a single controller that is accessible by all other components. The timing module follows the temporal discretization paradigm used in previous versions of MODFLOW, in which the total simulation time is divided by the user into stress periods and time steps. An adaptive time stepping approach based on Panday (2020) was added as an option to the timing module. Time step lengths can be shortened or lengthened based on simulation behavior, and if a Numerical Solution fails to converge, the program will retry the solution with a shorter time step.

Development of MODFLOW 6 has focused on the Numerical Solution of one or more numerical hydrologic models that may be connected (such as the example shown in Figure 1). This primary focus has resulted in generic simulation components, called Numerical Models, Numerical Exchanges, and Numerical Solutions, that are designed to work together to address many of the design requirements for MODFLOW 6. Each of the three numerical components is represented as an object in the program, which provides flexibility for the user to create and configure components according to the particular needs of a simulation. As described by Hughes et al. (2017), MODFLOW 6 introduced a new paradigm in which multiple Numerical Models, each with their own spatial discretization, can be solved simultaneously by a single Numerical Solution. This is a significant architectural advance over the traditional MODFLOW structure, in which the numerical solver was attached to a single model.

Configuring a Simulation: Coupling Models Using Exchanges

Hydrologic models and exchanges are written for MODFLOW 6 using the object-oriented concept of inheritance to extend the Numerical Model and Numerical Exchange classes to include the equations for a specific hydrologic process. The latest release of MODFLOW 6 as of this writing (Langevin et al. 2023) includes the GWF Model (Langevin et al. 2017) and the GWT Model (Langevin et al. 2022), which extend the generic Numerical Model class to include equations specific to groundwater flow and solute transport, respectively. The GWF Model and the GWT Model are fully functional groundwater flow and transport models, respectively. They each contain a well-documented set of packages (Langevin et al. 2017, 2022).

With the implementation of GWF and GWT as Numerical Models and the implementation of the GWF-GWF, GWT-GWT, and GWF-GWT exchanges, there are many different ways in which a user can configure a simulation, as shown in Figures 1 and 2. Simulation of a single groundwater flow model (Figure 2A) or a single groundwater transport model (Figure 2B) will likely remain popular configurations for most users. However, the ability to connect models with exchanges offers significant benefits in many applications. The ability to couple two GWF Models using the GWF-GWF Numerical Exchange (Figure 2C) incorporates LGR capabilities (Mehl and Hill 2013) into the core version of

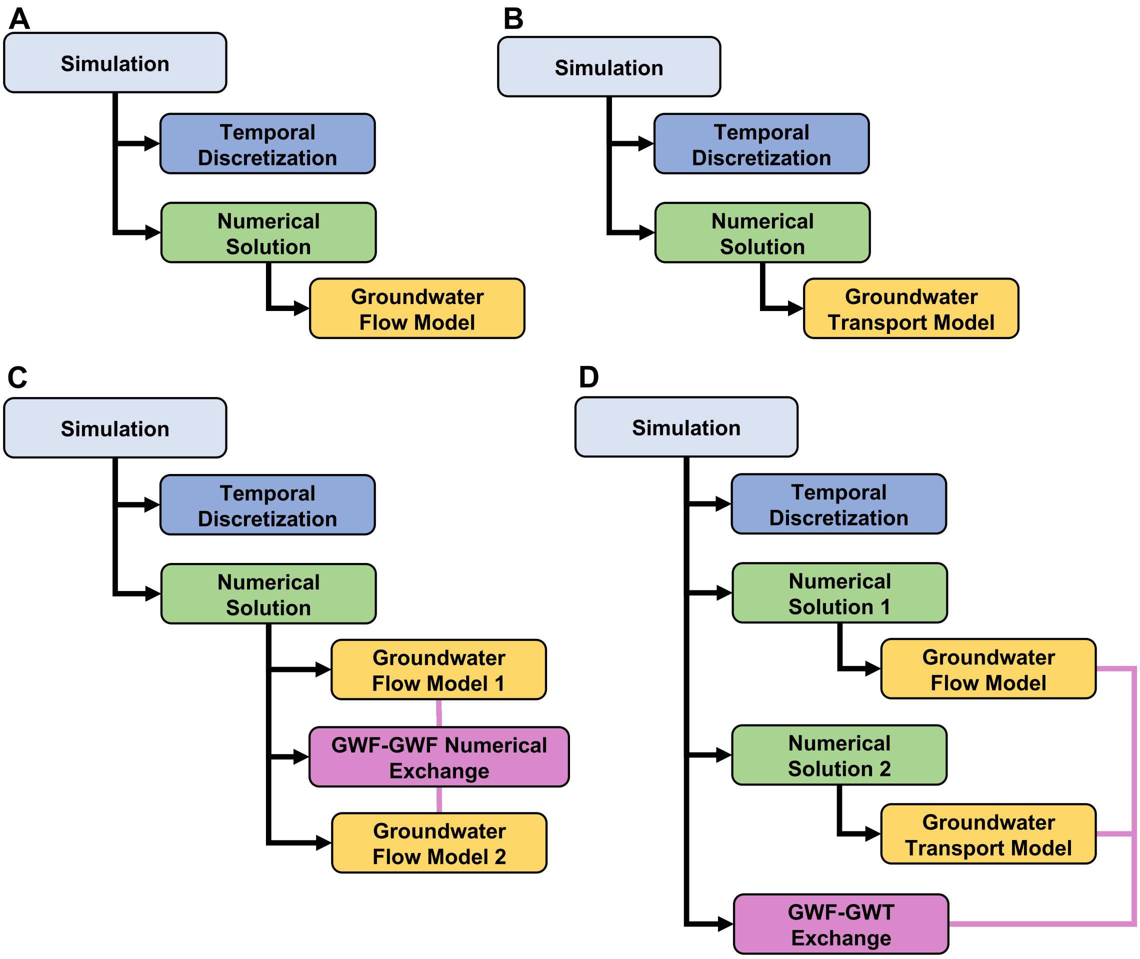

Figure 2. Schematic diagram showing several common ways in which the groundwater flow (GWF) and groundwater transport (GWT) models can be configured within a simulation. The common use case depicted in (A) consists of a single GWF model that is solved by a Numerical Solution. The simulation in (B) consists of a single GWT model that is solved by a Numerical Solution; in this case groundwater flows would come from a previous simulation, like the one shown in (A). The simulation in (C) shows a tightly coupled case in which two GWF models are connected by a GWF-GWF Exchange and solved simultaneously by one Numerical Solution. The simulation in (D) shows the case in which a GWF model and a GWT model are solved by separate Numerical Solutions, and flows are passed from the GWF model to the GWT model by the GWF-GWT exchange.

MODFLOW, and has been used, for example, to evaluate regional effects on local-scale lake fluctuations (Fienen et al. 2021, 2022b). Unlike in previous versions of MODFLOW (Mehl and Hill 2007, 2013), the LGR capabilities in MODFLOW 6 are not limited in the number of levels of nesting allowed; any number of parent, child, grandchild configurations are supported (Figure 1). The GWF-GWF Numerical Exchange is general in that it can connect GWF Models with different grid types. The LGR capabilities also support routing of streamflow from one GWF Model to another using the Water Mover (MVR) Package.

Figure 2D shows a common use case in which a single GWF Model and a single GWT Model are run together in the same simulation, and flows from the GWF Model are passed through memory to the GWT Model using the GWF-GWT Exchange. A coupled variable-density flow and solute transport simulation is possible using the configuration shown in Figure 2D. In this case, the Buoyancy Package must be activated for the GWF Model, and the GWT Model must simulate transport of a dissolved chemical species, such as salt (Langevin et al. 2020). This variable-density simulation capability incorporates SEAWAT functionality into the core version of MODFLOW and adds the benefits of unstructured grids and the Newton-Raphson formulation. Though not shown in Figure 2, it is also possible to simulate multiple chemical species by using a separate GWT Model for each chemical species, with each GWT Model coupled to the GWF Model through a separate GWF-GWT Exchange.

Due to the generality of the model and exchange implementation, more complex configurations are also possible, such as the one shown in Figure 3. In this case, two GWT Models are coupled together in the same Numerical Solution using the GWT-GWT Numerical Exchange. These two GWT Models receive flows from corresponding GWF Models using two different GWF-GWT Exchanges. This flexibility allows individual models to be developed and maintained separately from

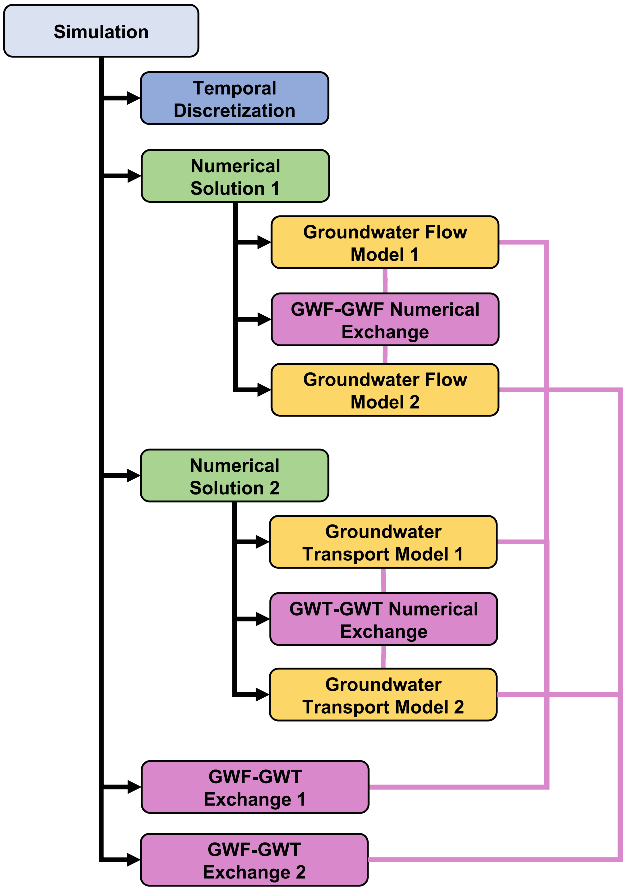

Figure 3. Schematic diagram showing a configuration in which two groundwater flow (GWF) models are solved by one Numerical Solution and two groundwater transport (GWT) models are solved by another Numerical Solution. Flows are passed from the GWF models to the GWT models using two separate GWF-GWT exchanges.

one another, and also tightly coupled at the matrix level with adjacent models.

Generalized Internal Framework for Formulating and Solving Numerical Solutions

Like many process-based simulators, MODFLOW solves a "balance equation" that mathematically describes the storage, movement, and sources and sinks of a conserved material (for example, water or solute) and is formulated in terms of a dependent variable (for example, hydraulic head or solute concentration). MODFLOW 6 uses the Control-Volume Finite-Difference (CVFD) method, which discretizes the model domain into a finite number of control volumes, or "cells," and formulates a discrete version of the balance equation over each cell. Associated with each cell is a specific point in space, or "node," at which the value of the dependent variable is calculated. The assemblage of model cells, nodes, and interconnections between them is called the model "grid."

Flows exchanged between a cell and the cells to which it is connected (its "neighbors") depend on the values of the dependent variable in (i.e., at the nodes of) that cell and its neighbors. For example, in the standard method of representing groundwater flow between two hydraulically connected cells in MODFLOW, the flow is proportional to the difference between the head values in those two cells. Considering all the neighbors to which a given cell is connected, the discrete balance equation for a particular cell, cell n, can be written in the algebraic form

$$A_{n,n}x_n + \sum_{m \in \eta_n} A_{n,m}x_m = b_n, \tag{1}$$

where $A_{n,n}$ is the coefficient for the dependent variable value in cell n; $A_{n,m}$ is the coefficient for the dependent variable value in neighboring cell m; x_n and x_m are the dependent variable values in cells n and m, respectively; b_n is the right-hand-side value, which is the sum of terms in the balance equation for cell n, including terms arising from boundary conditions, that do not involve the dependent variable values being solved for; and the summation is over the set of neighbors of cell n, which is denoted by η_n. For a regular MODFLOW structured grid, the set of neighbors, η_n, for cell n, is simply the overlying and underlying adjacent cells, adjacent cells to the left and right, and the adjacent cells to the front and back. In the general case of structured and unstructured grids, the set of neighbors of cell n includes adjacent cells that share a face with cell n. When a balance equation of the form shown in equation 1 is written for every cell in the grid, the resulting system of equations can be expressed in matrix-vector form as

$$\mathbf{Ax} = \mathbf{b}, \tag{2}$$

where $\mathbf{A}$ is a sparse, square matrix of coefficients with one row and one column for each cell in the grid, $\mathbf{x}$ is a vector of dependent variable values for each cell, and $\mathbf{b}$ is a vector of right-hand-side values for each cell.

Core versions of MODFLOW prior to MODFLOW 6 were designed primarily to solve a single groundwater flow model on a regular grid made up of layers, rows, and columns of cells. The regularity of the connections between cells resulted in a matrix with a regular, symmetric sparsity pattern (the pattern of non-zero entries), and equation 2 was solved using a linear solver that relied on the regularity and symmetry of the matrix structure. This limited the level of integration that could be employed in solving the model. For example, the Local Grid Refinement (LGR) capability introduced the ability to use multiple, nested grids. The grids were loosely coupled, however, and the sub-model on each grid was updated and solved repeatedly as a separate matrix problem within a Picard iteration loop until overall convergence of the solution was achieved (Mehl and Hill 2007, 2013). The Layer Variable-Direction Anisotropy (LVDA) capability enabled the simulation of hydraulic conductivity with anisotropy oriented arbitrarily within a model layer by drawing head information from other cells in addition to the connected neighbors of a given cell (Anderman et al. 2002). To avoid increasing the "stencil" for a cell, that is, the set of non-zero coefficients for dependent variables in equation 1, and allowing the use of existing MODFLOW linear solvers, a matrix-splitting scheme was used in LVDA, and Picard iterations were required to eliminate the associated truncation error. Nonlinearity resulting from the dependence of the matrix coefficients and right-hand-side values on the values of the dependent variables, as occurs in simulations of unconfined flow, for example, was likewise resolved using Picard iterations.

The numerical modeling framework in MODFLOW 6 is specifically designed to handle multiple models, arbitrary matrix sparsity patterns, and nonlinearities in model formulations. This allows efficient implementation, tight coupling, and robust solution of a wide variety of numerical representations of hydrologic processes. For example, LGR is achieved by defining multiple Numerical Models of the same type (e.g., two groundwater flow models) coupled through Numerical Exchanges within the same Numerical Solution. Each cell in each of the models is allocated a row and column in a "global" **A** matrix and an entry in a "global" **b** vector. In this expanded version of equation 2, the notion of a "neighboring" cell is extended to allow connections with cells in other models, including models that use a different grid type or represent a different hydrologic process. In accordance with the modular organization of MODFLOW, each Numerical Model is responsible for populating the matrix and right-hand-side vector with coefficients that characterize the cell-to-cell connections within that model. Each Numerical Exchange is responsible for coefficients that characterize connections between cells in different models, allowing the Numerical Models to focus exclusively on their own internal connections, without direct knowledge of the hydrologic processes represented in other models. The Numerical Solution then solves all the tightly coupled models simultaneously, which typically has performance benefits. The general sparse matrix formulation and storage scheme also allows generalization of "neighboring cells" to cells without a direct connection in the grid. For example, the XT3D capability, which is in part a generalization to three dimensions of the arbitrarily oriented anisotropy enabled by LVDA, uses head information interpolated from "neighbors of neighbors" to formulate a generalized expression for flow between two connected cells. Thus, equation 1 can accommodate terms associated with cells to which cell n is not directly connected, but which influence cell n through the XT3D head-gradient interpolation scheme. Finally, in cases that involve nonlinearities, a Newton-Raphson correction can be applied to accelerate convergence of the "outer" iterations. Use of the Newton-Raphson scheme and other options in MODFLOW 6 can result in an asymmetric **A** matrix, which can be accommodated by the sparse matrix storage scheme and handled by a suite of linear solvers that do not rely on a particular matrix sparsity pattern.

For each time step of the simulation, the Numerical Solution calculates the dependent variable values by looping through the Numerical Models and Numerical Exchanges according to the scheme shown in Figure 4, which results in tight, matrix-level coupling of connected models. The solution sequence for a time step is divided into three steps: Prepare Solve, Solve, and Finalize Solve. During the Prepare Solve step, each Numerical Exchange and each Numerical Model prepare information that is constant for the time step. The Solve step is embedded in an outer iteration loop so that it can be repeated multiple times until convergence is achieved. The Solve step is divided into two parts. First, the system of linear equations is built by directing Numerical Exchanges and Numerical Models to calculate their matrix coefficients and add terms to equation 2. Once all of the matrix terms have been added, the Linear Solve routine is then called to approximate **x**, and if the new value for **x** meets convergence requirements, then the outer iteration loop is terminated and the Numerical Solution proceeds

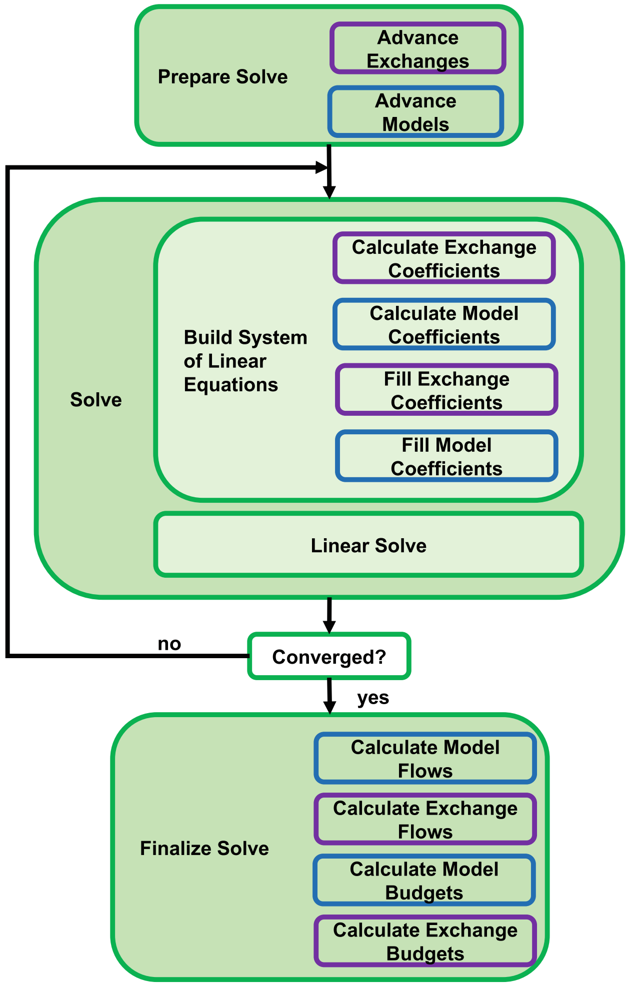

Figure 4. Schematic diagram showing the main sequence of steps used by a Numerical Solution to solve the dependent variable values (x) for a single time step. The sequence consists of three steps: prepare solve, solve, and finalize solve. Within each step, the Numerical Solution makes calls to each Numerical Exchange and each numerical model assigned to it. This figure is simplified from Hughes et al. (2017) to show the interaction between the Numerical Solution and the Numerical Models and Numerical Exchanges; there are additional Numerical Solution steps (addition of Newton–Raphson terms, nonlinear solution controls, etc.) that are not shown.

with Finalize Solve. During Finalize Solve, the Numerical Models and Numerical Exchanges calculate flows and budgets based on the converged value for **x**.

Coupling with External Programs: The MODFLOW API

The MODFLOW 6 architecture allows new types of models to be developed and incorporated into the program. If the new model is based on a CVFD scheme, it can inherit from the Numerical Model parent class and automatically leverage existing Numerical Solution routines. Exchanges can also be written so the new model can be coupled with other supported models.

To enable developers and advanced users to take advantage of modeling capabilities already available in other programs, or to program new capabilities without modifying MODFLOW 6 itself, the MODFLOW 6 program architecture was redesigned to support interoperability through an application programming interface (API) described by Hughes et al. (2022). The API was developed using the established Basic Model Interface (BMI) standard (Peckham et al. 2013). The API supports interoperability by allowing another modeling program, or a driver program written in a language like Python, to control and interact with MODFLOW during execution. This interaction is generally available for any MODFLOW 6 model or package. A key feature of the MODFLOW API is delegation of the calling sequence to a controlling program. This flexibility allows retrieval or modification of internal MODFLOW data between calls to Prepare Solve, Solve, and Finalize Solve (Figure 4). This fine-grained control, down to the outer iteration level, makes it possible to tightly couple MODFLOW with other models without having to implement those models directly in the MODFLOW program. As highlighted by Hughes et al. (2022), "The MODFLOW API provides a sustainable way to design and maintain software that relies on MODFLOW as a component. Software designed in this manner can take advantage of new MODFLOW features without having to modify and update the source code." A first reported use of the MODFLOW API is presented by White et al. (2023) to represent a closed-loop contaminant treatment system.

Discussion and Future Directions

The architecture of the current MODFLOW core version, MODFLOW 6, is designed to support multiple model instances and multiple types of models within a single simulation, Numerical Solution of generalized matrix equations with arbitrary sparsity patterns, and interoperability of the program through the MODFLOW API. This underlying object-oriented architecture provides a platform for consolidating many of the popular capabilities available in customized MODFLOW variants into a single program with consistent input and output formats, documentation, and simulation behavior. Table 3 summarizes the core capabilities available in MODFLOW 6 at the time of this writing (Langevin et al. 2023). As shown in Table 3, many of the popular capabilities released in MODFLOW variants (Table 2) are now available in MODFLOW 6. This includes many of the capabilities in MODFLOW-2005, MODFLOW-NWT, MODFLOW-CDSS, MODFLOW-USG, MODFLOW-LGR, MT3DMS, and SEAWAT. Through the interoperability afforded by the MODFLOW API, an even greater number of simulation capabilities are now possible, as demonstrated by Hughes et al. (2022), including capabilities first introduced in GSFLOW, MODFLOW-GWM, and MODSIM-MODFLOW.

Parallelization is an active area of development for MODFLOW. While there have been efforts to improve the performance of MODFLOW using both shared memory and distributed memory parallelization strategies, none of the efforts to date have to led to generalized functionality suitable for integration with the core version of MODFLOW. The multi-model architecture of MODFLOW 6 provides a natural avenue for parallel solution of models across multiple processors, with communication between processors as needed, using the message passing interface. A prototype of this capability was used by Verkaik et al. (2022) to simulate a global-scale groundwater model with nearly 300 million nodes across hundreds of cores. Current efforts are focusing on implementing the parallel routines in a manner consistent with the MODFLOW modular design approach so that existing and new types of process models can take advantage of the parallelization advantages with little additional work.

Development and support of new process models for MODFLOW 6, either through direct integration as a new model or through model coupling strategies that use the API, will likely remain a focus. For example, future work may focus on implementing energy transport, improved particle tracking, watershed processes, surface water flow and transport, and flow and transport through connected pipes and conduits. In the past, new process models and advanced capabilities for MODFLOW were often released as a new MODFLOW variant. The MODFLOW 6 modular platform provides a path for developing and releasing new and independent types of models in a way that is similar to how packages for groundwater flow have been developed and released. The underlying object-oriented and modular design of MODFLOW 6 allows ongoing development efforts to proceed relatively independently, with minimally invasive integration into the program as new capabilities reach maturity. New models that are directly integrated into MODFLOW 6 following established framework conventions will automatically be compatible with other models, through exchanges, the API, and multi-model parallelization, for example. For users, this means a substantial increase in capability, with complexity managed through the highly modular concepts that extend throughout the code, input, output, and documentation.

Software Availability

MODFLOW 6 is open source software developed and released by the USGS. The complementary FloPy package (Bakker et al. 2016; Hughes et al. 2023) contains

Table 3
Core Capabilities Available in MODFLOW 6

Capability	Simulation Component	Description
Grid flexibility	GWF, GWT	Structured and unstructured grids, patterned after Panday et al. (2013), can be used to simulate groundwater flow (Langevin et al. 2017) and groundwater transport (Langevin et al. 2022). IDOMAIN capability can be used to exclude cells and handle pinched layers. Applications include Davis et al. (2019), Goode and Senior (2020), Corson-Dosch et al. (2022), Fienen et al. (2022a), and Fiore and Colarullo (2023)
Newton–Raphson formulation	GWF	The Newton–Raphson formulation is available as an alternative to traditional wetting and drying (Langevin et al. 2017). Capability is patterned after Painter et al. (2008), Niswonger et al. (2011), and Panday et al. (2013). Applications include Ellis et al. (2023)
Advanced flow packages	GWF	The GWF Model includes advanced packages to represent multi-aquifer wells, lakes, streams, and unsaturated zone flow. Advanced packages capabilities are consolidated from Merritt and Konikow (2000); Halford and Hanson (2002); Prudic et al. (2004); Niswonger et al. (2006); Konikow et al. (2009); and Niswonger and Prudic (2005). Applications include Davis et al. (2019) and Fienen et al. (2021, 2022b)
Anisotropic groundwater flow and dispersion	GWF, GWT	XT3D multi-point flux approximation represents full three-dimensional anisotropic groundwater flow and dispersion on structured and unstructured grids (Provost et al. 2017). Flow capability is an extended alternative to the Model-Layer Variable-Direction Horizontal Anisotropy capability (Anderman et al. 2002). Applications include Goode and Senior (2020)
Water Mover	GWF, GWT	The Water Mover (MVR) can be used to route simulated flows and solute mass between packages in the GWF and GWT models (Langevin et al. 2017). Application of MVR is demonstrated by Morway et al. (2021)
Solute transport	GWT	One or more GWT models can be included in a single simulation in order to represent three-dimensional solute transport on structured or unstructured grids (Langevin et al. 2022). Capability is intended to extend the multi-species option in MT3DMS (Zheng and Wang 1999). Applications include Wu et al. (2022) and White et al. (2023)
Advanced transport packages	GWT	Solute transport can be represented within lakes, streams, multi-aquifer wells and the unsaturated zone, similar to earlier capabilities in MODFLOW (Merritt and Konikow 2000; Hornberger and Konikow 2006). The GWT Model includes balance equations for the advanced packages in the system of equations so that concentrations in advanced package features are solved as the dependent variable. Application of the Lake Transport (LKT) Package is demonstrated by Mancewicz et al. (2022)
Coupled variable-density flow and transport	GWF-GWT	Variable-density groundwater flow and solute transport can be represented using the GWF Model Buoyancy Package, which calculates density from solute concentrations in one or more GWT Models (Langevin et al. 2020, 2022). This capability is patterned after the variable-density capabilities available in SEAWAT (Guo and Langevin 2002; Langevin et al. 2003, 2008)
Local grid refinement (LGR)	GWF-GWF, GWT-GWT	LGR capabilities can be used to add spatial resolution in areas of interest for flow, transport, or flow and transport models in the same simulation. Flow capabilities are extended from the work of Mehl and Hill (2007, 2013). Transport capability is not available in any previous MODFLOW version. Applications include Fienen et al. (2021, 2022a, 2022b)
Interoperability	GWF, GWT	External programs can control and interact with MODFLOW during execution (Hughes et al. 2022). Applications include Guillaumot et al. (2022) and White et al. (2023)

full Python support for all MODFLOW 6 models and packages. We welcome input from the community through our public software repository.

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