



# Modelling groundwater flow with **MODFLOW: an introduction**

**Laura Foglia<sup>1</sup>, Iacopo Borsi<sup>2</sup>, Rudy Rossetto<sup>3</sup>**

- 1. Technical University Darmstadt (Germany)**
- 2. TEA Sistemi S.p.A. – Pisa (Italy)**
- 3. Scuola Superiore Sant’Anna – Pisa (Italy)**



## **FREEWAT**

Free and Open Source Software Tools for Water Resource Management  
EU HORIZON 2020 Project

**This lecture presents an introduction to MODFLOW, highlights the important features and mainly provides references to the most useful literature and webpages! It does not pretend to be a complete MODFLOW manual!**



# Overview of MODFLOW

MODFLOW: public-domain three-dimensional finite-difference groundwater simulation code by the U.S. Geological Survey.

MODFLOW can be run as a MS-DOS command line executable and reads several ASCII text files as input describing grid, properties, boundary conditions, initial conditions, time steps, stresses, solution and output options. Output is to ASCII text and binary files.

A graphical user interface such as FREEWAT can provide images of model features and can support visualization and graphical manipulation of model input and output. A GUI can create the MODFLOW input files and execute MODFLOW. You never need to see the text files or know the commands that are necessary to run MODFLOW ... until something goes wrong!



# MODFLOW

## Documentation and Reading

Read the MODFLOW documents in order

**MODFLOW 1988 1996 2000(GWProcess OBSProcess) 2005**

All these and much more can be downloaded at

<http://water.usgs.gov/software/lists/groundwater/>

Read for the essence of how the codes perform.

You do not need to read detailed descriptions of input or source code at this time, but can go back for those details when needed in the future

Note the conceptual model features of MODFLOW discussed in the 1988 are very important and are NOT repeated in later documents



# MODFLOW

## Documentation and Reading

### Further Reading for MODFLOW modelers

There are many additional simulation packages and many data-processing tools.

For example, Anderson and Woessner, 1992, *Applied Groundwater Modeling* is an excellent textbook for groundwater-flow modeling

And the new 2015 edition!!!



# KEEP UP-TO-DATE

**New Developments and MODFLOW Software updates**

**USGS Software Web Site**

**<http://water.usgs.gov/software/lists/groundwater/>**

**BOOKMARK THAT PAGE!**

**Let's open a new browser session there now**



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### Water Resources Groundwater Software

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- [Variably-Saturated Flow and Transport](#)
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#### Groundwater Flow, Transport, and Geochemical Reactions, including Groundwater/Surface-Water Interactions

- **NEW** [1DTempPro](#) (DOS) Version 1.0.1.1, 2013/02/04  
A graphical software package to visually calibrate one-dimensional VS2DH models at vertical groundwater/surface-water exchange.
- [BIOMOC](#) (DOS/DG/SIG/Sun) Version 1.0, 1999/03/10  
A multispecies solute-transport model with biodegradation
- [CFP](#) (Win) Version 1.8, 2011/02/23  
Conduit Flow Process for MODFLOW 2005
- [MODFLOW, MODFLOW-2005, and related programs](#)



## MODFLOW Core Version: MODFLOW-2005



The current core version of MODFLOW is [MODFLOW-2005 v.1.11.00](#). MODFLOW-2005 is the standard version of MODFLOW supported by the USGS Office of Groundwater and is the most stable and well-tested version of the code.

» [Download MODFLOW-2005](#)

» [New to MODFLOW? Start here.](#)

## MODFLOW Variants

The MODFLOW variants below are newer, specialized, or advanced versions of MODFLOW for use by experienced modelers.



### [MODFLOW-NWT: A Newton formulation for MODFLOW-2005 v.1.0.9](#)

MODFLOW-NWT uses a Newton-Raphson formulation to improve solution of unconfined groundwater-flow problems.



### [MODFLOW-USG v.1.2.00](#)

MODFLOW-USG uses an unstructured-grid approach to simulate groundwater flow and tightly coupled processes using a control volume finite-difference formulation.



### [GSFLOW: Coupled Ground-water and Surface-water FLOW model v.1.1.6](#)

GSFLOW is a coupled groundwater and surface-water flow model based on the USGS Precipitation-Runoff Modeling System (PRMS), MODFLOW-2005, and MODFLOW-NWT.

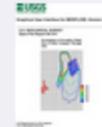


### [Groundwater Management \(GWM\) Process v.1.5.1](#)

GWM is used to simulate groundwater management.

## MODFLOW Utilities, Post Processors, and Graphical User Interfaces (GUIs)

The USGS software below are the most commonly used USGS MODFLOW utilities.



### [GW Chart](#)

GW\_Chart is a graphing application for MODFLOW, Zonebudget, and other codes. GW\_Chart also converts binary cell-by-cell flow files to text files.



### [ModelMuse](#)

ModelMuse is a GUI for MODFLOW-2005, MODFLOW-LGR, MODFLOW-NWT, MT3DMS, PHAST, MODPATH, and ZONEBUDGET.



### [ModelViewer](#)

Model Viewer is a program for 3D visualization of groundwater-model results.



### [ZONEBUDGET](#)

ZONEBUDGET is a program for computing subregional water budgets for MODFLOW.

[Additional MODFLOW Utilities »](#)



# And the new MODFLOW-OWHM, One-World-Hydrologic-model

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**Featured Science**

- NEW** Fractured Rock Geophysical Toolbox Method Selection Tool
- Groundwater availability in the United States: the value of quantitative regional assessments (Journal Article)
- USGS Groundwater Technical Procedures Videos
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- USGS Seeks National Groundwater Monitoring Network Proposals
- USGS Projects Large Loss of Alaska Permafrost by 2100

**USGS Groundwater Watch**

USGS maintains a network of active wells to provide basic

Water Software > Groundwater Software > MODFLOW and Related Programs > OWHM

## MODFLOW-OWHM: One Water Hydrologic Flow Model

- [Overview of MODFLOW-OWHM](#)
- [Program History](#)
- [Information and Downloads](#)
  - [General Information](#)
  - [Software Downloads](#)
  - [Documentation of MF-OWHM](#)
  - [MODFLOW-OWHM Process and Packages Support](#)
  - [Superseded Versions](#)
- [Example USGS Applications of MF-OWHM](#)
- [Point of Contact](#)
- [Additional USGS Software Resources and Disclaimers](#)

### Overview of MODFLOW-OWHM

The One-Water Hydrologic Flow Model (MF-OWHM) is a MODFLOW-based integrated hydrologic flow model (IHM). MF-OWHM is designed for the analysis of a broad range of conjunctive-use issues. Conjunctive use is the combined use of groundwater and surface water. **MF-OWHM allows the simulation, analysis, and management of human and natural water movement within a physically-based supply-and-demand framework.**

MF-OWHM is based on the Farm Process for MODFLOW-2005 (MF-FMP2, [Schmid and Hanson, 2009](#)) that is now combined with Local Grid Refinement (LGR, [Mehl and Hill, 2013](#)) for embedded models to allow use of the Farm Process (FMP) and Streamflow Routing (SFR) within embedded grids. MF-OWHM also now includes new features such as the Surface-Water Routing Process (SWR, [Hughes and others, 2012](#)), Seawater Intrusion (SWI, [Bakker and others, 2013](#)), and Riparian Evapotranspiration (RIP-ET, [Maddock III and others, 2012](#)). MF-OWHM contains all the previously available solvers and the new solvers such as Newton-Raphson (NWT, [Niswonger and others, 2011](#)) and the nonlinear preconditioned conjugate gradient (PCGN, [Naff and Banta, 2008](#)).

**New to MODFLOW? Start here!**



# ONLINE MODFLOW MANUAL

USGS Online Guide to MODFLOW-2000/2005

<http://water.usgs.gov/nrp/gwsoftware/modflow2000/MFDOC/guide.html>

## **ESSENTIAL BOOKMARK!**

**The online guide provides references to MODFLOW documents, definitions and formats for variables, and many helpful tips.**

**\*\*Note you can download this to your computer and use it off line, but it will not be updated unless you download and replace it**

## Online Guide to MODFLOW

Contents Index Search

- Introduction
- Beginner's Guide to MODFLOW
- Frequently Asked Questions
- Package Incompatibilities
- Suggestions on Compiling
- Miscellaneous
- Name File
- LGR Control File
- Array Reading Utility Modules
- List Utility Module
- SWR1 List Utility Subroutine SSWRLSTRD
- SWR1 Time Series Utility Subroutine SSWR\_RDTABDATA
- Input Files Supported in Various Versions of MODFLOW
- Ground-Water Flow Process
- Observation Process
- Sensitivity Process
- SWR - Surface-Water Routing Process
- Parameter Estimation Process
- Conduit Flow Process

2013 U.S. Geological Survey

»No topics above this level«

## Online Guide to MODFLOW



Compiled by [Richard B. Winston](#)

Revised: 3/7/2013

### Introduction

The purpose of these web pages is to provide a unified description of the formats for MODFLOW-2000, MODFLOW-2005, MODFLOW-LGR, MODFLOW-CFP, and MODFLOW-NWT input files. These descriptions have been copied from the original reports in which they were published and supplemented with materials found in the "doc" directory of the MODFLOW-2000, MODFLOW-2005, MODFLOW-LGR MODFLOW-CFP, and MODFLOW-NWT distribution files. *These web pages are not substitute for or a definitive guide to MODFLOW-2000, MODFLOW-2005, MODFLOW-LGR, MODFLOW-CFP, or MODFLOW-NWT. They may contain errors that are not in the original documents. In case of doubt, consult the original documents or examine the source code.*

In a few cases, obvious typographical errors in the original documents have been corrected in the version of the input instructions presented on these web pages. Such changes are not marked.

Some packages, such as the [Interbed Storage](#) package, were originally published as part of MODFLOW-88. In such cases, the instructions for including these package in a MODFLOW-2000, MODFLOW-2005, MODFLOW-LGR, MODFLOW-CFP, or MODFLOW-NWT model have been updated to reflect how the input is specified in MODFLOW-2000, MODFLOW-2005, MODFLOW-LGR, MODFLOW-CFP, or MODFLOW-NWT.

In a few cases, the instructions have been supplemented by additional material not found in the original input instructions. Such materials are shown in a different type face like **this**. The sources of such additional material include examination of the source code, correspondence with the authors of a package, and experience.

Keywords in the input files that must be entered exactly as shown (in a case-insensitive manner) are displayed in these web pages in bold and italics like *this*.



# What is MODFLOW?

Widely used ground-water flow simulation program that runs on any platform (Windows, Sun, Unix, Linux,...).

Mostly written in standard FORTRAN (GMG is C++)

Solves the ground-water flow equation with different possible properties, boundary conditions, and initial conditions

First version, 1983, McDonald and Harbaugh. Written to serve USGS needs. Education emphasized.

Public domain (Free)

Open source (Anyone can check and change the source code)

- Changed versions are sometimes commercial – it's up to the developer

Well documented - Modularly constructed (More later)



# What is MODFLOW?

Cited in statutes, legally tested

Many other programs use results from or are based on MODFLOW:

- Public domain/open source
  - MT3DMS (multi-species solute or heat transport, some reactions, dual porosity) (Chunmiao Zheng, U Alabama)
  - MODPATH (particle tracking) (Dave Pollock, USGS)
  - SEAWAT (density-dependent transport using MODFLOW and MT3DMS) (Chris Langevin, USGS)
  - PHT3D (= MT3DMS + PHREEQC) (Henning Prommer)
- Commercial
  - MODHMS, MODFLOW-Surfact (Integrated sw/gw/unsat)
  - GUI's: PMwin, VisualMF, Groundwater Vistas, GMS, Triwaco, ...



# What is MODFLOW?

Program organized into MODules

- Activate the capabilities you need; no overhead from other capabilities (execution time, RAM)
- The structure is clear and documented for adding additional capabilities such as new equations
- Modularity in 'Processes' and 'Packages'

## What is MODFLOW-2005?

- Internal computer storage redesigned to support storage of multiple models necessary for local grid refinement and facilitate linkages to other models (GSFLOW = MODFLOW + PRMS).
- Parameter-estimation, sensitivity analysis, uncertainty now done in UCODE\_2005



# Summary of MODFLOW capabilities

- Single Phase, Saturated Flow
- Constant Density
- Porous Media (Darcy's Law applies)
- 1, 2, Or 3 Dimensional (2D areal or cross-section OR Quasi-3D)
- Steady State or Transient Flow
- Heterogeneous, Anisotropic (aligned with grid), Layered Units
- Block-Centered Finite-Difference with variable grid spacing
- Layers can be Confined or Convertible
- Boundary conditions include: Dirichlet, Neuman, Cauchy, and Phreatic Surface
- Boundary condition packages include Wells, Recharge, Evapotranspiration, Rivers, Drains, Thin Barriers to Horizontal Flow, Re-wetting, and others.
- Many Solver options
- Monitoring of simulated values comparable to field observations
  
- Sensitivity analysis and parameter estimation to be accomplished by UCODE



# Selected USGS MODFLOW Capabilities

## Transport

- Link-MT3DMS (LMT). Produces files for use by MT3DMS (Zheng)
- SEAWAT v4. Variable density using MODFLOW and MT3DMS. Improvements in representation of viscosity, chemical diffusion, constant head boundaries.
- Ground-Water Transport (GWT) Package (currently for MF2000 only)

## Solvers

- Link-Multi-Grid (LMG). Typically up to 10 times faster than PCG2, but uses a lot of RAM. Free to USGS users.
- Geometric Multi-Grid (GMG). Can be very fast!
- PCG with Improved Nonlinear Control (PCGN).

## Packages for improved simulation of saturated-zone processes

- Multi-Node well (MNW)
- Hydrogeologic Unit Flow (HUF) Package updates: LVDA: Model-layer variable-direction horizontal anisotropy. KDEP: K varies with depth. SYTP: partial accounting for free surface; numerically stable.



# Selected USGS MODFLOW Capabilities, cont.

## Local Grid Refinement

- MODFLOW-LGR: Accurate local grid refinement. Can have multiple refined areas. Coming soon: LGR with particles tracked between regional and local grids.

## Interactions with processes above the water table and at land surface

- FARM Process: Sophisticated accounting for ET, diversions, etc related to agricultural demands.
- Streamflow-Routing with unsaturated flow beneath streams (SFR2)
- Unsaturated zone using (1) kinematic wave (UZF) and (2) Richard's equation (VSF)
- GSFLOW: Integrated surface processes represented using PRMS; separate program

## Optimization for ground-water management

- Ground-Water Management (GWM) Process



# Who is MODFLOW?

Collaborative open-source development with roots at the USGS

## *Some USGS developers*

- Arlen Harbaugh (MODFLOW, Reston, Virginia, USA)
- Ned Banta (MODFLOW-2000, Lakewood, Colorado, USA)
- Mary Hill (SA/PE/UA, MODFLOW-2000, UCODE, MMA, Boulder, Colorado, USA)
- Steffen Mehl (local grid refinement (LGR), SA/PE/UA, now at CalSU-Chico, USA)
- Stan Leake (compaction and subsidence, TMR, Tucson, Arizona, USA)
- John Hoffman (compaction and subsidence, TMR, Tucson, Arizona, USA)
- Dave Prudic (gw/sw interaction, STR, SFR, GSFLOW, Carson City, Nevada, USA)
- Rick Niswonger (gw/sw interactions, SFR, GSFLOW, Carson City, Nevada, USA)
- Paul Barlow (ground-water management, MODMAN, Reston, VA, USA)
- Randy Hanson (FARM Process, MNW, San Diego, USA)
- Alden Provost (HUF, Reston, VA)
- Dave Pollock (particle tracking, MODPATH, Reston, Virginia, USA)
- Chris Langevin (transport, saltwater intrusion, SEAWAT, Miami, Florida, USA)
- Lennie Konikow (transport extended from MOC3D, GWT, Reston, Virginia, USA)
- George Hornberger (transport extended from MOC3D, GWT, Reston, Virginia, USA)

## *Some non-USGS developers*

- Chunmiao Zheng (transport, MT3DMS, University of Alabama, USA)
- Eileen Poeter (UCODE, MMA, Colorado School of Mines, IGWMC, Golden, CO, USA)
- Evan Anderman (ADV, HUF, now at EvanAnderman.com, photography)
- Henning Prommer (MODFLOW+PHREEQC, CSIRO, Perth, Australia)
- Wolfgang Schmid (FARM Process, U. of Arizona, USA)
- David Ahlfeld (ground-water management, GWM, U. of Massachusetts, USA)
- You...???



# MODFLOW DEVELOPMENT

- Originally organized in modules
  - Modules grouped into packages that perform calculations either specific to the behavior of a geohydrologic feature or a numerical modeling task
  - Packages allow
    - examination of specific hydrologic features independently
    - facilitates development of additional capabilities
- Originally solely a ground-water flow model



# MODFLOW DEVELOPMENT

- Scope broadened to allow capabilities such as transport and parameter estimation
- Expansion of modular design required (MODFLOW-2000)
  - addition of “Process”
- MODFLOW-2005 is similar in design to MODFLOW-2000
  - Incorporates different approach for managing internal data
  - Fortran modules are used to declare data that can be shared among subroutines
  - MODFLOW subroutines were originally called modules
  - generic term module has been eliminated and replaced by the term subroutine



# ORIGINAL MODULAR STRUCTURE (1988):

- BAS - basic package
  - general tasks - gridding, constant head and no-flow boundaries, initial conditions, time stepping
- OC - output control package
  - controls the information and format of results
- BCF - block centered flow package
  - layer types, grid dimensions, material properties
- WEL - well package
  - locations and flow rates of wells
- RCH - recharge package
  - recharge rates and locations
- RIV - river package
  - locations, river bed material properties, and river stages
- DRN - drain package
  - location, material properties surrounding drains, and elevation of drains
- EVT - evapotranspiration package
  - parameters describing evapotranspiration rate with depth to water table
- GHB - general head boundary package
  - locations, local material properties, and elevation of specified heads
- SOLVERS
  - SIP - strongly implicit procedure package
  - SOR - slice-successive over-relaxation package



## PACKAGES WRITTEN AFTER ORIGINAL MODFLOW:

- PCG2 - preconditioned conjugate-gradient 2 package
  - alternative matrix solver
- STR1 - stream routing package
  - differs from the river package in that the surface water stage varies based on the surface water flow and the Manning equation
- BCF2 - block-centered flow 2 package
  - allows for re-wetting of cells that have gone dry
- BCF3 - block-centered flow 3 package
  - a supplement to the BCF2 package, allowing alternative interblock transmissivity formulations
- HFB1 - horizontal flow barrier package
  - simulation of thin, vertical, low permeability features that impede horizontal flow
- TLK1 - transient leakage package
  - simulates transient leakage and storage changes in confining units of quasi-3D models
- GFD1 - general finite difference flow package
  - substitutes for the BCF package, allows user to enter conductance rather than calculating with MODFLOW
- IBS1 - interbed storage package
  - simulates compaction of compressible, fine-grained units within or adjacent to aquifers in response to pumping
- CHD1 - time-variant specified head boundary package
  - allows time varying specified head



# PACKAGES WRITTEN FOR MODFLOW- 2000 and since:

- rapidly growing long list
- earlier packages are listed here,
- refer to the
  - [USGS MODFLOW and related programs](#) web page, OR
  - use the [USGS OnLine Guide for MODFLOW](#)

GWF1 - ground water flow process (GWF in name file)

finite difference simulation of saturated porous media flow

OBS1 - observation process (OBS in name file)

monitors value of head or flow at specified locations

SEN1 - sensitivity process (SEN in name file)

calculates the change in simulated head and flows at observation locations

PES1 - parameter estimation process (PES in name file)

estimates values of parameters by nonlinear regression to minimize the weighted sum of squared residuals for observations

DIS - discretization package (DIS in name file)

gridding, defining division of space and time for the numerical solution

MULT - multiplier file (MULT in name file)

defines the spatial distribution of multipliers in the grid that act on parameter values specified in those zone



# PACKAGES WRITTEN FOR MODFLOW-2000

## and since: (continued)

ZON - zone file (ZONE in name file)

defines the spatial distribution of zones in the grid where specified parameters apply

BAS6 - basic package (BAS6 in name file)

constant head and no-flow boundary conditions; and initial conditions

OC - output control package (OC in name file)

controls the information and format of results

BCF6 - block centered flow package (BCF6 in name file)

defines material properties with some parameters being dependent on grid dimensions (e.g. transmissivity), thus this package ignores the discretization information in DIS for some purposes -- the parameter method of inputting data cannot be used -- method of interblock conductance calculations can be selected

LPF1 - layer property flow package (LPFin name file)

an alternative to BCF6 defines material properties with all parameters independent of grid dimensions (e.g. hydraulic conductivity) -- the parameter method of inputting data can be used -- method of interblock conductance calculations can be selected

HFB6 - horizontal flow barrier package (HBF6 in name file)

represents thin barriers that occur between model cells by defining their hydraulic conductivity divided by their thickness and specifying where they occur



# PACKAGES WRITTEN FOR MODFLOW-2000 and since: (continued)

WEL6 - well package (WEL in name file)

locations and flow rates of wells

RCH6 - recharge package (RCH in name file)

recharge rates and locations

RIV6 - river package (RIV in name file)

locations, river bed material properties, and river stages

STR6 - stream routing package (STR in name file)

differs from the river package in that the surface water stage varies based on the surface water flow (calculated as specified flow and ground water flux to/from stream) and the Manning equation

DRN6 - drain package (DRN in name file)

location, material properties surrounding drains, and elevation of drains (this update allows a fraction [0-1] of the drain outflow to be returned to a specified cell)

EVT6 - evapotranspiration package (EVT in name file)

parameters describing evapotranspiration rate with depth to water table

GHB6 - general head boundary package (GHB in name file)

locations, local material properties, and elevation of specified heads

CHD6 - time-variant specified head boundary package (CHD in name file)

allows time varying specified head



# PACKAGES WRITTEN FOR MODFLOW-2000 and since: (continued)

SOLVERS (SIP SOR PCG DE4 LMG in name file)

SIP5 - strongly implicit procedure package

SOR5 - slice-successive over-relaxation package

PCG2 - preconditioned conjugate gradient package

DE45 - direct solution by alternating diagonal ordering package

LMG1 - multigrid solver speeds execution for large grids and high degree of heterogeneity

ADV2 - advective transport observation package (ADV2 in name file)

allows use of travel time observations for parameter observations

RES1 - reservoir package (RES in name file)

simulates leakage between reservoir and aquifer as reservoir area changes in response to stage changes

FHB1 - flow and head boundary package (FHB in name file)

allows flow and head boundary conditions that vary at times other than starting and ending times of stress periods

IBS6 - interbed storage (subsidence) (IBS in name file)

simulates compaction related to hydraulic head decline

HUF1 - hydrologic-unit flow package (HUF in name file)

calculates effective hydraulic properties for cells based on geometric description of hydrologic units



# PACKAGES WRITTEN FOR MODFLOW-2000 and since: (continued)

LAK3 - lake package (LAK in name file)

allows variation of lake stage based on water budgets

ETS1 - evapotranspiration package with segment ET function (ETS in name file)

allows function describing evapotranspiration rate with depth to water table to be piece-wise linear

DRT1 - drain package with return flows (DRT in name file)

allows user to allocate proportions of drain flow to be recharge to specified cells

LMT6 - link to MT3D (LMT in name file)

allows printing of file to be read by MT3D for contaminant transport

SFR - Streamflow-Routing package (SFR in name file)

is used to simulate streams in a model (provides greater flexibility in how streams are specified than STR)

UZF - Unsaturated Zone Flow Package (UZF in name file)

simulates vertical flow of water through the unsaturated zone to the saturated zone



# Basic MODFLOW input and output

## **BASIC INPUT ITEMS INCLUDE:**

- Grid
- Time stepping
- Hydraulic parameters
- Boundary Conditions
- Stresses
- Solution parameters

## **BASIC OUTPUT ITEMS:**

- Hydraulic Heads
- Drawdown
- Flow rates
- Mass Balance
- Optional info at specified times
- Iteration information

Underscore files describing various model inputs/outputs  
Binary files containing output in compressed form



# Main MODFLOW input file

## NAME file (.nam)

The NAME file specifies the names of the input and output files used for a MODFLOW simulation, associates each file name with a FORTAN unit number, and identifies the packages that will be used in the model.

An ASCII text file is needed for every process and package defined in the MODFLOW NAME file. This class will focus on the commonly used packages.



# MODFLOW basic: Finite-Difference Methods

For complex systems and boundary conditions, there are no analytical solutions to the groundwater-flow equation, and numerical methods are needed. MODFLOW uses finite-difference methods.

## User

- DISCRETIZE modeled area into N grid cells
- Assign aquifer properties to each grid cell
- Assign boundary conditions

## MODFLOW

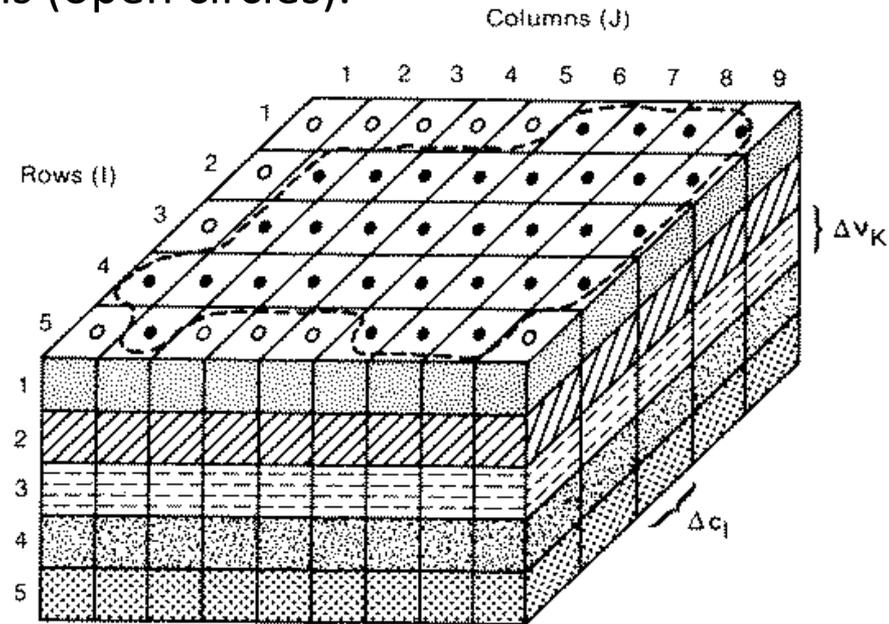
- Set up finite-difference solution to the GROUNDWATER-FLOW EQUATION for each grid cell (N EQUATIONS)
- Either H or Q will be KNOWN at each block N UNKNOWNNS
- SOLVE for H or Q in all blocks using matrix algebra and iterative solutions

$$\frac{\partial}{\partial x} \left( \mathbf{bK}_x \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left( \mathbf{bK}_y \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left( \mathbf{bK}_z \frac{\partial h}{\partial z} \right) = S_s \frac{\partial h}{\partial t} + \sum W(x, y, z, t)$$

# Finite-Difference Grids

Complex geologic material distributions are simplified.  
 Physical aquifer properties likely vary within and between layers.  
 Square or Rectangular grid cells arranged in Rows and Columns  
 Active (closed circle) and Inactive cells (open circles).

Values assigned to grid cells represent the geometry, aquifer properties, boundary conditions, initial condition, and stresses on a groundwater system to build a representation of field conditions.



Layers may correspond to horizontal geohydrologic intervals

- 
- 
- 
- $\Delta r_j$   
number)
- $\Delta c_i$   
number)
- $\Delta v_k$
- $\Delta r_j \Delta c_i \Delta v_k$

- Aquifer boundary
- Active cell
- Inactive cell
- Width of cell in row direction (j indicates column
- Width of cell in column direction (i indicates row
- Thickness of the cell
- Volume of cell with coordinates (i,j,k)

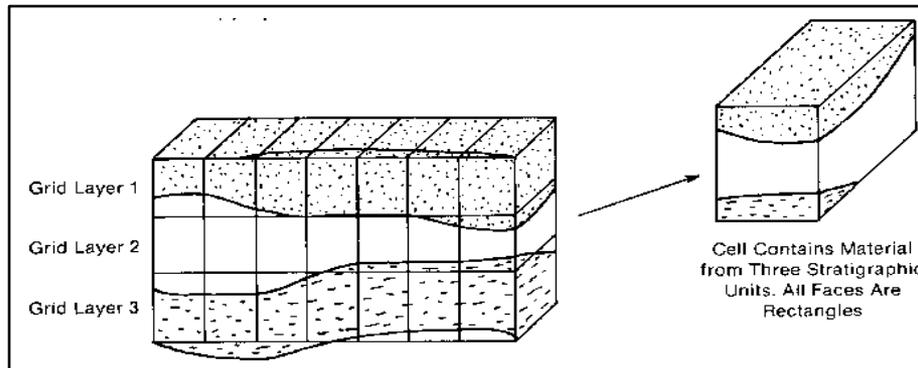
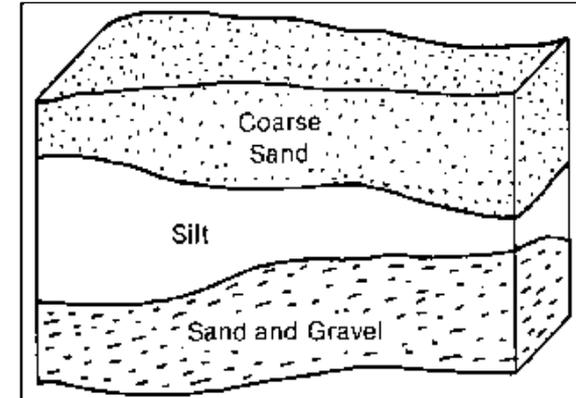


# Finite difference cells

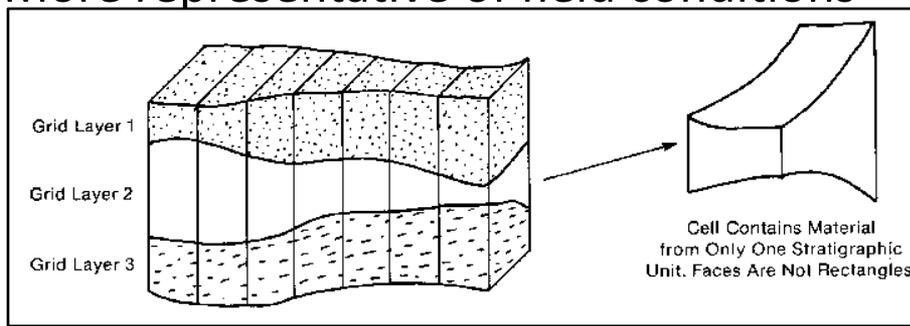
- Mesh-centered
- Block-centered
  - Easier math for boundaries
  - MODFLOW

# MODFLOW: DEFINING LAYERS

- Layer Representation Options
  - Constant layer thickness /variable properties
    - Expedites modeling
    - Rough approximation
    - Compatibility with another function



- Variable layer thickness /constant properties
  - More representative of field conditions





# MODFLOW: DEFINING LAYERS

- One layer
  - layer represents a single hydrostratigraphic unit or aquifer
- Quasi-3D
  - Hydrogeologic units horizontal
  - Leakance
- Fully 3D
  - Dipping units
  - Aquifers and Confining units explicit



# MODFLOW: GRID ORIENTATION

- Grid drawn on an overlay of a map of the area to be modeled
- If possible orient the grid so that the x and y axes are colinear with  $K_x$  and  $K_y$  and vertical axis is aligned with  $K_z$
- For finite difference, try to minimize the number of nodes that fall outside the boundaries of the modeled area
- Set boundaries far from the area of interest so imposed stresses to the interior of system don't reach the boundaries

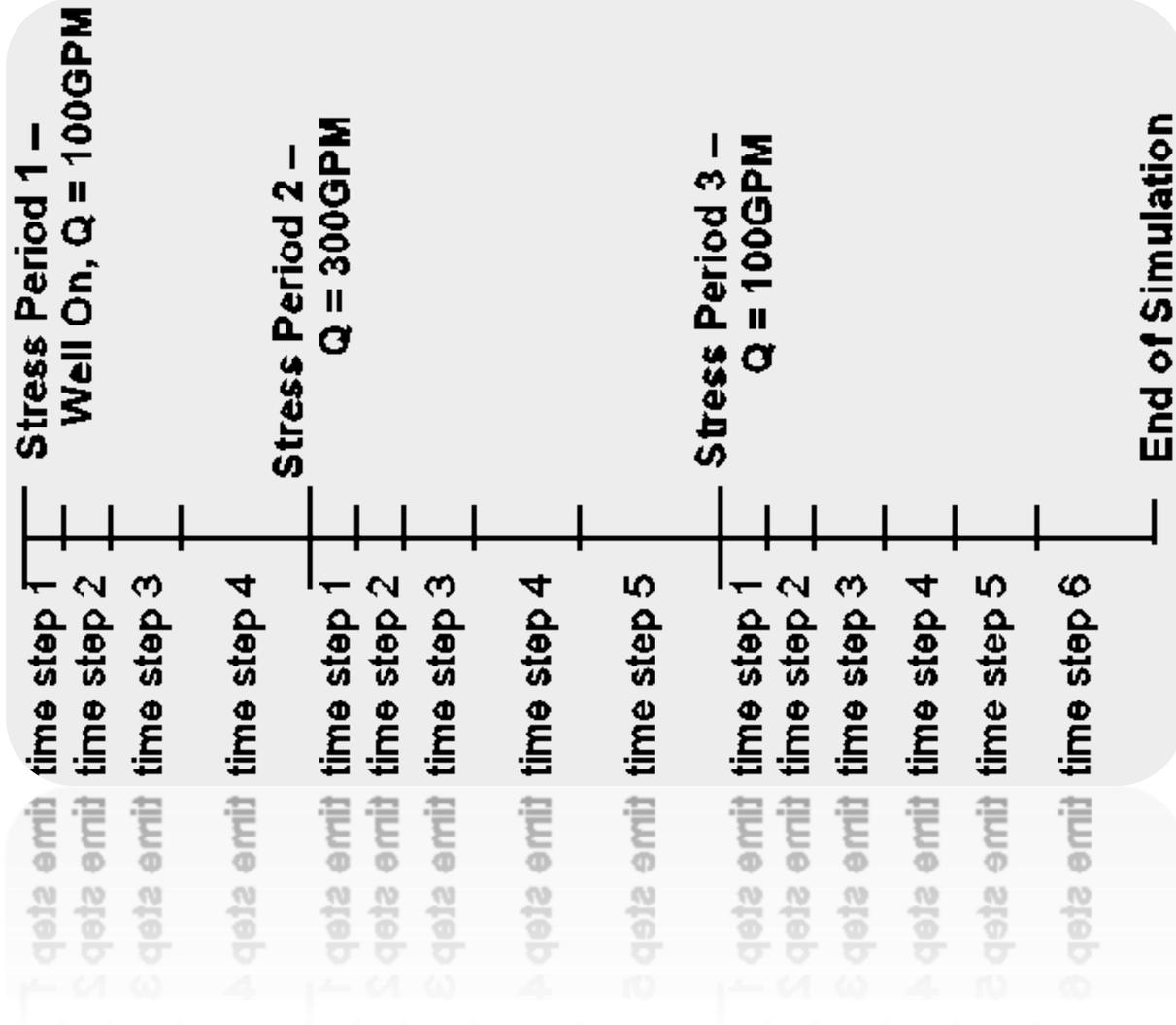


# MODFLOW: DISCRETIZE TIME

## Discretize Time

- TIME STEPS: temporal equivalent of grid cells
  - Small when stresses change and increase in length to a constant, convenient size until the stresses change
- STRESS PERIODS: groups of time steps during which stresses do not change
  - Temporal data compiled at these increments

# MODFLOW: DISCRETIZE TIME





# MODFLOW: DISCRETIZE TIME

- Difficult to decide on initial time step size
- MODFLOW requires the time period, number of steps and a multiplier to gradually increase steps

$$\text{initial time step size} = \text{period length} * \frac{1 - \text{time step multiplier}}{1 - (\text{time step multiplier})^{\text{number of steps}}}$$

Multiplier is typically 1.1 to 1.5



# Flow model creation: Time

## Steady state

- Inputs = outputs. No change in storage
- No time dimension: easier to visualize
- Errors in model setup more clear in results

## Transient

- Requires (often steady-state) initial conditions
- Requires a value for storage
- Stresses are defined using stress periods (time interval of input)
- Each stress period is divided into time steps (time interval of head calculation).
  
- Lengthy calculation times can produce large output files
  
- For some tips on when to “go transient”, see H.M.Haitjema (2006) Role of Hand Calculations in Ground Water Flow Modeling, Ground Water.



# How small is small enough?

- YOU KNOW YOUR DISCRETIZATION IS APPROPRIATE WHEN:

THE ANSWER REMAINS THE SAME FOR:  
SMALLER TIME STEPS, STRESS PERIODS,  
AND  
SMALLER CELL SIZES

- TIME
  - Easy to test smaller time steps
  - Stress periods require recompiling stress data (may be time consuming) and updating any packages with stresses specified
- SPATIAL
  - Unless you have an automated grid generator / input file creator, then the time requirements and logistics of rebuilding the model with smaller cell sizes renders the task unreasonable
  - Important to use smaller grid sizes from the beginning of numerical model development because you will never be able to test this issue.
  - In reality, few if any modelers check this.



# Solving the Finite-Difference Equations

The finite-difference equations for head are solved for each grid cell in a model resulting in a matrix of equations to be solved.

A variety of matrix solution techniques are utilized to solve the finite-difference equations. These techniques iteratively approximate the solution. There are a few essential concepts in order to use a solution wisely

## **DIRECT SOLVER – Exact solution of matrixes**

Direct solutions used rarely because the problems we solve are large and require direct solutions of the entire matrix with available computer memory.



# Finite difference solution (ctd)

## **ITERATIVE SOLVER** – Iterative (approximate) solution of equations starting from initial conditions

Iterative numerical solutions of the groundwater-flow equation matrix are usually employed, and several options are available with MODFLOW.

Iterative solvers begin from an input initial condition (initial head at  $n=0$ ) and repeatedly approximate (*iterate*) the solution to the matrix, until there is very little change from the previous approximation and **the solution converges**.

**Convergence tolerance** is often specified by the user. Sometimes results from subsequent iterations change very slowly, and there is a need to speed up the process. Other times the approximation causes large changes that repeatedly overshoot the answer in opposite directions, and there is a need to slow down the process.

Often the code provides the user the opportunity to specify an **acceleration or relaxation** (two terms for the same variable) parameter to **speed up or stabilize the convergence process**. Occasionally a particular solver requires specific input items and you will need to carefully read the manual to understand the options, but nearly all solvers require a tolerance and relaxation.



# Finite difference solution (ctd)

CONVERGENCE IS "ARBITRARY" i.e. it depends on the tolerance value:

GENERALLY we assume that the user specified a reasonable tolerance and that the solution will be fairly accurate (have a small mass balance) at that precision level

For heads A REASONABLE TOLERANCE is small relative to the total head change across the system and small relative to the head difference between cells in low gradient areas.



# Finite difference solution (ctd)

**IF TOLERANCE IS VERY SMALL, LACK OF CONVERGENCE MAY NOT BE SIGNIFICANT** because the solution may be very precise, that is the mass balance may be very small.

For example, a user may specify a tolerance for head change between iterations that is smaller than the precision of the computer ... this tolerance could never be met but the solution would be very precise. In a case like this, it is usually desirable to increase the tolerance so that the problem converges to avoid the unfounded concerns of those who feel uncomfortable with the words "did not converge!" In reality the solution will not be any better. One could simply look at the model output to see how much head change occurred for the last iteration and use a value just slightly larger. Then the solution would be identical but the output would say "solution converged!"



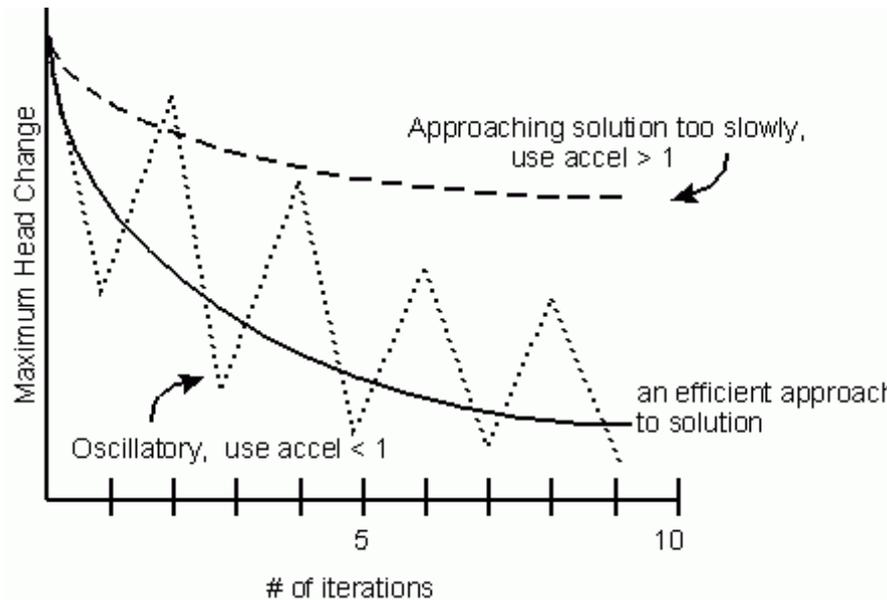
# Finite difference solution (ctd)

**IF TOLERANCE IS VERY LARGE, PRESENCE OF CONVERGENCE MAY NOT BE SIGNIFICANT because the solution may be very imprecise, that is the mass balance may be large.**

For example, a user may specify a tolerance for head change between iterations that is large compared to the total head change across the model or to the difference in head between cells in areas of low gradient. The model would converge after a small number of iterations but the flow field may appear erratic, even with flow apparently generated out of "nowhere" because one cell ends with a high head and flow moves out to all surrounding cells and there is no source to "feed" that radial outflow. Such conditions result in a poor mass balance.

# Acceleration or Relaxation

If progress toward convergence is proceeding too slowly, use a factor larger than one. If progress toward convergence is over shooting the answer (maximum head change alternates sign with each iteration), use a factor less than one.



Typically the maximum head change varies in location. A good code will report the node at which the maximum occurred. If your model is not converging efficiently, it can be useful to note where the maximum head change is occurring. Sometimes evaluation of your input will reveal that you have a "typo", for example you may have typed the exponent on a hydraulic conductivity incorrectly resulting in a large contrast of conductivity between adjacent cells, or you may have added an extra "0" to a boundary head for one cell causing a huge influx at one cell.



# Example excerpt from MODFLOW Output:

## BEGINNING OF SIMULATION

SOLVING FOR HEAD

ITER: 0 RES: 2.5980E+07 CFAC: 1.000

ITER: 1 RES: 1.8517E+06 CFAC: 0.071

ITER: 2 RES: 4.9647E+05 CFAC: 0.268

ITER: 3 RES: 9.6388E+04 CFAC: 0.194

ITER: 4 RES: 2.0855E+04 CFAC: 0.216

ITER: 5 RES: 5.9308E+03 CFAC: 0.284

-----  
PCG ITERATIONS : 5

DAMPING : 0.5662E-07

L2-NORM OF RESIDUAL : 5.9308E+03

MAX HEAD CHANGE : 1.7661E+07

MAX HEAD CHANGE AT (COL,ROW,LAY) : ( 24, 110, 12)

-----  
..

## .LATER TIME IN SIMULATION

ITER: 0 RES: 8.6464E+02 CFAC: 1.000

ITER: 1 RES: 7.0492E+01 CFAC: 0.082

-----  
PCG ITERATIONS : 1

DAMPING : 0.1000E+01

L2-NORM OF RESIDUAL : 7.0492E+01

MAX HEAD CHANGE : 8.5938E-01

MAX HEAD CHANGE AT (COL,ROW,LAY) : ( 11, 49, 6)

-----  
TIME STEP : 5

STRESS PERIOD : 2

GMG CALLS : 4

PCG ITERATIONS : 4

-----  
TOTAL PCG ITERATIONS : 17880



# MASS BALANCE – another consideration for convergence

## **ULTIMATELY THE SOLUTION MUST CONSERVE MASS**

Although your conceptual model may be based on a balanced hydrologic budget, the numerical model will have mass imbalances if the heads are not calculated accurately. The fluxes will be based on gradients between cells. If the heads are not accurate, the gradients will produce inconsistent fluxes, thus the inflows and outflows (note that flow into storage is an outflow and flow in from storage is an inflow) will not balance.

## **EXAMPLES of MODELING PROBLEMS THAT CAN LEAD TO MASS IMBALANCE INCLUDE:**

- large convergence tolerance
- poor conceptual model formulation (i.e. set up is hydraulic nonsense)
- large contrasts in properties between adjacent cells
- large difference in size of adjacent cells
- large time steps or time steps so small that the defined flows are below the accuracy of the computer solution



# MASS BALANCE (ctd)

## **MOST CODES PROVIDE A TABLE TO ASSESS MASS BALANCE**

Generally the table includes a summary of inflow and outflow to and from various types of features as well as the overall flow. This is another good place to pause and assess the model results to be sure everything makes sense. It is also valuable to evaluate the inflow or outflow to each cell where a head or head dependent flux has been specified. Such evaluation can reveal errors that could otherwise go unnoticed yet have negative repercussions on results. The mantra for this is repeated below, always monitor the flow at constant-head nodes and the flux at specified-flux nodes.

## **A SMALL MASS BALANCE IS REQUIRED**

**substantially <1% (0.5% is the high end of acceptable)**



# Example excerpt from MODFLOW Output:

VOLUMETRIC BUDGET FOR ENTIRE MODEL AT END OF TIME STEP 5 IN STRESS PERIOD 16

CUMULATIVE VOLUMES L\*\*3      RATES FOR THIS TIME STEP      L\*\*3/T

-----		-----		-----	
IN:				IN:	
---				---	
STORAGE	= 61384087785.7633	STORAGE	=	5644891.4979	
CONSTANT HEAD	= 0.0000	CONSTANT HEAD	=	0.0000	
WELLS =	0.0000	WELLS	=	0.0000	
DRAINS =	0.0000	DRAINS	=	0.0000	
RIVER LEAKAGE	= 105133899486.2039	RIVER LEAKAGE	=	3559330.3534	
HEAD DEP BOUNDS	= 0.0000	HEAD DEP BOUNDS	=	0.0000	
RECHARGE	= 2.7380E+12	RECHARGE	=	7194487.6472	
SPECIFIED FLOWS	= 0.0000	SPECIFIED FLOWS	=	0.0000	
STREAM LEAKAGE	= 69744176600.6383	STREAM LEAKAGE	=	1955526.7305	
ET SEGMENTS	= 0.0000	ET SEGMENTS	=	0.0000	
MNW =	321347679.5662	MNW	=	47991.3395	
TOTAL IN	= 2.9746E+12	TOTAL IN	=	88402227.5684	
OUT:		OUT:			
----		----			
STORAGE	= 42534787126.9181	STORAGE	=	729950.6762	
CONSTANT HEAD	= 0.0000	CONSTANT HEAD	=	0.0000	
WELLS =	40637515208.1547	WELLS	=	17999510.6501	
DRAINS =	16552965696.6484	DRAINS	=	373047.8186	
RIVER LEAKAGE	= 13184784416.5005	RIVER LEAKAGE	=	975905.1566	
HEAD DEP BOUNDS	= 18640052988.0677	HEAD DEP BOUNDS	=	399313.7562	
RECHARGE	= 0.0000	RECHARGE	=	0.0000	
SPECIFIED FLOWS	= 55214439264.0000	SPECIFIED FLOWS	=	1219104.0000	
STREAM LEAKAGE	= 725689791735.0275	STREAM LEAKAGE	=	7224961.1519	
ET SEGMENTS	= 1.8580E+12	ET SEGMENTS	=	48937653.1254	
MNW =	4123872601.1030	MNW	=	541647.0605	
TOTAL OUT =	2.9746E+12	TOTAL OUT =		88401093.3958	
IN - OUT =	10027659.6802	IN - OUT =		1134.1726	
PERCENT DISCREPANCY =	0.00	PERCENT DISCREPANCY =		0.00	



# MASS BALANCE (ctd)

## **SOMETIMES A LARGE MASS BALANCE IS NOT A PROBLEM:**

For example, if there is a large imbalance for an early time step, perhaps even 200%, it may not be important, because models generally start with very small time steps and gradually increase the length of each time step, so a 200% error in the first time step may only reflect lost accounting for a gallon of water while the problem as a whole involves 10s of thousands of gallons and subsequent time steps have reasonable mass balances.

**MOST IMPORTANTLY ONE MUST CAREFULLY EVALUATE THE MODEL OUTPUT TO DETERMINE WHERE WATER ENTERS AND LEAVES THE MODEL AND ASSESS IF THE FLOW PATTERN AND VOLUMES ARE REASONABLE**

**ALWAYS MONITOR:**

**Q @ CONSTANT H CELLS**

**AND**

**H @ SPECIFIED Q CELLS**



# MODFLOW: Defining Boundary Conditions

- Correct selection of boundary conditions is a critical step in model design.
- For steady-state simulations, the boundary conditions largely determine the resulting simulated flow patterns.
- For transient simulations, boundary conditions can effect simulation results when transient stresses reach the boundary, and realistic boundaries should be selected.
- Physical boundary examples and type:
  - Impermeable rock (no-flow or specified-flux)
  - Faults (no-flow or specified-flux)
  - Lakes (constant-head), constant-flux, or head-dependent)
  - Streams (constant-head, constant-flux, or head-dependent)
  - Springs (constant-head, constant-flux, or head-dependent)
  - Saltwater interface (no-flow)
- Hydraulic boundary examples and type:
  - Groundwater divides (no-flow)
  - Flow lines (no-flow)



It is most desirable to terminate a model extent at physical hydrologic boundaries.

However, model extents may need truncation to maintain the desired level of detail and still have the model execute in a reasonable amount of time. Consequently models sometimes have artificial boundaries. For example, heads may be fixed at known water-table elevations at a county line, or a flow line or groundwater divide may be set as a no-flow boundary.

<b>BOUNDARY TYPE</b>	<b>PHYSICAL EXAMPLES</b>	<b>ARTIFICIAL USES</b>
<b>CONSTANT or SPECIFIED HEAD</b>	<b>Fully Penetrating Surface- Water Features</b>	<b>Distant Boundary (Line of unchanging hydraulic- head contour)</b>
<b>SPECIFIED FLUX</b>	<b>Precipitation/Recharge Pumping/Injection Wells Impermeable material</b>	<b>Flow line Groundwater Divide Subsurface Influx</b>
<b>HEAD DEPENDENT FLUX</b>	<b>Rivers Springs (drains) Evapotranspiration Leakage From a Reservoir or Adjacent Aquifer</b>	<b>Distant Boundary (Line of unchanging hydraulic- head contour)</b>

# Type of Boundary Conditions

<b>BOUNDARY CONDITION NAME</b>	<b>BOUNDARY TYPE &amp; OTHER NAME</b>	<b>MATHEMATICAL NAME</b>	<b>MATHEMATICAL EXPRESSION</b>
<b>Constant/ Specified Head</b>	<b>Type 1 specified head</b>	<b>Dirichlet</b>	<b><math>H = C</math></b>
<b>No-Flow or Specified Flux</b>	<b>Type 2 specified flux</b>	<b>Neumann</b>	<b><math>\frac{\partial h}{\partial x} = C</math> (specified flux)  <b><math>C = 0</math>, No-flow</b></b>
<b>Head- dependent Flux</b>	<b>Type 3 mixed condition</b>	<b>Cauchy</b>	<b><math>Q = f(h, K, A)</math></b>

After:

Definition of Boundary and Initial Conditions in the Analysis of  
Saturated Ground-Water Flow Systems – An Introduction,

O. Lehn Franke, Thomas E. Reilly, and Gordon D. Bennett, USGS - TWRI Chapter B5, Book 3, 1987  
And Anderson and Woessner, 1992, *Applied Groundwater Modeling*



# Back to the world of users instead of programmers --

## What is required for a simulation? How do we start building the model?

Tell the program what capabilities to use

- Name file (NAM)

Package input files for each process (only the GWF Process is always required)

- Basic (BAS6) (can define constant head BC's here)
- Discretization (DIS)
- Hydrogeologic info (for example, LPF or BCF)

Solver. Here we use

- For example, Preconditioned Conjugate Gradient (PCG)



# Activating capabilities

Turn Packages on and define input files using the NAME file

Example:

```
# GW Flow process input files
bas6          41      test0.bas
lpf           42      test0.lpf
wel           43      test0.wel
pcg           44      ../data/test0.pcg
.
.
```

→ Using FREEWAT, the NAME file gets created automatically, but it is important to know that the NAME is the place where the names of all the files used in the model are stored.



# Basics of Data Input

Two types of input data: List data (for example as in the RIVER package that is presented later) and Array data (for example as in the RECHARGE package)

- List data

- Data input using lists of cells

layer row column .....

Example:

1 3 43 .....

2 62 53 .....

- Array data

- Data input in arrays with one row for each row of the model grid and one column for each column of the model grid. Sometimes repeat one array for each model layer.

# # # # # .....

# # # # # .....

# # # # # .....

# # # # # .....

.



# Before starting with the model development - Aspects of flow model creation

- Conceptual model
- Base map
- Grid design
  - Areal
  - Model layers (thickness can be variable)
- Boundary conditions
- Aquifer properties
- Pumping wells
- Recharge
- Time

# If you need any assistance, please contact

Laura Foglia, Technical University Darmstadt - [foglia@geo.tu-darmstadt.de](mailto:foglia@geo.tu-darmstadt.de)

Giovanna De Filippis – Scuola Superiore Sant’Anna (Pisa - Italy) - [g.defilippis@sssup.it](mailto:g.defilippis@sssup.it)

Iacopo Borsi , TEA Sistemi SpA – [iacopo.borsi@tea-group.com](mailto:iacopo.borsi@tea-group.com)

Rudy Rossetto, Scuola Superiore Sant’Anna (Pisa - Italy) – [r.rossetto@sssup.it](mailto:r.rossetto@sssup.it)

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- 1. Hydrological part has been developed starting from a former project, named SID&GRID, funded by Regione Toscana through EU POR-FSE 2007-2013 ([sidgrid.isti.cnr.it](http://sidgrid.isti.cnr.it)).*
- 2. Porting of SID&GRID under QGis has been performed through funds provided by Regione Toscana to Scuola Superiore S.Anna - Project Evoluzione del sistema open source SID&GRID di elaborazione dei dati geografici vettoriali e raster per il porting negli ambienti QGis e Spatialite in uso presso la Regione Toscana (CIG: ZA50E4058A)*
- 3. Latest Version of FREEWAT is under development within EU H2020 project FREEWAT - Free and Open Source Software Tools for Water Resource Management. FREEWAT project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement n. 642224 ([www.freewat.eu](http://www.freewat.eu))*



## FREEWAT

Free and Open Source Software Tools for Water Resource Management  
EU HORIZON 2020 Project

**EIP Water** Online Market Place  
Matchmaking for water Innovation  
**MAR Solutions - Managed Aquifer  
Recharge Strategies and Actions  
(AG128)**

 **ict4water.eu**