MODFLOW with Flopy (1): Intro & Installation

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MODFLOW

What is MODFLOW?

- MODFLOW is the U.S. Geological Survey's computer code
- It solves groundwater flow equation
- Public domain (i.e. free) open-source software written in Fortran
- the "de facto" software for aquifer simulation
- First version : 1983
- Latest version : MODFLOW 6 (Hughes et al., 2017)
- We will use MODFLOW-2005 (Harbaugh, 2005) until MODFLOW 6 becomes full-fledged
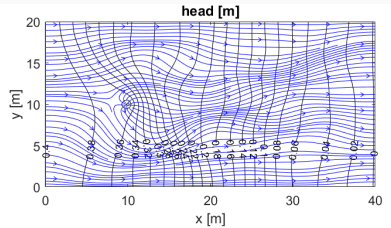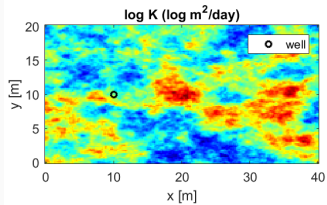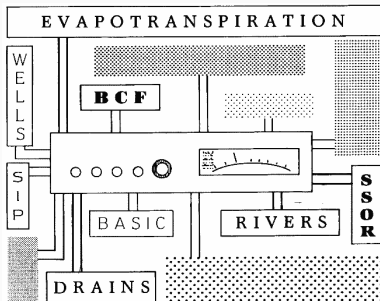
MODFLOW and Relevant Programs

Figure 1: Cover image from McDonald & Harbaugh (1983)

- MODFLOW is organized into "MODules"
- You can activate modules/packages for wells, rivers, drains based on your specific application.

Many other programs based on MODFLOW - so-called MODFLOW suite

- MT3DMS - transport
- MODPATH - particle tracking
- SEAWAT - density-dependent flow and transport in coastal aquifers
- Phreeqc - reaction
- PEST, UCODE - parameter estimation, sensitivity analysis

Some commercial programs (with GUI)

- Visual MODFLOW, GMS, PMWin, …

https://www.dropbox.com/s/64v7wk9ert6xa9h/
transport.avi?dl=0

Plotted using MATLAB (will use python to play the movie later)

Some Comments on MODFLOW

- Most widely used groundwater flow simulation software even accepted by regulatory agencies and cited in statutes
- Have undergone extensive review and improvements
- Many recent updates! - unstructured grid, better numerical convergence to nonlinear processes, and so on
- Still lack of Graphical User Interface (GUI) - unless you use commercial products (Visual MODFLOW, GMS)

Basic Groundwater Flow Equation

3D flow with constant density in porous media is described by

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial \phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_{yy}\frac{\partial \phi}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_{zz}\frac{\partial \phi}{\partial z}\right) + q = S_s\frac{\partial \phi}{\partial t} \qquad (1)$$

where

S is the specific storage $[L^{-1}]$

ϕ is the hydraulic head $[L]$

K is hydraulic conductivity $[L/T]$

q is source/sink term $[T^{-1}]$

MODFLOW

- MODFLOW uses a finite difference method (FDM) using block-centered grid scheme
- FDM solves groundwater flow equations by approximating partial differential equations with algebraic equations, by using finite differences to approximate derivatives
  - Eq. (1) is approximated through a finite set of discrete points in space and time
  - the partial derivatives are replaced by differences in head values at these point
- The domain is essentially discretized as cubic cells
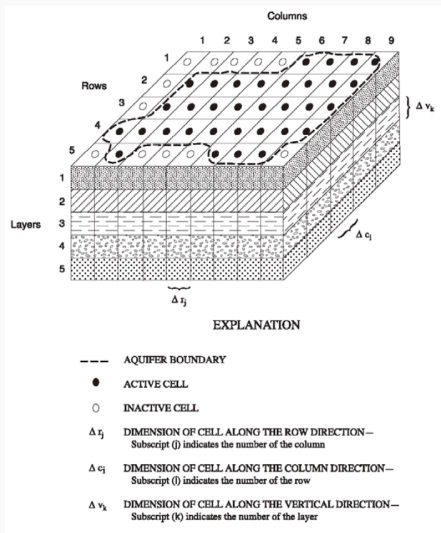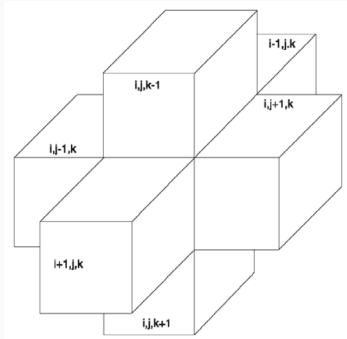- Mass balance is enforced for each cell
- http://pubs.usgs.gov/tm/2005/tm6A16/PDF.htm

Figure 2: Example grid from Fig. 2-1 Harbaugh (2005)

Finite Difference Equation

Water mass balance is accounted for by summing the water fluxes across each side of the cell and internal source/sinks

$$\sum Q_i = S_i \frac{\Delta \phi}{\Delta t} V_i \tag{2}$$

Figure 3: cell (i,j,k) configuration for mass balance equation (from Fig. 2-2 Harbaugh [2005])

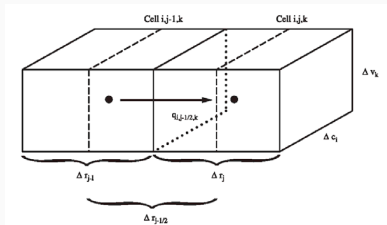$$q_{i,j-1/2,k} = K_{i,j-1/2,k} \Delta c_i \Delta v_k \frac{(\phi_{i,j-1,k} - \phi_{i,j,k})}{\Delta r_{j-1/2}} \tag{3}$$

Figure 4: Flow into cell i,j,k from cell i,j-1,k (from Fig. 2-3 Harbaugh [2005])

Each cell can be

- active cell : variable head
- inactive cell : outside the domain
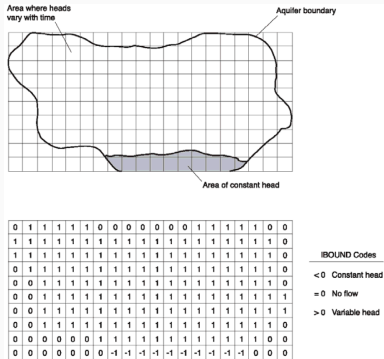- constant head (boundary)

Figure 5: Example of cell type (from Fig 4-1 Harbaugh [2005])

Ultimately, a linear system (matrix equation) is derived from finite difference equation

$$A\phi = f \tag{4}$$

where $\phi = (\phi_1, \phi_2, \cdots \phi_N)^\top$, A is the invertible matrix of coefficients and f the righ-hand-side vector.

MODFLOW provides several algorithms to solve Eq. (4) - like direct, pcg, $\cdots$

MODFLOW Packages

Numerous packages are available; some packages we will use in the class. We will learn how to use these packages by examples!

Package Name	Abbreviation	Description
Basic	BAS6	cell type, initial and boundary conditions
Discretization	DIS	spatial/temporal discretization
Output Control	OC	what and when information is to be output
Layer Property Flow	LPF	performs the (cell by cell) flow computation; K and Ss
Well	WEL	injection/extraction wells
Preconditioned Conjugate Gradient	PCG	solve matrix equation with PCG

References

Harbaugh, A.W., 2005, MODFLOW-2005, The U.S. Geological Survey modular ground-water model – the Ground-Water Flow Process: U.S. Geological Survey Techniques and Methods 6-A16

`http://pubs.usgs.gov/tm/2005/tm6A16/PDF.htm`

McDonald, M.G., and Harbaugh, A.W., 1983. A modular three-dimensional finite-difference ground-water flow model. Open-File Report 83-875. U.S. Geological Survey.

FLOPY

Python package for creating, running, and post-processing MDOFLOW-based models

- open software environment that combines Python with MODFLOW suite
- Flopy can generate input files for the MODFLOW family programs in a few lines of code!

Installation (1)

1. install Python 3.6, we will use ANACONDA Python
   (`https://www.anaconda.com/download/`)
2. install PyCharm Professional, plz apply for student license
   (`https://www.jetbrains.com/student`)
3. install numpy, matplotlib, flopy (in PyCharm,
   File-Settings-Project-Project Interpreter- click "+" on the right
   panel)
4. install MODFLOW
   4.1 (Windows) obtain MODFLOW-2005 executables from
       `https://water.usgs.gov/ogw/modflow/MODFLOW-2005_`
       `v1.12.00/MF2005.1_12.zip` - in the unzipped folder,
       executable file (mf2005.exe) is in "bin" directory
   4.2 (Mac, Linux) install MODFLOW programs
       `https://github.com/modflowpy/pymake`
5. Then copy your executable to your python working directory.
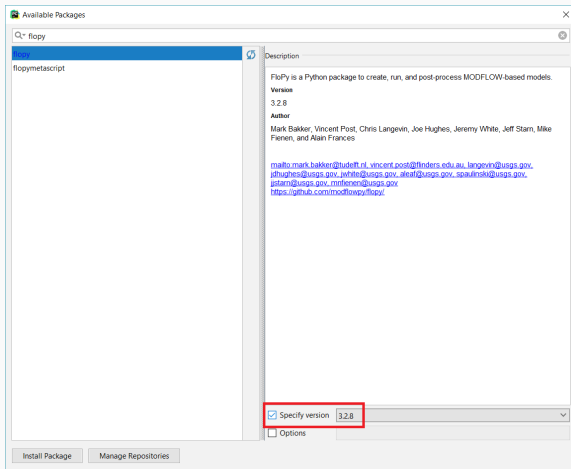
See next slide for more information

For Python, we use Anaconda, an open source Python distribution known for its simple package management. Python is your engine to help you create MODFLOW inputs.

To access and utilize your engine, you need an integrated development environment (IDE) that helps write and run your scripts. We will use PyCharm, which is one of widely used Python IDE.

PyCharm Installation `https://youtu.be/5rSBPGGLkW0`

```
>> import flopy
>> flopy.__version__
```

you should have flopy version '3.2.8' (as of 1/22/2018). If not, install
flopy version 3.2.8 and exit and start PyCharm again.

Please visit `https://water.usgs.gov/ogw/flopy/` for more information

Tutorial:
`https://modflowpy.github.io/flopydoc/index.html`

video by Konrad Hafen `https://youtu.be/kqEDaLR9rB0`

Also read Bakker et al. (2016), "Scripting MODFLOW model development using Python and FloPy", Groundwater. `http://onlinelibrary.wiley.com/doi/10.1111/gwat.12413/abstract`

- Download or copy tutorial01.py from
  `https://github.com/modflowpy/flopy/blob/master/examples/Tutorials/Tutorial01/tutorial01.py`
- Start a project in Pycharm
- Create tutorial01.py and copy the code or add downloaded tutorial01.py
- Run

> Exception: The program mf2005 does not exist or is not
> executable.

You have to install relevant MODFLOW program (mf2005) first and
provide the exact location