Hydraulic groundwater modeling

- Week 10

- Tools for numerical groundwater modeling

Selection of software

- What code is best in solving your particular problem ?
- How accurate will the code be in representing the real world ?
- What are the data requirements for both code and problem ?
- What computer hardware and supporting staff are required ?
- How much training is required to use the software?
- Are there possibilities for support?
- How much will the software cost ?

USGS Modflow

- Developed by USGS
- Based on finite differences (written in Fortran)
- Open source (can be modified)
  - Various extensions, modifications, derivatives
  - Can be linked for heat / mass transfer, pre- & post-processing
- Very popular for aquifer simulation
- GUI controlled and script-based
- Several specialized packages for hydrological situations

USGS Modflow (ctd.)

- Modflow variants: specialized versions for specific tasks
  - SEAWAT – variable density flow and transport
  - PEST++ – parameter estimation
  - FloPy – Python package to run Modflow
  - ModelMuse – GUI for Modflow and derivatives
- Controlling Modflow is usually done using scripts
  - Modflow has its own input/output structure
- Modflow is said to have a steep learning curve, especially if you are not familiar with Python or other kinds of programming

FeFlow

- Finite Element subsurface FLOW system
- Specifically for groundwater flow, mass transfer and heat transfer
- Based on finite elements
- Saturated and unsaturated conditions
- Horizontal and vertical 2D and 3D simulations
- including fluid density effects and chemical multi-component reaction systems
- Commercial software with graphical user interface (GUI)

Spring by Deltah

- Includes density driven flow, heat & contaminat transport
- Includes visualization tools
- Includes Geostatistics and interpolation algorithms
- Allows fracture flow stochastically or explicitly
- Smart meshing
- Sophisticated inclusion of discrete features such as tunnels or mines
- Considers if building crosses geological layers
- Limited version available to use for free

Hydrus

- Simulating water flow, heat and solute transport in variably saturated porous media
- Solution of Richard‘s equation
- Hydrus 1D (open-source) and Hydrus 2D/3D (commercial license)
- Based on FE
- Allows inverse(!) modeling for soil parameters

TOUGH

- Simulator for non-isothermal multiphase flow in porous media
- Primarily designed for geothermal reservoir studies and high-level nuclear waste isolation
- Derivatives: TOUGHREACT and TOUGH2 for reactive flow
- Precipitation and dissolution reactions can change formation porosity and permeability
- iTOUGH2 (inverse TOUGH2) provides inverse modeling capabilities

OpenGeoSys

- Open source project for coupled thermo-hydro-mechanical-chemical (THMC) processes in porous and fractured media
- Optimized for high-performance computing
- Includes GUI tools but also allows scripts using C++
- Focus on coupled processes and complex physics

DuMux

- DuMux = DUNE for Multi-{Phase, Component, Scale, Physics, ...} flow and transport in porous media,
- free and open-source simulator
- C++ research code
- Emphasis on coupled and multi-phase problems

Multi-purpose FE solver

- There is a great number of commercial multi-purpose FE solvers
  - e.g. COMSOL Multiphysics and ABAQUS
- FE based with parallelization options
- Controlled by GUI mainly, but also scriptable
- Not specifically for groundwater flow modeling but very useful for multi-physics problems
  - e.g. hydrogeology & geophysics & engineering
- Usually comparably expansive licensing

Libraries

- If you can programm, you can assemble your own software suite.
- There are several code libraries free to use:
  - help you to get started
  - use advanced High-performance computing (HPC) techniques.
- Go and check out: OpenFOAM, PetSc, Pflotran, …

Lessons learned

- There are many suitable software packages
  - Commercial & open source
- All require training but all rely on principles introduced in this course
- Make a smart choice!