Hydraulic groundwater modeling

- Week 9
- Inside r.gwflow

Groundwater Modeling in Grass GIS

- Groundwater modeling in Grass GIS not high-end
- Developed by Simon Gebbert in 2007 @TU Berlin (Germany)
- Other software maybe more convenient user experience
- Grass GIS allows options and insights hidden by professional software

Discretization in space

- Based on structured meshes
  - 2D: rectangles
  - 3D: rectangular Hexahedron
- Cell-centered finite volume method
  - Variable approximated in the center of control volume
- Chosen scheme valid for
  - Homogeneous (equal volume size in one space direction)
  - Linear, rectangular volumes

Discretization in time

- Implicit Euler backward scheme
  - Unconditionally stable
  - Error grows with increasing time step
- In r.solute.transport
  - If time step > CFL limit: Compute suitable time step and apply until input dt is reached

Numerical dispersion

- Chosen scheme less suitable for hyperbolic PDEs
  - Might cause numerical dispersion
- Check Peclet number for quantification of the effect
  - Reduce grid size if necessary

- To stabilize the advection term, weighting scheme is used
  - Full upwind: use only points upstream
  - Exponential upwind: exponential weighting of points with distance

Iterative solution methods

- Available in Grass GIS
  - Jacobi-Verfahren,
  - Gauß-Seidel Verfahren
  - Successive over-relaxation (sor)
  - Conjugated gradients (CG)
  - Bi-conjugated gradients (BCG)
- Memory efficient
- For groundwater flow: CG well suited based on matrix composition
- For solute transport: BCG well suited based on more complex matrix composition

Stopping criterion for iterations

- Two ways to stop an iteration
  - Convergence of solutions achieved
  - Maximum number of iterations reached
- Convergence error level
  - Solutions of two consecutive iterations differ by less than demanded error
- Maximum number of iterations
  - If solutions do not converge (or only very slowly)
  - Abort criteria to avoid deadlock of computer

Relaxation factor

- An adequate choice of the relaxation factor is non-trivial
- Depends on properties of generates arrays of linear system of equations
- In general < 2
- Related to convergence / can improve convergence
- Used in Jacobi or SOR (iterative) solver

Preconditioning

- Mathematically a transformation
- Making problem more suitable for iterative solver
- Increases the rate of convergence
  - A solution is optained within fewer iterations
- Condition number
  - Function to measure dependence of outcome w.r.t. small input variations
  - A measure of sensitivity
  - Preconditioning reduces condition number
- Calculating the Preconditioner also requires computational costs

Direct solvers

- Available in Grass GIS
    - Gauss-elimination
    - LU decomposition
- Here: Cholesky solver (kind of LU decomposition but more efficient)
- Requires significant amount of memory
- Rather uncommon choice

Super-computing

- Grass GIS supports parallel solution of PDE (gpde library)
- Based on OpenMP
  - Open multi-processing
  - Shared memory parallelization
- Threadsafe
  - Multi-processor execution without blocking or introducing errors

Lessons learned

- Grass GIS is not perfect for groundwater modeling
  - Limited functionality
  - Requires lot of user interaction
- Understanding benefits/drawbacks of solver types
- Functionality of iterative solvers and controling parameters associated with accuracy