InterFrost spread sheet for participant's code information

File is code related, if you use more than one code please provide one file per code …

Aims: 1°) provide pieces of information that will probably be essential to understand possible differences in the results or performances, 2°) provide info that will be essential to improve the codes from a "best practice" perspective.

Name of the code: COMSOL

Participant laboratory: British Geological Survey

Participant name(s): Johanna Scheidegger

Is the code used or developed by the team? COMSOL is a commercially available multiphysics software suite.

Numerical scheme, order of the numerical scheme:

-Linear solver: Direct

-Direct Solver: The MUMPS Solver

The MUMPS solver works on general systems of the form Ax = b and uses several preordering algorithms to permute the columns and thereby minimize the fill-in. MUMPS is multithreaded on platforms that support multithreading and also supports solving on distributed memory architectures through the use of MPI. The code is written in Fortran 90.

-Fully Coupled Solver: uses a damped version of Newton's method, or for stationary problems, a double dogleg method, to handle parameters for a fully coupled solution approach. Here, the constant Newton nonlinear method is used, with a damping factor of 1 (default), and limit on nonlinear convergence rate of 0.9 (default). The Jaobian update is minimal and reuses the Jacobian for several nonlinear systems whenever deemed possible. The Newton iterations are terminated when the estimated relative error is smaller than a specified tolerance. But when the maximum number of iterations have been performed, the Newton's method is terminated even if the tolerance is not fulfilled. Here, a maximum number of iterations of 4 is specified.

If the fully coupled solver does not converge, then the segregated solver is used. This was not necessary for TH1-TH3.

- The Segregated Solver:

The Segregated solver handles parameters for a segregated solution approach. This attribute makes it possible to split the solution process into substeps. Each substep uses a damped version of Newton's method. The segregated solver is terminated when the estimated relative error is smaller than a specified tolerance.

Time discretization strategy (fixed time steps / if adaptative, provide further information)

BDF method: Backward differentiation formula with free steps taken by solver. The maximum BDF order is set to 5 and the minimum BDF order set to 1.

The BDF solver uses backward differentiation formulas with order of accuracy varying from one (that is, backward Euler) to five. BDF methods have been used for a long time and are known for their stability. However, they can have severe damping effects, especially the lower-order methods. Backward Euler severely damps any high frequencies. Even if you are expecting a solution with sharp gradients, you might get a very smooth solution due to the damping in backward Euler.

Spatial discretization

- So far, only 1D and 2D have been implemented, although 3D should also be possible
- internal mesh generator
- Here, a structured quadrilateral mesh is used. Unstructured quadrilateral meshes, or unstructured triangular meshes are also available in COMSOL.

Treatment of non-linearities?

- Method used: damped Newton
- Convergence criterion expression and threshold value:
  Relative tolerance: 1e-6
  Absolute tolerance: 1e-4

Resolution of linear systems

- Linear solvers: The MUMPS Solver (Multifrontal Massively Parallel sparse direct Solver)
- pre-conditioner: are available for iterative linear system solver, but not used here.

How is the TH coupling managed?

- Damped Newton Methods. The nonlinear solver uses an affine invariant form of the damped Newton method

List of available boundary conditions options in the code

- Flux conditions, or Neumann boundary condition. The flux can be calculated based on local values of dependent variables and other parameters. This allows switching between Neumann and Dirichlet boundary condition.
- The Dirichlet Boundary Condition specifies a value of u on the boundary of the domain: u = r. By default, it is a unidirectional condition, applying reaction terms on u but not on any variables appearing in r.
- The Constraint boundary condition specifies an expression R which is constrained to be equal to zero on the selection, R = 0. By default, this is a bidirectional constraint, meaning that all variables in R are affected by reaction terms.

Sources of averaging (under relaxation, spatial averaging on variables …)

Constitutive laws implemented

- Saturation curve: the saturation curve can be easily specified and modified. So far, either a saturation curve after van Genuchten has been used, for which the pore water pressure is obtained via the Clausius-Clapeyron equation, as described by Kurylik 2013.

$$\Theta_w = \left[1 + (\frac{\Theta_s - \Theta_r}{(1 + (\alpha\, P_w)^n)^m})\right]$$

With $P_{wf} = L_f \rho_w \ln(\frac{T+273.15}{273.15})$ and $P_w = bx\, P_{wf}$, where b=1 for solid-liquid-solid contact soils and b=2.2 for solid-solid soils. A, n and m are van Genuchten parameters.

Alternatively, a smoothed Heaviside function, defined as follows is used:

$if\ T < T_r \rightarrow\ \Theta_w = \Theta_r$

$if\ T_r < T > 0 \rightarrow\ \Theta_w = \Theta_r + (\Theta_s - \Theta_r)(0.5 + 0.9375\left(\frac{T+0.5\,T_r}{0.5\,T_r}\right) - 0.625\left(\frac{T+0.5\,T_r}{0.5\,T_r}\right)^3 + 0.1875\left(\frac{T+0.5\,T_r}{0.5\,T_r}\right)^5)$

$if\ T > 0 \rightarrow\ \Theta_w = \Theta_s$

- Permeability as a function of temperature: relative permeability has been implemented either as a van Genuchten curve and related to the Clausius-Clapeyron equation:

$$k_r = \frac{(1 - \frac{(\alpha\, P_w)^{n-1}}{(1 + (\alpha\, P_w)^n)^m})^2}{(1 + (\alpha\, P_w)^n)^{m/2}}$$

Or else, the relative permeability is defined via an impedance law, defined as:

$$k_r = 10\text{^}(-10\left(\frac{\Theta_w}{\Theta_s}\right))$$

What kind of averaging for the properties (depending on water, ice, bulk parameters)?

Thermal conductivity is calculated as a weighted geometric mean from the thermal conductivities of rock, water and ice.

The volumetric heat capacity is calculated as a weighted average of the volumetric heat capacities of rock, water and ice.

Is (massively) parallel resolution implemented?

Not so far, although with the appropriate license Cluster computing should be possible.

Papers / reports / web site providing (further) information

The modelling in the following papers has not been dome with COMSOL, but with FlexPDE, together with Victor Bense

Scheidegger, J. M., and V. F. Bense, Impacts of glacially recharged groundwater flow systems on talik evolution, Journal of Geophysical Research: Earth Surface, doi:10.1002/2013JF002894, 2014.

Scheidegger, J. M., V. F. Bense, and S. E. Grasby, Transient nature of Arctic spring systems driven by subglacial meltwater, Geophysical Research Letters, 39, L12,405, doi:10.1029/2012GL051445, 2012.

Further pieces of information?

The modelling with COMSOL is under development since end of 2014 and mainly heat conduction modelling has been carried out so far.