InterFrost spread sheet for participant's code information

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: **HEATFLOW/3D**

Participant laboratory: ***Université Laval, Quebec City, Quebec, Canada***

Participant name(s): ***John Molson, René Therrien***

Is the code used or developed by the team? ***Code was developed by the team.***

Numerical scheme, order of the numerical scheme: ***Galerkin finite element, linear basis functions, 2nd order accurate Leismann time-weighting scheme (Leismann & Frind, WRR, 1989), Centred time-weighting of spatial derivatives***

Time discretization strategy (fixed time steps / if adaptive, provide further information)
User-defined variable time steps

Spatial discretization

- ***3D (can also be run in 1D or 2D)***
- ***Internal mesh generator or can read an external deformed brick mesh***
- ***Structured grid, 3D deformable hexahedral (8-node) brick elements***

Treatment of non-linearities?

- Method used (Newton, Picard …) ***Picard Iteration for free watertbale (using deformable mesh) and for flow-transport coupling***
- Convergence criterion expression and threshold value:
  User-defined convergence criteria and maximum iteration limits for free watertable, heads and temperature (as part of Picard iteration), and convergence tolerance for the iterative matrix solver.

Resolution of linear systems

- Linear solvers
- pre-conditioner : ***Pre-conditioning conjugate gradient symmetric matrix solver. Leismann scheme is adopted which generates a symmetric transport matrix, while maintaining 2nd order accuracy.***

How is the TH coupling managed?

- Sequential resolution / iterative process / simultaneous inversion?
  Sequential (iterative) resolution of heads and temperature. Picard iteration. Non-linear terms centered in time.

List of available boundary condition options in the code

1st, 2nd, 3rd-type conditions available for groundwater flow and heat transport

3rd -type heat transport boundary at ground surface applies a user-defined variable air-temperature and the model-generated temperature gradient across an exchange layer to allow heat transfer (gain or loss) across the top surface.

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

Under or over-relaxation during Picard iteration is possible. For assembly of element matrices, coefficients are spatially averaged onto elements, based on nodal temperatures and saturations.

Constitutive laws implemented

- Saturation curve
- Permeability as a function of temperature

These functions can be easily modified by the user; see User Guide. Currently, user can choose between 3 functions for the unfrozen water content (Wu) – temperature curve. An exponential relative permeability – Wu curve is used.

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

Volume averaging based on water/ice saturations

Is (massively) parallel resolution implemented?

No, however standard compiler-based optimization and parallelization can be performed.

- Which approach (domain decomposition, loop decomposition). **N/A**
- Indicative number of processors **N/A**

Papers / reports / web site providing (further) information

http://www.science.uwaterloo.ca/~molson/

1. Molson, J.W., E.O. Frind, *HEATFLOW-SMOKER 3D*, Density-dependent flow and advective-dispersive transport of mass, thermal energy or residence time in 3D fractured porous media, Version 5.0, Université Laval & University of Waterloo, 2015.
2. Kalbus, E., Schmidt, C., Molson, J.W., Reinstorf, F., and Schirmer, M., Influence of aquifer and streambed heterogeneity on the distribution of groundwater discharge, *Hydrol. Earth Syst. Sci.*, 13, 69-77, doi:10.5194/hess-13-69-2009, 2009.
3. Markle, J., Schincariol, R., Sass, J., Molson, J. Characterization of the two-dimensional thermal conductivity distribution in an unconfined sand and gravel aquifer, *Soil Science Society of America Journal*, vol.70: p.1281-1294, doi: 10.2136/sssaj2005.0293, 2006.
4. Molson, J.W., Frind, E.O., Palmer, C., Thermal energy storage in an unconfined aquifer 2. Model development, validation and application, *Water Resources Research*, 28(10), 2857-2867, 1992.
5. Molson, J.W., Pehme, P., Cherry, J., Parker, B., Numerical analysis of heat transport in fractured sedimentary rock: Implications for thermal probes, In Proceedings: 2007 NGWA/U.S. EPA Fractured Rock Conference: State of the Science and Measuring Success in Remediation (#5017), Portland, Maine, September 24-26, 2007
6. Yang, J., Edwards, R.N., Molson, J.W., Sudicky, E.A., Fracture-induced hydrothermal convection in the oceanic crust and the interpretation of heat-flow data, *Geophysical Research Letters*, vol. 23 (9), 929-932, 1996.

Further pieces of information? **Includes 1D or 2D discrete fractures. Options available for temperature-dependent geochemical equilibrium speciation and for simulating mean residence time (groundwater age). Direct or numerical integration for element matrices. Deformable mesh for adapting to a free watertable. Does not include solute exclusion during freezing or freeze-thaw induced deformation.**