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

MELT (**M**ultiphas**E** f**L**ow and **T**ransport)

Participant laboratory

Desert Research Institute, Reno, Nevada, USA

Participant name(s)

Jennifer M. Frederick, Ph.D.

Is the code used or developed by the team?

MELT is currently used as a research code by the developer (Dr. Frederick) to study multi-phase, variable-density, subsurface, and submarine flows at continental margins, to better understand the evolution of relict Arctic submarine permafrost and methane gas hydrates.

Numerical scheme, order of the numerical scheme

Finite Volume Method (FVM) scheme, using a 2nd order midpoint rule for surface integrals and gradients at cell faces, and 2nd order volume integrals
Automatic upwinding incorporated for advection

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

Forward difference, first order, explicit in time, used to solve for all time-varying properties, such as temperature field, solute fields (e.g., salinity, concentration of dissolves gases, etc), and phase saturations (e.g., ice, fluid, gas, hydrate).

Time steps are adaptive, and are chosen to satisfy the CFL conditions in each dimension:

$$r = \frac{D\Delta t}{\Delta x^2} \; or \; \frac{D\Delta t}{\Delta y^2} \qquad C = \frac{u_x \Delta t}{\Delta x} \; or \; \frac{u_y \Delta t}{\Delta y}$$

$$in\ each\ direction\ \ C \leq 2r \leq 1$$

and the most restrictive condition is satisfied.

Spatial discretization

2D, internal mesh generator, structured grid which is node centered and velocities are defined on cell faces (staggered gridding).

Treatment of non-linearities?

- Method used (Newton, Picard …)
- Convergence criterion expression and threshold value

Resolution of linear systems

Pressure is solved with an iterative scheme – General Minimum Residual Method (GMRES) or Conjugant Gradient Method (CG) with an Additive Schwarz Method (ASM) pre-conditioner or Incomplete Factorization (ILU) pre-conditioner implemented by PETSc, 3rd party library package (suite of data structures and routines) for the scalable (parallel) solution of scientific applications modeled by partial differential equations, developed and maintained by the Argonne National Laboratory, USA.

How is the TH coupling managed?

Sequential resolution of TH coupling.

List of available boundary conditions options in the code

Any form of boundary conditions can be implemented, but it requires manual modification within the source code.

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

Spatial variable (such as permeability, relative permeability, conductivity, diffusivity, etc.) are averaged using a harmonic averaging in space. Anisotropic permeability, conductivity, diffusivity, etc. are allowed.

Constitutive laws implemented

- Saturation curve
  Any ice saturation curve as a function of temperature can be implemented, as long as a suitable derivative (di/dT) can be defined. Most simulations impose a linear ice saturation function defined by the lower and upper melting temperature, and a minimum (or residual) fluid saturation.
- Permeability as a function of temperature
  Any permeability function can be imposed, but the default is to modify the local porosity, as a function of ice saturation (ice is assumed as solid), and then a Kozeny-Carman relationship is imposed to modify intrinsic permeability to a local permeability as a function of the local porosity.
  The Kozeny-Carman relationship is as follows:
  $K_i = K * [(\phi_i-\phi_c)^3 ((1+\phi_c)-\phi)^2] /[(\phi-\phi_c)^3 ((1+\phi_c)-\phi_i)^2]$
  where ϕ_i is local porosity, ϕ_c is percolation porosity, and ϕ is intrinsic porosity of sediment

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

The grid cell rho*Cp term is defined as a weighted average of the individual phase rho*Cp values:
rho*Cp [cell] = (1-ϕ)*s*rho_s*Cp_s + ϕ*f*rho_f*Cp_f + ϕ*i*rho_i*Cp_i + …

The grid cell thermal conductivity is defined as a mixture model (*not* a weighted average) of the individual phase thermal conductivity values, and can be made anisotropic:
K [cell] = K_s^(1-ϕ) x K_f^(ϕf) x K_i^(ϕi) x …

Is (massively) parallel resolution implemented?

A massively parallel resolution can be implemented, but it is only currently implemented for the pressure solver, using domain decomposition under the PETSc library package. Several hundred processors can be used, however, I have only personally used ~48 because the problem size did not justify a large number of processors. Typically, the PETSc parallel routines do best when the ratio of unknowns to processors is ~10,000 to 20,000.

Papers / reports / web site providing (further) information

Papers published using the MELT research code:

2015 **Frederick, J. M.** & B. A. Buffett (2015), Effects of submarine groundwater discharge on the present-day extent of relict submarine permafrost and gas hydrate stability on the Beaufort Sea continental shelf, *Journal of Geophysical Research Earth Surface*, 120, doi:10.1002/2014JF003349.

2014 **Frederick, J. M.** & B. A. Buffett (2014), Taliks in relict submarine permafrost and gas hydrate deposits: Pathways for methane escape under present and future conditions, *Journal of Geophysical Research Earth Surface*, 119, doi:10.10022013JF002987.

2013 **Frederick, J. M.** & B. A. Buffett (2013), Use of cosmogenic 129-I to constrain numerical models of fluid flow in marine sediments: Application to the Blake Ridge Hydrate Province, *Geochemistry*, *Geophysics*, *Geosystems*, 14, doi:10.1002/ggge.20059.

2011 **Frederick, J. M.** & B. A. Buffett (2011), Topography- and fracture-driven fluid focusing in layered ocean sediments, *Geophysical Research Letters*, 38, L08614, doi:10.1029/2010GL046027.

Further pieces of information?