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 : Arctic Terrestrial Simulator (ATS)

Participant laboratory: Los Alamos National Laboratory

Participant name(s): Ethan Coon

Is the code used or developed by the team? Developed

Numerical scheme, order of the numerical scheme: overall 1st order, see below

Time discretization strategy (fixed time steps / if adaptative, provide further information) : backward Euler, adaptive timestepping, where timestep grows/shrinks based upon number of nonlinear iterations required to solve the previous timestep. Additionally if a timestep fails (i.e. doesn't converge within some number of iterations) we cut the time step and try again.

Spatial discretization: spatial scheme is mimetic finite differences (MFD), which is a locally conservative 2nd order method generally, except that we use upwind relative permeability for flow, which degrades the result to 1st order (but allows kr → 0).

- 2D / 3D
- external/internal mesh generator
- structured or unstructured grids, what kind of polyhedral mesh (tetra ? hexa ?)

Treatment of non-linearities?

- Method used (Newton, Picard …) : Nonlinear Krylov Acceleration (i.e. Calef et al 2011), along with significant custom globalizations strategies that include backtracking, clipping of pressure/temperature updates, and variable changes to locally swap to a energy/water content (similar to Krabbenhoft 2007)
- Convergence criterion expression and threshold value:
  Several parts to the error norm, max of all of:
    - |err_w| / max(mass_w, rho_w * vol * poro * 0.05) where err_w is the error in mass conservation
    - Error in constraint on mass fluxes relative to a typical flux (user-provided) (This is because MFD includes a face unknown which is a constraint ensuring the flux through a face from the left equals the flux through the face from the right.)
    - |err_E| / max(energy_w, E_internal(T=0.01) * rho_w * vol * poro * 0.05

- constraint on energy fluxes as for mass

Tolerance for all runs was 1.e-6

Resolution of linear systems

- Linear solvers: NKA as a solver (like GMRES with a rolling restart)
- pre-conditioner: Boomer AMG

How is the TH coupling managed?

- Sequential resolution / iterative process / simultaneous inversion? Fully implicit coupling (simultaneous inversion)

List of available boundary conditions options in the code:

- Flow: Dirichlet pressure, Neumann flux, Robins, seepage face, "surface flow" BC (formulates diffusion wave equation as a Neumann BC to couple surface and subsurface flow)
- Energy: Dirichlet temperature, Neumann energy flux, "surface energy" BC (formulates advection/diffusion of surface energy as a Neumann BC, along with above enables fully coupled surface/subsurface flow and energy)

Sources of averaging (under relaxation, spatial averaging on variables …): None? Unsure of what you mean here.

Constitutive laws implemented

- Saturation curve: van Genuchten, Brooks-Corey, linear (for unfrozen media). Painter & Karra model for permafrost, along with several other unpublished tweaks to that model.
- Permeability as a function of temperature: We typically write permeability as a function of liquid saturation using the van Genuchten/Mualem relations. This works independently of whether there is ice or not – "freezing = drying" approximation.

What kind of averaging for the properties (depending on water, ice, bulk parameters)? None? Unsure of what you mean here.

Is (massively)parallel resolution implemented? yes

- Which approach (domain decomposition, loop decomposition). Domain decomposition
- Indicative number of processors: ATS has been run on up to 10k cores, more typical problems are 10-100 cores. The limiting factor is often not weak scaling but time step size (strong scaling).

Papers / reports / web siteproviding (further) information

http://software.lanl.gov/ats

Further pieces of information?