

InterFrost inter-comparison stand of July 2015

(CG 24th July 2015)

The final results are now almost all delivered. It really took us some more weeks to converge on the results. So it is time for me to send you an overview of the Performance Measures for the following 13 codes:

Cast3M, OpenFoam, COMSOL, DarcyTools, MELT, SMOKER, ATS, SUTRA, PFLOWTRAN, FEFLOW, GEOAN, FlexPDE, GINETTE

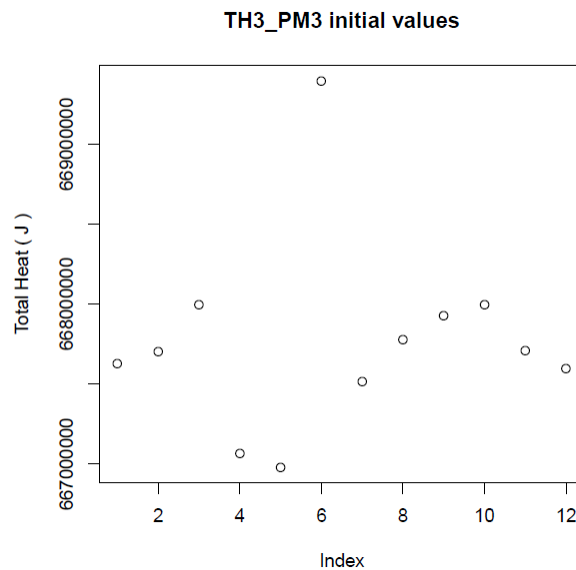
I had removed in between MarsFlo from the group of codes but I guess it should be back. My apologies! Their results are still the same as in April, limited to TH2.

I include here the plots for all Performance Measures. Due to the large amount of codes that are relative close to each other, it is hard to see each individual result. So that I have made special plots for all codes. These "special" plots include the results of this particular code in plain line while all other codes are represented as dotted lines. If you are willing to see particularly how CODE behaves, please download InterFrost_CODE.pdf

In case I still have some errors, of course mention them to me.

Some new analyses of the results are provided in these plots as well as the general plots InterFrost_Total2_meanvar.pdf :

1°) **Scatter plots of several initial conditions** are provided in pages 21-23 corresponding with TH2_PM3 (total volume of water), TH3_PM1 (equivalent hydraulic conductivity), TH3_PM3 (Total sensible heat). These differences are mean to be of interest because they are probably the result of different meshing strategies which might not exactly provide the accurate initial condition geometries. The order of the indices is the one of the codes provided above previously, see examples below.

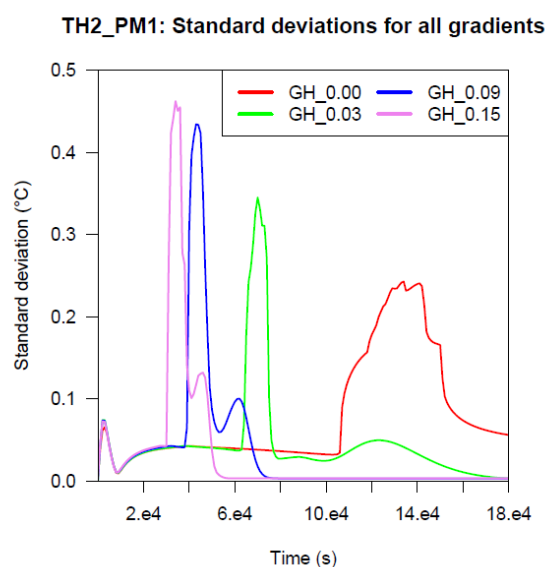


TH3_PM3 initial values for all codes from 1 to 13: 1-Cast3M, 2-OpenFoam, 3-COMSOL, 4-DarcyTools, 5-MELT, 6-SMOKER, 7-ATS, 8-SUTRA, 9-PFLOWTRAN, 10-FEFLOW, 11-GEOAN, 12-FlexPDE, 13-GINETTE

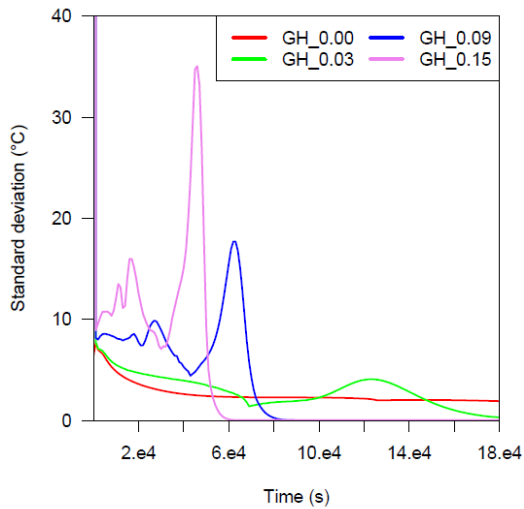
2°) Other analyses introduced here are the **mean curves as well as the standard deviations**. These curves are computed for each time step (I firstly projected all curves provided on a regular grid). This is a classical mean and the standard deviation. I then plot in plain black lines the evolution of the mean (limited here to TH2 results solely, in a first tentative way) and the mean - (2 times the standard deviation) and the mean + (2 times the standard deviation). All code results are plotted in dotted lines in the background.

The initial idea was to sum up all the 13 code information in a simple format for the next generation of modelers to come and compare their results with us and see if they are "within the bounds". But for some PMs, the mean curve is really different from any curve and the space between all 3 curves does not contain the simulations. Maybe the envelope of the curves will be a better information to propagate for future modelers willing to compare their results with us.

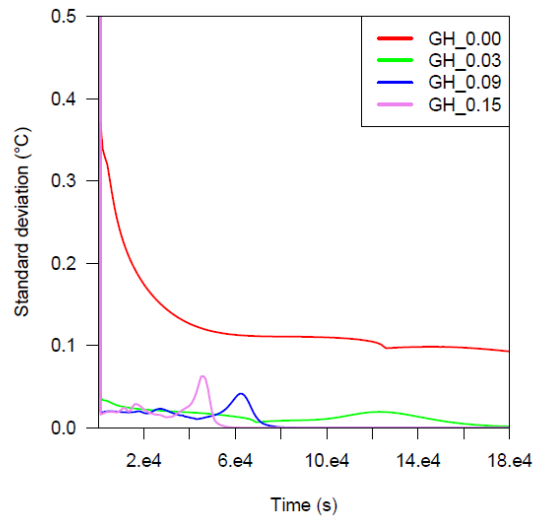
Another reason to provide this second analysis is to look at the standard deviations. The standard deviation provides indeed some information about the range of dispersion of the results. One of the immediate impression we had in April, looking at the first inter-comparison results was that the lower gradient cases are the cases where the dispersion of our results is maximum (we don't perform well there !?) and considering higher levels of advectons (larger head gradients) would kind of make us, closer, converge. The information contained in the standard deviation is intended to measure this. Plots as a function of head gradients however shows that this is not really the case (except in the case of TH2_PM2 maybe). In some cases where the mean has some evolution and does not get to zero, it is better to draw the standard deviation relative to (divided by) the mean. For TH2_PM1 moving from negative values to positive I did not find any way to introduce the mean while for the fluxes of TH2_PM2 the maximum level of the mean corrects the relative amplitude differences. For the total water volumes (TH2_PM3), dividing directly by the mean is the best option but does not change significantly the shape of the curves as compared with the direct plot of the standard deviation. As a conclusion to the question: "where do we perform the best (the least scattered), with high advection or low?" the answer is not straightforward, no so clear trend appears in my view. A major conclusion for me is however that we do not perform very differently as the head gradient increases while I would have initially guessed that the discrepancies would increase. We probably have similar numerical schemes when it comes to the advective component.



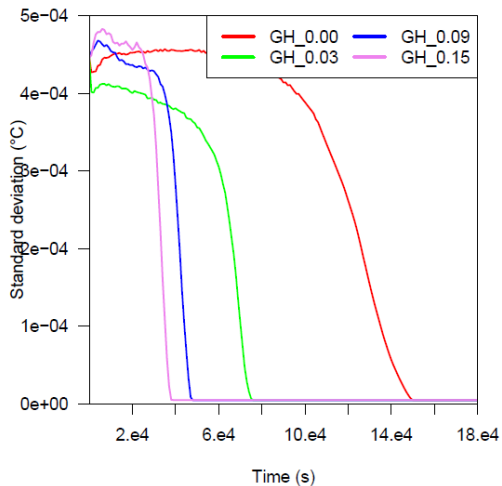
TH2_PM2: Standard deviations for all gradients



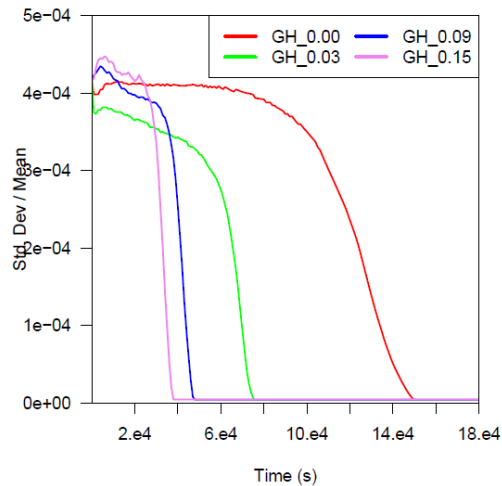
TH2_PM2: Std. Dev. / Max(Mean) for all grad.



TH2_PM3: Standard Deviation for all gradients



TH2_PM3: Standard Dev. / Mean evolution for all grad



Now I will carry on with some requirements useful for the further analysis and preparatory step for our common paper:

1. Please provide some information in the table below with simulation characteristics: meshing strategy (projected on regular mesh or dedicated mesh), number of elements ...
2. Please comment on the discrepancies in regard of your code results versus the group of results, especially
 - a. point out discrepancies that could result from differences in the implementations of the equations (e.g. other terms, volume change associated with liquid to solid water phases that was not included in the benchmark equations, other boundary conditions),
 - b. Are you using the reference characteristic laws (e.g. freezing function, intrinsic permeability curve),
 - c. If you carried on convergence tests, please mention how mesh refining changes the curve (for instance for me refining mesh means moving threshold time for TH2_PM1 to later times)

So I suggest you fill up the next page and send it back to the group per email.

I tried to prepare the framework for a forum on the InterFrost web site as well as a place to share documents. I was unfortunately too much in a rush this month to make it work properly. Sorry. We will have to exchange information per email. By the way, the suggestion of using google tools is appropriate by strictly forbidden at our lab for security reasons. One of the organizations supervising our lab is the French Atomic Commission ...

With all this I will be back I guess in September with some draft paper.

The questionnaires you filled in are still available on the web site (participant and lab pages) and provide a valuable complementary base of information. I enclose them all in zip form on the web site July Inter-comparison. Please mention to me in case I happened to forgot yours.

Questionnaire, July 2015

For the reference calculation you provided in TH2:

Code	Number of nodes	Number of elements	Element type	Further information?
Cast3M	31609	31104	Quadrilateral	2D simulation

For the reference calculation you provided in TH3:

Code	Number of nodes	Number of elements	Element type	Further information?
Cast3M	8848	17272	Triangular	2D simulation

Does your code differ from the reference cases? Did you identify features that would be a source of discrepancies of the results? (different terms in the equations, different simplifications, different freezing curve or intrinsic permeability curve implemented ...):

If you carried on convergence tests, please describe what influence the meshing has on the PMs (NB the case of TH3_PM2 was already identified: the more refined the grid the higher the fluxes, apparently with no limit, because of the close presence of imposed 5°C and -5°C points at adjacent nodes in the corners):

Any further comment?