pmd*RT: Coupled fluid, heat and chemical modelling

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Project F6-M9

Why Reactive Transport Models

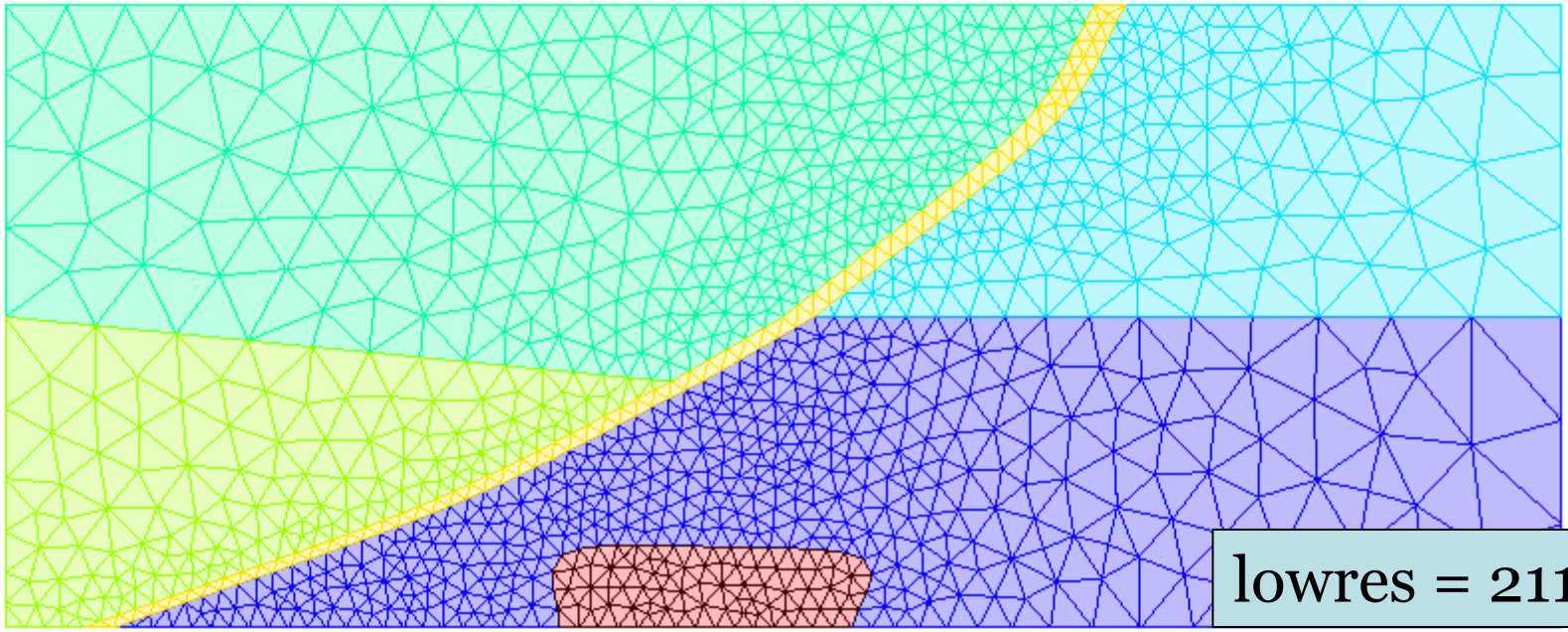
- RT Modelling simulates coupled fluid-flow, heat-chemical transfer, and fluid-rock reaction
- Modelling to understand the feedback, interaction and outcomes of coupled physical processes
- Progress towards modelling natural processes in 3D
  - predictive 3D boxes!

Summary

- pmd*CRC now has a usable reactive transport code
- Applied development stage at the moment
  - Some issues to be sorted but very serious progress being made
  - Benchmarking started
- GUI being developed (Chook-RT?)

*pmd*RT?*

- pmdCRC developed reactive transport code
  - Couples heat, fluid and chemical transport and chemical reaction – Mechanics being currently being considered!
  - Uses finite element – non-uniform mesh
  - Uses FastFlo4 to solve PDE's coupling of external modules (i.e. EOS)
- Running in windows environment
  - JCU Cluster – Win64 on multiprocessor AMD operton 2.6 (20% quicker than P4 3.2HT)
- Chemical Solving
  - Currently via the WinGibbs solver used in HCh
  - Log K solver capability being developed
- Easy to add extra functionality via Python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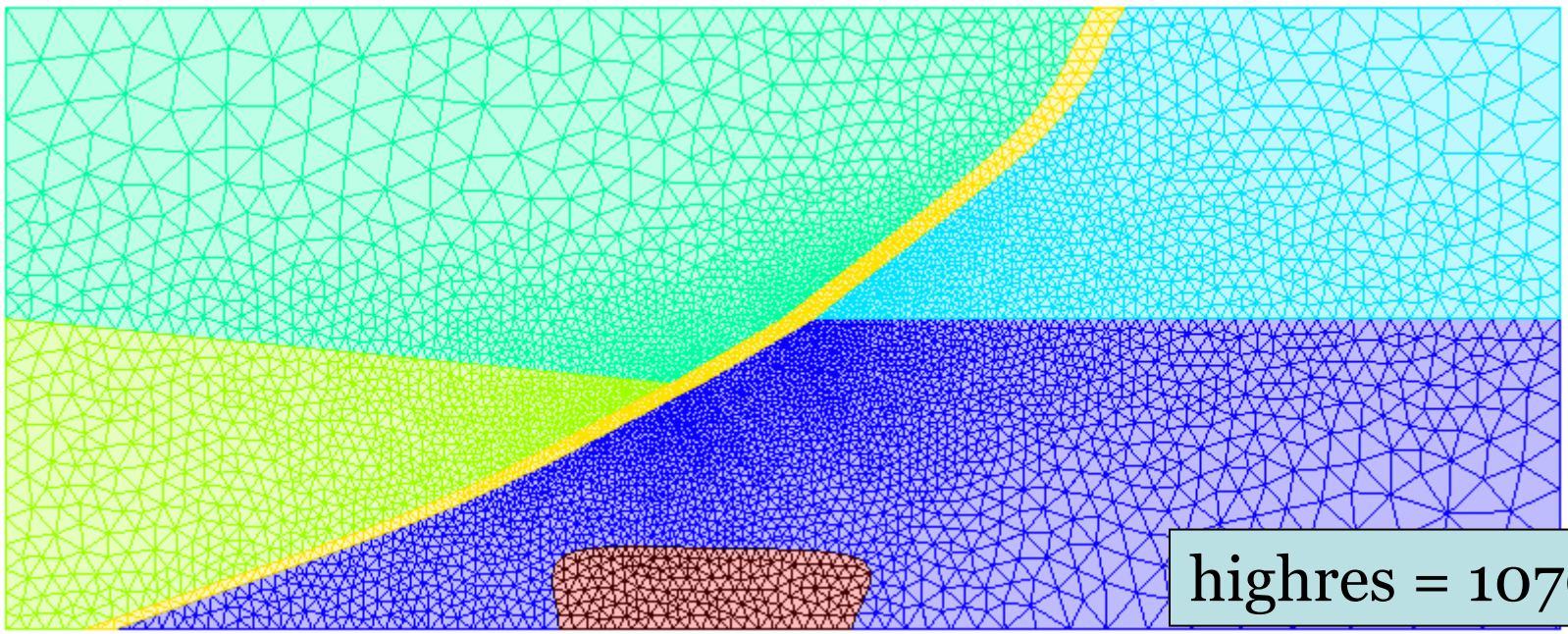
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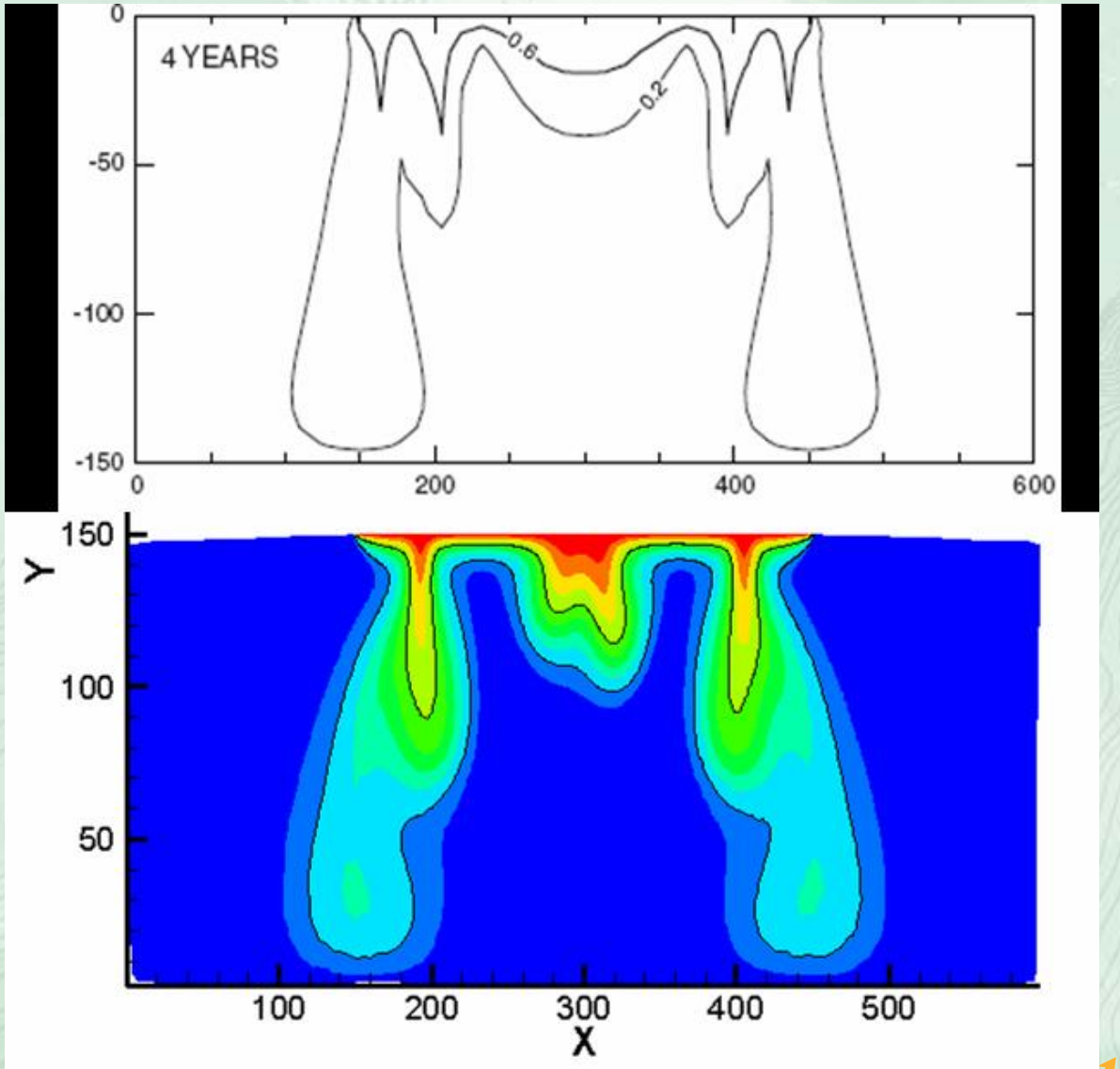
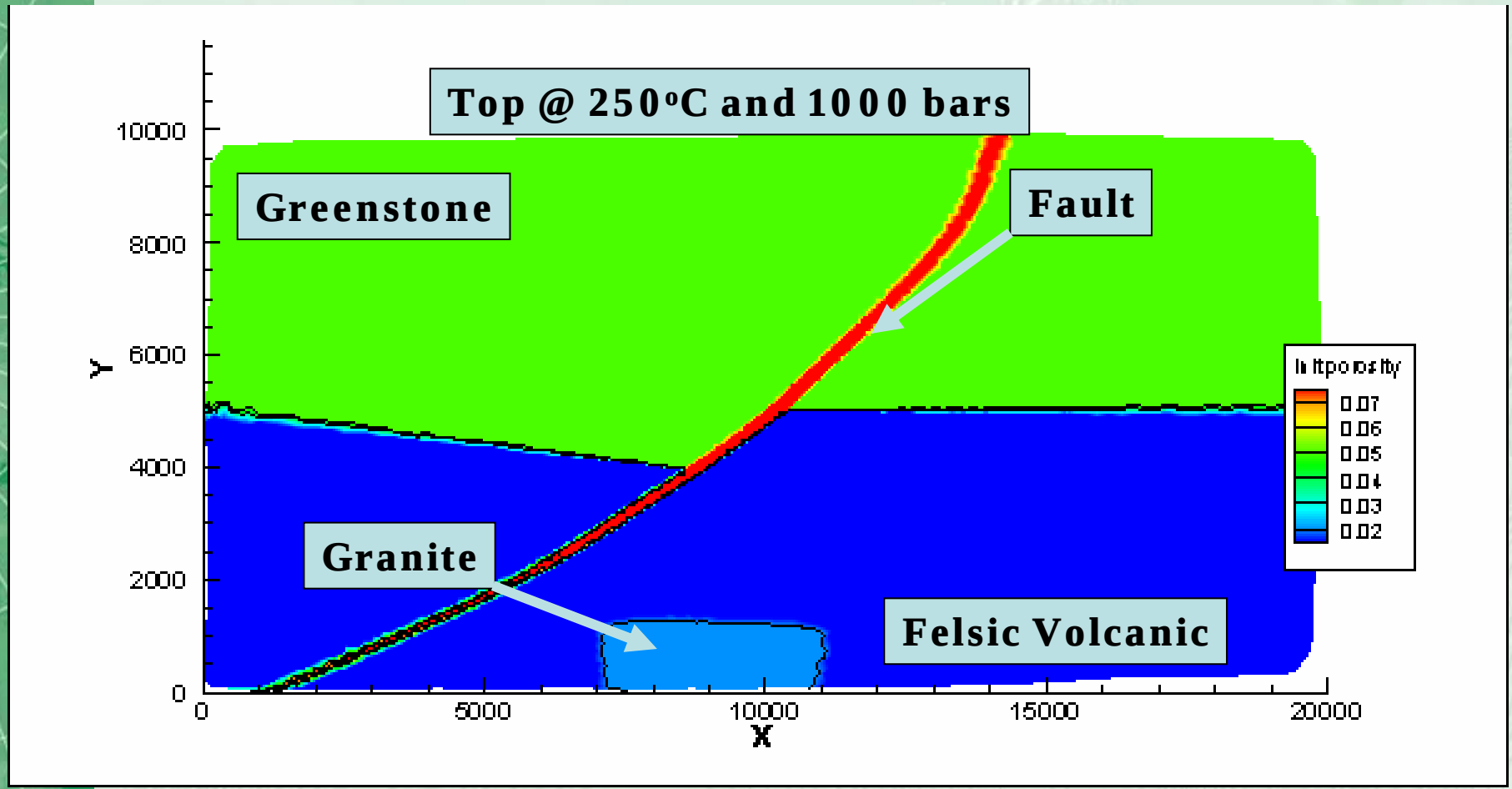
Benchmarking

Comparison of modified Elder problem with HST3D (USGS benchmark hydrological code)



Application and Testing



Physical Properties

Rock Unit	~mineralogy	Log permeability	porosity	ini gold in fluid (molal)
Greenstone	**qtz calcite albite tremolite chlorite pyrrhotite**	**-16**	**0.05**	**$1x10^{-9}$**
Felsic Volc	**qtz pyrite albite muscovite k-feldspar**	**-17**	**0.01**	**$1x10^{-9}$**
Fault Zone	**qtz albite muscovite calcite pyrite pyrrhotite**	**-15**	**0.08**	**-**
Granite	**qtz muscovite k-feldspar plagioclase (ab-an) pyrite magnetite biotite**	**-16**	**0.02**	**$1x10^{-6}$**

granite:

'NaCl (aq)' : 0.89,
'KCl (aq)' : 0.28,
'CaCl2 (aq)' : 0.02,
'FeCl2 (aq)' : 0.40,
'H2S (aq)' : 1e-3,
'Au+ (aq)' : 1e-6

fault_zone :

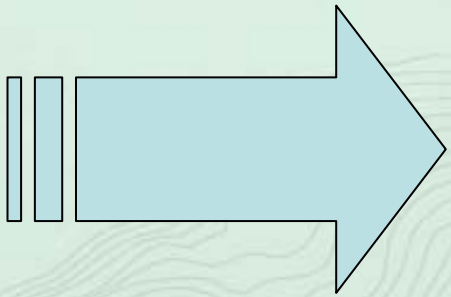
'NaCl (aq)' : 1,
'KCl (aq)' : 1

felsic volcanic:

'NaCl (aq)' : 1.32,
'KCl (aq)' : 0.40,
'CaCl2 (aq)' : 0.12,
'CO2 (aq)' : 4.7,
'H2S (aq)' : 2.86e-2,
'SO4-- (aq)' : 1e-5,
'Au+ (aq)' : 1e-9

greenstone :

'NaCl (aq)' : 0.78,
'KCl (aq)' : 0.16,
'CaCl2 (aq)' : 0.75,
'CO2 (aq)' : 0.05,
'H2S (aq)' : 5.6e-4,
'Au+ (aq)' : 1e-9



1) Aqueous components added to rock and fluid (vol by porosity)

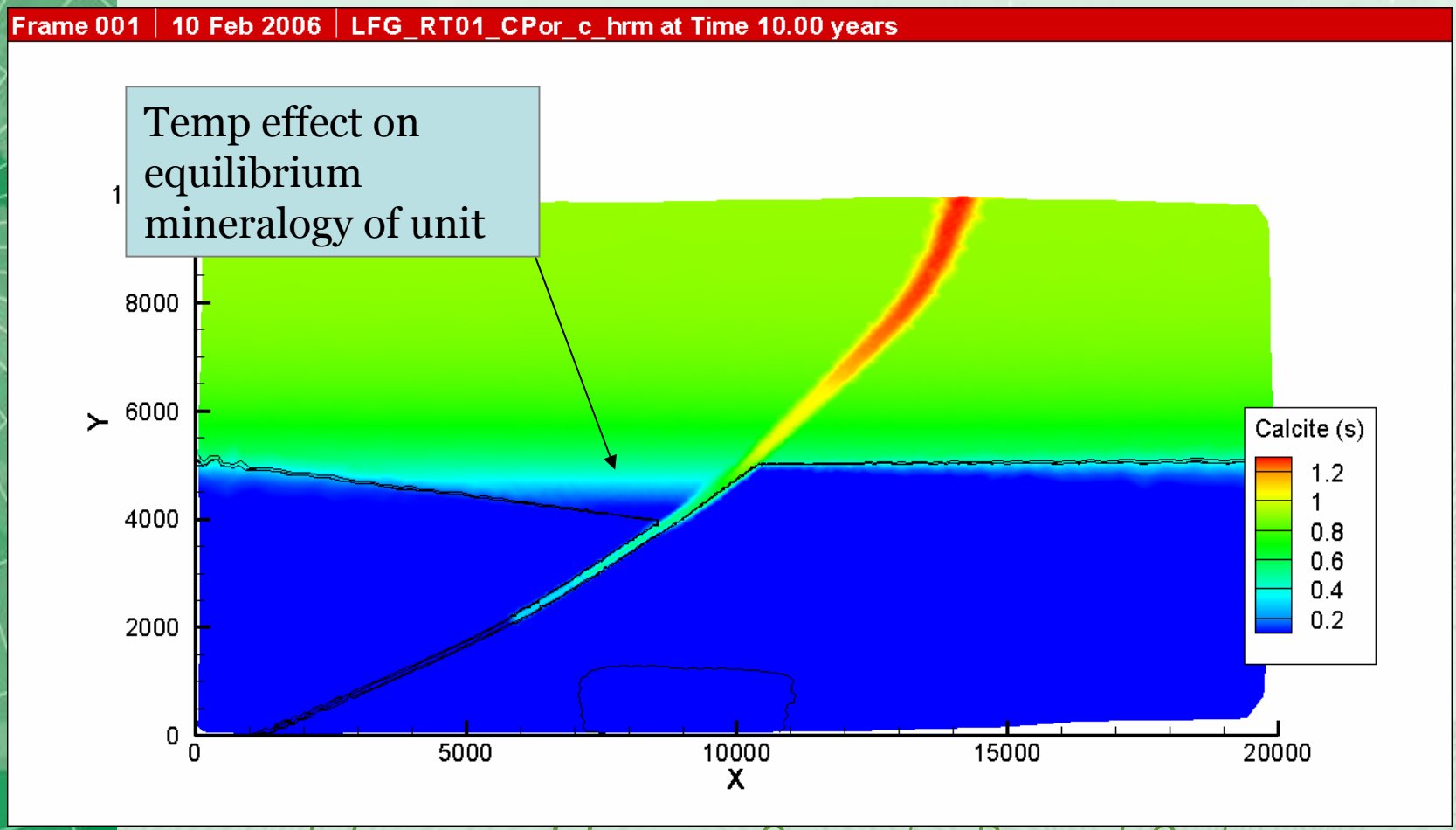
2)

-> Equilibrium step 0

-> Equilibrium step 1

Initialised Fluid-Rock System

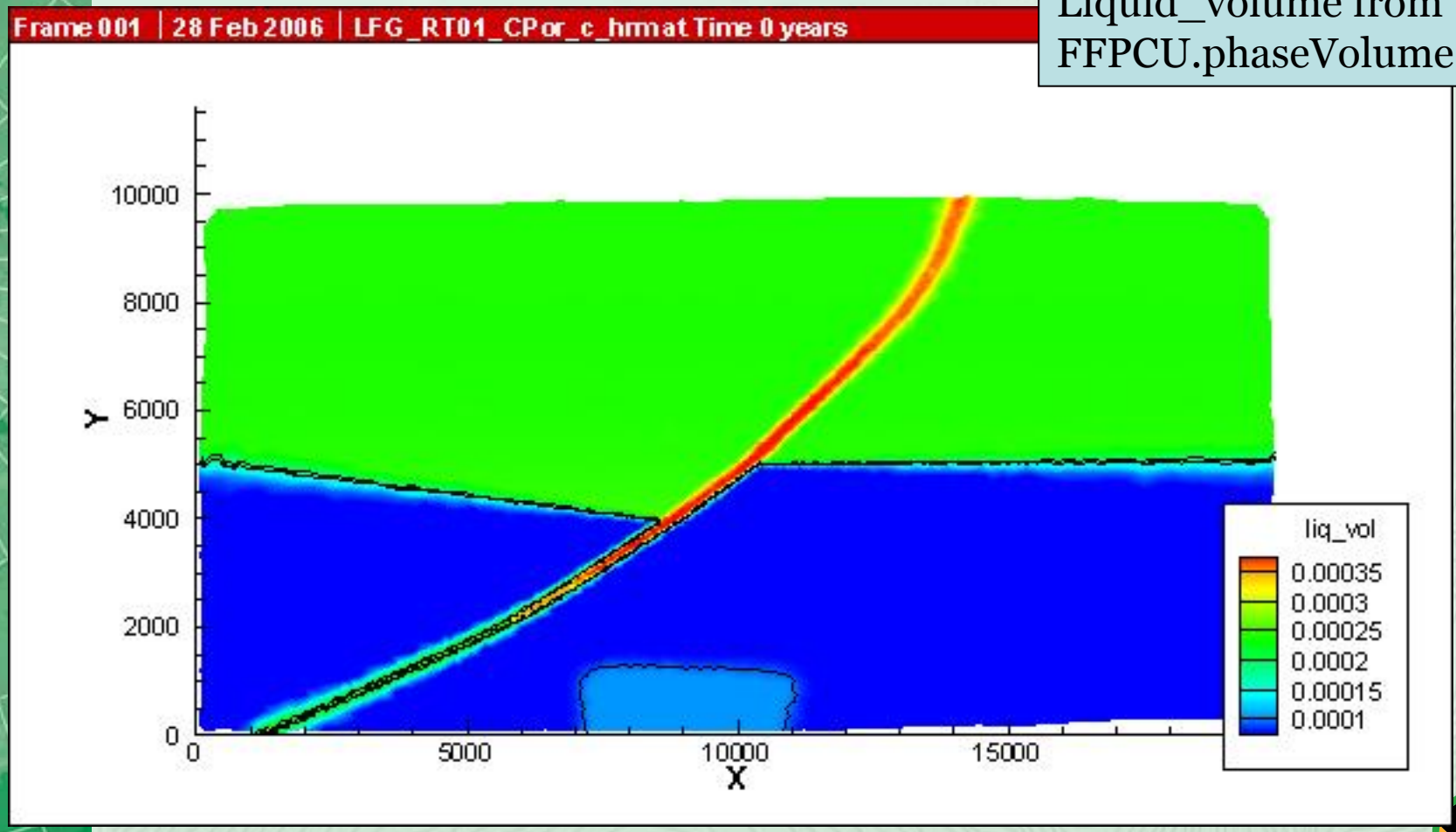
Initialisation of Chemistry



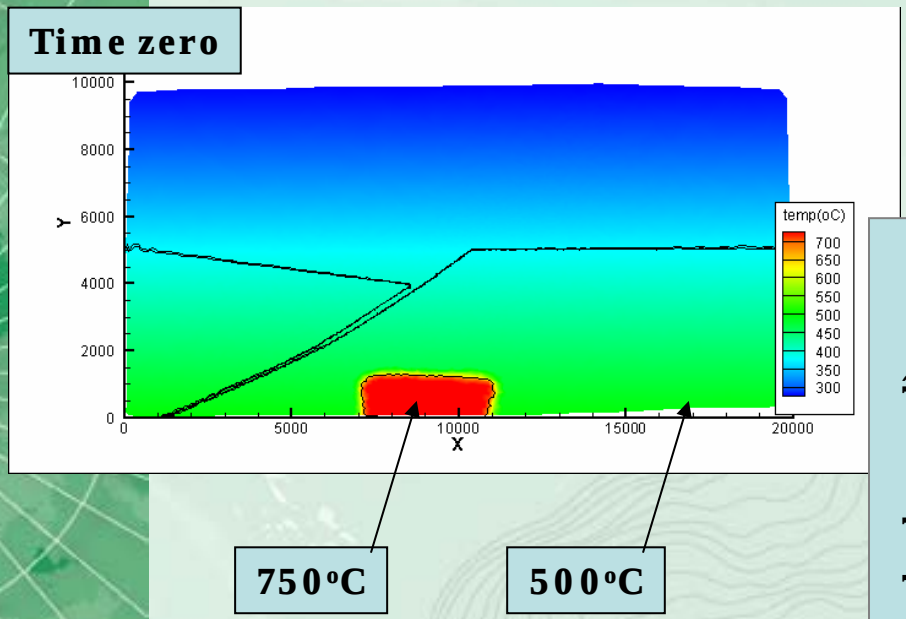
pmd*CRC

Liquid_volume @ step 0

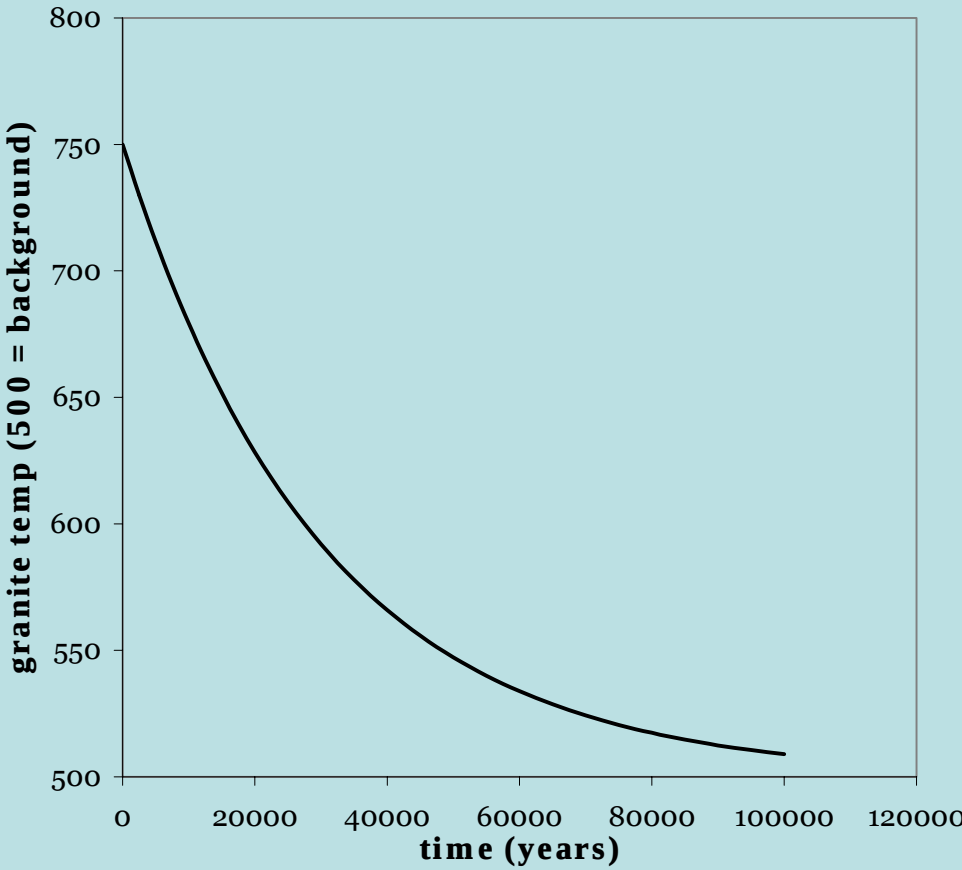
Liquid_volume from FFPCU.phaseVolume



Granite



Uses a dynamic boundary condition that allows the fluid to cool the granite further.

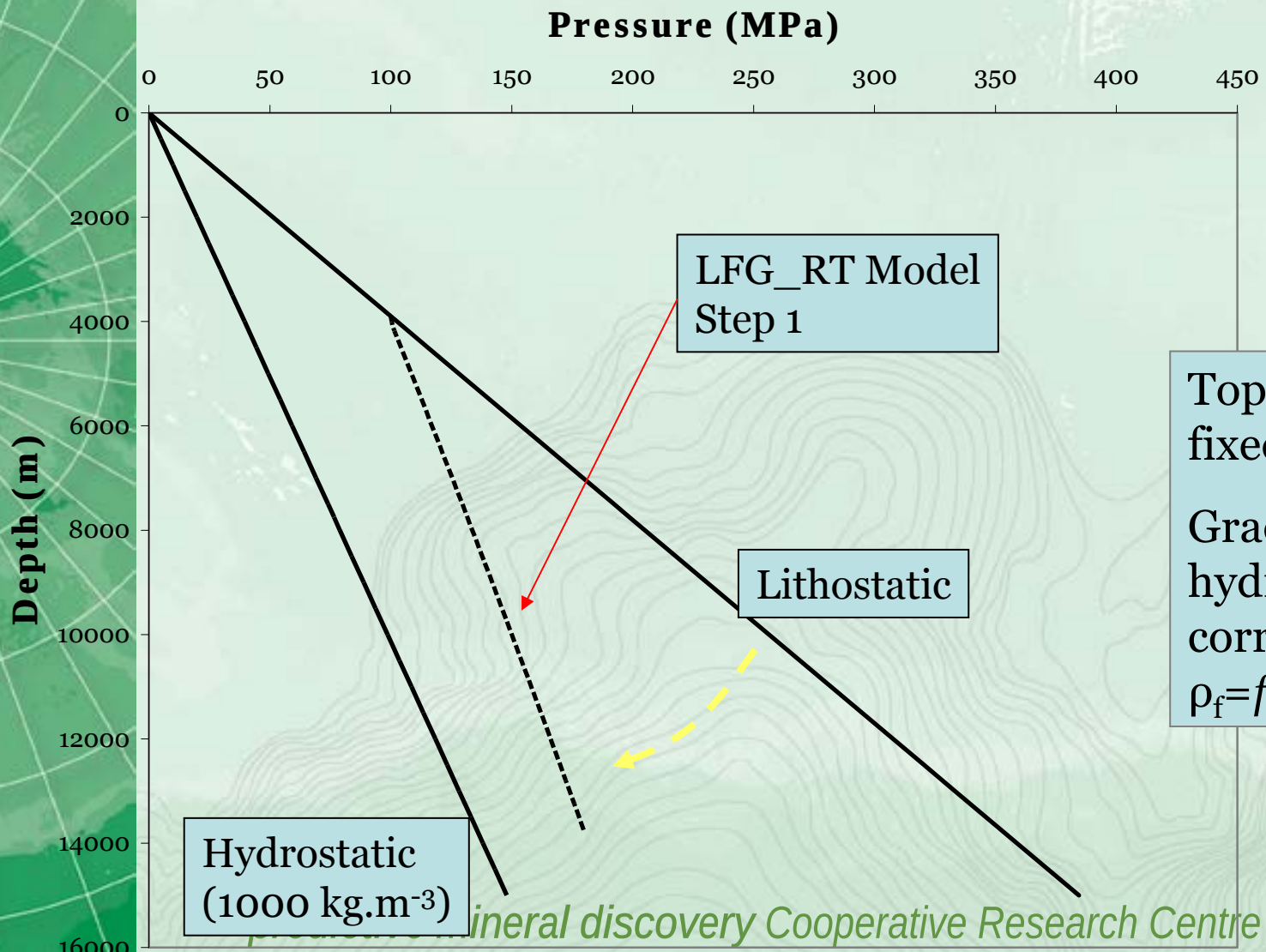


Granite cools by:

excess_t * $e^{(-time/event\_length)}$

event_length = 30,000

Pore Pressure



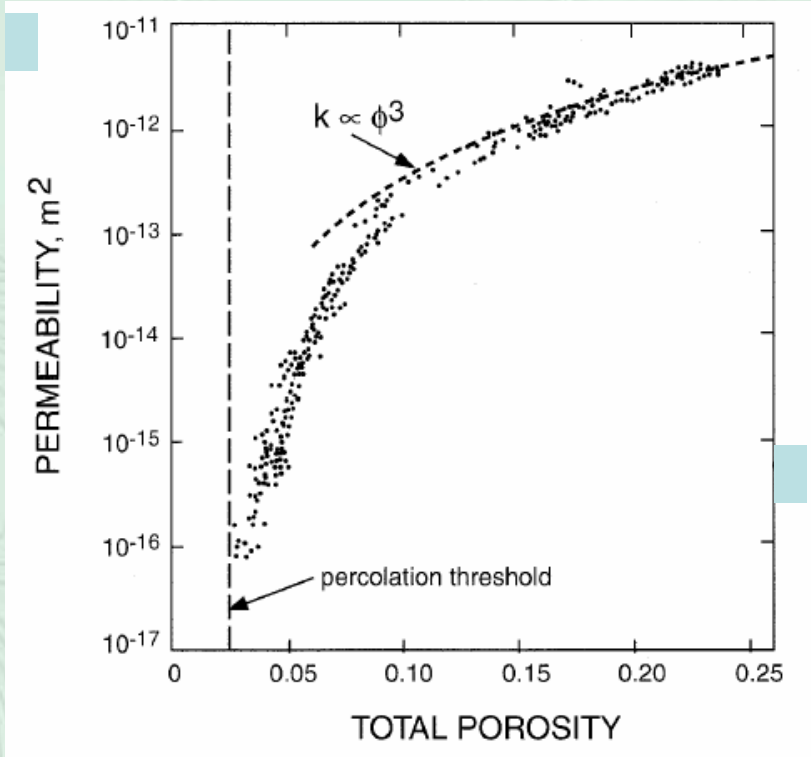
Top boundary is fixed porepn

Gradient is hydrostatic with correction for $\rho_f = f(T)$

Movie

Dynamic Porosity-Permeability

- Chemical reactions will dissolve of precipitate mass
  - Porosity increases or decreases
  - Permeability will change based on some relationship to porosity



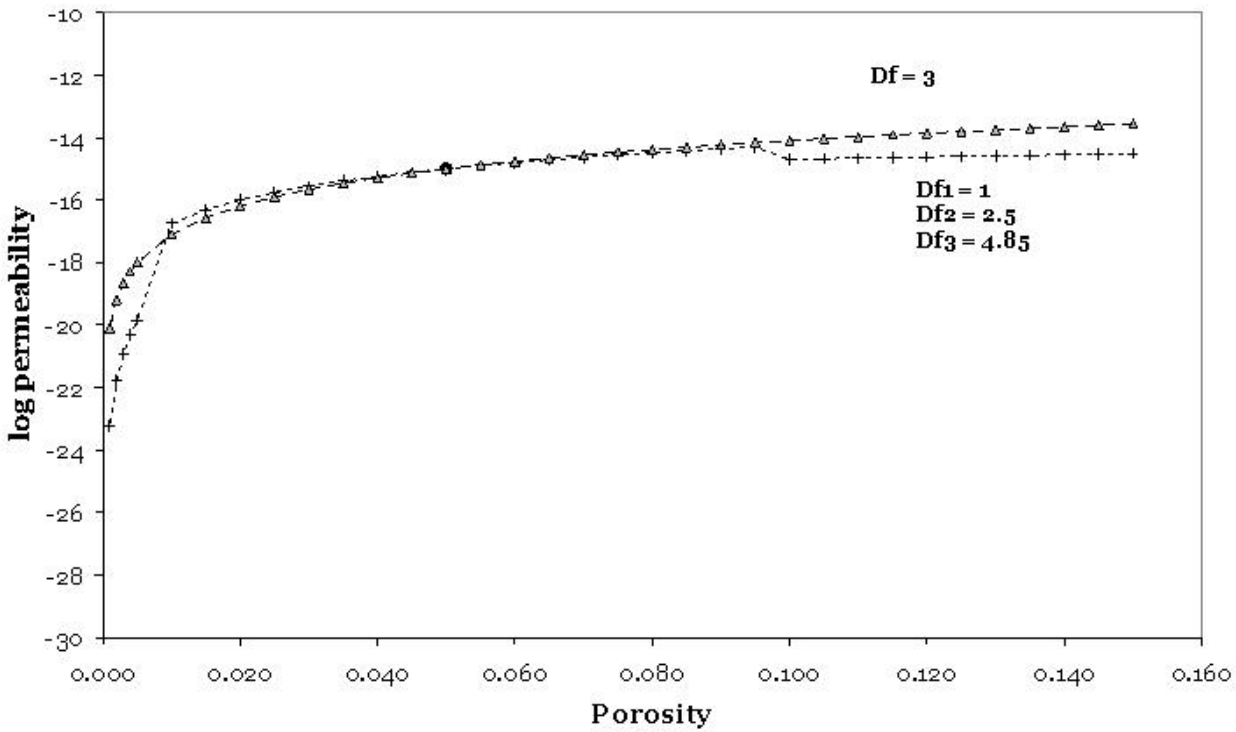
Cox et al., 2000

Dynamic Porosity-Permeability

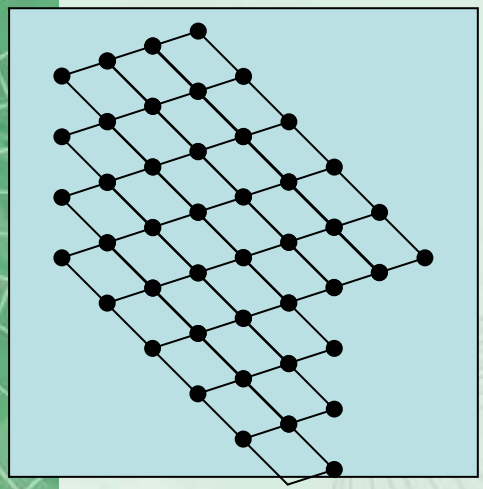
$$\phi = V_f$$

$$\kappa = \kappa_0 \left(\frac{\phi}{\phi_0} \right)^n$$

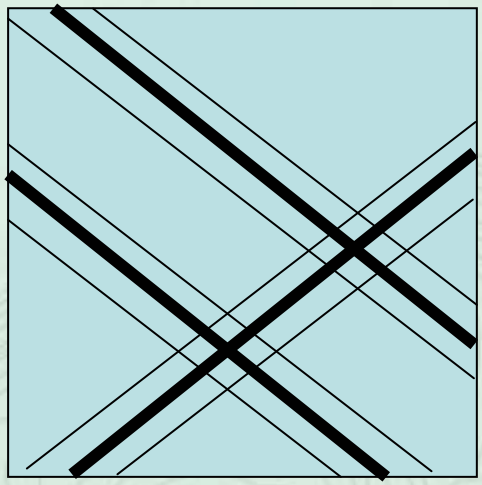
FFPyChemUtils.phaseVolume



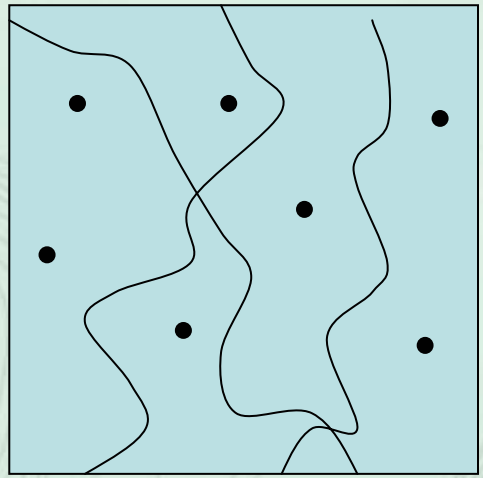
How much rock does my fluid know about?



Distributed effective porosity



Fracture porosity and percolation limited alteration



Limited effective porosity

unreactive solid fraction = changes the chemical f/r

Dynamic Chem Por-Perm

$$\phi_C = \frac{\phi}{(1-\omega)}$$

$$\omega = unreactive\_sol\_fraction$$

$$\phi = (\Delta\phi_C)\phi$$

If por = 0.08, ω = 0.80 then por_chem = 0.4

Equivalent to fracture porosity

The model stores two dynamically linked porosities

Thank-you

Reminder ..

More details about dynamic porosity-permeability in poster!