Thermal-Mechanical-Hydrological-Chemical simulations using escript, Abaqus and WinGibbs

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This paper presents our recent development of a numerical code to simulate Thermal-Mechanical-Hydrological-Chemical (TMHC) processes for geological applications within a unified multi-scale thermodynamical framework (Poulet et al 2010). This work follows the pioneering approach from Regenauer-Lieb (2009) who focuses on the importance of an energy based framework and of the consideration of direct and indirect feedbacks. The thermo-mechanical part of our framework derives directly from this approach and includes a temperature dependant elasto-visco-plastic constitutive behaviour which accounts for continuum damage and several creep mechanisms (Karrech et al 2009). The hydrological part follows the conventional Darcy flow assumption in porous media (Coussy 2004) and the fluid-rock chemical reactions are treated using WinGibbs, a component of the HCH software (Shvarov and Bastrakov (1999)) based on a Gibbs free energy minimiser. Chemical feedbacks are taken into account through their effect on material properties (density and specific heat) using PreMDB (Siret et al 2008) and we also use the equation of state of water adopted by the International Association for the Properties of Water and Steam (IAPWS) in 1997, as described by Wagner (2000). This implementation is consistent with the internal model used by WinGibbs.

Our Finite-Element implementation is based on the Escript modelling library (Gross 2005), which provides great flexibility with its robust and efficient numerical framework to solve partial differential equations in parallel. Its high-level Object Oriented interface uses the Python programming language and a user friendly modular structure which allows us to separate efficiently the physical description of the problem from its numerical implementation. Our software architecture also includes a connection to Abaqus™, hence allowing us to benefit from another powerful solver and make direct use of all recent advances developed using that platform (Karrech et al 2009).

To illustrate the capabilities of our code we present some results of a generic unconformity-type uranium deposit model. The continuum damage theory implemented in Abaqus is linked to an increase of permeability affecting the flow pattern and localising accordingly some precipitation and dissolution zones of uraninite based on the fluid-rock geochemical reactions.

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