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UNCONVENTIONAL GEOMECHANICS: CONSTITUTIVE MODELLING AND ENERGY-BASED BIFURCATION ANALYSIS OF MULTISCALE, MULTIPHYSICAL MECHANISMS DRIVING THE MACROSCOPIC RESPONSE OF GEOMATERIALS

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Summary. Geoscientists are confronted with the challenge of assessing nonlinear phenomena that result from multi-physics coupling across multiple scales from the quantum level to the scale of the earth and from femtosecond to the 4.5 Ga of history of our planet. Measuring Earth material behaviour on time scales of millions of years therefore transcends our current capability in the laboratory. We review an alternative path considering multiscale and multiphysics approaches with quantitative structure-property relationships. This approach allows a sound basis to incorporate physical principles such as chemistry, thermodynamics, diffusion and geometry-energy relations into simulations and data assimilation on the vast range of length and time scales encountered in the Earth. We identify key length scales for Earth systems processes and find a substantial scale separation between chemical, hydrous and thermal diffusion. We propose that this allows a simplified two-scale analysis where the outputs from the micro-scale model can be used as inputs for meso-scale simulations, which then in turn becomes the micro-model for the next scale up.

In this work we focus on four types of couplings that underpin fundamental instabilities in the Earth. These are thermal (T), hydraulic (H), mechanical (M) and chemical (C) processes, which are driven and controlled by the transfer of heat to the Earth's surface. Instabilities appear as faults, folds, compaction bands, shear/fault zones, plate boundaries and convective patterns. Convective patterns emerge from buoyancy overcoming viscous drag at a critical Rayleigh number. All other processes emerge as material bifurcations from non-conservative thermodynamic forces with a critical critical dissipative source term, which can be characterised by the modified Gruntfest number Gr. These dissipative processes reach a quasi-steady state when, at maximum dissipation, THMC diffusion (Fourier, Darcy, Biot, Fick) balance the source terms. The emerging steady state dissipative patterns are defined by the respective diffusion length scales. These length scales provide a fundamental thermodynamic yardstick for measuring instabilities in the Earth. The first step of an open-source implementation of a fully coupled THMC multiscale theoretical framework will be presented.

The fundamental challenges of coupling different processes will be reviewed and presented. A key aspect in this challenge is the presence of several fundamentally different lengths of the THMC engine, spanning micro-metre to tens of kilometres. These length scales are compounded by the additional necessity to consider microstructure information in the formulation of enriched continua for THMC feedback simulations (i.e., micro-structure enriched continuum formulation). Another challenge is to consider the important factor time, which implies that the geomaterial often is very far away from initial yield and flowing on a time scale that cannot be accessed in the laboratory. This leads to the requirement of adopting a thermodynamic framework in conjunction with flow theories of plasticity. This framework allows, unlike classical concepts of plasticity, the description of both solid mechanical and fluid dynamic instabilities. We show that the different length scales are always accompanied by different time-scales and we deduce that THMC systems self-organise in time around the Minimum Entropy Production threshold. This is a fundamental difference of multiphysics plasticity from the classical concepts, where systems obeying rate-independent associative flow laws axiomatically self-organise around the Maximum Entropy Production limit. In the applications we show the similarity of THMC feedback patterns across scales such as brittle and ductile folds and boudinage structures, faults and compaction bands.