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Modelling deformation dynamics across scales using LYNX: a massively parallel open-source simulator

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Understanding the key physical processes controlling the different deformation modes of sedimentary rocks is crucial to assess the strength and long-term behaviour of the lithosphere, as well as to characterize emplacement conditions and the evolution in space and time of its georesources. For example, the feasibility of successful targeting unconventional, high enthalpy geothermal resources in volcanic setting requires to understand of the non-linear dynamics controlling the brittle-to-ductile transition at depth under different tectonothermal conditions as also locally modified by operational activities. Due to the disparate length and temporal scales involved and to the high non-linearity of these processes, numerical simulators have become increasingly of help in such studies. Despite recent advances, models of the rheology and mechanical properties of the lithosphere remain particularly challenging due to the multiphysics coupling controlling the deformation of lithospheric rocks and their inherent multiscale behaviour ranging from the scales typical of grain size processes to the km scale of shear zone in the deep crust and mantle.

In this study, we present a new simulator LYNX (Lithospere dYnamic Numerical toolboX), which relies on an implicit multiphysics coupling of the physics describing the deformation modes as they occur in the rigid portion of lithosphere plates including thermal, mechanical and hydraulic feedback processes. The novelty of the study stems from it being inspired by a new theoretical understanding of the role that porosity and its evolution through time within porous rock compartments have in affecting and, to a large degree, controlling the dynamic responses of geological systems to external forcing of diverse nature (from natural, tectonic driven to anthropogenic ones). The numerical core of LYNX is based on the Multiphysics Object-Oriented Simulation Environment (MOOSE), which provides a powerful and flexible platform to solve for multiphysics problems implicitly and in a tightly coupled manner on unstructured meshes which is of interest for the considered non-linear context. In addition, the use of high-level nonlinear solvers allow us to tackle these complex multiphysics problems with high accuracy in three dimensions.

After reviewing the physical framework for coupled thermal, hydraulic and poro-viscoplastic (damage) physics, we describe basics of its numerical implementation in LYNX focusing mainly on aspects related to the tight, across-scale coupling among the different processes. In a second part, we present a suite of applications to show the robustness and capability of the newly developed simulation environment to (1) consistently integrate physical processes as observed in the field and/or in the laboratory and reconcile these observations across different scales, (2) to investigate the first order processes responsible for the present thermo-mechanical states of natural systems and, (3) its dynamic evolutions due to different forcing conditions.