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Multi-phase multi-component reactive flow in Geodynamics

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Multi-phase multi-component reactive flow (MPMCRF) controls a number of important complex geodynamic/geochemical problems, such as melt generation and percolation, metasomatism, rheological weakening, magmatic differentiation, ore emplacement, and fractionation of chemical elements, to name a few. These interacting processes occur over very different spatial and temporal scales and under very different physico-chemical conditions. Therefore, there is a strong motivation in geodynamics for investigating the equations governing MPMCRF, their mathematical structure and properties, and the numerical techniques necessary to obtain reliable and accurate results.
In this contribution we present results from a novel numerical framework to solve multiscale MPMCRF problems in geodynamic contexts. Our approach is based on the effective tracking of the most basic building blocks: internal energy and chemical composition. This is achieved through the combination of rigorous solutions to the conservation equations (mass, energy and momentum) for each dynamic phase (instead of the more common "mixture-type" approach) and the transport equation for the chemical species, within the context of classical irreversible thermodynamics. Interfacial processes such as phase changes, chemical diffusion+reaction, and surface tension effects are explicitly incorporated in the context of ensemble averaging. Phase assemblages, mineral and melt compositions, and all other physical parameters of multi-phase systems are obtained through dynamic free-energy minimization procedures.