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An autonomous phase diagram database to take thermodynamic melting models into account during chemically evolving geodynamic simulations of magmatic systems

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Self-consistent geodynamic models of magmatic systems are a challenge as rocks continuously change their chemical compositions, which may affect the mechanical behavior of the system. Melt extraction events create new rocks by injecting magma into fractures while depleting the source region. As the chemistry of these source rocks changes locally depending on the conditions of melt extraction, new phase diagrams are required to track the future rock evolution for each chemical state. This will change density, melt fraction as well as the mineralogical and chemical compositions, which has a direct feedback on the mechanical processes. As a consequence, a sufficiently large number of phase diagrams is required to study the evolution of magmatic systems in detail. As each of the melting diagrams may depend on 10 oxides as well as pressure and temperature, this is a 12-dimensional computational problem. Since computing a single phase diagram for a fixed chemical composition (as a function of pressure and temperature) may take several hours, computing new phase diagrams during an ongoing numerical simulation is computationally unfeasible. One strategy to avoid such a problem is to precompute diagrams and create a phase diagram database, which contains all bulk rock compositions that could emerge during petro-thermo-mechanical simulations. Establishing such a comprehensive database would requires repeating geodynamic simulations many times while collecting all requested compositions that occur during a typical simulation, while continuously updating the database until no further compositions are required.
Alternatively, this issue can be resolved by applying a forecast method that uses the entries of the existing database to predict possible requests of chemical composition. This involves the computation of new bulk rock compositions. They can be computed within boundaries that are defined manually or through principal component analysis (PCA) in a parameter space consisting of clustered database entries. We have implemented both methods within a massively parallel computational framework, while using the Gibbs free energy minimization program Perple_X. Results show that the autonomous forecast approach has a very good predictive power. Our predicted models focus well on physically realistic parts of the oxide parameter domain, which is spanned by the requested rock compositions of the forward models. This thus opens new perspectives in modelling magmatic systems.