Grain Growth Prediction Based on Data Assimilation by Implementing 4DVar on Phase-Field Models

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Macroscopic mechanical properties of rocks or alloys are largely affected by micro grain structures in them. Thus, accurately predicting the temporal evolution of grain structure is essential to control the macroscopic properties.
Phase-field (PF) models are often used to simulate growth of micro grain structures. However, the PF models generally contain many phenomenological parameters that are not directly observable in experiments. Thus, in order to predict the temporal evolutions of the grain structures quantitatively, it is essential to establish a methodology to estimate such parameters together with their uncertainties from limited observational/experimental data, and then to investigate how the estimates affect the results of the PF simulations.
We propose a method to predict growth of grain structure based on a four-dimensional variational method (4DVar), which is one of the data assimilation methods. Our method utilizing a second-order adjoint method can estimate model parameters together with their uncertainties, and enables us to analyze how the uncertainties influence temporal evolutions of model variables, even when using large-scale simulation models such as PF models. When implemented on a multi-phase-field model, the proposed method allows us to calculate the predicted grain structures and uncertainties in them that depend on the quality and quantity of the observational data. We confirm through numerical tests involving synthetic data that the proposed method correctly reproduces the true grain structure assumed in advance. Furthermore, it successfully quantifies uncertainties in the predicted grain structures, where such uncertainty quantifications provide valuable information to optimize experimental design.

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