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Grain growth prediction and its uncertainty based on multi-phase-field model with 4DVar and second-order adjoint method

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Phase-field models have often been used to simulate temporal evolution of grain structures in rocks or metals by modeling interactions among grains. However, the phase-field models need many phenomenological parameters that are not directly observable. Thus, establishing a methodology to estimate these parameters from limited observational/experimental data is necessary to predict the dynamics of grain structures. We emphasize here that an evaluation of the uncertainties in the estimated parameters also provides valuable information, since the uncertainties affect the results of the simulated grain structures.

The number of computations needed to obtain optimum initial states does not depend on the degree of freedom of the system such that a four-dimensional variational method (4DVar) is applicable to even massive simulation models, such as the phase-field models. Although the conventional 4DVar has a serious disadvantage in that it only provides estimates of initial states but cannot evaluate their uncertainties, Ito et al. (Physical Review E, 2016) solved this problem by establishing a new 4DVar that enables us to obtain not only the optimum, but also the associated uncertainty using a second-order adjoint method (Le Dimet et al., 2002). This new 4DVar is appropriate for data assimilation based on the phase-field models because it can quantify several uncertainties of interest within a practical number of computations.

We propose a method to predict grain growth based on data assimilation by using 4DVar. The method utilizing the second-order adjoint method, compared with conventional data assimilation methods, can drastically save the computational cost needed to obtain the estimates and uncertainties of parameters involved in the phase-field 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 phase-field assumed in advance. Furthermore, it successfully quantifies uncertainties in the predicted grain structures, where such uncertainty quantifications provide valuable information to optimize the experimental design.

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