Bayesian inference of grain growth prediction via multi-phase-field models

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We propose a Bayesian inference methodology to evaluate unobservable parameters involved in multi-phase-field models with the aim of accurately predicting the observed grain growth, such as in metals and rocks. This approach integrates models and a set of observational image data of grain structures. Since the set of image data is not a time series, directly applying conventional inference techniques that require time series as the input data is difficult. The key idea in our methodology to overcome this difficulty is to construct a time series with an appropriate statistic that characterizes static image data of grain structures. Our methodology implements the empirical Bayes method. It can estimate not only a probability density function of the parameters but also an initial phase-field, which is generally unobservable in real experiments. After validating the proposed method through numerical tests using synthetic data, we apply it to real experimental images of grain structures in a steel alloy. The proposed method properly estimates unobservable parameters together with their uncertainties, and successfully selects the initial phase-field that best explains the experimental data from among candidate initial phase-fields.

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