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Data assimilation for phase-field models based on the ensemble Kalman filter

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ABSTRACT

We have developed a data assimilation (DA) methodology based on the ensemble Kalman filter (EnKF) for estimating unknown parameters involved in a phase-field model from observational/experimental data. The DA methodology based on Bayesian statistics is able to estimate parameters by incorporating observational/experimental data into the phase-field model and evaluate the uncertainty of the estimated parameters. In this paper, we apply the EnKF-based DA method to estimate the phase-field mobility for a phase-field simulation of the isothermal austenite-to-ferrite transformation in a Fe–C–Mn alloy. Our DA method is validated through numerical experiments called "twin experiments" to verify that the DA method can estimate a priori assumed-true phase-field mobility from synthetic observational data. The results of the twin experiments using various initial phase-field mobilities show that our DA methodology can successfully estimate the true phase-field mobility, even when the initial value largely deviates from the true value. Furthermore, our DA method reveals the sampling interval for observational data necessary to accurately estimate the parameter and its uncertainty.

1. Introduction

Recently, numerical simulations have been extensively applied to study microstructural evolution in materials with the goal of realizing high-throughput material design [1]. The phase-field method has attracted considerable attention because it allows the simulation of microstructural evolutions based on the total free energy of the material [2–4]. The phase-field method has already been used to simulate various types of microstructural evolution including solidification in alloys [5–7], phase transformations in steels [8–11], grain growth [12,13], and recrystallization [14,15]. However, the phase-field method often requires immeasurable material constants, unknown parameters, initial conditions, and boundary conditions to simulate realistic microstructural evolution processes. One of these parameters is the mobility of the phase field (hereinafter called the phase-field mobility), which characterizes the rate of interfacial migration. In previous studies, the optimal value of phase-field mobility has been determined from experimental data. For example, the phase-field mobility used in the phase-field simulation of the austenite-to-ferrite ($\gamma \rightarrow \alpha$) transformation in a Fe–C–Mn alloy was selected to reproduce the experimentally measured phase fraction curves [8]. However, such trial-and-error identification of the parameter is a time-consuming task, and the uncertainty in the resulting parameter has not been evaluated.

Data assimilation (DA) has been employed as a computational technique for estimating model parameters and states of target systems as well as for efficiently improving simulation models by embedding experimental data into the models [16]. DA begins with the definition of a stochastic variable called a state vector, which contains all of the physical variables of a target system and sometimes includes model parameters involved in a given simulation model. The state variable follows a probability density function (PDF), which reasonably provides an optimum solution that maximizes values such as a likelihood or a posterior distribution. The PDF also provides the uncertainty in the optimum state variables based on the broadness of the PDF in the neighborhood of the optimum. DA continuously updates the PDFs, starting from a given

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prior PDF, by incorporating experimental data into the existing PDF based on Bayes' theorem [17,18]. As explained in many studies [16–18], the DA algorithm is generally categorized into two types: sequential (or online) DA based on a sequential Bayesian filter such as a Kalman filter, EnKF [19,20], or particle filter [21,22] and non-sequential (or offline) DA based on a method such as the adjoint method [23,24].

DA has mainly been used in natural sciences such as meteorology [25], oceanography [26,27], seismology [28], and fluid dynamics [29]. Recently, some DA methodologies have been applied to phase-field simulation, representing the first application of DA in materials science. Koyama et al. used a particle filter to identify the gradient energy coefficient in a phase-field model of the spinodal decomposition in Cu–Ag alloy [30]. They estimated the composition gradient energy coefficient to fit the experimental data. The particle filter, which is based on the Monte Carlo method, numerically computes integrals of PDFs (see Section 3.4). Although the particle filter is easy to implement, degeneracy becomes a problem as the dimension of the state variable increases (i.e., as the number of variables increases). Therefore, the particle filter is generally applicable only to small problems. Ito et al. developed a new adjoint method for non-sequential DA [31]. Unlike conventional adjoint methods, this second-order adjoint method allows the evaluation of uncertainty even in the case of a massive autonomous system. This method was validated through numerical tests called twin experiments using synthetic observational data related to a two-dimensional phase-field model of solidification in a pure material. The twin experiments showed that the a priori assumed-true initial condition and model parameter were completely reproduced with a practical computational cost. When an adjoint method is implemented in a simulation model, the computational cost needed to complete DA is usually much smaller than when a particle filter is used. However, implementing the adjoint method requires complex programming, and slight changes in the simulation model require extensive modifications to the DA code.

In this paper, we develop an EnKF-based DA methodology for estimating unknown parameters along with initial and boundary conditions used in phase-field simulations from experimental/observational data. In principle, the EnKF eliminates the degeneracy problem inherent in the particle filter, and considerably less programming effort is required compared to when using the adjoint method. To validate our DA method, twin experiments were performed to determine whether the DA method works properly as a parameter optimizer. The twin experiments performed in this study attempt to reproduce the a priori assumed phase-field mobility in a one-dimensional phase-field simulation of the isothermal austenite-to-ferrite ($\gamma \rightarrow \alpha$) transformation in a Fe–C–Mn ternary alloy. Through the twin experiments, we clarified the influences of the initial value of phase-field mobility and an observation frequency, which is the time interval to obtain observational data, on the estimation accuracy of the true phase-field mobility.

2. Phase-field model

The phase-field model of the $\gamma \rightarrow \alpha$ transformation in Fe–C–Mn alloy used in this study is based on the models proposed by Wheeler et al. [32] and Yeon et al. [33]. The phase-field variable ϕ ($\boldsymbol{r}$, τ) is defined as a non-conserved order parameter denoting the local volume fraction of the γ phase. Here $\boldsymbol{r}$ and τ represent coordinates and a unit of time, respectively. ϕ ($\boldsymbol{r}$, τ) takes the value of 1 at coordinates inside the γ phase and 0 inside the α phase. ϕ ($\boldsymbol{r}$, τ) varies from 1 to 0 at the interface between phases γ and α. The concentrations of manganese (Mn) and carbon (C) atoms, $c_{\mathrm{Mn}}(\boldsymbol{r}, \tau)$ and $c_{\mathrm{C}}(\boldsymbol{r}, \tau)$, respectively, are defined as conserved order parameters. Hereafter, ($\boldsymbol{r}$, τ) is eliminated for a simple description.

The total free energy of the system is defined as the Gibbs free energy functional using the order parameters ϕ and c_i (i = Mn or C) as

$$G = \int_V \left(g_{\mathrm{chem}} + g_{\mathrm{doub}} + g_{\mathrm{grad}}\right) dV, \tag{1}$$

where g_{chem} is the chemical free energy density and is expressed by

$$g_{\mathrm{chem}} = \{1 - g(\phi)\} g^{\alpha}(c_i, T) + g(\phi) g^{\gamma}(c_i, T), \tag{2}$$

where g^{α} and g^{γ} are the chemical free energy densities of phases α and γ, respectively, which are functions of temperature and the local concentrations of solute elements. The chemical free energies are given by the sub-lattice model [34], and its parameters are assessed by the calculation of phase diagrams using CALPHAD [35–39]. $g(\phi)$ is the energy density distribution function, which determines the distribution of chemical free energy density in an interface and is given by the following equation:

$$g(\phi) = \phi^3 (10 - 15\phi + 6\phi^2). \tag{3}$$

In Eq. (1), g_{doub} is the double-well potential function, which is given as

$$g_{\mathrm{doub}} = W h(\phi) = W \phi^2 (1 - \phi)^2, \tag{4}$$

where W is the height of the double-well potential. W is a function of the interfacial energy ω and the thickness of the interface η:

$$W = \frac{6\omega b}{\eta}, \tag{5}$$

where b is a parameter related to η and is defined as $b = 2\tanh^{-1}(1 - 2\lambda)$, where λ defines the interfacial region as $\lambda < \phi < 1 - \lambda$. In this study, we use $\lambda = 0.1$, giving $b = 2.19$.

In Eq. (1), g_{grad} is the gradient energy density, which is given by

$$g_{\mathrm{grad}} = \frac{a^2}{2} |\nabla \phi|^2, \tag{6}$$

where a is the gradient energy coefficient and is given by

$$a = \sqrt{\frac{3\omega\eta}{b}}. \tag{7}$$

The evolution equation of the phase-field variable is derived from the Allen–Cahn equation as [40]

$$\begin{aligned} \frac{\partial \phi}{\partial \tau} &= -M_{\phi} \frac{\delta G}{\delta \phi} \\ &= -M_{\phi} \left\{ \left(g^{\gamma}(c_i, T) - g^{\alpha}(c_i, T)\right) \frac{\partial g(\phi)}{\partial \phi} + W \frac{\partial h(\phi)}{\partial \phi} - a^2 \nabla^2 \phi \right\}, \end{aligned} \tag{8}$$

where M_{ϕ} is the phase-field mobility, which is estimated by EnKF-based DA in this paper.

The evolution equation of the concentration field c_i (i = Mn or C) is derived from the Cahn–Hilliard equation [41]:

$$\frac{\partial c_i}{\partial \tau} = \nabla \cdot \left(M_i \nabla \frac{\delta G}{\delta c_i} \right) = \nabla \cdot \left(M_i \nabla \frac{\partial g_{\mathrm{chem}}}{\partial c_i} \right), \tag{9}$$

where M_i is the diffusion mobility of atom i (i = Mn or C) and is expressed as

$$M_i = (1 - \phi) M_i^{\alpha} + \phi M_i^{\gamma}, \tag{10}$$

where M_i^j represents the diffusion mobility of atom i (i = Mn or C) in phase j (j = α or γ) and is given by

$$M_i^j = \frac{D_i^j}{\left(\frac{\partial^2 g^j}{\partial c_i^2} \right)}. \tag{11}$$