Spatiotemporal Thermal Field Modeling Using Partial Differential Equations With Time-Varying Parameters

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***Abstract*—Accurate modeling of a thermal field is one of the fundamental requirements in engineering thermal management in numerous industries. Existing studies have shown that using differential equations to model a thermal field delivers good performance when the parameters are predetermined through physical or experimental analysis. However, due to variations of the inner medium affected by certain latent factors, the parameters in differential equation models may not be treated as constants while the thermal field is estimated, and this fact poses a new challenge to field estimation by directly solving the differential equation models. In this study, a novel approach to thermal field modeling is developed by considering the parameters as functional variables that vary temporally in partial differential equations (PDEs). This approach provides a new perspective to model the dynamic thermal field by fully using the collected sensor data from the thermal system. Specifically, time-varying parameters can be constructed through a combination of basis functions whose coefficients can be efficiently estimated through the sensor data. A two-level iterative parameter estimation algorithm is also tailored to obtain the parameters in the PDE model. Both simulation and real case studies show that our proposed approach provides satisfactory estimation performance compared with the benchmark method that uses the constant parameter estimation.**

***Note to Practitioners*—The proposed method aims to model a thermal field using PDEs with time-varying parameters. To better implement this method in practice, three things are noteworthy: first, the proposed method models a thermal field by fully considering physics-specific engineering knowledge using PDEs and the collected sensor data from thermal systems. Second, because time-varying parameters in PDEs cannot be estimated directly, the proposed model represents the time-varying parameters by a combination of B-spline basis functions in terms of time. Estimating time-varying parameters is converted into estimating the constant coefficients of the basis functions. Because the derivatives of a thermal field might not have an analytical expression, the proposed model represents the thermal field by a combination of B-spline basis functions. Taking the derivatives of the thermal field is converted into taking the derivatives of the corresponding basis functions. Third, the proposed method can not only model a thermal field but can also be applied in other physics-specific engineering cases.**

***Index Terms*—Sensor data, spatiotemporal thermal field, time-varying parameters, two-level regression model.**

I. Introduction

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ENGINEERING thermal management (ETM) plays an important role in ensuring the stable system operation of many industrial systems. Advanced technologies in ETM can be found in different industries, including intelligent refrigerated warehouses [1], thermal conductors in nuclear plants [2], cooling equipment in supercomputer centers [3], and so on. One of the prerequisites to effectively implement these technologies in various industrial systems is to accurately obtain the thermal distribution with spatial and temporal variations. In current practice, differential equations, which are used to describe dynamic systems, are generally employed to acquire the underlying dynamic thermal distribution. This set of differential equations is usually developed by experts with a wealth of industrial experience. The associated parameters in such equations, which represent the dynamic properties of engineering systems, are important measures to characterize the intrinsic mechanism. In many cases, the parameters can be determined by experts in engineering systems or through a large number of experiments. However, in some other cases, the associated parameters are unknown due to a lack of thorough understanding on complex thermal systems or limited budgets for conducting experiments. Estimating the associated parameters is necessary when using partial differential equations (PDEs) to model a thermal field, but it remains a challenging task. In addition, in some cases, due to the variation of the thermal conductor under certain unknown conditions, such as physical property changes of the medium or environmental surroundings, the parameters in PDEs cannot be treated as static ones. When modeling thermal fields in such cases, the parameters should be considered as fundamental variables that vary over time, which is also consistent with

ETM这个技术很重要

要控制好ETM，就要知道它的dynamic system。

一般这个dynamic system会用differential equation刻画。

一般这个PDE会由experts给出；但是当training data比较少的时候，experts也很难给出PDE。就需要去identify PDE了。

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the underlying truth in engineering applications. Estimating time-varying parameters when using PDEs to model a thermal field poses a new challenge.

The advancement of sensor technology and network infrastructure provides a new round of opportunity to acquire the thermal distribution in various engineering fields. A large number of thermal data can be collected through the multiple interconnected sensors mounted on the heat-conducting medium. These sensors are sparsely distributed to *in situ* measure the temperature and may have great potential in thermal field estimation. To take full advantage of the acquired sensor data, empirical methods such as advanced statistical models are used for field estimation in various engineering domains [4], [5]. Linear statistical models are the first to be used to describe dynamic fields. For example, Xu and Huang [6] applied a multivariate linear function to capture the 2-D spatial field of nanostructures. Chen and Yang [7] described a cardiac electrical field by using a combination of linear kernel regression models. These models are purely data-driven and show good capabilities for capturing the dynamic profiles of spatial fields. However, for complex fields such as 3-D thermal fields, these models lack substantial explanations and sometimes deliver poor fitting because numerous parameters are required simultaneously for estimation. Kriging is another widely used method for field estimation. For example, Inoue *et al.* [8] introduced a spatiotemporal kriging model to describe solar radiation about the direction and the speed of cloud movement. Zhang *et al.* [9] proposed a kriging model by integrating sparse matrix algorithms and reduced rank techniques to provide high-quality estimation of a 2-D field. Our previous work integrated kriging into a Gaussian random field framework to model the dynamic thermal field using a sensor network [10]. However, the kriging model is computationally intractable for a complex field with a large set of sensor data. Hence, dynamic thermal field estimation cannot be properly handled when only data-driven methods are developed.

Inspired by data-driven methods, some researchers have attempted to model dynamic fields by using differential equations. For example, Wang and Zhang [11] simulated a thermodynamic process in a cubic granary using the differential equation of heat transmission. Yin *et al.* proposed a multi-variable fractional-order extremum seeking control strategy to obtain the optimal design of lighting systems based on differential equations [12]. In addition, optimal algorithms are proposed to solve differential equations. For example, the finite element method has been used extensively to obtain numerical solutions to differential equations [13]. Other algorithms including the Bayesian inference [14], adaptive hierarchical sparse grid collocation algorithm [15], multivariate extremum seeking control method with Newton algorithm [16] have also been developed to solve differential equations in recent years. These approaches are applied by assuming the associated parameters in the differential equations are known. However, in some engineering cases, the parameters in differential equations are unknown because of a lack of expert knowledge or limited budgets for conducting experiments.

To solve this problem, researchers have attempted to estimate parameters in differential equations when modeling dynamic systems through analyzing the observed data. Traditional differential evolution approaches borrowed a standard nonlinear regression method to estimate parameters in differential equations [17], [18]. To improve parameter estimation performance, Ho and Chan [19] developed hybrid Taguchi-differential evolution method to provide robust optimal solutions. Kaschek and Timmer [20] proposed a variational approach to improve the accuracy of parameter estimation. These methods essentially require solving the differential equations repeatedly using numerical approaches, leading to a heavy computational burden. To resolve this problem, Hall and Ma [21] proposed a fast one-step parameter cascade method for the parameter estimation of differential equations, which provides a tradeoff between the model accuracy and the computational cost. Meanwhile, Sun *et al.* [22] proposed a penalized maximum likelihood framework that can improve the accuracy and computational efficiency of parameter estimates. To guarantee parameter robustness, smoothing approaches were borrowed for parameter estimation in ordinary differential equation (ODE) models [23]. Liang and Wu [24] proposed the local smoothing approach and a pseudoleast squares regression to estimate parameters. The two-step approach is another strategy for estimating the parameters in ODE models [25]. Chang *et al.* [26] applied a two-step parameter estimation method for ODE models. The method estimates the dynamic process and its derivatives using observations in the first step and then uses least squares to estimate parameters in ODE models in the second step. These methods can estimate the parameters of differential equations with simple structures but have difficulty dealing with complex dynamic systems with multiple variables, such as parameter estimation in PDEs.

Fundamental studies in field modeling with PDEs through estimated parameters can be found in the last decade [27], [28]. To improve parameter estimation in PDEs, which is one of the most important tasks in field modeling, Xun *et al.* [29] estimated constant parameters in PDEs by using a parameter cascading method. Guo *et al.* [30] introduced a residual-based recursive parameter estimation algorithm. Asiri and Laleg-Kirati [31] proposed the modulating function-based method to estimate parameters in 1-D spatiotemporal-dependent PDEs. The methods of [29]–[31] assume parameters of PDE models as constants, that is, parameters will not change over time once they are estimated from the observed data. Such estimated parameters are analogous to those predetermined parameters through expertise and cannot reflect the truth while physical properties change in the system.

For field modeling using differential equations with time-varying parameters, Hong and Lian [32] proposed two-step estimators using quadratic regression functional theory to model an ODE with time-varying parameters. Cao *et al.* [33] proposed a nonlinear least squares method for ODEs, where penalized splines are used to model the functional parameters. Torkamani and Butcher [34] adopted the extended Kalman–Bucy filter to model an ODE with time-varying parameters. However, in most of the engineering practices, multiple variables coexist in the thermal systems, and traditional ODE models that only consider the single variable and few parameters are incapable of capturing the dynamics. Hence, it is desirable to develop a solvable method to deal with the dynamic thermal field with multiple variables using time-varying parameters.

In conclusion, existing approaches for thermal field modeling have gaps in the following: first, most existing methods model a thermal field by data-driven models using sensor data. However, for complex thermal systems, pure data-driven methods cannot achieve an accurate result. Second, some approaches are adopted to model a thermal field by ODEs with estimated time-varying parameters. These methods can estimate time-varying parameters of thermal systems with simple structures but have difficulty handling complex spatiotemporal thermal systems with multiple variables. Third, some researchers use differential equations to model a thermal field by assuming that the associated parameters in the differential equations are known or propose optimal algorithms to estimate parameters in differential equations by assuming the associated parameters as constants. However, in some engineering cases, where the associated parameters may not be treated as constants, these models fail to model a thermal field. Therefore, modeling a thermal field still faces several challenges as follows: first, physical mechanism of the thermal conductivity should be considered to model an accurate thermal field. Second, a thermal field generally has complex spatiotemporal correlated structures, and such spatiotemporal correlation must be considered in the modeling of the thermal field. Third, when modeling a thermal field using a PDE, the parameters in the PDE should be considered as fundamental variables that vary over time due to the variation of the thermal conductor. Estimating time-varying parameters in PDEs remains a challenging task.

To fill in the research gap and address the challenges for the thermal field modeling, in this article, we develop a thermal field modeling method using PDEs with time-varying parameters. Specifically, to resolve the parameter estimation problem, we treat the time-varying parameters as functional variables and use a combination of B-spline basis functions to characterize them. To parameterize the PDE model using observed sensor data, we borrow a combination of B-spline functions to characterize the thermal process. To accurately obtain the underlying thermal field, a two-level regression method is proposed to estimate coefficients of time-varying parameters and the thermal process by simultaneously considering the time-varying parameter model fitting and the PDE model fitting.

Compared with existing methods, the proposed method addresses the challenges of thermal field modeling by estimating time-varying parameters in PDEs in the following aspects. First, compared with purely data-driven methods, our proposed method leverages the physical mechanism of thermal conductivity by using a PDE model to achieve an accurate thermal field. Second, our method can model complex thermal systems and capture spatiotemporal correlation of the thermal systems by using a PDE with estimated time-varying parameters. Third, our method can estimate time-varying parameters in PDEs using sensor data for thermal field modeling.

The rest of this article is organized as follows. Section II introduces the PDE models for field modeling and the main approach for parameter estimation, including the modeling of time-varying parameters, the modeling of the dynamic process, and the associated parameter estimation method. Both simulation and real case studies are discussed in Section III to validate our proposed method. Section IV provides the discussion and conclusion.

II. Research Methodology

Given that 3-D spatiotemporal fields are commonly used in engineering domains, without loss of generality, we take a general 3-D spatiotemporal thermal field as an example to introduce our method in this section. We consider a 3-D spatiotemporal thermal field $u(\mathbf{x})$, in which $\mathbf{x} = \{t, x, y, z\}^T$ denotes a vector of independent variables in terms of t in the time domain and x, y, and z in the space domain. We assume that the 3-D spatiotemporal field can be represented by a PDE model with time-varying parameters as follows:

$$\mathcal{G}\left(\mathbf{x}, u(\mathbf{x}), \frac{\partial u(\mathbf{x})}{\partial t}, \ldots, \frac{\partial u(\mathbf{x})}{\partial z}, \frac{\partial^2 u(\mathbf{x})}{\partial t^2}, \ldots, \frac{\partial^2 u(\mathbf{x})}{\partial t \partial z}, \ldots; \Theta(t)\right) = \mathbf{0} \quad (1)$$

where $\Theta(t) = \{\theta_l(t)\}_{l=1:L}$ is a vector of time-varying parameters of the PDE model. We obtain the observed data of $u(\mathbf{x})$ from sensor networks embedded in the thermal conducting medium, and the observed data of $u(\mathbf{x})$ are denoted as ζ, that is, $\zeta_i = u(\mathbf{x}_i) + \epsilon_i$, where $\epsilon_i, i = 1, \ldots, n$ are corresponding measurement errors. We aim to estimate the unknown time-varying parameters of the PDE model in (1) from the observed data $\{(\zeta_i, \mathbf{x}_i), i = 1, \ldots, n\}$.

Two assumptions are made prior to the introduction of the proposed method.

Assumption 1: The modeled thermal field varies smoothly over space and time and is continuously differentiable.

Assumption 2: The parameters of the PDE model vary smoothly with time and are continuously differentiable.

Fig. 1 illustrates the framework of the research methodology. First, because the parameters of PDE models vary over time, they cannot be estimated directly. To solve this problem, we represent the time-varying parameters by a combination of basis functions in terms of time. Estimating time-varying parameters is converted into estimating the coefficients of the basis functions. Second, the derivatives of the thermal field in PDEs might not have an analytical expression because the thermal field is a nonlinear multidimensional dynamic process, and thus we model the dynamic process by a combination of basis functions in terms of space and time. Taking the derivatives of the process is converted into taking the derivatives of the corresponding basis functions. Compared with directly handling the derivatives of the process, obtaining the derivatives of basis functions is more convenient, which has an analytical expression. Then, according to the structure of the established model, we tailor a two-level regression method to estimate the coefficients of the time-varying parameters and the dynamic process. Finally, we can obtain the time-varying parameters and underlying thermal field.

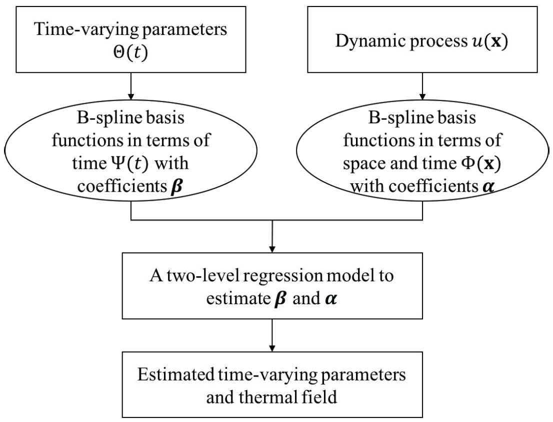


Fig. 1. Framework of the research methodology.

It is noted that the basis functions in our proposed method should satisfy the following requirements. First, the basis functions are smooth and continuously differentiable. Second, the derivatives of the basis functions have analytical expressions. In the proposed method, we select B-spline functions as the basis functions. Any other basis functions that satisfy the requirements are also applicable.

Following this idea, Section II-A introduces the modeling of the time-varying parameters $\Theta(t)$, and Section II-B introduces the modeling of the dynamic process $u(\mathbf{x})$. In Section II-C, we propose a two-level regression model by considering the time-varying parameter model fitting and PDE model fitting simultaneously to accurately model the thermal field. In Section II-D, we introduce the parameter estimation Algorithm to the PDE models.

A. Modeling of Time-Varying Parameters

Any continuous function can be expressed as a combination of spline basis functions. We represent the time-varying parameters in the PDE model $\Theta(t) = \{\theta_l(t)\}_{l=1,\ldots,L}$ through a combination of B-spline basis functions in terms of time as follows:

$$\theta_l(t) = \sum_{m_l=1}^{M_l} \Psi_{l,m_l}(t)\beta_{l,m_l} = \Psi_l^T(t)\boldsymbol{\beta}_l \tag{2}$$

where $\Psi_l(t) = (\Psi_{l,1}(t), \ldots, \Psi_{l,m_l}(t), \ldots, \Psi_{l,M_l}(t))^T$ is a vector of the basis functions for the lth parameter, $\boldsymbol{\beta}_l = (\beta_{l,1}, \ldots, \beta_{l,m_l}(t), \ldots, \beta_{l,M_l})^T$ is a vector of basis coefficients for the lth parameter, and M_l is the number of the basis functions for the lth parameter. Each $\Psi_l(t), l = 1, \ldots, L$, satisfies

$$\Psi_{l(i_l,1)}(t) = \begin{cases} 1, & T_{i_l} < t < T_{i_l+1} \\ 0, & \text{otherwise} \end{cases} \tag{3}$$

$$\begin{aligned}\Psi_{l(i_l,p_l)}(t) = {} & \frac{t - T_{i_l}}{T_{i_l+p_l-1} - T_{i_l}}\Psi_{l(i_l,p_l-1)}(t) \\ & + \frac{T_{i_l+p_l} - t}{T_{i_l+p_l} - T_{i_l+1}}\Psi_{l(i_l+1,p_l-1)}(t)\end{aligned} \tag{4}$$

where i_l denotes the index of knots for the lth parameter, T_{i_l} is the location of the knot i_l, and p_l denotes the order of basis functions for the lth parameter. We denote I_l to be the number of knots for the lth parameter, and then we obtain $I_l = M_l - p_l + 1$. We express the vector of the basis functions for the time-varying parameters $\Psi_l(t)$ from $\Psi_{l(i_l,p_l)}(t)$, with $i_l = 1, \ldots, I_l$. Without loss of generality, identical basis functions are selected for the time-varying parameters, that is, $\Psi_l(t) = \Psi(t)$, for $l = 1, \ldots, L$. To simplify the notation, we represent the basis coefficients as $\boldsymbol{\beta}$, where $\boldsymbol{\beta} = \{\boldsymbol{\beta}_1, \boldsymbol{\beta}_2, \ldots, \boldsymbol{\beta}_L\}$.

B. Modeling of the Dynamic Process

Most PDE models in engineering domains have no analytical solutions since the derivatives of the dynamic process $u(\mathbf{x})$ might not have an analytical expression. Thus, we model the dynamic process $u(\mathbf{x})$ in (1) by a combination of B-spline basis functions. We choose B-splines as basis functions for the PDEs because B-splines are nonzero only in short subintervals, which achieve computational efficiency and numerical stability. In addition, the derivatives of B-spline functions have analytical expressions. $u(\mathbf{x})$ can be represented as follows:

$$u(\mathbf{x}) = \sum_{k=1}^{K} \Phi_k(\mathbf{x})\alpha_k = \Phi^T(\mathbf{x})\boldsymbol{\alpha} \tag{5}$$

where $\Phi^T(\mathbf{x}) = (\Phi_1(\mathbf{x}), \Phi_2(\mathbf{x}), \ldots, \Phi_K(\mathbf{x}))^T$ denotes a vector of basis functions for the dynamic process, $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_K)^T$ denotes a vector of basis coefficients for the dynamic process, and K is the total number of basis functions. For a multivariate dynamic process, we employ a tensor product of B-spline basis functions to form the multivariate basis functions, in which the basis functions can be obtained using the similar approach in (3) and (4). We provide a detailed elaboration on the tensor product of B-splines in Appendix A.

C. Two-Level Regression Model

We represent $u(\mathbf{x})$ and $\Theta(t)$ by the combinations of B-spline basis functions obtained in (2) and (5), respectively. Then, the PDE model can be expressed as

$$\mathcal{G}\left(\mathbf{x}, \Phi^T(\mathbf{x})\boldsymbol{\alpha}, \frac{\partial\Phi^T(\mathbf{x})}{\partial t}\boldsymbol{\alpha}, \frac{\partial\Phi^T(\mathbf{x})}{\partial x}\boldsymbol{\alpha}, \ldots; \Psi(t), \boldsymbol{\beta}\right) = \mathbf{0}. \tag{6}$$

To simplify the notation, we denote $\mathcal{G}\{\mathbf{x}, \Phi^T(\mathbf{x})\boldsymbol{\alpha}, \partial\Phi^T(\mathbf{x})/\partial t\boldsymbol{\alpha}, \partial\Phi^T(\mathbf{x})/\partial x\boldsymbol{\alpha}, \ldots; \Psi(t), \boldsymbol{\beta}\}$ by $\mathcal{G}\{\Phi(\mathbf{x}), \boldsymbol{\alpha}; \boldsymbol{\beta}\}$

We propose a two-level regression model to estimate the basis coefficients of the time-varying parameters and the dynamic process by considering the time-varying parameter model fitting and PDE model fitting simultaneously. In the first level of optimization, we estimate the basis coefficients $\boldsymbol{\alpha}$ for the dynamic process with the fixed $\boldsymbol{\beta}$ by minimizing the regression function $\mathcal{I}(\boldsymbol{\alpha}|\boldsymbol{\beta})$ with the roughness penalty as follows:

$$\mathcal{I}(\boldsymbol{\alpha}|\boldsymbol{\beta}) = \sum_{i=1}^{n}\{\zeta_i - \Phi^T(\mathbf{x}_i)\boldsymbol{\alpha}\}^2 + \lambda\int \mathcal{G}\{\Phi(\mathbf{x}), \boldsymbol{\alpha}; \boldsymbol{\beta}\}^2 d\mathbf{x} \tag{7}$$

where λ is the penalty parameter. A common practice is to estimate the basis coefficients $\boldsymbol{\alpha}$ for the dynamic process

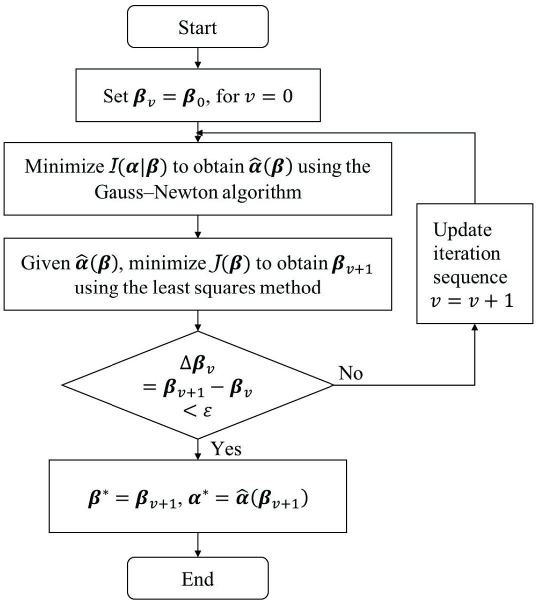


Fig. 2. Flowchart of the two-level iterative parameter estimation algorithm.

by penalized splines, which performs a penalty to achieve smoothness of the estimated function. We model a roughness penalty as $\int \mathcal{G}\{\Phi(\mathbf{x}), \boldsymbol{\alpha}; \boldsymbol{\beta}\}^2 d\mathbf{x}$ for a fixed $\boldsymbol{\beta}$, which integrates the PDE model into (7). The roughness penalty regularizes the fitting of the dynamic process and shows the accuracy of the fitting to the PDE model; specifically, a small value indicates an accurate fitting of the spline approximation to the PDE model. The integration in (7) can be approximated by numerical integration methods [33].

Then, we propose a second level of optimization to estimate the coefficients of the time-varying parameters $\boldsymbol{\beta}$. We represent the estimate of $\boldsymbol{\alpha}$ for the fixed $\boldsymbol{\beta}$ as $\hat{\boldsymbol{\alpha}}(\boldsymbol{\beta})$, which is a function of $\boldsymbol{\beta}$. Given that the estimator $\hat{\boldsymbol{\alpha}}(\boldsymbol{\beta})$ has been regularized, we minimize the residual sum of squares $\mathcal{J}(\boldsymbol{\beta})$ to estimate $\boldsymbol{\beta}$

$$\mathcal{J}(\boldsymbol{\beta}) = \sum_{i=1}^{n}\{\zeta_i - \Phi^T(\mathbf{x}_i)\hat{\boldsymbol{\alpha}}(\boldsymbol{\beta})\}^2. \quad (8)$$

D. Parameter Estimation Algorithm

1) Estimating Parameters in PDE Models: We develop a two-level iterative algorithm to estimate parameters in PDE models, in which we minimize the objective functions $\mathcal{I}(\boldsymbol{\alpha}|\boldsymbol{\beta})$ and $\mathcal{J}(\boldsymbol{\beta})$ iteratively until convergence to a solution is achieved (Fig. 2). Initially, we set $\boldsymbol{\beta}$ as $\boldsymbol{\beta}_0$. In the v_{th} iteration, we minimize $\mathcal{I}(\boldsymbol{\alpha}|\boldsymbol{\beta})$ to obtain $\hat{\boldsymbol{\alpha}}$ using the Gauss–Newton algorithm that updates $\boldsymbol{\alpha}$ iteratively until convergence

$$\boldsymbol{\alpha}_w = \boldsymbol{\alpha}_{w-1} - \left(\frac{\partial^2\mathcal{I}(\boldsymbol{\alpha}|\boldsymbol{\beta})}{\partial\boldsymbol{\alpha}\partial\boldsymbol{\alpha}^T}\Big|_{\boldsymbol{\alpha}_{w-1}}\right)^{-1}\left(\frac{\partial\mathcal{I}(\boldsymbol{\alpha}|\boldsymbol{\beta})}{\partial\boldsymbol{\alpha}}\Big|_{\boldsymbol{\alpha}_{w-1}}\right) \quad (9)$$

where w denotes the iteration index for the estimation of $\boldsymbol{\alpha}$, and $(\partial\mathcal{I}(\boldsymbol{\alpha}|\boldsymbol{\beta})/\partial\boldsymbol{\alpha}|_{\boldsymbol{\alpha}_{w-1}})$ and $(\partial^2\mathcal{I}(\boldsymbol{\alpha}|\boldsymbol{\beta})/\partial\boldsymbol{\alpha}\partial\boldsymbol{\alpha}^T|_{\boldsymbol{\alpha}_{w-1}})$ denote the first-order and second-order derivatives of $\mathcal{I}(\boldsymbol{\alpha}|\boldsymbol{\beta})$ in terms of $\boldsymbol{\alpha}$ given $\boldsymbol{\alpha}_{w-1}$, respectively.

After $\hat{\boldsymbol{\alpha}}(\boldsymbol{\beta})$ is obtained, we can linearize $\hat{\boldsymbol{\alpha}}(\boldsymbol{\beta})$ given $\boldsymbol{\beta}_v$ and then replace the criterion of (8) as follows:

$$\mathcal{J}(\boldsymbol{\beta}) = \sum_{i=1}^{n}\left\{\left(\zeta_i - \Phi^T(\mathbf{x}_i)\hat{\boldsymbol{\alpha}}(\boldsymbol{\beta}_v) + \frac{\hat{\boldsymbol{\alpha}}(\boldsymbol{\beta})}{\partial\boldsymbol{\beta}}\Big|_{\boldsymbol{\beta}_v}\boldsymbol{\beta}_v\right) - \frac{\hat{\boldsymbol{\alpha}}(\boldsymbol{\beta})}{\partial\boldsymbol{\beta}}\Big|_{\boldsymbol{\beta}_v}\boldsymbol{\beta}\right\}^2 \quad (10)$$

in which the first-order derivative of $\hat{\boldsymbol{\alpha}}(\boldsymbol{\beta})$ in terms of $\boldsymbol{\beta}$ can be analytically expressed as follows:

$$\frac{\partial\hat{\boldsymbol{\alpha}}(\boldsymbol{\beta})}{\partial\boldsymbol{\beta}} = -\left\{\frac{\partial^2\mathcal{I}(\boldsymbol{\alpha}|\boldsymbol{\beta})}{\partial\boldsymbol{\alpha}\partial\boldsymbol{\alpha}^T}\Big|_{\hat{\boldsymbol{\alpha}}(\boldsymbol{\beta})}\right\}^{-1} \times \left\{\frac{\partial^2\mathcal{I}(\boldsymbol{\alpha}|\boldsymbol{\beta})}{\partial\boldsymbol{\alpha}\partial\boldsymbol{\beta}^T}\Big|_{\hat{\boldsymbol{\alpha}}(\boldsymbol{\beta})}\right\}. \quad (11)$$

Given that $\hat{\boldsymbol{\alpha}}(\boldsymbol{\beta})$ is obtained by minimizing $\mathcal{I}(\boldsymbol{\alpha}|\boldsymbol{\beta})$, we have $\partial\mathcal{I}(\boldsymbol{\alpha}|\boldsymbol{\beta})/\partial\boldsymbol{\alpha}|_{\hat{\boldsymbol{\alpha}}(\boldsymbol{\beta})} = 0$. By taking the derivative in terms of $\boldsymbol{\beta}$ on the left side of $\partial\mathcal{I}(\boldsymbol{\alpha}|\boldsymbol{\beta})/\partial\boldsymbol{\alpha}|_{\hat{\boldsymbol{\alpha}}(\boldsymbol{\beta})} = 0$ and assuming that $\partial^2\mathcal{I}(\boldsymbol{\alpha}|\boldsymbol{\beta})/\partial\boldsymbol{\alpha}\partial\boldsymbol{\alpha}^T|_{\hat{\boldsymbol{\alpha}}(\boldsymbol{\beta})}$ is nonsingular, we obtain the analytical expression of the first-order derivative of $\hat{\boldsymbol{\alpha}}(\boldsymbol{\beta})$ in (11). The nonsingularity of $\partial^2\mathcal{I}(\boldsymbol{\alpha}|\boldsymbol{\beta})/\partial\boldsymbol{\alpha}\partial\boldsymbol{\alpha}^T|_{\hat{\boldsymbol{\alpha}}(\boldsymbol{\beta})}$ can be guaranteed when the number of observed data is larger than the dimension of $\boldsymbol{\alpha}$. After inserting (11) into (10), we minimize $\mathcal{J}(\boldsymbol{\beta})$ by the least squares method to update the estimate of $\boldsymbol{\beta}$ as $\boldsymbol{\beta}_{v+1}$. The estimator $\boldsymbol{\beta}^*$ is achieved until the difference between $\boldsymbol{\beta}_{v+1}$ and $\boldsymbol{\beta}_v$ is negligible.

In the special case of linear PDEs, parameters can not only be estimated by the aforementioned iterative method but can also be estimated by an analytical method in the following. The expression of linear PDE models is linear for $\boldsymbol{\alpha}$, that is,

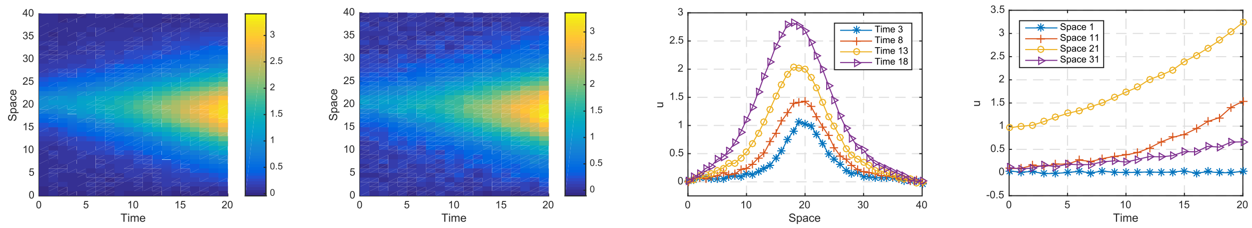
$$\mathcal{G}\left(\mathbf{x}, \Phi^T(\mathbf{x})\boldsymbol{\alpha}, \frac{\partial\Phi^T(\mathbf{x})}{\partial t}\boldsymbol{\alpha}, \frac{\partial\Phi^T(\mathbf{x})}{\partial x}\boldsymbol{\alpha}, \ldots; \Psi(t), \boldsymbol{\beta}\right) = \mathbf{g}^T\left(\Phi(\mathbf{x}), \frac{\partial\Phi(\mathbf{x})}{\partial t}, \frac{\partial\Phi(\mathbf{x})}{\partial x}, \ldots; \Psi(t), \boldsymbol{\beta}\right)\boldsymbol{\alpha} = \mathbf{0} \quad (12)$$

where $\mathbf{g}\{\Phi(\mathbf{x}), \partial\Phi(\mathbf{x})/\partial t, \partial\Phi(\mathbf{x})/\partial x, \ldots; \Psi(t), \boldsymbol{\beta}\}$ denotes a function of the basis functions and their derivatives. To simplify the notation, we represent $\mathbf{g}\{\Phi(\mathbf{x}), \partial\Phi(\mathbf{x})/\partial t, \partial\Phi(\mathbf{x})/\partial x, \ldots; \Psi(t), \boldsymbol{\beta}\}$ by $\mathbf{g}\{\mathbf{x}; \boldsymbol{\beta}\}$. In linear PDEs, $\hat{\boldsymbol{\alpha}}(\boldsymbol{\beta})$ can be solved as an analytical expression. By substituting into (2), (5), and (12), $\mathcal{I}(\boldsymbol{\alpha}|\boldsymbol{\beta})$ in (7) can be written as

$$\mathcal{I}(\boldsymbol{\alpha}|\boldsymbol{\beta}) = \sum_{i=1}^{n}\{\zeta_i - \Phi^T(\mathbf{x}_i)\boldsymbol{\alpha}\}^2 + \lambda\int\boldsymbol{\alpha}^T\mathbf{g}(\mathbf{x}; \boldsymbol{\beta})\mathbf{g}^T(\mathbf{x}; \boldsymbol{\beta})\boldsymbol{\alpha}d\mathbf{x}.$$

We denote $\boldsymbol{\zeta} = (\zeta_1, \zeta_2, \ldots, \zeta_n)^T$, and $\boldsymbol{\Phi}$ as the $K \times n$ basis matrix with the ith column $\Phi(\mathbf{x}_i)$. The $K \times K$ penalty matrix is represented by $\boldsymbol{\Omega}(\boldsymbol{\beta}) = \int\mathbf{g}(\mathbf{x}; \boldsymbol{\beta})\mathbf{g}^T(\mathbf{x}; \boldsymbol{\beta})d\mathbf{x}$. $\boldsymbol{\Omega}(\boldsymbol{\beta})$ is calculated by the numerical integration method, which we introduce in Appendix B in detail. $\mathcal{I}(\boldsymbol{\alpha}|\boldsymbol{\beta})$ is a quadratic function of $\boldsymbol{\alpha}$, and we express $\mathcal{I}(\boldsymbol{\alpha}|\boldsymbol{\beta})$ as the matrix notation as follows:

$$\mathcal{I}(\boldsymbol{\alpha}|\boldsymbol{\beta}) = (\boldsymbol{\zeta} - \boldsymbol{\Phi}^T\boldsymbol{\alpha})^T(\boldsymbol{\zeta} - \boldsymbol{\Phi}^T\boldsymbol{\alpha}) + \lambda\boldsymbol{\alpha}^T\boldsymbol{\Omega}(\boldsymbol{\beta})\boldsymbol{\alpha}. \quad (13)$$



(a) (b) (c) (d)

Fig. 3. Numerical solution to the PDE model with time-varying parameters in the simulation case. (a) 2-D view ($\sigma = 0.02$). (b) 2-D view ($\sigma = 0.05$). (c) Examples of temporal profiles in a space domain ($\sigma = 0.02$). (d) Examples of spatial profiles in a time domain ($\sigma = 0.02$).

By minimizing (13), the estimate of $\boldsymbol{\alpha}$ can be obtained as a close form for the fixed $\boldsymbol{\beta}$

$$\hat{\boldsymbol{\alpha}}(\boldsymbol{\beta}) = \{\boldsymbol{\Phi}\boldsymbol{\Phi}^T + \lambda\boldsymbol{\Omega}(\boldsymbol{\beta})\}^{-1}\boldsymbol{\Phi}\boldsymbol{\zeta}. \tag{14}$$

Then, by substituting $\hat{\boldsymbol{\alpha}}(\boldsymbol{\beta})$ into $\mathcal{J}(\boldsymbol{\beta})$ in (8), $\mathcal{J}(\boldsymbol{\beta})$ can be written as the matrix notation

$$\mathcal{J}(\boldsymbol{\beta}) = \|\boldsymbol{\zeta} - \boldsymbol{\Phi}^T\{\boldsymbol{\Phi}\boldsymbol{\Phi}^T + \lambda\boldsymbol{\Omega}(\boldsymbol{\beta})\}^{-1}\boldsymbol{\Phi}\boldsymbol{\zeta}\|_2^2. \tag{15}$$

We minimize the criterion (15) to obtain an estimate of $\boldsymbol{\beta}$ as $\boldsymbol{\beta}^*$. The estimated basis coefficients of $u(\mathbf{x})$, $\boldsymbol{\alpha}^*$, can be obtained by substituting $\boldsymbol{\beta}^*$ into (14).

2) Selection of Penalty Parameter: The estimated basis coefficients of time-varying parameters $\boldsymbol{\beta}^*$ and the dynamic process $\boldsymbol{\alpha}^*$ can be obtained given any value of the penalty parameter λ. In other words, both the estimated basis coefficients for time-varying parameters and the dynamic process can be considered as functions of λ and are denoted as $\boldsymbol{\beta}^*(\lambda)$ and $\boldsymbol{\alpha}^*(\lambda)$. As our goal is to estimate time-varying parameters in the PDE model and make the solution of the PDE close to the truth, we consider the time-varying parameter model fitting and PDE model fitting simultaneously and minimize the following criterion to obtain an optimal λ:

$$\mathcal{O}(\lambda) = \sum_{i=1}^{n}(\zeta_i - \Phi^T(\mathbf{x}_i)\boldsymbol{\alpha}^*(\lambda)))^2 + \mathcal{G}^2\{\Phi(\mathbf{x}_i), \boldsymbol{\alpha}^*(\lambda); \boldsymbol{\beta}^*(\lambda)\}. \tag{16}$$

The first part in $\mathcal{O}(\lambda)$, which measures the accuracy of the estimated dynamic process, tends to choose a small penalty parameter value. The second part in $\mathcal{O}(\lambda)$, which assesses the estimated PDE modeling errors, tends to choose a large penalty parameter value. We consider these two parts when selecting an optimal penalty parameter value, thereby making the best tradeoff between the time-varying parameter model fitting and the PDE model fitting. We use cross validation to choose the penalty parameter.

III. Case Study

A. Simulation Study

We used the PDE model with time-varying parameters in (17) to simulate the data. The PDE model is called a 1-D linear reaction convection–diffusion equation

$$\frac{\partial u(t,z)}{\partial t} - \theta_1(t)\frac{\partial^2 u(t,z)}{\partial z^2} - \theta_2(t)\frac{\partial u(t,z)}{\partial z} - \theta_3(t)u(t,z) = 0. \tag{17}$$

TABLE I
Coefficient Values of the PDE Model in the Simulation Case

Coefficient	Value				
β_1	0.4303	0.4807	0.5263	0.5762	0.5899
β_2	0.0988	0.0968	0.1082	0.1049	0.1077
β_3	0.1127	0.0975	0.0980	0.0780	0.0923

We described the time-varying parameters in (17) by B-spline basis functions as follows:

$$\theta_l(t) = \sum_{m=1}^{M_l}\Psi_{lm}(t)\beta_{lm} = \Psi_l^T(t)\boldsymbol{\beta}_l, \quad l = 1, 2, 3.$$

We considered B-spline basis functions $\boldsymbol{\beta}_l, l = 1, 2, 3$ with $M_l = 5$, which is sufficient in most of engineering practices. Then, the coefficients of the B-spline basis functions $\boldsymbol{\beta}_l, l = 1, 2,$ and 3 were set randomly (Table I). The PDE model was numerically solved using the finite difference method by setting the boundary conditions as $u(t, 0) = 0$ and $u(t, 40) = 0$ and the initial values as $u(0, z) = \{1 + 0.1(20 - z)^2)\}$ in the time domain $t \in [0, 20]$ and the space domain $z \in [0, 40]$. The meshgrid has a grid size of 0.005 in the time domain and 0.01 in the space domain. Fig. 3 shows the numerical solution of the PDE model with time-varying parameters. We obtained a 20×40 meshgrid-based simulation data in the spatiotemporal domain $[0, 20] \times [0, 40]$. To validate the effectiveness of our proposed method for parameter estimation of the PDE model given the observed data, we conducted simulations in which the observed data were simulated by adding Gaussian white noises with standard deviation (SD) $\sigma = 0.01$, 0.02, and 0.05, which are independent and identically distributed in the spatiotemporal domain, to the numerical solution of the PDE model at each time and space unit.

The order of basis functions is determined from two aspects: first, because the proposed method needs to take the derivatives of the basis functions, the order of basis functions should be larger than the order of derivatives. Second, fivefold cross validation is used to determine the order of basis functions in the proposed method. The PDE model in (17) indicated that the second partial derivatives in terms of t and z were continuously differentiable, respectively. Therefore, the order of basis functions should be larger than 2, and we chose the order of basis functions as three in the time and space domain, respectively, by using fivefold cross validation. We used a

TABLE II
SIMULATION RESULTS OF ESTIMATED COEFFICIENTS $\boldsymbol{\beta}^*$

Noise	$\sigma = 0.01$				$\sigma = 0.02$				$\sigma = 0.05$			
	Mean values	Bias ($\times 10^{-3}$)	SD ($\times 10^{-4}$)	RMSE ($\times 10^{-3}$)	Mean values	Bias ($\times 10^{-3}$)	SD ($\times 10^{-4}$)	RMSE ($\times 10^{-3}$)	Mean values	Bias ($\times 10^{-3}$)	SD ($\times 10^{-4}$)	RMSE ($\times 10^{-3}$)
$\boldsymbol{\beta}_1^*$	0.4302	-0.1720	0.3485	0.1755	0.4302	-0.1784	0.7181	0.1932	0.4301	-0.2343	2.0001	0.3080
	0.4723	-8.4000	2.4007	8.4034	0.4722	-8.4707	5.5533	8.4888	0.4717	-8.9481	15.7032	9.0847
	0.4870	-39.2406	9.4882	39.2521	0.4868	-39.5093	23.0013	39.5761	0.4853	-40.9386	63.4289	41.4265
	0.5772	1.0071	4.3784	1.0981	0.5771	0.9445	8.6876	1.2830	0.5767	0.5316	23.8192	2.4394
	0.5926	2.6427	0.7832	2.6439	0.5926	2.6466	1.5852	2.6513	0.5925	2.6172	4.4917	2.6554
$\boldsymbol{\beta}_2^*$	0.0992	0.3915	0.6339	0.3966	0.0992	0.3827	1.3286	0.4051	0.0992	0.3359	3.2887	0.4700
	0.1036	6.7696	1.3912	6.7710	0.1035	6.7469	2.7046	6.7523	0.1033	6.5507	6.4271	6.5821
	0.0931	-15.1182	0.3263	15.1183	0.0931	-15.1184	0.6706	15.1185	0.0931	-15.1242	1.6096	15.1251
	0.0922	-12.7024	0.3946	12.7025	0.0922	-12.6971	0.7889	12.6973	0.0923	-12.6424	1.6920	12.6435
	0.1087	0.9984	0.4170	0.9993	0.1087	1.0001	0.8456	1.0036	0.1087	1.0165	2.1555	1.0391
$\boldsymbol{\beta}_3^*$	0.1127	-0.0094	0.0489	0.0106	0.1127	-0.0085	0.1042	0.0135	0.1127	-0.0039	0.2621	0.0265
	0.0973	-0.1627	0.1080	0.1631	0.0973	-0.1613	0.2298	0.1630	0.0973	-0.1527	0.5547	0.1624
	0.0988	0.8706	0.1093	0.8707	0.0988	0.8725	0.2382	0.8728	0.0988	0.8808	0.6233	0.8830
	0.0781	0.0816	0.0691	0.0819	0.0781	0.0819	0.1396	0.0831	0.0781	0.0837	0.3219	0.0896
	0.0921	-0.1357	0.0296	0.1358	0.0921	-0.1361	0.0493	0.1362	0.0921	-0.1354	0.1221	0.1360

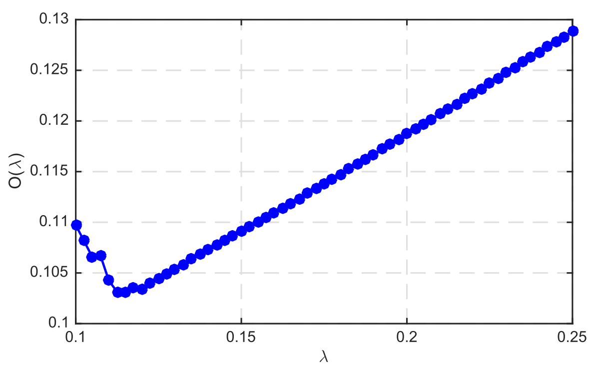


Fig. 4. Selection of the penalty parameter.

tensor product of basis functions in the time and space domains to form the basis functions for $u(t, z)$ with four and ten equally spaced knots in the time and space domains, respectively.

To validate the performance of our proposed parameter estimation method, we used the SD of the discrepancy between the true and estimated values as the criterion in assessing the accuracy of our proposed method, that is,

$$\text{STD} = \left[\frac{\sum_{j=1}^{N_t}\sum_{k=1}^{N_z}(\hat{u}(t_j, z_k) - u(t_j, z_k))^2}{N_t N_z}\right]^{\frac{1}{2}} + \left[\frac{\sum_{j=1}^{N_t}\sum_{k=1}^{N_z}\hat{\mathcal{G}}^2(\hat{u}(t_j, z_k); \boldsymbol{\beta}^*)}{N_t N_z}\right]^{\frac{1}{2}} \quad (18)$$

where N_t and N_z are the numbers of grid points in the time and space domains, respectively; and t_j and z_k are the grid points with $j = 1, \ldots, N_t$ and $k = 1, \ldots, N_z$. The first term in STD assesses the accuracy of the estimated dynamic process $\hat{u}(t, z)$, and the second term assesses the estimated PDE modeling errors $\hat{\mathcal{G}}(\hat{u}(t, z); \boldsymbol{\beta}^*)$, where $\hat{\mathcal{G}}(\hat{u}(t, z); \boldsymbol{\beta}^*) = (\partial\hat{u}(t, z)/\partial t) - \Psi_1^T(t)\boldsymbol{\beta}_1^*(\partial^2\hat{u}(t, z)/\partial z^2) - \Psi_2^T(t)\boldsymbol{\beta}_2^*(\partial\hat{u}(t, z)/\partial z) - \Psi_3^T(t)\boldsymbol{\beta}_3^*\hat{u}(t, z)$ and $\hat{u}(t, z) = \Phi^T(t, z)\boldsymbol{\alpha}^*$.

We initially addressed the selection of the penalty parameter λ. Fig. 4 shows the curve of $\mathcal{O}(\lambda)$ using the cross validation given a series of λ values. Considering the minimization of $\mathcal{O}(\lambda)$, we selected $\lambda^* = 0.1125$ as the appropriate penalty parameter. Then, we estimated the time-varying parameters in the PDE model of (17) using the proposed method and implemented it with 1000 replicates. The simulation results of the estimated coefficients $\boldsymbol{\beta}^*$ are summarized in Table II, including the mean values, bias, SD, and root-mean-squared errors (RMSEs) of the estimated coefficients when the SD of the data noises σ was 0.01, 0.02, and 0.05. Here, the bias represents the difference between the estimated coefficient values and the true coefficient values. The SD quantifies the amount of dispersion for the estimated coefficients. The RMSE is a measure of accuracy that represents the square root of the quadratic mean of the differences between the estimated values and true values of the coefficients. As shown in Table II, our proposed method obtains the coefficients with small bias, SD, and RMSE values, indicating that the estimated coefficients from our proposed method are acceptable. In addition, the mean values of STDs of our proposed method stay in low levels, which are equal to 0.0234 (when $\sigma = 0.01$), 0.0311 (when $\sigma = 0.02$), and 0.0598 (when $\sigma = 0.05$). Hence, the results of the estimated coefficients indicate our proposed method performs well for both the time-varying parameters and the PDE model.

To further validate the effectiveness of our method, we compared the performance of our method with that of another alternative method [29], in which the parameters of the PDE model were considered to be constants. As shown in Fig. 5, our proposed method exhibits superior performance in terms of STDs by treating the parameters time-varying. The alternative method assumes the constant parameters in the PDE model to simplify the modeling of parameter estimation, thus failing to obtain good fitting results.

We obtained the field using the PDE model with estimated time-varying parameters and calculated the root mean square errors between the estimated field values and the true values, which are 0.0147, 0.0148, and 0.0151 for the noise with $\sigma = 0.01$, 0.02, and 0.05, respectively. The small values of the root mean square errors show that our proposed method can model the field accurately using a PDE with time-varying parameters.

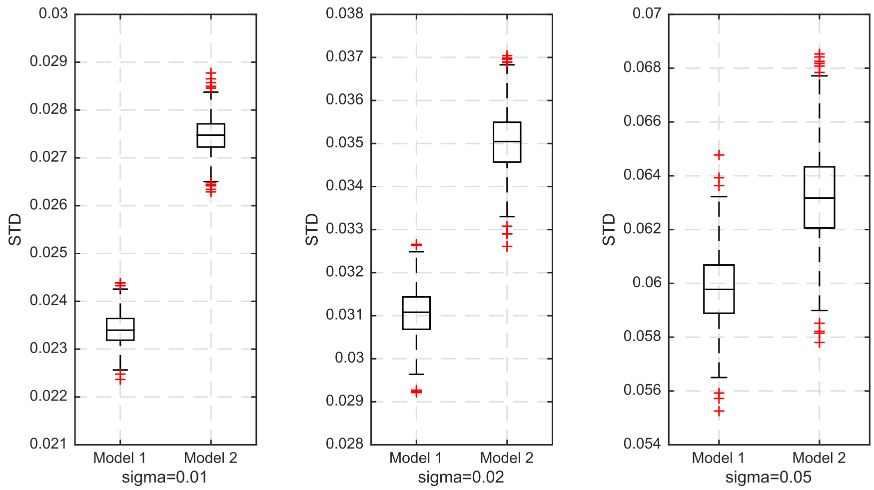
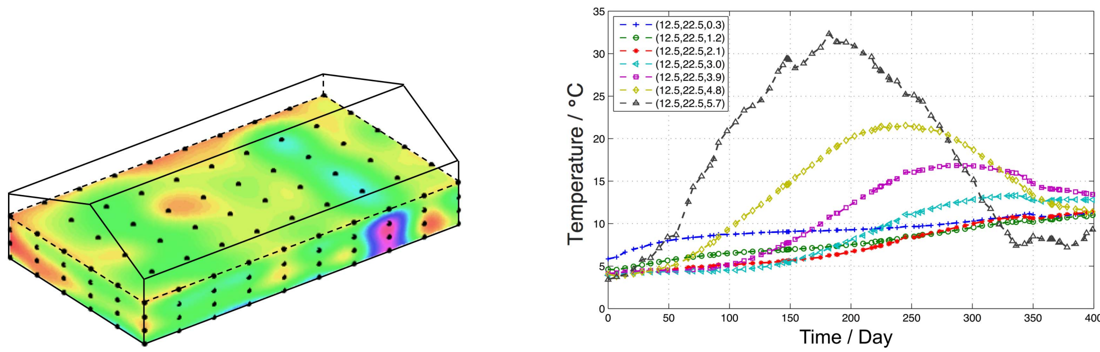


Fig. 5. Boxplots of STDs using the proposed method (Model 1) and constant parameter estimation method (Model 2) from 1000 data sets.



(a) (b)

Fig. 6. Observations of the thermodynamic model in a national granary. (a) Anatomic view of the granary with the locations of the sensors (note that the cloud represents the grain temperature field, and black dots represent the sensor locations). (b) Grain temperature profiles at various locations.

B. Real Case Study

We also tested our proposed method by estimating the time-varying parameters of a thermodynamic model in granaries. We considered the thermodynamic process of grain in a national granary in the middle of China. Fig. 6 shows an anatomic view of the granary and examples of grain temperature profiles at various locations. We can observe that grain temperature varies across both space and time. The PDE model of the thermodynamic process in the granary can be expressed as a 3-D unsteady heat transfer function as follows:

$$\frac{\partial u(t,x,y,z)}{\partial t} = \theta_x(t)\frac{\partial^2 u(t,x,y,z)}{\partial x^2} + \theta_y(t)\frac{\partial^2 u(t,x,y,z)}{\partial y^2} + \theta_z(t)\frac{\partial^2 u(t,x,y,z)}{\partial z^2} \quad (19)$$

where $u(t,x,y,z)$ denotes the grain temperature in the granary at location (x,y,z) and time t; x, y, z, and t denote the indexes of the 3-D space domain and the time domain, respectively; and the parameters $\theta_x(t)$, $\theta_y(t)$, and $\theta_z(t)$ denote the physical properties of the grain stored in the granary, which are usually unknown. Given that the physical properties of the grain are affected by many factors, such as grain temperature and humidity, $\theta_x(t)$, $\theta_y(t)$, and $\theta_z(t)$ vary with time. We estimated the time-varying parameters $\theta_x(t)$, $\theta_y(t)$, and $\theta_z(t)$ using the grain temperature sensing data we collected at least every 7 days from the grain temperature sensor networks, and the data were gathered from January 31 in one year to January 30 in the next year. There are 240 evenly spaced temperature sensors distributed in a cubic granary with 46 m in length, 26 m in width, and 6 m in height. The sensors are placed every 5 m in the x- and y-directions and every 1.8 m in the z-direction. We obtained 15 600 samples of $10 \times 6 \times 4$ meshgrid-based sensing data. As shown in Fig. 6, the observations of grain temperature are spatiotemporally correlated in a 3-D field, which increases the difficulty of solving a multidimensional thermodynamic model. We can also observe in Fig. 6 that noise occurs in the grain temperature field owing to uncertain factors that increase the difficulty of the parameter estimation for the thermodynamic model.

For the B-spline basis functions in modeling the thermodynamic model, we chose the order of basis functions as three in the x-, y-, and z-directions of the space domain and the time domain t, respectively, by using fivefold cross validation. We used a tensor product of 1-D basis functions in the x-, y-, and z-directions of the space domain and the time domain t to form the basis functions for $u(t,x,y,z)$. We selected the basis functions with five, seven, and four

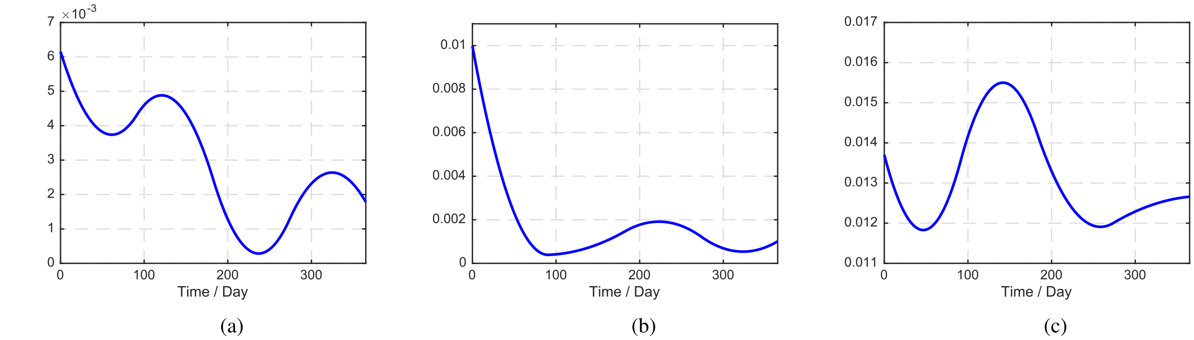


Fig. 7. Time-varying parameters estimated by our method in the real case. (a) $\theta_x(t)$. (b) $\theta_y(t)$. (c) $\theta_z(t)$.

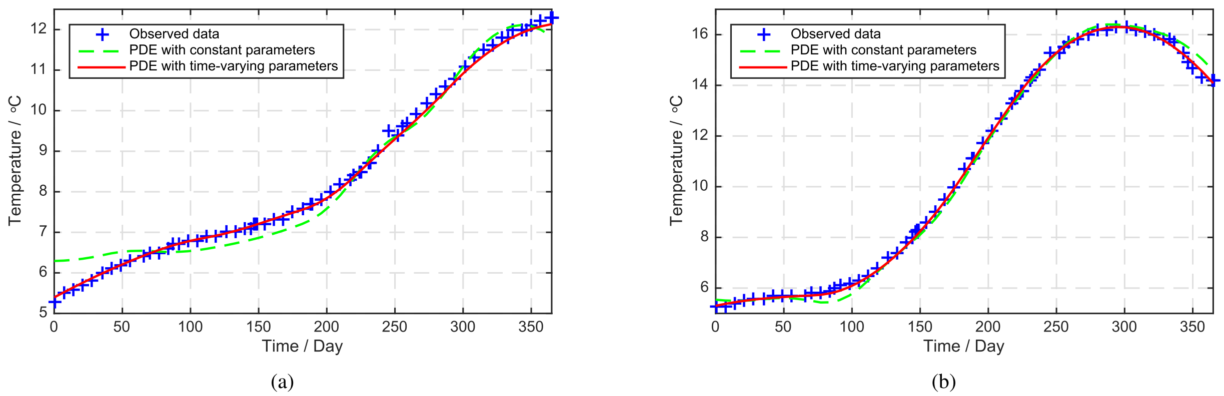


Fig. 8. Examples of the estimated 3-D grain temperature field. (a) and (b) Coordinates (5.5, 5.5, 2.1) and (5.5, 10.5, 3.9), respectively.

TABLE III
REAL CASE RESULTS OF ESTIMATED COEFFICIENTS $\boldsymbol{\beta}^*$

Coefficient	Estimated value ($\times 10^{-2}$)					
β_1^*	0.9750	0.2561	0.6062	-0.1176	0.3720	-0.0156
β_2^*	1.9658	0.0311	0.0469	0.2469	-0.0029	0.2050
β_3^*	1.7370	1.0035	1.7062	1.1438	1.2568	1.2751

equally spaced knots in the respective x-, y-, and z-directions of the space domain and five evenly spaced knots in the time domain t by using fivefold cross validation. The procedure of modeling the basis functions for $u(t, x, y, z)$ is the same as $u(t, z)$ in the simulation case. Due to the limited space of this article, the details are omitted here.

We applied the proposed method to estimate the time-varying parameters in the thermodynamic model. We summarized the estimated coefficients of the time-varying parameters in the PDE model in Table III and presented the estimated time-varying parameters of the thermodynamic model in Fig. 7. We can see that the parameters vary slowly over time and present with various patterns, which is coincident with the physical properties of the stored grains, that is, the physical properties of grains vary slowly during storage and have various thermal transmission effects in different directions of the granary. To show the superiority of the estimated time-varying parameters of the PDE model, we borrowed the method with constant parameters in the thermodynamic model (STD $= 0.6939$) as a benchmark. The STD of the proposed method is 0.6483, which shows the better performance of our proposed method than the benchmark method. Fig. 8 shows the profiles of the grain temperature field at two locations obtained by our proposed method and the benchmark method. We can see in Fig. 8 that our proposed method captures the profiles of the grain temperature field more accurately than the benchmark method. Given that the physical properties of stored grains are affected by many latent factors, the parameters of the thermodynamic model may vary at each time epoch. Our method achieves good performance by applying the spline functions to successfully characterize the time-varying parameters of the thermodynamic model.

IV. DISCUSSION AND CONCLUSION

Parameters in PDE models are important measures to characterize the intrinsic changes of thermal fields. Given that the intrinsic changes in thermal fields vary in terms of time with the extrinsic factors, constant parameters cannot characterize the intrinsic changes of thermal fields accurately. Thus, a PDE model should be used with time-varying parameters to characterize the dynamics of thermal fields. In most cases, the parameters in PDEs are unknown and cause difficulty when modeling thermal fields. Therefore, estimating the time-varying parameters in PDE models is necessary for thermal fields.

In this article, we propose a thermal field modeling method using PDEs with time-varying parameters. Because time-varying parameters in the PDE are unknown, we first estimate the time-varying parameters in the PDE, and then model the thermal field using the PDE with the estimated time-varying parameters. To resolve the parameter estimation problem, we treat the time-varying parameters as functional variables and use a combination of B-spline basis functions in terms of time to characterize them. Because the thermal field is a nonlinear multidimensional dynamic process, the derivatives of the dynamic process might not have an analytical expression. We model the dynamic process by a combination of B-spline basis functions. Thus, taking the derivatives of the thermal field is converted into taking the derivatives of the corresponding B-spline basis functions, which generates an analytical expression. A two-level regression method is developed to estimate the coefficients of the time-varying parameters and the dynamic process by considering the time-varying parameter model fitting and the PDE model fitting simultaneously. Then, we obtain the time-varying parameters and underlying thermal field. Simulation and real case studies are conducted to validate our proposed method, and the results show that our proposed method provides satisfactory performance.

In the future, we intend to investigate a parameter calibration method for PDE models by combining physical mechanisms and statistical analysis of thermal systems.

Appendix A
Tensor Product of Basis Functions

In the simulation case, two independent variables are used, namely, a space variable z and a time variable t. In the space domain, we employ a combination of basis functions in terms of z as follows:

$$\Phi_{i_z,1}(z) = \begin{cases} 1, & Z_{i_z} < z < Z_{i_z+1} \\ 0, & \text{otherwise} \end{cases}$$
$$\Phi_{i_z,p_z}(z) = \frac{z - Z_{i_z}}{Z_{i_z+p_z} - Z_{i_z}}\Phi_{i_z,p_z-1}(z) + \frac{Z_{i_z+p_z} - z}{Z_{i_z+p_z} - Z_{i_z+1}}\Phi_{i_z+1,p_z-1}(z)$$

where p_z denotes the order of basis functions in terms of space, i_z denotes the index of knots in terms of space, and Z_{i_z} denotes the location of the knot i_z. We denote M_z to be the number of basis functions in terms of space, and then we obtain $M_z = I_z + p_z - 1$, in which I_z is the number of knots in the space domain. To simplify the notation, we express the basis functions in the space domain $\Phi_{i_z,p_z}(z), i_z = 1, \ldots, I_z$ as $\Phi_z(z) = \{\Phi_{z,1}(z), \ldots, \Phi_{z,m_z}(z), \ldots, \Phi_{z,M_z}(z)\}$, in which $\Phi_{z,m_z}(t), Z_{i_z} < z < Z_{i_z+1}$ is a piecewise function for all $m_z = 1, \ldots, M_z$. Similarly, in the time domain, we obtain $\Phi_t(t) = \{\Phi_{t,1}(t), \ldots, \Phi_{t,m_t}(t), \ldots, \Phi_{t,M_t}(t)\}$, where M_t is the number of basis functions in terms of t. The tensor product of the basis functions for $u(z, t)$ is expressed as follows:

$$u(t, z) = \sum_{m_t=1}^{M_t}\sum_{m_z=1}^{M_z} \alpha_{m_t,m_z}\Phi_{m_t,m_z}(t, z) = \mathbf{\Phi}^T\boldsymbol{\alpha} \tag{20}$$

in which

$$\Phi_{m_t,m_z}(t, z) = \Phi_{t,m_t}(t)\Phi_{z,m_z}(z), \quad (m_t = 1, \ldots, M_t, m_z = 1, \ldots, M_z)$$

where $\mathbf{\Phi}$ denotes a vector of basis functions for $u(t, z)$, and $\boldsymbol{\alpha}$ denotes a vector of basis coefficients for $u(t, z)$.

Appendix B
Calculation of Penalty Matrix $\mathbf{\Omega}(\boldsymbol{\beta})$

$\mathbf{\Omega}(\boldsymbol{\beta})$ is a $K \times K$ penalty matrix, in which (h, j)th element is calculated by $\int \mathbf{g}_h(\mathbf{x}; \boldsymbol{\beta})\mathbf{g}_j^T(\mathbf{x}; \boldsymbol{\beta})d\mathbf{x}$. In our simulation and real cases, $\mathbf{\Omega}(\boldsymbol{\beta})$ is the summation of matrix integrals; it is introduced in Appendix B-A and Appendix B-B.

A. $\mathbf{\Omega}(\boldsymbol{\beta})$ in Simulation Case

$$\begin{aligned}
&\mathbf{\Omega}(\boldsymbol{\beta}) \\
&= \int_z\int_t \mathbf{g}(t, z, \boldsymbol{\beta})\mathbf{g}^T(t, z, \boldsymbol{\beta})dtdz \\
&= \int_z\int_t \boldsymbol{\beta}_1^T\Psi_1(t)\Psi_1^T(t)\boldsymbol{\beta}_1\frac{\partial^2\mathbf{\Phi}}{\partial z^2}\frac{\partial^2\mathbf{\Phi}^T}{\partial z^2}dtdz \\
&\quad + \int_z\int_t \boldsymbol{\beta}_2^T\Psi_2(t)\Psi_2^T(t)\boldsymbol{\beta}_2\frac{\partial\mathbf{\Phi}}{\partial z}\frac{\partial\mathbf{\Phi}^T}{\partial z}dtdz \\
&\quad + \int_z\int_t \boldsymbol{\beta}_3^T\Psi_3(t)\Psi_3^T(t)\boldsymbol{\beta}_3\mathbf{\Phi}\mathbf{\Phi}^T dtdz \\
&\quad + \int_z\int_t \boldsymbol{\beta}_2^T\Psi_2(t)\Psi_1(t)\boldsymbol{\beta}_1^T\left(\frac{\partial^2\mathbf{\Phi}}{\partial z^2}\frac{\partial\mathbf{\Phi}^T}{\partial z} + \frac{\partial\mathbf{\Phi}}{\partial z}\frac{\partial^2\mathbf{\Phi}^T}{\partial z^2}\right)dtdz \\
&\quad + \int_z\int_t \boldsymbol{\beta}_3^T\Psi_3(t)\Psi_1(t)\boldsymbol{\beta}_1^T\left(\frac{\partial^2\mathbf{\Phi}}{\partial z^2}\mathbf{\Phi}^T + \mathbf{\Phi}\frac{\partial^2\mathbf{\Phi}^T}{\partial z^2}\right)dtdz \\
&\quad + \int_z\int_t \boldsymbol{\beta}_2^T\Psi_2(t)\Psi_3(t)\boldsymbol{\beta}_3^T\left(\frac{\partial\mathbf{\Phi}}{\partial z}\mathbf{\Phi}^T + \mathbf{\Phi}\frac{\partial\mathbf{\Phi}^T}{\partial z}\right)dtdz \\
&\quad - \int_z\int_t \boldsymbol{\beta}_1^T\Psi_1(t)\left(\frac{\partial^2\mathbf{\Phi}}{\partial z^2}\frac{\partial\mathbf{\Phi}^T}{\partial t} + \frac{\partial\mathbf{\Phi}}{\partial t}\frac{\partial^2\mathbf{\Phi}^T}{\partial z^2}\right)dtdz \\
&\quad - \int_z\int_t \boldsymbol{\beta}_2^T\Psi_2(t)\left(\frac{\partial\mathbf{\Phi}}{\partial z}\frac{\partial\mathbf{\Phi}^T}{\partial t} + \frac{\partial\mathbf{\Phi}}{\partial t}\frac{\partial\mathbf{\Phi}^T}{\partial z}\right)dtdz \\
&\quad - \int_z\int_t \boldsymbol{\beta}_3^T\Psi_3(t)\left(\frac{\partial\mathbf{\Phi}}{\partial t}\mathbf{\Phi}^T + \mathbf{\Phi}\frac{\partial\mathbf{\Phi}^T}{\partial t}\right)dtdz \\
&\quad + \int_z\int_t \frac{\partial\mathbf{\Phi}}{\partial t}\frac{\partial\mathbf{\Phi}^T}{\partial t}dtdz.
\end{aligned} \tag{21}$$

B. $\mathbf{\Omega}(\boldsymbol{\beta})$ in Real Case

$$\begin{aligned}
&\mathbf{\Omega}(\boldsymbol{\beta}) \\
&= \int \mathbf{g}(t, x, y, z, \boldsymbol{\beta})\mathbf{g}^T(t, x, y, z, \boldsymbol{\beta})d\mathbf{x} \\
&= \int \boldsymbol{\beta}_1^T\Psi_1(t)\Psi_1(t)^T\boldsymbol{\beta}_1\frac{\partial^2\mathbf{\Phi}}{\partial x^2}\frac{\partial^2\mathbf{\Phi}^T}{\partial x^2}d\mathbf{x} \\
&\quad + \int \boldsymbol{\beta}_2^T\Psi_2(t)\Psi_2(t)^T\boldsymbol{\beta}_2\frac{\partial^2\mathbf{\Phi}}{\partial y^2}\frac{\partial^2\mathbf{\Phi}^T}{\partial y^2}d\mathbf{x} \\
&\quad + \int \boldsymbol{\beta}_3^T\Psi_3(t)\Psi_3(t)^T\boldsymbol{\beta}_3\frac{\partial^2\mathbf{\Phi}}{\partial z^2}\frac{\partial^2\mathbf{\Phi}^T}{\partial z^2}d\mathbf{x} \\
&\quad + \int \boldsymbol{\beta}_2^T\Psi_2(t)\Psi_1(t)^T\boldsymbol{\beta}_1\left(\frac{\partial^2\mathbf{\Phi}}{\partial y^2}\frac{\partial^2\mathbf{\Phi}^T}{\partial x^2} + \frac{\partial^2\mathbf{\Phi}}{\partial x^2}\frac{\partial^2\mathbf{\Phi}^T}{\partial y^2}\right)d\mathbf{x} \\
&\quad + \int \boldsymbol{\beta}_3^T\Psi_3(t)\Psi_1(t)^T\boldsymbol{\beta}_1\left(\frac{\partial^2\mathbf{\Phi}}{\partial z^2}\frac{\partial^2\mathbf{\Phi}^T}{\partial x^2} + \frac{\partial^2\mathbf{\Phi}}{\partial x^2}\frac{\partial^2\mathbf{\Phi}^T}{\partial z^2}\right)d\mathbf{x}
\end{aligned}$$

$$
\begin{aligned}
&+\int \boldsymbol{\beta}_3^T \Psi_3(t)\Psi_2(t)^T \boldsymbol{\beta}_2\left(\frac{\partial^2 \boldsymbol{\Phi}}{\partial z^2}\frac{\partial^2 \boldsymbol{\Phi}^T}{\partial y^2}+\frac{\partial^2 \boldsymbol{\Phi}}{\partial y^2}\frac{\partial^2 \boldsymbol{\Phi}^T}{\partial z^2}\right)d\mathbf{x}\\
&-\int \boldsymbol{\beta}_1^T \Psi_1(t)\left(\frac{\partial \boldsymbol{\Phi}}{\partial t}\frac{\partial^2 \boldsymbol{\Phi}^T}{\partial x^2}+\frac{\partial^2 \boldsymbol{\Phi}}{\partial x^2}\frac{\partial \boldsymbol{\Phi}^T}{\partial t}\right)d\mathbf{x}\\
&-\int \boldsymbol{\beta}_2^T \Psi_2(t)\left(\frac{\partial \boldsymbol{\Phi}}{\partial t}\frac{\partial^2 \boldsymbol{\Phi}^T}{\partial y^2}+\frac{\partial^2 \boldsymbol{\Phi}}{\partial y^2}\frac{\partial \boldsymbol{\Phi}^T}{\partial t}\right)d\mathbf{x}\\
&-\int \boldsymbol{\beta}_3^T \Psi_3(t)\left(\frac{\partial \boldsymbol{\Phi}}{\partial t}\frac{\partial^2 \boldsymbol{\Phi}^T}{\partial z^2}+\frac{\partial^2 \boldsymbol{\Phi}}{\partial z^2}\frac{\partial \boldsymbol{\Phi}^T}{\partial t}\right)d\mathbf{x}\\
&+\int \frac{\partial \boldsymbol{\Phi}}{\partial t}\frac{\partial \boldsymbol{\Phi}^T}{\partial t}d\mathbf{x} \qquad (22)
\end{aligned}
$$

where $\mathbf{x} = \{t, x, y, z\}$.

C. Numerical Integration for $\boldsymbol{\Omega}(\boldsymbol{\beta})$

$\boldsymbol{\Omega}(\boldsymbol{\beta})$ usually does not have an analytical expression and needs to be evaluated using the numerical method. $\boldsymbol{\Omega}(\boldsymbol{\beta})$ is composed of integrations of basis functions with the same structures, which are calculated using the same rule. We use the composite Simpson's rule repeatedly to calculate the integrals [29]. For a univariate function $\varphi(x)$, the composite Simpson's rule approximates the integral as

$$
\begin{aligned}
\int_a^b \varphi(x)dx &\approx \frac{C}{3}\left(\varphi(x_0)+4\sum_{d=1}^{D/2}\varphi(x_{2d-1}) + 2\sum_{d=1}^{D/2-1}\varphi(x_{2d})+\varphi(x_D)\right)\\
&= \frac{C}{3}\sum_{d=0}^{D} w_d\varphi(x_d) \qquad (23)
\end{aligned}
$$

where $C = (b-a)/D$, $x_d = a + dC$, with $d = 0, 1, \ldots, D$, denote quadrature knots, and $(w_0, w_1, w_2 \ldots, w_{D-2}, w_{D-1}, w_D) = (1, 4, 2, 4, \ldots, 2, 4, 2, 1)$ denotes the weight of the quadrature knots, in which D is an even integer.

We take the calculation of the penalty matrix $\int_z \int_t (\partial\boldsymbol{\Phi}/\partial t)(\partial\boldsymbol{\Phi}^T/\partial t)dtdz$ in the simulation case as an example. We denote $D_1 + 1$ as the number of quadrature knots in the time domain, $(t_0, \ldots, t_{D_1})$ as the vector of knots, and $\boldsymbol{w}_1 = (w_{1,0}, w_{1,1}, \ldots, w_{1,D_1})$ as the vector of weights. Similarly, $D_2 + 1$, $(z_0, \ldots, z_{D_2})$, and $\boldsymbol{w}_2 = (w_{2,0}, w_{2,1}, \ldots, w_{2,D_2})$ are the number of quadrature knots, knot vector, and weight vector in the space domain, respectively. The (h, j)th element of the penalty matrix $\int_z \int_t (\partial\boldsymbol{\Phi}/\partial t)(\partial\boldsymbol{\Phi}^T/\partial t)dtdz$ is as follows:

$$
\begin{aligned}
&\int_z\int_t \frac{\partial}{\partial t}\Phi_h(t,z)\frac{\partial}{\partial t}\Phi_j(t,z)dtdz\\
&\approx \left(\frac{C}{3}\right)^2\sum_{d_1=0}^{D_1}\sum_{d_2=0}^{D_2} w_{1,d_1}w_{2,d_2}\frac{\partial}{\partial t}\Phi_h(t_{d_1}, z_{d_2})\frac{\partial}{\partial t}\Phi_j(t_{d_1}, z_{d_2})
\end{aligned}
$$

where D_1 and D_2 need to be reasonably large to ensure the accuracy of the numerical integration approximation, i.e., $D_1 D_2 = 10K$, in which K is the number of basis functions used in (5).

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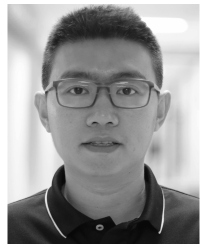

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