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Variational data assimilation with finite-element discretization for second-order parabolic interface equation

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In this paper, we propose and analyze a finite-element method of variational data assimilation for a second-order parabolic interface equation on a two-dimensional bounded domain. The Tikhonov regularization plays a key role in translating the data assimilation problem into an optimization problem. Then the existence, uniqueness and stability are analyzed for the solution of the optimization problem. We utilize the finite-element method for spatial discretization and backward Euler method for the temporal discretization. Then based on the Lagrange multiplier idea, we derive the optimality systems for both the continuous and the discrete data assimilation problems for the second-order parabolic interface equation. The convergence and the optimal error estimate are proved with the recovery of Galerkin orthogonality. Moreover, three iterative methods, which decouple the optimality system and significantly save computational cost, are developed to solve the discrete time evolution optimality system. Finally, numerical results are provided to validate the proposed method.

Keywords: data assimilation; second-order parabolic interface equation; finite-element method optimization; gradient-based iterative method.

1. Introduction

One major type of data assimilation aims to identify an initial condition by incorporating distributed observations over a time period into a dynamic system in order to improve the performance of the forecast. Such problems arise, for instance, in weather prediction (Brandt & Zaslavsky, 1997; Bruneau *et al.*, 1997; Rihan *et al.*, 2005; Fisher *et al.*, 2009), ocean state forecast (Rozier *et al.*, 2007; Agoshkov *et al.*, 2008; Agoshkov & Ipatova, 2010; Ipatova *et al.*, 2010; Tinka *et al.*, 2010; Le Dimet *et al.*, 2017; García-Archilla *et al.*, 2020), geoscience (Marchuk & Zalesny, 1993; Le Dimet *et al.*, 2004; Auroux, 2007; Vo & Durlofsky, 2015; Gesho *et al.*, 2016; Tarrahi *et al.*, 2016; Tang *et al.*, 2020), chemistry (Veersé *et al.*, 2000; Triantafyllou *et al.*, 2005; Le Dimet *et al.*, 2017) and so on. Currently there are several main categories of data assimilation techniques. First, statistical methods are based on the Bayes' theorem and consider the data assimilation as a recursive Bayesian estimation, see, e.g., Hansen & Penland (2007); Apte *et al.* (2008); Dimitriu (2008); Li & Xiu (2008); Mandel *et al.* (2008); Evensen (2009); Mandel *et al.* (2009); Stroud *et al.* (2010); Zamani *et al.* (2010); Iglesias *et al.* (2013); Fossum & Mannseth (2014); Bergou *et al.* (2016); González *et al.* (2017); Meldi & Poux (2017); Abarbanel *et al.* (2018); Reich (2019). Second, variational methods are based on optimal control theory and minimize an appropriately designed cost functional which measures the distance between the state variable and the distributed observations, see, e.g., Daescu & Navon (2003); Auroux (2007); Daescu & Navon (2007); Agoshkov *et al.* (2008); Apte *et al.* (2008); Jiang & Douglas (2009); Korn (2009); Rhodes & Hollingsworth (2009); Fehrenbach *et al.* (2010); Gronskis *et al.* (2013); Ştefănescu *et al.* (2015); Mons *et al.* (2016); Binev *et al.* (2017); Taddei (2017); Arcucci *et al.* (2019); Funke *et al.* (2019). Besides, nudging method and continuous data assimilation approach have also become popular in a lot of research fields recent years, see, e.g., Zou *et al.* (1992); Auroux & Nodet (2012); Rebholz & Zerfas (2021) and (Olson & Titi, 2003; Azouani *et al.*, 2014; Markowich *et al.*, 2016).

Over the past few decades, a vast amount of literature employing variational methods has been contributed to investigate the data assimilation problem for parabolic equations. In Lions (1971), J. L. Lions provided an elementary introduction of the adjoint method to recover parameters for parabolic partial differential equations. Motivated by this approach, researchers afterwards employed similar thoughts on the initial recovery of parabolic types of dynamics systems. In Yamamoto & Zou (2001); Burman *et al.* (2018), thorough analysis and efficient numerical methods were developed to attain the optimal initial condition of the heat equation. In Clason & Hepperger (2009), a forward approach to reconstruct the initial state was presented for the convection-diffusion equation and a practical algorithm is established. Moreover, the nonlinear parabolic equations, such as in water movement and in radiative heat transfer problems, were studied in Le Dimet & Shutyaev (2001); Pereverzyev *et al.* (2008) by reducing nonlinearity. However, to our current knowledge, few studies have investigated data assimilation for parabolic interface equations, which describe a variety of physical phenomena and have extensive applications.

Parabolic interface equations model physical or engineering problems when two or more distinct materials or fluids with different conductivities or diffusions are involved. Unlike a normal parabolic equation, many important features, such as the lower global regularity, interface jump conditions and discontinuous coefficients, need to be addressed more both theoretically and numerically, see, e.g., Babuska (1970); Chen & Zou (1998); Vaughan *et al.* (2006); He *et al.* (2011, 2013).

The main interest of this paper is to investigate the variational data assimilation for a second-order parabolic interface equation. A conventional way for solving such a problem is through optimization techniques. Under the constraint of the parabolic interface equation, we formulate the data assimilation problem as an optimization problem and minimize a cost functional that consists of a regularization term and the misfit between the state variable and the distributed observations. The regularization term and the misfitting term use weighted L^2 norm to account for the background and observations error covariance. Existence and uniqueness of such a minimization problem are established. We further demonstrate the stability analysis of the optimal solution and investigate the stability behavior affected by the error covariance operators and the regularization parameter. We also provide the first order necessary optimality system in continuous level with a weak and strong form.

In order to numerically approximate the proposed data assimilation problem, a finite-element method (FEM) is constructed for the spatial approximation to handle the interface and the discontinuous coefficient in the constraint equation, while the backward Euler scheme is utilized as a temporal discretization. A fully discrete optimality system is then derived by applying the Lagrange multiplier rule. *A priori* error estimation between the numerical approximation and the solution to the continuous data assimilation problem is carried out by introducing a variety of auxiliary equations to overcome the analysis gaps between the classical FEM (Chen & Zou, 1998) and the FEM in data assimilation. Moreover, we develop three decoupled iterative methods based on the conjugate gradient method, the BFGS method and the steepest descent method, in order to reduce the computational cost of solving the discrete optimality system.

The rest of this article is organized as follows: in Section 2, we introduce the second-order parabolic interface equation and provide the necessary mathematical preliminaries. In Section 3, we prove the wellposedness of the continuous data assimilation problem and derive the optimality system. In Section 4, we discuss the finite-element approximation to the continuous data assimilation problem and show its convergence analysis. In Section 5, three iterative methods are illustrated in detail that address the extreme computational cost. In Section 6, numerical experiments are presented to verify the expected performance. In Section 7, we draw some conclusions.

2. The second-order parabolic interface equation and preliminaries

We consider the following second-order parabolic interface equation:

$$\begin{cases} u_t - \nabla \cdot (\beta(x,y)\nabla u) = f, \quad \text{in } \Omega \times (0,T], \\ u(\cdot,0) = u_0, \quad \text{in } \Omega, \\ u = 0, \quad \text{on } \partial\Omega \times (0,T], \end{cases} \tag{2.1}$$

together with the jump interface condition,

$$[u]|_\Gamma = 0, \quad \left[\beta(x,y)\frac{\partial u}{\partial \vec{n}}\right]|_\Gamma = 0. \tag{2.2}$$

Here $\Omega \subset \mathbb{R}^2$ is an open bounded domain, the curve Γ is a smooth interface that separates Ω into two subdomains Ω^+ and Ω^- such that $\Omega = \Omega^+ \cup \Omega^- \cup \Gamma$, $[u]|_\Gamma = u^+|_\Gamma - u^-|_\Gamma$ is the jump of function u across the interface Γ, where $u^+ = u|_{\Omega^+}$ and $u^- = u|_{\Omega^-}$, $\vec{n}$ is the unit normal vector along interface Γ pointing to Ω^-, $\frac{\partial u}{\partial \vec{n}}$ is the normal derivative of u and $\beta(x,y)$ is assumed to be a positive piecewise constant function

$$\beta(x,y) = \begin{cases} \beta^+ & \text{if } (x,y) \in \Omega^+, \\ \beta^- & \text{if } (x,y) \in \Omega^-, \end{cases}$$

and the source term f is given discontinuously as

$$f(x,y,t) = \begin{cases} f^+ & \text{if } (x,y) \in \Omega^+, \\ f^- & \text{if } (x,y) \in \Omega^-. \end{cases}$$

We now introduce necessary preliminaries for the discussion of the data assimilation problem concerning equations (2.1)-(2.2). Let $\|\cdot\|$ denote norm of bounded linear operators, $(\cdot,\cdot)$ denote inner product in a Hilbert space, $\|\cdot\|_0$ denote the L^2-norm, $\|\cdot\|_\infty$ denote the L^∞-norm and $\|\cdot\|_m$ denote the standard norm in the Sobolev space $W^{m,2}(\Omega)$, which is also written as $H^m(\Omega)$. For the temporal–spatial function spaces over $(0,T)\times\Omega$, we define

$$\text{for } 1\leqslant p<\infty,\quad W^{m,p}(0,T;\mathscr{B})=\left\{u(t)\in\mathscr{B} \text{ for a.e. } t\in(0,T) \text{ and } \sum_{j=0}^{m}\int_0^T \|u^{(j)}(t)\|_{\mathscr{B}}^p\,\mathrm{d}t<\infty\right\};$$

$$\text{for } p=\infty,\quad W^{m,\infty}(0,T;\mathscr{B})=\left\{u(t)\in\mathscr{B} \text{ for a.e. } t\in(0,T) \text{ and } \max_{0\leqslant j\leqslant m}\left(ess\sup_{0\leqslant t\leqslant T}\|u^{(j)}(t)\|_{\mathscr{B}}\right)<\infty\right\};$$

which are equipped with corresponding norms

$$\|u\|_{W^{m,p}(0,T;\mathscr{B})}=\left(\sum_{j=0}^{m}\int_0^T \|u^{(j)}(t)\|_{\mathscr{B}}^p\,\mathrm{d}t\right)^{\frac{1}{p}},$$

$$\|u\|_{W^{m,\infty}(0,T;\mathscr{B})}=\max_{0\leqslant j\leqslant m}\left(ess\sup_{0\leqslant t\leqslant T}\|u^{(j)}(t)\|_{\mathscr{B}}\right),$$

where $\mathscr{B}$ is a general Banach space. As usual, we let $L^p(0,T;\mathscr{B})=W^{0,p}(0,T;\mathscr{B})$ and $H^m(0,T;\mathscr{B})=W^{m,2}(0,T;\mathscr{B})$.

We shall also need the following spaces:

$$X=H^1(\Omega)\cap H^2(\Omega^+)\cap H^2(\Omega^-),$$
$$Y=L^2(\Omega)\cap H^1(\Omega^+)\cap H^1(\Omega^-),$$

equipped with norms

$$\|u\|_X=\|u\|_{H^1(\Omega)}+\|u\|_{H^2(\Omega^+)}+\|u\|_{H^2(\Omega^-)},$$
$$\|u\|_Y=\|u\|_{L^2(\Omega)}+\|u\|_{H^1(\Omega^+)}+\|u\|_{H^1(\Omega^-)}.$$

We write $Y(0,T)=L^2(0,T;X)\cap H^1(0,T;Y)$.

To introduce a weak form of the interface problem (2.1)–(2.2), we define the continuous bilinear form $a(\cdot,\cdot)$: $H_0^1(\Omega)\times H_0^1(\Omega)\to\mathbb{R}$ and the associated operator $A: H_0^1(\Omega)\to H^{-1}(\Omega)$ as follows:

$$a(u,v)=\int_\Omega \beta(x,y)\nabla u\cdot\nabla v\,\mathrm{d}x\,\mathrm{d}y=\int_{\Omega^+}\beta^+\nabla u\cdot\nabla v\,\mathrm{d}x\,\mathrm{d}y+\int_{\Omega^-}\beta^-\nabla u\cdot\nabla v\,\mathrm{d}x\,\mathrm{d}y,$$
$$a(u,v)=\langle Au,v\rangle,$$

where $\langle\cdot,\cdot\rangle$ defines the duality pairing between $H^{-1}(\Omega)$ and $H_0^1(\Omega)$. We may also use $\langle\cdot,\cdot\rangle$ to refer a general duality pairing in other Banach space. As usual, $a(\cdot,\cdot)$ has been assumed to be coercive and continuous, i.e.,

$$a(u,u) \geqslant C_c\|u\|_1^2 \quad \forall u \in H_0^1(\Omega), \tag{2.3}$$

$$a(u,v) \leqslant C\|u\|_1\|v\|_1 \quad \forall u,v \in H_0^1(\Omega). \tag{2.4}$$

Setting $W(0,T) = L^2(0,T;H_0^1(\Omega)) \cap H^1(0,T;H^{-1}(\Omega))$, the weak formulation can be stated as follows Chen & Zou (1998):

$$\begin{aligned}
&\text{Given } f \in L^2(0,T;H^{-1}(\Omega)), \quad \text{find } u \in W(0,T) \ \text{ satisfying} \\
&\left\langle \frac{\partial u}{\partial t}, v \right\rangle + a(u,v) = \langle f, v\rangle, \quad \forall v \in H_0^1(\Omega), \\
&u(\cdot,0) = u_0 \quad \text{at } t=0 \quad \text{in } L^2(\Omega).
\end{aligned} \tag{2.5}$$

Note that (2.5) can be expressed in the form:

$$\begin{aligned}
&\frac{\partial u}{\partial t} + Au - f = 0 \quad \text{in } H^{-1}(\Omega), \\
&u(\cdot,0) = u_0 \quad \text{in } L^2(\Omega).
\end{aligned}$$

Throughout this paper, C is a generic positive constant that is independent of the mesh parameter h and the time step τ and is not necessarily the same at each occurrence.

3. Variational data assimilation

Let U denote the admissible solutions set that could be either $L^2(\Omega)$ or a closed convex subset of $L^2(\Omega)$. Given $T > 0$, $\alpha > 0$, a distributed observation $\hat{u} \in L^2(0,T;L^2(\Omega_o))$, a nonzero measure subset $\Omega_o \subseteq \Omega$, and a background information $u_0^b \in L^2(\Omega)$, the variational data assimilation for the second-order parabolic interface equation is given by

$$\min_{u_0\in U} F(u_0) = \frac{1}{2}\int_0^T \|\hat{u} - \mathscr{G}u(u_0)\|_{0,R,\Omega_o}^2 \,\mathrm{d}t + \frac{\alpha}{2}\left\|u_0 - u_0^b\right\|_{0,B}^2 \tag{3.1}$$

subject to

$$\begin{cases}
\left\langle \dfrac{\partial u}{\partial t}, v \right\rangle + a(u,v) = \langle f, v\rangle \quad \forall v \in H_0^1(\Omega), \\
u(\cdot,0) = u_0 \quad \text{at } t=0 \quad \text{in } \ L^2(\Omega).
\end{cases} \tag{3.2}$$

Here the mapping $u(u_0) : L^2(\Omega) \to W(0,T)$ is defined as the solution of (3.2) with the initial value u_0. The mapping $\mathscr{G} : L^2(\Omega) \mapsto L^2(\Omega_o)$ is a restriction of function $v(\cdot,t) \in L^2(\Omega)$, i.e.,

$$\mathscr{G}v = v|_{\Omega_o} = v \quad \text{for points } \ (x,y) \in \Omega_o.$$

Also $\mathscr{G}$ has the following basic properties

$$\|\mathscr{G}\| \leqslant 1, \quad \mathscr{G}^* = \chi_{\Omega_o},$$

where $\mathscr{G}^*$ is the adjoint operator of $\mathscr{G}$, and χ_{Ω_o} is the characteristic function. We also give the notations $\|\cdot\|^2_{0,R,\Omega_o} = (R\cdot,\cdot)_{\Omega_o} = (\cdot,\cdot)_{0,R,\Omega_o}$ and $\|\cdot\|^2_{0,B} = (B\cdot,\cdot) = (\cdot,\cdot)_{0,B}$. $R(\cdot,t) : L^2(\Omega_o) \mapsto L^2(\Omega_o)$ and $B : L^2(\Omega) \mapsto L^2(\Omega)$ are all bounded, self-adjoint and positive definite operators accounting for the observations and background error covariance. Further discussion for R and B will be provided in the numerical approximation Section 4. Here we interpret the boundedness and positive definiteness as follows:

$$\left|(p,q)_{0,R(\cdot,t),\Omega_o}\right| \leqslant \lambda^R(t)\|p\|_{0,\Omega_o}\|q\|_{0,\Omega_o} \quad \forall p,q \in L^2(\Omega_o), \tag{3.3}$$

$$(R(\cdot,t)p,p)_{0,\Omega_o} \geqslant \lambda_R(t)\|p\|^2_{0,\Omega_o} \quad \forall p \in L^2(\Omega_o), \tag{3.4}$$

$$|(p,q)_{0,B}| \leqslant \lambda^B\|p\|_0\|q\|_0 \quad \forall p,q \in L^2(\Omega), \tag{3.5}$$

$$(Bp,p) \geqslant \lambda_B\|p\|^2_0 \quad \forall p \in L^2(\Omega), \tag{3.6}$$

where $\lambda_R(t), \lambda^R(t)$ and λ_B, λ^B are all positive real numbers. We further assume that

$$\sup_{0<t\leqslant T} \lambda^R(t) = \lambda^R > 0, \quad \inf_{0<t\leqslant T} \lambda_R(t) = \lambda_R > 0. \tag{3.7}$$

The minimization of $\frac{1}{2}\int_0^T \|\hat{u} - \mathscr{G}(u_0)\|^2_{0,R,\Omega_o}\,\mathrm{d}t$ in (3.1) is the primary goal, which tries to drive the state variable $u(u_0)$ close to the distributed observations $\hat{u}$ over $(0,T) \times \Omega_o$ via adjusting the initial condition u_0. The second term $\frac{\alpha}{2}\|u_0 - u_0^b\|^2_{0,B}$ incorporates the background information, also works as a Tikhonov regularization and plays a key role in guaranteeing the uniqueness and stability of the optimal solution for the data assimilation problem. The α is a regularization parameter to balance the minimizing in the cost functional according to the reliability of observations and background information. It is well-known that the identification of initial conditions of diffusion equations such as heat equation is severely ill-posed because of the smoothing property of solutions. That is, the solution does not depend continuously on the data so that small noise in data may cause huge errors in the initial temperature. This lack of stability can be alleviated by investigating the deviations in solutions in an admissible set that is usually defined to be a bounded set in some appropriate function space. This so-called conditional stability of initial value identifications was extensively studied in the literature and provides some insightful guidance to numerical solutions of practical inverse problems, we refer to Li *et al.* (2009) and Yamamoto & Zou (2001) for more details. In practical computations, the choice of the regularization parameter α is important and tricky and usually makes use of statistical information about the noise level δ in the observation information $\hat{u}$. Roughly speaking, the approaches include *a priori* choice $\alpha = \alpha(\delta)$, *a posteriori* choice $\alpha = \alpha(\delta, \hat{u})$ and heuristic rules $\alpha = \alpha(\hat{u})$, we refer to Engl *et al.* (1996) and Vogel (2002, Chap. 7) for a comprehensive study. In our problem setting in (3.1)–(3.2), the noise information can be incorporated into the error covariance operators R and B contained in the norms $\|\cdot\|_{0,R,\Omega_o}$ and $\|\cdot\|_{0,B}$, respectively, thus the regularization parameter α can be simply chosen as 1.

For the minimization problem (3.1)–(3.2), provided that $\partial\Omega$ and Γ are smooth enough, $f \in L^2(0,T;L^2(\Omega))$, $\hat{u} \in L^2(0,T;L^2(\Omega_o))$, and $u_0^b \in L^2(\Omega)$, we have the following existence and uniqueness result.

THEOREM 3.1 (Lions, 1971, Theorem 1.1) There exists a unique solution $u_0 \in U$ for the data assimilation problem (3.1)–(3.2). Furthermore, the solution u_0 is characterized by

$$F'(u_0)(v-u_0) = \int_0^T \left(\mathscr{G}u(u_0) - \hat{u}, \mathscr{G}u(v) - \mathscr{G}u(u_0)\right)_{0,R,\Omega_o} \mathrm{d}t + \alpha \left(u_0 - u_0^b, v - u_0\right)_{0,B} \geqslant 0 \quad \forall v \in U. \tag{3.8}$$

Next, we show that the solution of problem (3.1)–(3.2) is stable with respect to the perturbations on the distributed observations and the regularization parameter α.

THEOREM 3.2 The solution of problem (3.1)–(3.2) continuously depends on the regularization parameter α, observations $\hat{u}$, and background information u_0^b. I.e., let $\bar{u}_0$ be the optimal solution with regularization parameter $\alpha + \epsilon_1$, perturbed observations $\hat{u} + \epsilon_2$, and background information $u_0^b + \epsilon_3$, where $\epsilon_1 \in \mathbb{R}$, $\epsilon_2 \in L^2(0,T;L^2(\Omega_o))$ and $\epsilon_3 \in L^2(\Omega)$. Assume C is a positive constant and $\frac{\|\epsilon_3\|_0}{|\epsilon_1|} \leqslant C$, we then have the following estimate:

$$\alpha\|u_0 - \bar{u}_0\|_0^2 \leqslant \left(\frac{\lambda^R}{\sqrt{2\lambda_R\lambda_B}}\right)^2 \|\epsilon_2\|^2_{L^2(0,T;L^2(\Omega_o))} + \left(\frac{\lambda^B}{\lambda_B}\right)^2 \left(\|u_0\|_0^2 + \|u_0^b\|_0^2\right)|\epsilon_1| + C\left(\frac{\lambda^B}{\lambda_B}\right)^2 (\alpha + |\epsilon_1|)^2 \|\epsilon_3\|_0.$$

Proof. Using the optimality condition (3.8) gives us

$$\int_0^T \left(\mathscr{G}u(\bar{u}_0) - \hat{u} - \epsilon_2, \mathscr{G}u(v) - \mathscr{G}u(\bar{u}_0)\right)_{0,R,\Omega_o} \mathrm{d}t + (\alpha + \epsilon_1)\left(\bar{u}_0 - u_0^b - \epsilon_3, v - \bar{u}_0\right)_{0,B} \geqslant 0 \quad \forall v \in U. \tag{3.9}$$

Taking $v = u_0$ in (3.9) and $v = \bar{u}_0$ in (3.8) provides us

$$\int_0^T \left(\mathscr{G}u(\bar{u}_0) - \hat{u} - \epsilon_2, \mathscr{G}u(u_0) - \mathscr{G}u(\bar{u}_0)\right)_{0,R,\Omega_o} \mathrm{d}t + (\alpha + \epsilon_1)\left(\bar{u}_0 - u_0^b - \epsilon_3, u_0 - \bar{u}_0\right)_{0,B} \geqslant 0,$$

$$\int_0^T \left(\mathscr{G}u(u_0) - \hat{u}, \mathscr{G}u(\bar{u}_0) - \mathscr{G}u(u_0)\right)_{0,R,\Omega_o} \mathrm{d}t + \alpha\left(u_0 - u_0^b, \bar{u}_0 - u_0\right)_{0,B} \geqslant 0.$$

Adding the two inequalities together leads to

$$\begin{aligned}&\int_0^T \|\mathscr{G}u(u_0) - \mathscr{G}u(\bar{u}_0)\|^2_{0,R,\Omega_o} \mathrm{d}t + (\alpha + \epsilon_1)\|u_0 - \bar{u}_0\|^2_{0,B} \\ &\leqslant \int_0^T \left(\epsilon_2, \mathscr{G}u(\bar{u}_0) - \mathscr{G}u(u_0)\right)_{0,R,\Omega_o} \mathrm{d}t + \epsilon_1\left(u_0 - u_0^b, u_0 - \bar{u}_0\right)_{0,B} + (\alpha + \epsilon_1)\left(\epsilon_3, u_0 - \bar{u}_0\right)_{0,B}.\end{aligned} \tag{3.10}$$

For terms in the left-hand side of (3.10), we use (3.4) and (3.7) to have

$$\begin{aligned}&\int_0^T \|\mathscr{G}u(u_0) - \mathscr{G}u(\bar{u}_0)\|^2_{0,R,\Omega_o} \mathrm{d}t + (\alpha + \epsilon_1)\|u_0 - \bar{u}_0\|^2_{0,B} \\ &\qquad \geqslant \lambda_R \int_0^T \|u(u_0) - u(\bar{u}_0)\|^2_{0,\Omega_o} \mathrm{d}t + \lambda_B(\alpha - |\epsilon_1|)\|u_0 - \bar{u}_0\|_0^2.\end{aligned} \tag{3.11}$$

For terms in the right-hand side (3.10), we use (3.3), (3.5), (3.7), and apply Cauchy–Schwarz and Young's inequality,

$$
\begin{aligned}
&\int_0^T (\epsilon_2, \mathscr{G}u(\bar{u}_0) - \mathscr{G}u(u_0))_{0,R,\Omega_o}\,\mathrm{d}t + \epsilon_1\left(u_0 - u_0^b, u_0 - \bar{u}_0\right)_{0,B} + (\alpha+\epsilon_1)\,(\epsilon_3, u_0 - \bar{u}_0)_{0,B} \\
&\leqslant \lambda^R \int_0^T \|\epsilon_2\|_{0,\Omega_o}\|u(u_0) - u(\bar{u}_0)\|_{0,\Omega_o}\,\mathrm{d}t + \lambda^B|\epsilon_1|\left\|u_0 - u_0^b\right\|_0 \|u_0 - \bar{u}_0\|_0 + \lambda^B(\alpha + |\epsilon_1|)\|\epsilon_3\|_0\|u_0 - \bar{u}_0\|_0 \\
&\leqslant \lambda_R \int_0^T \|u(u_0) - u(\bar{u}_0)\|^2_{0,\Omega_o}\,\mathrm{d}t + \frac{(\lambda^R)^2}{4\lambda_R}\int_0^T \|\epsilon_2\|^2_{0,\Omega_o}\,\mathrm{d}t + \frac{\lambda_B}{2}|\epsilon_1|\|u_0 - \bar{u}_0\|_0^2 + \frac{(\lambda^B)^2}{2\lambda_B}\left(\|u_0\|_0^2 + \|u_0^b\|_0^2\right)|\epsilon_1| \\
&\quad + \frac{\lambda_B}{2}|\epsilon_1|\|u_0 - \bar{u}_0\|_0^2 + \frac{(\lambda^B)^2\|\epsilon_3\|_0^2}{2\lambda_B|\epsilon_1|}(\alpha + |\epsilon_1|)^2.
\end{aligned}
\tag{3.12}
$$

Combining (3.10)–(3.12) leads to

$$
\lambda_B(\alpha - 2|\epsilon_1|)\|u_0 - \bar{u}_0\|_0^2 \leqslant \frac{(\lambda^R)^2}{4\lambda_R}\int_0^T \|\epsilon_2\|^2_{0,\Omega_o}\,\mathrm{d}t + \frac{(\lambda^B)^2}{2\lambda_B}\left(\|u_0\|_0^2 + \|u_0^b\|_0^2\right)|\epsilon_1| + \frac{(\lambda^B)^2\|\epsilon_3\|_0^2}{2\lambda_B|\epsilon_1|}(\alpha + |\epsilon_1|)^2.
$$

Setting $|\epsilon_1| \leqslant \frac{\alpha}{4}$, we have the inequality

$$
\alpha\|u_0 - \bar{u}_0\|_0^2 \leqslant \left(\frac{\lambda^R}{\sqrt{2\lambda_R\lambda_B}}\right)^2 \|\epsilon_2\|^2_{L^2(0,T;L^2(\Omega_o))} + \left(\frac{\lambda^B}{\lambda_B}\right)^2\left(\|u_0\|_0^2 + \|u_0^b\|_0^2\right)|\epsilon_1| + C\left(\frac{\lambda^B}{\lambda_B}\right)^2(\alpha + |\epsilon_1|)^2\|\epsilon_3\|_0,
\tag{3.13}
$$

which implies that the solution of problem (3.1)–(3.2) continuously depends on the observational data $\hat{u}$, u_0^b, and α. □

The inequality (3.13) indicates that the solution stability would depend on α and the property of operators R and B, the property of B especially matters more. Once R and B have been prescribed, the regularization parameter α will dominate the stability.

With guarantee of the wellposedness, we next derive the optimality system to solve for the optimal initial condition. For presentation convenience, we consider the admissible set $U = L^2(\Omega)$ in the rest of paper, we also give remarks for specific cases of $U \subseteq L^2(\Omega)$.

There are multiple ways to work out the optimality system, such as dual method and the Lagrange multiplier rule. The core idea behind them are all essentially based on fundamental calculus of variation. In our case, we consider the variational data assimilation problem (3.1)–(3.2) as a PDE-constrained optimization, and adopt the Lagrange multiplier rule to relax the constraint. We first introduce the Lagrange multiplier $\begin{pmatrix} u^* \\ u^*(\cdot,0)\end{pmatrix} \in W(0,T) \times L^2(\Omega)$ and form the Lagrange functional:

$$
\begin{aligned}
\mathscr{L}(u, u_0, u^*, u_0^*) &= \frac{1}{2}\int_0^T \|\hat{u} - \mathscr{G}u(u_0)\|^2_{0,R,\Omega_o}\,\mathrm{d}t + \frac{\alpha}{2}\left\|u_0 - u_0^b\right\|^2_{0,B} \\
&+ \int_0^T \left(\left\langle \frac{\partial u}{\partial t}, u^*\right\rangle + a(u,u^*) - \langle f, u^*\rangle\right)\mathrm{d}t + \left(u(\cdot,0) - u_0, u^*(\cdot,0)\right).
\end{aligned}
\tag{3.14}
$$

Calculus of variation of (3.14) with respect to the multiplier $\begin{pmatrix} u^* \\ u^*(\cdot,0) \end{pmatrix}$ recovers the constraint equation (3.2). Calculus of variation of (3.14) with respect to $\begin{pmatrix} u \\ u(\cdot,0) \end{pmatrix}$, we obtain

$$\begin{aligned}
\frac{\partial \mathscr{L}(u,u_0,u^*,u_0^*)}{\partial u} v &= \int_0^T (\hat{u} - \mathscr{G}u(u_0), -\mathscr{G}v)_{0,R,\Omega_o}\,\mathrm{d}t + \int_0^T \left(\left\langle \frac{\partial v}{\partial t}, u^* \right\rangle + a(v,u^*) \right) \mathrm{d}t + (v(\cdot,0), u^*(\cdot,0)) \\
&= \int_0^T \left(\mathscr{G}^* \left(\hat{u} - \mathscr{G}u(u_0)\right), -v\right)_{0,R,\Omega_o}\,\mathrm{d}t + \int_0^T \left(\left\langle \frac{\partial v}{\partial t}, u^* \right\rangle + a(v,u^*) \right) \mathrm{d}t + (v(\cdot,0), u^*(\cdot,0)) \\
&= 0, \\
\frac{\partial \mathscr{L}(u,u_0,u^*,u_0^*)}{\partial u_0} z &= \alpha \left(u_0 - u_0^b, z\right)_{0,B} - (z, u^*(\cdot,0)) = 0.
\end{aligned} \tag{3.15}$$

Taking integration by part in time on the first equation of (3.15), we have

$$\begin{aligned}
&\int_0^T \left(\hat{u} - \mathscr{G}u(u_0), -\mathscr{G}v\right)_{0,R,\Omega_o}\,\mathrm{d}t + (v(\cdot,T), u^*(\cdot,T)) - (v(\cdot,0), u^*(\cdot,0)) \\
&+ \int_0^T \left(-\left\langle \frac{\partial u^*}{\partial t}, v \right\rangle + a(v,u^*) \right) \mathrm{d}t + (v(\cdot,0), u^*(\cdot,0)) = 0.
\end{aligned}$$

By imposing $u^*(\cdot,T) = 0$, we have

$$\int_0^T \left(-\left\langle \frac{\partial u^*}{\partial t}, v \right\rangle + a(u^*,v) \right) \mathrm{d}t = \int_0^T \left(\hat{u} - \mathscr{G}u(u_0), \mathscr{G}v\right)_{0,R,\Omega_o}\,\mathrm{d}t, \tag{3.16}$$

recall that $a(v,u^*) = a(u^*,v)$ from the definition of the bilinear form $a(\cdot,\cdot)$.

We now summarize the above operations (3.14)–(3.16) and conclude the optimality system:

$$\begin{cases}
\left\langle \dfrac{\partial u}{\partial t}, v \right\rangle + a(u,v) = \langle f, v\rangle \quad \forall v \in H_0^1(\Omega), \\
u(\cdot,0) = u_0 \quad \text{in } L^2(\Omega), \\
-\left\langle \dfrac{\partial u^*}{\partial t}, v \right\rangle + a(u^*,v) = \left(\hat{u} - \mathscr{G}u(u_0), \mathscr{G}v\right)_{0,R,\Omega_o} \quad \forall v \in H_0^1(\Omega), \\
u^*(\cdot,T) = 0 \quad \text{in } L^2(\Omega), \\
\alpha \left(u_0 - u_0^b, z\right)_{0,B} - (u^*(\cdot,0), z) = 0 \quad \forall z \in L^2(\Omega).
\end{cases} \tag{3.17}$$

Taking integration by part in space of Ω^+, Ω^- and following a density argument, the optimality system (3.17) can also be stated as a strong form:

$$
\begin{cases}
\dfrac{\partial u}{\partial t} - \nabla \cdot (\beta(x,y)\nabla u) = f \quad \text{in } \Omega \times (0,T], \\
u(\cdot,0) = u_0 \quad \text{in } \Omega, \\
u = 0 \quad \text{on } \partial\Omega \times (0,T], \\
[u]|_\Gamma = 0 \quad \text{on } \Gamma \times (0,T], \\
\left[\beta(x,y)\dfrac{\partial u}{\partial \vec{n}}\right]|_\Gamma = 0 \quad \text{on } \Gamma \times (0,T], \\
-\dfrac{\partial u^*}{\partial t} - \nabla \cdot (\beta(x,y)\nabla u^*) = \chi_{\Omega_o} R\left(\hat{u} - \mathscr{G}u(u_0)\right) \quad \text{in } \Omega \times [0,T), \\
u^*(\cdot,T) = 0 \quad \text{in } \Omega, \\
u^* = 0 \quad \text{on } \partial\Omega \times [0,T), \\
[u^*]|_\Gamma = 0 \quad \text{on } \Gamma \times [0,T), \\
\left[\beta(x,y)\dfrac{\partial u^*}{\partial \vec{n}}\right]|_\Gamma = 0 \quad \text{on } \Gamma \times [0,T), \\
\alpha B\left(u_0 - u_0^b\right) - u^*(\cdot,0) = 0 \quad \text{in } \Omega.
\end{cases} \tag{3.18}
$$

Since the minimization problem (3.1)–(3.2) is strictly convex, the first order necessary condition above is also sufficient. The latter optimality system with strong form can provide more options on the numerical solving.

REMARK 3.3 If the admissible set is considered as $U = \{u_0 \in L^2(\Omega) : a \leqslant u_0 \leqslant b\}$, then the optimal solution is an orthogonal projection of $\frac{B^{-1}u^*(\cdot,0)}{\alpha} + u_0^b$ onto U, i.e., $u_0 = \max\left\{a, \min\left\{b, \frac{B^{-1}u^*(\cdot,0)}{\alpha} + u_0^b\right\}\right\}$.

REMARK 3.4 For the interface conditions with jump $[\beta(x,y)\frac{\partial u}{\partial \vec{n}}]|_\Gamma = g$ and $[u]|_\Gamma = 0$, the constraint equation in (3.1)–(3.2) can be replaced by

$$
\begin{cases}
\left\langle \dfrac{\partial u}{\partial t}, v \right\rangle + a(u,v) = \langle f, v\rangle + \langle g, v\rangle \quad \forall v \in H_0^1(\Omega), \\
u(\cdot,0) = u_0 \quad \text{at } t = 0 \quad \text{in } L^2(\Omega).
\end{cases}
$$

We are still able to apply the Lagrange multiplier rule as shown above to attain the corresponding optimality system.

If the interface conditions with jump $[\beta(x,y)\frac{\partial u}{\partial \vec{n}}]|_\Gamma = g$ and $[u]|_\Gamma = p$ are both nonhomogeneous, the solution u is no longer in $H^1(\Omega)$ space, and we cannot define classical weak formulations and weak solutions. However, assume Γ is smooth and $p \in H^{1/2}(\Gamma)$, we can use the extension theorem to do a homogenization. We have an extended function w_1 such that $w_1|_\Gamma = p$ and satisfies

$$\begin{cases} \dfrac{\partial w_1}{\partial t} - \nabla \cdot (\beta^+ \nabla w_1) = 0 \quad \text{in } \Omega^+ \times (0,T], \\ w_1(\cdot,0) = w_0^1 \quad \text{in } \Omega^+, \\ w_1 = \begin{cases} p & \text{on } \Gamma \times (0,T], \\ 0 & \text{on } \partial\Omega^+ \setminus \Gamma \times (0,T]. \end{cases} \end{cases}$$

We can further extend w_1 from Ω^+ to Ω

$$w_2 = \begin{cases} w_1 & \text{in } \Omega^+, \\ 0 & \text{in } \Omega^-, \end{cases}$$

which gives a function w_2 with $[w_2]|_\Gamma = p$. Set $w = u - w_2$, we have a nonhomogeneous jump parabolic interface equation

$$\begin{cases} \dfrac{\partial w}{\partial t} - \nabla \cdot (\beta \nabla w) = f \quad \text{in } \Omega \times (0,T], \\ w(\cdot,0) = w_0 = \begin{cases} u_0 - w_0^1 & \text{in } \Omega^+, \\ u_0 & \text{in } \Omega^-, \end{cases} \\ [w]|_\Gamma = 0 \quad \text{on } \Gamma \times (0,T], \\ \left[\beta(x,y) \dfrac{\partial w}{\partial \vec{n}}\right]|_\Gamma = g - \dfrac{\partial w_2}{\partial \vec{n}} \quad \text{on } \Gamma \times (0,T]. \end{cases} \tag{3.19}$$

So far, we are available to introduce the weak formulation for equation (3.19) and formulate the data assimilation problem as:

$$\min_{w_0 \in U} F(w_0) = \frac{1}{2}\int_0^T \left\| \left(\hat{u} - \mathscr{G} w_2\right) - \mathscr{G} w(w_0) \right\|_{0,R,\Omega_o}^2 \, \mathrm{d}t + \frac{\alpha}{2} \left\| w_0 - \left(u_0^b - w_2(\cdot,0)\right) \right\|_{0,B}^2$$

subject to

$$\begin{cases} \left\langle \dfrac{\partial w}{\partial t}, v \right\rangle + a(w,v) = \langle f, v \rangle + \left\langle g - \dfrac{\partial w_2}{\partial \vec{n}}, v \right\rangle, \quad \forall v \in H_0^1(\Omega), \\ w(\cdot,0) = w_0 \quad \text{at } t = 0 \quad \text{in } L^2(\Omega). \end{cases}$$

To obtain u_0 and u, we first solve for w_0 and w, then have $u_0 = w_0 + w_2(\cdot,0)$ and $u = w + w_2$.

4. A finite-element approximation and convergence analysis

To numerically compute the solution discussed in Section 3, we present a fully discrete approximation to the data assimilation problem (3.1)–(3.2), that uses a piecewise linear finite-element method in space and the backward Euler scheme in time.

For the spatial discretization, we first approximate the smooth interface Γ and boundary $\partial\Omega$ with line segments, the union of such line segments forms an approximated interface Γ_h and boundary $\partial\Omega_h$. The domain circumscribed by $\partial\Omega_h$ is denoted with Ω_h, which is an approximation of Ω. Γ_h divides Ω_h into two subdomains Ω_h^+ and Ω_h^-, which forms an approximation of Ω^+ and Ω^-, respectively.

Let $\mathscr{T}_h^+$ denote a family of triangulation of Ω_h^+ and $\mathscr{T}_h^-$ denote a family of triangulation of Ω_h^- such that

$$\mathscr{T}_h = \mathscr{T}_h^+ \cup \mathscr{T}_h^-.$$

We need the vertices on $\partial\Omega_h$ or Γ_h of a triangle $\tau_h \in \mathscr{T}_h$ to be vertices of $\partial\Omega_h$ or Γ_h, respectively. We also assume the triangulation $\mathscr{T}_h$ satisfies the usual sort of quasi-uniformity condition.

Associated with $\mathscr{T}_h$ is the finite-element space $V_h = \mathrm{span}\{\phi_i\}_{i=1}^{i=N_b}$, where ϕ_i is piecewise linear polynomials and N_b is the number of finite-element nodes. The admissible set of discrete optimal solutions is then denoted by $U_h = V_h \cap U$.

For the time discretization we uniformly construct a time grid $0 = t_0 < t_1 < t_2 < t_3 ... < t_n ... < t_N = T$ with time step $\tau = \frac{T}{N}$. Let $I_n = (t_{n-1}, t_n]$ denote the n^{th} sub-interval. We use the finite-dimensional space

$$V_{\tau,h} = \{v : [0,T] \to V_h : v|_{I_n} \in V_h \quad \text{is constant in time}\}.$$

Let v^n be the value of $v \in V_{\tau,h}$ at t_n and $V_{\tau,h}^n$ be the restriction to I_n of the functions in $V_{\tau,h}$.

Given specific h, τ and $\alpha > 0$, the fully discrete approximation of problem (3.1)–(3.2) is stated as

$$\min_{u_{0,h} \in U_h} F_h(u_{0,h}) \tag{4.1}$$

subject to

$$\begin{cases} \left\langle \dfrac{u_h^{n+1} - u_h^n}{\tau}, v_h \right\rangle + a\left(u_h^{n+1}, v_h\right) = \langle f_{n+1}, v_h\rangle \quad \forall v_h \in V_h, \\ u_h^0 = u_{0,h}, \end{cases} \tag{4.2}$$

where

$$F_h(u_{0,h}) = \frac{1}{2}\tau \sum_{n=1}^{N} \left\| \hat{u}_h^n - \mathscr{G}_h^n u_h^n \right\|_{0,R_h^n,\Omega_o}^2 + \frac{\alpha}{2}\left\| u_{0,h} - u_{0,h}^b \right\|_{0,B_h}^2. \tag{4.3}$$

Here, $\hat{u}_h^n$ and $u_{0,h}^b$ can be viewed as finite-element interpolations or projections of $\hat{u}^n = \hat{u}(\cdot, t_n)$ and u_0^b, respectively. Mimicking the definition in the continuous case, we define $\mathscr{G}_h^n : L_h^2(\Omega) \mapsto L_h^2(\Omega_o)$ as the restriction mapping and $\mathscr{G}_h = \sum_{n=1}^{N} \mathscr{G}_h^n \chi_{I_n}$ as a piecewise constant function in time. We also have $\|\cdot\|^2_{0,R_h^n,\Omega_o} = (R_h^n \cdot, \cdot)_{\Omega_o} = (\cdot,\cdot)_{0,R_h^n,\Omega_o}$, and $\|\cdot\|^2_{0,B_h} = (B_h\cdot,\cdot) = (\cdot,\cdot)_{0,B_h}$. $R_h^n = R_h(\cdot,t_n) : L_h^2(\Omega_o) \mapsto L_h^2(\Omega_o)$ and $B_h : L_h^2(\Omega) \mapsto L_h^2(\Omega)$ are all bounded, self-adjoint and positive definite operators accounting for the observation and background error covariance. The operator $R_h = \sum_{n=1}^{N} R_h^n \chi_{I_n}$ is a piecewise constant function in time. $L_h^2(\Omega_o)$ and $L_h^2(\Omega)$ are L^2 spaces consisting of the span of the finite-element basis $\{\phi_i\}_{i=1}^{N_b}$. We also have the following operator properties:

$$\left|(p,q)_{0,R_h^n,\Omega_o}\right| \leqslant \lambda^{R_h^n} \|p\|_{0,\Omega_o} \|q\|_{0,\Omega_o} \quad \forall p,q \in L_h^2(\Omega_o), \tag{4.4}$$

$$\left(R_h^n p, p\right)_{0,\Omega_o} \geqslant \lambda_{R_h^n} \|p\|^2_{0,\Omega_o} \quad \forall p \in L_h^2(\Omega_o), \tag{4.5}$$

$$|(p,q)_{0,B_h}| \leqslant \lambda^{B_h} \|p\|_0 \|q\|_0 \quad \forall p,q \in L_h^2(\Omega), \tag{4.6}$$

$$(B_h p, p) \geqslant \lambda_{B_h} \|p\|_0^2 \quad \forall p \in L_h^2(\Omega), \tag{4.7}$$

where $\lambda_{R_h^n}, \lambda^{R_h^n}$ and $\lambda_{B_h}, \lambda^{B^h}$ are all positive real numbers. Recall the operator: $R_h(t) = \sum_{n=1}^{N} R_h^n \chi_{(t\in((n-1)\tau, n\tau])}$ and denote $\{\lambda^{R_h} = \sup_{0<t\leqslant T} \lambda^{R_h(t)} : |(p,q)_{0,R_h(t),\Omega_o}| \leqslant \lambda^{R_h(t)} \|p\|_{0,\Omega_o} \|q\|_{0,\Omega_o}$ $\forall p,q \in L_h^2(\Omega_o)\}$ and $\{\lambda_{R_h} = \inf_{0<t\leqslant T} \lambda_{R_h(t)} : |(p,q)_{0,R_h(t),\Omega_o}| \geqslant \lambda_{R_h(t)} \|p\|_{0,\Omega_o} \|q\|_{0,\Omega_o}$ $\forall p,q \in L_h^2(\Omega_o)\}$, we note that

$$\lambda^{R_h} = \sup_{1\leqslant n\leqslant N} \lambda^{R_h^n} > 0, \;\; \lambda_{R_h} = \inf_{1\leqslant n\leqslant N} \lambda_{R_h^n} > 0. \tag{4.8}$$

We also notice that, if we restrict the discussion of $R(\cdot,t_n), R_h^n, B$ and B_h in the finite dimensional space, i.e., $R(\cdot,t_n), R_h^n : L_h^2(\Omega_o) \mapsto L_h^2(\Omega_o)$ and $B, B_h : L_h^2(\Omega) \mapsto L_h^2(\Omega)$, then $R(\cdot,t_n) = R_h^n$, $B = B_h$, and R distinguishes from R_h only with a time approximation. In other words, the spatial approximation for operators R and B cannot be necessarily applied in the context of finite-element methods. The operator $\mathscr{G}_h$ is slightly different, the temporal approximation to $\mathscr{G}$ is not in need automatically, we can assume there is no spatial difference neither, i.e., $\mathscr{G} = \mathscr{G}_h$ when defined in space $L_h^2(\Omega)$. For clarity, we will remark more about the difference between the cost functions with and without spatial approximation of operators R and B in the following.

Remark 4.1 For case without spatial approximation of operators $R(\cdot,t_n)$ and B, the cost functional (4.3) is equivalent to the following matrix–vector formulation:

$$\min_{\vec{u}_{0,h}\in\mathbb{R}^{N_b}} F_h(\vec{u}_{0,h}) = \frac{1}{2}\tau \sum_{n=1}^{N} \left(\vec{\hat{u}}_h^n - \mathscr{G}_h^n \vec{u}_h^n\right)^T M_{R_h^n} \left(\vec{\hat{u}}_h^n - \mathscr{G}_h^n \vec{u}_h^n\right) + \frac{\alpha}{2}\left(\vec{u}_{0,h}^b - \vec{u}_{0,h}\right)^T M_{B_h} \left(\vec{u}_{0,h}^b - \vec{u}_{0,h}\right). \tag{4.9}$$

In (4.9), the matrix representation of the operator $\mathscr{G}_h^n$ is still denoted by $\mathscr{G}_h^n$, $\mathscr{G}_h^n$ gives the values of $\vec{u}_h^n$ at mesh grids within the observation domain Ω_o. $\vec{u}_{0,h}, \vec{u}_{0,h}^b, \vec{\hat{u}}_h^n$ and $\vec{u}_h^n$ are vector representations of $u_{0,h}, u_{0,h}^b, \hat{u}_h^n$ and u_h^n with finite-element basis $\{\phi_i\}_{i=1}^{N_b}$. The observation error covariance R_h^n and background error covariance B_h are incorporated into the weighted mass matrix $M_{R_h^n}$ and M_{B_h}, which are assembled from the finite-element method:

$$M_{R_h^n} = \left[\int_{\Omega_o} R_h^n \phi_j \phi_i \,\mathrm{d}x\,\mathrm{d}y\right]_{supp\{\phi_i,\phi_j\}\subset\Omega_o}, \qquad M_{B_h} = \left[\int_{\Omega} B_h \phi_j \phi_i \,\mathrm{d}x\,\mathrm{d}y\right]_{i,j=1}^{N_b}.$$

For case with spatial approximation for operators $R(\cdot, t_n)$ and B, the cost functional (4.3) can be equivalent to the following matrix–vector formulation:

$$\min_{\vec{u}_{0,h}\in\mathbb{R}^{N_b}} F_h(\vec{u}_{0,h}) = \frac{1}{2}\tau \sum_{n=1}^{N} \left(Q_h^n\left(\vec{\hat{u}}_h^n - \mathscr{G}_h^n \vec{u}_h^n\right)\right)^T M_o \left(Q_h^n\left(\vec{\hat{u}}_h^n - \mathscr{G}_h^n \vec{u}_h^n\right)\right)$$
$$+ \frac{\alpha}{2}\left(P_h\left(\vec{u}_{0,h}^b - \vec{u}_{0,h}\right)\right)^T M \left(P_h\left(\vec{u}_{0,h}^b - \vec{u}_{0,h}\right)\right). \tag{4.10}$$

In (4.10), M_o and M are mass matrices assembled as $M_o = \left[\int_{\Omega_o} \phi_j\phi_i \,\mathrm{d}x\,\mathrm{d}y\right]_{supp\{\phi_i,\phi_j\}\subset\Omega_o}$ and $M = \left[\int_{\Omega} \phi_j\phi_i \,\mathrm{d}x\,\mathrm{d}y\right]_{i,j=1}^{N_b}$. We still denote the matrix representation of operators R_h^n and B_h with R_h^n and B_h, R_h^n and B_h correspond to the inverse of the observation and background error covariance matrix. Since R_h^n and B_h are symmetric and positive definite, we have the decompositions $R_h^n = (Q_h^n)^T Q_h^n$ and $B_h = P_h^T P_h$ for some invertible matrices Q_h^n and P_h.

In real applications, the cost functional (4.10) is more often to be used since the observations $\{\hat{u}_h^n\}_{n=1}^N$ is usually evaluated at a set of discrete time moments $\{t_n\}_{n=1}^N$ and of spatial mesh grids.

Similar to the proof for the wellposedness of the continuous data assimilation problem, one can prove the wellposedness of the fully discrete data assimilation problem (4.1)–(4.3). Due to the page limitation, the details are omitted here.

THEOREM 4.2 Given $\tau = \frac{T}{N}$ and mesh size h, for each fixed regularization parameter α, there exists a unique optimal solution $u_{0,h} \in U_h$ such that the cost functional (4.3) is minimized.

Proof. First, note that the L^2-norm is continuous, the operators $\mathscr{G}_h^n$, R_h^n and B_h are all bounded, and the solution mapping $\mathscr{H}_h^n : u_{0,h} \mapsto u_h^n := \mathscr{H}_h^n(u_{0,h})$ is continuous by using the stability of the discretized parabolic interface equation (4.2). The cost functional (4.3) is composed by all these continuous mappings and thus is also continuous. Next, we show that the cost functional (4.3) is strictly convex by calculating its second-order derivative. The first order derivative of $F_h(u_{0,h})$ is

$$\frac{\partial F_h(u_{0,h})}{\partial u_{0,h}} z = \tau \sum_{n=1}^{N} \left(\hat{u}_h^n - \mathscr{G}_h^n u_h^n, -\frac{\partial\left(\mathscr{G}_h^n u_h^n\right)}{\partial u_{0,h}} z\right)_{0,R_h^n,\Omega_o} + \alpha\left(u_{0,h} - u_{0,h}^b, z\right)_{0,B_h} \quad \forall z \in U_h. \tag{4.11}$$

From (4.11), we calculate the second-order derivative of $F_h(u_{0,h})$:

$$\frac{\partial^2 F_h(u_{0,h})}{\partial {u_{0,h}}^2}(z,v) = \tau \sum_{n=1}^{N} \left(-\frac{\partial\left(\mathscr{G}_h^n u_h^n\right)}{\partial u_{0,h}} v, -\frac{\partial\left(\mathscr{G}_h^n u_h^n\right)}{\partial u_{0,h}} z\right)_{0,R_h^n,\Omega_o} + \tau \sum_{n=1}^{N} \left(\hat{u}_h^n - \mathscr{G}_h^n u_h^n, -\frac{\partial^2\left(\mathscr{G}_h^n u_h^n\right)}{\partial {u_{0,h}}^2}(z,v)\right)_{0,R_h^n,\Omega_o}$$
$$+ \alpha(v,z)_{0,B_h} \quad \forall z, v \in U_h. \tag{4.12}$$

Furthermore, we have $\frac{\partial^2(\mathscr{G}_h^n u_h^n)}{\partial {u_{0,h}}^2}(z,v) = \frac{\mathscr{G}_h^n \partial^2(u_h^n)}{\partial {u_{0,h}}^2}(z,v)$ due to the linearity of $\mathscr{G}_h^n$, and $\frac{\partial^2 u_h^n}{\partial {u_{0,h}}^2}(z,v) = 0$ because of the linearity of the parabolic interface equation (4.2). Therefore, with (4.12) we have

$$\frac{\partial^2 F_h(u_{0,h})}{\partial {u_{0,h}}^2}(z,z) = \tau \sum_{n=1}^{N} \left(\frac{\partial \left(\mathscr{G}_h^n u_h^n\right)}{\partial u_{0,h}} z, \frac{\partial \left(\mathscr{G}_h^n u_h^n\right)}{\partial u_{0,h}} z \right)_{0,R_h^n,\Omega_o} + \alpha (z,z)_{0,B_h} \geqslant \lambda_{B_h} \|z\|_0^2 \quad \forall z \in U_h, \quad (4.13)$$

which concludes the strictly convexity of (4.3). The convexity and continuity indicate that (4.3) is lower-semi-continuous. Then, similar to the proof in (Lions, 1971, Theorem 1.1), by arguing a constructed minimizing sequence on the lower-semi-continuous cost functional (4.3), we can conclude that there exist an optimal solution $u_{0,h}$. Using the strictly convexity again, we claim that the optimal solution is unique. This completes the proof. □

THEOREM 4.3 The solution of problem (4.1)–(4.3) continuously depends on the observational data $\{\hat{u}_h^n\}$, the background information $u_{0,h}^b$, and the parameter α. I.e., let $\bar{u}_{0,h}$ be the optimal solution for regularization parameter $\alpha+\epsilon_1$, perturbed observations $\{\hat{u}_h^n+\epsilon_{(n)}\}$, and background information $u_{0,h}^b+\epsilon_3$. where $\epsilon_1 \in \mathbb{R}$, $\epsilon_{(n)} \in L^2(\Omega_o)$ and $\epsilon_3 \in L^2(\Omega)$. Assume C is a positive constant and $\frac{\|\epsilon_3\|_0}{|\epsilon_1|} \leqslant C$ and $\sup_{1\leqslant n\leqslant N} \epsilon_{(n)} \leqslant \epsilon_2$, we then have the following estimate:

$$\alpha \|u_{0,h} - \bar{u}_{0,h}\|_0^2 \leqslant T\left(\frac{\lambda^{R_h}}{\sqrt{2\lambda_{R_h}\lambda_{B_h}}}\right)^2 \|\epsilon_2\|_{0,\Omega_o}^2 + \left(\frac{\lambda^{B_h}}{\lambda_{B_h}}\right)^2 \left(\|u_{0,h}\|_0^2 + \|u_{0,h}^b\|_0^2\right) |\epsilon_1| + C\left(\frac{\lambda^{B_h}}{\lambda_{B_h}}\right)^2 (\alpha + |\epsilon_1|)^2 \|\epsilon_3\|_0.$$

Proof. With (4.11), the first order optimality condition of problem (4.1)–(4.3) is given by

$$\begin{aligned} \frac{\partial F_h(u_{0,h})}{\partial u_{0,h}}(z - u_{0,h}) &= \tau \sum_{n=1}^{N} \left(\hat{u}_h^n - \mathscr{G}_h^n u_h^n, -\frac{\mathscr{G}_h^n \partial u_h^n}{\partial u_{0,h}}(z - u_{0,h}) \right)_{0,R_h^n,\Omega_o} + \alpha (u_{0,h} - u_{0,h}^b, z)_{0,B_h} \\ &= \tau \sum_{n=1}^{N} \left(\hat{u}_h^n - \mathscr{G}_h^n u_h^n, \mathscr{G}_h^n \left(u_h^n(u_{0,h}) - u_h^n(z)\right)\right)_{0,R_h^n,\Omega_o} + \alpha \left(u_{0,h} - u_{0,h}^b, z - u_{0,h}\right)_{0,B_h} \geqslant 0. \end{aligned} \quad (4.14)$$

Similar to Theorem 3.2, inequality (4.14) is the key to prove the stability. We can apply the same techniques as in the proof of Theorem 3.2 to complete the proof. □

REMARK 4.4 In finite dimensional spaces, bounded operators are all compact. Therefore, λ^{R_h}, λ_{R_h} and λ^{B_h}, λ_{B_h} are all determined by the max-min eigenvalues of $\{R_h^n\}$ and B_h.

In order to derive the discrete optimality system and solve for $u_{0,h}$, we apply the Lagrange multiplier rule and form the Lagrange functional:

$$\begin{aligned} \mathscr{L}\left(\bar{u}_h, u_{0,h}, \bar{u}_h^*\right) = &\frac{1}{2}\tau \sum_{n=1}^{N} \left\|\hat{u}_h^n - \mathscr{G}_h^n u_h^n\right\|_{0,R_h^n,\Omega_o}^2 + \frac{\alpha}{2}\left\|u_{0,h} - u_{0,h}^b\right\|_{0,B_h}^2 \\ &+ \tau \sum_{n=0}^{N-1} \left\langle \frac{u_h^{n+1} - u_h^n}{\tau} + A u_h^{n+1} - f_{n+1}, u_h^{*n} \right\rangle + \left(u_h^0 - u_{0,h}, u_h^{*0}\right), \end{aligned} \quad (4.15)$$

where $\bar{u}_h = (u_h^1, u_h^2, u_h^3, ..., u_h^N)$ and $\bar{u}_h^* = (u_h^{*0}, u_h^{*1}, u_h^{*2}, u_h^{*3}, ..., u_h^{*N-1})$. Recall that $\langle Au, v\rangle = a(u, v)$, and A is self-adjoint in the sense of $\langle Au, v\rangle_{H^{-1}\times H_0^1} = \langle Av, u\rangle_{H^{-1}\times H_0^1}$. Then we rewrite (4.15) as

$$\begin{aligned}
\mathscr{L}\left(\bar{u}_h, u_{0,h}, \bar{u}_h^*\right) &= \frac{1}{2}\tau \sum_{n=1}^{N} \left\|\hat{u}_h^n - \mathscr{G}_h^n u_h^n\right\|_{0,R_h^n,\Omega_o}^2 + \frac{\alpha}{2}\left\|u_{0,h} - u_{0,h}^b\right\|_{0,B_h}^2 + \left(u_h^N, u_h^{*N}\right) - \left(u_h^N, u_h^{*N}\right) + \left(u_h^0 - u_{0,h}, u_h^{*0}\right) \\
&\quad + \tau \sum_{n=0}^{N-1}\left(\left\langle \frac{u_h^{n+1} - u_h^n}{\tau}, u_h^{*n}\right\rangle + \left\langle Au_h^{n+1}, u_h^{*n}\right\rangle - \left\langle f_{n+1}, u_h^{*n}\right\rangle\right) \\
&= \frac{1}{2}\tau \sum_{n=1}^{N} \left\|\hat{u}_h^n - \mathscr{G}_h^n u_h^n\right\|_{0,R_h^n,\Omega_o}^2 + \frac{\alpha}{2}\left\|u_{0,h} - u_{0,h}^b\right\|_{0,B_h}^2 + \tau \sum_{n=1}^{N}\left\langle \frac{u_h^{*n-1} - u_h^{*n}}{\tau}, u_h^n\right\rangle \\
&\quad + \tau \sum_{n=1}^{N}\left\langle Au_h^{*n-1}, u_h^n\right\rangle - \tau \sum_{n=1}^{N}\left\langle f_n, u_h^{*n-1}\right\rangle + \left(u_h^N, u_h^{*N}\right) - \left(u_{0,h}, u_h^{*0}\right).
\end{aligned} \tag{4.16}$$

Using standard techniques of calculus of variations, we derive equations that correspond to rendering (4.16) stationary. Variations in the Lagrange multiplier $\bar{u}_h^*$ recover the constraint equation (4.2). Variations with respect to $u_{0,h}$ and u_h^n, for $n = 1, 2, 3....N - 1$ yield

$$\begin{aligned}
\frac{\partial \mathscr{L}\left(\bar{u}_h, u_{0,h}, \bar{u}_h^*\right)}{\partial u_{0,h}} z_h &= \alpha\left(u_{0,h} - u_{0,h}^b, z_h\right)_{0,B_h} - \left(u_h^{*0}, z_h\right) = 0, \\
\frac{\partial \mathscr{L}\left(\bar{u}_h, u_{0,h}, \bar{u}_h^*\right)}{\partial u_h^n} v_h &= \tau\left\langle \frac{u_h^{*n-1} - u_h^{*n}}{\tau}, v_h\right\rangle + \tau\left\langle Au_h^{*n-1}, v_h\right\rangle - \tau\left(\hat{u}_h^n - \mathscr{G}_h^n u_h^n, \mathscr{G}_h^n v_h\right)_{0,R_h^n,\Omega_o} = 0.
\end{aligned} \tag{4.17}$$

Imposing $u_h^{*N} = 0$ when calculating the variation with respect to u_h^N results in the discrete optimality system:

$$\begin{cases}
\left\langle \dfrac{u_h^{n+1} - u_h^n}{\tau}, v_h\right\rangle + a\left(u_h^{n+1}, v_h\right) = \langle f_{n+1}, v_h\rangle, \\
u_h^0 = u_{0,h}, \\
-\left\langle \dfrac{u_h^{*n+1} - u_h^{*n}}{\tau}, v_h\right\rangle + a\left(u_h^{*n}, v_h\right) = \left(\chi_{\Omega_o} R_h^n\left(\hat{u}_h^{n+1} - \mathscr{G}_h^{n+1}u_h^{n+1}\right), v_h\right), \\
u_h^{*N} = 0, \\
\left(\alpha B_h\left(u_{0,h} - u_{0,h}^b\right) - u_h^{*0}, z_h\right) = 0,
\end{cases} \tag{4.18}$$

for $n = 0, 1, 2, 3.....N - 1$.

We shall expect the discrete solution in (4.18) to converge to the solution of (3.17). That is, given fixed α, $u_{0,h} \to u_0$, $u_h \to u$ and $u_h^* \to u^*$ should be attained while the time step τ and finite-element mesh size h diminish (Yamamoto & Zou, 2001).

THEOREM 4.5 For each fixed regularization parameter α, let $\{u_{0,h}\}_{h>0}$ be the corresponding sequence of minimizer of the discrete data assimilation problem (4.1)–(4.3). Then $\{u_{0,h}\}_{h>0}$ converges to the optimal solution u_0 of the continuous problem (3.1)–(3.2) as $h, \tau \to 0$.

Proof. It is not difficult to see $F_h(u_{0,h}) \leqslant C$ for some constant C independent of h and τ. This can be verified by noticing that $F_h(u_{0,h}) \leqslant F_h(u^b_{0,h})$ while $F_h(u^b_{0,h})$ can be uniformly bounded by $\hat{u}, f$ and u^b_0. Then we can show that $\|u_{0,h}\|_0 \leqslant \sqrt{\frac{2}{\alpha\lambda_{B_h}} F_h(u_{0,h})} + \|u^b_{0,h}\|_0$ by using the cost functional $F_h(u_{0,h})$ in (4.3):

$$\sqrt{\frac{\alpha\lambda_{B_h}}{2}}\left(\|u_{0,h}\|_0 - \left\|u^b_{0,h}\right\|_0\right) \leqslant \sqrt{\frac{\alpha\lambda_{B_h}}{2}}\left\|u_{0,h} - u^b_{0,h}\right\|_0 \leqslant \sqrt{\frac{\alpha}{2}}\left\|u_{0,h} - u^b_{0,h}\right\|_{0,B_h} \leqslant \sqrt{F_h(u_{0,h})}.$$

Hence we can extract a subsequence $\{u_{0,h'}\}$ from $\{u_{0,h}\}$ such that $\{u_{0,h'}\}$ weakly converges to μ^* in $L^2(\Omega)$. We conclude furthermore

$$\lim_{h',\tau\to 0} \frac{1}{2}\tau \sum_{n=1}^{N} \left\|\hat{u}^n_h - \mathscr{G}^n_h u^n_h(u_{0,h'})\right\|^2_{0,R^n_h,\Omega_o} \to \frac{1}{2}\int_0^T \|\hat{u} - \mathscr{G}u(\mu^*)\|^2_{0,R,\Omega_o}\,\mathrm{d}t.$$

Thus, for $\forall v \in U$, by the weakly lower semicontinuity we deduce

$$\begin{aligned} F(\mu^*) &\leqslant \liminf_{h',\tau\to 0} \frac{1}{2}\tau \sum_{n=1}^{N} \left\|\hat{u}^n_{h'} - \mathscr{G}^n_h u^n_{h'}(u_{0,h'})\right\|^2_{0,R^n_{h'},\Omega_o} + \frac{\alpha}{2}\liminf_{h',\tau\to 0}\left\|u_{0,h'} - u^b_{0,h'}\right\|^2_{0,B_{h'}} \\ &\leqslant \liminf_{h',\tau\to 0} F_{h'}(u_{0,h'}) \leqslant \liminf_{h',\tau\to 0} F_{h'}(\pi_{h'}(v)) \\ &= \frac{1}{2}\int_0^T \|\hat{u} - \mathscr{G}u(v)\|^2_{0,R,\Omega_o}\,\mathrm{d}t + \frac{\alpha}{2}\|v - u^b_0\|^2_{0,B} = F(v), \end{aligned} \tag{4.19}$$

where π_h is the L^2 projection operator from U to U_h.

Then (4.19) and the uniqueness result in Theorem 3.1 imply that μ^* is the optimal solution of the problem (3.1)–(3.2) and thus the theorem is proved. □

Besides a general convergence result in Theorem 4.5, under appropriate assumptions, we can obtain the optimal finite-element convergence rate for $u_0 - u_{0,h}$, $u - u_h$ and $u^* - u^*_h$.

Compared with the classical FEM analysis, the difficulties in our case lie in the undetermined initial condition from the forward state equation and the Galerkin orthogonality we miss on the backward adjoint equation, both of which would lead to the invalidity of the classical analysis framework. In order to overcome these difficulties, we introduce the following auxiliary equations to bridge the analysis in the data assimilation problem and the classical FEM approximation results (Chen & Zou, 1998):

$$\begin{cases} \left\langle \dfrac{\partial u(u_{0,h})}{\partial t}, v\right\rangle + a(u(u_{0,h}), v) = \langle f, v\rangle, \\ u(u_{0,h})(\cdot, 0) = u_{0,h}, \end{cases} \tag{4.20}$$

$$\begin{cases} \left\langle -\dfrac{\partial u^*_{R_h}(u_h)}{\partial t}, v \right\rangle + a\left(u^*_{R_h}(u_h), v\right) = \left(\mathscr{G}^* R_h(\hat{u}_h - \mathscr{G}_h u_h), v\right), \\ u^*_{R_h}(u_h)(\cdot, T) = 0, \end{cases} \tag{4.21}$$

$$\begin{cases} \left\langle -\dfrac{\partial u^*_R(u_{0,h})}{\partial t}, v \right\rangle + a\left(u^*_R(u_{0,h}), v\right) = \left(\mathscr{G}^* R(\hat{u} - \mathscr{G} u(u_{0,h})), v\right), \\ u^*_R(u_{0,h})(\cdot, T) = 0. \end{cases} \tag{4.22}$$

The motivation of the constructions for (4.20) and (4.21) is to remove the uncertainties on the initial condition and source term. We then convert the target error estimate into an intermediate error that can be controlled by using (4.22) and the additional equalities $\alpha B(u_0 - u_0^b) - u^*(\cdot, 0) = 0$ and $\alpha B_h(u_{0,h} - u_{0,h}^b) - u_h^{*0} = 0$ in the optimality systems. The details will be demonstrated in the following theorem and lemmas.

THEOREM 4.6 Let $(u, u^*, u_0) \in W(0,T) \times W(0,T) \times U$ and $(u_h, u_h^*, u_{0,h}) \in V_{\tau,h} \times V_{\tau,h} \times U_h$ be solutions of the continuous optimality system (3.18) and discrete optimality system (4.18), respectively. Assuming u, u^* and u_0 are smooth enough, the observation $\hat{u}_h \in L^2(0,T; L^2(\Omega_o)) \cap L^\infty(0,T; L^2(\Omega_o))$, and the operators R, R_h, $\hat{u}$, $\hat{u}_h$, u_0^b, $u_{0,h}^b$ satisfy the following approximation:

$$\int_t^T ((R - R_h)p, q)_{0,\Omega_o}\, \mathrm{d}s \leqslant C\tau \|p\|_{L^2(t,T;L^2(\Omega_o))} \|q\|_{L^2(t,T;L^2(\Omega_o))},$$

$$\left\| u_0^b - u_{0,h}^b \right\|_0 \leqslant Ch^2, \quad \|\hat{u} - \hat{u}_h\|_{L^2(0,T;L^2(\Omega_o))} \leqslant C\left(\tau + h^2\right)$$

for any $p, q \in L^2(0,T; L_h^2(\Omega_o))$ and $T > t \geqslant 0$. Then we have the optimal finite-element convergence rate

$$\|u_0 - u_{0,h}\|_0 + \|u - u_h\|_{L^2(0,T;L^2(\Omega))} + \left\|u^* - u_h^*\right\|_{L^2(0,T;L^2(\Omega))} \leqslant C\left(\Omega, \alpha, \lambda_B, \lambda^R\right)(h^2 + \tau),$$

where $C(\Omega, \alpha, \lambda_B, \lambda^{R_h})$ is a constant that depends on Ω, and is proportional to $\frac{1}{\alpha}$, $\frac{\lambda^B}{\lambda_B}$ and $\frac{\lambda^R}{\lambda_B}$ as well.

This is the major theorem we are going to show in this section. To prove it, some useful inequalities need to be derived based on the auxiliary equations first.

LEMMA 4.7 Let $(u(u_{0,h}), u^*_{R_h}(u_h), u^*_R(u_{0,h})) \in W(0,T) \times W(0,T) \times W(0,T)$ be solutions for equations (4.20), (4.21) and (4.22), let $(u, u^*, u_0) \in W(0,T) \times W(0,T) \times U$ be the solution of (3.17), and let $(u_h, u_h^*, u_{0,h}) \in V_{\tau,h} \times V_{\tau,h} \times U_h$ be the solution of (4.18). Assume that the observations $\hat{u}_h \in L^2(0,T; L^2(\Omega_o)) \cap L^\infty(0,T; L^2(\Omega_o))$ and, for $\forall p, q \in L^2(0,T; L_h^2(\Omega_o))$, $R - R_h$ satisfies the approximation:

$$\int_t^T ((R - R_h)p, q)_{0,\Omega_o}\, \mathrm{d}s \leqslant C\tau \|p\|_{L^2(t,T;L^2(\Omega_o))} \|q\|_{L^2(t,T;L^2(\Omega_o))},$$

then we have the following inequalities

$$\|u - u(u_{0,h})\|_{L^2(0,T;L^2(\Omega))} \leqslant C\|u_0 - u_{0,h}\|_0, \tag{4.23}$$

$$\sup_{0\leqslant t\leqslant T} \left\| \left(u^*_{R_h}(u_h) - u^*_R(u_{0,h})\right)(\cdot,t)\right\|_{L^2(\Omega)} \leqslant C\left(\lambda^R\|\hat{u}_h - \hat{u}\|_{L^2(0,T;L^2(\Omega_o))} + \lambda^R\|u(u_{0,h}) - u_h\|_{L^2(0,T;L^2(\Omega))} + \tau\right), \tag{4.24}$$

$$\left\|u^*_{R_h}(u_h) - u^*_R(u_{0,h})\right\|_{L^2(0,T;L^2(\Omega))} \leqslant C\left(\lambda^R\|u(u_{0,h}) - u_h\|_{L^2(0,T;L^2(\Omega))} + \lambda^R\|\hat{u}_h - \hat{u}\|_{L^2(0,T;L^2(\Omega_o))} + \tau\right), \tag{4.25}$$

$$\left\|u^* - u^*_R(u_{0,h})\right\|_{L^2(0,T;L^2(\Omega))} \leqslant C\lambda^R\|u_0 - u_{0,h}\|_0. \tag{4.26}$$

Proof. By subtractions between the forward equation in (3.17) and (4.20), (4.21) and (4.22), and the backward equation in (3.17) and (4.22), respectively, we obtain the following new equations

$$\begin{cases} \left\langle \dfrac{\partial(u - u(u_{0,h}))}{\partial t}, v\right\rangle + a(u - u(u_{0,h}), v) = 0, \\ (u - u(u_{0,h}))(\cdot,0) = u_0 - u_{0,h}, \end{cases} \tag{4.27}$$

$$\begin{cases} \left\langle -\dfrac{\partial\left(u^*_{R_h}(u_h) - u^*_R(u_{0,h})\right)}{\partial t}, v\right\rangle + a\left(u^*_{R_h}(u_h) - u^*_R(u_{0,h}), v\right) \\ = \left(\mathcal{G}^*R_h(\hat{u}_h - \mathcal{G}_h u_h) - \mathcal{G}^*R(\hat{u} - \mathcal{G}u(u_{0,h})), v\right), \\ \left(u^*_{R_h}(u_h) - u^*_R(u_{0,h})\right)(\cdot,T) = 0, \end{cases} \tag{4.28}$$

$$\begin{cases} \left\langle -\dfrac{\partial\left(u^* - u^*_R(u_{0,h})\right)}{\partial t}, v\right\rangle + a\left(u^* - u^*_R(u_{0,h}), v\right) \\ = \left(\mathcal{G}^*R(\hat{u} - \mathcal{G}u) - \mathcal{G}^*R(\hat{u} - \mathcal{G}u(u_{0,h})), v\right), \\ \left(u^* - u^*_R(u_{0,h})\right)(\cdot,T) = 0. \end{cases} \tag{4.29}$$

Taking $v = u - u(u_{0,h})$ in (4.27) and integrating from 0 to t, we find out

$$\int_0^t \frac{1}{2}\frac{d\|u - u(u_{0,h})\|_0^2}{\mathrm{d}s}\,\mathrm{d}s + \int_0^t a(u - u(u_{0,h}), u - u(u_{0,h}))\,\mathrm{d}s = 0. \tag{4.30}$$

Using the coercivity of the bilinear form $a(\cdot,\cdot)$, equation (4.30) infers

$$\|(u - u(u_{0,h}))(\cdot,t)\|_0^2 + 2C_c\int_0^t \|u - u(u_{0,h})\|_1^2\,\mathrm{d}s \leqslant \|u_0 - u_{0,h}\|_0^2.$$

Thus, we have the inequality

$$\|u - u(u_{0,h})\|_{L^2(0,T;L^2(\Omega))} \leqslant C\|u_0 - u_{0,h}\|_0. \tag{4.31}$$

For equation (4.28), we need to rewrite the right-hand side terms as follows:

$$\left\langle -\frac{\partial\left(u^*_{R_h}(u_h) - u^*_R(u_{0,h})\right)}{\partial t}, v\right\rangle + a\left(u^*_{R_h}(u_h) - u^*_R(u_{0,h}), v\right) = \left(\mathscr{G}^*R_h(\hat{u}_h - \mathscr{G}_h u_h) - \mathscr{G}^*R(\hat{u} - \mathscr{G}u(u_{0,h})), v\right)$$
$$= \left(\mathscr{G}^*R_h(\hat{u}_h - \mathscr{G}_h u_h) - \mathscr{G}^*R(\hat{u}_h - \mathscr{G}_h u_h) + \mathscr{G}^*R(\hat{u}_h - \mathscr{G}_h u_h) - \mathscr{G}^*R(\hat{u} - \mathscr{G}u_h) + \mathscr{G}^*R(\hat{u} - \mathscr{G}u_h)\right.$$
$$\left. -\mathscr{G}^*R(\hat{u} - \mathscr{G}u(u_{0,h})), v\right)$$
$$= \left((R_h - R)(\hat{u}_h - \mathscr{G}_h u_h) + R(\hat{u}_h - \hat{u}) + R(\mathscr{G}u(u_{0,h}) - \mathscr{G}u_h), \mathscr{G}v\right)_{0,\Omega_o}.$$

Taking $v = u^*_{R_h}(u_h) - u^*_R(u_{0,h})$ on the previous equation, we have

$$-\frac{1}{2}\frac{\mathrm{d}\|u^*_{R_h}(u_h) - u^*_R(u_{0,h})\|_0^2}{\mathrm{d}t} + a\left(u^*_{R_h}(u_h) - u^*_R(u_{0,h}), u^*_{R_h}(u_h) - u^*_R(u_{0,h})\right)$$
$$= \left((R_h - R)(\hat{u}_h - \mathscr{G}_h u_h) + R(\hat{u}_h - \hat{u}) + R(\mathscr{G}u(u_{0,h}) - \mathscr{G}u_h), \mathscr{G}\left(u^*_{R_h}(u_h) - u^*_R(u_{0,h})\right)\right)_{0,\Omega_o}.$$

Integrating both sides from t to T implies

$$\frac{1}{2}\left\|(u^*_{R_h}(u_h) - u^*_{R_h}(u_{0,h}))(\cdot,t)\right\|_0^2 + \int_t^T a\left(u^*_{R_h}(u_h) - u^*_R(u_{0,h}), u^*_{R_h}(u_h) - u^*_R(u_{0,h})\right)\,\mathrm{d}t$$
$$= \int_t^T \left((R_h - R)(\hat{u}_h - \mathscr{G}_h u_h) + R(\hat{u}_h - \hat{u}) + R(\mathscr{G}u(u_{0,h}) - \mathscr{G}u_h), \mathscr{G}\left(u^*_{R_h}(u_h) - u^*_R(u_{0,h})\right)\right)_{0,\Omega_o}\,\mathrm{d}s. \tag{4.32}$$

Note that $(u^*_{R_h}(u_h) - u^*_R(u_{0,h}))(\cdot,T) = 0$ has been used in (4.32). Applying the coercivity of the bilinear form $a(\cdot,\cdot)$, the boundedness of operators R and R_h, the Cauchy–Schwarz inequality, Poincaré's inequality and Young's inequality on the previous equation, we have

$$\frac{1}{2}\left\|\left(u^*_{R_h}(u_h) - u^*_R(u_{0,h})\right)(\cdot,t)\right\|_0^2 + C_c\int_t^T \left\|u^*_{R_h}(u_h) - u^*_R(u_{0,h})\right\|_1^2\,\mathrm{d}s$$
$$\leqslant C_1\tau\|\hat{u}_h - \mathscr{G}_h u_h\|_{L^2(t,T;L^2(\Omega_o))}\left\|u^*_{R_h}(u_h) - u^*_R(u_{0,h})\right\|_{L^2(t,T;H^1(\Omega))}$$
$$+ C_2\lambda^R\|\hat{u}_h - \hat{u}\|_{L^2(t,T;L^2(\Omega_o))}\left\|u^*_{R_h}(u_h) - u^*_R(u_{0,h})\right\|_{L^2(t,T;H^1(\Omega))}$$
$$+ C_3\lambda^R\|u(u_{0,h}) - u_h\|_{L^2(t,T;L^2(\Omega))}\left\|u^*_{R_h}(u_h) - u^*_R(u_{0,h})\right\|_{L^2(t,T;H^1(\Omega))}$$
$$\leqslant C_c\left\|u^*_{R_h}(u_h) - u^*_R(u_{0,h})\right\|^2_{L^2(t,T;H^1(\Omega))} + \frac{3C_1^2\tau^2}{4C_c}\|\hat{u}_h - \mathscr{G}_h u_h\|^2_{L^2(t,T;L^2(\Omega_o))}$$
$$+ \frac{3\left(C_3\lambda^R\right)^2}{4C_c}\|\hat{u}_h - \hat{u}\|^2_{L^2(t,T;L^2(\Omega_o))} + \frac{3\left(C_3\lambda^R\right)^2}{4C_c}\|u(u_{0,h}) - u_h\|^2_{L^2(t,T;L^2(\Omega))}. \tag{4.33}$$

Reorganizing inequality (4.33) provides us

$$\left\| \left(u^*_{R_h}(u_h) - u^*_R(u_{0,h})\right)(\cdot,t)\right\|_0^2 \leqslant \frac{3C_1^2\tau^2}{2C_c}\int_t^T \|\hat{u}_h - \mathscr{G}_h u_h\|_{0,\Omega_o}^2 \,\mathrm{d}s$$
$$+ \frac{3\left(C_2\lambda^R\right)^2}{2C_c}\int_t^T \|\hat{u}_h - \hat{u}\|_{0,\Omega_o}^2\,\mathrm{d}s + \frac{3\left(C_3\lambda^R\right)^2}{2C_c}\int_0^T \|u(u_{0,h}) - u_h\|_0^2\,\mathrm{d}s. \tag{4.34}$$

Since $\hat{u}_h, u_h \in L^\infty(0,T;L^2(\Omega_o))$, we have a supremum over time t for the term $\|\hat{u}_h - \mathscr{G}_h u_h\|_{0,\Omega_o}^2$, which allows us to bound this term from above. Therefore, (4.34) further implies:

$$\left\|u^*_{R_h}(u_h) - u^*_R(u_{0,h})\right\|_{L^2(0,T;L^2(\Omega))} \leqslant C\left(\lambda^R\|u(u_{0,h}) - u_h\|_{L^2(0,T;L^2(\Omega))} + \lambda^R\|\hat{u}_h - \hat{u}\|_{L^2(0,T;L^2(\Omega_o))} + \tau\right), \tag{4.35}$$

$$\sup_{0\leqslant t<T}\left\|\left(u^*_{R_h}(u_h) - u^*_R(u_{0,h})\right)(\cdot,t)\right\|_{L^2(\Omega)} \leqslant C\left(\lambda^R\|u(u_{0,h}) - u_h\|_{L^2(0,T;L^2(\Omega))} + \lambda^R\|\hat{u}_h - \hat{u}\|_{L^2(0,T;L^2(\Omega_o))} + \tau\right). \tag{4.36}$$

For equation (4.29), we take $v = u^* - u^*_R(u_{0,h})$, use the coercivity, the Cauchy–Schwarz inequality, Poincaré's inequality and Young's inequality, and proceed similarly as (4.33)–(4.34), to obtain the following inequality:

$$\left\|\left(u^* - u^*_R(u_{0,h})\right)(\cdot,t)\right\|_0^2 \leqslant C(\lambda^R)^2\|u(u_{0,h}) - u\|^2_{L^2(0,T;L^2(\Omega))}. \tag{4.37}$$

(4.37) gives us

$$\left\|u^* - u^*_R(u_{0,h})\right\|_{L^2(0,T;L^2(\Omega))} \leqslant C\lambda^R\|u(u_{0,h}) - u\|_{L^2(0,T;L^2(\Omega))}. \tag{4.38}$$

Finally, combining (4.38) and (4.31) leads to

$$\left\|u^* - u^*_R(u_{0,h})\right\|_{L^2(0,T;L^2(\Omega))} \leqslant C\lambda^R\|u_0 - u_{0,h}\|_0.$$

The proof of Lemma 4.7 is completed. □

Now we are in position to connect the inequalities derived above with the classical FEM convergence results Chen & Zou (1998). Using the triangle inequality and inequality (4.23), we can bound $\|u - u_h\|_{L^2(0,T;L^2(\Omega))}$ as follows:

$$\begin{aligned}\|u - u_h\|_{L^2(0,T;L^2(\Omega))} &\leqslant \|u - u(u_{0,h})\|_{L^2(0,T;L^2(\Omega))} + \|u(u_{0,h}) - u_h\|_{L^2(0,T;L^2(\Omega))}\\ &\leqslant C\|u_0 - u_{0,h}\|_0 + \|u(u_{0,h}) - u_h\|_{L^2(0,T;L^2(\Omega))}.\end{aligned} \tag{4.39}$$

From inequalities (4.25) and (4.26), $\|u^* - u_h^*\|_{L^2(0,T;L^2(\Omega))}$ can be bounded similarly:

$$\begin{aligned}\|u^* - u_h^*\|_{L^2(0,T;L^2(\Omega))} &\leqslant \|u^* - u_R^*(u_{0,h})\|_{L^2(0,T;L^2(\Omega))}\\ &+ \left\|u_R^*(u_{0,h}) - u_{R_h}^*(u_h)\right\|_{L^2(0,T;L^2(\Omega))} + \left\|u_{R_h}^*(u_h) - u_h^*\right\|_{L^2(0,T;L^2(\Omega))}\\ &\leqslant C\lambda^R\|u_0 - u_{0,h}\|_0 + \left\|u_{R_h}^*(u_h) - u_h^*\right\|_{L^2(0,T;L^2(\Omega))}\\ &+ C\left(\lambda^R\|u(u_{0,h}) - u_h\|_{L^2(0,T;L^2(\Omega))} + \lambda^R\|\hat{u}_h - \hat{u}\|_{L^2(0,T;L^2(\Omega_o))} + \tau\right). \end{aligned} \tag{4.40}$$

Note that u_h and u_h^* are the classical FEM approximations of $u(u_{0,h})$ and $u_{R_h}^*(u_h)$, convergence and error estimates between them are obtained immediately while traditional regularities are satisfied.

From inequalities (4.39) and (4.40), we observe that the convergence analysis now points to the only undetermined term $\|u_0 - u_{0,h}\|_0$. Another two conditions $\alpha B(u_0 - u_0^b) - u^*(\cdot,0) = 0$ and $\alpha B_h(u_{0,h} - u_{0,h}^b) - u_h^{*0} = 0$ will be used to work on $\|u_0 - u_{0,h}\|_0$.

LEMMA 4.8 Under the same conditions for $u, u^*, u_0, u_{0,h}, u_R^*(u_{0,h})$ and $u(u_{0,h})$ as in Lemma 4.7, we have the following error estimate:

$$\|u_0 - u_{0,h}\|_0 \leqslant \frac{1}{\alpha\lambda_B}\left(\left\|u_R^*(u_{0,h})(\cdot,0) - u_h^{*0}\right\|_0 + \alpha\lambda^B\left\|u_{0,h}^b - u_0^b\right\|_0\right). \tag{4.41}$$

Proof. Recalling the property of the operator B and using the equalities $\alpha B_h(u_{0,h} - u_{0,h}^b) - u_h^{*0} = 0$ and $\alpha B(u_0 - u_0^b) - u^*(\cdot,0) = 0$, we find out

$$\lambda_B\|u_0 - u_{0,h}\|_0^2 \leqslant \left(B(u_0 - u_{0,h}), u_0 - u_{0,h}\right) = \frac{1}{\alpha}\left(u^*(\cdot,0) - BB_h^{-1}u_h^{*0} + \alpha B\left(u_0^b - u_{0,h}^b\right), u_0 - u_{0,h}\right). \tag{4.42}$$

Recall $B = B_h$ when they both act on the finite dimensional space $L_h^2(\Omega)$, hence $B^{-1}B_h = I$, where $I: L_h^2(\Omega) \mapsto L_h^2(\Omega)$. Therefore, we can rewrite (4.42) and manipulate it further

$$\begin{aligned}\lambda_B\|u_0 - u_{0,h}\|_0^2 &\leqslant \frac{1}{\alpha}\left(u^*(\cdot,0) - u_h^{*0} + \alpha B\left(u_0^b - u_{0,h}^b\right), u_0 - u_{0,h}\right)\\ &= \frac{1}{\alpha}\left(u^*(\cdot,0) - u_R^*(u_{0,h})(\cdot,0) + u_R^*(u_{0,h})(\cdot,0) - u_h^{*0} + \alpha B\left(u_0^b - u_{0,h}^b\right), u_0 - u_{0,h}\right)\\ &= \frac{1}{\alpha}\Big((u^*(\cdot,0) - u_R^*(u_{0,h})(\cdot,0), u_0 - u_{0,h}) + (u_R^*(u_{0,h})(\cdot,0) - u_h^{*0}, u_0 - u_{0,h})\\ &+ \left(\alpha B\left(u_0^b - u_{0,h}^b\right), u_0 - u_{0,h}\right)\Big). \end{aligned} \tag{4.43}$$

Our focus next is to handle the first term in the right-hand side of (4.43). We first need equations (4.27) and (4.29) from the proof in Lemma 4.7. Taking $v = u^* - u_R^*(u_{0,h})$ in (4.27) gives us

$$\int_0^T \left\langle \frac{\partial(u - u(u_{0,h}))}{\partial t}, u^* - u_R^*(u_{0,h}) \right\rangle \mathrm{d}t + \int_0^T a(u - u(u_{0,h}), u^* - u_R^*(u_{0,h}))\,\mathrm{d}t = 0.$$

Applying integration by parts with respect to t on the previous equation, we obtain

$$\begin{aligned}&-\int_0^T \left\langle \frac{\partial\left(u^* - u_R^*(u_{0,h})\right)}{\partial t}, u - u(u_{0,h}) \right\rangle \mathrm{d}t + \int_0^T a\left(u^* - u_R^*(u_{0,h}), u - u(u_{0,h})\right)\,\mathrm{d}t \\ &+ \left((u^* - u_R^*(u_{0,h}))(\cdot,T), (u - u(u_{0,h}))(\cdot,T)\right) - \left((u^* - u_R^*(u_{0,h}))(\cdot,0), (u - u(u_{0,h}))(\cdot,0)\right) = 0. \quad (4.44)\end{aligned}$$

To work on equation (4.44), we take $v = u - u(u_{0,h})$ on equation (4.29) to have

$$\begin{cases} \left\langle -\dfrac{\partial(u^* - u_R^*(u_{0,h}))}{\partial t}, u - u(u_{0,h}) \right\rangle + a(u^* - u_R^*(u_{0,h}), u - u(u_{0,h})) \\ = \left(\mathscr{G}^* R(\mathscr{G}u(u_{0,h}) - \mathscr{G}u), u - u(u_{0,h})\right), \\ (u^* - u_R^*(u_{0,h}))(\cdot,T) = 0. \end{cases} \quad (4.45)$$

Using (4.45) the equation (4.44) is simplified as follows:

$$\left((u^* - u_R^*(u_{0,h}))(\cdot,0), (u - u(u_{0,h}))(\cdot,0)\right) = -\int_0^T \left(R\left(\mathscr{G}u - \mathscr{G}u(u_{0,h})\right), \mathscr{G}u - \mathscr{G}u(u_{0,h})\right)_{0,\Omega_o}\,\mathrm{d}t.$$

We know that $\int_0^T \left(R\left(\mathscr{G}u - \mathscr{G}u(u_{0,h})\right), \mathscr{G}u - \mathscr{G}u(u_{0,h})\right)_{0,\Omega_o}\,\mathrm{d}t$ is non-negative due to the positive definiteness of the operator R, which then tells us

$$\left(u^*(\cdot,0) - u_R^*(u_{0,h})(\cdot,0), u_0 - u_{0,h}\right) \leqslant 0. \quad (4.46)$$

Combining (4.46) with (4.43), we find out

$$\begin{aligned}\lambda_B\|u_0 - u_{0,h}\|_0^2 &\leqslant \frac{1}{\alpha}\left((u_R^*(u_{0,h})(\cdot,0) - u_h^{*0}, u_0 - u_{0,h}) + \left(\alpha B\left(u_0^b - u_{0,h}^b\right), u_0 - u_{0,h}\right)\right) \\ &\leqslant \frac{1}{\alpha}\left(\left\|u_R^*(u_{0,h})(\cdot,0) - u_h^{*0}\right\|_0 \|u_0 - u_{0,h}\|_0 + \alpha\lambda^B \left\|u_{0,h}^b - u_0^b\right\|_0 \|u_0 - u_{0,h}\|_0\right). \end{aligned} \quad (4.47)$$

Hence

$$\|u_0 - u_{0,h}\|_0 \leqslant \frac{1}{\alpha\lambda_B}\left(\left\|u_R^*(u_{0,h})(\cdot,0) - u_h^{*0}\right\|_0 + \alpha\lambda^B \left\|u_{0,h}^b - u_0^b\right\|_0\right).$$

The proof is completed. □

By using the triangle inequality and (4.24), the last step necessary for Theorem 4.6 is provided by

$$
\begin{aligned}
&\left\| u_h^{*0} - u_R^*(u_{0,h})(\cdot,0) \right\|_0 \\
&\leqslant \left\| u_h^{*0} - u_{R_h}^*(u_h)(\cdot,0) \right\|_0 + \left\| u_{R_h}^*(u_h)(\cdot,0) - u_R^*(u_{0,h})(\cdot,0) \right\|_0 \\
&\leqslant \max_{0\leqslant i\leqslant N-1} \left\| u_h^{*i} - u_{R_h}^*(u_h)(\cdot,t_i) \right\|_0 + \sup_{0\leqslant t<T} \left\| u_{R_h}^*(u_h) - u_R^*(u_{0,h}) \right\|_0 \\
&\leqslant \max_{0\leqslant i\leqslant N-1} \left\| u_h^{*i} - u_{R_h}^*(u_h)(\cdot,t_i) \right\|_0 + C\left(\lambda^R \| u(u_{0,h}) - u_h \|_{L^2(0,T;L^2(\Omega))} + \lambda^R \| \hat{u}_h - \hat{u} \|_{L^2(0,T;L^2(\Omega_o))} + \tau \right).
\end{aligned} \tag{4.48}
$$

We have nearly achieved our goal of connecting the convergence in the data assimilation problem with classical FEM convergence results. Rearranging inequalities (4.39), (4.40), (4.41) and (4.48), we conclude

$$
\begin{aligned}
&\|u_0 - u_{0,h}\|_0 + \|u - u_h\|_{L^2(0,T;L^2(\Omega))} + \|u^* - u_h^*\|_{L^2(0,T;L^2(\Omega))} \\
&\leqslant \left(C + C\lambda^R + 1\right) \|u_0 - u_{0,h}\|_0 + (C\lambda^R + 1)\|u(u_{0,h}) - u_h\|_{L^2(0,T;L^2(\Omega))} + C\tau + \left\| u_{R_h}^*(u_h) - u_h^* \right\|_{L^2(0,T;L^2(\Omega))} \\
&\quad + \frac{C\lambda^B\left(C + C\lambda^R + 1\right)}{\alpha\lambda_B} \|\hat{u} - \hat{u}_h\|_{L^2(0,T;L^2(\Omega_o))} \\
&\leqslant \left(C\lambda^R + 1 + \frac{C\lambda^R\left(C + C\lambda^R + 1\right)}{\alpha\lambda_B} \right) \|u(u_{0,h}) - u_h\|_{L^2(0,T;L^2(\Omega))} + \left(C + \frac{C\left(C + C\lambda^R + 1\right)}{\alpha\lambda_B} \right)\tau \\
&\quad + \frac{C + C\lambda^R + 1}{\alpha\lambda_B} \max_{0\leqslant i\leqslant N-1} \left\| u_h^{*i} - u^*(u_h)(\cdot,t_i) \right\|_0 + \frac{\left(C + C\lambda^R + 1\right)\lambda^B}{\lambda_B} \left\| u_0^b - u_{0,h}^b \right\|_0 + \left\| u_{R_h}^*(u_h) - u_h^* \right\|_{L^2(0,T;L^2(\Omega))} \\
&\quad + \frac{C\lambda^R\left(C + C\lambda^R + 1\right)}{\alpha\lambda_B} \|\hat{u} - \hat{u}_h\|_{L^2(0,T;L^2(\Omega_o))}.
\end{aligned}
$$

Using results in Chen & Zou (1998), the following classical error bounds hold:

$$
\begin{aligned}
\max_{0\leqslant i\leqslant N-1} \left\| u_h^{*i} - u_{R_h}^*(u_h)(\cdot,t_i) \right\| &\leqslant C(h^2|\log h| + \tau), \\
\left\| u_{R_h}^*(u_h) - u_h^* \right\|_{L^2(0,T;L^2(\Omega))} &\leqslant C(h^2|\log h| + \tau), \\
\|u(u_{0,h}) - u_h\|_{L^2(0,T;L^2(\Omega))} &\leqslant C(h^2|\log h| + \tau).
\end{aligned}
$$

Finally, we have the convergence result

$$
\|u_0 - u_{0,h}\|_0 + \|u - u_h\|_{L^2(0,T;L^2(\Omega))} + \|u^* - u_h^*\|_{L^2(0,T;L^2(\Omega))} \leqslant C\left(\alpha, \lambda_B, \lambda^R\right)(h^2 + \tau),
$$

which completes the proof of Theorem 4.6.

Also, the dependence of the constant C indicates that the property of B, R and the small regularization parameters may cause the numerical accuracy to degenerate. Hence, in practice one needs to use more refined mesh size h and time step τ to reduce the finite-element approximation error caused by small α, λ_B, or large ratio $\frac{\lambda^R}{\lambda_B}$.

REMARK 4.9 If the discrete cost function is given as (4.9), that means we have both temporal and spatial approximations for operators R and B. In this case, the approximation $R - R_h$ in Theorem 4.6 needs to satisfy, for $\forall\, p, q \in L^2_h(\Omega_o)$,

$$\int_t^T ((R - R_h)p, q)_{0,\Omega_o}\, \mathrm{d}s \leqslant C(\tau + h^2)\|p\|_{L^2(t,T;L^2(\Omega_o))}\|q\|_{L^2(t,T;L^2_h(\Omega_o))}.$$

In addition, we need to modify the proof of step (4.43) in Lemma 4.8:

$$\begin{aligned}
&\lambda_B\|u_0 - u_{0,h}\|_0^2 \leqslant \frac{1}{\alpha}\left(u^*(\cdot,0) - BB_h^{-1}u_h^{*0} + \alpha B\left(u_0^b - u_{0,h}^b\right), u_0 - u_{0,h}\right)\\
&= \frac{1}{\alpha}\left(u^*(\cdot,0) - u_R^*(u_{0,h})(\cdot,0) + u_R^*(u_{0,h})(\cdot,0) - u_h^{*0} + u_h^{*0} - BB_h^{-1}u_h^{*0} + \alpha B\left(u_0^b - u_{0,h}^b\right), u_0 - u_{0,h}\right)\\
&= \frac{1}{\alpha}\left(\left(u^*(\cdot,0) - u_R^*(u_{0,h})(\cdot,0), u_0 - u_{0,h}\right) + \left(u_R^*(u_{0,h})(\cdot,0) - u_h^{*0}, u_0 - u_{0,h}\right)\right.\\
&\quad \left. + \left(B\left(B^{-1} - B_h^{-1}\right)u_h^{*0}, u_0 - u_{0,h}\right) + \left(\alpha B\left(u_0^b - u_{0,h}^b\right), u_0 - u_{0,h}\right)\right).
\end{aligned} \tag{4.49}$$

So far, we realize that one more condition for Theorem 4.6 is in need:

$$\left|\left(\left(B^{-1} - B_h^{-1}\right)p, q\right)\right| \leqslant Ch^2\|p\|_0\|q\|_0 \quad \forall p, q \in L^2_h(\Omega). \tag{4.50}$$

Then using (4.50) and doing the same manipulations as steps (4.44)–(4.46), we end up with

$$\begin{aligned}
\lambda_B\|u_0 - u_{0,h}\|_0^2 \leqslant \frac{1}{\alpha}&\left(\left\|u_R^*(u_{0,h})(\cdot,0) - u_h^{*0}\right\|_0\|u_0 - u_{0,h}\|_0 + C\lambda^B h^2\left\|u_h^{*0}\right\|_0\|u_0 - u_{0,h}\|_0\right.\\
&\left. + \alpha\lambda^B\left\|u_{0,h}^b - u_0^b\right\|_0\|u_0 - u_{0,h}\|_0\right).
\end{aligned} \tag{4.51}$$

The result of Lemma 4.8 will be given as

$$\|u_0 - u_{0,h}\|_0 \leqslant \frac{C}{\alpha\lambda_B}\left(\left\|u_R^*(u_{0,h})(\cdot,0) - u_h^{*0}\right\|_0 + \lambda^B h^2 + \alpha\lambda^B\left\|u_{0,h}^b - u_0^b\right\|_0\right).$$

Then the optimal finite-element convergence rate can still be achieved.

REMARK 4.10 One can prove that the solution u_0 of the regularized problem (3.1)–(3.2) converges to the unique solution (if exist) or minimum norm solution of the original ill-posed problem (i.e., problem (3.1)–(3.2) with $\alpha = 0$), with even convergence rates with respect to the regularization parameter α if we assume certain source conditions (cf. (Engl *et al.*, 1996, Chap. 5.4)). Combined with the *a priori* finite-element error estimate established in Theorem 4.6, this will enable us to choose the appropriate parameters coupling the regularization parameter α, the noise level δ, the mesh sizes h and τ, to achieve an optimal convergence. We refer to von Daniels & Hinze (2020) and the references therein for a similar idea. Once the noise level is given and fixed, the regularization parameter can be chosen with either *a priori* or a posterior rule, while the discretization parameters can be chosen accordingly by using the error estimates established in Theorem 4.6.

5. Iterative methods solving the discrete optimality system

Due to the forward in time nature in the state equation and backward in time nature of the adjoint equation, solving the discrete optimality system directly would produce a massive linear system and encounters computational difficulties. Considering the stability in data assimilation problem, in this section we develop three iterative algorithms, based on the BFGS method, the conjugate gradient(CG) method, and the steepest descent method, to decouple the discrete optimality system, which improve the computation efficiency significantly.

5.1 *Matrix–vector calculation*

To show a concrete implementation of these gradient-based iterative methods, we first provide a finite-element assembling and give readers a matrix-vector calculation of the gradient at each iteration.

Recall the discrete optimality system, for $n = 0, 1, 2, 3, ..., N-1$,

$$\begin{cases} \left\langle \dfrac{u_h^{n+1} - u_h^n}{\tau}, v_h \right\rangle + a\left(u_h^{n+1}, v_h\right) = \langle f_{n+1}, v_h \rangle, \\ u_h^0 = u_{0,h}, \\ -\left\langle \dfrac{u_h^{*n+1} - u_h^{*n}}{\tau}, v_h \right\rangle + a\left(u_h^{*n}, v_h\right) = \left(\chi_{\Omega_o} R_h^n \left(\hat{u}_h^{n+1} - \mathscr{G}_h^{n+1} u_h^{n+1}\right), v_h\right), \\ u_h^{*N} = 0, \\ \left(\alpha B_h \left(u_{0,h} - u_{0,h}^b\right) - u_h^{*0}, z_h\right) = 0. \end{cases} \tag{5.1}$$

Considering the integral formula of the forward equation in (5.1), we have

$$\int_\Omega \frac{u_h^{n+1} - u_h^n}{\tau} v_h \,\mathrm{d}x\,\mathrm{d}y + \int_{\Omega^+} \beta^+ \nabla u_h^{n+1} \nabla v_h \,\mathrm{d}x\,\mathrm{d}y + \int_{\Omega^-} \beta^- \nabla u_h^{n+1} \nabla v_h \,\mathrm{d}x\,\mathrm{d}y = \int_{\Omega^+} f_{n+1}^+ v_h \,\mathrm{d}x\,\mathrm{d}y + \int_{\Omega^-} f_{n+1}^- v_h \,\mathrm{d}x\,\mathrm{d}y. \tag{5.2}$$

For each time moment n, $u_h^n = \sum_{j=1}^{N_b} u_j^n \phi_j$, plugging u_h^n into (5.2) and using $v_h = \{\phi_i\}_{i=1}^{N_b}$ to test (5.2), we obtain

$$\int_\Omega \frac{\sum_{j=1}^{N_b}\left(u_j^{n+1} - u_j^n\right)}{\tau} \phi_j \phi_i \,\mathrm{d}x\,\mathrm{d}y + \int_{\Omega^+} \sum_{j=1}^{N_b} u_j^{n+1} \beta^+ \frac{\partial \phi_j}{\partial x}\frac{\partial \phi_i}{\partial x} \,\mathrm{d}x\,\mathrm{d}y + \int_{\Omega^+} \sum_{j=1}^{N_b} u_j^{n+1} \beta^+ \frac{\partial \phi_j}{\partial y}\frac{\partial \phi_i}{\partial y} \,\mathrm{d}x\,\mathrm{d}y$$
$$+ \int_{\Omega^-} \sum_{j=1}^{N_b} u_j^{n+1} \beta^- \frac{\partial \phi_j}{\partial x}\frac{\partial \phi_i}{\partial x} \,\mathrm{d}x\,\mathrm{d}y + \int_{\Omega^-} \sum_{j=1}^{N_b} u_j^{n+1} \beta^- \frac{\partial \phi_j}{\partial y}\frac{\partial \phi_i}{\partial y} \,\mathrm{d}x\,\mathrm{d}y = \int_{\Omega^+} f_{n+1}^+ \phi_i \,\mathrm{d}x\,\mathrm{d}y + \int_{\Omega^-} f_{n+1}^- \phi_i \,\mathrm{d}x\,\mathrm{d}y.$$

Then the matrix–vector formulation of the forward equation is

$$\begin{cases} M\dfrac{\vec{u}_h^{n+1}-\vec{u}_h^{n}}{\tau}+Q\vec{u}_h^{n+1}=\vec{f}^{n+1}, \\ \vec{u}_h^{0}=\vec{u}_{0,h}, \end{cases} \tag{5.3}$$

where

$$\begin{aligned} M&=\left[\int_{\Omega}\phi_j\phi_i\,\mathrm{d}x\,\mathrm{d}y\right]_{i,j=1}^{N_b}, \quad \vec{f}^{n+1}=\left[\int_{\Omega^+}f_{n+1}^{+}\phi_i\,\mathrm{d}x\,\mathrm{d}y\right]_{i=1}^{N_b}+\left[\int_{\Omega^-}f_{n+1}^{-}\phi_i\,\mathrm{d}x\,\mathrm{d}y\right]_{i=1}^{N_b}, \\ Q&=\left[\int_{\Omega^+}\beta^{+}\frac{\partial\phi_j}{\partial x}\frac{\partial\phi_i}{\partial x}\,\mathrm{d}x\,\mathrm{d}y\right]_{i,j=1}^{N_b}+\left[\int_{\Omega^+}\beta^{+}\frac{\partial\phi_j}{\partial y}\frac{\partial\phi_i}{\partial y}\,\mathrm{d}x\,\mathrm{d}y\right]_{i,j=1}^{N_b} \\ &\quad+\left[\int_{\Omega^-}\beta^{-}\frac{\partial\phi_j}{\partial x}\frac{\partial\phi_i}{\partial x}\,\mathrm{d}x\,\mathrm{d}y\right]_{i,j=1}^{N_b}+\left[\int_{\Omega^-}\beta^{-}\frac{\partial\phi_j}{\partial y}\frac{\partial\phi_i}{\partial y}\,\mathrm{d}x\,\mathrm{d}y\right]_{i,j=1}^{N_b}. \end{aligned} \tag{5.4}$$

Similarly, the matrix–vector formulation of the discrete backward equation can be written as

$$\begin{cases} -M\dfrac{\vec{u}_h^{*n+1}-\vec{u}_h^{*n}}{\tau}+Q\vec{u}_h^{*n}=\vec{b}^{*n+1}, \\ \vec{u}_h^{*N}=\vec{0}, \end{cases} \tag{5.5}$$

where

$$\vec{b}^{*n+1}=\left[\int_{\Omega}\chi_{\Omega_o}R_h^{n+1}\left(\hat{u}_h^{n+1}-\mathscr{G}_h^{n+1}u_h^{n+1}\right)\phi_i\,\mathrm{d}x\,\mathrm{d}y\right]_{i=1}^{N_b}.$$

Now the gradient at k^{th} iteration, $\vec{F}_h'\left(u_{0,h}^{(k)}\right)$, is calculated as follows:

$$\begin{cases} M\dfrac{\vec{u}_h^{n+1(k)}-\vec{u}_h^{n(k)}}{\tau}+Q\vec{u}_h^{n+1(k)}=\vec{b}^{n+1}, \\ \vec{u}_h^{0(k)}=\vec{u}_{0,h}^{(k)}, \end{cases} \tag{5.6}$$

$$\begin{cases} -M\dfrac{\vec{u}_h^{*n+1(k)}-\vec{u}_h^{*n(k)}}{\tau}+Q\vec{u}_h^{*n(k)}=\vec{b}^{*n+1(k)}, \\ \vec{u}_h^{*N(k)}=\vec{0}, \end{cases} \tag{5.7}$$

$$\vec{F}_h'\left(u_{0,h}^{(k)}\right)=\alpha\left(\vec{u}_{0,h}^{B_h(k)}-\vec{u}_{0,h}^{b,B_h}\right)-\vec{u}_h^{*0(k)}, \tag{5.8}$$

where $\vec{u}_{0,h}^{B_h(k)}$ and $\vec{u}_{0,h}^{b,B_h}$ satisfy $M\vec{u}_{0,h}^{B_h(k)}=M_{B_h}\vec{u}_{0,h}^{B_h(k)}$ and $M\vec{u}_{0,h}^{b,B_h}=M_{B_h}\vec{u}_{0,h}^{b}$.

Solving equations (5.6)–(5.7) with initial condition $\vec{u}_{0,h}^{(k)}$ forward and backward to obtain $\vec{F}_h'\left(u_{0,h}^{(k)}\right)$ will be a basic ingredient for all our algorithms. Note that n and k in above represent steps for the time evolution and the gradient iteration, we will keep these notations in the rest of presentation.

REMARK 5.1 We also need to remind readers that $\vec{p}$ is the vector representation of an element p in a Hilbert space with finite-element basis $\{\phi_i\}_{i=1}^{N_b}$. Especially, $\|\vec{p}\|_0^2$ will refer $\|\vec{p}\|_0^2 = (\vec{p},\vec{p})_M = \vec{p}^T M\vec{p}$, where M is the mass matrix.

5.2 *The conjugate gradient method*

Conjugate gradient method (CG) is a popular algorithm to solve variational problems, it can achieve a superlinear convergence rate only considering the first order derivative. The main feature of CG is that the current descent direction d^k is conjugate orthogonal to all previous descent directions $d^0, d^1, d^2, ...d^{k-1}$, which allows a convergence within finite iterations for the finite dimension optimization. A standard CG algorithm update is given as follows:

- Initialize $\vec{u}_{0,h}^{(0)}$ and $\vec{d}^0 = -\vec{F}_h'\left(u_{0,h}^{(0)}\right)$.
- Update $\vec{u}_{0,h}^{(k+1)} = \vec{u}_{0,h}^{(k)} + \gamma^k \vec{d}^k$ with

$$\vec{d}^k = \begin{cases} -\vec{F}_h'\left(u_{0,h}^{(0)}\right) & k=0, \\ -\vec{F}_h'\left(u_{0,h}^{(k)}\right) + \beta^k \vec{d}^{k-1} & k \geqslant 1, \end{cases} \qquad \beta^k = \frac{\left(\vec{F}_h'\left(u_{0,h}^{(k)}\right), \vec{F}_h'\left(u_{0,h}^{(k)}\right)\right)}{\left(\vec{F}_h'\left(u_{0,h}^{(k-1)}\right), \vec{F}_h'\left(u_{0,h}^{(k-1)}\right)\right)}.$$

- γ_k is a positive number determined with exact line search by minimizing the functional $\gamma_k = \text{argmin}_{\gamma\in\mathbb{R}} F_h(u_{0,h}^{(k)} + \gamma^k d^k)$ or using inexact line search methods, such as the Armijo or Wolfe condition.

The CG method Marchuk & Shutyaev (2002, 2004) can also be understood as an accelerated steepest descent method based on fixed point theorem, and a natural CG variant is expressed as follows.

- Initialize $\vec{u}_{0,h}^{(0)}$ and $\vec{u}_{0,h}^{(1)}$.
- Update $\vec{u}_{0,h}^{(k+1)} = \vec{u}_{0,h}^{(k)} - \zeta^k \vec{F}_h'\left(u_{0,h}^{(k)}\right) + \eta^k \left(\vec{u}_{0,h}^{(k)} - \vec{u}_{0,h}^{(k-1)}\right)$.

the term $\vec{u}_{0,h}^{(k)} - \vec{u}_{0,h}^{(k-1)}$ is called a momentum term accounting for the acceleration.

We will adopt the first CG version as our presentation and provide an exact line search method to optimally determine the step sizes γ^k and β^k.

Recall that the CG method Hestenes & Stiefel (1952) was originally developed to solve linear system

$$\mathscr{A}x = b, \quad \text{where } \mathscr{A} \text{ is a positive definite operator (or matrix)}, \tag{5.9}$$

or equivalently to find out the minima of the quadratic functional

$$J(x) = \frac{1}{2}(\mathscr{A}x, x) - (b, x). \tag{5.10}$$

The standard CG algorithm with exact line search to solve (5.9) or (5.10) is illustrated as:

Algorithm 1 Classic Conjugate Gradient Algorithm

Input: $x^{(0)}$, tol;
Compute the gradient at $x^{(0)}$: $J'(x^{(0)}) = \mathscr{A}x^{(0)} - b$, initialize $r_0 = -J'(x^{(0)})$ and $d_0 = -J'(x^{(0)})$, set error $= 1$ and $k = 0$;
while error $>$ tol **do**
  Compute $\bar{d}^k = \mathscr{A} d_k$;
  Compute $\gamma_k = \dfrac{(r_k, r_k)}{(d_k, \bar{d}_k)}$;
  Update $x^{(k+1)} = x^{(k+1)} + \gamma_k d_k$;
  Compute $r_{k+1} = r_k - \gamma_k \mathscr{A} d_k$;
  Compute $\beta_k = \dfrac{(r_{k+1}, r_{k+1})}{(r_k, r_k)}$;
  Compute $d_{k+1} = r_{k+1} + \beta_k d_k$;
  Set $k = k + 1$ and error $= \|r_{k+1}\|$;
end while
Output: $x^{(k+1)}$;

For purpose of implementing the Algorithm 1 into our data assimilation problem, we first rewrite the optimization problem (3.1)–(3.2) as a reduced form:

$$\begin{aligned} \min_{u_0 \in U} F(u_0) =& \frac{1}{2}\int_0^T \|\hat{u} - \mathscr{G}u\|^2_{0,R,\Omega_o}\,\mathrm{d}t + \frac{\alpha}{2}\left\|u_0 - u_0^b\right\|^2_{0,B} \\ \text{s.t.}\ \ u =& S_f u_0, \end{aligned} \tag{5.11}$$

where the operator $S_f : L^2(\Omega) \mapsto W(0,T)$ is defined by the parabolic interface constraint (3.2) and the subscript f corresponds to the source term. Since the equation (3.2) is a linear PDE, the operator S_f is an affine mapping. Hence, $S_f'(u_0)$, the derivative of S_f at u_0, does not depend on u_0 and f. More concretely, we have

$$S_f'(u_0)z = S_0 z \ \ \forall z \in L^2(\Omega), \ \ \text{or} \ \ S_f'(u_0) = S_0. \tag{5.12}$$

We then denote by $S_0^* = (S_f'(u_0))^* : W(0,T)' \mapsto L^2(\Omega)'$ the adjoint operator of S_0 or $S_f'(u_0)$. That is,

$$\langle q, S_0 z\rangle_{(W(0,T)',W(0,T))} = \langle S_0^* q, z\rangle_{(L^2(\Omega)',L^2(\Omega))} \tag{5.13}$$

for $\forall (q,z) \in W(0,T)' \times L^2(\Omega)$. Recall (3.14)–(3.16), we have $S_0^* q = \Phi(\cdot,0)$, where Φ solves the following backward parabolic equation

$$\begin{cases} -\left\langle \dfrac{\partial \Phi}{\partial t}, v \right\rangle + a(\Phi, v) = \langle q, v \rangle, \\ \Phi(\cdot, T) = 0. \end{cases} \tag{5.14}$$

For convenience, we always keep the discussion in the continuous level, the solving of the discrete data assimilation will be a straightforward discretization of the continuous one.

By doing a calculus of variation, we derive the optimality condition

$$\begin{aligned} \langle F'(u_0), z\rangle &= \left(\alpha B\left(u_0 - u_0^b\right), z\right) - \left(R(\hat{u} - \mathscr{G} S_f u_0), \left(\mathscr{G} S_f\right)'(u_0) z\right) \\ &= \left(\alpha B_h\left(u_0 - u_0^b\right), z\right) - \left(\left(\left(\mathscr{G} S_f\right)'(u_0)\right)^* R(\hat{u} - \mathscr{G} S_f u_0), z\right) \\ &= 0 \quad \forall\, z \in L^2(\Omega), \end{aligned} \tag{5.15}$$

Using the linearity of $\mathscr{G}$ and (5.12), we update the optimality condition (5.15) as

$$\begin{aligned} \left(\alpha B\left(u_0 - u_0^b\right), z\right) - \left(S_0^* \mathscr{G}^* R(\hat{u} - \mathscr{G} S_f u_0), z\right) = 0 \quad \forall z \in L^2(\Omega), \text{ i.e.} \\ \alpha B\left(u_0 - u_0^b\right) - S_0^* \mathscr{G}^* R(\hat{u} - \mathscr{G} S_f u_0) = 0. \end{aligned} \tag{5.16}$$

For clarity, we remind readers that the operator S_0^* acting on $\mathscr{G}^* R(\hat{u} - \mathscr{G} S_f u_0)$ is equivalent to solve the backward adjoint equation in (3.17) with source term $\mathscr{G}^* R(\hat{u} - \mathscr{G} S_f u_0)$, which exactly gives $u^*(\cdot, 0)$.

Note that $\alpha B u_0^b$ and $S_0^* \mathscr{G}^* R\hat{u}$ are known variables, therefore, (5.16) can be temporarily written as

$$\alpha B u_0 + S_0^* \mathscr{G}^* R \mathscr{G} S_f u_0 = S_0^* \mathscr{G}^* R\hat{u} + \alpha B u_0^b. \tag{5.17}$$

For S_f, we can decompose it as:

$$S_f u_0 = S_f 0 + S_0 u_0. \tag{5.18}$$

Apparently, S_0 is a linear operator and $S_f 0$ is a known variable, this finally allows us to rewrite (5.17) as:

$$\alpha B u_0 + S_0^* \mathscr{G}^* R \mathscr{G} S_0 u_0 = S_0^* \mathscr{G}^* R\hat{u} - S_0^* \mathscr{G}^* R \mathscr{G} S_f 0 + \alpha B u_0^b. \tag{5.19}$$

We now claim that the operator $\alpha B + S_0^* \mathscr{G}^* R \mathscr{G} S_0$ is positive definite. First, $\left(\alpha B + S_0^* \mathscr{G}^* R \mathscr{G} S_0\right)^* = \alpha B + S_0^* \mathscr{G}^* R \mathscr{G} S_0$ is obviously true. Second, for $\forall\, 0 \neq z \in L^2(\Omega)$, we have

$$\left(\left(\alpha B + S_0^* \mathscr{G}^* R \mathscr{G} S_0\right) z, z\right) = \alpha (Bz, z) + \left(S_0^* \mathscr{G}^* R \mathscr{G} S_0 z, z\right) = \alpha (Bz, z) + \left(R \mathscr{G} S_0 z, \mathscr{G} S_0 z\right) > \alpha \lambda_B \|z\|_0^2. \tag{5.20}$$

In (5.20), we have used the positive definiteness of the operators B and R.

So far, we can write the optimality condition (5.16) in form of (5.9),

$$\mathscr{A} u_0 = \left(\alpha B + S_0^* \mathscr{G}^* R \mathscr{G} S_0\right) u_0, \;\; b = S_0^* \mathscr{G}^* R \hat{u} - S_0^* \mathscr{G}^* R \mathscr{G} S_f 0 + \alpha B u_0^b.$$

We here further clarify the operation of $\mathscr{A}$ acting on an element $u_0 \in L^2(\Omega)$. First, recall that $S_0 z$ is to solve the parabolic interface equation with initial z and source term 0. Second, the operator S_0^* acting on $\mathscr{G}^* R \mathscr{G} S_0 z$ is equivalent to solve the backward adjoint equation with initial 0 and source term $\mathscr{G}^* R \mathscr{G} S_0 z$. Therefore, $\mathscr{A} z$ is obtained by sequentially solving the following forward and backward equations:

$$\begin{cases} \left\langle \dfrac{\partial \psi}{\partial t}, v \right\rangle + a(\psi, v) = \langle 0, v \rangle, \\ \psi(\cdot, 0) = z, \end{cases} \tag{5.21}$$

$$\begin{cases} -\left\langle \dfrac{\partial \psi^*}{\partial t}, v \right\rangle + a(\psi^*, v) = \left(\mathscr{G}^* R \mathscr{G} \psi, v\right), \\ \psi^*(\cdot, T) = 0, \end{cases} \tag{5.22}$$

$$\mathscr{A} z = \alpha B z + \psi^*(\cdot, 0). \tag{5.23}$$

In discrete level, (5.21)–(5.23) can be written in matrix–vector form as follows:

$$\begin{cases} M \dfrac{\vec{\psi}_h^{n+1} - \vec{\psi}_h^n}{\tau} + Q \vec{\psi}_h^{n+1} = \vec{0}, \\ \vec{\psi}_h^0 = \vec{z}, \end{cases} \tag{5.24}$$

$$\begin{cases} -M \dfrac{\vec{\psi}_h^{*n+1} - \vec{\psi}_h^{*n}}{\tau} + Q \vec{\psi}_h^{*n} = \vec{b}_{\psi_h}^{n+1}, \\ \vec{\psi}_h^{*N} = \vec{0}, \end{cases} \tag{5.25}$$

$$\overrightarrow{\mathscr{A} z} = \alpha \vec{z}^{B_h} + \vec{\psi}_h^{*0}, \tag{5.26}$$

where $M_{B_h} \vec{z} = M \vec{z}^{B_h}$ and $\vec{b}_{\psi_h}^{n+1} = \left[\int_\Omega \chi_{\Omega_o} R_h^{n+1} \mathscr{G}_h^{n+1} \psi_h^{n+1} \phi_i \,\mathrm{d}x\,\mathrm{d}y\right]_{i=1}^{N_b}$.

All work in (5.15)–(5.26) essentially have provided us all of the information to update the CG iterations. We summarize these ingredients into Algorithm 2 to solve our data assimilation problem.

REMARK 5.2 We never use the information $b = S_0^* \left(\mathscr{G}^* R \hat{u} - \mathscr{G}^* R \mathscr{G} S_f 0\right) + \alpha B u_0^b$. Because $b - \mathscr{A} u_0$ essentially is the negative gradient $-F'(u_0)$, we can use (5.6)–(5.8) to find it out.

Algorithm 2 Conjugate Gradient Algorithm

Input: $\vec{u}_{0,h}^{(0)}$ and tol;
Compute $\vec{F}'_h(u_{0,h}^{(0)})$, initialize $\vec{r}_0 = -\vec{F}'_h(u_{0,h}^{(0)})$ and $\vec{d}_0 = -\vec{F}'_h(u_{0,h}^{(0)})$, set error = 1, and start the iteration step $k = 0$;
while error $>$ tol **do**
Compute $\vec{\bar{d}}_k = \overrightarrow{\mathscr{A}d_k}$ by solving equations (5.24)–(5.26) sequentially;
Compute $\gamma_k = \dfrac{\|\vec{r}_k\|_0^2}{(\vec{d}_k, \vec{\bar{d}}_k)_M}$;
Compute $\vec{r}_{k+1} = \vec{r}_k - \gamma_k \overrightarrow{\mathscr{A}d_k}$;
Update $\vec{u}_{0,h}^{(k+1)} = \vec{u}_{0,h}^{(k)} + \gamma_k \vec{d}_k$;
Compute $\beta_k = \dfrac{\|\vec{r}_{k+1}\|_0^2}{\|\vec{r}_k\|_0^2}$;
Compute $\vec{d}_{k+1} = \vec{r}_{k+1} + \beta_k \vec{d}_k$;
Set $k = k + 1$ and error $= \|\vec{r}_{k+1}\|_0$;
end while
Output: $\vec{u}_{0,h}^{(k+1)}$;

5.3 *The BFGS method*

For gradient-based iterative algorithm, the descent direction d^k at each step is the key component to determine its effectiveness, which is generally written as

$$d^{k+1} = -D_k F'_h\left(u_{0,h}^{(k)}\right).$$

Choosing D_k as an identity operator gives the steepest descent method that usually has a global convergence, but possibly with slow convergence rate. For $D_k = \left(F''_h(u_{0,h}^{(k)})\right)^{-1}$ the Newton's method is obtained with a fast (locally quadratic) convergence rate. Unfortunately, Newton method involves the calculation of the second-order derivative and its inverse, which are not an easy task in data assimilation due to the complexity of the constraints and the large-scale dimension of unknowns. To address this issue, the BFGS method was developed as a replacement of the Newton method, since it can achieve a superlinear or nearly quadratic local convergence rate without much effort to compute the second-order derivative and its inverse. The BFGS method essentially tries to approximate the inverse of the second-order derivative in the following way:

$$D_k = \left(I - \theta^k (s^k \otimes g^k)\right) D_{k-1} \left(I - \theta^k (g^k \otimes s^k)\right) + \theta^k (s^k \otimes s^k), \tag{5.27}$$

where $s^k = u_{0,h}^{(k)} - u_{0,h}^{(k-1)}$, $g^k = F'_h(u_{0,h}^{(k)}) - F'_h(u_{0,h}^{(k-1)})$, and $\theta^k = \frac{1}{(s^k, g^k)}$. The operator $\otimes$ is defined as, for $p, q \in L_h^2(\Omega)$,

$$(p \otimes q)z = (q, z)p, \quad \forall z \in L_h^2(\Omega). \tag{5.28}$$

The above update is based on a continuity assumption for the second-order derivative of the cost functional. The expression (5.27) is obtained by searching a bounded operator D_k that is as close as possible to the previous D_{k-1} in the sense of a weighted Hilbert–Schmidt norm Hinze *et al.* (2009); Vuchkov *et al.* (2020):

$$\min_{D\in\mathscr{L}\left(L_h^2(\Omega),L_h^2(\Omega)\right)} \frac{1}{2}\left\| W^{\frac{1}{2}}\left(D-D_{k-1}\right)W^{\frac{1}{2}}\right\|_{HS} \quad \text{subject to } Dg^k = s^k.$$

Here, $\mathscr{L}$ represents a general linear bounded operator, W is a weighted operator satisfying $Ws^k = g^k$, and the constraint $Dg^k = s^k$ comes from a secant approximation of the second-order derivative of $F_h(u_{0,h})$ at $u_{0,h}^{(k)}$.

The BFGS algorithm can now be briefly described as follows:

- Initialize $u_{0,h}^{(0)}$ and a bounded positive definite operator D_0.
- Update $u_{0,h}^{(k+1)} = u_{0,h}^{(k)} - \gamma^k D_k F_h'\left(u_{0,h}^{(k)}\right)$ with

$$D_k = \begin{cases} D_0, & k=0,\\ \left(I-\theta^k(s^k\otimes g^k)\right)D_{k-1}\left(I-\theta^k(g^k\otimes s^k)\right)+\theta^k(s^k\otimes s^k), & k\geqslant 1.\end{cases}$$

- γ^k is determined with exact line search or an inexact line search method.

Next, we show how to compute the matrix form of D_k in a more explicit way with the operation $\otimes$ working on the $L_h^2(\Omega)$ space. Based on the definition in (5.28), for $p,q\in L_h^2(\Omega)$, we deduce

$$(p\otimes q)z = (q,z)p = \vec{q}^T M\vec{z}p = (M^T\vec{q})^T\vec{z}p = \vec{p}(M^T\vec{q})^T z, \quad \forall z\in L_h^2(\Omega). \tag{5.29}$$

Therefore, the matrix representation of $p\otimes q$ acting on $L_h^2(\Omega)$ is $\vec{p}(M^T\vec{q})^T$. Meanwhile, the calculation of θ^k is straightforward

$$\theta^k = \frac{1}{(s^k,g^k)} = \frac{1}{\vec{s}^{kT}M\vec{g}^k}.$$

Now we can rewrite (5.27) as a matrix and vector multiplication form:

$$D_k = \left(I - \frac{\vec{s}^k(M^T\vec{g}^k)^T}{\vec{s}^{kT}M\vec{g}^k}\right)D_{k-1}\left(I-\frac{\vec{g}^k(M^T\vec{s}^k)^T}{\vec{s}^{kT}M\vec{g}^k}\right)+\frac{\vec{s}^k(M^T\vec{s}^k)^T}{\vec{s}^{kT}M\vec{g}^k}. \tag{5.30}$$

We summarize the BFGS iterative algorithm in Algorithm 3. Note that the γ^k is simply picked as 1 in the Algorithm 3, reader can also apply the inexact line search method introduced in Subsection 5.4 to update γ^k at each step and obtain faster convergence.

5.4 *The steepest descent method with inexact line search*

The BFGS and CG methods can provide fast convergence rate and solve the discrete optimality system (4.18) effectively for most of cases. However, for any numerical scheme, there exists a trade-off between

Algorithm 3 BFGS Algorithm

Input: $\vec{u}_{0,h}^{(0)}$, a positive definite matrix D_0, and tol;
Compute $\vec{F}_h'(u_{0,h}^{(0)})$, the first descent direction $-D_0\vec{F}_h'(u_{0,h}^{(0)})$, and the first update $\vec{u}_{0,h}^{(1)} = \vec{u}_{0,h}^{(0)} - D_0\vec{F}_h'(u_{0,h}^{(0)})$. Set error=1 and start the iteration step $k = 1$;
while error $>$ tol **do**
Compute $\vec{F'}_h(u_{0,h}^{(k)})$;
Compute $\vec{s}^k = \vec{u}_{0,h}^{(k)} - \vec{u}_{0,h}^{(k-1)}$, $\vec{g}^k = \vec{F}_h'(u_{0,h}^{(k)}) - \vec{F}_h'(u_{0,h}^{(k-1)})$;
Compute $D_k = \left(I - \frac{\vec{s}^k(M^T\vec{g}^k)^T}{\vec{s}^{kT}M\vec{g}^k}\right) D_{k-1} \left(I - \frac{\vec{g}^k(M^T\vec{s}^k)^T}{\vec{s}^{kT}M\vec{g}^k}\right) + \frac{\vec{s}^k(M^T\vec{s}^k)^T}{\vec{s}^{kT}M\vec{g}^k}$;
Update $\vec{u}_{0,h}^{(k+1)} = \vec{u}_{0,h}^{(k)} - D_k\vec{F}_h'(u_{0,h}^{(k)})$;
Set $k = k + 1$ and error $= \|\vec{F}_h'(u_{0,h}^{(k)})\|_0$;
end while

its stability and convergence rate. In other words, the BFGS and CG methods are relatively less stable and hence may cause the algorithms to diverge for some of the data assimilation scenarios that have low stability, e.g., small regularization parameter α in the cost functional (4.1).

To tackle this numerical problem, we present the steepest descent method Hinze *et al.* (2009); De Reyes (2015) in this section to gain more stability at the cost of a lower convergence rate. With the gradient information $\vec{F}_h'(u_{0,h}) = \alpha B_h(\vec{u}_{0,h} - \vec{u}_0^b) - \vec{u}_h^{*0}$ shown in (4.17), a simple steepest descent method to solve the discrete data assimilation problem is illustrated as follows:

- Initialize $\vec{u}_{0,h}^{(0)}$.
- Update $\vec{u}_{0,h}^{(k+1)} = \vec{u}_{0,h}^{(k)} - \gamma^k\vec{F}_h'\left(u_{0,h}^{(k)}\right)$.
- γ^k is determined with exact line search or an inexact line search method.

We here present an inexact line search algorithm using Armijo backtracking method to update the γ^k: find γ^k via repeatedly solving the forward equation (5.6) with initial value

$$\vec{u}_{0,h}^{(k+1)} = \vec{u}_{0,h}^{(k)} - \gamma^k\vec{F}_h'\left(u_{0,h}^{(k)}\right) \quad \text{by updating} \quad \gamma^k = \rho\gamma^k, \tag{5.31}$$

until the following inequality is satisfied

$$F_h\left(u_{0,h}^{(k+1)}\right) \leqslant F_h\left(u_{0,h}^{(k)}\right) + \delta\gamma^k\left(F_h'\left(u_{0,h}^{(k)}\right), -F_h'\left(u_{0,h}^{(k)}\right)\right), \tag{5.32}$$

where γ^k is typically initialized as a constant equal or greater than 1, and δ and ρ are chosen in $(0, 1)$.

The straight line

$$y(\gamma^k) = F_h\left(u_{0,h}^{(k)}\right) + \delta\gamma^k\left(F_h'\left(u_{0,h}^{(k)}\right), -F_h'\left(u_{0,h}^{(k)}\right)\right) \tag{5.33}$$

is a search line, which evaluates the decreasing of the cost functional (4.3). If the point $\left(\gamma^k, F_h(u_{0,h}^{(k)} + \gamma^k(u_h^{*0(k)} - \gamma u_{0,h}^{(k)}))\right)$ is underneath the line (5.33), γ^k is a good candidate of descent step size, otherwise, we need to go through step (5.31) until the inequality (5.32) is satisfied.

We now summarize the steepest descent method algorithm:

Algorithm 4 Steepest Descent Algorithm

Input: $\gamma, \delta, \rho, \vec{u}_{0,h}^{(0)}$, and tol;
Set $k = 0$;
while error $>$ tol **do**
  Compute $\vec{F}'_h(u_{0,h}^{(k)})$;
  Inexact line search for γ^k:
  while $F_h(u_{0,h}^{(k)} - \gamma {F_h}'(u_{0,h}^{(k)})) > F_h(u_{0,h}^{(k)}) + \delta\gamma \left({F_h}'(u_{0,h}^{(k)}), -{F_h}'(u_{0,h}^{(k)})\right)$ **do**
    Reduce γ: $\gamma = \rho\gamma$;
    Solve (5.6) with initial condition $\vec{u}_{0,h}^{(k)} - \gamma \vec{F}'_h(u_{0,h}^{(k)})$ to compute
    $F_h(u_{0,h}^{(k)} - \gamma {F_h}'(u_{0,h}^{(k)}))$;
  end while
  Output γ as γ^k;
  Update $\vec{u}_{0,h}^{(k+1)} = \vec{u}_{0,h}^{(k)} - \gamma^k \vec{F}'_h(u_{0,h}^{(k)})$;
  Set $k = k + 1$ and error $= \|\vec{F}'_h(u_{0,h}^{(k)})\|_0$;
end while
Output: $\vec{u}_{0,h}^{(k+1)}$;

6. Numerical experiments

In this section, we use the methods developed in this paper to numerically show the data assimilation performance. The finite-element space is chosen on continuous piecewise linear polynomials, and the backward Euler scheme is used for time discretization. L^∞ and L^2 norm errors will be used to evaluate the numerical results. But we focus more on the L^2 norm error, since the way we measure the distance between observations and state variable in the cost functional is in an L^2 norm sense.

6.1 *Verification of the finite-element convergence rate*

Before discussing the data assimilation performance, we first provide an example to verify the optimal FEM convergence rate from Theorem 4.6. Given a set of smooth observations and for each fixed regularization parameter α, we expect to observe that the finite-element approximation converges in a second order regarding to L^2 norm. Mesh sizes of $1/8$, $1/16$, $1/32$ and time steps of $1/32$, $1/128$, $1/512$ are used, respectively. For each fixed α, the discrete solution with $h = 1/64$ and $\tau = 1/2048$ will be considered as the analytical solution.

TABLE 1 *The finite-element convergence rate of the recovered initial solution u_0*

Finite-element convergence rate					
α	$\|\|u_0 - u_{0,\frac{1}{8}}\|\|$	$\|\|u_0 - u_{0,\frac{1}{16}}\|\|$	rate	$\|\|u_0 - u_{0,\frac{1}{32}}\|\|$	rate #
1	7.1×10^{-2}	1.7×10^{-2}	2.06	3.3×10^{-3}	2.35
$\frac{1}{10}$	6.1×10^{-2}	1.4×10^{-2}	2.12	2.7×10^{-3}	2.37
$\frac{1}{50}$	5.9×10^{-2}	1.3×10^{-2}	2.17	2.6×10^{-3}	2.32
$\frac{1}{200}$	5.8×10^{-2}	1.3×10^{-2}	2.15	2.5×10^{-3}	2.37
$\frac{1}{1000}$	5.9×10^{-2}	1.3×10^{-2}	2.15	2.5×10^{-3}	2.37

For the setup of the parabolic interface equation, we consider u as follows:

$$u = \begin{cases} u^+ = \sin(\pi \cdot x)\sin(\pi \cdot y)\sin(t+1) & \text{in } \Omega^+ \times (0,T], \\ u^- = 2\sin(\pi \cdot x)\sin(\pi \cdot y)\sin(t+1) & \text{in } \Omega^- \times (0,T]. \end{cases}$$

Other relevant parameters are set as: $\beta^+ = 1$, $\beta^- = \frac{1}{2}$, $\Omega^+ = (0,1) \times (0,1)$, $\Omega^- = (1,2) \times (0,1)$ and $\Gamma : x = 1$. The boundary condition and jump interface condition satisfy $u = 0$ on $\partial\Omega$, $[u]|_\Gamma = 0$ on Γ, and $[\beta(x,y)\frac{\partial u}{\partial \vec{n}}]|_\Gamma = 0$. Both f^+ and f^- can be computed by using u^+, u^-, β^+, and β^-.

For the observation function $\hat{u}$, we use

$$\hat{u} = \begin{cases} \frac{11}{10}\sin(\pi \cdot x)\sin(\pi \cdot y)\sin(t+1) & \text{in } \Omega^+ \times (0,T], \\ \frac{22}{10}\sin(\pi \cdot x)\sin(\pi \cdot y)\sin(t+1) & \text{in } \Omega^- \times (0,T]. \end{cases}$$

We consider the background information as:

$$u_0^b = \begin{cases} 2\sin(\pi \cdot x)\sin(\pi \cdot y)\sin(1) & \text{in } \Omega^+, \\ 4\sin(\pi \cdot x)\sin(\pi \cdot y)\sin(1) & \text{in } \Omega^-. \end{cases}$$

The observations window is $\Omega_o = [0,2] \times [0,1]$ and $(0,T]$, where $T = 1$. In this scenario, we assume the error covariance related operators for observations and background information are $R = 10$ and $B = 1$.

Numerical results are displayed in Table 1, where the L^2 norm errors appear to satisfy the optimal second-order convergence rate for different α.

6.2 *Data assimilation performance I*

We now investigate the data assimilation performance utilizing the methods proposed in Section 5. The model setup for experiments are given as follows: $\Omega^+ = (0,1) \times (0,1)$, $\Omega^- = (1,2) \times (0,1)$, Γ : $x = 1$, $\beta^+ = 1$ and $\beta^- = \frac{1}{2}$. The analytical solution u is: $u^+ = \sin(\pi \cdot x)\sin(\pi \cdot y)\sin(t+1)$ and $u^- = 2\sin(\pi \cdot x)\sin(\pi \cdot y)\sin(t+1)$, and f^+ and f^- can be computed based on β^+, β^-, u^+ and u^-. The space and time observations windows are considered in $\Omega_o = [0.25, 1.75] \times [0.25, 0.75]$ and $(0,T]$, where

TABLE 2 *Data assimilation with BFGS method*

Data assimilation performance: BFGS method			
α	$\|\|u-u_h\|\|_{L^2(0,T)}$	$\|\|u-u_h\|\|_{L^\infty(0,T)}$	Iteration #
10	3.84×10^{-3}	2.41×10^{-3}	25
1	3.19×10^{-3}	2.33×10^{-3}	13
$\frac{1}{10}$	2.76×10^{-3}	2.09×10^{-3}	20
$\frac{1}{50}$	2.81×10^{-3}	2.07×10^{-3}	28
$\frac{1}{500}$	3.76×10^{-3}	2.11×10^{-3}	63
$\frac{1}{10^6}$	–	–	∞

$T=1$. We introduce the observations and background noises by adding multivariate normal distributions $e_{ob}^n \sim \mathcal{N}(0, (\frac{1}{100}I)^2), n=1,2,3,\cdots,N$ and $e_b \sim \mathcal{N}(0, (\frac{1}{10}I)^2)$ into the exact solution (discrete values of u at mesh grids along time moment t_n) as our observations and background information. Note that the covariance matrix are now uniform diagonal matrix $(\frac{1}{100}I)^2$ and $(\frac{1}{10}I)^2$, and R_h^n and B_h are $100I$ and $10I$. We test the expected performance by adjusting the regularization parameter α. The spatial and temporal step sizes are set to be $1/50$ and $1/200$, respectively.

By the way, we evaluate the data assimilation performance based on the $L^2(0,T)$ and $L^\infty(0,T)$ norm relative errors, which are defined as follows:

$$\|u-u_h\|_{L^2(0,T)} = \sqrt{\sum_{n=1}^{N} \tau \frac{\|u^n-u_h^n\|_0^2}{\|u^n\|_0^2}}, \quad \|u-u_h\|_{L^\infty(0,T)} = \sum_{n=1}^{N} \tau \frac{\|u^n-u_h^n\|_{L^\infty(\Omega)}}{\|u^n\|_{L^\infty(\Omega)}}.$$

Here, N is the number of time steps according to τ and T.

In Tables 2–4, the numerical simulations show accurate forecasting results which match the practical expectation. In addition, the convergence comparison among the three iterative methods indicates that the CG and BFGS methods are preferred for the well-conditioning or the moderate-conditioning data assimilation cases because of their higher convergence rate, and the steepest descent method is a backup for some extreme ill-conditioning scenarios only because of its stability advantage.

6.3 *Data assimilation performance II*

In this subsection, we further verify our proposed data assimilation methods with more diversified experiments, which are based on different time and space observation windows and conductivity jumps across the interface Γ in the parabolic interface equation (3.2). The model setup for experiments are given as follows: $\Omega^+ = (0,1)\times(0,1)$, $\Omega^- = (1,2)\times(0,1)$ and $\Gamma : x=1$. The boundary condition and jump interface condition satisfy $u=0$ on $\partial\Omega$, $[u]|_\Gamma = 0$, $[\beta(x,y)\frac{\partial u}{\partial \vec{n}}]|_\Gamma = 0$, and the source term $f^+ = f^- = 4xy+9$. The spatial and temporal step sizes are set to be $1/50$ and $1/200$, respectively. Also, based on the numerical test in Subsection 6.2, we empirically choose a fixed regularization parameter $\alpha = \frac{1}{5}$ for all cases and alternatively use the BFGS and CG methods to compute simulation results in the following.

TABLE 3 *Data assimilation with conjugate gradient method*

Data assimilation performance: conjugate gradient method			
α	$\|\|u - u_h\|\|_{L^2(0,T)}$	$\|\|u - u_h\|\|_{L^\infty(0,T)}$	Iteration #
10	3.84×10^{-3}	2.41×10^{-3}	5
1	3.19×10^{-3}	2.33×10^{-3}	8
$\frac{1}{10}$	2.76×10^{-3}	2.09×10^{-3}	17
$\frac{1}{50}$	2.79×10^{-3}	2.08×10^{-3}	28
$\frac{1}{500}$	3.73×10^{-3}	2.10×10^{-3}	78
$\frac{1}{10^6}$	–	–	∞

TABLE 4 *Data assimilation with steepest descent method*

Data assimilation performance: steepest descent method			
α	$\|\|u - u_h\|\|_{L^2(0,T)}$	$\|\|u - u_h\|\|_{L^\infty(0,T)}$	Iteration#
10	3.83×10^{-3}	2.41×10^{-3}	18
1	3.18×10^{-3}	2.32×10^{-3}	67
$\frac{1}{10}$	2.76×10^{-3}	2.08×10^{-3}	453
$\frac{1}{50}$	2.79×10^{-3}	2.08×10^{-3}	672
$\frac{1}{500}$	3.71×10^{-3}	2.09×10^{-3}	843
$\frac{1}{10^6}$	2.45×10^{-3}	2.03×10^{-3}	1263

TABLE 5 *The BFGS method is used to compute the numerical results, Ite = Iteration*

Data assimilation performance: $\beta^+ = 0.5, \beta^- = 2, T = 1$			
Space window	$\|\|u - u_h\|\|_{L^2(0,T)}$	$\|\|u - u_h\|\|_{L^\infty(0,T)}$	Ite#
$\Omega_o = [0, 2] \times [0, 1]$	2.00×10^{-3}	5.92×10^{-4}	52
$\Omega_o = [1, 2] \times [0, 1]$	2.40×10^{-3}	4.20×10^{-3}	53
$\Omega_o = [0, 1] \times [0, 1]$	2.50×10^{-3}	7.57×10^{-4}	49
$\Omega_o = [0.2, 1.2] \times [0, 1]$	2.50×10^{-3}	7.25×10^{-4}	49
$\Omega_o = [0.8, 1.8] \times [0, 1]$	3.40×10^{-3}	1.70×10^{-3}	52
$\Omega_o = [0.2, 1.2] \times [0.2, 0.8]$	2.29×10^{-3}	3.27×10^{-3}	43
$\Omega_o = [0.8, 1.8] \times [0.2, 0.8]$	3.40×10^{-3}	1.50×10^{-3}	52

We will consider $\beta^+ = 0.5$ and $\beta^- = 2$ for the moderate conductivity jump test and $\beta^+ = 0.5$ and $\beta^- = 20$ for the large conductivity jump test. For both cases, we firstly numerically run the corresponding parabolic interface model on the time period (0,1.125] based on an initial condition $w_0 = \sin(\pi \cdot x)\sin(\pi \cdot y)$ (note that this initial condition w_0 is only used to generate data, not the one we intend to recover). We

TABLE 6 *The CG method is used to compute the numerical results, Ite = Iteration*

Data assimilation performance: $\beta^+ = 0.5, \beta^- = 20, T = 1$			
Space window	$\|\|u - u_h\|\|_{L^2(0,T)}$	$\|\|u - u_h\|\|_{L^\infty(0,T)}$	Ite#
$\Omega_o = [0,2] \times [0,1]$	2.20×10^{-3}	6.16×10^{-4}	17
$\Omega_o = [1,2] \times [0,1]$	5.70×10^{-2}	2.90×10^{-3}	5
$\Omega_o = [0,1] \times [0,1]$	2.30×10^{-3}	6.17×10^{-4}	19
$\Omega_o = [0.2,1.2] \times [0,1]$	2.50×10^{-3}	7.35×10^{-4}	22
$\Omega_o = [0.8,1.8] \times [0,1]$	4.20×10^{-3}	1.90×10^{-3}	13
$\Omega_o = [0.2,1.2] \times [0.2,0.8]$	2.90×10^{-3}	8.72×10^{-4}	21
$\Omega_o = [0.8,1.8] \times [0.2,0.8]$	4.20×10^{-3}	1.80×10^{-3}	12

TABLE 7 *The BFGS method is used to compute the numerical results, Ite = Iteration*

Data assimilation performance without background information: $\beta^+ = 0.5, \beta^- = 2, T = 1$			
Space window	$\|\|u - u_h\|\|_{L^2(0,T)}$	$\|\|u - u_h\|\|_{L^\infty(0,T)}$	Ite#
$\Omega_o = [0,2] \times [0,1]$	1.90×10^{-3}	6.83×10^{-4}	81
$\Omega_o = [1,2] \times [0,1]$	7.82×10^{-2}	4.75×10^{-2}	80
$\Omega_o = [0,1] \times [0,1]$	1.25×10^{-2}	4.43×10^{-3}	85
$\Omega_o = [0.2,1.2] \times [0,1]$	7.40×10^{-2}	2.50×10^{-3}	76
$\Omega_o = [0.8,1.8] \times [0,1]$	3.23×10^{-2}	1.93×10^{-2}	79
$\Omega_o = [0.2,1.2] \times [0.2,0.8]$	7.70×10^{-3}	2.60×10^{-3}	72
$\Omega_o = [0.8,1.8] \times [0.2,0.8]$	3.32×10^{-2}	1.99×10^{-2}	79

TABLE 8 *The CG method is used to compute the numerical results, Ite = Iteration*

Data assimilation performance without background information: $\beta^+ = 0.5, \beta^- = 20, T = 1$			
Space window	$\|\|u - u_h\|\|_{L^2(0,T)}$	$\|\|u - u_h\|\|_{L^\infty(0,T)}$	Ite#
$\Omega_o = [0,2] \times [0,1]$	2.70×10^{-3}	1.30×10^{-3}	16
$\Omega_o = [1,2] \times [0,1]$	1.95×10^{-1}	9.70×10^{-2}	6
$\Omega_o = [0,1] \times [0,1]$	2.50×10^{-3}	7.14×10^{-4}	33
$\Omega_o = [0.2,1.2] \times [0,1]$	2.50×10^{-3}	9.26×10^{-4}	35
$\Omega_o = [0.8,1.8] \times [0,1]$	4.82×10^{-2}	2.49×10^{-2}	18
$\Omega_o = [0.2,1.2] \times [0.2,0.8]$	3.20×10^{-3}	1.20×10^{-3}	34
$\Omega_o = [0.8,1.8] \times [0.2,0.8]$	4.96×10^{-2}	2.56×10^{-2}	19

add Gaussian noise $e_{ob}^n \sim \mathscr{N}(0, (\frac{1}{100}I)^2)$ to the numerical solution on the time period $(0.125, 1.125]$ as observation data $\{\hat{u}_h^n\}$ (noise size compared to data with respect to L^2 norm is around 11.2% for moderate jump test and 9.3% for large jump test) and add Gaussian noise $e_b \sim \mathscr{N}(0, (\frac{1}{5}I)^2)$ onto the numerical solution at $t = 0.125$ as background information $u_{0,h}^b$. In other words, the solution at $t = 0.125$ will be the real initial condition we target on recovering, which will also be used to achieve better state predictions.

Tables 5 and 6 display decent state simulation results for different observation windows while both moderate and large conductivity jump models are considered. The numerical tests show that it is more efficient to collect observations from small conductivity region to have better simulation result, which makes sense that the state in small conductivity region is less diffusive and more sensitive to initial conditions compared with the larger conductivity region. In general, the more data we use, the more accurate the data assimilation result is. In Tables 7 and 8, we test our data assimilation methods while the background information is absent (i.e., the regularization term in the objective function is simply $\frac{\alpha}{2}\|u_{0,h}\|_0^2$ and other setup are the same). We are still able to achieve accurate assimilation results once observations are provided relevant or sufficient enough. However, the simulation performance without background information is generally poorer than experiments with background information, which emphasizes the importance of background information in data assimilation, especially for cases of only partial observations available. This is expected in the sense of the balance between the accuracy and the available information. In addition, the numbers of iterations in Tables 5–8 again demonstrate the efficiency of the developed CG and BFGS methods. All of these validate the proposed methods in this paper.

7. Conclusion

In this paper we propose a variational data assimilation method for a second-order parabolic interface equation and demonstrate the wellposedness of such a problem by using weighted L^2 norms. The Lagrange multiplier rule is used in the derivation of the optimality systems. By utilizing a finite-element method we develop a numerical approximation and analyze its convergence properties with respect to the continuous data assimilation. The optimal convergence rate is established by recovering the Galerkin orthogonality in the optimality systems. Based on the efficient iterative algorithms developed in Section 5, the numerical experiments validate the proposed methods in this paper and display promising results.

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