

A Cubic B-spline Finite Element Method for Optimal Control Problem Governed by Nonlinear Parabolic Equation Describing Crystal Surface Growth

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Abstract—We propose a cubic B-spline finite element method to solve the optimal control problem governed by nonlinear parabolic equation depicting crystal surface growth. Considering that both the state equation and the adjoint equation are fourth-order nonlinear parabolic equations, we select the cubic B-spline functions as shape functions. We establish a fully-discrete scheme of the optimality system and use an iterative method to solve it. In the end, a numerical example is demonstrated for the purpose of verifying the feasibility and effectivity of the suggested method.

Index Terms—Optimal control problem, cubic B-spline, fourth-order nonlinear parabolic equation, finite element method, iterative method.

I. INTRODUCTION

OPTIMAL control problems have received more and more attention from the researchers. Generally speaking, an optimal control problem (OCP) is aimed at finding a control variable within an admissible set, so that the state tends to the desired state during the course of minimizing the objective functional, and at the same time both the control and state variables are subject to the differential equations. A host of practical problems can be boiled down to optimal control problems governed by differential equations, such as heating processes, fluid flows and chemical engineering. The basic theory and numerical methods for OCP can refer to the monographs by Lions [1]. Details of the adaptive finite element method (FEM) can be found in [2].

In [3], the crystal surface growth model is expressed by the following fourth-order nonlinear parabolic equation in the case of 1D:

$$\begin{cases} \frac{\partial u}{\partial t} + au_{xxxx} + \mu \left(\frac{u_x}{1 + |u_x|^2} \right)_x = 0, \\ u_x(0, t) = u_x(1, t) = u_{xxx}(0, t) = u_{xxx}(1, t) = 0, \\ u(x, 0) = u_0(x), \quad x \in \Omega, \end{cases} \quad (x, t) \in \Omega \times (0, T], \quad t \in (0, T], \quad (1)$$

Manuscript received February 24, 2022; revised August 4, 2022. This work was supported by the National Natural Science Foundation of China (Grant Nos. 11871312 and 12131014).

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where $a > 0$, $\mu > 0$ and $\Omega = (0, 1)$. Here $u(x, t)$ which is an unknown quantity to be solved represents the displacement of height of the crystal surface at the point x . The highest order item au_{xxxx} means the surface diffusion of adatoms resulted from the deviation of the chemical potential. Additionally, nonlinear term $\mu(u_x/(1 + |u_x|^2))_x$ indicates the effect of surface roughening [3]–[5].

Reference [3] considered the OCP governed by fourth-order nonlinear parabolic differential equation (1). It was proved that the optimal solution existed, and then the optimality system was established. However, they didn't design numerical method to solve it. Due to the fact that it is hard to obtain the exact solutions for optimal control problems directly, there emerge some methods to obtain the numerical solutions like the finite difference method (FDM), finite element method (FEM) [6]–[10] and so on. An important step of FEM is to establish the finite element space for the state variable, which needs to select appropriate shape functions. When we choose m -order polynomials as shape functions, the smoothness of approximate solutions may be unsatisfactory. The k th-order B-spline functions can just make up for this deficiency, since it is continuously differentiable of order $k - 2$. The B-spline method has been widely applied to derive numerical solutions of partial differential equations [11]–[18]. In [11], a bicubic B-spline interpolation method was proposed to solve two-dimensional heat equations. In [12], the authors proposed a two-dimensional bicubic B-spline FEM to deal with MHD-duct flow model. [14] developed a quadratic B-spline FEM to solve the coupled Schrödinger-Boussinesq equations numerically. Qin et al. [18] presented a cubic B-spline FEM to solve equation (1) with homogeneous Dirichlet boundary condition. They showed that the approximate solution obtained by cubic B-spline FEM had better smoothness than that obtained by Hermite FEM [19], but the convergence rates of these two methods were the same. However, there are few studies on the application of B-splines to solve optimal control problems numerically.

Invoked by the work of [18], we develop a cubic B-spline FEM for fourth-order nonlinear parabolic OCP. The remainder of the article is organized as follows. The optimality system of OCP governed by equation (1) is obtained in Section II. In Section III, the B-spline functions are introduced first. After that the piecewise cubic B-spline finite element space is established. We construct a numerical example in Section IV to demonstrate that our suggested approach is feasible and efficient. Here, a fully-discrete scheme is established

for the optimality system and the calculation is performed by using an iterative method to avoid solving large systems of the coupled algebraic equations. Finally, we make some conclusions in Section V.

II. MODEL

We will employ the normal notations of Sobolev spaces and norms, see [20]. Let $V = H_E^2(\Omega) = \{u : u \in H^2(\Omega), u_x|_{\partial\Omega} = 0\}$. For fixed $T > 0$, we define the state space as

$$W(0, T; V) = \{u : u \in L^2(0, T; V), u_t \in L^2(0, T; V^*)\},$$

where V^* represents the dual space of V . We denote L^2 -, H^k - norms in Ω by $\|\cdot\|$ and $\|\cdot\|_k$ respectively.

We are concerned about the following nonlinear parabolic OCP governed by equation (1) in this article:

$$\min_{w \in L^2(Q_0)} J(u, w) = \frac{1}{2} \int_0^T (\|u - z_d\|^2 + \lambda \|w\|^2) dt \quad (2)$$

subject to

$$\begin{cases} \frac{\partial u}{\partial t} + au_{xxxx} + \mu \left(\frac{u_x}{1 + |u_x|^2} \right)_x = Bw + f, \\ u_x(0, t) = u_x(1, t) = u_{xxx}(0, t) = u_{xxx}(1, t) = 0, \\ u(x, 0) = u_0(x), \quad x \in \Omega, \end{cases} \quad (x, t) \in \Omega \times (0, T], \quad t \in (0, T], \quad (3)$$

where J is referred to as the objective functional and w is the control variable defined on $Q_0 \subseteq Q = \Omega \times (0, T)$. Equation (3) is termed as the state equation. Moreover, u denotes the state variable and z_d represents the desired state variable. $f(x, t) \in L^2(0, T; L^2(\Omega))$ is a known function and $u_0(x) \in V$ is a pre-defined data. λ is a positive constant serving as a regularization parameter. Let B be a linear continuous operator from $L^2(Q_0)$ to $L^2(0, T; L^2(\Omega))$. Our target is to find w in $L^2(Q_0)$ to make u tend to z_d during the course of optimizing the objective functional J .

We write the variational formulation of the state equation (3) as the following: For all $v \in V$, $t \in (0, T]$, find $u(x, t) \in W(0, T; V)$ such that

$$\begin{cases} (u_t, v)_{V^*, V} + a(D^2u, D^2v) - \mu \left(\frac{Du}{1 + |Du|^2}, Dv \right) \\ = (Bw + f, v), \quad \forall v \in V, \\ u(x, 0) = u_0(x), \quad x \in \Omega, \end{cases} \quad (4)$$

where $Du = u_x$, $D^2u = u_{xx}$ and

$$(v, w)_{V^*, V} = \int_{\Omega} vw \, dx \quad \forall v \in V^*, w \in V.$$

For fixed f, w and u_0 , equation (4) exists a unique weak solution according to reference [3].

Therefore, we restate the optimal control problem (2)-(3) as follows:

$$\min_{w \in L^2(Q_0)} J(u, w) = \frac{1}{2} \int_0^T (\|u - z_d\|^2 + \lambda \|w\|^2) dt \quad (5)$$

subject to

$$\begin{cases} (u_t, v)_{V^*, V} + a(D^2u, D^2v) - \mu \left(\frac{Du}{1 + |Du|^2}, Dv \right) \\ = (Bw + f, v), \quad \forall v \in V, \\ u(x, 0) = u_0(x), \quad x \in \Omega. \end{cases} \quad (6)$$

According to reference [3], the solution of control problem (5)-(6) is uniquely determined. Furthermore, a pair (u, w) satisfies (5)-(6) when and only when there exists a co-state $p \in W(0, T; V)$ such that the triplet (u, p, w) is the solution of the following optimality system:

$$\begin{cases} (u_t, v)_{V^*, V} + a(D^2u, D^2v) - \mu \left(\frac{Du}{1 + |Du|^2}, Dv \right) \\ = (Bw + f, v), \quad \forall v \in V, \\ u(0) = u_0, \end{cases} \quad (7)$$

$$\begin{cases} -(p_t, \eta)_{V^*, V} + a(D^2p, D^2\eta) \\ - \mu \left(\frac{1 - |Du|^2}{(1 + |Du|^2)^2} Dp, D\eta \right) = (u - z_d, \eta), \\ \forall \eta \in V, \\ p(T) = 0, \end{cases} \quad (8)$$

$$(B^*p + \lambda w, \tilde{w} - w)_{L^2(Q_0)} \geq 0, \quad \forall \tilde{w} \in L^2(Q_0), \quad (9)$$

where B^* is the adjoint operator of B . The equation (8) is called as the adjoint equation of (7) and p is the co-state variable. Moreover, the inequality (9) is referred to as first-order necessary optimality condition. As a result, solving the distributed optimal control problem (5)-(6) is equivalent to solving the optimality system (7)-(9).

III. FINITE ELEMENT SPACE

In this section, the B-spline functions are introduced first. After that, the piecewise cubic B-spline finite element space is established.

Let $N_k(x)$ represent the k th-order B-spline function whose support is $[0, k]$, where k is a positive integer. To be more precise, $N_k(x)$ can be defined recursively by [18]

$$N_k(x) = (N_{k-1} * N_1)(x) = \int_0^1 N_{k-1}(x-t) dt \quad (10)$$

with

$$N_1(x) = \chi_{[0,1]} = \begin{cases} 1, & x \in [0, 1], \\ 0, & \text{else.} \end{cases} \quad (11)$$

According to (10)-(11), we derive that $N_4(x)$ is the fourth-order cubic B-spline function and its specific form is

$$N_4(x) = \begin{cases} \frac{1}{6}x^3, & x \in [0, 1], \\ -\frac{1}{2}x^3 + 2x^2 - 2x + \frac{2}{3}, & x \in [1, 2], \\ \frac{1}{2}x^3 - 4x^2 + 10x - \frac{22}{3}, & x \in [2, 3], \\ -\frac{1}{6}(x-4)^3, & x \in [3, 4], \\ 0, & \text{else.} \end{cases} \quad (12)$$

It's well known that $N_k(x)$ belongs to $C^{k-2}(-\infty, +\infty)$.

Assume that L is a positive integer, the interval $0 = x_0 < x_1 < \dots < x_L = 1$ is partitioned equally by step size $h = 1/L$. Let $\phi_i(x) = N_4(\frac{x-x_i}{h})$ denote the cubic B-spline basis function at x_i . Each cubic B-spline basis function is nonzero over four adjacent elements so that on each interval $[x_i, x_{i+1}]$ there are four cubic B-spline functions, namely $\phi_{i-3}(x)$, $\phi_{i-2}(x)$, $\phi_{i-1}(x)$ and $\phi_i(x)$, as shown in Figure 1. Based on this, we need to introduce virtual nodes x_{-3}, x_{-2}

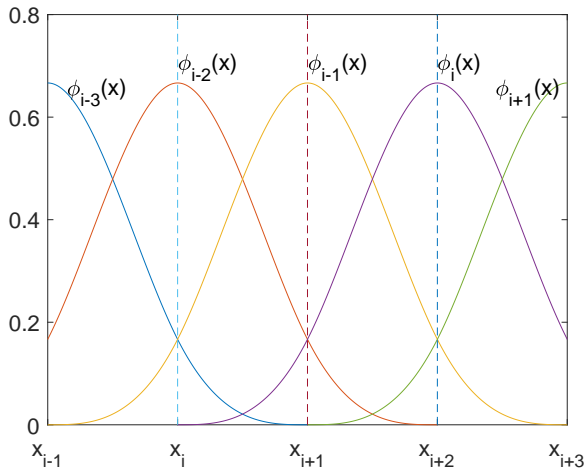


Fig. 1. A family of cubic B-spline basis functions

and x_{-1} to deal with the boundary conditions. Moreover, there are three nonzero cubic B-spline basis functions at x_i , namely $\phi_{i-3}(x)$, $\phi_{i-2}(x)$ and $\phi_{i-1}(x)$. This can be seen from Figure 1. The nonzero values are given in the following,

$$\phi_{i-3}(x_i) = \frac{1}{6}, \phi_{i-2}(x_i) = \frac{2}{3}, \phi_{i-1}(x_i) = \frac{1}{6}. \quad (13)$$

The set of $\phi_{-3}, \phi_{-2}, \dots, \phi_{L-2}, \phi_{L-1}$ forms a basis for piecewise cubic B-spline space associated with the partition $\{x_i, 0 \leq i \leq L\}$. By using these splines as trial functions, we can express the approximation solution $u_h(x, t)$ as

$$u_h(x, t) = \sum_{i=-3}^{L-1} \delta_i(t) \phi_i(x), \quad (14)$$

where $\delta_i(t)$ is time-dependent quantity. However, $u_h(x, t)$ must satisfy the essential boundary conditions $u_{h,x}(0, t) = u_{h,x}(1, t) = 0$. A straightforward calculation yields

$$\begin{aligned} \phi'_j(x_i) &= \frac{1}{h} N'_4 \left(\frac{x_i - x_j}{h} \right) \\ &= \begin{cases} \frac{1}{h} N'_4(3) = -\frac{1}{2h}, & j = i - 3, \\ \frac{1}{h} N'_4(1) = \frac{1}{2h}, & j = i - 1, \\ 0, & \text{else.} \end{cases} \end{aligned} \quad (15)$$

Therefore, from

$$\begin{aligned} u_{h,x}(x_0, t) &= \delta_{-3}(t) \phi'_{-3}(x_0) + \delta_{-1}(t) \phi'_{-1}(x_0) \\ &= -\frac{1}{2h} \delta_{-3}(t) + \frac{1}{2h} \delta_{-1}(t) \\ &= 0, \\ u_{h,x}(x_L, t) &= \delta_{L-3}(t) \phi'_{L-3}(x_L) + \delta_{L-1}(t) \phi'_{L-1}(x_L) \\ &= -\frac{1}{2h} \delta_{L-3}(t) + \frac{1}{2h} \delta_{L-1}(t) \\ &= 0, \end{aligned} \quad (16)$$

we have $\delta_{-3}(t) = \delta_{-1}(t)$, $\delta_{L-3}(t) = \delta_{L-1}(t)$. These conditions are not easily satisfied when the system of equations is subsequently solved. To deal with this problem, we make some adjustments to the cubic B-spline basis functions. Let

$$\begin{aligned} \tilde{\phi}_{-1}(x) &= \phi_{-3}(x) + \phi_{-1}(x), \\ \tilde{\phi}_{L-3}(x) &= \phi_{L-3}(x) + \phi_{L-1}(x), \end{aligned}$$

and other basis functions remain unchanged. After modification, we obtain

$$\begin{aligned} u_{h,x}(x_0, t) &= \delta_{-3}(t) \phi'_{-3}(x_0) = -\frac{1}{2h} \delta_{-3}(t), \\ u_{h,x}(x_L, t) &= \delta_{L-1}(t) \phi'_{L-1}(x_L) = \frac{1}{2h} \delta_{L-1}(t). \end{aligned} \quad (17)$$

Hence, in order to satisfy $u_{h,x}(0, t) = u_{h,x}(1, t) = 0$, we just need to take $\delta_{-3}(t) = \delta_{L-1}(t) = 0$. Eventually, cubic B-spline basis functions are established in the following:

$$\begin{aligned} &\{\phi_{-3}(x), \phi_{-2}(x), \tilde{\phi}_{-1}(x), \phi_0(x), \dots \\ &\dots, \phi_{L-4}(x), \tilde{\phi}_{L-3}(x), \phi_{L-2}(x), \phi_{L-1}(x)\}. \end{aligned}$$

Let U_h be the linear space of functions v such that

- (1) $v \in C^2([0, 1])$,
- (2) $v|_{[x_{i-1}, x_i]}$ is a cubic B-spline function, $i = 1, \dots, L$,
- (3) $v'(0) = v'(1) = 0$.

Based on the above analysis, we have

$$U_h = \text{span}\{\phi_{-2}(x), \tilde{\phi}_{-1}(x), \phi_0(x), \dots, \phi_{L-4}(x), \tilde{\phi}_{L-3}(x), \phi_{L-2}(x)\} \subset V.$$

The approximation solutions $u_h(x, t)$ and $p_h(x, t)$ satisfy

$$\begin{aligned} u_h(x, t) &= \sum_{i=-2}^{L-2} \delta_i(t) \phi_i(x), \\ p_h(x, t) &= \sum_{i=-2}^{L-2} \beta_i(t) \phi_i(x). \end{aligned}$$

IV. NUMERICAL EXAMPLE

We construct a numerical example in this section to demonstrate that the cubic B-spline FEM mentioned from the above section is effective and feasible.

We consider the model (2)-(3) by choosing $\lambda = 1, a = \mu = 1$ and $T = 1$. Let $Q_0 = Q$ and B is an identity operator, that is, the control w is unconstrained. We can derive the following optimality condition by (9):

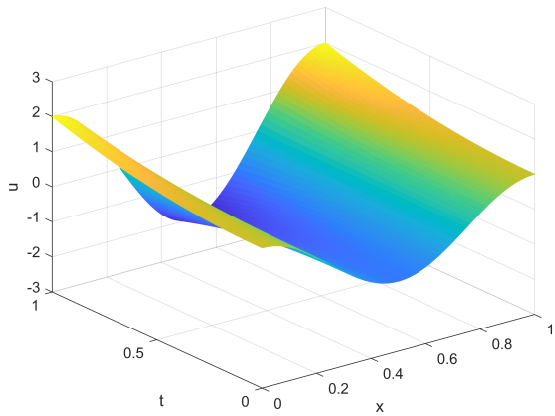
$$p + w = 0. \quad (18)$$

Substituting (18) into the state equation (7) leads to the optimality system

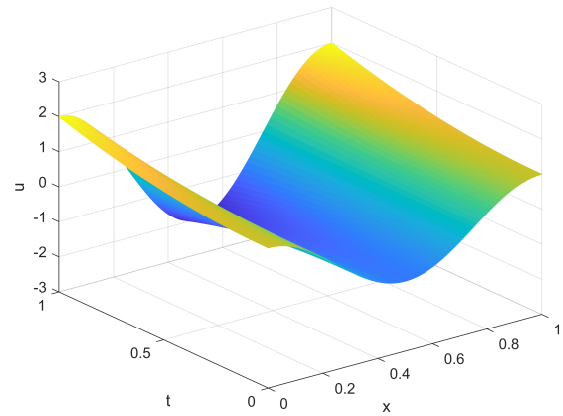
$$\begin{cases} (u_t, v) + (D^2 u, D^2 v) - \left(\frac{Du}{1 + |Du|^2}, Dv \right) \\ \quad = (-p + f, v), \quad \forall v \in V, \\ u(x, 0) = u_0(x), \quad x \in \Omega, \\ -(p_t, \eta) + (D^2 p, D^2 \eta) - \left(\frac{1 - |Du|^2}{(1 + |Du|^2)^2} Dp, D\eta \right) \\ \quad = (u - z_d, \eta), \quad \forall \eta \in V, \\ p(x, T) = 0, \quad x \in \Omega. \end{cases} \quad (19)$$

This is a coupled system of two parabolic differential equations for u and p . Once p has been found, the optimal control w can be obtained from (18).

On the strength of the cubic B-spline basis, the semi-discrete finite element formulation for (19) reads as follows:

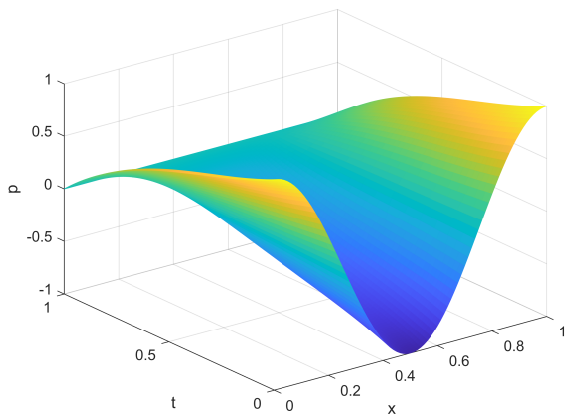


(a) Exact solution of u

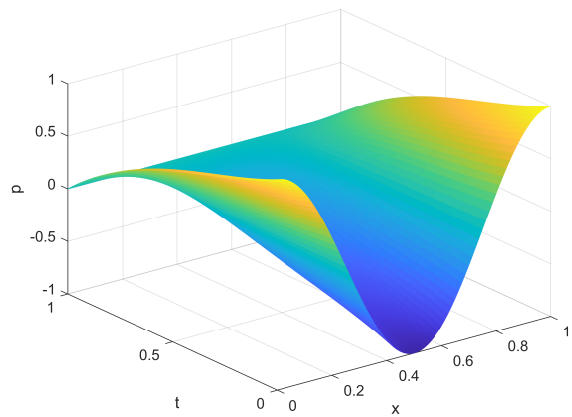


(b) Approximate solution of u

Fig. 2. Comparison figures of state variable u

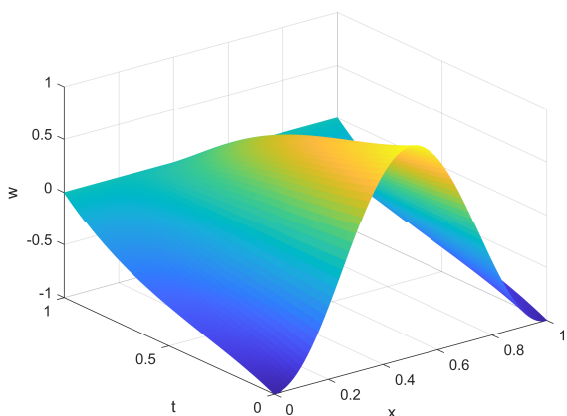


(a) Exact solution of p

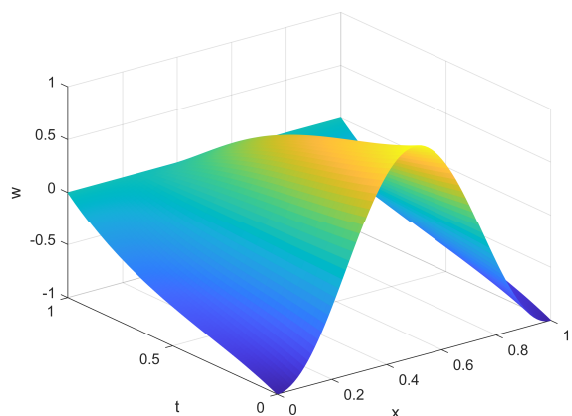


(b) Approximate solution of p

Fig. 3. Comparison figures of co-state variable p



(a) Exact solution of w



(b) Approximate solution of w

Fig. 4. Comparison figures of control variable w

lished. Finally, the numerical example has demonstrated that our proposed approach is efficient and valid.

In this paper, the parabolic equations are nonlinear, and the objective functional is defined over the whole time interval.

In fact, our method can be extended to the situation of other types of boundary conditions with the objective functional at the final state. The results for this case will be presented in a forthcoming paper.

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