周期热传导方程优化控制问题的一种迭代解法

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摘 要：本文研究了一类以时间周期热传导方程为约束条件的优化控制问题，该优化问题旨在寻求使得目标泛函达到最小的源项. 本文提出了一种迭代求解算法. 该算法应用最优性条件将问题转化为两个耦合的时间周期热传导方程，然后将这两个方程迭代解耦，再以 Gauss-Seidel 模式交替求解. 数值算例显示，算法的收敛速度对离散参数是稳健的.

关键词：周期热传导方程；优化控制；迭代
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An iterative solver for time-periodic heat optimal control problems

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Abstract: In this paper, an iterative algorithm is introduced for solving a class of optimal control problems constrained by time-periodic heat equation, where the optimization is concerned by searching a best source term of the heat equation to minimize the objective function. By applying the optimality condition, the problem is firstly transformed into two coupled time-periodic heat equations. Then the iterative algorithm is applied to decouple the coupled PDE system. Finally, the equations are separately solved in the Gauss-Seidel pattern. Numerical examples are presented to illustrate the robustness of the convergence rate of algorithm with respect to the discretization parameters.

Keywords: Time-periodic heat equation; Optimal control; Iteration
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1 Introduction

In this paper, we consider the optimal control problems constrained by time-periodic heat partial differential equation (PDE)[1-20]. Applications of such problems include the design of reverse flow reactors[12], cyclically steered (bio-) reactors[5] and energy-producing kites[4], etc. Meanwhile, such optimal control problems also arise in a variety of chemical engineering applications[3, 8, 9, 15, 18, 19] such as the moving bed processes[14] which find widespread use in the pharmaceutical and food industry.

Different from the usual setting for linear parabolic control systems in the literature, a par-

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ticular feature of the time-periodic parabolic control problems is the constraint that the solution of the underlying dynamical system is periodic in time. This kind of optimal control problems appear as the sub-problems in inexact Newton or inexact sequential quadratic programming methods for the solution of nonlinear optimization problems with time-periodic partial differential equation (PDE) constraints.

The computation of optimal controls is based on the optimal conditions and their approximate solutions using some numerical discretization. The applicability and the accuracy of this strategy depend on the availability of structure of the discretized optimality systems. If accurate solutions are required, the resulting discretized problems will inevitably be of large scale, because in this case we often need to use small discretization sizes. Thus, it is an important issue to design efficient solvers to treat the optimal control problems with time-periodic PDE constraint. Existing numerical methods for this kind of control problems include the relaxation techniques[6], the multigrid method[2] and the interesting pre-conditioning technique which attract considerable attention in the past years (see, *e. g.*, Refs. [1,7,10,11,13,16,20]). However, these existing approaches are more complicated than the one proposed in this paper. In a word, the new iterative algorithm studied here has essential difference with respect to mechanism, computational cost and complexity with the just mentioned algorithms.

In this paper, we propose a new approach to solve the time-periodic heat optimal control problems. We firstly reformulate the optimal control problem as two coupled time-periodic heat equations. Then we solve this coupled PDE system via an iteration process. By picking up an initial guess for the control variable (chosen randomly in practical computation), we solve the state equation and the solution plays a role of source term for the adjoint equation. Then we solve the adjoint equation and with the solution we can prepare for the next iteration. We show that the convergence rate of the proposed iterative algorithm is robust with respect to the space and time discretization parameters.

The rest of this paper is organized as follows. In Section 2, we present the optimal control problem studied in this paper. The optimality system is also derived in detail in this section. Section 3 presents the algorithm and the details concerning implementation in practice. In Section 4, we show numerical results which indicate that the convergence rate of the proposed algorithm is robust with respect to the change of discretization parameters. Section 5 concludes this paper.

2 The optimal control problem

The model that we are interested in is the following optimal control problem:

$$\min_{y,u} J(y,u), \text{with}$$

$$J(y,u) = \frac{1}{2}\int_0^1\int_\Omega (y(x,t)-\bar{y}(x,t))^2\mathrm{d}x\mathrm{d}t + \frac{\eta}{2}\int_0^1\int_\Omega u^2(x,t)\mathrm{d}x\mathrm{d}t \tag{1a}$$

where y (the state variable) and u (the control variable) satisfy the following constraints

$$\begin{cases}\partial_t y-\mu\Delta y=-u,\ (x,t)\in\Omega\times(0,1),\\ y(x,0)=y(x,1),\ x\in\Omega,\\ y(x,t)=0,\ (x,t)\in\partial\Omega\times(0,1)\end{cases} \tag{1b}$$

Here $\Omega\subseteq\mathbb{R}^d$ is a general space domain, $\bar{y}(x,t)$ is a known function and $\eta>0$.

In order to solve (1a~1b), we now derive the optimality system. Denote by $y(u)$ the solution of the state equation in (1b) and by $y'(u;\delta u)$ the first-order directional derivative of y at u along the direction δu. Let

$$e(y,u)=\partial_t y-\mu\Delta y-u.$$

Then, a routine calculation yields

$$e_y(y,u)y'(u;\delta u)+e_u(y,u)\delta u=0 \tag{2}$$

It is easy to get $e_y(y,u)=\partial_t-\mu\Delta$ and $e_u(y,u)=I$, where I is the identity operator. Substituting these results in to (2) gives

$$\partial_t y'(u;\delta u)-\mu\Delta y'(u;\delta u)-\delta u=0 \tag{3}$$

Let e_y^* and e_u^* be the dual operators of e_y and e_u, defined as follows: $\forall v,u$,

$$\langle e_y v, u\rangle = \langle v, e_y^* u\rangle, \langle e_u v, u\rangle = \langle v, e_u^* u\rangle \tag{4}$$

where $\langle\cdot\rangle$ denotes the standard inner product in the space and time domain $\Omega\times(0,1)$. Since $e_u = I$, it is easy to see $e_u^* = I$. We now derive the expression of e_y^*. We have

$$\langle e_y v, u\rangle = \int_0^1\int_\Omega (\partial_t v - \mu\Delta v) u \,\mathrm{d}x\mathrm{d}t =$$
$$\int_0^1\int_\Omega \partial_t v u \,\mathrm{d}x\mathrm{d}t - \mu\int_0^1\int_\Omega \Delta v u\,\mathrm{d}x\mathrm{d}t =$$
$$\int_\Omega\left(\int_0^1 \partial_t v u\,\mathrm{d}t\right)\mathrm{d}x - \mu\int_0^1\left(\int_\Omega \Delta v u\,\mathrm{d}x\right)\mathrm{d}t =$$
$$-\int_\Omega\int_0^1 v\,\partial_t u\,\mathrm{d}t\mathrm{d}x + \mu\int_0^1\int_\Omega \nabla v\cdot\nabla u\,\mathrm{d}x\mathrm{d}t =$$
$$-\int_\Omega\int_0^1 v\,\partial_t u\,\mathrm{d}t\mathrm{d}x - \mu\int_0^1\int_\Omega v\Delta u\,\mathrm{d}x\mathrm{d}t =$$
$$-\int_\Omega\int_0^1 v(\partial_t + \mu\Delta)u\,\mathrm{d}x\mathrm{d}t.$$

This gives $e_y^* = \partial_t + \mu\Delta$. In summary, the dual operators implied by (4) are

$$e_y^* = \partial_t + \mu\Delta, e_u^* = I \tag{5}$$

Let $\hat{J}(u) = J(y(u), u)$. Then we have

$$\hat{J}'(u;\delta u) = \lim_{r\to 0}\frac{\hat{J}(u + r\delta u) - \hat{J}(u)}{r} =$$
$$\frac{1}{2}\int_0^1\int_\Omega \lim_{r\to 0}\frac{[y(u(x,t) + r\delta u(x,t)) - \bar{y}(x,t)]^2 - (y(u(x,t)) - \bar{y}(x,t))^2}{r}\mathrm{d}x\mathrm{d}t +$$
$$\frac{\eta}{2}\int_0^1\int_\Omega \lim_{r\to 0}\frac{[u(x,t) + r\delta u(x,t)]^2 - u^2(x,t)}{r}\mathrm{d}x\mathrm{d}t.$$

This gives

$$\hat{J}'(u;\delta u) = \int_0^1\int_\Omega y'(u;\delta u)[y(u) - \bar{y}]\mathrm{d}x\mathrm{d}t + \eta\int_0^1\int_\Omega u\delta u\,\mathrm{d}x\mathrm{d}t \tag{6}$$

In (3) and (6), by letting $\delta u = v - u$ with some suitable v we have

$$\hat{J}'(u;v-u) = \int_0^1\int_\Omega y'(u;v-u)[y(u) - \bar{y}]\mathrm{d}x\mathrm{d}t + \eta\int_0^1\int_\Omega u(v-u)\mathrm{d}x\mathrm{d}t, \partial_t y'(u;v-u) - \mu\Delta y'(u;v-u) - (v-u) = 0,$$

which is equivalent to

$$\hat{J}'(u;v-u) = \langle y'(u;v-u), y-\bar{y}\rangle + \eta\langle u, v-u\rangle$$
$$e_y(y,u)y'(u;v-u) + e_u(y,u)(v-u) = 0 \tag{7}$$

where $y := y(u)$.

Let p (the so-called co-state variable) be the solution of the following equation

$$e_y^*(y,u)p = -(y-\bar{y}) \tag{8}$$

Then it follows by using (8) and the second equation in (7) that

$$\langle e_y(y,u)y'(u;v-u), p\rangle = -\langle e_u(y,u)(v-u), p\rangle.$$

Now, by using (5) and (8) we have

$$\langle v-u, e_u^*(y,u)p\rangle = \langle y'(u;v-u), e_y^*(y,u)p\rangle = -\langle y'(u;v-u), y-\bar{y}\rangle = \langle y'(u;v-u), -(y-\bar{y})\rangle \tag{9}$$

Since (9) holds for arbitrary directional variable v, it holds

$$e_y^*(y,u)p = -(y-\bar{y}).$$

This together with $e_y^* = \partial_t + \mu\Delta$ (cf. (5)) implies the following equation for the co-state variable p:

$$(\partial_t + \mu\Delta)p = -(y-\bar{y}) \tag{10a}$$

Moreover, since (9) holds for all $x\in\Omega$ and $t\in[0,1]$, by letting $x\in\partial\Omega$ and $t = 0, 1$ we get the following conditions for (10a)

$$p(0,x) = p(1,x) \text{ for } x\in\Omega,\ p(t,x) = 0 \text{ for } (x,t)\in\partial\Omega\times(0,1) \tag{10b}$$

Substituting (8) and (9) into (7) gives

$$\hat{J}'(u;v-u) = -\langle v-u, e_u^*(y,u)p\rangle + \eta\langle u, v-u\rangle = \langle \eta u - e_u^*(y,u)p, v-u\rangle \tag{11}$$

By the so-called first-order optimality condition, the minimization of $\hat{J}$ implies that $\hat{J}'(u;v-u) = 0$ holds all directional variable v, i.e.,

$$\langle \eta u - e_u^*(y,u)p, v-u\rangle = 0, \forall v.$$

Since $e_u^* = I$ (cf. (5)), this gives

$$\langle \eta u - p, v - u \rangle = 0, \forall v.$$

Hence, it must hold that $\eta u = p$, *i. e.*, $u = \frac{p}{\eta}$. Substituting this algebraic condition into the right hand-side of the first equation in (1b)

$\partial_t y - \mu \Delta y = -\frac{p}{\eta}$ follows. In summary, we get the following optimality system for (1a~1b):

$$\begin{cases} \partial_t y - \mu \Delta y = -\frac{p}{\eta}, & (x,t) \in \Omega \times (0,1), \\ y(x,0) = y(x,1), & x \in \Omega, \\ y(x,t) = 0, & (x,t) \in \partial\Omega \times (0,1), \end{cases}$$

$$\begin{cases} \partial_t p + \mu \Delta p = -(y - \bar{y}), & (x,t) \in \Omega \times (0,1), \\ p(x,0) = p(x,1), & x \in \Omega, \\ p(x,t) = 0, & (x,t) \in \partial\Omega \times (0,1) \end{cases} \tag{12}$$

When the co-state variable p is ready, the control variable u can be chosen as $u = \eta p$.

3 The algorithm

We now propose an iterative algorithm for solving (12) as follows.

$$\begin{cases} \partial_t y^{k+1} - \mu \Delta y^{k+1} = -\frac{p^k}{\eta}, \ (x,t) \in \Omega \times (0,1), \\ y^{k+1}(x,0) = y^{k+1}(x,1), \ x \in \Omega, \\ y^{k+1}(x,t) = 0, \ (x,t) \in \partial\Omega \times (0,1), \end{cases}$$

$$\begin{cases} \partial_t p^{k+1} + \mu \Delta p^{k+1} = -(y^{k+1} - \bar{y}), \\ \quad (x,t) \in \Omega \times (0,1), \\ p^{k+1}(x,0) = p^{k+1}(x,1), \ x \in \Omega, \\ p^{k+1}(x,t) = 0, \ (x,t) \in \partial\Omega \times (0,1) \end{cases} \tag{13}$$

where $k \geqslant 0$ is the iteration index and for $k=0$ we need to pick an initial guess $p^0(x,t)$ for the co-state variable. In practical computation, such an initial guess is chosen randomly subject to the periodic condition and the boundary condition. In (13), with $p^k(x,t)$ known from the previous iteration, we can first solve $y^{k+1}(x,t)$ from the first PDE and then solve $p^{k+1}(x,t)$ from the second PDE. The algorithm is therefore of the Gauss-Seidel type.

Both the first and second PDEs in (13) are time-periodic heat equations and many existing numerical methods can be directly applied. As an illustration, we consider the case $\Omega = (0,1)^d$ with $d=1,2,3$ as follows. By a mesh with m nodes and denoting the value of $y(x,t)$ (resp. $p(x,t)$) at the i-th node x_i by $y_i(t)$ (resp. $p_i(t)$), the discrete solution

$$y^{k+1}(t) \approx (y^{k+1}(x_1,t), \cdots, y^{k+1}(x_M,t))^T$$

and

$$p^{k+1}(t) \approx (p^{k+1}(x_1,t), \cdots, p^{k+1}(x_M,t))^T$$

satisfy

$$\begin{cases} \frac{\mathrm{d}\, y^{k+1}(t)}{\mathrm{d}t} + \mu A\, y^{k+1}(t) = -\frac{p^k(t)}{\eta}, t \in (0,T), \\ y^{k+1}(0) = y^{k+1}(t) \end{cases} \tag{14a}$$

and

$$\begin{cases} \frac{\mathrm{d}\, p^{k+1}(t)}{\mathrm{d}t} - \mu A\, p^{k+1}(t) = -(y^{k+1}(t) - \bar{y}(t)), \\ \quad t \in (0,T), \\ p^{k+1}(0) = p^{k+1}(t) \end{cases} \tag{14b}$$

where $\bar{y}(t) = (\bar{y}_1(t), \cdots, \bar{y}_M(t))^T$. The matrix A in (14) denotes an approximation of the negative Laplacian $-\Delta$ under homogeneous Dirichlet boundary conditions. A concrete example of the matrix A is the one derived through the centered finite difference scheme subjected with Dirichlet boundary condition:

$$\begin{cases} A = \Lambda_{\Delta x} := \frac{1}{\Delta x^2} \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{bmatrix}_{m \times m}, \ d=1, \\ A = I_x \otimes \Lambda_{\Delta x} + \Lambda_{\Delta x} \otimes I_x, \ d=2, \\ A = I_x \otimes I_x \otimes \Lambda_{\Delta x} + I_x \otimes \Lambda_{\Delta x} \otimes I_x + \Lambda_{\Delta x} \otimes I_x \otimes I_x, \ d=3 \end{cases} \tag{15}$$

where Δx denotes the mesh size, m denotes the number of spatial grids and $I_x \in \mathbf{R}^{M \times M}$ is the identity matrix with $M=m^d$ in the d-dimensional case ($d=1,2,3$). We can also consider other boundary conditions and spatial discretizations, such as finite element and finite volume, etc.

For temporal discretization, we consider the backward-Euler method for the state equation concerning $y^{k+1}(t)$ and the forward-Euler method for the co-state equation concerning $p^{k+1}(t)$. This numerical setting leads to the following full discrete formula:

$$\begin{cases} \dfrac{y_n^{k+1}-y_{n-1}^{k+1}}{\Delta t}+\mu A\, y_n^{k+1}=-\dfrac{p_n^k}{\eta}, \\ \quad n=1,2,\cdots,N_t, \\ y_0^{k+1}=y_{N_t}^{k+1} \end{cases} \tag{16a}$$

and

$$\begin{cases} \dfrac{p_n^{k+1}-p_{n-1}^{k+1}}{dt}-\mu A\, p_{n-1}^{k+1}=-(y_{n-1}^{k+1}-\bar{y}_{n-1}), \\ \quad n=N_t,N_t-1,\cdots,1, \\ p_0^{k+1}=p_{N_t}^{k+1} \end{cases} \tag{16b}$$

where Δt denotes the time step-size and $N_t=\dfrac{T}{\Delta t}$. Define

$$Y^k=(y_1^k,y_2^k,\cdots,y_{N_t}^k)^T,$$
$$P^k=(p_{N_t-1}^k,\cdots,p_1^k,p_0^k)^T,$$
$$\widetilde{Y}^k=(u_{N_t-1}^k,\cdots,u_1^k,u_0^k)^T,$$
$$\bar{Y}=(\bar{y}_{N_t-1},\cdots,\bar{y}_1,\bar{y}_0)^T,\widetilde{P}^k=(p_1^k,p_2^k,\cdots,p_{N_t}^k)^T$$

and

$$M=\begin{bmatrix} I+\mu\Delta tA & & & -I \\ -I & I+\mu\Delta tA & & \\ & \ddots & \ddots & \\ & & -I & I+\mu\Delta tA \end{bmatrix} \tag{17}$$

Then, we can represent (1b) as the following linear algebraic system:

$$\begin{cases} MY^{k+1}=-\dfrac{1}{\eta}\widetilde{P}^k, \\ MP^{k+1}=\widetilde{Y}^k-\bar{Y} \end{cases} \tag{18}$$

Note that the matrix M given by (17) takes the form of block circulant and therefore a p-cyclic SOR (successive over-relaxation) iterative method [17] can be applied as an inner solver to handle each of the two linear systems in (18), which yields very efficient computation of the two systems in (18).

4　Numerical examples

In this section, we present numerical results to validate the efficiency of the proposed iterative algorithm in Section 3. For all numerical results, the initial guess $p^0(x,t)$ for the proposed algorithm is chosen randomly under the periodic condition and the zero boundary condition. We consider the 1D case together with centered finite difference discretization for the Laplacian. We use the following data:

$$\bar{y}(x,t)=2\sin\left(7tx\arcsin\left(\frac{tx}{1+tx}\right)\right),\mu=1,$$
$$\eta=0.08,T=2.5 \tag{19}$$

With this data, the solution of the optimality system (12) $y(x,t)$ (left subfigure) and $p(x,t)$ (right subfigure) is shown in Fig. 1.

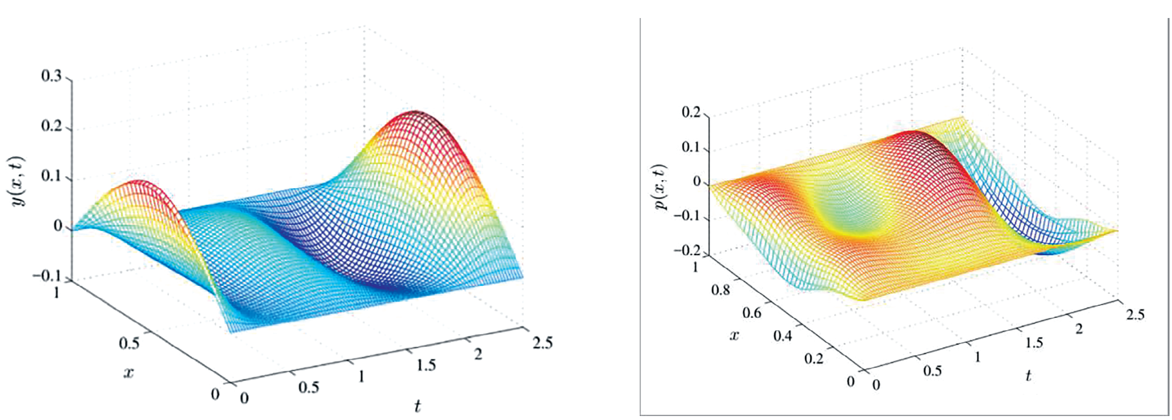

Fig. 1　Numerical solution of the optimality system (12) with the data given by (19)

We now study whether or not the convergence rate of the full discrete version of the proposed iterative algorithm in Section 3 is robust with respect to the discretization parameters Δt and Δx. In Fig. 2, we show the measured convergence rates of the algorithm in two situations: in the left subfigure we fix $\Delta t = 0.02$ and choose for Δx three values and in the right subfigure we fix $\Delta x = 0.025$ and choose for Δt three values. In both situations, we see clearly that the convergence rate is insensitive to the change of Δx and Δt.

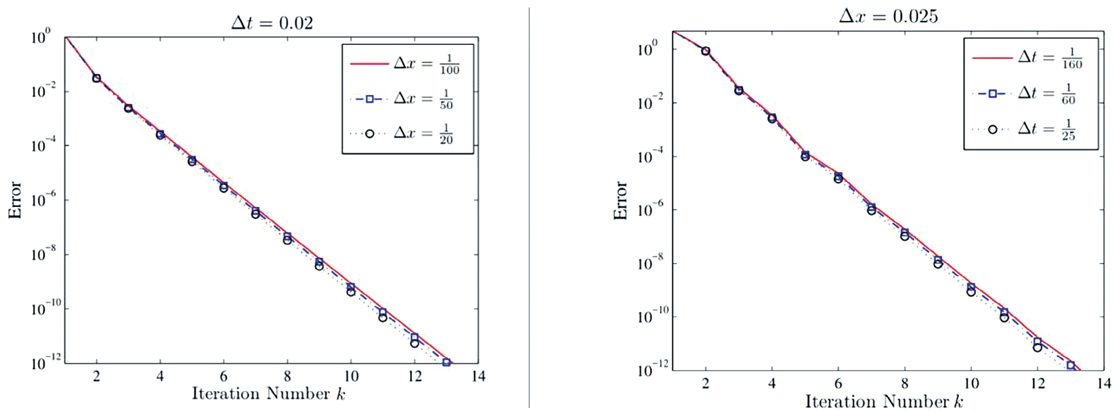

Fig. 2　Convergence rate of the iterative algorithm (18) with different space mesh size (left) and time step size (right)

5　Conclusions

We have proposed an iterative algorithm for solving the optimal control problems with time-periodic heat equations as the constraint. We first derive the optimality system of such an optimal control problem, which consists of two coupled time-periodic heat equations. Then we apply the Gauss-Seidel iteration to such an optimality system, that is to say, we firstly solve the state equation and then solve the co-state equation in an iteration pattern. The full discrete version of the proposed iterative algorithm is also presented. Numerical results indicate that the proposed algorithm possesses robust convergence rate with respect to both the space and the time discretization parameters.

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