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Handling state constraints and economics in feedback control of transport-reaction processes

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ABSTRACT

Transport-reaction processes, which are typically described by parabolic partial differential equations (PDEs), play an important role within the chemical process industries. Therefore, it is important to develop feedback control techniques that operate transport-reaction processes in an economically optimal fashion in the presence of constraints in the process states and manipulated inputs. Economic model predictive control (EMPC) is a predictive control scheme that combines process economics and feedback control into an integrated framework with the potential of improving the closed-loop process economic performance compared to traditional control methodologies. In this work, we focus on systems of nonlinear parabolic PDEs and propose a novel EMPC design integrating adaptive proper orthogonal decomposition (APOD) method with a high-order finite-difference method to handle state constraints. The computational efficiency and constraint handling properties of this design are evaluated using a tubular reactor example modeled by two nonlinear parabolic PDEs.

1. Introduction

The development of computationally efficient control methods for partial differential equation (PDE) systems has been a major research topic in the past 30 years (e.g., [6]). The design of feedback control algorithms for PDE systems is usually achieved on the basis of finite-dimensional systems (i.e., sets of ordinary differential equations (ODEs) in time) obtained by applying a variety of spatial discretization and/or order reduction methods to the PDE system. The classification of PDE systems, which is based on the properties of the spatial differential operator into hyperbolic, parabolic, or elliptic, typically determines the finite-dimensional approximation approaches employed to derive finite-dimensional models (e.g., [6,24]). A class of processes described by PDEs within chemical process industries is transport-reaction processes. For example, tubular reactors are typically described by parabolic PDEs since both convective and diffusive transport phenomena are significant.

For parabolic PDE systems (e.g., diffusion-convective-reaction processes) whose dominant dynamics can be adequately represented by a finite number of dominant modes, Galerkin's method with spatially global basis functions is a good way among many weighted residual methods (e.g., [9,21]) to construct a reduced-order model (ROM) of the PDE system. Specifically, it can be used to derive a finite-dimensional ODE model by applying approximate inertial manifolds (AIMs) (e.g., [10]) that capture the dominant dynamics of the original PDE system. The basis functions used in Galerkin's method may either be analytical or empirical eigenfunctions. After applying Galerkin's method to the PDE system and a low-order ODE system is derived, the control system can be designed by utilizing control methods for linear/nonlinear ODE systems [6].

One way to construct the empirical eigenfunctions is by applying proper orthogonal decomposition (POD) (e.g., [23,12,15]) to PDE solution data. This data-based methodology for constructing the basis eigenfunctions has been widely adopted in the field of model-based control of parabolic PDE systems (e.g., [5,25,4,17,15]). However, to achieve high accuracy of the ROM derived from the empirical eigenfunctions of the original PDE system, the POD method usually needs a large ensemble of solution data (snapshots) to contain as much local and global process dynamics as possible. Constructing such a large ensemble of snapshots becomes a significant challenge from a practical point of view; because currently, there is no general way to realize a representative ensemble. Based on this consideration, an adaptive proper orthogonal decomposition (APOD) methodology was proposed to recursively update the ensemble of snapshots and compute on-line the new empirical

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eigenfunctions in the on-line closed-loop operation of PDE systems (e.g., [20,22,26,19]). While the APOD methodology of [26,19] demonstrated its ability to capture the dominant process dynamics by a relatively small number of snapshots which reduces the overall computational burden, these works did not address the issue of computational efficiency with respect to optimal control action calculation and input and state constraint handling. Moreover, the ROM accuracy is limited by the number of the empirical eigenfunctions adopted for the ROM; in practice, when a process faces state constraints, the accuracy of the ROM based on a limited number of eigenfunctions may not be able to allow the controller to avoid a state constraint violation.

Economic model predictive control (EMPC) is a practical optimal control-based technique that has recently gained widespread popularity within the process control community and beyond because of its unique quality of effectively integrating process economics and feedback control (see [8] for an overview of recent results and references). It deals with a reformulation of the conventional MPC quadratic cost function in which an economic (not necessarily quadratic) cost function is used directly as the cost in MPC, and, it may, in general, lead to time-varying process operation policies (instead of steady-state operation), which directly optimize process economics. However, most of previous EMPC systems have been designed for lumped parameter processes described by linear/nonlinear ODE systems (e.g., [1,2,14,11,13]). In our previous work ([16,15]), an EMPC system with a general economic cost function for parabolic PDE systems was proposed which operates the closed-loop system in a dynamically optimal fashion. Specifically, the EMPC scheme was developed on the basis of low-order nonlinear ODE models derived through Galerkin's method using analytical eigenfunctions [16] and empirical eigenfunctions derived by POD [15], respectively. However, no work has been done on applying APOD techniques for model order reduction to parabolic PDE systems under EMPC. Typically, EMPC will operate a system at its constraints in order to achieve the maximum closed-loop economic performance benefit. Thus, the challenge is to formulate EMPC schemes that can handle state constraints (i.e., prevent state constraint violation).

Motivated by the above considerations, in this work, we apply APOD to parabolic PDE systems by considering process control system computational efficiency and some specific constraints imposed on the process (i.e., state and input constraints), and propose a novel EMPC design integrating APOD method with a high-order finite-difference method. The proposed EMPC method is applied to a non-isothermal tubular reactor where a second-order chemical reaction takes place and the computational efficiency, state and input constraint satisfaction, and closed-loop economic performance are evaluated.

2. Preliminaries

2.1. Parabolic PDEs

We consider parabolic PDEs of the form:

$$\frac{\partial x}{\partial t} = A\frac{\partial x}{\partial z} + B\frac{\partial^2 x}{\partial z^2} + Wu(t) + f(x) \tag{1}$$

with the boundary conditions:

$$\frac{\partial x}{\partial z}|_{z=0} = g_0 x(0, t), \quad \frac{\partial x}{\partial z}|_{z=1} = g_1 x(1, t) \tag{2}$$

for $t \in [0, \infty)$ and the initial condition:

$$x(z, 0) = x_0(z) \tag{3}$$

where $z \in [0, 1]$ is the spatial coordinate, $t \in [0, \infty)$ is the time, $x(z, t) = [x_1(z, t) \ldots x_{n_x}(z, t)]^T \in \mathbb{R}^{n_x}$ is the vector of the state variables (x^T denotes the transpose of x), and $f(x)$ denotes a nonlinear vector function. The notation A, B, W, g_0 and g_1 is used to denote (constant) matrices of appropriate dimensions. The control input vector is denoted as $u(t) \in \mathbb{R}^{n_u}$ and is subject to the following constraints:

$$u_{\min} \le u(t) \le u_{\max} \tag{4}$$

where u_{min} and u_{max} are the lower and upper bound vectors of the manipulated input vector, $u(t)$. Moreover, the system states are also subject to the following state constraints:

$$x_{i,\min} \le \int_0^1 r_{x_i}(z) x_i(z, t) dz \le x_{i,\max} \tag{5}$$

for $i = 1, \ldots, n_x$ where $x_{i,min}$ and $x_{i,max}$ are the lower and upper state constraint for the i-th state, respectively. The function $r_{x_i}(z) \in L_2(0, 1)$ where $L_2(0, 1)$ is the space of measurable square-integrable functions on the interval [0, 1], is the state constraint distribution function.

2.2. Galerkin's method with POD-computed basis functions

To reduce the PDE model of Eq. (1) into an ODE model, we take advantage of the orthogonality of the empirical eigenfunctions obtained from POD ([23,12]). Specifically, using Galerkin's method ([7,10]), a low-order ODE system for the PDEs of Eq. (1) describing the temporal evolution of the amplitudes corresponding to the first m_i eigenfunctions of the i-th PDE state in Eq. (1) has the following form:

$$\begin{aligned} \dot{a}_s(t) &= \mathcal{A}_s a_s(t) + \mathcal{F}_s(a_s(t)) + \mathcal{W}_s u(t) \\ x_i(z, t) &\approx \sum_{j=1}^{m_i} a_s^{ij}(t)\phi_{ij}(z), \quad i = 1, \ldots, n_x \end{aligned} \tag{6}$$

where $a_s(t) = [a_{s,1}^T(t) \ldots a_{s,n_x}^T(t)]^T$ is a vector of the total eigenmodes, $a_{s,i}(t) = [a_s^{i1}(t) \ldots a_s^{im_i}(t)]^T$ is a vector of the amplitudes of the first m_i eigenfunctions, $a_s^{ij}(t)$ is the $j-th$ eigenmode of $i-th$ PDE, $\mathcal{A}_s$ and $\mathcal{W}_s$ are constant matrices, $\mathcal{F}_s(a_s(t))$ is a nonlinear smooth vector function of the modes obtained by applying weighted residual method to Eq. (1), and $\{\phi_{ij}(z)\}_{j=1:m_i}$ are the first m_i dominant empirical eigenfunctions computed from POD for the i-th PDE state, $x_i(z, t)$.

3. EMPC of parabolic PDE systems with state and control constraints

3.1. Adaptive proper orthogonal decomposition

Compared with POD, APOD is a more computationally efficient algorithm because it only needs an ensemble of a small number of snapshots in the beginning. It can complete the recursive update of the computation of the dominant eigenfunctions, while keeping the size of the ensemble small to reduce the computational burden of updating the ensemble once a new process state measurement is available. Moreover, APOD can also adaptively adjust the number of the basis eigenfunctions under a desired energy occupation requirement, η. Out of N possible eigenvalues from the covariance matrix of the ensemble, the most dominant m eigenvalues of the covariance matrix occupies η energy of the whole ensemble, i.e., $\sum_{j=1}^{m}\lambda_j / \sum_{j=1}^{N}\lambda_j \le \eta$. Then, the computational efficiency of the control system whose construction is based on the ROM with the dominant eigenfunctions will be improved due to the adaptive property of APOD [26]. Since the basis eigenfunctions are