

Predictive control of PDEs via using adaptive reduced order modeling

Sivakumar Pitschaiah and Antonios Armaou[†], *Senior Member IEEE & AIChE*

Abstract—This work employs adaptive reduced order models (ROMs) in the design of model predictive controllers for stabilization of processes that are mathematically expressed as parabolic partial differential equation (PDE) systems. Initially, we construct a locally valid ROM of the PDE system employing the basis functions computed by applying an adaptive model reduction methodology called APOD on a small data ensemble. This ROM is then utilized in the design of model predictive controllers (MPC) under constraints on the control action. As periodic closed-loop process data becomes available (during closed-loop operation under the constructed MPC), we recursively update the ROM by employing our computationally efficient adaptive model reduction methodology thus extending the validity of ROM over the current operating region. The effects of employing the adaptive methodology on performance of MPC is studied. The design of such MPC controllers is illustrated by employing the methodology on numerical simulations.

I. INTRODUCTION

A significant research effort in recent years has focused on designing efficient tools for both the analysis and control of spatially varying processes that can be mathematically expressed as nonlinear distributed parameter systems (DPS). The research activity in this area has been motivated by a wealth of industrially important processes (e.g., chemical vapor deposition & etching, catalytic reaction & polymerization processes) [4] which exhibit significant spatial variations due to the presence of strong diffusive and convective mechanisms. Such distributed chemical processes with significant diffusive phenomena can be described by systems of linear/nonlinear parabolic partial differential equations (PDEs). The long-term dynamic behavior of such parabolic PDEs is characterized by a finite-number of degrees of freedom [15]. An important issue in the design of controllers for PDE system is the presence of constraints in the process operation.

Model predictive control (MPC), also known as receding horizon control, is one of the powerful tools for handling these process constraints with an optimal control setting. Even though most of the research in MPC seems to be focused on systems modeled by ODEs, the question of MPC designs for PDEs [6] is also gaining interest in the research community. Motivated by this, Galerkin's method was successfully used to derive ROMs, leading to MPC designs that were computationally less expensive [5], [11], [10]. However, the above formulation of ROMs cannot be directly applied to systems which have nonlinear spatial

differential operators or complicated spatial domains as one cannot obtain the required eigenfunctions analytically.

To overcome this limitation researchers have focused on data-driven methods such as proper orthogonal decomposition (POD) also known as the method of snapshots [14], [8]. This method has been widely used in model reduction [7], [9], optimization [16] and geometric control [1], [13] of distributed processes without considering process constraints. Above data-driven methods though assume an *a priori* availability of a large ensemble of snapshots to correctly capture the incidence of new trends during the process evolution using the basis functions computed off-line from that snapshot ensemble. However, generating such an ensemble is not straightforward (and experimentally infeasible) as it necessitates using suitably designed inputs to excite all the modes [7]. Furthermore, currently no methodology exists to synthesize such an ensemble.

Recently, we presented a methodology in [12], [18] to recursively compute empirical eigenfunctions of a given PDE system in a computationally inexpensive and robust way and derive reduced order models for control purposes. This approach is based on the computation of an approximation of the eigenspace of the covariance matrix corresponding to its significant eigenvalues. This dominant eigenspace is updated recursively as new snapshots from the process are added to the ensemble, simultaneously increasing or decreasing its dimensionality if required. In this work, we extend the previous method by designing MPC controllers, that respect the process constraints, to stabilize the processes than can be modeled by nonlinear parabolic partial differential equation systems. We utilize the adaptive model reduction methodology for the design and update of ROM. This updated ROM is then utilized in the design and implementation of MPC controllers. Note that we do not require the availability of spectral eigenfunctions or well constructed data ensemble (see [13], [17]) as required in the literature. Rather we recursively update the initially computed ROM of the process, using the closed-loop measurements of the process.

II. MATHEMATICAL PRELIMINARIES

We focus on designing model predictive controllers for nonlinear parabolic PDEs of the following form:

$$\frac{\partial \bar{x}}{\partial t} = \mathcal{L}(\bar{x}) + b(z)u + f(\bar{x}). \quad (1)$$

subject to the following boundary and initial conditions:

$$q \left(\bar{x}, \frac{d\bar{x}}{d\eta}, \dots, \frac{d^{n_o-1}\bar{x}}{d\eta^{n_o-1}} \right) = 0 \text{ on } \Gamma \quad (2)$$

$$\bar{x}(z, 0) = \bar{x}_0(z)$$

Financial support from the National Science Foundation, CAREER Award # CBET 06-44519 is gratefully acknowledged.

[†]Department of Chemical Engineering, The Pennsylvania State University, University Park, PA 16802, USA, Tel: (814) 865-5316, Email: armaou@engr.psu.edu.

and the following input constraints

$$u^{min} \leq u \leq u^{max} \quad (3)$$

where $\bar{x}(z, t) \in \mathbb{R}^n$ denotes the vector of state variables, $z = [z_1, z_2, z_3] \in \Omega \subset \mathbb{R}^3$ is the vector of spatial coordinates, $u \in \mathbb{R}^l$ denotes the vector of manipulated inputs; u^{min} and u^{max} denotes the lower and upper bounds on the manipulated input, Ω is the domain of definition of the process and Γ is its boundary. $\mathcal{L}(\bar{x})$ is a dissipative, possibly nonlinear, spatial differential operator, $f(\bar{x})$ is a nonlinear vector function, $q(\bar{x}, \frac{d\bar{x}}{d\eta}, \dots, \frac{d^{n_o-1}\bar{x}}{d\eta^{n_o-1}})$ is a nonlinear vector function which is assumed to be sufficiently smooth, $\frac{d\bar{x}}{d\eta}|_{\Gamma}$ denotes the derivative in the direction perpendicular to the boundary and $\bar{x}_0(z)$ is the initial condition. $b(z) \in \mathbb{R}^l$ is a known vector of z of the form $[b_1(z) b_2(z) \dots b_l(z)]$, where $b_i(z)$ describes how the i^{th} control action $u_i(t)$ is distributed in the spatial domain Ω .

The parabolic PDE system of Eq. 1 can be recast as an infinite dimensional system in an appropriate Hilbert space $\mathcal{H}(\Omega, \mathbb{R}^n)$, \mathcal{H} being the space of n -dimensional vector functions defined on Ω that satisfy the boundary conditions in Eq. 2.

$$\mathcal{H} = \left\{ x \in L_2[\Omega, \mathbb{R}^n]; q\left(x, \frac{dx}{d\eta}, \dots, \frac{d^{n_o-1}x}{d\eta^{n_o-1}}\right) = 0 \text{ on } \Gamma \right\} \quad (4)$$

We define the inner product and norm in \mathcal{H} as follows:

$$(\phi_1, \phi_2) = \int_{\Omega} \phi_1^*(z) \phi_2(z) dz, \|\phi_1\|_2 = (\phi_1, \phi_1)^{1/2} \quad (5)$$

where $\phi_1, \phi_2 \in \mathcal{H}[\Omega, \mathbb{R}^n]$. Defining the state function x on \mathcal{H} as $x(t) = \bar{x}(z, t), t > 0, z \in \Omega$, the operator \mathcal{A} in $\mathcal{H}[\Omega, \mathbb{R}^n]$ as $\mathcal{A}(x) = \mathcal{L}(\bar{x})$, the input, controlled output and measured output operators as $\mathcal{B}u = bu$, the system of Eqs. 1-2 acquires the following form in the Hilbert space, \mathcal{H} :

$$\dot{x} = \mathcal{A}(x) + \mathcal{B}u + f(x), x(0) = x_0 \quad (6)$$

$$u^{min} \leq u \leq u^{max}.$$

where $f(x) = f(\bar{x}(z, t))$ and $x_0 = \bar{x}_0(z)$.

Assumption 1: The long-term dynamics of the above PDE system is finite dimensional.

III. FORMULATION AND UPDATE OF ROM

In this section, we formulate and update the ROM for the system in Eqs.1-2 using an adaptive model reduction methodology which we name APOD. We initially compute the empirical basis functions, by employing APOD off-line on the available off-line process data of Eq.1-2. We utilize these basis functions in a Galerkin method framework to derive the ROM for the above system. The validity of these models is confined to a small region of the entire state space, $\mathcal{H}(\Omega)$, spanned by the available initial process data. During the closed loop process evolution APOD updates these models (using the closed loop process data) extending the region of validity of these models. These updated ROMs will be utilized in the section IV for the design of model predictive controllers to stabilize the processes in Eqs.1-2.

A. Computation of initial basis functions

We use the initially available collection of off-line data snapshots of the system in Eqs. 1-2 to construct the initial basis functions using proper orthogonal decomposition. We first construct the covariance matrix C_N [12] then solve the following eigenvalue-eigenvector problem

$$C_N \Psi = \lambda \Psi$$

to compute N eigenvalues. We partition the eigenspace of the covariance matrix, C_N , into two subspaces; the dominant one containing the modes which capture at least ε percent of energy in the ensemble (denoted as \mathbb{P}) and the orthogonal complement to \mathbb{P} containing the rest of the modes (denoted as \mathbb{Q}). Such a partition is possible due to the fact that the dominant dynamics of dissipative PDEs are finite (typically small) dimensional [15]. Note that we define ε as the percentage energy of the ensemble captured by dominant eigenfunctions. We assume that out of N possible eigenvectors of C_N , m have the corresponding eigenvalues such that $\sum_{i=1}^m \lambda_i / \sum_{i=1}^N \lambda_i \leq \frac{\varepsilon}{100}$; m eigenmodes of C_N capture ε percent of energy in the ensemble. These eigenvectors are then used in the following equation

$$\phi_i(z) = \sum_k \Psi_i^k v_k(z), i = 1, \dots, m.$$

to compute N eigenfunctions; here ϕ_i represents the i^{th} eigenfunction and Ψ_i^k is the k^{th} eigenvector of C_N . An orthonormal basis for the subspace \mathbb{P} can be obtained as:

$$Z = [\Psi_1, \Psi_2, \dots, \Psi_m], Z \in \mathbb{R}^{N \times m} \quad (7)$$

where $\Psi_1, \Psi_2, \dots, \Psi_m$ denote the eigenvectors of C_N that correspond to the eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_m$. Note that the eigenfunctions computed by these eigenvectors capture the dominant dynamics of the PDE system of Eq.1-2. The orthogonal projection operators P and Q onto subspaces \mathbb{P} and \mathbb{Q} can be computed as

$$P = ZZ^T, Q = I - ZZ^T \quad (8)$$

where I denotes the identity matrix of dimension N .

B. Derivation of ROM

In this section, we derive a locally valid ROM of the system of Eq. 6 using the above local basis functions. Using assumption 1, the Hilbert space \mathcal{H} is partitioned into two subspaces \mathcal{H}_s & \mathcal{H}_f respectively. \mathcal{H}_s includes the slow evolving modes whereas \mathcal{H}_f includes fast evolving stable process modes. Clearly $\mathcal{H} = \mathcal{H}_s \oplus \mathcal{H}_f$ and \mathcal{H}_f is an infinite-dimensional subspace, while \mathcal{H}_s is a finite-dimensional one. Using the orthogonal projection operator Q the state $x \in \mathcal{H}(\Omega)$ can be decomposed as $x_s = Px \in \mathcal{H}_s$ and $x_f = Qx \in \mathcal{H}_f$. The state x of the system of Eq. 6 now can be expressed as:

$$x = x_s + x_f = Px + Qx \quad (9)$$

Applying projection operators \mathcal{P} and \mathcal{Q} to the system of Eq. 6 and using the above decomposition of x the system of Eq. 6 can be equivalently expressed as:

$$\begin{aligned} \frac{dx_s}{dt} &= \mathcal{A}_s(x_s, x_f) + \mathcal{B}_s u + f_s(x_s, x_f) \\ \frac{\partial x_f}{\partial t} &= \mathcal{A}_f(x_s, x_f) + \mathcal{B}_f u + f_f(x_s, x_f) \\ y_c &= Cx_s + Cx_f, y_m = S_m x_s + S_m x_f \\ x_s(0) &= Px(0) = Px_0, x_f(0) = Qx(0) = Qx_0 \end{aligned} \quad (10)$$

where $\mathcal{A}_s = \mathcal{P}\mathcal{A}(x_s + x_f)$, $\mathcal{B}_s = \mathcal{P}\mathcal{B}$, $f_s = \mathcal{P}f$, $\mathcal{A}_f = \mathcal{Q}\mathcal{A}(x_s + x_f)$, $\mathcal{B}_f = \mathcal{Q}\mathcal{B}$ and $f_f = \mathcal{Q}f$ and the notation $\partial x_f / \partial t$ is used to denote that the state x_f belongs in an infinite dimensional subspace (\mathcal{H}_f).

Using singular perturbation arguments for infinite dimensional systems [4], we neglect the infinite dimensional fast and stable x_f subsystem in Eq. 10. The following m -dimensional x_s subsystem is obtained:

$$\begin{aligned} \frac{dx_s}{dt} &= \mathcal{A}_s(x_s, 0) + \mathcal{B}_s u + f_s(x_s, 0) \\ x_f &\equiv 0 \end{aligned} \quad (11)$$

Under the assumptions already stated, the above finite dimensional system is an accurate approximation of the dominant dynamics of the infinite dimensional system of Eq. 6.

Note that we use the basis functions, ϕ , computed in step A to define the subspaces \mathcal{H}_s & \mathcal{H}_f , i.e., $\mathcal{H}_s = \text{span}\{\phi_1, \phi_2, \dots, \phi_m\}$ and $\mathcal{H}_f = \mathcal{H} \setminus \mathcal{H}_s$. As these basis functions have a small range of validity the ROM (Eq. 11) computed using these basis functions may not remain valid during the course of closed-loop process evolution. To avoid this situation, we periodically update the basis functions, ϕ , using APOD thus extending it's validity over the current operational space.

C. Online refinement of ROM

To ensure the validity of the ROM in Eq. 11 during the closed-loop process evolution, we update [12] the ROM using "periodically" available closed-loop snapshots. Initially, the closed-loop snapshots are used to update the orthonormal basis for the subspace \mathbb{P} possibly by increasing or decreasing the size of the basis if required and by maintaining the accuracy of the basis by performing orthogonal power iteration. We then use these updated basis functions to update the ROM in Eq. 11. We maintain that the extra work required for the above process is small as long as the dimension of \mathbb{P} is small (a fact that is expected for parabolic PDEs).

The algorithm outlined below computes an approximation to Z without requiring the solution of the eigenvalue-eigenvector problem of the covariance matrix, C_N . To simplify the algorithm, we also assume that the dimensionality of the covariance matrix C_N remains constant. This is achieved by discarding the oldest snapshot from the ensemble as a new one is obtained. As a new snapshot from the process becomes available, the subspace \mathbb{P} may change in the following three ways:

- The dimension of the dominant subspace \mathbb{P} may increase i.e., one mode corresponding from \mathcal{Q} becomes

necessary to capture the desired percentage of energy in the ensemble. This is ascertained by monitoring the contribution of the dominant eigenvalue of $c_q = \mathcal{Q}C_N\mathcal{Q}$, which is the eigenvalue λ_{m+1} of C_N towards the total energy of the ensemble, i.e.,

$$\xi = \frac{\lambda_{m+1}}{\sum_{i=1}^{m+1} \lambda_i}$$

If ξ increases to more than $(100 - \epsilon)$ percent we append Z , the basis of subspace \mathbb{P} , with the corresponding eigenvector associated with λ_{m+1} .

- Some of the eigenmodes of the subspace \mathbb{P} may no longer be necessary to capture the required ϵ percent of the energy. In this case, the basis Z should be updated and its dimension should be simultaneously decreased. To test this the following $m \times m$ matrix $H = Z^T C_N Z$ is introduced. If only \hat{m} , with $\hat{m} < m$, eigenvalues of H are dominant then the basis Z is updated and its dimension is decreased.
- The dimensionality of \mathbb{P} remains unchanged. However the basis Z is updated, whenever the current basis is not accurate, to maintain the accuracy of the basis. The following one step power iteration $Z = \text{orth}(C_N Z)$ is executed (if necessary after analyzing the accuracy of the current basis) to maintain the accuracy of the basis after each addition of a snapshot.

Based on the new values of Z , we now compute the revised basis functions $\phi_1, \phi_2, \dots, \phi_m$ as a linear combination of the snapshots given by the following equation

$$\phi_i(z) = \sum_{k=1}^N \psi_i^k v_k(z), \quad i = 1, \dots, m \quad (12)$$

where ψ_i^k denotes the k^{th} element of vector ψ_i and $\{v_k\}_{k=1}^N$ is the collection of N snapshots. These updated basis functions are then utilized to update the ROM of Eq.11. In between the periodic updates of ROM, we assume that the updated ROM computed in Eq. 11 remains as a valid representation of the original system in Eq. 6.

IV. DESIGN OF MODEL PREDICTIVE CONTROLLERS

In this section, we utilize the recursively updated ROMs in the synthesis of model predictive controllers to stabilize the system given by Eqs. 1-2. We assume that the full state measurements from the process becomes available periodically. The control law is obtained by formulating and solving the following open-loop optimal control problem with a receding control horizon.

$$u^o = \arg \min_u J(x_s, u)$$

s. t.

$$\frac{dx_s}{dt} = \mathcal{A}_s(x_s, 0) + \mathcal{B}_s u + f_s(x_s, 0), x_s(t_0) = Px_0, \quad (13)$$

$$u \in \mathcal{U},$$

We employed a standard performance index J

$$J(x_s, u) = \int_t^{t+T_p} (q_s \|x_s\|_2^2 + u^T R u) d\tau + g_s (x_s(t+T_p))^2 \quad (14)$$

where T_p denotes the prediction horizon, q_s & g_s are strict positive numbers. \mathcal{U} denotes the set of admissible input values which is assumed to be compact. Thus $\mathcal{U} = \{u(t) \in \mathbb{R}^l : u_i^{min} \leq u(t) \leq u_i^{max}, i = 1, \dots, l\}$, where u_i^{min} & u_i^{max} are the maximum & minimum bounds on u_i .

We discretize the temporal domain into m_t intervals with a step length of $\delta t_i = t_i - t_{i-1}$, $\forall i = 1, \dots, m_t$. The control action $u(t)$ is then expressed as a series of the form

$$u(t) = \sum_{i=0}^{m_t-1} u_{i+1} [H(t-t_i) - H(t_{i+1}-t)] \quad (15)$$

where $H(\cdot)$ is the standard Heaviside function. Using control vector parametrization (CVP) methodology and the above discretized form of the control vector, we reformulate the dynamic optimization problem in Eq.13 as an algebraic nonlinear one. CVP involves the temporal discretization of the control vector only, and the solution of the dynamic equality constraints through direct integration, keeping track of constraint violations during the process evolution [19]. Solution of the optimization problem yields an optimal input sequence u^o at each sampling instance and only the first input vector in the sequence is actually implemented. Subsequently, the prediction horizon is moved forward by one time-step, and the above problem is re-solved using new process measurements.

V. APPLICATIONS

A. Application 1 - Diffusion-reaction processes

In this section, we apply the proposed adaptive model reduction and control methodology to a typical diffusion-reaction process that exhibits nonlinear dynamic behavior. Specifically, we consider an elementary exothermic reaction $A \rightarrow B$ taking place on a thin catalytic rod. The temperature of the rod is adjusted by means of an actuator located along the length of the rod. Assuming that the reactant A is present in excess, the spatial profile of the dimensionless temperature of the rod is described by the following parabolic PDE:

$$\frac{\partial x}{\partial t} = \frac{\partial}{\partial z} \left(k(x) \frac{\partial x}{\partial z} \right) + \beta_T(z) (e^{-\gamma/(1+x)} - e^{-\gamma}) + \beta_U (b(z)u(t) - x) \quad (16)$$

subject to the following boundary conditions:

$$x(0, t) = 0, x(\pi, t) = 0 \quad (17)$$

and the initial condition $x(z, 0) = x_0(z)$.

Here x denotes the dimensionless rod temperature, z is the spatial coordinate along the axis of the rod, $\beta_T(z)$ denotes the dimensionless heat of reaction and is an explicit function of the spatial coordinate z , γ denotes the dimensionless activation energy, β_U denotes the dimensionless heat transfer coefficient, $u(t)$ denotes the magnitude of actuation, and $b(z)$ accounts for the spatial profile of the actuator. A spatially distributed actuator with $b(z) = H(z - 0.3\pi) - H(z - 0.6\pi)$,

where $H(\cdot)$ again denotes the standard Heaviside function, was considered. The nominal values and expressions of the process parameters used in the presented simulations are: $k = 0.5 + 0.7/(x+1)$, $x_0(z) = 0.5$, $\beta_T(z) = 13[\cos(z) + 1]$, $\gamma = 2$, and $\beta_U = 2$. Figure 1(a) presents the evolution of the PDE for $u(t) = 0$ from an initial condition of $x(z, 0) = 0.5$. It is observed that the system evolves away from the above steady-state to another steady-state characterized by a non-uniform distribution of temperature across the rod. Hence, we conclude that the steady-state $x(z, t) = 0$ is an unstable one. As a result we formulate the control problem as the one that stabilizes the rod temperature around the spatially open-loop unstable steady-state. We initially collected an ensemble of 100 open-loop snapshots of the system of Eq.16 with $u(t) = 0$, without performing an exhaustive sampling of the state-space of the PDE. This ensemble of snapshots is presented in Figure 1(a). Applying the APOD step resulted in a single dominant basis function which captured more than 99% of the energy embedded in the ensemble.

We utilized the MPC formulation presented in section IV to stabilize the unsteady steady-state $x(z, t) = 0$. A prediction horizon of $T_p = 6$, with time step $\delta t = 0.25$ and penalty parameters $q_s = 100$, $R = 20$, $g_s = 300$ were used. $\mathcal{U} = \{u(t) \in \mathbb{R}^1 : -0.6 \leq u(t) \leq 0.6\}$. The control vector was discretized using $m_t = 4$ intervals over a control horizon of $T_c = 4$ and the resulting discretized control vector was utilized for the solution of the above optimization problem using CVP methodology. The optimization problem was solved using the MATLAB subroutine `fmincon`. The first input vector from the obtained optimal control sequence u_o was actually implemented in the plant Eq.16. Subsequently, the prediction horizon was moved forward by one time-step, the ROM was updated by using the obtained closed-loop measurement & APOD methodology and the above optimization problem was re-solved using the new ROM & process measurements. Figure 1(b) presents the closed-loop profile of the state $x(z, t)$; it is clear that the controller successfully drives the process to the spatially uniform steady state of $x(z, t) = 0$. Figure 2(a) presents the corresponding control action that drives the process to the steady state. We note that the computed control action stays within the constraint set \mathcal{U} . We also observe that the objective function J (computed at discrete time-steps of $t = 0.25$) converges to zero upon the achievement of the desired control objective.

As more process measurements from the closed-loop operation were included in the ensemble while simultaneously old snapshots were removed, a new basis function became dominant and joined the dominant eigenspace \mathbb{P} at $t = 0.75$. Consequently, the dimensionality of the ROM of Eq.16 increased from $m = 1$ to $m = 2$. Following the update of ROM the constraints of the MPC were revised and the optimization problem in section IV was re-solved using the new ROM & new process measurements.

To test the robustness of the methodology, we varied the process parameters, initial conditions and actuator distribution functions. In all the cases the process successfully converged to desired steady state. Figure 2(b) presents the

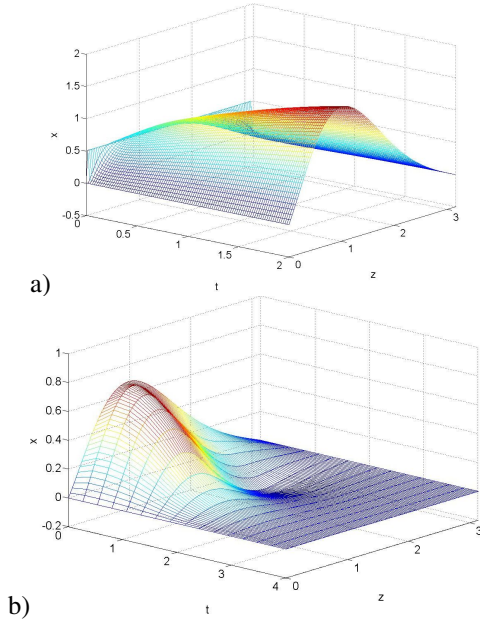


Fig. 1. a) Open-loop profile of the state of the diffusion-reaction process (Eq.16). b) Closed-loop profile of the state of the diffusion-reaction process (Eq.16).

computed control action for a -12.5% variation in β_T and -20% variation in initial condition. We observe that in the both cases the system is driven to the spatially uniform steady state $x(z,t) = 0$ faster and with less control action, since in these two cases the effect of destabilizing nonlinearity is smaller in the first case of variation in β_T and in the second case the system starts closer to the spatially uniform steady state.

B. Application 2 - Wave suppression

In this section, we illustrate the proposed methodology to Kuramoto-Sivashinsky equation (KSE) with distributed actuation.

$$\frac{\partial x}{\partial t} = -v \frac{\partial^4 x}{\partial z^4} - \frac{\partial^2 x}{\partial z^2} - x \frac{\partial x}{\partial z} + \sum_{i=1}^l b_i u_i(t) \quad (18)$$

subject to the periodic boundary conditions:

$$\frac{\partial^j x}{\partial z^j}(-\pi, t) = \frac{\partial^j x}{\partial z^j}(\pi, t), j = 0, \dots, 3 \quad (19)$$

and the initial condition

$$x(z, 0) = x_0(z) \quad (20)$$

where the x is the state of the system $x \in \mathcal{H}([-\pi, \pi], \mathbb{R})$ and is considered to be sufficiently smooth (i.e., differentiable 4 times), z is the spatial coordinate, t is the time and $u_i(t)$ is the i^{th} manipulated input. The spatial differential operator of system of Eq. 1, for this problem is of the form:

$$\mathcal{A}(x) = -v \frac{\partial^4 x}{\partial z^4} - \frac{\partial^2 x}{\partial z^2} - x \frac{\partial x}{\partial z} \quad \left\{ x \in \mathcal{H}([-\pi, \pi], \mathbb{R}); \frac{\partial^j x}{\partial z^j}(-\pi) = \frac{\partial^j x}{\partial z^j}(\pi), j = 0, \dots, 3 \right\} \quad (21)$$

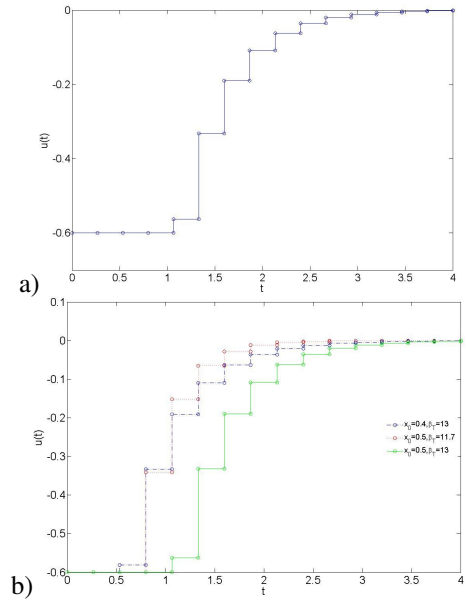


Fig. 2. a) Temporal profile of the control action. b) Temporal profile of the manipulated control action for nominal parameters and for -20% variation of the initial condition and for a -12.5% variation of β_T .

where the length of the spatial domain is 2π and the diffusion parameter in Eq. 18 was set as $v = 0.25$. Three control actuators were assumed to be available at the following locations $L = [0.4\pi, 0.6\pi, -0.3\pi]$; the corresponding spatial distribution functions at these locations are $b_i(z) = \delta(z - L_i); i = 1, \dots, 3$. In these simulation runs, the following spatially non-uniform initial condition was considered:

$$x_0 = \sum_{i=1}^4 \sin(iz)$$

Figure 3(a), presents the wave pattern observed in the open-loop evolution of KSE wherein we observe the formation of persistent waves. Thus the control objective was set to stabilize the process in a optimal way in the neighborhood of the spatially uniform steady state $x(z,t) = 0$.

For the design of controller, an initial ensemble of 100 open-loop snapshots ($N = 100$) was collected by simulating the process with $u(t) \equiv 0$ till $t = 2$. Note that no exhaustive sampling of state space as performed in [2] was not required. Application of POD to this ensemble resulted in $m = 3$ basis functions that captured 99.99% of the energy of the ensemble. These basis functions were then employed in the computation of the local ROM (Eq. 11) for the above process.

We then utilized the MPC formulation presented in section IV to stabilize the unsteady steady-state $x(z,t) = 0$. A prediction horizon of $T_p = 7$, with the time step $\delta t = 0.2$ and $q_s = 100$, $R = 20I^{3 \times 3}$, $g_s = 300$ were used. $\mathcal{U} = \{u(t) \in \mathbb{R}^3 : -3 \leq u_i(t) \leq 3, i = 1 \dots 3\}$.

Figure 3(b) presents the closed-loop profile of the state $x(z,t)$; the controller successfully drives the process to a neighborhood around the spatially uniform steady state of $x(z,t) = 0$ in a finite time. Figure 4(a) presents the corresponding control action that drives the process to the steady

state. We note that the computed control action stays within the constraint set \mathcal{U} . Also the value of the objective function

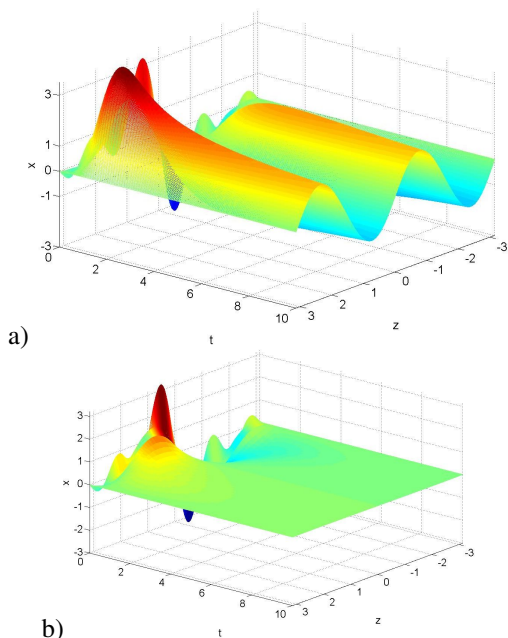


Fig. 3. a) Open-loop profile of the state of the diffusion-reaction process (Eq.18). b) Closed-loop profile of the state of the diffusion-reaction process (Eq.18).

J converges to zero upon achieving the control objective (Figure 4(b)).

APOD increases the dimensionality of ROM from 3 to 4 at $t = 0.6$ as more basis functions were needed to capture the emerging new trends of the closed-loop process. To maintain the accuracy of the basis functions and the ROM we updated the ROM using the step 3 of the APOD methodology (section III C).

We also stabilized the above KSE process using a lower energy criterion of 99%. For this case APOD was found to have a superior performance compared to just utilizing POD methodology. For the reasons of brevity we do not present these results in this manuscript. Further reduction of ϵ lead to deterioration of performance. However the MPC controller designed based on APOD still stabilized the process while a POD designed one failed.

REFERENCES

- [1] A. ARMAOU AND P. D. CHRISTOFIDES, *Wave suppression by nonlinear finite-dimensional control*, Chem. Eng. Sci., 55 (2000), pp. 2627–2640.
- [2] ———, *Dynamic optimization of dissipative PDE systems using nonlinear order reduction*, Chem. Eng. Sci., 57 (2002), pp. 5083–5114.
- [3] E. BALSACANTO, A. A. ALONSO, AND J. R. BANGA, *Dynamic optimization of complex distributed process systems*, Chem. Eng. R&D., 83 (2005), pp. 724–729.
- [4] P. D. CHRISTOFIDES, *Nonlinear and Robust Control of PDE Systems*, Birkhäuser, New York, 2001.
- [5] S. DUBLJEVIC, P. MHASKAR, N. H. EL-FARRA, AND P. D. CHRISTOFIDES, *Predictive control of parabolic pdes with state and control constraints*, Int. J. Rob. & Nonl. Contr., 16 (2006), pp. 749–772.

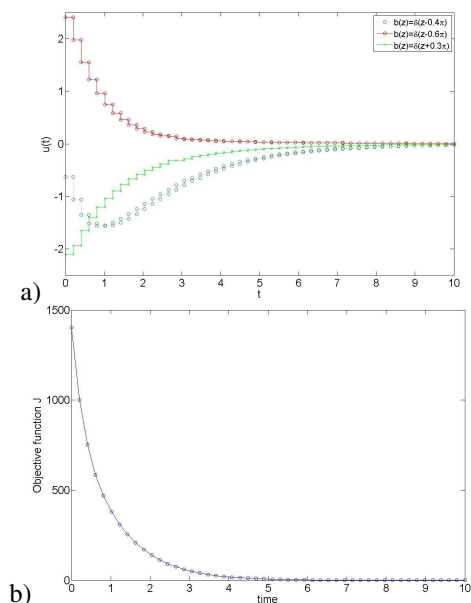


Fig. 4. a) Temporal profile of the manipulated control action with 3 control actuators. b) Temporal profile of the MPC objective function. b)Temporal profile of the dimensionality of the ROM

- [6] P. DUFOUR, Y. TOURE, D. BLANC, AND P. LAURENT, *On nonlinear distributed parameter model predictive control strategy: on-line calculation time reduction and application to an experimental drying process*, Comp. & Chem. Eng., 27 (2003), pp. 1533–1542.
- [7] M. D. GRAHAM AND I. G. KEVREKIDIS, *Alternative approaches to the Karhunen-Loève decomposition for model reduction and data analysis*, Comp. & Chem. Eng., 20 (1996), pp. 495–506.
- [8] P. HOLMES, J. L. LUMLEY, AND G. BERKOOZ, *Turbulence, Coherent Structures, Dynamical Systems and Symmetry*, Cambridge University Press, New York, 1996.
- [9] C. HOMESCU, L. R. PETZOLD, AND R. SERBAN, *Error estimation for reduced-order models of dynamical systems*, SIAM Review., 49 (2007), pp. 277–299.
- [10] Y. LOU, G. HU, AND P. D. CHRISTOFIDES, *Model predictive control of nonlinear stochastic pdes with application to a sputtering process*, AIChE J., 54 (2008), pp. 2065–2081.
- [11] M. MAHMOOD AND P. MHASKAR, *Safe-parking framework for fault-tolerant control of transport-reaction processes*, Ind. Eng. Chem. Res., 49 (2010), pp. 4285–4296.
- [12] S. PITCHAI AH AND A. ARMAOU, *Output feedback control of distributed parameter systems using adaptive proper orthogonal decomposition*, Ind. & Eng. Chem. Res., 49 (2010), pp. 10496–10509.
- [13] S. Y. SHVARTSMAN AND I. G. KEVREKIDIS, *Nonlinear model reduction for control of distributed systems: a computer-assisted study*, AIChE J., 44 (1998), pp. 1579–1595.
- [14] L. SIROVICH, *Turbulence and the dynamics of coherent structures: part I, II and III*, Quarterly of Applied Mathematics, XLV (1987), pp. 561–590.
- [15] R. TEMAM, *Infinite-Dimensional Dynamical Systems in Mechanics and Physics*, Springer-Verlag, New York, 1988.
- [16] A. THEODOROPOULOU, R. A. ADOMAITIS, AND E. ZAFIRIOU, *Model reduction for optimization of rapid thermal chemical vapor deposition systems*, IEEE Transactions on Semiconductor Manufacturing, 11 (1998), pp. 85–98.
- [17] A. VARSHNEY AND A. ARMAOU, *Multiscale optimization using hybrid PDE/kMC process systems with application to thin film growth*, Chem. Eng. Sci., 60 (2005), pp. 6780–6794.
- [18] A. VARSHNEY, S. PITCHAI AH, AND A. ARMAOU, *Feedback control of dissipative distributed parameter systems using adaptive model reduction*, AIChE J., 55 (2008), pp. 906–918.
- [19] W. H. VASSILIADIS, V. S. SARGENT AND C. C. PANTELIDES, *Solution of a class of multistage dynamic optimization problems, parts I & II*, Ind. Eng. Chem. Res., 33 (1994), pp. 2111–2133.