



Computation of Empirical Eigenfunctions and Order Reduction for Nonlinear Parabolic PDE Systems with Time-Dependent Spatial Domains ^{*}

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Abstract

This article presents a methodology for the computation of empirical eigenfunctions and the construction of accurate low-dimensional approximations for nonlinear parabolic partial differential equation (PDE) systems with time-dependent spatial domains. The method is successfully applied to a diffusion-reaction process with nonlinearities, spatially-varying coefficients and time-dependent spatial domain, and is shown to lead to the construction of accurate low-order models that are robust with respect to variations in the model parameters and different initial conditions.

Keywords: Karhunen-Loève expansion, Empirical eigenfunctions, Galerkin's method, Diffusion-convection-reaction processes with moving domains

1 Introduction

In this paper, we consider the problem of deriving low-order dynamic models for nonlinear parabolic PDE systems with the following description:

$$\frac{\partial \bar{x}}{\partial t} = L(\bar{x}) + f(t, \bar{x}), \quad \bar{x}(z, 0) = \bar{x}_0(z) \quad (1)$$

subject to the following mixed-type boundary conditions:

$$C_1 \bar{x}(0, t) + D_1 \frac{\partial \bar{x}}{\partial z}(0, t) = R_1, \quad C_2 \bar{x}(l(t), t) + D_2 \frac{\partial \bar{x}}{\partial z}(l(t), t) = R_2 \quad (2)$$

where the rate of change of the length of the domain, $l(t)$, is typically governed by an ordinary differential equation of the following general form:

$$\frac{dl}{dt} = \mathcal{G}(t, l, \int_0^{l(t)} \bar{a}(z, t, l, \bar{x}, \frac{\partial \bar{x}}{\partial z}) dz), \quad l(0) = l_0 \quad (3)$$

^{*}Financial support from an NSF CAREER award, CTS-9733509, is gratefully acknowledged.

In the above system of equations, $\bar{x}(z, t) = [\bar{x}_1(z, t) \cdots \bar{x}_n(z, t)]^T$ denotes the vector of state variables, $[0, l(t)] \subset \mathbb{R}$ is the domain of definition of the process, $z \in [0, l(t)]$ is the spatial coordinate, $t \in [0, \infty)$ is the time, $L(\bar{x})$ is a nonlinear differential operator which involves first- and second-order spatial derivatives, $f(t, \bar{x})$ is a nonlinear vector function, $\mathcal{G}(t, l, \int_0^{l(t)} \bar{a}(z, t, l, \bar{x}, \frac{\partial \bar{x}}{\partial z}) dz)$, $\bar{a}(z, t, l, \bar{x}, \frac{\partial \bar{x}}{\partial z})$ are nonlinear scalar functions, C_1, D_1, C_2, D_2 are constant matrices, R_1, R_2 are column vectors, and $\bar{x}_0(z)$ and l_0 are the initial conditions of the state and the domain size, respectively. In order to simplify the notation of this manuscript, we assume that $l(t)$ is a known and smooth function of time which satisfies $l(t) \in (0, l_{max}]$, $\forall t \in [0, \infty)$, where l_{max} denotes the maximum length of the spatial domain.

2 Methodology for model reduction

The main obstacles in developing a general model reduction method for systems of the form of Eq.1 are: a) the spatial differential operator is nonlinear, and b) the domain of definition of the process is generally time-varying. These issues do not allow the computation of analytic expressions for the eigenvalues and eigenfunctions of the spatial differential operator of the system, and thus, they prohibit the direct use of Galerkin's methods or orthogonal collocation methods with the eigenfunctions as basis functions, to derive finite dimensional approximations of the PDE system. To overcome these problems, we employ the following methodology for the computation of empirical eigenfunctions and the construction of accurate low-dimensional approximations for systems of the form of Eq.1.

- (i) Initially, the nonlinear parabolic PDE system is expressed with respect to an appropriate time-invariant spatial coordinate and a representative (with respect to different initial conditions and input perturbations) ensemble of solutions of the resulting time-varying PDE system is constructed by computing and solving a high-order discretization of the PDE.
- (ii) Then, the Karhunen-Loève expansion (and in particular the method of snapshots [1]) is directly applied to the ensemble of solutions to derive a small set of empirical eigenfunctions (dominant spatial patterns) that capture almost all the energy of the ensemble of solutions.
- (iii) Finally, the empirical eigenfunctions are used as basis functions within a Galerkin's model reduction framework to derive low-order ordinary differential equation (ODE) systems that accurately describe the dominant dynamics of the PDE system.

Owing to space limitations, the detailed theoretical development of the above method as well as a presentation of its use in the design of nonlinear low-order feedback controllers can be found in [2]. We also note that the use of empirical eigenfunctions as basis functions in Galerkin's method has been shown to lead to the derivation of accurate nonlinear low-dimensional approximations of

several dissipative PDE systems arising in the modeling of diffusion-reaction processes [3,4]. Furthermore, the Karhunen-Loève expansion was recently employed to construct empirical eigenfunctions for transport-reaction processes whose solutions contain traveling structures exploiting symmetry concepts [5]. In the next section, we present an application of the method to a diffusion-reaction process.

3 Application to a diffusion-reaction process

We consider a diffusion-reaction process with moving domain and spatially-varying coefficients described by the following parabolic PDE:

$$\frac{\partial \bar{x}}{\partial t} = \frac{\partial}{\partial z} \left(k(z) \frac{\partial \bar{x}}{\partial z} \right) + \beta_T(z) \left(e^{-\frac{\gamma}{1+\bar{x}}} - e^{-\gamma} \right) + \beta_U(b(z,t)u(t) - \bar{x}) \quad (4)$$

$$\bar{x}(z, 0) = 0.5, \quad \bar{x}(0, t) = 0, \quad \bar{x}(l(t), t) = 0$$

where \bar{x} is the state of the system, γ, β_u are constant dimensionless process parameters, $\beta_T(z), k(z)$ are dimensionless process parameters that are explicit functions of the spatial coordinate z , $u(t) = [u_1(t) \ u_2(t)]^T$ is the vector of the inputs (which will be used in the construction of the ensemble of solutions), and $b(z, t) = [b_1(z, t) \ b_2(z, t)]$ is a vector function which determines how the inputs $u_1(t), u_2(t)$ are distributed in space. The values and expressions of the process parameters that were used in our calculations are: $\beta_U = 2.0$, $\gamma = 4.0$, $\beta_T(z) = 45(1.5 - e^{-0.5z})$, $k(z) = e^{-0.5z}$ and $l(t) = \pi[1.4 - 0.4exp(-0.02t^{2.7})]$.

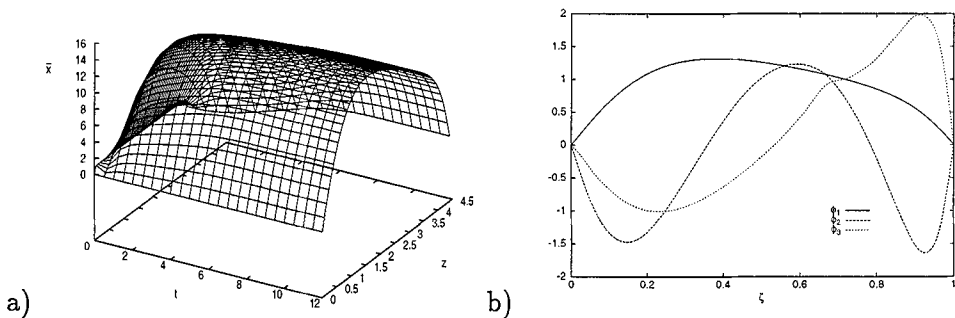


Fig. 1. a) Profile of \bar{x} for spatially varying $\beta_T(z), k(z)$ ($u(t) = 0$), and b) First three empirical eigenfunctions.

An accurate high-order discretization of the PDE of Eq.4 was constructed using Galerkin’s method with the following set of basis functions:

$$\phi_j(z, t) = \sqrt{\frac{2}{l(t)}} \sin \left(j \pi \frac{z}{l(t)} \right), \quad j = 1, \dots, \infty \quad (5)$$

It was found that a 30-th order Galerkin truncation of the system of Eq.4 using the above basis functions leads to an accurate solution of the PDE (it was verified that further increase in the order of the Galerkin model as well as reduction in the temporal discretization step provide no substantial

improvement on the accuracy of the simulation results). Figure 1a shows the evolution of the state of the PDE for $u(t) = 0$ starting from initial conditions which are very close to the steady-state $\bar{x}(z, t) = 0$. We observe that the system moves to another steady-state which is characterized by a maximum at $z = 0.375 l(t)$. This implies that the steady-state $\bar{x}(z, t) = 0$ is unstable (this was also verified through linearization) and the spatially non-uniform steady-state is stable.

We now continue with the computation of the set of empirical eigenfunctions. We initially constructed an ensemble of solutions by solving the high order discretization of the Eq.4 for four different initial conditions and five different time-profiles of the manipulated variables. This led to a total of 20 spatiotemporal solution profiles. Subsequently, 51 “snapshots” of the profile of the state of Eq.4 as a function of the spatial coordinate, z , for 51 fixed time instants during the process time were taken from each solution data set and were combined, to generate an ensemble of 1020 solutions. To apply Karhunen-Loève expansion we first expressed the developed ensemble of solutions into an appropriate spatial coordinate $\zeta = z/l(t)$ whose domain of definition is time-invariant. The Karhunen-Loève expansion was then applied to the developed ensemble of solutions to compute seven empirical eigenfunctions that describe the dominant spatial solution patterns embedded in the ensemble (they account for more than 99.9% of the energy included in the entire ensemble). The first three of these empirical eigenfunctions are presented in Figure 1b. Note that they are not symmetric with respect to the center of the system, $\zeta = 0.5$, owing to the spatial nonuniformity of β_T and k .

We now proceed with the use of the computed empirical eigenfunctions to construct accurate low-dimensional ODE approximations of the PDE. To accomplish this, the parabolic PDE system of Eq.4 is equivalently expressed in terms of $\zeta = z/l(t)$ as follows:

$$\frac{\partial \bar{x}}{\partial t} = \frac{1}{l(t)^2} \frac{\partial}{\partial \zeta} \left(k(\zeta) \frac{\partial \bar{x}}{\partial \zeta} \right) + \frac{i}{l(t)} \zeta \frac{\partial \bar{x}}{\partial \zeta} + \beta_T(\zeta) \left(e^{-\frac{\gamma}{1+\bar{x}}} - e^{-\gamma} \right) \quad (6)$$

$$+\beta_U(b(\zeta, t)u(t) - \bar{x}), \quad \bar{x}(\zeta, 0) = 0.5, \quad \bar{x}(0, t) = 0, \quad \bar{x}(1, t) = 0$$

We initially applied Galerkin’s method with the first three of the seven empirical eigenfunctions as basis functions to the PDE of Eq.6 to construct a third-order model. Figure 2a shows the discrepancy between the third-order ODE model and the high-order discretization of the PDE; we observe a very good agreement between the two models for all times, with the maximum deviation being lower than 0.5% (the deviation is computed to be the maximum error in the solution profile divided by the value of the state at that point).

For the sake of comparison, we also constructed a third-order approximation of the PDE using Galerkin’s method with basis functions the first three functions

of Eq.5 (this set of functions is the solution of the eigenvalue problem of the spatial operator of Eq.4 for the constant value of $k = 1$). We observe that the error (Figure 2b) between this third-order model and the high-order discretization of the PDE is significant (about 11%), which is mainly a result of the fact that this approach does not account for the spatial non-uniformity of the diffusion coefficient $k(z)$. We note that higher-order approximations computed using this approach result in more accurate models; specifically, we found that a 7th order model is needed to produce the same error of 3.4% as a second order model based on empirical eigenfunctions, and a 10th order model is needed to have the same error of 0.5% as the third order model based on empirical eigenfunctions.

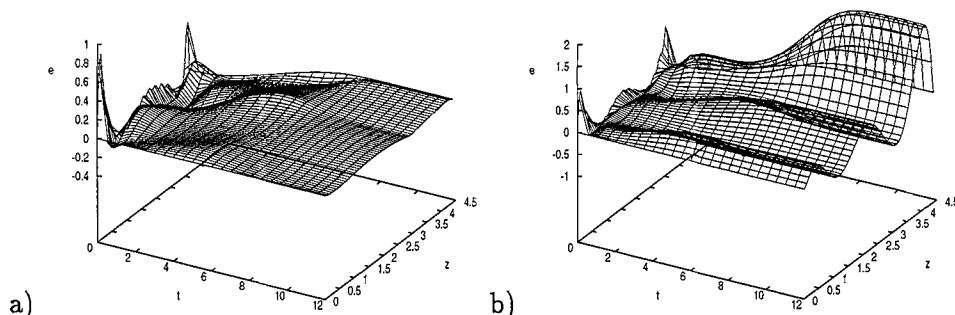


Fig. 2. Deviation between the third-order model and the high-order discretization of the PDE using as basis functions: a) empirical eigenfunctions, and b) sinusoidal functions.

We also tested the ability of the third-order model to give accurate predictions when the process parameters have values which are different from the ones used in the construction of the ensemble of solutions for the computation of the empirical eigenfunctions. Specifically, for $\beta_T = 55(1.5 - e^{-0.5z})$ (which corresponds to an about +20% variation with respect to the nominal value of β_T), the maximum error between the third-order model and the high-order discretization of the PDE is less than 0.5% for all times. On the other hand, for $\beta_T = 45(1.5 - e^{-0.4z})$ (which corresponds to an about -20% variation with respect to the nominal value of β_T), the error between the these two models remains under 0.7% for all times as can be seen in Figure 3a. We also tested the robustness of the third-order model for a +20% ($k = e^{-0.4z}$) and -20% ($k = e^{-0.6z}$) variation in the spatial dependence of k . The corresponding errors between the third-order model and the high-order discretization of the PDE remain small for all times, being under 0.6% in the first and 1.6% in the second case (which is shown in Figure 3b).

Finally, we tested the robustness of the third-order model for two initial conditions which are different from the ones used for the construction of the empirical eigenfunctions. Specifically, for the initial condition $\bar{x}_0(z) = 0.5 + 0.5\sin(z)$, the deviation between the third-order model and the high-order discretization of the PDE is presented in Figure 4a, while for $\bar{x}_0(z) = 0.4 + 0.6\sin(3z)$,

the same deviation is shown in Figure 4b. In both cases, the maximum error between the two models is less than 1.6% for all times, implying the robustness of the proposed model reduction procedure with respect to significant variations in the initial conditions.

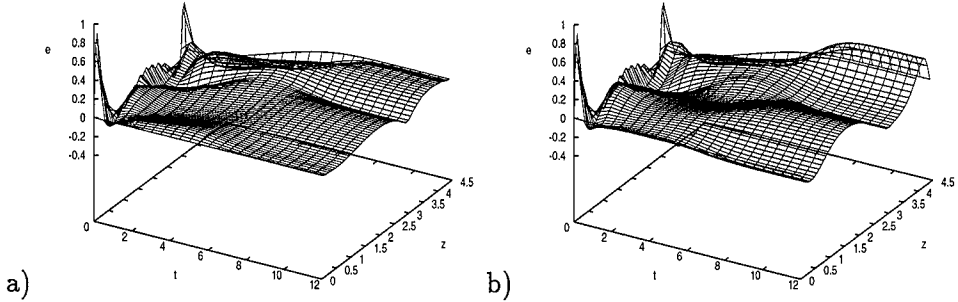


Fig. 3. Deviation between the third-order model and the high-order discretization of the PDE for a) $\beta_T(z) = 45(1.5 - e^{-0.4z})$, and b) $k(z) = e^{-0.6z}$.

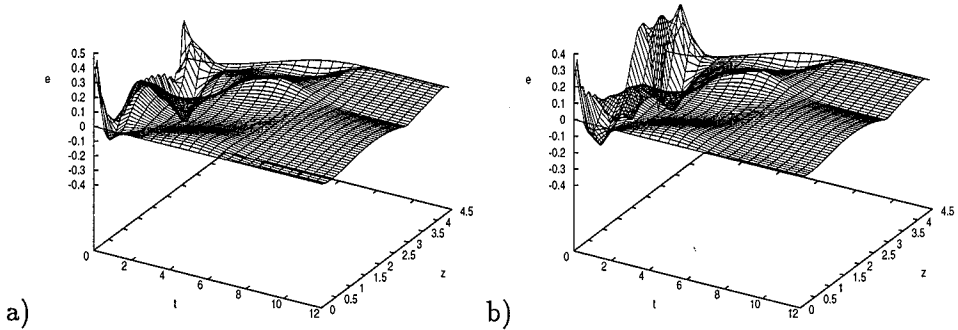


Fig. 4. Deviation between the third-order model and the high-order discretization of the PDE for a) $\bar{x}_0(z) = 0.5 + 0.5\sin(z)$, and b) $\bar{x}_0(z) = 0.4 + 0.6\sin(3z)$.

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