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Low-order empirical modeling of distributed parameter systems using temporal and spatial eigenfunctions

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Abstract

We provide a methodology for retrieving spatial and temporal eigenfunctions from an ensemble of data, using Proper Orthogonal Decomposition (POD). Focusing on a Newtonian fluid flow problem, we illustrate that the efficiency of these two families of eigenfunctions can be different when used in model reduction projections. The above observation can be of critical importance for low-order modeling of Distributed Parameter Systems (DPS) in on-line control applications, due to the computational savings that are introduced. Additionally, for the particular fluid flow problem, we introduce the use of the entropy of the data ensemble as the criterion for choosing the appropriate eigenfunction family.

Keywords: Empirical modeling; Distributed parameter systems; Eigenfunctions

1. Introduction

Proper orthogonal decomposition (POD) is based on second-order statistical properties, which result in a set of empirical eigenfunctions (also called spatial modes) from a collection of data. These modes are used in a weighted residual method (WRM) (Finlayson, 1972) to obtain a finite dimensional low-order dynamical system which has the smallest degree of freedom possible. Detailed analysis of the POD-Galerkin projection is provided in Holmes, Lumely, and Berkooz (1996). Although the theory behind POD dates back to 1933 (Hotelling, 1933), recently this method has received substantial attention, primarily because of two factors. Firstly, extracting structural information from large amounts of data has become of growing importance and POD is the optimal empirical method for capturing these features. Secondly, for the application of feedback control to infinite-dimensional distributed parameter systems (DPS) (Christophides, 2001a, 2001b), an attractive approach is to approximate the model by some reduced order model and develop control algorithms for the simplified model.

The properties of POD make this method popular for modeling, identification, control and optimization of distributed parameter systems. In Shvartsman and Kevrekidis (1998), a computer-assisted study was presented for nonlinear model reduction towards application of control to DPS. Alternative approaches to POD for model reduction and data analysis were provided in Graham and Kevrekidis (1996). A low-order model identification of DPS was provided in Zheng and Hoo (2002). The POD-Galerkin projection was used as a model reduction technique for compressible flows in Rowley, Colonius, and Murray (2003) and the stability properties were investigated in Iollo, Lanteri, and Désidéri (1998). The method of empirical eigenfunctions used to construct nonlinear low-order approximation of parabolic PDE and nonlinear controllers was initially proposed in Baker and Christofides (2000). The two-time-scale behavior of dissipative PDEs and the use of singular perturbation to construct very small basis functions sets that accurately capture the dominant dynamics of parabolic PDE was proposed in Christofides and Daoutidis (1997). An application of nonlinear control to Burgers equation and 2D channel incompressible fluid flow was

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examined in Baker, Armaou, and Christofides (2000). Another application was the boundary control of the Navier–Stokes equations by empirical reduction of modes (Park & Lee, 2000). The method has also been applied for the optimal control of turbulent fluid flows governed by Navier–Stokes equations (Ravindran, 1999), and the control of flow separations over a forward-facing step (Ravindran, 2002). Finally, the POD-Galerkin procedure was used for the optimization of transport-reaction systems (Armaou & Christofides, 2002; Bendersky & Christofides, 2000).

Even though the efficiency of POD is dependent on the initial data ensemble, there are no a priori rules for the generation of the ensemble. In order to obtain the eigenfunctions, a basic assumption is made that the data are fully representative of the temporal progression of the system. Under this assumption (when working in one dimension in space and in time), the pre-dominant approach (Alonso, Kevrekidis, Banga, & Frouzakis, 2003; Atwell & King, 2001; Banks, del Rosario, & Tran, 2002; Hung & Senturia, 1999; Park, Lee, & Jang, 1998) is to obtain spatial eigenfunctions and proceed with the model reduction. In this article, we assume that the data ensemble spans the domain both temporally and spatially; thus, we can obtain two families of empirical eigenfunctions from the initial data ensemble. One family characterizes the changes in the spatial profile (the spatial eigenfunctions φ) and the other characterizes changes in time (the temporal eigenfunctions ψ). With the use of an example, we reveal that the temporal eigenfunctions can provide better results in reducing the size of the original model. We also illustrate that the entropy of the spatiotemporal data can provide valuable information about the complexity of the spatial and temporal variations (of the original ensemble) separately.

This paper is organized as follows. In Section 2, we give a brief introduction of the control problems encountered in microchemical systems and the relevance of the analysis presented in this paper. The main theoretical aspects of POD and a framework for retrieving the spatial and temporal eigenfunctions are provided in Section 3. Section 4 contains the examined geometry, the model equations and the Finite Element Method (FEM) simulation results used for the creation of the data ensemble. The details of the model reduction technique are given in Section 5. In Section 6, we examine an alternative quantitative measure of the complexity of the data ensemble, the entropy. We then apply the model reduction using the spatial and temporal eigenfunctions, and we provide the simulation results in Section 7. We conclude the paper with remarks on our presented research results and an analysis of unresolved issues that are currently under investigation.

2. Motivation

Our research effort is centered on eventually developing and embedding a controller in a catalytic reformer and separator microchemical system that can operate as a sustained source of hydrogen fuel for proton exchange membrane (PEM) fuel cells. Microchemical systems (Brenchley & Wegeng, 1998; Jensen, 1999; Jensen et al., 1998; Pattekar & Kothare, 2004) are a new generation of miniature chemical Systems-on-a-Chip (SoC) that carry out chemical reactions and separations, in precisely fabricated three-dimensional microreactor configurations. The examined SoC will be used potentially as an alternative to conventional portable sources of electricity such as batteries for laptop computers and mobile phones due to its ability to provide an uninterrupted supply of electricity as long as a supply of methanol, water and heat can be provided. The system states such as temperature, concentration, pressure and velocity are functions of space and time. Thus, we have a distributed parameter system with combined distributed boundary sensing and actuation.

Applying control in a microchemical system may include efficient mixing of different laminar streams, manipulating microflows and adjusting the temperature distribution. From a control perspective, we face the following challenges. Firstly, the development of an efficient controller capable of handling the high dimensional models of these SoC and secondly, reducing its complexity so that it can be implemented on a chip and subsequently embedded with the rest of the system. While the control of fluid flows has been an active research area (see el Hak & Bushnell, 1991for results and references), there is very little work in literature on the dynamics and control of microflows in these highly functional and versatile SoC. Given the ability to accurately measure velocity profiles within microchannels (Meinhart, Wereley, & Santiago, 1999; Sinton, Escobedo-Canseco, Ren, & Li, 2002), active manipulation of microflows can be achieved by applying control both at the macroscopic level or within the microchannels. The simplest approach is to apply control at specific inlets and outlets at the macroscopic level. Within the microchannels, control can be applied using different kinds of external fields. There are applications reported that use electrostatic fields, electromagnetic forces, sound and capillary effects (Ho & Tai, 1998).

We use FEMLAB (FEMLAB Reference Manual, 2001) to design the microchemical system geometry, to appropriately place the sensors and the actuators and to obtain FEM simulation results of fluid flows and heat transfer in these complex geometries. We have proposed (Bleris, Kothare, Garcia, & Arnold, 2004) the design framework and custom arithmetic architecture details for a microcontroller that can provide optimal sensing–control–actuation performance, for temperature control applications, in microchemical systems. For the control of microflows, using the FEMLAB-obtained data ensemble, we intend to apply the POD-Galerkin projection, in order to derive low-order Ordinary Differential Equations (ODE) approximations of the Navier–Stokes. These ODE systems will be subsequently used for the design of low-order feedback controllers that can be embedded in the microchemical system and control on-line the flow field.

In this direction, we examine the details behind the POD-Galerkin projection method. We have proposed the use of