MODEL REDUCTION OF NONLINEAR SYSTEMS: A GREY-BOX MODELING APPROACH [1]

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Abstract: We present a novel model reduction methodology for the approximation of large-scale nonlinear systems. The methodology stems from the need to find computationally efficient substitute models for nonlinear systems. The nonlinear system is viewed as a grey-box model with a mechanistic (first-principle) component and an empirical (black-box) component identified for the computationally intensive parts of the nonlinear system. The mechanistic part is approximated using proper orthogonal decompositions whereas the empirical part is identified as polynomial functions by parameter estimation using the reduced order mechanistic part.

Keywords: Model Reduction, Parameter Estimation, Proper Orthogonal Decomposition, Distributed Parameter Systems

1. INTRODUCTION

Distributed parameter systems represented by partial differential equations (PDE's) are abundant in applications such as the modeling of flow phenomena in distillation columns, chemical reactors, heat exchangers, or in glass manufacturing. The numerical simulation of such models invariably involves the discretization of equations using numerical techniques such as finite differences, finite volume methods or finite element methods. In fact, all commercial computational tools for distributed parameter systems are based on these discretization techniques. Although these computational tools yield satisfactory and accurate solutions, the computational time required to accurately approximate system responses from boundary conditions, input variables and system parameters is often quite large. In spite of the tremendous advancements in computing power, the use of simulation tools for on-line and real-time applications such as model-based control, dynamic optimization, plant monitoring or parameter estimation, is often limited by the simulation time of these models. This makes it necessary to find computationally more efficient approximate models that retain the accuracy of the complex models. This need has led to the development and implementation of various model reduction techniques for distributed parameter systems (Gay and Ray, 1995), (Mahadevan and Hoo, 2000),

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(Hoo and Zheng, 2001), (Shvartsman *et al.*, 2000), (Shvartsman and Kevrekidis, 1998).

Most model reduction techniques are based on projection methods where high dimensional (state-) variables are projected on low dimensional manifolds so as to define a reduced order dynamical system. The technique of proper orthogonal decomposition (POD), combined with Galerkin projections is particularly popular in the fluid dynamics community and has been extensively discussed and applied in the literature as a model reduction tool for nonlinear and distributed parameter systems.

Most of the projection based model reduction techniques aim to reduce the state dimension of the system while preserving the input-output behavior as good as possible. It is often silently assumed that a significant state-dimension reduction implies a significant enhancement of computational speed. However, recent studies have shown that this is not necessarily the case for the reduction of nonlinear distributed parameter systems. See, e.g., (Schlegel *et al.*, 2002), (Rathinam and Petzold, 2003),(Astrid, 2004),(van den Berg, 2005).

This work is motivated to develop a model approximation technique with the explicit aim to improve the computational efficiency while keeping desirable model properties intact. We introduce a new methodology, a *grey-box modeling* approach to obtain substitute models. In grey-box modeling, sometimes also referred to as *hybrid modeling*, the system to be approximated is assumed to consist of the interconnection of a known system component (mechanistic part, white-box part) with a (partly) unknown component (black-box). Model reduction is performed on one of the interconnecting components (the mechanistic, white-box part), while system identification techniques will be applied to the other component (the empirical part). There are a number of reasons that motivate such an approach.

Firstly, finite element discretization of the spatial geometry of nonlinear distributed parameter systems typically leads to performing nonlinear function evaluations in each of the mesh elements. As a consequence, the computational load per nonlinear function evaluation is critical for the total computational load of solving the discretized model. By *separating* computationally intensive nonlinear functions in a model *before* performing any kind of model reduction, a structure is created in which computationally intensive functions can be substituted by simpler ones that are faster to evaluate. In this work, polynomial functions are considered for replacing the computationally intensive nonlinear functions. This procedure may lead to computationally more efficient approximate models.

Secondly, issues such as sparsity of the resulting models and model uncertainty can be easily addressed within this approach. A more detailed discussion on the methodological aspects of this approach can be found in (Romijn *et al.*, n.d.)

The paper is structured as follows: Section 2 presents some preliminaries on grey-box modeling and POD reduction. Section 3 provides some background on the reduction methodology. In Section 4, the proposed methodology is implemented on a dynamical system. Finally, conclusions are deferred to section 5.

2. PRELIMINARIES

2.1 Grey-Box Modeling

A *grey-box model* consists of a combination of a mechanistic (*first principle*) model and an empirical (*black-box*) model. Several grey-box model structures have been proposed in the literature (Psichogios and Ungar, 1992), (Thompson and Kramer, 1994),(Abonyi *et al.*, 2002). The most general form is based on the ordinary differential equation

$$\dot{x} = f_{\mathrm{FP}}\left(x, u, f_{\mathrm{EM}}\left(x, u\right)\right) \tag{1}$$

which contains first principle equations f_{FP} which describe the interaction of the model states x, inputs u and the outputs of an empirical model f_{EM}. Such models are usually derived from conservation laws and balance equations but are, without exception, reduced to lumped models of low order. A grey-box model that is governed by a partial differential equation (PDE) including an empirical term has not been investigated before to the knowledge of the authors. In this work the general partial differential equation

$$\frac{\partial T}{\partial t} = \mathcal{A}(T) + \mathcal{B}(u) + \mathcal{F}(T, u) \tag{2}$$

is considered. Here $T(., t)$ denotes the state variable at position x in some spatial geometry Ω and at time t, $u(x, t)$ denotes the input. For all t, $T(., t)$ is assumed to belong to a Hilbert space $\mathcal{H}$; $\mathcal{A}$ is a linear operator $\mathcal{A} : D(\mathcal{A}) \to \mathcal{H}$ where $D(\mathcal{A}) \subset \mathcal{H}$ is the domain of $\mathcal{A}$; $\mathcal{B}$ denotes the input operator and $\mathcal{F}$ represents nonlinear terms and model mismatch. The system (2) is separated in two parts

$$\frac{\partial T}{\partial t} = \mathcal{A}(T) + \mathcal{B}(u) + q \tag{3a}$$

$$q = \mathcal{F}(T, u) \tag{3b}$$

where the nonlinear function $\mathcal{F}(T, u)$ is viewed as the (known or unknown) empirical part of the