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Stabilized reduced order models for the advection–diffusion–reaction equation using operator splitting

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ABSTRACT

Reduced order modeling (ROM) coupled with finite element methods has been used effectively in many disciplines to efficiently solve complex problems. However, for advection-dominated flows numerical simulations often contain spurious, nonphysical oscillations which will also be apparent in the ROM simulations. In this work we consider stabilization methods for ROM for the advection–diffusion–reaction (ADR) equation when it is solved both with and without operator splitting. Specifically we consider the streamline-upwind Petrov–Galerkin (SUPG) stabilization method and the spurious oscillations at layers diminishing (SOLD) stabilization method. We build on these methods by constructing a coherent framework which successfully integrates these model reduction, stabilization, and operator splitting approaches, and we provide numerical examples detailing the application of this framework in the ADR setting. The stabilized ROM results are compared numerically with their corresponding full finite element simulations.

1. Introduction

In many complex models understanding the behavior of the system requires obtaining many realizations of the state equations which necessitates performing simulations over a range of model parameter values. Because performing many simulations for complex partial differential equations (PDEs) is typically computationally expensive, methods have been developed to reduce the work. One such class of methods is reduced order modeling (ROM).

The idea of using a reduced basis for computation was first introduced by Noor in structural analysis [1]. Interest in model reduction has expanded to an array of applications such as fluid dynamics [2], aeronautics [3], and climate modeling [4]. The goal of the model reduction method used here is to determine a low-dimensional approximation space over which to pose the state equations. The basis for this space is typically found by generating realizations of the state equations for a range of parameter values and then compressing the data; this procedure is typically implemented as a preprocessing step. In this work we used proper orthogonal decomposition (POD) to compress the data so the method is often referred to as POD-ROM. In Section 2 we present a brief overview of the ROM procedure that we use.

The advection–diffusion–reaction (ADR) equation is of importance because it models reactive solute transport. If the problem being modeled is diffusion dominated, then standard methods can be used to generate the ROM basis and the corresponding ROM solution. However, if the problem is advection dominated it is well known that standard finite element or finite difference approximations contain spurious, nonphysical oscillations unless a fine enough discretization is used. For this reason there has been considerable research into developing methods for adding stabilization to remove these nonphysical oscillations.

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Early attempts to remove spurious oscillations in finite element simulations used upwind discretizations but these tended to add too much diffusion. A method called SUPG which added diffusion only in the streamline direction was introduced in a paper in 1982 [5]. This method was a significant improvement over earlier attempts. Subsequently, there have been many extensions and analytical results published for SUPG; see [6–8] and the references therein. For some problems nonphysical oscillations also occur in the vicinity of steep gradients in the solution which SUPG does not address. To reduce these spurious oscillations a class of methods have been developed which are called SOLD methods; see [9] for a review of these methods. In Section 3 we briefly review these two stabilization methods and discuss how to implement them into the ROM setting and provide numerical results. A third stabilization method, flux correction transport, is also discussed but we argue that it is not easily implemented in the ROM setting. Much of the underlying theoretical analysis supporting the use of streamline diffusion methods in POD-based ROM was introduced in [10], and a recent paper contains further theoretical analysis of streamline diffusion ROM methods applied to convection–diffusion problems and studies the optimal selection of stabilization parameters in this setting [11]. In contrast, the goal of our work is to construct and demonstrate a framework incorporating these methods which can be applied to a variety of ADR problems, including both advection-dominated and diffusion-dominated cases.

Even after stabilization is added to the problem, the computational costs of generating solutions to the full and reduced equations can be significant. To reduce this cost, operator splitting is often used, especially for the case where the reactions are nonlinear. For example, in the ADR equation the transport phase can be solved followed by the reaction phase; in addition, the transport phase can be broken down into advection and diffusion phases creating a three-step process at each time step. For a nonlinear reaction an advantage is that once the reaction phase is separated from the transport phase, the PDE describing transport becomes linear. Moreover, the reaction phase can be solved as an initial value problem at each node thus simplifying computations. Another advantage of operator splitting is that one can tailor the numerical scheme to the phase. The stability of operator splitting for the ADR equation was studied in [12]. In Section 4 we present a novel construction which incorporates model reduction, operator splitting, and stabilization in an integrated framework. This framework accommodates both SUPG and SOLD stabilization strategies, and can be used to apply both two- and three-phase operator splitting for the ADR equation. In this manner, our approach is a strategy for improving both the computational cost of generating realizations as well as the numerical stability of the realizations. We provide numerical examples which allow us to study the accuracy and the computational cost of our approach.

2. Brief overview of POD-based ROM

In the context of solving partial differential equations (PDEs) using reduced order modeling, one generates a set of reduced basis vectors as a preprocessing step. The goal is for the dimension of the reduced space to be much smaller than the size of the system used to solve the PDE by standard methods such as finite elements or finite differences. Once the basis is chosen, the ROM solution is sought as a linear combination of these basis vectors and so the state equations are posed as a Galerkin problem in a standard way.

In this section we give a brief overview of the model reduction procedure and then describe it for the ADR equation. We also indicate how inhomogeneous initial and boundary conditions are handled in the ROM setting.

2.1. Model reduction procedure

In the model reduction process we generate a set of particular solutions to a differential equation which contains one or more parameters; we call these solutions "snapshots" and they are obtained by using standard methods which typically require solving large systems, which may be banded under certain circumstances (such as when a structured computational grid is used). Throughout this work we use standard finite elements methods to generate the snapshots. We sample the solution space along both the parameter domain and time domain, such that each snapshot is a solution of the PDE corresponding to a single parameter set and a particular time, assuming the PDE is time dependent. We assemble the vector representations of these snapshots as columns in a snapshot matrix, S.

Because the columns of the snapshot matrix contain a great deal of redundant information, we compress the information to obtain a set of reduced basis vectors. In this work we do this by using a proper orthogonal decomposition (POD). However, there are alternative methods which may be used to compress the snapshot data, such as CVT [2]. In POD one determines the singular value decomposition of the snapshot matrix S and the first d left singular vectors, ψ_i, of this matrix form the orthonormal reduced basis set. The reduced order solution u^n_{ROM} at time t_n is sought as a linear combination of these basis vectors and the problem is posed as a Galerkin problem over the reduced space.

In general, these basis functions have global support over the domain, which leads to a dense system of equations. Thus the only way ROM is feasible is if $d \ll m$, where m is the dimension of the system of algebraic equations using a high dimensional method.

One can show that the error of the d-dimensional POD space is given by the sum of the squares of the singular values corresponding to the unused left singular vectors of S [13]. We may compute this relative error as

$$e_{\text{POD}} = \sum_{i=d+1}^{l} \sigma_i^2 \Big/ \sum_{i=1}^{l} \sigma_i^2, \tag{1}$$