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Reduction procedure for parametrized fluid dynamics problems based on proper orthogonal decomposition and calibration

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ABSTRACT

In this paper an extension of the proper orthogonal decomposition to a multi-parameter domain is proposed. The method produces a low-order model after three consequent steps: construction of an optimal basis functions set with respect to model error; computing the model coefficients with the Galerkin approach; calibration of the coefficients to minimize the model error. As a particular example the 2D square cylinder wake flow is used to show the potential of the extended method for different laminar flow regimes. The proposed method shows good interpolation properties of the reduced model with respect to the defined range of Reynolds numbers.

1. Introduction

Detailed modeling of physical and chemical processes based on conservation laws often leads to nonlinear spatially distributed models. Such models possess good predictive qualities and can be used for offline-applications like process design tasks. However, for some applications spatially distributed nonlinear models are often too complex. The first example is an advanced model based control concepts that requires a solution of the model in real time. The second example is dynamic optimization and parameter identification problems, where one calculation of the objective function requires several solutions of the model equations.

For such applications reduced order models are desirable. Among a number of various order reduction techniques, the focus in this work is on the reduction process based on a construction of a low-order model that minimizes the defined error between the solution of the detailed reference model and the reduced low-order one. For example, Grepl et al. (2007) propose the efficient reduced-basis method for nonlinear elliptic and parabolic problems based on the empirical interpolation. Another possible reduction approach will lead to proper orthogonal decomposition (POD) type methods with spatially distributed basis functions and time-dependent coefficients (Sirovich, 1987; Kunisch and Volkwein, 2003; Nguyen et al., 2008; Bergmann et al., 2009) or, vice versa, time-distributed basis functions and coefficients of a reduced model that are spatially distributed (Lumley, 1967). In applications it is also quite important to estimate the approximation quality of the reduced model with some quantitative measure.

In this contribution, we propose an extension of the model reduction based on the POD-like approach that differs from the original one in a way that the reduction is performed for snapshot solutions distributed not only in time and space but also in a multi-parameter space. The developed extension resembles model order reduction approaches of parametrized systems that have been intensively developed during the last decade (Haasdonk et al., 2008; Haasdonk and Ohlberger, 2008; Knezevic and Patera, 2010). The reduction method consists of three steps:

- Finding the optimal basis set of spatially orthonormal functions that is a *best approximation* of the model reference data from a set of orthonormal functions.
- Computing coefficient matrices of the reduced model with a Galerkin approximation in the optimal basis.
- Optimization or *calibration* of the model coefficients to minimize the approximation error.

The necessity of the calibration is shown in recent studies (Galletti et al., 2004; Kalb and Deane, 2007; Cordier et al., 2010).

The contributions this paper are summarized as follows:

- An approach for the multi-parameter POD method is proposed.
- The necessity of calibration is shown and a method for the reduction of the total model reduction error is proposed.

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- Model reduction is demonstrated on the confined square cylinder wake flow with spatial basis functions that provide a best approximation basis for model coefficients in the (t,Re)-domain.

The structure of the paper is as follows. In the next section, a test system is presented that will be used to illustrate the reduction method. Sections 3–5 present three steps of the proposed reduction method. Section 6 presents results of the application of the reduction procedure to the example system for different laminar flow regimes: steady-state flow with the Reynolds number $10 \le Re \le 50$; periodic flow with $100 \le Re \le 150$; and combination of both regimes with $50 \le Re \le 150$.

2. Reference model

The reference model used to illustrate the method is the confined square cylinder wake flow that recently has become a testing benchmark for CFD model reduction (Noack et al., 2003, 2010; King et al., 2005; Bergmann et al., 2009; Cordier et al., 2010), to name but a few. The model consists of the continuity equation and the momentum balance in an incompressible medium that are expressed by the following system of dimensionless Navier–Stokes equations:

$$\frac{\partial \mathbf{u}}{\partial t}+(\mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla p+\frac{1}{Re}\Delta\mathbf{u}$$

$$\nabla\cdot\mathbf{u}=0, \tag{1}$$

where $\mathbf{u} := (u,\ v)$ is the vector of flow velocities in x_1 and x_2 directions, p is the pressure, Re is the Reynolds number. The spatial Ω–domain shown in Fig. 1 is a rectangle with dimensionless side lengths 32×8 with a unit square cylinder inside it. Boundary conditions in space subject to the geometry in Fig. 1 are as follows. The inlet Γ_{in} has a parabolic velocity profile $\mathbf{u}=(x_2(8-x_2)/16,\ 0)$ with the unit maximal velocity in x_1-direction. The outlet Γ_{out} shows convective outflow of the fluid with a zero reference pressure. Other boundary conditions are modeled with the no-slip condition for a viscous fluid. The initial condition is a zero velocity field. Simulation of the reference model is performed in the CFD tool OpenFOAM (Jasak, 1996) that is based on the second order finite volume method. Model simulations in OpenFOAM produce a set of N_s snapshots for the defined set of parameter points $\mu_i=(t_i,Re_i)\in\mathcal{M}\subset\mathbb{R}^{N_p}$ for $i=1,\ldots,N_s$. The snapshots in the test example are space distributed functions on an equidistant rectangular mesh with 131 904 cells and define the velocity components of solutions $\mathbf{u}_i=(u(t_i,Re_i),\ v(t_i,Re_i))$ in the parameter domain $\mathcal{M}$ with $0\le t\le 300$ and $5\le Re\le 150$. One snapshot for $Re=150$ is shown in Fig. 1 as an iso-vorticity plot with solid lines for positive vorticity values, dashed lines for negative values, and bold solid lines for zero values.

3. Basis functions computation

The proposed method is similar to the continuous proper orthogonal decomposition procedure proposed by Kunisch and Volkwein (2003) and Henri and Yvon (2005). In this section we recall statements of the POD method.

Let $\mathbf{u}_i(x)=\mathbf{u}(\mu_i,x)$ be given piecewise continuous solutions or snapshots of the reference problem for N_s parameter values $\mu_i\in\mathcal{M}\subset\mathbb{R}^{N_p}$ with spatial variables $x\in\Omega$. In the classical POD method, $\mathcal{M}$ contains the time variable only, and $N_p=1$. In this work we consider the case that snapshots are not only available for different time points, but also for different values of the model parameters, i.e. $\mathcal{M}$ consists of the time variable and N_p-1 physical parameters.

Let $\boldsymbol{\psi}_i|_1^{N_b}$ be continuous functions in Ω that form an unknown orthonormal basis. The POD method considers a constrained minimization of the average mean square error E between the reference and projected data with respect to $\boldsymbol{\psi}_i|_1^{N_b}$

$$\min_{\substack{(\boldsymbol{\psi}_i,\boldsymbol{\psi}_j)_\Omega=\delta_{ij}\\ 1\le i,j\le N_b}} E(\boldsymbol{\psi}_i) := \frac{1}{V}\sum_{j=1}^{N_s}\left\|\mathbf{u}_j-\sum_{i=1}^{N_b}(\mathbf{u}_j,\boldsymbol{\psi}_i)_\Omega\boldsymbol{\psi}_i\right\|_\Omega^2\cdot w_j, \tag{2}$$

where δ_{ij} is the Kronecker delta, V is a volume of $\mathcal{M}$–domain, and an inner product with induced norm are

$$(\mathbf{f},\mathbf{h})_\Omega=\int_\Omega \mathbf{f}^T\mathbf{h}\,\mathrm{d}x \quad\text{and}\quad \|\mathbf{f}\|_\Omega=(\mathbf{f},\mathbf{f})_\Omega^{1/2}. \tag{3}$$

In (2) w_j are non-negative weights that correspond to a quadrature rule in the parameter domain $\mathcal{M}$

$$\int_{\mathcal{M}} f(\mu)\,\mathrm{d}\mu \approx \sum_{i=1}^{N_s} f(\mu_i)\cdot w_i \tag{4}$$

for a suitable choice of sampling points μ_i. The choice of the points μ_i may be reformulated as a search of quadrature points in the parameter domain to minimize the quadrature error in (4). Methods to minimize the quadrature error by choosing suitable sampling points μ_i can be found in literature, e.g. based on optimality conditions (Kunisch and Volkwein, 2010), greedy empirical procedures (Maday et al., 2009), sparse grids (Klimke, 2007), etc. In this work, a greedy sampling method that refines the points selection based on the reduced model error after a calibration step (see Section 5) is applied. The set of sampling points is a rectangular mesh in the N_p-dimensional parameters domain that is used with a trapezoidal quadrature rule in (4). The corresponding weights are defined as $w_i=\prod_{p=1}^{N_p}\Delta_{p,i}$ with parameter differences

$$\Delta_{p,i}=\frac{1}{2}\cdot\begin{cases}\mu_{p,i+1}-\mu_{p,i}, & i=1,\\ \mu_{p,i+1}-\mu_{p,i-1}, & i=2,\ldots,N_s^p-1,\\ \mu_{p,i}-\mu_{p,i-1}, & i=N_s^p\end{cases}$$

where $\mu_{p,i}$ is a p-component of a snapshot μ_i and N_s^p is a number of mesh points in p-dimension. With this definition, the weight w_i is a volume of a hyper-rectangle surrounding the sampling point μ_i.

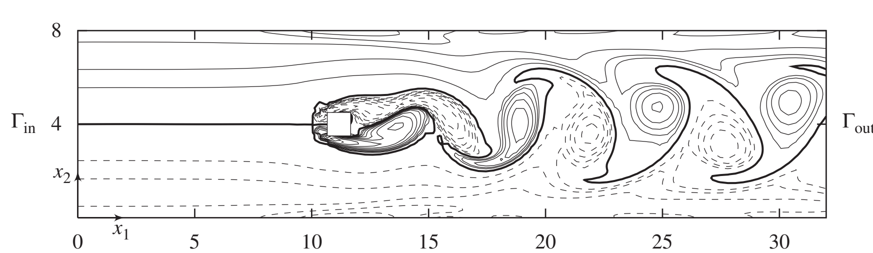

Fig. 1. Reference model geometry and iso-vorticity plot at $Re=150$.