Towards Physically Admissible Reduced-Order Solutions for Convection-Diffusion Problems

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Abstract

This note proposes, analyzes, and studies numerically a regularization approach in the computation of the initial condition for reduced-order models (ROMs) of convection-diffusion equations. The aim of this approach consists in reducing significantly spurious oscillations in the ROM solutions.

Keywords: Reduced order models (ROMs); Proper orthogonal decomposition; Convection-dominated equations; ROM initial condition; Differential filter

1. Introduction

Convection-diffusion equations are part of many models for natural phenomena and industrial processes. They model the behavior of, e.g., temperature (energy balance) or concentrations. Often, convection dominates diffusion. In this situation, it is well known that so-called stabilized discretizations have to be employed to perform stable numerical simulations [8]. From the practical point of view, not only the accuracy of a discretization, measured in some norm, is of interest but also that the numerical solution possesses admissible values. For instance, a computed concentration with strong negative spurious oscillations is useless in practice. However, there are relatively few discretizations that lead to solutions without spurious oscillations, like the FEM-FCT schemes [5, 6].

ROM is usually applied if simulations with nearly the same setup have to be repeated over and over again and if the efficiency is of more importance than the accuracy, like in the simulation of optimization problems. Based on a set of snapshots and the proper orthogonal decomposition (POD) approach [9], one may compute a basis that already captures important features of the solution.

Standard ROM simulations of convection-diffusion equations suffer from strong spurious oscillations. The reasons for them are twofold: the construction

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of the ROM's initial condition and the used discretization. This note addresses the first issue. In addition to using the standard definition by an L^2 projection, a regularization is applied. To the best of the authors' knowledge, this approach has not been proposed in the literature so far. It will be analyzed briefly and numerical studies show that spurious oscillations are damped significantly.

2. Reduced-Order Models for Convection-Diffusion Equations

Consider the convection-diffusion-reaction equation

$$\partial_t u - \varepsilon \Delta u + \boldsymbol{b} \cdot \nabla u + cu = f \quad \text{in } (0, T] \times \Omega \tag{1}$$

with homogeneous Dirichlet boundary conditions $u = 0$ and the initial condition $u^0(\boldsymbol{x})$. In (1), Ω is a bounded domain in $\mathbb{R}^d$, $d \in \{2, 3\}$, with boundary Γ, $\boldsymbol{b}(t, \boldsymbol{x})$ and $c(t, \boldsymbol{x})$ denote convection and reaction fields, respectively, $\varepsilon > 0$ is a constant diffusion coefficient, and T is the length of the time interval.

Let $X = H_0^1(\Omega)$. To compute the POD basis functions, the centered-trajectory method is utilized, i.e., the POD modes are computed from the fluctuation of the snapshots $u_i - \bar{u}_h$, $i = 1, \ldots, M$, where $\bar{u}_h$ is the average of the snapshots. For a detailed description of performing the POD and computing the POD modes, it is referred to [10]. Let the ROM approximation u_{ro} of the solution u be given by $u(t, \boldsymbol{x}) \approx u_{\text{ro}}(t, \boldsymbol{x}) = \bar{u}_h(\boldsymbol{x}) + u_r(t, \boldsymbol{x})$, where $u_r(t, \boldsymbol{x}) = \sum_{i=1}^r \alpha_i(t) \varphi_{\text{ro},i}(\boldsymbol{x})$ with the unknown coefficients $\{\alpha_i\}_{i=1}^r$ and the POD basis functions $\{\varphi_{\text{ro},i}\}_{i=1}^r$. The standard Galerkin reduced-order model (G-ROM) is built by projecting the continuous problem into the finite-dimensional POD space $X_r = \text{span}\{\varphi_{\text{ro},i}, i = 1, \ldots, r\}$. Numerical investigations in [1] asserted that the stabilization of a ROM was necessary in order to obtain stable simulations for arbitrary POD dimensions r in the convection-dominated regime. The stabilized Streamline-Upwind Petrov–Galerkin reduced-order model (SUPG-ROM) was used, which is presented in the following.

Let the superscript n of a function denote the evaluation of the function at the time instance t_n and let Δt denote the fixed time step. The SUPG-ROM combined with the backward Euler method reads as follows: For $n = 1, 2, \ldots$ find $u_r^n = u_{\text{ro}}^n - \bar{u}_h \in X_r$ such that $\forall v_r \in X_r$

$$\begin{aligned} &\left(u_r^n - u_r^{n-1}, v_r\right) + \Delta t a_{\text{SUPG},r}\left(u_r^n, v_r\right) = \Delta t \left(f^n, v_r\right) - \Delta t\, a_{\text{SUPG},r}\left(\bar{u}_h, v_r\right) \\ &+ \Delta t \sum_{K \in \mathcal{T}_h} \delta_{r,K} \left(f^n, \boldsymbol{b}^n \cdot \nabla v_r\right)_K - \sum_{K \in \mathcal{T}_h} \delta_{r,K} \left(u_r^n - u_r^{n-1}, \boldsymbol{b}^n \cdot \nabla v_r\right)_K, \end{aligned} \tag{2}$$

where $\delta_{r,K}$ is a stabilization parameter to be chosen and

$$\begin{aligned} a_{\text{SUPG},r}(u_r, v_r) = &\left(\varepsilon \nabla u_r, \nabla v_r\right) + \left(\boldsymbol{b}^n \cdot \nabla u_r, v_r\right) + \left(c^n u_r, v_r\right) \\ &+ \sum_{K \in \mathcal{T}_h} \delta_{r,K} \left(-\varepsilon \Delta u_r + \boldsymbol{b}^n \cdot \nabla u_r + c^n u_r, \boldsymbol{b}^n \cdot \nabla v_r\right)_K \end{aligned}$$

for all $u_r, v_r \in X_r \subset X_h$. Setting $\delta_{r,K} = 0$ in (2) recovers the Galerkin ROM. In [1], numerical analysis was utilized to derive the appropriate scalings of the stabilization parameter $\delta_{r,K}$ for the case of a family of uniform triangulations. In the study, the finite element version of the SUPG stabilization parameter $\delta_r = \mathcal{O}(h)$, with h being the finite element mesh width, was recommended and therefore this choice will be employed in the numerical simulations in Section 4.

3. Computation of the ROM's Initial Condition

The coefficients $\{\alpha_i^0\}_{i=1}^r$ of the initial condition for a projection-based ROM such as (2) are usually obtained by projecting $u^0 - \bar{u}_h$ in the L^2 sense onto the POD basis: $\alpha_i^0 = \left(u^0 - \bar{u}_h, \varphi_{\mathrm{ro},i}\right)$, $i = 1, \ldots, r$. Consequently, the reduced-order approximation u_{ro}^0 of the initial condition u^0 has the form

$$u^0 \approx u_{\mathrm{ro}}^0 = \bar{u}_h + \sum_{i=1}^{r} \alpha_i^0 \varphi_{\mathrm{ro},i}, \tag{3}$$

which is the best approximation of u^0 in the POD space X_r in the L^2 sense.

However, there might be different goals than this. Depending on the origin of the POD basis, the initial condition (3), although optimal in the L^2 sense, can be polluted by spurious oscillations, e.g., see Fig. 2. From the point of view of physical applications, it is desirable to be able to construct a ROM initial condition that suppresses spurious oscillations as well as possible but still approximates well the function u^0.

A possible way to achieve this goal originates from turbulence modeling. In some turbulence models, like Approximate Deconvolution Models and the Leray α-model, a regularized velocity is defined by solving a Helmholtz equation

$$-\mu^2 \Delta u_{\mathrm{fil}} + u_{\mathrm{fil}} = u, \tag{4}$$

where μ is the filter width usually chosen to be $\mu \sim h$, see [4, 7] for more details on this so-called differential filter. Thus, the ROM initial condition (3) can be filtered in a post-processing step by computing the Galerkin approximation of (4) with respect to the POD basis. Finally, the following problem has to be solved: Find $u_{\mathrm{ro,fil}}$ with $u_{\mathrm{ro,fil}} - \bar{u}_h = \sum_{i=1}^r \tilde{\alpha}_i^0 \varphi_{\mathrm{ro},i} \in X_r$ such that

$$\mu^2 \left(\nabla u_{\mathrm{ro,fil}}, \nabla \varphi_{\mathrm{ro},i}\right) + \left(u_{\mathrm{ro,fil}}, \varphi_{\mathrm{ro},i}\right) = \left(u_{\mathrm{ro}}^0, \varphi_{\mathrm{ro},i}\right), \quad i = 1, \ldots, r, \tag{5}$$

where u_{ro}^0 is the ROM approximation (3). It should be noted that the differential filter was used in ROM simulations of turbulent flows [11].

Next, the convergence of $u_{\mathrm{ro,fil}}^0$ for the special case of a family of uniform triangulations will be investigated. Using the triangle inequality yields

$$\left\|u^0 - u_{\mathrm{ro,fil}}\right\|_0 \leq \left\|u^0 - u_{\mathrm{ro}}^0\right\|_0 + \left\|u_{\mathrm{ro}}^0 - u_{\mathrm{ro,fil}}^0\right\|_0.$$

The first term on the right-hand side can be expected to be small by the construction of u_{ro}^0 as the best approximation in L^2. To obtain an estimation of the second term on the right-hand side, the difference $u_{\mathrm{ro}}^0 - u_{\mathrm{ro,fil}}^0$ can be utilized as a test function in (5). By shifting the second term on the left-hand side to the

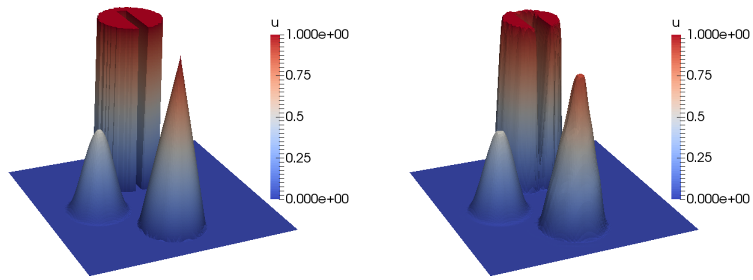

Figure 1: Interpolated continuous initial condition (left) and solution at $t = 6.28$ for the FEM-FCT scheme (right).

right-hand side of the equation, by using the Cauchy–Schwarz inequality and the standard inverse estimate, one obtains

$$\begin{aligned}\left\|u_{\mathrm{ro}}^0 - u_{\mathrm{ro,fil}}^0\right\|_0^2 &\le \mu^2 \left\|\nabla u_{\mathrm{ro,fil}}^0\right\|_0 \left\|\nabla\left(u_{\mathrm{ro}}^0 - u_{\mathrm{ro,fil}}^0\right)\right\|_0 \\ &\le C h^{-1}\mu^2 \left\|\nabla u_{\mathrm{ro,fil}}^0\right\|_0 \left\|u_{\mathrm{ro}}^0 - u_{\mathrm{ro,fil}}^0\right\|_0,\end{aligned}$$

such that for $\mu \sim h$ it holds

$$\left\|u_{\mathrm{ro}}^0 - u_{\mathrm{ro,fil}}^0\right\|_0 = \mathcal{O}(h). \tag{6}$$

On the one hand, the filtering procedure (5) yields a solution that does not represent the best approximation of u^0 in the L^2 sense anymore. But because of (6) the function $u_{\mathrm{ro,fil}}^0$ is still a good approximation of u^0 with the convergence of at least first order in the L^2 sense. On the other hand, $u_{\mathrm{ro,fil}}^0$ can lead to a better approximation of u^0 with respect to spurious oscillations.

4. Numerical Studies

In this section, it will be numerically investigated to which extent the Galerkin ROM and SUPG-ROM based on oscillation-free snapshots are able to compute admissible ROM solutions. Moreover, the impact of the filtering procedure (5) of the ROM initial condition on the ROM results will be studied. The code MooNMD [2] was utilized to perform the numerical studies.

For the sake of brevity, numerical results are presented only for one example, the standard rotating body example. A detailed description of this example can be found, e.g., in [3]. Initially, three bodies are given, see Fig. 1, which are rotated counter clock wise. The coefficients of (1) are $\Omega = (0,1)^2$, $T = 6.28$, $\varepsilon = 10^{-20}$, $\boldsymbol{b} = (0.5 - y, x - 0.5)^T$, and $c = f = 0$. Because of the very small diffusion, the result after one revolution should recover the initial solution.

To evaluate the results of the simulations, several measures of interest will be monitored. Besides considering plots of the obtained solutions, the $L^2(\Omega)$ error $\|u^n - u_{\mathrm{ro}}^n\|_0$ at certain times and the discrete analog of the $L^1(0,T;L^2(\Omega))$ error $\frac{1}{N+1}\sum_{n=0}^{N}\|u^n - u_{\mathrm{ro}}^n\|_0$, respectively, will be considered, where u^n denotes the

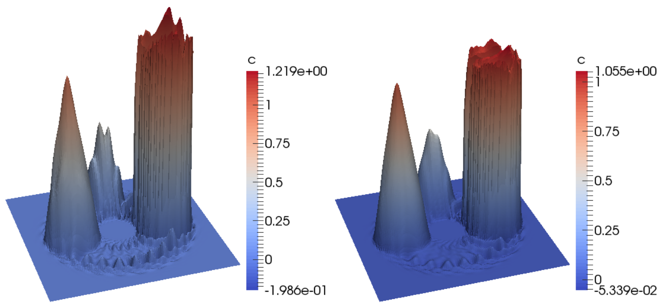

Figure 2: Standard ROM initial condition (3) (left) and regularized ROM initial condition (5) (right) based on physically admissible snapshots from the FEM-FCT approach for $r = 50$.

solution of the continuous problem at time t_n. In addition, the minimum and the maximum values of the solution will be computed in the vertices of the mesh cells. The $L^2(\Omega)$ error gives some idea of the accuracy of the methods and the smearing in the numerical solutions. The minimum and the maximum values indicate the under- and overshoots of the numerical solution. The reference minimum and maximum values of the solution are 0 and 1, respectively.

The snapshots were obtained by approximating the solution of (1) with the nonlinear flux-corrected transport (FEM-FCT) scheme with the Crank–Nicolson method as time integrator, e.g., see [5, 6]. Piecewise linear finite elements P_1 and the length of the time step $\Delta t = 10^{-3}$ were utilized. The computations were carried out using 16641 degrees of freedom with the mesh width $h = 1.1 \cdot 10^{-2}$. Then, 1257 snapshots, corresponding to every fifth numerical solution, were used to compute the POD basis. In Fig. 1, the FEM-FCT solution for the final time is shown. By construction of the scheme, the solution does not exhibit any spurious oscillations. The POD basis was computed from the fluctuating part of the snapshots with respect to the L^2 inner product by the method of snapshots [9].

G-ROM and SUPG-ROM simulations were carried out with the backward Euler scheme (2) using $\Delta t = 10^{-3}$. Note that the spatial error usually dominates in ROM simulations such that the choice of the time integrator is of only minor importance. The ROMs with the standard ROM initial condition are denoted by G-ROM and SUPG-ROM and the ones equipped with the regularized ROM initial condition (5) by G-ROM(reg) and SUPG-ROM(reg). Simulations with different values of μ were performed. The best results were obtained with $\mu = 0.8\,h$ and for the sake of brevity only these will be presented. Figure 2 shows the standard and the regularized initial conditions for $r = 50$. It can be seen that the standard ROM initial condition is polluted by spurious oscillations even if the FEM-FCT snapshots are free of oscillations. The post-processing filtering procedure is able to suppress them significantly.

Computational results are presented in Figs. 3 and 4. The results for all $r \in \{50, 150\}$ are qualitatively similar. With G-ROM, the $L^1(0,T;L^2(\Omega))$ error is a little bit smaller than with SUPG-ROM. However, the spurious oscillations

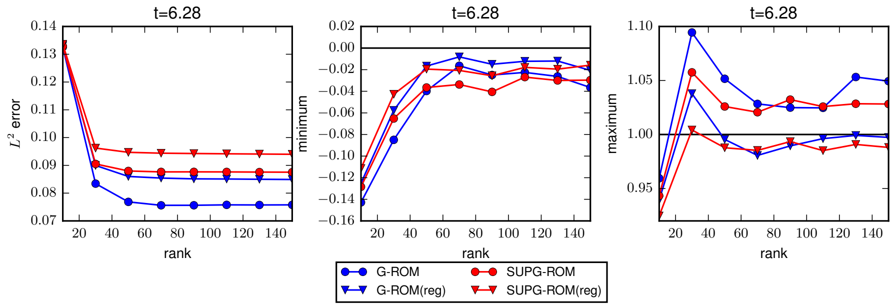

Figure 3: Measures of interest at $t = 6.28$.

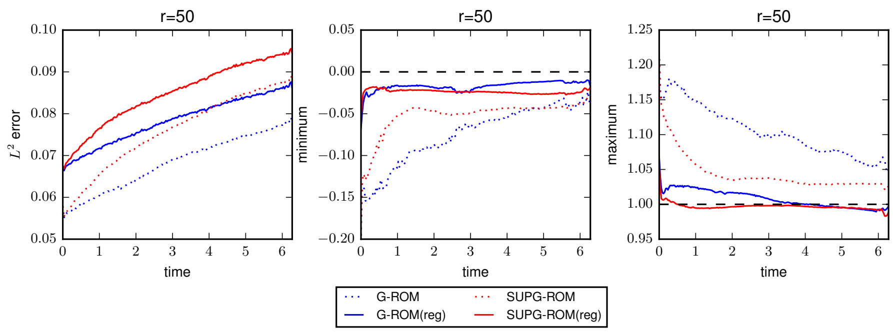

Figure 4: Time evolution of the measures of interest for G-ROMs and SUPG-ROMs for $r = 50$.

in the first part of the time interval are considerably larger. Using the regularized initial condition $u_{\text{ro,fil}}$ leads to a significant damping of the undershoots and particularly of the overshoots. This desired property can be observed in the whole time interval. But, the $L^1(0, T; L^2(\Omega))$ error is somewhat larger than with the standard initial condition u^0.

5. Summary and Outlook

This note proposed a regularization of the ROM's initial condition for convection-diffusion equations. Numerical studies showed a significant damping of spurious oscillations in the computed solutions. The main open question for future research is the construction of a ROM discretization that ensures numerical solutions without spurious oscillations.

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