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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.

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 [1]. 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 [2,3].

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

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problems. Based on a set of snapshots and the proper orthogonal decomposition (POD) approach [4], 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 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 $u_i - \bar{u}_h$, $i = 1, \dots, M$, 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 [5]. Let the ROM approximation u_{ro} of the solution u be given by $u(t, \boldsymbol{x}) \approx u_{\mathrm{ro}}(t, \boldsymbol{x}) = \bar{u}_h(\boldsymbol{x}) + u_r(t, \boldsymbol{x})$, where $u_r(t, \boldsymbol{x}) = \sum_{i=1}^{r} \alpha_i(t) \varphi_{\mathrm{ro},i}(\boldsymbol{x})$ with the unknown coefficients $\{\alpha_i\}_{i=1}^r$ and the POD basis functions $\{\varphi_{\mathrm{ro},i}\}_{i=1}^r$. The standard Galerkin reduced-order model (G-ROM) is built by projecting the continuous problem into the finite-dimensional POD space $X_r = \mathrm{span}\{\varphi_{\mathrm{ro},i}, i = 1, \dots, r\}$. Numerical investigations in [6] 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 $n = 1, 2, \dots$ find $u_r^n = u_{\mathrm{ro}}^n - \bar{u}_h \in X_r$ such that $\forall v_r \in X_r$

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

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

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

for all $u_r, v_r \in X_r \subset X_h$. Setting $\delta_{r,K} = 0$ in (2) recovers the Galerkin ROM. In [6], 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 this 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.