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On the stable solution of transient convection–diffusion equations

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HIGHLIGHTS

- We consider transient convection–diffusion equation with dominating convection.
- The model has an application in optimal control of the asymmetric flow field-flow fractionation process.
- For a stable discretization we propose a monotone edge-averaged finite element (EAFE) scheme.
- EAFE is generalized to a time-dependent case and a new error estimate is proved.
- We present numerical results for comparison with a popular SUPG method.

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ABSTRACT

A transient convection–diffusion equation is considered, which particularly arises in optimization problems for the asymmetric flow field-flow fractionation (AF4) process. A time-dependent generalization of the monotone edge-averaged finite element (EAFE) scheme is used to obtain a stable discretization in the convection-dominated regime. New error estimates are proved for this scheme and a comparison with the popular SUPG method is presented. Numerical experiments demonstrate that the EAFE method is more suitable for problems where boundary layers are formed.

1. Introduction

The dynamics of the concentration of small particles ruled by an external velocity flow field plays an important role in various applications in natural sciences and industry. Typically such problems are described mathematically by convection–diffusion equations coupled with Stokes or Navier–Stokes equations, see e.g., [1,2].

It is well known that in the convection-dominated regime standard Galerkin approximations suffer from a loss of monotonicity, which may result in spurious oscillations and instabilities [3,2]. These difficulties have already been observed in context of finite difference approximations in the early 1960s. Pioneering works on the analysis of stable numerical schemes for one-dimensional convection-dominated convection–diffusion equations has been conducted by Samarskii [4] in context of finite difference and by Christie et al. [5] in context of finite element discretizations.

The Streamline-Upwind Petrov–Galerkin (SUPG) or Streamline-Diffusion (SD) finite element method, introduced by Hughes and Brooks [6], see also [7–9], can be viewed as a multidimensional generalization of such optimal one-dimensional upwind schemes. By adding a consistent diffusion term in streamline direction, this method provides a stable discretization

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tool for convection dominated transport equations. However, SUPG approximations may still develop boundary or internal layers in the crosswind direction (orthogonal to the flow direction) resulting in numerical crosswind layers [10]. Several so-called spurious oscillations at layers diminishing (SOLD) methods have been proposed since the mid 1980s with the aim to remove this drawback [11,12], for an overview see also [13].

Other approaches to a stable numerical solution of (evolutionary) convection–diffusion–reaction equations include discontinuous Galerkin (DG) finite element methods, see, e.g., [14,15] and the references therein, local projection stabilization (LPS) schemes [16,17], which are based on a scale separation and local projections into a larger-scale space, and finite element flux corrected transport schemes (FEM-FCT) [18,19]. Unlike in SUPG, SOLD, DG, or LPS schemes, FEM-FCT achieves the stabilization by modifying the system matrix and the right hand side vector on the algebraic level. For an overview and performance comparison of the above mentioned approaches see [20,21].

There are many applications, for example in semi-conductor device modeling [22,23] or in field-flow fractionation processes [24], where it is desirable that the numerical scheme is monotone, which means that it preserves the maximum principle. Here we consider a transient convection–diffusion problem arising in the optimal control of the asymmetric flow field-flow fractionation (AF4) process, see [25]. The simulation of the AF4 process plays an important role in a number of different applications in medicine, biology, and chemistry.

We study the edge-averaged finite element (EAFE) scheme, which has been proposed in [26] and generalized to problems with tensor coefficients in [27], for transient convection–diffusion problems with a main focus on the aforementioned application. The main contribution of this work concerns the application of this monotone scheme to time-dependent problems, the derivation of a new error estimate (for the transient case), and an experimental comparison with the SUPG method.

The remainder of the paper is organized as follows. In Section 2 we introduce a mathematical description of the problem. Two stable discretizations (SUPG and EAFE schemes) of the state equation are discussed in Section 3, where we also present a new error estimate for the EAFE scheme and comment on some more general convection–diffusion problems. Section 4 is devoted to numerical experiments.

2. Mathematical model

2.1. Problem statement

We consider a flow that satisfies the following Stokes equation:

$$\begin{cases} \triangle\vec{V} - \nabla p = 0, & \text{in } \Omega, \\ \nabla\cdot\vec{V} = 0, & \text{in } \Omega, \\ \vec{V} = \vec{g}(u(t)), & \text{on } \partial\Omega. \end{cases} \tag{1}$$

Here $\vec{V}$ is the velocity field, p is the pressure, $\vec{g}(u)$ is a certain prescribed boundary velocity function (depending on a vector parameter u) and Ω is a bounded polygonal domain in $\mathbb{R}^d$. One can see that, determined by the Dirichlet boundary data $\vec{g}(u(t))$, the velocity flow $\vec{V}(\cdot) = \vec{V}(\cdot; u(t))$ is a function of a time-dependent control parameter $u = u(t)$.

We study a mass-conserving convection–diffusion equation for the concentration $c(x, t)$ of particles or a substance driven by the velocity flow $\vec{V}(x; u(t))$ satisfying the system (1), that is,

$$\begin{cases} \frac{\partial}{\partial t}c + \nabla\cdot\left(\vec{V}c - \varepsilon\nabla c\right) = 0, & (x, t) \in \Omega\times(0, T) \\ c(x, 0) = c_0(x), & x \in \Omega \\ \left(\varepsilon\nabla c - \vec{V}c\right)\cdot\vec{n} = 0, & (x, t) \in \partial\Omega\times(0, T) \end{cases} \tag{2}$$

where ε is a diffusion coefficient and $\vec{n}$ is the outward unit vector normal to the boundary $\partial\Omega$.

According to the boundary condition (last equation in (2)) an appropriate choice of the space for a variational formulation of problem (2) is $V = H^1(\Omega)$. In other words we are looking for a function $c(\cdot, t) \in V$ which satisfies the system (2) at any time moment $t \in (0, T)$.

Multiplying the first equation in (2) by an arbitrary test function $\varphi \in V$, integrating over Ω, using the divergence theorem, and taking into account the incompressibility of the flow $\vec{V}$ (i.e., $\nabla\cdot\vec{V} = 0$) yields

$$\begin{aligned} 0 &= \langle \tfrac{\partial}{\partial t}c, \varphi\rangle_{L^2(\Omega)} + \langle\nabla\cdot(\vec{V}c - \varepsilon\nabla c), \varphi\rangle_{L^2(\Omega)} \\ &= \tfrac{\partial}{\partial t}\langle c, \varphi\rangle_{L^2(\Omega)} + \langle\varphi, (\vec{V}c - \varepsilon\nabla c)\cdot\vec{n}\rangle_{L^2(\partial\Omega)} - \langle\vec{V}c - \varepsilon\nabla c, \nabla\varphi\rangle_{L^2(\Omega)}. \end{aligned}$$

Further, by using the boundary condition we obtain

$$\begin{cases} \frac{\partial}{\partial t}\langle c(t), \varphi\rangle_{L^2(\Omega)} + \left\langle\varepsilon\nabla c(t) - \vec{V}c(t), \nabla\varphi\right\rangle_{L^2(\Omega)} = 0 \quad \forall\varphi \in V, \\ c(0) = c_0, \end{cases} \tag{3}$$

where the first equation in (3) should be understood in the sense of distributions in $(0, T)$, that is, for a.e. $t \in (0, T)$, and the initial condition is regarded as an equivalence of two elements of $L^2(\Omega)$.