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Preserving nonnegativity of an affine finite element approximation for a convection–diffusion–reaction problem

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HIGHLIGHTS

- We present a monotone FEM scheme for a convection–diffusion–reaction problem in 2, 3D.
- The considered equation does not possess an underlying maximum principle.
- Sufficient conditions are given to ensure the nonnegativity of the approximations.
- Numerical examples confirm the necessity and sufficiency of the conditions.

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ABSTRACT

An affine finite element scheme approximation of a time dependent linear convection–diffusion–reaction problem in 2D and 3D is presented. For these equations which do not satisfy an underlying maximum principle, sufficient conditions are given in terms of the coefficient functions, the computational grid and the discretization parameters to ensure that the nonnegativity property of the true solution is also satisfied by its approximation. Numerical examples are given which confirm the necessity and sufficiency of the discretization conditions to guarantee the nonnegativity of the approximation.

1. Introduction

In this paper we consider the finite element approximation of the linear convection–diffusion–reaction problem: *Determine* $u(\mathbf{x}, t)$ *satisfying*

$$\frac{\partial u(\mathbf{x}, t)}{\partial t} - \nabla \cdot a(\mathbf{x}, t)\nabla u(\mathbf{x}, t) + \mathbf{b}(\mathbf{x}, t) \cdot \nabla u(\mathbf{x}, t) + g(\mathbf{x}, t)u(\mathbf{x}, t) = f(\mathbf{x}, t), \quad (\mathbf{x}, t) \in \Omega \times (0, T], \tag{1.1}$$

$$u(\mathbf{x}, t) = 0, \quad (\mathbf{x}, t) \in \partial\Omega \times (0, T], \tag{1.2}$$

$$u(\mathbf{x}, 0) = u_0(\mathbf{x}), \quad \mathbf{x} \in \overline{\Omega}, \tag{1.3}$$

whose well-posedness in the sense of the existence of a classical solution can be found in [1, Theorem 10 p. 206]. Such equations arise in modeling many physical phenomena. Often the unknown quantity u in (1.1)–(1.3) represents a nonnegative physical quantity. In such cases, it is highly desirable that the numerical approximation to u also be nonnegative.

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This paper distinguishes itself by proposing a numerical scheme which preserves the nonnegativity of the solution to the fairly general convection–diffusion–reaction equation (1.1) which does not possess an underlying maximum principle. Moreover, the provided proof brings together the 2D and 3D setting into a single framework, allowing for a simple verification of the computational parameters required to guarantee the nonnegativity of the numerical approximations. Our interest in this problem is motivated by the finite element approximation of the generalized (nonlinear) Burgers–Huxley equation [2], a model that arises in several fields. For example, in electrodynamics, the Burgers–Huxley equation describes the motion of the domain wall of a ferroelectric material in an electric field [3], in biology it is used to model the nerve pulse propagation in nerve fibers [4], and it is also used as a prototype model in the study of interactions between diffusion transport, convection and reaction [5].

For the system of equations (1.1)–(1.3) we assume $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, is a bounded domain, $a(\mathbf{x}, t) \in L^\infty((0, T); L^\infty(\Omega))$, $0 < a_{\min} \le a(\mathbf{x}, t) \le a_{\max}$, $\mathbf{b}(\mathbf{x}, t) \in L^\infty((0, T), H^1(\Omega))$, $g(\mathbf{x}, t), f(\mathbf{x}, t) \in L^\infty((0, T); L^\infty(\Omega))$ and $u_0(\mathbf{x}) \in L^2(\Omega)$, $u_0(\mathbf{x}) \ge 0$. It is straightforward to show that under the additional assumption of smooth coefficients and $\varepsilon g + f > 0$ in $\Omega \times [0, T]$ for all $\varepsilon \in (0, \varepsilon_0)$, the classical solution $u(\mathbf{x}, t)$ is nonnegative [6]. This is the content of the following proposition.

Proposition 1. *Let $u_0 \ge 0$ and all the functions arising in (1.1) be smooth, with the additional constraint that $\varepsilon g + f > 0$ for all $\varepsilon \in (0, \varepsilon_0)$. Then, $u(\mathbf{x}, t) \ge 0$ for all $(\mathbf{x}, t) \in \overline{\Omega} \times [0, T]$.*

Proof. Rewriting (1.1) as

$$\frac{\partial u(\mathbf{x}, t)}{\partial t} - a(\mathbf{x}, t)\Delta u(\mathbf{x}, t) = f(\mathbf{x}, t) - g(\mathbf{x}, t)u(\mathbf{x}, t) + \nabla a(\mathbf{x}, t) \cdot \nabla u(\mathbf{x}, t) - \mathbf{b}(\mathbf{x}, t) \cdot \nabla u(\mathbf{x}, t), \tag{1.4}$$

one can proceed by contradiction by choosing $t = t_0$ to be the first time when u attains the value $u(\mathbf{x}_0, t_0) = -\varepsilon$ for some $\varepsilon \in (0, \varepsilon_0)$ and $\mathbf{x}_0 \in \Omega$. This implies that $u(\mathbf{x}_0, t_0) = \min_{(\mathbf{x},t)\in\overline{\Omega}\times[0,t_0]} u(\mathbf{x}, t)$. Thus, one can conclude that the left hand side of (1.4) is nonpositive, while the right hand side is positive since all the spatial derivatives vanish and $f - u(\mathbf{x}_0, t_0)\, g = f + \varepsilon g > 0$ by assumption. Therefore, we get a contradiction which implies that the function u could not have attained a negative value. □

Hence, it is important for physical relevance, that under such conditions the numerical approximation also should be nonnegative on $\overline{\Omega}$.

Over the years there has been considerable work done on numerical approximation schemes for elliptic and parabolic differential equations that inherit a maximum principle satisfied by the continuous equation being approximated. Here we refer to an equation as satisfying a maximum principle if the maximum of the solution (approximation) can be bounded by the maximum of the initial data, the boundary data, and a constant multiple of the right hand side function (See [7, Def. 2.1]). The following definition makes the previous statement precise.

Definition 1. Define $\mathcal{C} = C^1((0, T); C^2(\Omega))$. For $u \in \mathcal{C}$ set f to be the corresponding function that arises after evaluating u in (1.1). Let $t \in (0, T)$ and define the following sets: $Q_t = \Omega \times (0, t]$, $\Gamma_t = (\partial\Omega \times [0, t]) \cup (\Omega \times \{0\})$. We say that (1.1) satisfies a maximum principle if

$$\min_{\Gamma_t} u + t \min\left\{0, \inf_{Q_t} f\right\} \le u(\mathbf{x}, t) \le \max_{\Gamma_t} u + t \max\left\{0, \sup_{Q_t} f\right\} \tag{1.5}$$

holds for all $u \in \mathcal{C}$ and $(\mathbf{x}, t) \in \Omega \times (0, T)$. Additionally, we say that u is nonnegative if $u(\mathbf{x}, t) \ge 0$ for all $(\mathbf{x}, t) \in \overline{\Omega} \times [0, T]$.

In such cases where a maximum principle holds, the nonnegativity of the solution (approximation) typically follows from the nonnegativity of the data. The equivalence of having the (discrete) nonnegative property and a (discrete) maximum principle has been studied in [7].

Under the assumptions stated above for the parameters in (1.1), Eq. (1.1) does not satisfy an underlying maximum principle as given in Definition 1. To illustrate that, let $\Omega = (0, 1) \times (0, 1) \subset \mathbb{R}^2$, $\mathbf{x} = (x_1, x_2)$ and consider the following linear partial differential equation

$$\begin{aligned} \frac{\partial u(\mathbf{x}, t)}{\partial t} - \Delta u(\mathbf{x}, t) - au(\mathbf{x}, t) &= f(\mathbf{x}, t), \quad (\mathbf{x}, t) \in \Omega \times (0, T), \\ u(\mathbf{x}, 0) &= \sin(\pi x_1)\sin(\pi x_2), \quad \mathbf{x} \in \overline{\Omega}, \\ u(\mathbf{x}, t) &= 0, \quad (\mathbf{x}, t) \in \partial\Omega \times (0, T), \end{aligned}$$

where $a > 0$. Setting $a = 2\pi^2 + 1$ and $f(\mathbf{x}, t) = 0$ implies that the $C^\infty((0, T); C^\infty(\Omega))$ solution is the nonnegative function $u(\mathbf{x}, t) = \sin(\pi x_1)\sin(\pi x_2)\exp(t)$, whose maximum occurs in the interior. However, the maximum cannot be bounded using (1.5).

Herein we determine sufficient conditions on the temporal and spatial discretization parameters, Δt and h, respectively, such that the computed approximation is nonnegative. In the following, we give a brief summary of recent work on discrete maximum principles for the approximation of elliptic and parabolic differential equations. A detailed description of the development in this area is given in [8,9].