Computers and Mathematics with Applications 71 (2016) 1875–1897

Contents lists available at ScienceDirect

Computers and Mathematics with Applications

journal homepage: www.elsevier.com/locate/camwa

An exponential integrator for finite volume discretization of a reaction–advection–diffusion equation

Antoine Tambue *

The African Institute for Mathematical Sciences (AIMS) and Stellenbosch University, 6-8 Melrose Road, Muizenberg 7945, South Africa
Center for Research in Computational and Applied Mechanics (CERECAM), University of Cape Town, 7701 Rondebosch, South Africa
Department of Mathematics and Applied Mathematics, University of Cape Town, 7701 Rondebosch, South Africa

ARTICLE INFO

Article history:
Received 19 August 2015
Received in revised form 1 March 2016
Accepted 3 March 2016
Available online 2 April 2016

Keywords:
Parabolic partial differential equation
Finite volume method
Exponential integrators
Errors estimate

ABSTRACT

We consider the numerical approximation of a general second order semi-linear parabolic partial differential equation. Equations of this type arise in many contexts, such as transport in porous media. Using the finite volume with two-point flux approximation on regular mesh combined with exponential time differencing of order one (ETD1) for temporal discretization, we derive the L^2 estimate under the assumption that the non linear term is locally Lipschitz. Numerical simulations to sustain the theoretical results are provided.

1. Introduction

Flow and transport are fundamental in many geo-engineering applications, including oil and gas recovery from hydrocarbon reservoirs, groundwater contamination and sustainable use of groundwater resources, storing greenhouse gases (e.g. CO_2) or radioactive waste in the subsurface, or mining heat from geothermal reservoirs. Mathematical models of such processes are coupled systems of nonlinear equations with possibly degeneracy appearing in the diffusion and transport terms. The focus of this paper is only on advection–diffusion problem below, involving a nonlinear reaction term,

$$\frac{\partial X}{\partial t} = \nabla \cdot (\mathbf{D}(\mathbf{x})\nabla X) - \nabla \cdot (\mathbf{q}(\mathbf{x})X) + f(\mathbf{x}, X) \quad (\mathbf{x}, t) \in \Omega \times [0, T], \tag{1}$$

where Ω is an open domain of $\mathbb{R}^d$, $d \in \{2, 3\}$, $\mathbf{D}$ is the symmetric dispersion tensor, X is the unknown concentration of the contaminant, $\mathbf{q}$ the Darcy's velocity and f the reaction and source term. For the sake of simplicity, without loss of generality, we assume that f is explicitly independent of time. The model equation (1) finds interest in many engineering problems with specific coefficients. Finite element, finite volume or the combination finite element-finite volume methods are mostly used for space discretization of the problem (1) while explicit, semi implicit and fully implicit methods are usually used for time discretization (see [1–7]). Due to time step size constraints, fully implicit schemes are more popular for time discretization for quite a long time compared to explicit Euler schemes. However, implicit schemes need at each time step a solution of large systems of nonlinear equations. This can be the bottleneck in computations. Improving the efficiency of implicit schemes is currently a major interest in many applications. Recently [8,9] have proposed some alternative techniques to solve the

* Correspondence to: The African Institute for Mathematical Sciences (AIMS) and Stellenbosch University, 6-8 Melrose Road, Muizenberg 7945, South Africa.
E-mail address: antonio@aims.ac.za.

http://dx.doi.org/10.1016/j.camwa.2016.03.001
0898-1221/

corresponding nonlinear equations in implicit schemes based on fixed point iterations in [9], and fixed point iterations coupled with high order splitting technique in [8]. Although the convergence of fixed points methods is generally linear, a quadratic convergence has been obtained in [9]. Recent years, exponential integrators have become an attractive alternative in many evolutions equations (see [10–16,15,17]). In contrast to classical methods, they are robust with respect to the Péclet number, they do not require the solution of large linear systems. Instead they make explicit use of the matrix exponential and related matrix functions. The price to pay is the computing of the matrix exponential functions of the non diagonal matrices, which has revived interest and significance progresses nowadays (see [14,13,15,16,15]).

In this work, we combine a finite volume method with the first order exponential time differencing scheme of order 1 (ETD1). Although both discretization techniques have been together used for solving evolutionary problems like (1) (see [10–12]), a proper combination of rigorous convergence proof of them has been lacking so far. Furthermore the nonlinear term is assumed to be locally Lipschitz, which covers many reaction functions in geo-engineering applications.

The paper is organized as follows. In Section 2, we present the semigroup formulation of (1), the existence and uniqueness of the solution along with some proprieties of the mild solution. In Section 3, we present the finite volume space discretization of (1), the existence and the uniqueness of the corresponding semi-discrete problem, and the L^2 error estimate between the exact solution and the semi-discrete solution. Section 4 presents the time discretization of the semi-discrete problem based on ETD1 scheme, along with the convergence proof of the fully discrete scheme based on finite volume method and ETD1 scheme. We end by providing numerical simulations to sustain the theoretical results in Section 5. These results also show the efficiency of the ETD1 scheme compared to the standard time integrators, from which ETD1 scheme is ten times faster than the standard implicit scheme.

2. Semigroup formulation and well posedness

Let us start by presenting briefly the notation of the main function spaces and norms that we will use in this paper. We denote by $\|\cdot\|$ the norm associated to the inner product $(\cdot,\cdot)$ of the Hilbert space $H = L^2(\Omega)$. The norms in the Sobolev spaces $H^m(\Omega)$, $m \geqslant 0$ will be denoted by $\|.\|_m$. The space $H^{-1}(\Omega)$ is the dual of $H_0^1(\Omega)$ equipped with the norm $\|u\|_{-1} = \sup_{v\in H_0^1(\Omega)} \frac{|(u,v)|}{\|u\|_1}$. For a Banach space $\mathcal{V}$, we denote by $L(\mathcal{V})$ the set of bounded linear mapping from $\mathcal{V}$ to $\mathcal{V}$ and by $L^2(0,T,\mathcal{V})$ the set of all functions v defined on $\Omega \times (0,T)$ for which $v(.,t) \in \mathcal{V}$, $l \in L^2(0,T)$ with $l : t \to \|v(.,t)\|_{\mathcal{V}}$.

We assume that the domain Ω is bounded, has a smooth boundary or is a convex polygon. For the sake of simplicity, without loss of generality, we use the homogeneous Dirichlet boundary condition and also assume that the Darcy velocity $\mathbf{q}$ is known, and satisfies the mass conservation for incompressible fluids without internal source, that is $\nabla\cdot\mathbf{q} = 0$. However for $\nabla\cdot\mathbf{q} \neq 0$, our analysis also works when $\nabla\cdot\mathbf{q} > 0$. The comments on how to extend to the case $\nabla\cdot\mathbf{q} < 0$ are given at Remarks 3.2 and 2.1.

For a given initial condition $X_0 \in H$, the model problem (1) is reformulated as: find the function $X \in L^2(0,T,H^1(\Omega))$ such that

$$\begin{cases} \partial X/\partial t + \mathcal{A}X = f(\mathbf{x},X) & (\mathbf{x},t) \in \Omega \times [0,T] \\ X(\mathbf{x},0) = X_0 & \mathbf{x} \in \Omega \\ X(\mathbf{x},t) = 0 & (\mathbf{x},t) \in \partial\Omega \times (0,T], \end{cases} \tag{2}$$

where

$$\begin{aligned} \mathcal{A}X &= -\nabla\cdot(\mathbf{D}\nabla X) + \nabla\cdot(\mathbf{q}(\mathbf{x})X) \\ &= -\sum_{i,j=1}^{d} \frac{\partial}{\partial x_i}\left(D_{i,j}(\mathbf{x})\frac{\partial X}{\partial x_j}\right) + \sum_{i=1}^{d} q_i(\mathbf{x})\frac{\partial X}{\partial x_i}. \end{aligned}$$

For well posedness of (2), we assume that $\mathbf{D}$ is symmetric, $D_{i,j} \in L^\infty(\Omega)$, $q_i \in L^\infty(\Omega)$ and there exist two positive constants $c_1 > 0$ and $L > 0$ such that

$$\sum_{i,j=1}^{d} D_{i,j}(\mathbf{x})\xi_i\xi_j \geq c_1|\xi|^2 \quad \forall \xi \in \mathbb{R}^d \ \mathbf{x} \in \overline{\Omega} \ c_1 > 0, \tag{3}$$

and

$$|f(\mathbf{x},u) - f(\mathbf{x},v)| \leq L\left(1 + |u|^\gamma + |v|^\gamma\right)|u - v| \quad \forall u, v \in \mathbb{R} \ x \in \overline{\Omega}, \tag{4}$$

where $\gamma = 2$ for $d = 3$ and $\gamma \in [0,\infty)$ for $d = 2$.

Set $V = H_0^1(\Omega)$, the bilinear form associated to the operator $\mathcal{A}$ is given by

$$a(u,v) = \int_\Omega \left(\sum_{i,j=1}^{d} D_{i,j}\frac{\partial u}{\partial x_j}\frac{\partial v}{\partial x_i} + \sum_{i=1}^{d} q_i\frac{\partial u}{\partial x_j}v\right)dx \quad u, v \in V. \tag{5}$$