Journal of Computational and Applied Mathematics 241 (2013) 30–44

Contents lists available at SciVerse ScienceDirect

Journal of Computational and Applied Mathematics

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

An adaptive splitting approach for the quenching solution of reaction–diffusion equations over nonuniform grids

Matthew A. Beauregard *, Qin Sheng

Department of Mathematics and Center for Astrophysics, Space Physics and Engineering Research, Baylor University, One Bear Place # 97328, Waco, TX 76798, United States

ARTICLE INFO

Article history:
Received 26 April 2011
Received in revised form 2 October 2012

Keywords:
Reaction–diffusion equations
Quenching singularity
Degeneracy
Splitting method
Adaptation
Nonuniform grids

ABSTRACT

The numerical solution of a nonlinear degenerate reaction–diffusion equation of the quenching type is investigated. While spatial derivatives are discretized over symmetric nonuniform meshes, a Peaceman–Rachford splitting method is employed to advance solutions of the semidiscretized system. The temporal step is determined adaptively through a suitable arc-length monitor function. A criterion is derived to ensure that the numerical solution acquired preserves correctly the positivity and monotonicity of the analytical solution. Weak stability is proven in a von Neumann sense via the ∞-norm. Computational examples are presented to illustrate our results.

1. Introduction

Nonlinear degenerate reaction–diffusion equations of the quenching type play a vital role in modeling many important physical and engineering processes such as with the modeling of internal combustion [1–4]. These mathematical models may develop singularities in solutions or their derivatives in finite time [2,5–7]. The phenomena can be physically observed when certain environmental parameters exceed their limits in applications. A mathematical interpretation of such singularities is that the nonlinear forcing terms in the differential equations become unbounded when certain critical values are reached in finite time [2,8–10,7]. It has been extremely meaningful to estimate these critical values and the time upon which a quenching may occur through efficient and effective numerical algorithms [6,11–13].

Consider a two-dimensional solid fuel ignition model where the activation energy method has decoupled, that is, the dynamics of temperature is independent of the single-species mass fraction [14]. Let $D = (0, a) \times (0, b)$ for $a, b > 0$, ∂D be its boundary, and let $\Omega = D \times (0, T)$, $S = \partial D \times (0, T)$ where $T \in (0, \infty)$. A degenerate reaction–diffusion problem of the quenching type modeling the anticipated internal combustion process is [5,9,10]

$$\left(x^2 + y^2\right)^{q/2} u_t = u_{xx} + u_{yy} + f(u), \quad q \ge 0, (x, y, t) \in \Omega, \tag{1.1}$$

$$u(x, y, t) = 0, \quad (x, y, t) \in S, \tag{1.2}$$

$$u(x, y, 0) = u_0(x, y), \quad (x, y) \in D, \tag{1.3}$$

where the nonlinear source function, $f(u)$, is strictly increasing for $0 \le u < 1$ with

$$f(0) = f_0 > 0, \qquad \lim_{u \to 1^-} f(u) = \infty.$$

* Corresponding author.
E-mail address: Matthew_Beauregard@baylor.edu (M.A. Beauregard).

0377-0427/$ – see front matter © 2012 Elsevier B.V. All rights reserved.
doi:10.1016/j.cam.2012.10.005

The function $u(x, y, t)$ represents the temperature in the rectangular channel, and x and y are coordinates in the perpendicular and parallel directions to the channel walls, respectively. The function $\left(x^2+y^2\right)^{q/2}$ represents a singularity in the temperature transportation speed causing a degeneracy in Eq. (1.1) [2,15,16]. The parameter $q \in [0, 2)$, for which values close to two indicate a stronger degeneracy in the modeling equation, that is, a stronger defect in the transportation of heat throughout the channel, thus breaking symmetry. The upper bound on q ensures that the inverse of the degeneracy is integrable in the $L^2(D)$ space. The initial temperature $0 \le u_0 \ll 1$. The solution of (1.1)–(1.3) is said to *quench* if there exists a finite time T_c such that

$$\sup\left\{|u_t(x, y, t)| : (x, y) \in \overline{D}\right\} \to \infty, \quad \text{as } t \to T_c^-. \tag{1.4}$$

The value of T_c is referred as the *quenching time*. A necessary condition for this to occur is

$$\max\left\{|u(x, y, t)| : (x, y) \in \overline{D}\right\} \to 1^-, \quad \text{as } t \to T_c^-. \tag{1.5}$$

It has been shown that if f, f_u are nonnegative, then, for any fixed ratio a/b, there exists a unique critical domain D_c, the *quenching domain*, for which the solution of (1.1)–(1.3) quenches and is unique prior to T_c [17,18,9].

Although considerable efforts have been devoted to the field in recent years [5,19,20,10,11,21,22], the development of the theory and computation of quenching solutions, including estimations of quenching domains for (1.1)–(1.3), is still in its infancy. The complication in the numerical study is owed primarily to the following two facts. First, the strong nonlinear singularity may cause rapid changes in the gradient and time derivatives of u as quenching is approached. This requires fine resolution in the spatial and temporal grids. Adaptation of the underlying grids in space and time are often necessary for capturing the singularity precisely. Second, quenching type models are often multi-dimensional and attention needs to be given to the efficiently in singular computations. Splitting techniques have an edge on this issue as they offer efficient and effective means of advancing the numerical solution despite the Sheng–Suzuki barrier [23].

Motivated by aforementioned concerns, this paper focuses on a highly efficient algorithm that employs temporal adaptation coupled with nonuniform meshes. In particular, a suitable criterion is derived that preserves both positive and monotonic properties of the numerical solution while a weak stability is maintained in the presence of perturbations. Additionally, we motivate the use of specially-tailored exponentially graded grids, that is, static nonuniform grids focused about the quenching location. These grids are developed from a priori knowledge of the quenching location and solution shape. Our computational experiments indicate that the employment of such grids allow the computation to be accomplished with fewer grid points while maintaining an excellent agreement with prior results that used larger fixed, fine, and uniform meshes [5,10].

This paper is organized as follows. In Section 2, a second order Peaceman–Rachford splitting scheme is introduced for solving the singular problem (1.1)–(1.3) directly. Temporal steps are determined adaptively through a suitable arc-length monitor function [5]. Finite differences for approximating the spatial derivatives are introduced over a symmetric nonuniform mesh. In Section 3, it is shown that the monotonic property is conserved by the sequence of discrete solutions. Section 4 is devoted to a study of the numerical stability of the adaptive splitting method implemented. Further, Section 5 provides two illustrative examples from computational experiments calculating quenching domains and respective quenching times with the proposed decomposition algorithm. It is found that our results match existing calculations and theoretical predictions satisfactorily. Moreover, the agreement between the theoretical and numerical predications are improved. Finally, a brief summary about the results obtained, as well as some concerns and expectations, are given in Section 6. In the ensuing discussion all lowercase bold letters indicate vectors, uppercase letters are used for matrices. The infinity-norm is used throughout discussions unless otherwise specified.

2. Variable step splitting scheme

The problem (1.1)–(1.3) is rescaled, namely,

$$\begin{aligned} &u_t = \frac{1}{a^2\phi(x, y)}u_{xx} + \frac{1}{b^2\phi(x, y)}u_{yy} + \frac{f(u)}{\phi(x, y)}, \quad (x, y, t) \in \Omega, \\ &0 = u(0, y, t) = u(1, y, t) = u(x, 0, t) = u(x, 1, t), \quad (x, y, t) \in S, \\ &u(x, y, 0) = u_0(x, y), \quad (x, y) \in D, \end{aligned}$$

where $\phi(x, y) = \left(a^2x^2 + b^2y^2\right)^{q/2}$, $q \ge 0$, and $D = (0, 1) \times (0, 1)$.

Utilizing the nonuniform central difference approximation formulas discussed in [24], for given $N > 1$, we may replace spatial derivatives in the differential equation on any variable step mesh (x_i, y_j), for $i, j = 0, \ldots, N$. Let $h_k = x_{k+1} - x_k = y_{k+1} - y_k$ be the spatial step-size in both x and y directions. Consider a set of nonuniform step-sizes defined by

$$h_k = \frac{1}{2\sqrt{N^*}}\left[\sqrt{N^* + \frac{1}{2} - \left|k - \left(N^* - \frac{1}{2}\right)\right|} - \sqrt{N^* - \frac{1}{2} - \left|k - \left(N^* - \frac{1}{2}\right)\right|}\right], \tag{2.1}$$