Numerical Studies of a Nonlinear Heat Equation with Square Root Reaction Term

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Interest in calculating numerical solutions of a highly nonlinear parabolic partial differential equation with fractional power diffusion and dissipative terms motivated our investigation of a heat equation having a square root nonlinear reaction term. The original equation occurs in the study of plasma behavior in fusion physics. We begin by examining the numerical behavior of the ordinary differential equation obtained by dropping the diffusion term. The results from this simpler case are then used to construct nonstandard finite difference schemes for the partial differential equation. A variety of numerical results are obtained and analyzed, along with a comparison to the numerics of both standard and several nonstandard schemes.

Keywords: Mickens discretization; nonstandard finite difference scheme; nonlinear heat equation; numerical solutions; positivity

I. INTRODUCTION

We became interested in the topic of this article after reading a paper by Wilhelmsson et al. [1] on the study of a highly nonlinear parabolic partial differential equation. This equation models the plasma physics of a burning fuel for the generation of energy by means of nuclear fusion. The particular form of this equation they considered can be expressed as:

$$\frac{\partial T}{\partial t} = \frac{1}{10}\frac{\partial^2 (T^{5/2})}{\partial r^2} + \frac{1}{10r}\frac{\partial (T^{5/2})}{\partial r} + (1 - r^2)(aT^2 - bT^{1/2}) \tag{1.1}$$

where a and b are positive parameters, and the boundary conditions are

$$T(1, t) = 0, \quad T(0, t) < \infty. \tag{1.2}$$

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The variable T is the absolute temperature and therefore satisfies the positivity condition $T(r,t) \geq 0$ for $0 \leq r \leq 1$ and $t \geq 0$. The initial condition can take many forms; a realistic analytic possibility is

$$T(r,0) = A(r+B)(r-1)^2 \tag{1.3}$$

where $A > 0$ and $0 < B < 1$.

It should be noted that Eq. (1.1) has both nonlinear diffusion and reaction terms. Further, the $T^{1/2}$ term, in the reaction function, appears with a negative coefficient and, as a consequence, gives rise to dissipation. Prior to now, our efforts [2–7], along with those of Pedro Jordan [8], have not been successful in constructing positivity-preserving nonstandard finite difference schemes for the full equation given in Eq. (1.1). Thus, in order to better understand the dynamics of Eq. (1.1), we undertake in this article the study of some related, simplified differential equations having only the square root term. The first "toy equation" to be examined is the first-order, nonlinear ordinary differential equation

$$\frac{dT}{dt} = -\lambda T^{1/2}, \quad T(t_0) = T_0. \tag{1.4}$$

where λ is a positive parameter. This equation neglects both nonlinear diffusion and the $a(1-r^2)T^2$ term in the reaction function. Next, we examine a nonlinear partial differential equation having linear diffusion but also containing the square-root term, i.e.,

$$\frac{\partial T}{\partial t} = D\frac{\partial^2 T}{\partial x^2} - \lambda T^{1/2}, \tag{1.5}$$

where $D > 0$,

$$T(x,0) = f(x) \quad \text{and } T(0,t) = T(1,t) = 0.$$

and $f(x)$ is a given initial condition. Our major reason for studying these two "toy equations" is the belief that their analysis can provide fundamental understandings into how one should proceed with the construction of finite difference schemes for Eq. (1.1).

In the next section, we construct several nonstandard finite difference schemes for Eq. (1.4). The corresponding numerical solutions are obtained and compared to both a standard discretization and the exact solution. An important feature of the exact solution is that from an initial positive value at $t = 0$, the solution goes to zero in finite time. Because the exact solution is known, an exact finite difference scheme can be written down and this will allow us to also make comparisons between the numerical solutions of our constructed discretizations and the numerical values from the exact solution. Thus, by studying reasonable nonstandard finite difference schemes for Eq. (1.4) and carrying out comparative analyses to the exact numerical solutions of this equation, valuable insight can be obtained as to how one should select the best numerical approximation techniques for when the differential equation being solved does not possess a known exact solution. One example of such an equation is the nonlinear partial differential equation given in Eq. (1.5).

In the third section, we show how to construct positivity preserving schemes for Eq. (1.5) and carry out numerical experiments for a particular initial and boundary value problem. We also find an important functional relationship between the time and space time-sizes. Numerical results for different approximations are also given.

Finally, in the last section, we present a summary of our results detailed earlier in the paper. We also present plans for future work.

Certain expressions are used frequently in this paper. Therefore, it is useful to use the following abbreviations:

FD:	finite difference
IVP:	initial value problem
NSFD:	nonstandard finite difference
ODE:	ordinary differential equation
PDE:	partial differential equation.

II. THE SIMPLIFIED ODE

In this section of the article we analyze the simplified ODE found in Eq. (1.4). It is a separable, first-order ODE and an explicit expression can be found for its solution. In Section IIA, we give this solution. Next, in Section IIB we derive the exact FD scheme, a standard FD scheme and several NSFD schemes. Section IIC presents a short comparative analysis of the numerical solutions for these discretizations.

A. Exact Solution

With $T_0 > 0$, the IVP

$$\frac{dT}{dt} = -\lambda T^{1/2}, \quad T(t_0) = T_0, \tag{2.1}$$

can be solved to give

$$T(t) = \frac{1}{4}\left[2T_0^{1/2} - \lambda(t - t_0)\right]^2. \tag{2.2}$$

Because $\frac{dT}{dt} \leq 0$, it follows from Eq. (2.2) that $T(t)$ reaches zero at some time t^*, i.e. $T(t^*) = 0$, and that for $t > t^*$, it must be that $T(t) = 0$. The value for t^* is easily obtained from Eq. (2.2) and is given by

$$t^* = \left(\frac{1}{\lambda}\right)\left[2T_0^{1/2} + \lambda t_0\right], \tag{2.3}$$

or for $t_0 = 0$,

$$t^* = \frac{2T_0^{1/2}}{\lambda}. \tag{2.4}$$

As a consequence of these results, we conclude that the exact solution to the IVP given by Eq. (2.1), is

$$T(t) = \begin{cases} \frac{1}{4}\left[2T_0^{1/2} - \lambda(t - t_0)\right]^2, & 0 \leq t_0 \leq t < t^* \\ 0, & t \geq t^*. \end{cases} \tag{2.5}$$

For Eq. (2.1), $T(t) = 0$ is a singular solution and the composite solution given in Eq. (2.5) is also a classical solution since both it and its first derivative are continuous. For more details, see Kaplan [9, pp. 328].

Note that (take $t_0 = 0$) t^* is the time scale for the problem. By choosing T_0 as a scaling for $T(t)$, a scaled version of Eq. (2.1) can be written as

$$\frac{dS}{ds} = -2S^{1/2}, \quad S(0) = 1, \tag{2.6}$$

where $S = \frac{T}{T_0}$ and $s = \frac{t}{t^*}$ and the exact solution to the scaled problem given in (2.6) is

$$S(s) = \begin{cases} (1-s)^2, & 0 \le s < 1 \\ 0, & s \ge 1. \end{cases} \tag{2.7}$$

An interesting observation is that Eq. (2.1) can also be regarded as a special case of Chrystal's equation which arises in nonlinear poroacoustics. See, for example, Section VI6 of Jordan [10].

B. Discretizations

An exact FD scheme for the simplified ODE can be constructed from the general solution given in Eq. (2.5). This involves discretizing the exact solution given in Eq. (2.5) by applying the following transformations:

$$\begin{aligned} t &\to t_{k+1} \\ t_0 &\to t_k \\ T_0 &\to T_k \\ T(t) &\to T_{k+1} \end{aligned}$$

where $t_k = hk$, $h = \Delta t$, and $T_k = T(t_k)$. The resulting exact standard FD scheme can then be obtained as follows:

$$\begin{aligned} T_{k+1} &= \frac{1}{4}\left[2T_k^{1/2} - \lambda(t_{k+1} - t_k)\right]^2 \\ &= \frac{1}{4}\left[2T_k^{1/2} - \lambda h\right]^2 \\ &= \frac{1}{4}\left[4T_k - 4T_k^{1/2}\lambda h + \lambda^2 h^2\right] \\ T_{k+1} &= T_k - (\lambda h)T_k^{1/2} + \frac{\lambda^2 h^2}{4}, \end{aligned}$$

and this can be rewritten as

$$\frac{T_{k+1} - T_k}{h} = -\lambda T_k^{1/2} + \frac{\lambda^2 h}{4}. \tag{2.8}$$

Observe that in the above expression an extra term appears on the right-side compared to the standard forward-Euler approximation of (2.1) which is

$$\frac{T_{k+1} - T_k}{h} = -\lambda T_k^{1/2}. \tag{2.9}$$

A first NSFD scheme [4, 5, 7] can be derived by manipulating the right-side of (2.1), i.e. writing it as

$$\frac{dT}{dt} = -\lambda T^{1/2} = -\lambda \frac{T}{T^{1/2}} \tag{2.10}$$

and then discretizing this expression to give

$$\frac{T_{k+1} - T_k}{h} = -\lambda \left(\frac{T_{k+1}}{T_k^{1/2}} \right). \tag{2.11}$$

Solving for T_{k+1} gives

$$T_{k+1} = \left(\frac{T_k^{1/2}}{\lambda h + T_k^{1/2}} \right) T_k. \tag{2.12}$$

Since $\lambda h > 0$ the term in the bracket is always less than one in magnitude and thus it follows that

$$0 \leq T_{k+1} \leq T_k. \tag{2.13}$$

and it can be concluded that the solution to Eq. (2.12) monotonically decreases to zero.

A second NSFD scheme can be constructed by use of the following discretization

$$T^{1/2} \to \left(\frac{2T_{k+1}}{T_{k+1} + T_k} \right) T_k^{1/2}, \tag{2.14}$$

which gives

$$\frac{T_{k+1} - T_k}{h} = -\lambda T_k^{1/2} \left(\frac{2T_{k+1}}{T_{k+1} + T_k} \right). \tag{2.15}$$

This equation is quadratic in T_{k+1}. Solving for the non-negative solution gives the expression

$$T_{k+1} = -(\lambda h) T_k^{1/2} + \sqrt{T_k^2 + (\lambda h)^2 T_k}, \tag{2.16}$$

and this can be re-written as

$$\frac{T_{k+1} - T_k}{h} = -\lambda T_k^{1/2} + \left\{ \frac{\sqrt{T_k^2 + (\lambda h)^2 T_k} - T_k}{h} \right\}. \tag{2.17}$$

In the numerical calculations, the FD schemes in Eqs. (2.12) and (2.16) were denoted as NSFD(1) and NSFD(2).

C. Numerical Experiments

We now have four FD schemes which can be used to obtain numerical solutions to the IVP given in Eq. (2.1). They are (i) the exact scheme, Eq. (2.8); (ii) the standard scheme, Eq. (2.9); (iii) NSFD(1), the nonstandard scheme of Eq. (2.12); and (iv) NSFD(2), the nonstandard scheme of Eq. (2.16).

In the numerical experiments, the following parameter values were selected: $t_0 = 0$, $T_0 = 1$, $\lambda = 1$, and $h = W/N$ where $N = 100$ and W is the maximum value of the t variable; thus

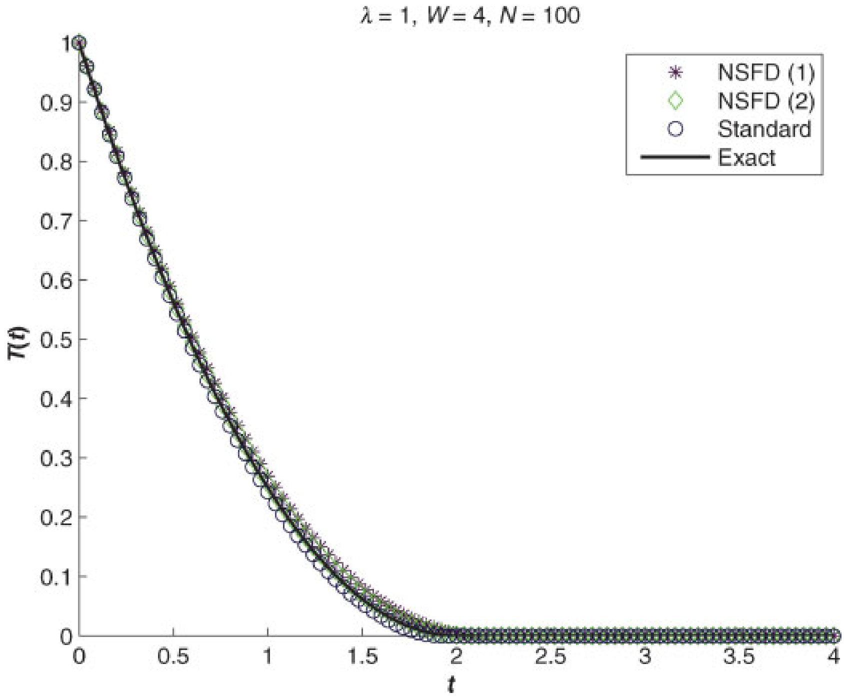

FIG. 1. Comparison of NSFD(1), NSFD(2), the standard scheme, and the exact scheme for Eq. (2.1). [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

$W = \mathcal{O}(1)$ and, in general, was chosen to be $W = 4$ for our numerical simulations. Note that for these choice of parameter values, $t^* = 2$.

Inspection of Figs. 1 and 2 allows the following conclusions to be made:

- (i) All four FD schemes give good numerical representations of the actual solution to Eq. (2.1).
- (ii) The largest numerical errors occur in the NSFD(1).
- (iii) The error in the NSFD(2) and standard FD schemes are essentially the same except for t values near $t^* = 2$.
- (iv) All schemes give a numerically zero solution for t greater than about t^*. Note that the standard scheme goes to zero (at least computationally) at $t = t^*$, while NSFD(2) does so at a slightly higher value than t^*, and NSFD(1), the worst of the three schemes, achieves zero for its solution at a still larger value of t^*. Thus, in terms of accuracy, the three schemes are ranked as follows: standard (most accurate), NSFD(2), and NSFD(1) (least accurate).

Although the results listed in (iv) may come as something of a surprise, it should be kept in mind that we have not tried to optimize the NSFD schemes with regard to their numerical accuracy. Our main goal in this article is to see what viable methods exist, so that when NSFD schemes are constructed for a nonlinear PDE containing a $T^{1/2}$ term, the positivity conditions will hold for the discretization.

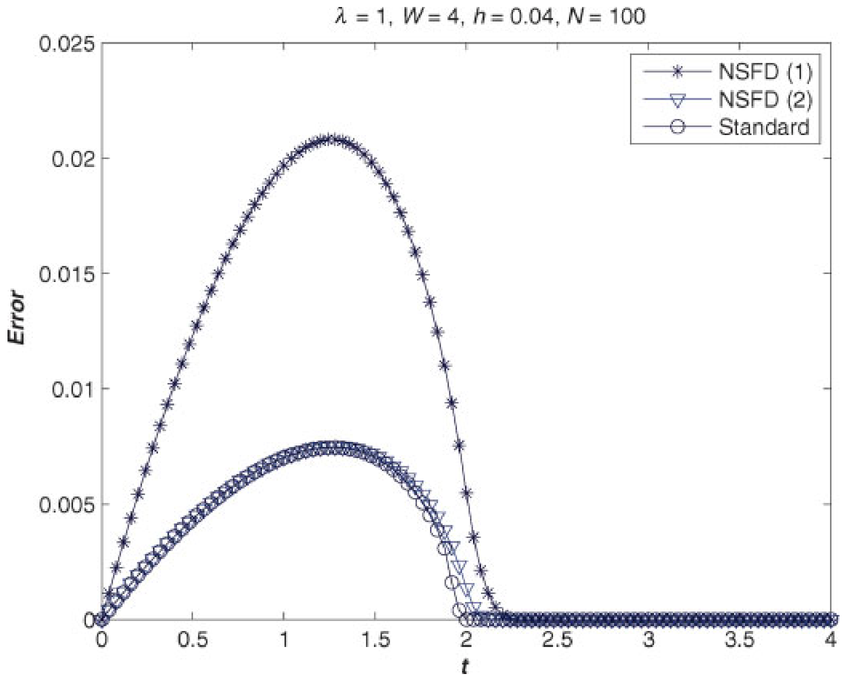

FIG. 2. Plot of the differences between the NSFD(1), NSFD(2), the standard scheme, and the exact FD scheme. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

It should be indicated that the replacement given by Eq. (2.14) is one of many possible forms. Another possibility is

$$T^{1/2} \to \frac{T_{k+1}}{\sqrt{\frac{T_{k+1}+T_k}{2}}}. \tag{2.18}$$

III. HEAT PDE WITH $T^{1/2}$ TERM

The work of the last section provides hints as to how the (much) simplified PDE of Wilhelmsson et al.

$$\frac{\partial T}{\partial t} = D\frac{\partial^2 T}{\partial x^2} - \lambda T^{1/2}; \quad 0 \le x \le 1, t > 0 \tag{3.1}$$

$$T(x,0) = f(x) = \text{ given}, \quad T(0,t) = T(1,t) = 0, \tag{3.2}$$

could be discretized. Note that a standard FD scheme for Eq. (3.1) is given by the expression

$$\frac{T_m^{k+1} - T_m^k}{\Delta t} = D\left[\frac{T_{m+1}^k - 2T_m^k + T_{m-1}^k)}{(\Delta x)^2}\right] - \lambda\left(\tilde{T}_m^k\right)^{1/2} \tag{3.3}$$

where $\tilde{T}_m^k$ can take a variety of forms such as

$$\left(\tilde{T}_m^k\right)^{1/2} = \left(T_m^k\right)^{1/2}, \tag{3.4a}$$

$$\left(\tilde{T}_m^k\right)^{1/2} = \sqrt{\frac{T_{m+1}^k + T_m^k + T_{m-1}^k}{3}}, \tag{3.4b}$$

$$\left(\tilde{T}_m^k\right)^{1/2} = \frac{\sqrt{T_{m+1}^k} + \sqrt{T_m^k} + \sqrt{T_{m-1}^k}}{3}. \tag{3.4c}$$

In the above discretizations, we use the notation $t \to t_k = k(\Delta t)$, $x \to x_m = m(\Delta x)$, and $T(x,t) \to T_m^k$. Thus, k and m are, respectively, the discrete time and space variables, and T_m^k is an approximation to $T(x_m, t_k)$.

Solving Eq. (3.3) for T_m^{k+1} gives

$$T_m^{k+1} = DR\left(T_{m+1}^k + T_{m-1}^k\right) + (1 - 2DR)T_m^k - (\lambda \Delta t)\left(\tilde{T}_m^k\right)^{1/2} \tag{3.5}$$

where $R = \frac{\Delta t}{(\Delta x)^2}$. If T_m^k satisfies a positivity condition, i.e.

$$T_m^k \geq 0 \quad (k\text{-fixed, all relevant } m) \tag{3.6}$$

then T_m^{k+1} is not necessarily non-negative. To obtain an assured positivity preserving scheme, we apply what was learned in the previous section and use the following discretization

$$\frac{T_m^{k+1} - T_m^k}{\Delta t} = D\left[\frac{T_{m+1}^k - 2T_m^k + T_{m-1}^k}{(\Delta x)^2}\right] - \lambda\left[\frac{T_m^{k+1}}{\left(\tilde{T}_m^k\right)^{1/2}}\right] \tag{3.7}$$

where $(\tilde{T}_m^k)$ takes one of the forms given in Eq. (3.4) or any such equivalent expression. Examination of this last equation shows that it is linear in T_m^{k+1}; therefore solving for it gives

$$T_m^{k+1} = DR\left[DR\left(T_{m+1}^k + T_{m-1}^k\right) + (1 - 2DR)T_m^k\right]\left[\frac{\left(\tilde{T}_m^k\right)^{1/2}}{(\lambda \Delta t) + \left(\tilde{T}_m^k\right)^{1/2}}\right]. \tag{3.8}$$

Inspection of Eq. (3.8) shows that positivity of the evolved solutions is certain if the following condition holds:

$$1 - 2DR \geq 0. \tag{3.9}$$

As in previous work [5, 7], we let

$$1 - 2DR = \gamma DR, \quad \gamma \geq 0, \tag{3.10}$$

where γ is a non-negative number. This gives us, first, a relationship between the time and space step-sizes, i.e.

$$\Delta t = \frac{(\Delta x)^2}{(2 + \gamma)D}, \tag{3.11}$$

and allows the following representation for this NSFD scheme:

$$T_m^{k+1} = DR\big[T_{m+1}^k + \gamma T_m^k + T_{m-1}^k\big]\left[\frac{\big(\tilde{T}_m^k\big)^{1/2}}{(\lambda\Delta t) + \big(\tilde{T}_m^k\big)^{1/2}}\right]. \tag{3.12}$$

To use this scheme, the following steps should be carried out:

(i) Select values for D, λ, and Δx.
(ii) Determine Δt from Eq. (3.11).
(iii) Select a set of boundary values and initial conditions.
(iv) Use the NSFD scheme of Eq. (3.12) to calculate the numerical solutions of Eq. (3.1).

We have carried out simulations using FD schemes. They are indicated by the following notations:

(a) Standard: Eq. (3.3) with $\tilde{T}_m^k = T_m^k$.
(b) NSFD(1): Eq. (3.12) with $\tilde{T}_m^k$ given by Eq. (3.4a).
(c) NSFD(2): Eq. (3.12) with $\tilde{T}_m^k$ given by Eq. (3.4b).
(d) NSFD(3): Eq. (3.12) with $\tilde{T}_m^k$ given by Eq. (3.4c).

The initial condition was selected to be

$$T(x,0) = \sin(\pi x), \quad 0 \le x \le 1, \tag{3.13}$$

with the boundary conditions

$$T(0,t) = T(1,t) = 0, \quad t > 0. \tag{3.14}$$

Typical results from our numerical experiments are given in Figs. 3–5. The representative numerics for NSFD(2) and NSFD(3) are presented in, respectively, Figs. 3 and 4. Note that in each case, the solution decreases monotonically with an increase in time as, as expected, the solutions are smooth and positive. No known exact solutions of Eq. (3.1) exist; consequently we cannot make a comparison with such a solution. However, in Fig. 5 we show the difference between the standard scheme and NSFD(1). These differences are small and decrease with time.

IV. DISCUSSION AND CONCLUSION

Our primary goal in studying the discretizations given in Sections I and II was to gain insight that could aid us in the formulation of improved FD schemes for more complex differential equations such as Eq. (1.1). The major difficulty is how to construct discrete models that also satisfy a condition of positivity as required by the physical principles operating as constraints on the structure of the mathematical (usually differential) equations. This issue is important and its importance derives from the fact that many numerical instabilities arise from violation of some physical principle by the FD equations [5–7]. In this article, we have demonstrated one possible mechanism for dealing effectively with terms of the form T^α where $0 < \alpha < 1$. The case when $\alpha < 1$

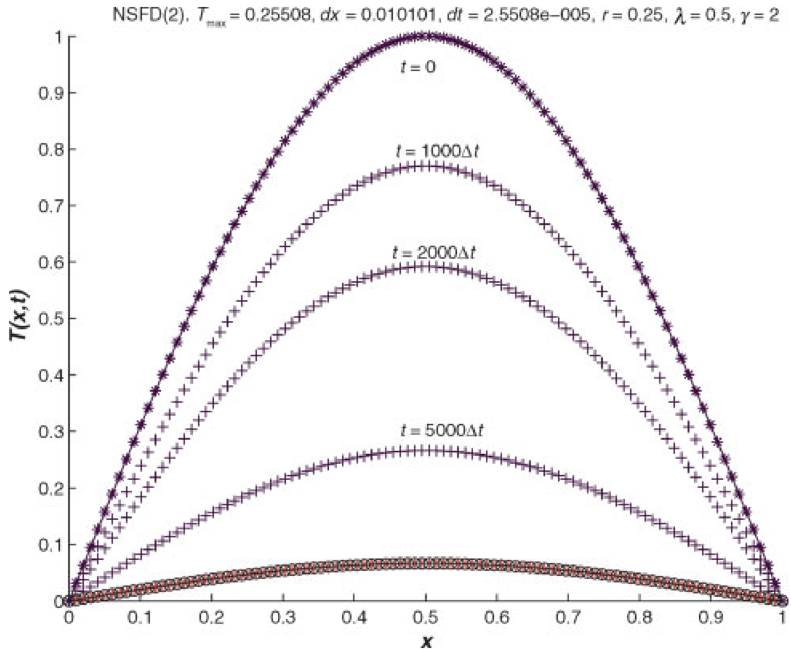

FIG. 3. Plots of the NSFD(2) scheme at various times. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

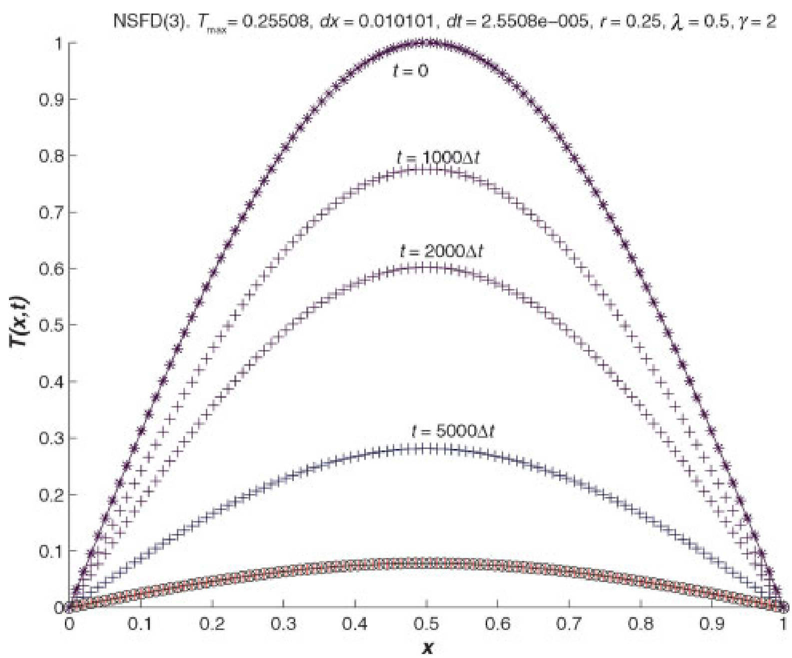

FIG. 4. Plots of the NSFD(3) scheme at various times. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

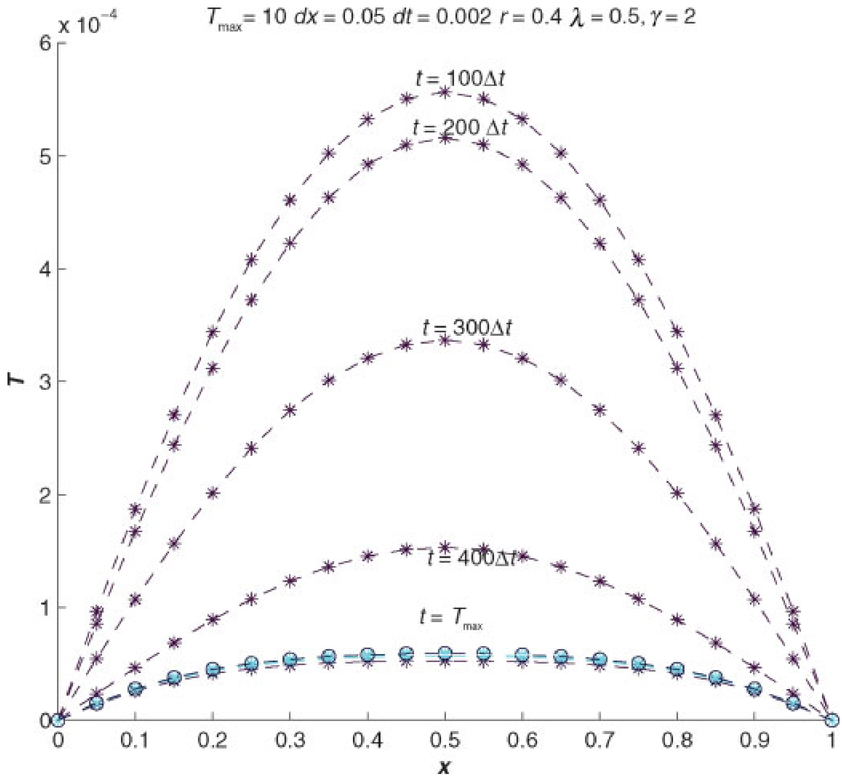

FIG. 5. Plot of the differences between the standard scheme and the NSFD(1) scheme. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

presently offers no fundamental problems within the framework of the current NSFD scheme methodology [5–7]. The work presented in Sections II and III illustrate one possibility for this resolution. Clearly, alternative methods may also exist to eliminate these issues.

The major conclusions from the calculations and constructions we have given here are:

(i) positivity can be satisfied in FD schemes where fractional power terms appear;
(ii) the study of rather elementary or "toy model" differential equations can provide insight into what should be done for more complex ODEs and PDEs;
(iii) currently, no principle exists to restrict possible discretizations for terms such as T^{α}, $0 < \alpha < 1$.

This last point is one of the topics of research that we are currently studying. Finally, based on the work done in this article, we are extending these results to the full version of Eq. (1.1).

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