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

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November 12, 2008

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

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I. Introduction

Wilhelmsson *et al* [1] consider a highly nonlinear parabolic partial differential equation to model the plasma physics of a burning fuel for the generation of energy by means of nuclear fusion:

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

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

$$T(1,t) = 0, \qquad T(0,t) < \infty. \tag{2}$$

The variable T is the absolute temperature and therefore satsifies 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

$$T(r,0) = A(r+B)(r-1)^2 \tag{3}$$

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

It should be noted that Equation (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

II. The Simplified ODE

In order to better understand the dynamics of Equation (1), we first 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

$$\frac{dT}{dt} = -\lambda T^{1/2}, \qquad T(t_0) = T_0, \tag{4}$$

where $\lambda > 0$ and $T_0 > 0$.

A. Exact Solution

The exact solution to Equation (4) is

$$T(t) = \begin{cases} \frac{1}{4}\left[2T_0^{1/2} - \lambda(t - t_0)\right]^2, & 0 \le t_0 \le t < t^* \\ 0, & t \ge t^*. \end{cases} \tag{5}$$

where

$$t^* = \frac{2T_0^{1/2}}{\lambda}. \tag{6}$$

Of course $T(t) = 0$ is also a singular solution of Equation (4).

B. Discretizations

An exact finite difference scheme for the simplified ODE in Equation (4) can be constructed from the general solution given in Equation (5) by discretizing the exact solution and applying the following transformations:

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

where $t_k = hk$, $h = \Delta t$, and $T_k = T(t_k)$, to produce

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

The resulting exact standard finite difference scheme is

$$\frac{T_{k+1} - T_k}{h} = -\lambda T_k^{1/2} + \frac{\lambda^2 h}{4}. \tag{7}$$

Observe that in the above expression an extra term appears on the right-side compared to the standard forward-Euler approximation of (4) which is

$$\frac{T_{k+1} - T_k}{h} = -\lambda T_k^{1/2}. \tag{8}$$

B.1 First NSFD Scheme

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

$$\frac{dT}{dt} = -\lambda T^{1/2} = -\lambda \frac{T}{T^{1/2}} \tag{9}$$

and then discretizing this expression to give

$$\frac{T_{k+1} - T_k}{h} = -\lambda \left(\frac{T_{k+1}}{T_k^{1/2}} \right). \tag{10}$$

Solving for T_{k+1} gives

$$T_{k+1} = \left(\frac{T_k^{1/2}}{\lambda h + T_k^{1/2}} \right) T_k. \tag{11}$$

This first nonstandard finite difference scheme is denoted NSFD(1) in the numerical experiments

B.2 Second NSFD Scheme

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

$$T^{1/2} \rightarrow \left(\frac{2T_{k+1}}{T_{k+1} + T_k} \right) T_k^{1/2}, \qquad (12)$$

which gives

$$\frac{T_{k+1} - T_k}{h} = -\lambda T_k^{1/2} \left(\frac{2T_{k+1}}{T_{k+1} + T_k} \right). \qquad (13)$$

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

$$\frac{T_{k+1} - T_k}{h} = -\lambda T_k^{1/2} + \left\{ \frac{\sqrt{T_k^2 + (\lambda h)^2 T_k} - T_k}{h} \right\}. \qquad (14)$$

The nonstandard finite difference scheme in Equation (14) is denoted NSFD(2) in the numerical experiments

III. Numerical Experiments

We now have four FD schemes which can be used to obtain numerical solutions to the IVP given in Equation (4). They are (i) the exact scheme, Equation (7); (ii) the standard scheme, Equation (8); (iii) NSFD(1), the nonstandard scheme of Equation (11); and (iv) NSFD(2), the nonstandard scheme of Equation (14).

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 $W = \mathcal{O}(1)$ 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 Figure 1 and Figure 2 allows the following conclusions to be made:

(i) All four FD schemes give good numerical representations of the actual solution to Equation (4).

(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).

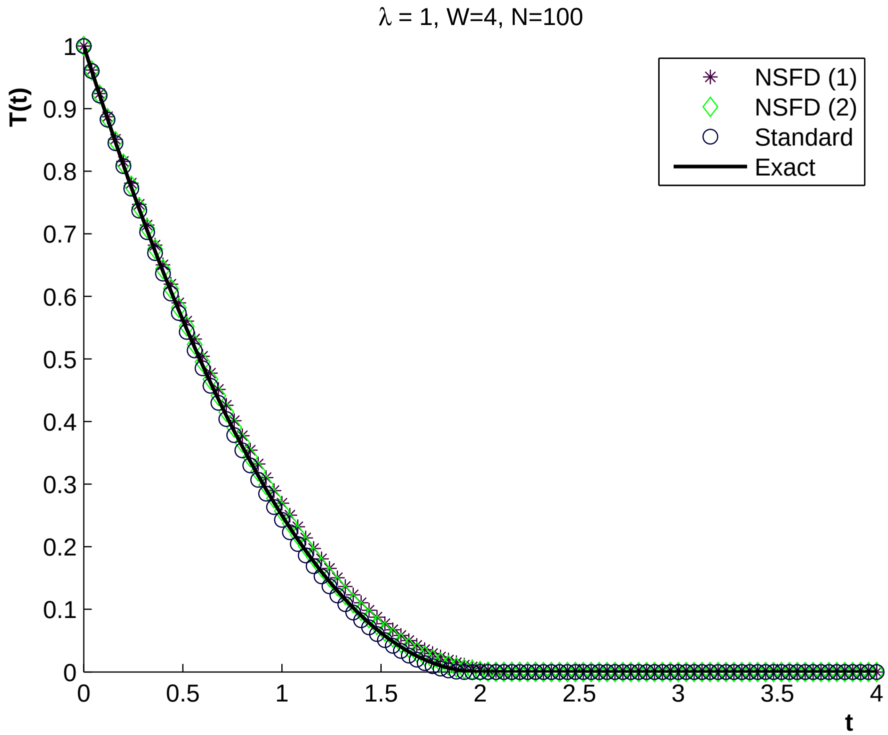

Figure 1: Comparison of NSFD(1), NSFD(2), the standard scheme, and the exact scheme for Equation (4).

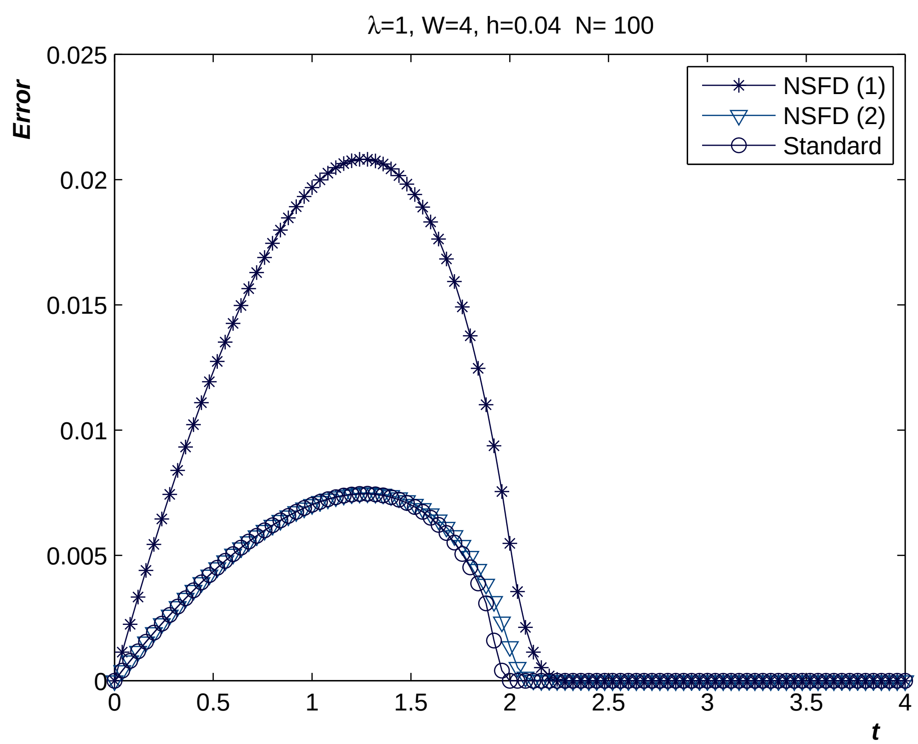

Figure 2: Plot of the differences between the NSFD(1), NSFD(2), the standard scheme, and the exact FD scheme

IV. The Simplified PDE

Our previous work with the "toy problem" provides hints for how to discretize the Simplified PDE given by

$$\frac{\partial T}{\partial t} = D\frac{\partial^2 T}{\partial x^2} - \lambda T^{1/2}; \quad 0 \le x \le 1, t > 0 \tag{15}$$

$$T(x,0) = f(x) = \text{given}, T(0,t) = T(1,t) = 0. \tag{16}$$

A standard finite difference scheme for Equation (15) is given by the expression

$$\frac{T_m^{k+1} - T_m^k}{\Delta t} = D\left[\frac{T_{m+1}^k - 2T_m^k + T_{m-1}^k)}{(\Delta x)^2}\right] - \lambda(\tilde{T}_m^k)^{1/2} \tag{17}$$

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

$$(\tilde{T}_m^k)^{1/2} = (T_m^k)^{1/2}, \tag{18a}$$

$$(\tilde{T}_m^k)^{1/2} = \sqrt{\frac{T_{m+1}^k + T_m^k + T_{m-1}^k}{3}}, \tag{18b}$$

$$(\tilde{T}_m^k)^{1/2} = \frac{\sqrt{T_{m+1}^k} + \sqrt{T_m^k} + \sqrt{T_{m-1}^k}}{3}. \tag{18c}$$

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 Equation (17) for T_m^{k+1} gives

$$T_m^{k+1} = DR(T_{m+1}^k + T_{m-1}^k) + (1-2DR)T_m^k - (\lambda\Delta t)(\tilde{T}_m^k)^{1/2} \tag{19}$$

where $R = \dfrac{\Delta t}{(\Delta x)^2}$. If $T_m^k \geq 0$(k-fixed, all relevant m) then T_m^{k+1} is not necessarily non-negative.

$$\frac{T_m^{k+1} - T_m^k}{\Delta t} = D\left[\frac{T_{m+1}^k - 2T_m^k + T_{m-1}^k}{(\Delta x)^2}\right] - \lambda\left[\frac{T_m^{k+1}}{(\tilde{T}_m^k)^{1/2}}\right] \tag{20}$$

where $(\tilde{T}_m^k)$ takes one of the forms given in Equation (18) 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

$$T_m^{k+1} = [DR(T_{m+1}^k + T_{m-1}^k) + (1-2DR)T_m^k]\left[\frac{(\tilde{T}_m^k)^{1/2}}{(\lambda\Delta t) + (\tilde{T}_m^k)^{1/2}}\right]. \tag{21}$$

Inspection of Equation (21) shows that positivity of the evolved solutions is certain if the following condition holds:

$$1 - 2DR \geq 0. \tag{22}$$

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

$$1 - 2DR = \gamma DR, \quad \gamma \geq 0, \tag{23}$$

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

$$\Delta t = \frac{(\Delta x)^2}{(2+\gamma)D}, \tag{24}$$

and allows the following representation for this NSFD scheme:

$$T_m^{k+1} = DR[T_{m+1}^k + \gamma T_m^k + T_{m-1}^k]\left[\frac{(\tilde{T}_m^k)^{1/2}}{(\lambda\Delta t) + (\tilde{T}_m^k)^{1/2}}\right]. \tag{25}$$

V. Numerical Results

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

(i) Select values for D, λ and Δx.

(ii) Determine Δt from Equation (24).

(iii) Select a set of boundary values and initial conditions.

(iv) Use the NSFD scheme of Equation (25) to calculate the numerical solutions of Equation (15).

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

(a) Standard: Equation (17) with $\tilde{T}_m^k = T_m^k$.

(b) NSFD(1): Equation (25) with $\tilde{T}_m^k$ given by Equation (18a).

(c) NSFD(2): Equation (25) with $\tilde{T}_m^k$ given by Equation (18b).

(d) NSFD(3): Equation (25) with $\tilde{T}_m^k$ given by Equation (18c).

The initial condition was selected to be

$$T(x,0) = \sin(\pi x), \qquad 0 \le x \le 1, \tag{26}$$

with the boundary conditions

$$T(0,t) = T(1,t) = 0, \qquad t > 0. \tag{27}$$

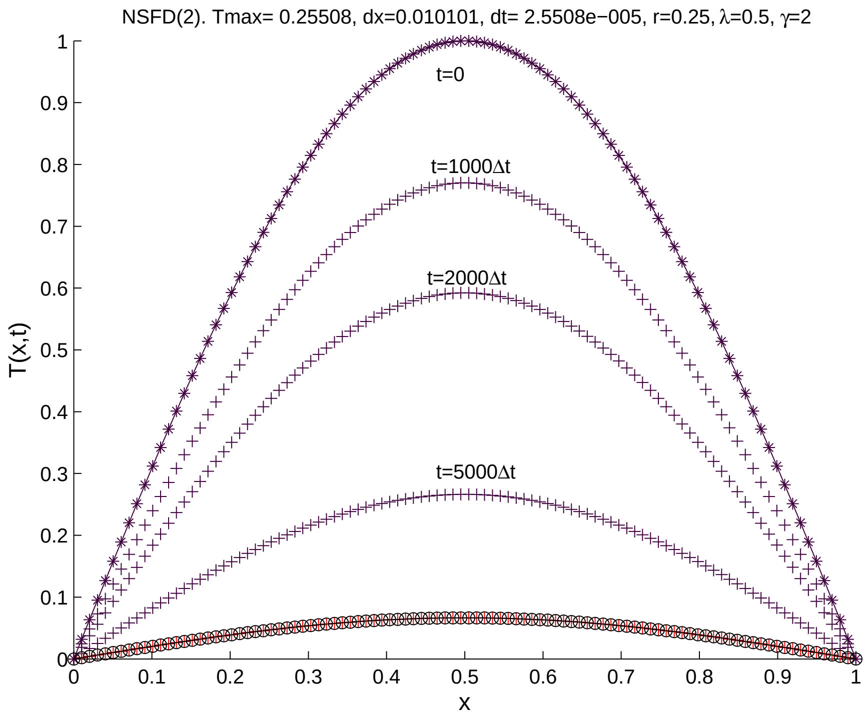

Figure 3: Plots of the NSFD(2) scheme at various times.

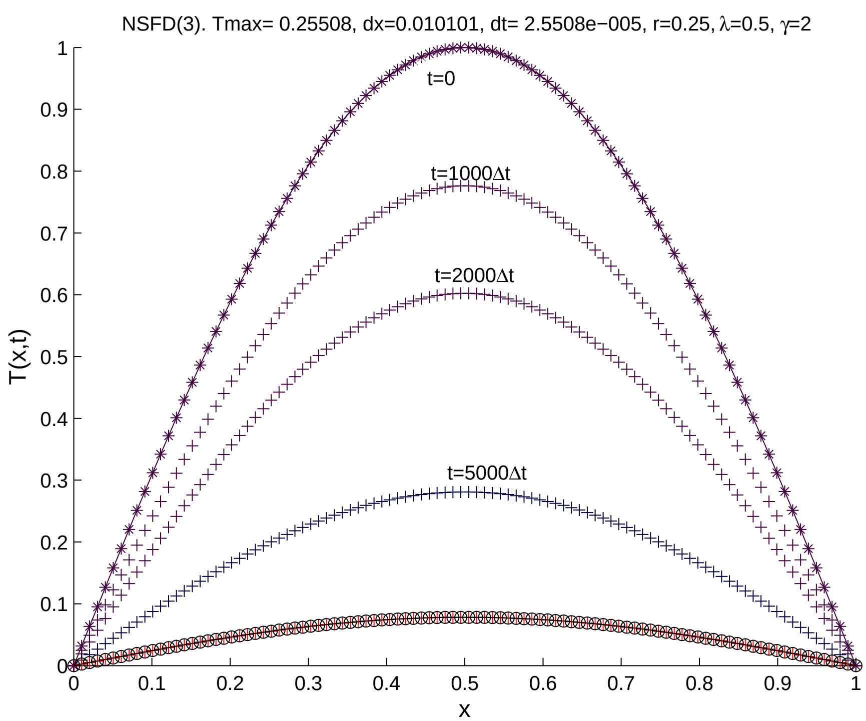

Figure 4: Plots of the NSFD(3) scheme at various times

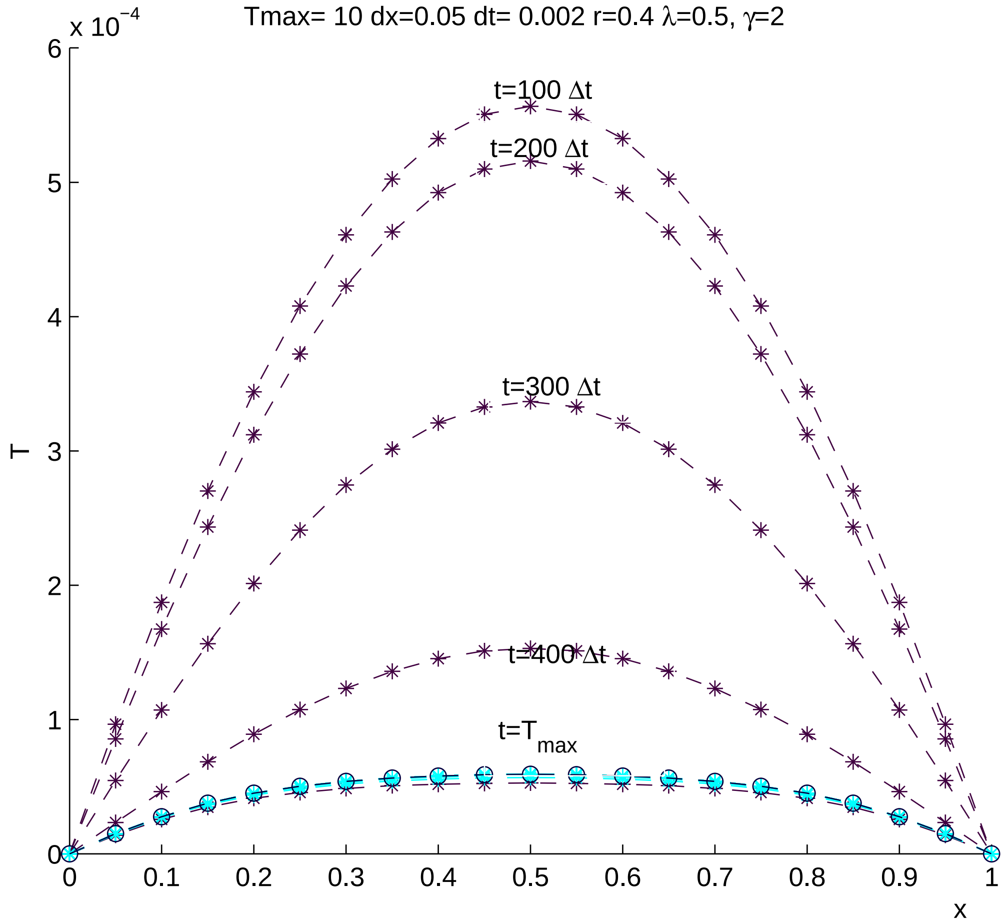

Figure 5: Plot of the differences between the standard scheme and the NSFD(1) scheme.

VI. Discussion and Conclusion

Our primary goal in studying the discretizations given in Sections 1 and 2 was to gain insight that could aid us in the formulation of improved FD schemes for more complex differential equations such as Equation (1). The major difficulty is how to construct discrete models that also satiisfy 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, 6, 7]. In this paper, we have demonstrated one possible mechanism for dealing effectively with terms of the form T^{α} where $0 < \alpha < 1$. The case when $\alpha < 1$ presently offers no fundamental problems within the framework of the current NSFD scheme methodology [5, 6, 7]. The work presented in Sections 2 and 3 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 comples ODEs and PDEs;

(iii) currently, no principle exists to restrict possible discretizations for terms such as T^{α}, $0 < \alpha < 1$.

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