DIFFERENT DIFFERENCES

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ABSTRACT

From calculus we know that a derivative of a a function can be approximated using a difference quotient. There are different forms of the difference quotient, such as the forward difference (most common), backward difference and centered difference. I will introduce and discuss "Mickens differences," which are decidedly different differences for approximating the derivatives in differential equations. Professor Ronald Mickens is an African-American Physics Professor at Clark Atlanta University who has written nearly 300 journal articles on this and related topics. These nonstandard finite differences can produce discrete solutions to a wide variety of differential equations with improved accuracy over standard numerical techniques. Applications drawn from first-semester Calculus to advanced computation fluid dynamics will be given.

Students are very welcome to attend. Knowledge of elementary derivatives/anti-derivatives and Taylor Approximations will be assumed.

OUTLINE

SECTION 1: Introduction and Applications of Different Differences to ODEs

- 1. Pop Quiz!
- 2. Briefly Revisit Calculus 1
- 3. A Short Primer on Numerical Analysis
 - An Intro to Difference Equations
 - A Simple Example
 - Computing Numerical Error
- 4. Different Differences (i.e. Mickens Differences or NSFD)
 - A Simple Example Revisited
 - A Slightly Harder NSFD example (the m = 0 boundary value problem)
 - Another NSFD example (the m > 0 boundary value problem)
- 5. Other Interesting Applications of NSFD
 - A problem in Theoretical Aerodynamics
 - The 1-d Bratu Problem
 - The Bratu Problem in Radial Coordinates

SECTION 2: Application of Different Differences to PDEs

- 6. A Problem from Plasma Physics Suggested by Mickens
 - Reduce The Problem To a Simple ODE
 - Convert the Simple ODE Into a Simple $O\Delta E$
 - \bullet Develop NSFD Schemes for the O ΔE
 - Some Numerical Experiments
 - Consider a Simplified PDE
 - Develop NSFD Schemes for the Simplified PDE
 - Some More Numerical Experiments
 - Conclusions

SECTION 1: Introduction and Applications of Different Differences to ODEs

Pop Quiz!

What's *the* primary difference between a **curve** and a **line**? (This is not a "trick" question)



QUESTION

The name of the property of a graph which determines whether that graph will be a line or a curve is called the

(*Choose one of the following to complete the previous sentence*):

- A. tangent
- B. slope
- C. vertical line test
- D. horizontal line test

ANSWER to Pop Quiz

The name of the property of a graph which determines whether that graph will be a line or a curve is called the **slope**.

A. tangent

B. slope \leftarrow CORRECT ANSWER!

- C. vertical line test
- D. horizontal line test

(RECALL from Calculus 1) The **slope** of a graph (or derivative of the function being graphed) is CONSTANT for a line. For a curve, the slope CHANGES VALUE at every point and is given by the derivative function. The slope of a tangent line to a graph equals the slope of the graph at the point of tangency.

We can find the slope of a *line* by computing $\frac{\Delta y}{\Delta x}$

We can find the slope of a curve by ... ?

Calculus 1, Revisited

The forward difference formula for f'(x) is given by

$$f'(x) \approx \frac{f(x+h) - f(x)}{(x+h) - x} = \frac{f(x+h) - f(x)}{h}$$

The backward difference formula is

$$f'(x) \approx \frac{f(x) - f(x - h)}{h}$$

The centered difference formula is

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

One way to show that these formulas "work" is to apply Taylor Expansions...

If a function f(x) is infinitely differentiable at a point x = a then the **Taylor Expansion** for the value f(t) about the point (a, f(a)) is given by...

$$f(t) \approx f(a) + f'(a)(t-a) + f''(a)\frac{(t-a)^2}{2} + \dots$$

With a change of variables $t \to x \pm h$ and $a \to x$

$$f(x+h) \approx f(x) + f'(x)h + f''(x)\frac{h^2}{2} + \dots$$
$$f(x-h) \approx f(x) - f'(x)h + f''(x)\frac{h^2}{2} + \dots$$

A Short Primer On Numerical Analysis (Let's Be Discrete!)

Split up an interval $a \leq x \leq b$ into N equal pieces, so

$$h = \frac{b-a}{N}$$
 and $x_k = a + kh$ for $k = 1, 2, \dots, N$

Let

$$u_{k} = f(x_{k})$$

$$u_{k+1} = f(x_{k+1}) = f(x_{k} + h)$$

$$u_{k-1} = f(x_{k-1}) = f(x_{k} - h)$$

Discrete Forward Difference

$$\frac{du}{dx} \approx \frac{u_{k+1} - u_k}{h}$$

Discrete Backward Difference

$$\frac{du}{dx} \approx \frac{u_k - u_{k-1}}{h}$$

Discrete Centered Difference

$$\frac{du}{dx} \approx \frac{u_{k+1} - u_{k-1}}{2h}$$

We can use these formulas to approximate derivatives in differential equations to produce difference equations **The Calculus Student's Favorite Function** Consider the initial value problem (IVP)

$$\frac{dy}{dx} = y, \quad y(0) = 1$$

We know the exact solution is $y(x) = e^x$

The discrete version of the exact solution is $y_k = e^{x_k}$

We can solve the IVP by **discretizing** the initial value problem.

Using a standard finite-difference scheme the discrete form of the IVP becomes

$$\frac{y_{k+1} - y_k}{h} = y_k$$
, for $k = 1, 2, \dots, N$ and $y_0 = 1$

which when rearranged or solved becomes

 $y_{k+1} - y_k = y_k h \Rightarrow y_{k+1} = y_k + h y_k = y_k (1+h)$ Applying the initial condition at k = 0

$$y_1 = y_0(1+h) = 1+h$$

when k = 1

$$y_2 = y_1(1+h) = (1+h)(1+h) = (1+h)^2$$

when k = 2

$$y_3 = y_2(1+h) = (1+h)(1+h)^2 = (1+h)^3$$

Therefore

$$y_k = (1+h)^k, \qquad k = 0, 1, 2, \dots N$$

Computing Numerical Error

How accurate was the solution generated by the standard finite difference scheme?

The exact solution to the differential equation (ODE) y' = y, y(0) = 1 is

$$y(x) = e^x$$

which has a discrete analogue given by

$$y_k = e^{kt}$$

The solution to the related difference equation $(O\Delta E)$ was

$$y_k = (1+h)^k, k = 0, 1, 2, \dots N$$

The error ϵ_k at any point $x_k = kh$ is given by

$$\epsilon_k = y(x_k) - y_k = e^{hk} - (1+h)^k$$

At k = 0 there is no error:

$$\epsilon_0 = e^0 - (1+h)^0 = 1 - 1 = 0$$

At k = 1

$$\epsilon_1 = e^h - (1+h)^1 = (1+h+\frac{h^2}{2}+...) - (1+h)$$
$$= \frac{h^2}{2} + ...$$

At k = 2 $\epsilon_2 = e^{2h} - (1+h)^2 = (1+2h+\frac{(2h)^2}{2}+...) - (1+h)^2$ $= (1+2h+2h^2+...) - (1+2h+h^2)$ $= h^2 + ...$

Numerical Results for N = 10



Discrete Error as N Increases (h decreases)



Visualization Of Numerical Solution of ODEs Using $O \Delta Es$

$$\begin{array}{cccc} \text{ODE} & \longrightarrow & (\text{approximated discretely}) \longrightarrow & & \text{O}\Delta \text{E} \\ \downarrow & & & \downarrow \\ (\text{solved}) & & & (\text{solved}) \\ \downarrow & & & \downarrow \\ y(x) & \longrightarrow & (\text{approximated discretely}) \longrightarrow & y(x_k) \approx & y_k \end{array}$$

Different Differences

Professor Ronald Mickens of Clark Atlanta University has suggested a different way to approximate the derivative

$$f'(x) \approx \frac{f(x + \phi_1(h)) - f(x)}{\phi_2(h)}, \quad \text{where } \phi_n = h + \dots$$

Note that as $h \to 0$ the above difference quotient yields f'(x) exactly as the standard formulae do.

The discrete analogue of Mickens' suggestion is

 $\frac{dy}{dx} \approx \frac{y_{k+1} - \psi y_k}{\phi(h)}$, where $\psi = 1 + \dots$ and $\phi(h) = h + \dots$

The beauty of this idea is that it gives us more flexibility to tailor our approximation technique to the particular differential equation we're trying to discretize.

Most often $\psi = 1$ and we need to choose a **denominator function** $\phi(h)$

$$\phi(h) = \begin{cases} h, \\ \sin(h), \\ e^{h} - 1, \\ 1 - e^{-h}, \\ \frac{h}{1 - h}, \\ \frac{1 - e^{-\lambda h}}{\lambda}, \\ \vdots \end{cases}$$

Application of a Mickens Difference To A Simple Example

Suppose we reconsider the ODE $\frac{dy}{dx} = y$, y(0) = 1. How do we make our choice of denominator function? There are no firm rules which direct you in every case. In this simple example we know the exact solution looks exponential so we should try a choice with this functional behavior

$$\phi(h) = e^h - 1$$

Our related difference equation $(O\Delta E)$ would become

$$\frac{y_{k+1} - y_k}{e^h - 1} = y_k, \qquad y_0 = 1$$

which can be rearranged to be

 $y_{k+1} = y_k + \phi(h)y_k = y_k + y_k(e^h - 1) \Rightarrow y_{k+1} = e^h y_k$ Applying the initial condition at k = 0

$$y_1 = y_0 e^h$$

When k = 1,

$$y_2 = y_1 e^h = e^h e^h = e^{2h}$$

When k = 2,

$$y_3 = y_2 e^h = e^h e^{2h} = e^{3h}$$

Therefore,

$$y_k = e^{kh}, \qquad k = 0, 1, 2, \dots, N$$

is the discrete version of the solution to the ODE produced using the Mickens finite difference scheme. **Error due to the Mickens Difference Method** Recall that the error ϵ_k at any point $x_k = kh$ is given by

 $\epsilon_k = y(x_k) - y_k$

The exact solution to the ODE is $y(x) = e^x$

The solution to the difference equation generated by using a standard finite-difference discretization of the ODE was $y_k = (1+h)^k$

The solution to the difference equation generated by using the nonstandard discretization of the ODE is $y_k = e^{kh}$.

Thus the numerical error of the Mickens scheme is given by

$$\epsilon_k = e^{x_k} - e^{kh} = e^{kh} - e^{kh} = 0$$

In other words, by making a good choice of denominator function one can produce a difference equation which represent an **exact** discrete version of the solution of the differential equation.

We have been able to "approximate" the differential equation exactly!

Was this a fluke? No!

Application of Mickens Differences To A Slightly Harder Problem

Consider the following boundary value problem in cylindrical coordinates for the function u(r)

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{du}{dr}\right) - m^{2}u = 0, \qquad m \text{ constant}$$
$$r\frac{du}{dr}\Big|_{r=0} = S,$$
$$u(1) = G.$$

When m = 0 the ODE becomes

$$\frac{d}{dr}\left(r\frac{du}{dr}\right) = 0$$

with the conditions u(r) = G at r = 1 and $r\frac{du}{dr} = S$ at r = 0Recall, if $\frac{d}{dr}(\heartsuit) = 0 \Leftrightarrow \heartsuit = \text{constant}$ Therefore $r\frac{du}{dr} = \text{constant}$. But our boundary condition tells us when r = 0, $r\frac{du}{dr} = S$ So, we know $r\frac{du}{dr} = S$ or $\frac{du}{dr} = \frac{S}{r}$

which means that $u = S \log r + C$ where C is a constant So, the exact solution u(r) of our given boundary value problem is

$$u(r) = S\log(r) + G$$

Applying Standard Finite Differences To The Same Problem

We can write our boundary value problem from before as the initial value problem that we actually solved and then use our discretization technique....

$$r\frac{du}{dr} = S, \qquad u(1) = G$$

First we split up the interval $0 < r_0 \le r \le 1$ into N pieces, so $r_k = r_0 + kh, k = 0, 1, 2, \dots N$ and $h = \frac{1 - r_0}{N}$

The discrete version of the ODE using standard differences will be

$$r_k \frac{u_{k+1} - u_k}{h} = S, \qquad u_N = G$$

which can be rearranged to produce

$$u_k = u_{k+1} - \frac{Sh}{r_k}, \qquad k = 0, 1, 2, \dots N - 1$$

We can find every value of u_k on the grid by starting at k = N since $u_N = G$.

Then u_{N-1} can be computed in terms of u_N , and u_{N-2} can be computed in terms of u_{N-1} and so on.

This process is called a (backward) marching scheme.

Applying Nonstandard Finite Differences To Another Problem

Consider again the ODE

$$r\frac{du}{dr} = S, \qquad u(1) = G$$

"Buckmire's Method" (Ph.D. Thesis, RPI, 1994) By manipulating the differential equation and approximating the derivatives

$$r\frac{du}{dr} = \frac{du}{\frac{dr}{r}} = \frac{du}{d(\log(r))} \approx \frac{\Delta u}{\Delta(\log(r))}$$

 Δu is defined as $u_{k+1} - u_k$ and $\Delta \log(r)$ is $\log(r_{k+1}) - \log(r_k)$.

The discrete version of the ODE using Buckmire's Method will be

 $\frac{u_{k+1} - u_k}{\log(r_{k+1}) - \log(r_k)} = S \text{ for } k = 0, 1, \dots N - 1, \text{ with } u_N = G$

which can be rearranged to be

$$u_{k} = u_{k+1} - S[\log(r_{k+1}) - \log(r_{k})]$$

= $u_{k+1} - S \log(r_{k+1}/r_{k})$

This is also a backward marching scheme for determining all values of u_k from k = N - 1, N - 2, ..., 1, 0 with $u_N = G$

How do the two competing numerical methods compare?



The m > 0 problem Recall the boundary value problem is

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{du}{dr}\right) - m^{2}u = 0, \qquad m \text{ constant}$$

$$r\frac{du}{dr}\Big|_{r=0} = S,$$

$$u(1) = G.$$

We can simplify the derivative terms to obtain

$$\frac{d^2u}{dr^2} + \frac{1}{r}\frac{du}{dr} - m^2u = 0$$

which becomes

$$r^2 \frac{d^2 u}{dr^2} + r \frac{du}{dr} - m^2 r^2 u = 0$$

If we let z = mr then this equation can be transformed into

$$z^2 \frac{d^2u}{dz^2} + z\frac{du}{dz} - z^2u = 0$$

$$z^2u'' + zu' + (m^2 - z^2)u = 0$$

The m = 0 case is known as the modified Bessel's Equation of zeroth order.

It's such a well-known equation that its solutions u(z) are functions called the **modified Bessel's functions of the first and second kind** $K_0(z)$ and $I_0(z)$ There are numerous functions whose name we know who are really just solutions of a differential equation. For example, the equation

$$\frac{d^2u}{dz^2} + u = 0$$

has two famous solutions: $\sin(z)$ and $\cos(z)$

When m > 0 the exact solution to our boundary value problem can be written in terms of $I_0(mr)$ and $K_0(mr)$

$$u(r) = -SK_0(rm) + (G + SK_0(m))\frac{I_0(rm)}{I_0(m)}$$

Since we have an exact solution we can compare it to numerical results generated from using standard finite difference approximations to the modified Bessel's equation versus using a nonstandard (Buckmire) finite difference approximation Comparing Results for m > 0Let S = G = 1 and choose N = 100 and $r_0 = 10^{-4}$ or 10^{-8} . Then $h = \frac{1-r_0}{100}$



Motivation: A Problem From Computational Fluid Dynamics)



Figure 1: Plot of Contours Around Transonic Shock Free Body

More Recent Motivations: The Bratu Problem

$$\Delta u + \lambda e^u = 0, \qquad u = 0 \text{ on } \partial U$$

In one-dimension the problem becomes

$$\frac{d^2}{dx^2}u(x) + \lambda e^{u(x)} = 0, \qquad u(0) = u(1) = 0$$

and there is an exact solution

$$u(x) = -2\ln\left(\frac{\cosh[(x-\frac{1}{2})\frac{\theta}{2}]}{\cosh(\frac{\theta}{4})}\right)$$

which we can check satisfies the boundary conditions

When
$$x = 0$$
, $u(x)$ becomes $u(0) = 0$ \checkmark

and

When
$$x = 1$$
, $u(x)$ becomes $u(1) = 0$ \checkmark

and u(x) satisfies the differential equation $u'' = -\lambda e^u$ if

$$\theta = \sqrt{2\lambda} \cosh\left(\frac{\theta}{4}\right)$$

because the LHS

$$u''(x) = -2 \operatorname{sech}^2 \left[\left(x - \frac{1}{2} \right) \frac{\theta}{2} \right] \frac{\theta^2}{4}$$

while the RHS

$$-\lambda e^{u(x)} = -\lambda \operatorname{sech}^2\left[\left(x - \frac{1}{2}\right)\frac{\theta}{2}\right] \cosh^2\left(\frac{\theta}{4}\right)$$



We want to get the unique solution when

$$\theta = \sqrt{2\lambda} \cosh\left(\frac{\theta}{4}\right)$$
$$1 = \sqrt{2\lambda_c} \sinh\left(\frac{\theta_c}{4}\right) \frac{1}{4}$$

which means that if we divide these two equations

$$\theta_c = \coth\left(\frac{\theta_c}{4}\right) 4$$
$$\frac{\theta_c}{4} = \coth\left(\frac{\theta_c}{4}\right)$$

So θ_c is 4 times the fixed point of the hyperbolic cotangent function, so $\theta_c = 4.479871456$ and $\lambda_c = 3.513830719$

The Bratu Problem In Radial Coordinates: a.k.a. "The Bratu-Gel'fand Problem"

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{du}{dr}\right) + \lambda e^{u(r)} = 0, \qquad u(1) = 0 \text{ and } u(0) < \infty$$

An exact solution to the **Bratu-Gelfand Problem in Cylindrical Coordinates** is known. It is

$$u(r;\lambda) = \ln \left[\frac{\frac{32}{\lambda^2} \left\{ 1 - \frac{\lambda}{4} \pm \sqrt{1 - \frac{\lambda}{2}} \right\}}{\left(1 + \frac{4r^2}{\lambda} \left\{ 1 - \frac{\lambda}{4} \pm \sqrt{1 - \frac{\lambda}{2}} \right\} \right)^2} \right]$$

My work on this problem is discussed in [2, 3].

The Bratu-Gelfand Problem in Spherical Coordinates is

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{du}{dr}\right) + \lambda e^{u(r)} = 0, \qquad u(1) = 0 \text{ and } u(0) < \infty$$

This problem does not have a known exact solution to my knowledge. If you think you can solve it, or know of an exact solution, come talk to me afterwards!

SECTION 2: Application of Different Differences to PDEs

A Problem In Plasma Physics

Wilhelmsson $et \ al \ [10]$ 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:

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

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

$$T(1,t) = 0,$$
 $T(0,t) < \infty.$ (2)

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

$$T(r,0) = A(r+B)(r-1)^2$$
(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.

The Simplified ODE

In order to better understand the dynamics of Equation (1), we first study some related, simplified ordinary differential equations having only the square root term.

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

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

The exact solution to Equation (4) is

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

where

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

Of course T(t) = 0 is also a singular solution of Equation (4). See [4] for discussion of singular solutions.

Discretizing the Simplified ODE Into a $\mathbf{O} \Delta \mathbf{E}$

Apply the following transformations to Equation (5):

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

where $t_k = hk$, $h = \Delta t$, and $T_k = T(t_k)$. The exact solution, Equation (5), was:

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

By applying the above discretization we construct an exact difference scheme:

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

The resulting *exact* finite difference scheme for the Simplified ODE is

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

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

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

Deriving The First NSFD Scheme

A first **nonstandard finite difference scheme** [6, 7, 9] 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

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

Solving for T_{k+1} gives

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

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

Deriving A Second NSFD Scheme

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

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

which gives

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

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

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

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

Some Numerical Experiments

We now have four FD schemes which can be used to obtain numerical solutions to the IVP given in Equation (4).

(i) the exact scheme Equation (7);

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

(ii) the standard scheme, Equation (8);

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

(iii) **NSFD(1)**, the nonstandard scheme of Equation (11);

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

(iv) NSFD(2), the nonstandard scheme of Equation (14).

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

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, $t^* = 2$.

The results of the numerical experiments are given in Figure 2 and Figure 3.



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



Figure 3: Plot of the differences between the NSFD(1), NSFD(2), the standard scheme, and the exact FD scheme

Interpreting The Results of the Numerical Experiments

Inspection of Figure 2 and Figure 3 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).

RECALL: our goal is to produce numerical solutions of the nonlinear Plasma Physics problem, not this "toy problem." However, insight gained from solving the toy problem assists us in coming up with a method to use to solve the Wilhemsson problem.

The Simplified PDE

Our previous work with the Simplified **ODE** provides hints for how to discretize the Simplified PDE given by

$$\frac{\partial T}{\partial t} = D \frac{\partial^2 T}{\partial x^2} - \lambda T^{1/2}; \quad 0 \le x \le 1, t > 0$$
(15)
$$T(x,0) = f(x) = \text{given}, T(0,t) = T(1,t) = 0.$$
(16)

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

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

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

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

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

$$(\tilde{T}_m^k)^{1/2} = \frac{\sqrt{T_{m+1}^k} + \sqrt{T_m^k} + \sqrt{T_{m-1}^k}}{3}.$$
 (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 $T_m^{k+1} = DR(T_{m+1}^k + T_{m-1}^k) + (1 - 2DR)T_m^k - (\lambda \Delta t)(\tilde{T}_m^k)^{1/2}$ (19)

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

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

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

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

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

As in previous work [7, 9], we let

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

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:

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

An Algorithm To Solve The Problem We Want To Solve

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 four 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

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

with the boundary conditions

$$T(0,t) = T(1,t) = 0, t > 0.$$
 (27)



Figure 4: Plots of the NSFD(2) scheme at various times.



Figure 5: Plots of the NSFD(3) scheme at various times



Figure 6: Plot of the differences between the standard scheme and the NSFD(1) scheme.

Discussion and Conclusions

Our primary goal in studying the discretizations of the Simplified ODE and the Simplified PDE was to gain insight that could aid us in the formulation of improved FD schemes for more complex differential equations such as Equation (1).

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 [7, 8, 9].

The work presented here illustrates 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} , $0 < \alpha < 1$.
- See [1] for a more involved discussion of the details of this work.

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Questions?