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Difference Equation Models of Differential Equations

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Table of Contents

Cover Page	1
Introduction	3
APPENDIX	5
A. Major Conferences Attended	5
B. Major Presentations	6
C. Abstracts	7
D. Publications	8
E. Honors, Awards, Etc.	8
F. Student Related Activities	9
G. Research Results	10

Introduction

Much of modern science and technology depends upon the ability to obtain solutions to differential equations that arise in the modeling of various systems [1, 2, 3]. In most instances the complexities of these equations do not permit the existence of analytic solutions that can be represented in terms of a finite number of the elementary functions [4]. Consequently, numerical integration methods must be used. An important technique to obtain numerical solutions is the use of finite-differences. However, an issue of great importance is the relationship between the numerical solutions and the actual (not known, *a priori*) analytical solutions to the differential equations. This leads the researcher to various questions related to local truncation errors, consistency, convergence, and stability [5, 6, 7].

The major thrust of this proposal was to continue our investigations of so-called non-standard finite-difference schemes as formulated by the PI [8]. These schemes do not follow the standard rules used to model continuous differential equations by discrete difference equations. The two major aspects of this procedure consist of generalizing the definition of the discrete derivative and using a nonlocal model (on the computational grid or lattice) for nonlinear terms that may occur in the differential equations.

Our aim was to investigate the construction of nonstandard finite-difference schemes for several classes of ordinary and partial differential equations. These equations are simple enough to be tractable, yet, have enough complexity to be both mathematically and scientifically interesting. It should be noted that all of these equations differential equations model some physical phenomena under an appropriate set of experimental conditions.

The major goal of the project was to better understand the process of constructing finite-difference models for differential equations. In particular, it demonstrates the value of using nonstandard finite-difference procedures. A secondary goal was to construct and study a variety of analytical techniques that can be used to investigate the mathematical properties of the obtained difference equations. These mathematical procedures are of interest in their own right [9] and should be a valuable contribution to the mathematics research literature in difference equations.

All of the results obtained from the research done under this project have been pub-

lished in the relevant research/technical journals or submitted for publication. Our expectation is that these results will lead to improved finite difference schemes for the numerical integration of both ordinary and partial differential equations.

Section G of the Appendix gives a concise summary of the major results obtained under funding by the grant. References to abstracts, published papers, and submitted manuscripts are also indicated. The other sections of the Appendix provide a breakdown of the PI's other research and professional activities which relate directly to the grant.

References

1. D. Potter, *Computational Physics* (Wiley, New York, 1973).
2. W. M. Washington and C. L. Parkinson, *An Introduction to Three-Dimensional Climate Modeling* (University Science Books; Mill Valley, CA; 1986).
3. M. Holt, *Numerical Methods in Fluid Dynamics* (Springer-Verlag, Berlin, 1984, 2nd edition).
4. D. Zwillinger, *Handbook of Differential Equations* (Academic Press, Boston, 1989).
5. F. B. Hildebrand, *Finite-Difference Equations and Simulations* (Prentice-Hall; Englewood Cliffs, NJ; 1968).
6. D. Greenspan and V. Casulli, *Numerical Analysis for Applied Mathematics, Science and Engineering* (Addison-Wesley; Redwood City, CA; 1988).
7. K. W. Morton and D. F. Mayers, *Numerical Solution of Partial Differential Equations* (Cambridge University Press, Cambridge, 1994).
8. R. E. Mickens, *Nonstandard Finite Difference Models of Differential Equations* (World Scientific; River Edge, NJ; 1994).
9. R. E. Mickens, *Difference Equations: Theory and Applications* (Van Nostrand Reinhold, New York, 1990).

APPENDIX

A. Major Conferences Attended

* Contributed presentation given.

** Invited presentation given and/or Chair-Organizer of a session.

*** Invited contributed presentation

- **1. International Conference on Scientific Computing and Modeling
Eastern Illinois University; Charleston, IL
October 12-14, 1995
- 2. Dynamical Numerical Analysis Conference
Georgia Institute of Technology; Atlanta, GA
December 14-16, 1995
- *3. American Mathematical Society - Mathematical Association of
America Joint Meetings
Orlando, FL
January 10-13, 1996
- **4. American Association for the Advancement of Science
Annual Meeting and Science Innovation Exposition
Baltimore, MD
February 8-12, 1996
- **5. Southeastern Section Meeting of the American Mathematical Society
Baton Rouge, LA
April 19-21, 1996
- 6. National Security Agency's Fourth Invitational Mathematics Conference
Fort Meade, MD
November 17-19, 1996
- *7. The Georgia Tech-UAB International Conference on Differential Equations and Math-
ematical Physics
Atlanta, GA
March 23-29, 1997
- *8. 1997 Joint Meeting of the American Physical Society and the American Association
of Physics Teachers with The Canadian Association of Physicists and the Sociedad
Mexicana de Fisica
- **9. American Mathematics Society Meeting
Wayne University; Detroit, MI
May 2-4, 1997

- ***10. 26th Annual Meeting of the Southeastern Theoretical Chemistry Association
University of Alabama at Birmingham; Birmingham, AL
May 16-17, 1997
- **11. 3rd CAARMS
Morgan State University (Baltimore, MD) and National Security Agency (Fort Meade, MD)
June 18-20, 1997
- ***12. Third International Conference on Theoretical and Computational Acoustics
Holiday Inn North; Newark, NJ
July 14-18, 1997

B. Major Presentations

- 1. "Spurious Limit-Cycles in Higher-Order Averaging Methods"
School of Electrical Engineering, Cornell University; Ithaca, NY
September 19, 1995
- 2. "Discrete Models of Continuous Systems: The Details Matter"
International Conference on Scientific Computing and Modeling;
Eastern Illinois University; Charleston, IL
October 12, 1995
- 3. "The Qualitative Theory of Ordinary Differential Equations"
Department of Mathematics, Xavier University; New Orleans, LA
October 26, 1995
- 4. "Relations Between Time and Space Step-Sizes in Numerical Schemes for PDE's that Follow from Positivity Conditions"
Fisk University; Nashville, TN
March 28, 1996
- 5. "Asymptotic Properties of Solutions to Discrete Coulomb Equations"
Southeastern Section Meeting of the American Mathematical Society;
Baton Rouge, LA
April 19, 1996
- 6. "Existence of Periodic Solutions for a Generalized Conservative Oscillator"
Georgia Tech International Conference on Differential Equations and Mathematical Physics; Atlanta, GA
March 24, 1997
- 7. "Nonstandard Finite-Difference Schemes"
Department of Mathematics, Howard University; Washington, DC
April 18, 1997

8. "Finite-Difference Schemes for a Scalar Reaction-Convection PDE"
Joint Meeting of the American Physical Society and the American Association of Physics Teachers; Washington, DC
April 20, 1997
9. "Relations Between Time and Space Step-Sizes in Numerical Schemes for PDE's that Follow from a Positivity Condition"
Detroit American Mathematical Society Meeting;
Wayne State University; Detroit, MI
May 3, 1997
10. "Numerical Tests of a New Finite-Difference Scheme for the Time-Dependent Schrödinger Equation"
The 26th Southeastern Theoretical Chemistry Association Meeting;
University of Alabama at Birmingham; Birmingham, AL
May 17, 1997
11. "Nonlinear Oscillations: Qualitative Theory"
3rd CAARMS, Morgan State University; Baltimore, MD
June 18, 1997
12. "Nonstandard Finite Difference Schemes: A Status Report"
Third Conference on Theoretical and Computational Acoustics, Holiday Inn North;
Newark, NJ
July 14, 1997

C. Abstracts

1. O. Oyediji and R. E. Mickens, "Discrete Modelling of Continuous Systems: The Details Matter," *Bulletin of the American Physical Society* 41, 1155 (1996).
2. R. E. Mickens, "Spurious Limit-Cycles in Higher Order Averaging Methods," *Abstracts of Papers Presented to the American Mathematical Society* 17, 145 (1996). Abstract 908-82-38.
3. R. E. Mickens, "Frontier Applications in Computer Methods for Dynamic Systems," *AMSIE '96* (The 1996 AAAS Annual Meeting and Science Innovation Exposition; Baltimore, MD; February 8-13, 1996). See pps. S-42 and A-47.
4. R. E. Mickens, "Asymptotic Solutions to Discrete Coulomb Equations," *Programs of the 911th AMS Meeting: Louisiana State University; Baton Rouge, Louisiana* (American Mathematical Society, 1996). Abstract 911-39-59.
5. K. Oyediji and R. E. Mickens, "Numerical Integration Schemes for the Dissipative Complex Equation," *Bulletin of the American Physical Society* 41, 1667 (1996).

6. R. E. Mickens, "Finite-Difference Schemes for a Scalar Reaction-Convection PDE," *Bulletin of the American Physical Society* 42, 1110 (1997).

D. Publications

1. R. E. Mickens, "Relations Between the Time and Space Step-Sizes for Finite-Difference Models of PDE's," *Journal of Applied Science and Computation* 1, 520 (1995).
2. J. Burnette and R. E. Mickens, "Spurious Limit-Cycles Arising in Higher-Order Averaging Methods," *Journal of Sound and Vibration* 193, 743 (1996).
3. R. E. Mickens, "Comments on the Shohat Expansion," *Journal of Sound and Vibration* 193, 747 (1996).
4. R. E. Mickens, "Exact Finite Difference Scheme for the Wave Equation with Spherical Symmetry," *Journal of Difference Equations and Applications* 2, 423 (1996).
5. R. E. Mickens and O. Oyediji, "Discrete Models of Continuous Systems: The Details Matter," in S. K. Dey and J. Ziebarth, editors, *Proceedings of Advances in Scientific Computing and Modeling* (Eastern Illinois University; Charleston, IL; October 12-14, 1995); pps. 91-95.
6. R. E. Mickens, "Asymptotic Properties of Solutions to Discrete Coulomb Equations," *Computers and Mathematics with Applications* (accepted for publication).
7. R. E. Mickens, "Asymptotic Properties of Solutions to Two Discrete Airy Equations," *Journal of Difference Equations and Applications* (accepted for publication).
8. R. E. Mickens, "Relation Between the Time and Space Step-Sizes in Nonstandard Finite-Difference Schemes for the Fisher Equation," *Numerical Methods for Partial Differential Equations* 13, 51 (1997).
9. R. E. Mickens, "Nonstandard Finite Difference Scheme for a Scalar Reaction-Convection PDE," *Journal of Difference Equation and Applications* (accepted for publication).
10. R. E. Mickens and K. O. Oyediji, "Numerical Integration of the Dissipative Complex Equation," *International Journal of Science and Computations* 4, 99 (1997).

Book

R. E. Mickens, *Oscillations in Planar Dynamic Systems* (World Scientific, Singapore, 1996).

E. Honors, Awards, Professional Activities

1. I serve on the editorial boards of the following research journals:
 - * *Journal of Applied Sciences and Computation*
 - * *Journal of Difference Equations and Applications*

2. I have reviewed books for

- * Mathematical Association of America
- * Kluwer Academic Publishers
- * Gordon and Breach Science Publisher

3. I reviewed research manuscripts for the following journals:

- * *Journal of Computational Physics*
- * *Computers and Mathematics with Applications*
- * *Journal of Difference Equations and Applications*
- * *Journal of Applied Sciences and Applications*
- * *Journal of Sound and Vibration*
- * *The Fibonacci Quarterly*

4. Honors

- * **Listed in**, *Breakthrough: The Changing Face of Science in America* (Blackside, Inc.; Boston, MA; 1996); pp. 23.
- * **Biography in** *Distinguished African American Scientists of the 20th Century*, editors, James H. Kessler et al. (Onyx Press; Phoenix, Arizona; 1996); pps. 253-256.
- * **Received**, National Association of Mathematicians Distinguished Service Award (March 22, 1996).

5. Professional Activities

- * **Chair**, Pegram Awards Committee, Southeastern Section of the American Physical Society
- * **Organizer and Chair**, session: "Frontier Applications in Computer Methods for Dynamic Systems," American Association for the Advancement of Science and Science Innovation Exposition; Baltimore, MD; February 9, 1996.
- * **Member**, Council of the Edward A. Bouchet-International Centre for Theoretical Physics Institute; Trieste, Italy.
- * **Organizer and Chair**, Session BA: "Recent Results in Computational Physics," Southeastern Section of the American Physical Society; Decatur, GA; November 14, 1996.

F. Student Related Activities

1. I served as a member of the Master-of-Science thesis committees for the following graduate students:

- * Donald Hollaway (Physics Department)
Thesis Title: "Numerical Analysis of Steady Two-Dimensional Heat Conduction with Heat Source Under Various Boundary Conditions"
- * Suzan B. Abdu (Department of Biological Sciences)
Thesis Title: "Model Study of an Origin of Life Hypothesis"
- * Dwight L. Mosby, Jr. (Physics Department)
Thesis Title: "Coadsorption of Sodium and Elemental Sulfur on Nickel (100) Surfaces"

2. I directed one Senior B.S. Honors Thesis:

* Monique K. Pryce (Physics Department)

Thesis Title: "Investigation of the Maxwell-Bloch Equations"

3. I direct/directed the research activities of the following students:

* Denise Brewly (graduate student, Department of Mathematics) Topics in nonlinear dynamics

* Monique Pryce (undergraduate student, Physics Department)

* Dennis Semwogerere (graduate student, Physics Department) Nonlinear oscillations

* Venita Bush (8th grade student; Peachtree Jr. High School; Atlanta, GA)

Ms. Bush won 3rd place in the 8th grade science contest for her project: "Does the Type of Music have an Effect on a Person's Physiological State?"

* Michael Turner (9th grade student; Therrell High School; Atlanta, GA)

Mr. Turner received the grade of "A" for his science project: "Comparing the Gravitational Attractions of the Moon and Earth"

4. Other student related activities:

* **Chair**, Advisory Committee, and **Member**, Executive Committee of the National Conference of Black Physics Students (NCBPS^T).

* **Panelist**, DOE Undergraduate Computational Engineering and Sciences Project Faculty Awards (1996).

* **Panelist**, National Science Foundation Graduate Fellowship Program (1997).

* **Moderator**, Undergraduate Session I: "Preparing for Graduate School," 11th Annual National Conference of Black Physics Students, Massachusetts Institute of Technology; Cambridge, MA; February 28, 1997.

* **Judge**, Mathematics and Physics Projects, "Science, Engineering, and Mathematics Day 1997"; Spelman College; Atlanta, GA; March 21, 1997.

* **Judge**, Science Fair Projects - 8th Grade; The Paideia School; March 24, 1997.

G. Research Results

This section gives a concise summary of the major research results obtained under the DOE grant. Except for the very recent results, all of these findings have been published in refereed journals, submitted for publication in such journals, and/or presented at scientific meetings.

1. Positivity and Nonstandard Finite Difference Schemes

Many dynamical systems can be modeled by partial differential equations (PDE) and the physical relevant solutions have the property of being non-negative. We have used this condition of "positivity" to obtain restrictions on the step-sizes. For nonlinear PDE's, having one space dimension, the functional relations between the step-sizes arise only for

nonstandard finite-difference schemes. Standard schemes generally give functional relations that not only involve the step-sizes, but also the local value of the solution. This technique has been applied to the Fisher, linear advection-diffusion, Burgers, and linearized Euler PDE's.

As an example, consider the Fisher equation

$$(1.1) \quad \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + u(1 - u).$$

For initial data

$$(1.2) \quad u(x, 0) = f(x), \quad 0 \leq f(x) \leq 1,$$

it can be shown that

$$(1.3) \quad 0 \leq u(x, t) \leq 1.$$

The nonstandard scheme

$$(1.4) \quad \frac{u_m^{n+1} - u_m^n}{\Delta t} = \frac{u_{m+1}^n - 2u_m^n + u_{m-1}^n}{(\Delta x)^2} + u_m^n - \left(\frac{u_{m+1}^n + u_m^n + u_{m-1}^n}{3} \right) u_m^{n+1},$$

has the property

$$(1.5) \quad 0 \leq u_m^n \leq 1 \Rightarrow 0 \leq u_m^{n+1} \leq 1,$$

provided

$$(1.6) \quad \Delta t = \frac{(\Delta x)^2}{3} \left[\frac{1}{1 - \frac{(\Delta x)^2}{3}} \right].$$

(Note that Δx satisfies the inequality $0 < \Delta x < \sqrt{3}$. In practice, this condition is easy to obtain since for the normalized Fisher equation the numerical procedure would use step-sizes such that $0 < \Delta x \ll 1$.) With this restriction, the finite-difference scheme of Eq. (1.4) becomes

$$(1.7) \quad u_m^{n+1} = \frac{R(u_{m+1}^n + u_m^n + u_{m-1}^n)}{1 + \left(\frac{\Delta t}{3}\right)(u_{m+1}^n + u_m^n + u_{m-1}^n)},$$

where $R = \Delta t / (\Delta x)^2$.

It should be noted that the condition, given by Eq. (1.5), does not hold in standard finite-difference schemes for the Fisher PDE, such as

$$(1.8) \quad \frac{u_m^{n+1} - u_m^n}{\Delta t} = \frac{u_{m+1}^n - 2u_m^n + u_{m-1}^n}{(\Delta x)^2} + u_m^n(1 - u_m^n).$$

The results of this section have been published. The reference is: R. E. Mickens, "Relations Between the Time and Space Step-Sizes in Nonstandard Finite-Difference Schemes for the Fisher Equation," *Numerical Methods for Partial Differential Equations* 13, 51-55 (1997).

2. A Scalar Reaction-Convection Equation

Nonlinear scalar reaction-convection partial differential equations (SRCPDE) have been used to investigate the existence and stability of spurious steady-state numerical solutions and how they are affected by various discretizations with regard to the space and time variables [1, 2, 3]. In particular, the report by Yee and Sweby [3] provided a detailed study of the equation

$$(2.1) \quad u_t + bu_x = \alpha S(u), \quad 0 \leq x \leq 1,$$

where α and b are positive parameters, and the nonlinear source term $S(u)$ is taken to be a cubic function. They studied spurious asymptotes and steady-states, nonphysical wave propagation speeds, and numerical basins of attraction as a function of varying how the derivatives and source term are discretely represented.

We also investigated this class of PDE's. In particular, we selected the following normalized, symmetric form of SRCPDE

$$(2.2) \quad u_t + u_x = u(1 - u^2), \quad -\infty < x < \infty.$$

Note that Eq. (2.2) has three constant solutions

$$(2.3) \quad \bar{u}_1 = 0, \quad \bar{u}_2 = +1, \quad \bar{u}_3 = -1.$$

The first solution is linearly unstable, while the other two are linearly stable.

Both the space-independent and the time-independent equations, in this case ordinary differential equations, also have these solutions as fixed-points. For example, the space-independent equation is

$$(2.4) \quad \frac{dw}{dt} = w(1 - w^2).$$

In previous work [4], we showed that the following nonstandard finite-difference scheme for Eq. (2.4)

$$(2.5) \quad \frac{w^{n+1} - w^n}{\left(\frac{1-e^{-2h}}{2}\right)} = \left(\frac{4}{3+e^{-2h}}\right) w^n \left[1 - \left(\frac{3w^{n+1} - w^n}{2}\right) w^n\right],$$

has only the three fixed-points of Eq. (2.3); each fixed-point has exactly the same linearly stability properties as the corresponding fixed-point of the differential equation (2.4); and for a given initial condition, always produces a solution which converges monotonically to the correct stable fixed-point. Of importance is the fact that *these results hold for arbitrary step-size, $h = \Delta t > 0$.*

In a recent paper [5, 6], we have used this result to construct a nonstandard scheme for the SRCPDE given by Eq. (2.2):

$$(2.6) \quad \frac{u_m^{n+1} - u_m^n}{\left(\frac{1-e^{-2\Delta t}}{2}\right)} + \frac{u_m^n - u_{m-1}^n}{\left(\frac{1-e^{-2\Delta x}}{2}\right)} = \left(\frac{4}{3+e^{-2\ell}}\right) u_{m-1}^n \left[1 - \left(\frac{3u_m^{n+1} - u_{m-1}^n}{2}\right) u_{m-1}^n\right],$$

where the following relation holds between the step-sizes

$$(2.7) \quad \Delta t = \Delta x = \ell.$$

The above scheme can be rewritten to the form

$$(2.8) \quad u_m^{n+1} = \left[\frac{(1 + \Sigma) + \left(\frac{1}{2}\right)\Sigma(u_{m-1}^n)^2}{1 + \left(\frac{3}{2}\right)\Sigma(u_{m-1}^n)^2} \right] u_{m-1}^n,$$

where

$$(2.9) \quad \Sigma = \frac{2(1 - e^{-2\ell})}{3 + e^{-2\ell}}.$$

It was shown that the solutions to this scheme has, in general, the same mathematical properties as the original PDE given by Eq. (2.2). For example, there are (only) three

constant solutions, given by Eq. (2.3), and they have the same linear stability properties as the corresponding solutions of the SRCPDE for all values of the step-sizes.

Finally, it is of interest to note that all of the eleven schemes constructed by Yee and Sweby [3] gave spurious asymptotes and steady-states as the step-sizes were varied.

References

1. R. J. LeVeque and H. C. Yee, "A study of numerical methods for hyperbolic conservation laws with stiff source terms," *J. Computational Physics* **86**, 187-210 (1990).
2. D. F. Griffiths et al., "Numerical wave propagation in an advection equation with a nonlinear source term," *SIAM J. Numerical Analysis* **29**, 1244-1260 (1992).
3. H. C. Yee and P. K. Sweby, "Nonlinear dynamics and numerical uncertainties in CFD," NASA Technical Memorandum 110398 (April 1996), Ames Research Center; Moffett Field, CA.
4. R. E. Mickens, "Comment on 'A second-order, chaos-free, explicit method for the numerical solutions of a cubic reaction problem in neurophysiology'," *Numerical Methods for Partial Differential Equations* **10**, 587-590 (1994).
5. R. E. Mickens, "Nonstandard finite-difference scheme for a scalar reaction-convection PDE," *Journal of Difference Equations and Applications* (accepted for publication).
6. R. E. Mickens "Finite-difference schemes for a scalar reaction-convection PDE," *Bulletin of the American Physical Society* **42**, 1110 (1997).

3. Two-Dimension Unidirectional Wave Equation

The unidirectional, linear wave equation in two-dimensions is

$$(3.1) \quad u_t + au_x + bu_y = 0, \quad u = u(x, y, t),$$

where a and b are constants. With initial data, $u(x, y, 0) = u_0(x, y)$, the solution is

$$(3.2) \quad u(x, y, t) = u_0(x - at, y - bt).$$

This equation has been used as a model equation to test the properties of various numerical integration schemes for PDE's.

We have derived the following exact finite-difference scheme for Eq. (3.1):

$$(3.3) \quad u_{m,n}^{k+1} = u_{m-1,n-1}^k,$$

where

$$(3.4) \quad t_k = (\Delta t)k, \quad x_m = (\Delta x)m, \quad y_n = (\Delta y)n,$$

and where the following two relations must hold among the step-sizes

$$(3.5) \quad \Delta x = a\Delta t, \quad \Delta y = b\Delta t.$$

The scheme of Eq. (3.3) is exact in that

$$(3.6) \quad u_{m,n}^k \equiv u(x_m, y_n, t_k)$$

for all step-sizes that satisfy Eq. (3.5). The expression of Eq. (3.3) can be rewritten to the form

$$(3.7) \quad \frac{u_{m,n}^{k+1} - u_{m,n}^k}{\Delta t} + \left(\frac{a}{\Delta x}\right) \left[\left(\frac{u_{m,n}^k + u_{m,n-1}^k}{2}\right) - \left(\frac{u_{m-1,n}^k + u_{m-1,n-1}^k}{2}\right) \right] \\ + \left(\frac{b}{\Delta y}\right) \left[\left(\frac{u_{m-1,n}^k + u_{m,n}^k}{2}\right) - \left(\frac{u_{m-1,n-1}^k + u_{m,n-1}^k}{2}\right) \right] = 0.$$

This scheme has the following features:

- (i) The discrete time-derivative is given by a forward Euler representation.
- (ii) The discrete x -derivative is obtained by applying a backward Euler scheme to the dependent function averaged over the grid points y_n and y_{n-1} .
- (iii) A similar statement applies to the discrete y -derivative.

A paper giving the details of the above work has been submitted to and accepted for publication in the *Journal of Sound and Vibration*, "Exact finite difference schemes for two-dimensional advection equations."

4. Douglas-Type Approximations for Derivatives

An important class of ordinary differential equations (ODE) is the so-called time-independent Schrödinger equation (TISE). These equations model a variety of physical systems, in particular some which arise in atomic/molecular physics. For our purposes, we select the following form for the TISE [1]:

$$(4.1) \quad -\left(\frac{m}{2}\right) \frac{d^2\psi}{dx^2} + V(x)\psi = E\psi,$$

where m = “mass” of the particle acted on by the known “potential” $V(x)$, and E is the constant “energy.”

A large number of standard finite-difference schemes have been constructed for the TISE. One of the more popular schemes is the Numerov method [2]. This method has been combined with the nonstandard scheme of Mickens and Ramadhani [3] to give the so-called combined Numerov-Mickens scheme (CNMS) [4].

Over four decades ago, Douglas [5] constructed a higher-order difference equation model for the linear diffusion PDE. We have shown that if this procedure is applied to the TISE the resulting finite-difference equation is exactly the one obtained by the Numerov method.

In more detail, the Douglas approximation for the second-order space derivative is

$$(4.2) \quad \frac{d^2}{dx^2} \rightarrow \frac{\delta_x^2}{h^2 \left(1 + \frac{\delta_x^2}{12}\right)} + O(h^4), \quad h = \Delta x,$$

where

$$(4.3) \quad \delta_x^2 \psi_m \equiv \psi_{m+1} - 2\psi_m + \psi_{m-1}.$$

Substitution of Eq. (4.2) into Eq. (4.1) and simplifying the resulting expression gives

$$(4.4) \quad \begin{aligned} & - \left(\frac{m}{2}\right) \left[\frac{\psi_{m+1} - 2\psi_m + \psi_{m-1}}{h^2} \right] \\ & + \left(\frac{1}{12}\right) [V_{m+1}\psi_{m+1} + 10V_m\psi_m + V_{m-1}\psi_{m-1}] \\ & = E \left(\frac{1}{12}\right) (\psi_{m+1} + 10\psi_m + \psi_{m-1}). \end{aligned}$$

This is precisely the Numerov scheme for Eq. (4.1). Hence, the Douglas representation for the second-order derivative gives for the TISE the same finite-difference equation as that obtained by the Numerov method. To the best of our knowledge, this interesting result has not appeared previously in the published scientific literature.

We have initiated an investigation using the Douglas representation to construct finite-difference models for the time-dependent Schrödinger equation

$$(4.5) \quad i \frac{\partial \psi}{\partial t} = -\frac{\partial^2 \psi}{\partial x^2} + V(x)\psi, \quad \psi = \psi(x, t).$$

This leads to a second-order scheme, in both Δt and Δx . However, no conclusive results have been obtained to date. We plan to continue with this investigation.

References

1. R. E. Mickens, *Nonstandard Finite Difference Models of Differential Equations* (World Scientific, 1994). See Chapter 8.
2. S. E. Koonin, *Computational Physics* (Addison-Wesley, 1986). See Section 3.1.
3. R. E. Mickens and I. Ramadhani, "Finite-difference scheme for the numerical solution of the Schrödinger equation," *Physical Review A* **45**, 2074–2075 (1992).
4. R. Chen et al., "Finite-difference scheme to solve Schrödinger's equation," *Physical Review E* **47**, 3799–3802 (1993).
5. J. Douglas, "The solution of the diffusion equation by a higher-order correct difference equation," *Journal of Mathematics and Physics* **35**, 145–151 (1956).

5. New Finite-Difference Scheme for the TDSE

We constructed a new finite-difference scheme for the time-dependent Schrödinger equation (TDSE) based on a discrete form of the Hamiltonian suggested by the Numerov method. The novel feature is that the scheme makes an $O(h^2)$ approximation to the potential energy term. The new scheme was applied to both the Morse oscillator and the soft-core potential and the numerical results were compared to those obtained by a conventional central-difference scheme.

The TDSE

$$(5.1) \quad i \frac{\partial \psi(x, t)}{\partial t} = H \psi(x, t),$$

has the formal solution

$$(5.2) \quad \psi(x, t) = \exp(-iHt)\psi(x, 0),$$

provided the Hamiltonian H does not depend on time. A standard time discretization is the Cayley form

$$(5.3) \quad \exp(-iH\tau) = \frac{1 - iH\tau/2}{1 + iH\tau/2} + O(H^3\tau^3).$$

The Hamiltonian, $H = T + V$, is the sum of the kinetic-energy operator T and the potential energy operator V . In the coordinate representation, we have

$$(5.4) \quad T = -\left(\frac{m}{2}\right) \frac{\partial^2}{\partial x^2}, \quad V = V(x).$$

The conventional central finite-difference scheme for the Hamiltonian is obtained by using the representations

$$(5.5) \quad \mathbf{H}\psi(x, t) \approx \mathbf{T}'\psi(x, t) + V(x)\psi(x, t)$$

where

$$(5.6) \quad \mathbf{T}'\psi(x, t) \equiv -\left(\frac{m}{2}\right) \frac{\psi(x+h, t) - 2\psi(x, t) + \psi(x-h, t)}{h^2}.$$

Our new finite-difference scheme uses the following discretization

$$(5.7) \quad \mathbf{H}\psi(x, t) \approx \mathbf{T}'\psi(x, t) + \mathbf{V}'\psi(x, t),$$

where the potential energy operator is defined by

$$(5.8) \quad \mathbf{V}'\psi(x, t) \equiv \frac{V(x+h)\psi(x+h, t) + 10V(x)\psi(x, t) + V(x-h)\psi(x-h, t)}{12}.$$

This expression is suggested by the Numerov method which is used to numerically integrate the TISE. (See Eq. (4.4).)

From Eqs. (5.2), (5.3), (5.6) and (5.8), the following scheme is obtained for the TDSE of Eq. (5.1):

$$(5.9) \quad (1 + i\mathbf{H}'\tau/2)\psi(x, t + \tau) = (1 - i\mathbf{H}'\tau/2)\psi(x, t),$$

where

$$(5.10) \quad \mathbf{H}' = \mathbf{T}' + \mathbf{V}'.$$

The above scheme was used to calculate both stationary (eigenstates and eigenvalues) and the time evolution (a Gaussian wave packet time-dependent state and associated correlation function) for both the Morse potential

$$(5.11) \quad V(x) = De^{-\beta x}(e^{-\beta x} - 2),$$

D and β are constants, and the soft-core potential

$$(5.12) \quad V(x) = -\frac{1}{\sqrt{1+x^2}}.$$

In comparison with the standard central-difference method, our new scheme does not provide any significant improvement for time step-sizes small enough to make the results converge. However, this initial result does indicate that alternatives may exist for improving the accuracy of schemes to numerically integrate the TDSE. Such new schemes will not only rely on modifications to $T\psi$, but, also modifications (nonlocal representations) to $V\psi$. We are currently investigating further this possibility.

These preliminary results are summarized in the following unpublished manuscript:

R. E. Mickens, "Numerical tests of a new finite-difference scheme for the time-dependent, Schrödinger equation."

6. Burgers PDE: Traveling Wave Solutions

Among the class of one-space dimension PDE's the Burgers equation plays an especially important role as a model equation that can be used to test numerical integration methods:

$$(6.1) \quad u_t + uu_x = u_{xx}.$$

Among its possible solutions are traveling wave solutions. These are solutions that take the form

$$(6.2) \quad u(x, t) = f(x - ct),$$

where the wave velocity is *a priori* unknown, and are determined by the solutions to the ODE

$$(6.3) \quad -cf' + ff' = f'',$$

where $z = x - ct$ and $f' = df/dz$. This equation can be solved to obtain the traveling wave solutions [1]. However, a search of the literature indicates that no finite-difference scheme exists for Eq. (6.3) such that it can be solved exactly. Using our nonstandard schemes, we have constructed a difference equation model of Eq. (6.3) that can be *solved for its exact solution*.

To proceed, let

$$(6.4) \quad z \rightarrow \frac{z}{2}, \quad f(z) \rightarrow y(z).$$

Then, Eq. (6.3) becomes, after one integration,

$$(6.5) \quad y' = y^2 - 2cy + 2A,$$

where A is the integration constant. A nonstandard scheme for Eq. (6.5) is [2]

$$(6.6) \quad \frac{y_k - y_{k-1}}{\phi(h)} = y_k y_{k-1} - 2cy_{k-1} + 2A,$$

where the function $\phi(h)$ has the property

$$(6.7) \quad \phi(h) = h + O(h^2), \quad h = \Delta z.$$

By operating on each term with the Δ operator ($\Delta y_k \equiv y_{k+1} - y_k$), we obtain the corresponding scheme for the ODE

$$(6.8) \quad y'' = 2yy' - 2cy',$$

which is

$$(6.9) \quad \frac{y_{k+1} - 2y_k + y_{k-1}}{\phi(h)\eta(h)} = 2y_k \left[\frac{y_{k+1} - y_{k-1}}{2\eta(h)} \right] - 2c \left[\frac{y_k - y_{k-1}}{\eta(h)} \right],$$

where $\eta(h)$ is a function such that

$$(6.10) \quad \eta(h) = h + O(h^2).$$

Equation (6.6) can be solved exactly [3]. Just as for the ODE of Eq. (6.5), we require [1]

$$(6.11) \quad \lim_{k \rightarrow \infty} y_k = u_1, \quad \lim_{k \rightarrow -\infty} y_k = u_2, \quad u_2 > u_1 > 0.$$

This gives

$$(6.12) \quad c = \frac{u_1 + u_2}{2}, \quad A = \frac{u_1 u_2}{2}.$$

Thus, the wave propagation velocity and the integration constant are determined by the asymptotic values of y_k . Note that these relations are *exactly* those gotten for the ODE [1].

The solution to Eq. (6.6), subject to the conditions given by Eq. (6.11) is

$$(6.13) \quad y_k = \frac{\alpha \lambda^k + D\beta}{r_+ \lambda^k + Dr_-},$$

where D is an arbitrary constant and

$$(6.14) \quad \alpha \equiv \frac{\phi u_2}{1 - u_1 \phi}, \quad \beta \equiv \frac{\phi u_1}{1 - u_2 \phi},$$

$$(6.15) \quad r_+ \equiv \frac{\phi}{1 - u_1 \phi}, \quad r_- \equiv \frac{\phi}{1 - u_2 \phi}.$$

To maintain positivity of the solution, y_k , we require

$$(6.16) \quad 0 < \phi(h) < \left(\frac{1}{u_2} \right), \quad h > 0.$$

A possible form for $\phi(h)$ that has this property is

$$(6.17) \quad \phi(h) = \frac{1 - e^{-hu_2}}{u_2}.$$

An elementary calculation shows that Eq. (6.13), with the condition of Eq. (6.16), gives solutions y_k that have all of the properties of the solutions of the ODE in Eq. (6.5).

The full details of the above calculations are in a manuscript submitted to *Numerical Methods for Partial Differential Equations*, where it is currently under review.

References

1. J. D. Logan, *Numerical Partial Differential Equations* (Wiley-Interscience, 1994). See Section 4.5.
2. R. E. Mickens, *Nonstandard Finite Difference Models of Differential Equations* (World Scientific, 1994). See Section 3.4.
3. R. E. Mickens, *Difference Equations: Theory and Applications* (Chapman and Hall, 1990). See Section 6.3.

7. Dissipative Complex Equation

The so-called dissipative complex equation

$$(7.1) \quad \frac{dz}{dt} = z[(1 - |z|^2) + i], \quad z = u + iv,$$

has been used to test the genesis of numerical instabilities for most of the standard integration methods applied to ODE's. (See references [1] and [3] of section 2.) This complex equation can be rewritten in terms of two real equations:

$$(7.2) \quad \frac{du}{dt} = u - v - u(u^2 + v^2),$$

$$(7.3) \quad \frac{dv}{dt} = u + v - v(u^2 + v^2).$$

In the (u, v) phase-plane, all trajectories to Eqs. (7.2) and (7.3) approach the limit-cycle, $u^2 + v^2 = 1$.

We have constructed a nonstandard finite-difference scheme for these equations. Our numerical studies show that the scheme gives solutions, for all $h > 0$, such that asymptotically they approach the correct limit-cycle located at $u_k^2 + v_k^2 = 1$. None of the schemes investigated by Yee and Sweby (see reference [3] of section 2) has this property.

The Figures on the next two pages show numerical results for $x_0 = u(0) = 0$, $y_0 = v(0) = 0.1$. Note that the step-sizes for the two figures are $h = 0.1$ and $h = 50!$ This work is summarized in the following abstract and publication:

1. K. Oyediji and R. E. Mickens, "Numerical integration schemes for the dissipative complex equation," *Bulletin of the American Physical Society* **41**, 1667 (1996).
2. R. E. Mickens and K. Oyediji, "Numerical integration of the dissipative complex equation," *International Journal of Applied Science and Computations* **4**, 99-103 (1997).

Figure 1. Dissipative complex equation.
 $x_0 = u(0) = 0$, $y_0 = v(0) = 0.1$, $h = 0.1$.

Figure 2. Dissipative complex equation.
 $x_0 = u(0) = 0$, $y_0 = v(0) = 0.1$, $h = 50$.