FINAL TECHNICAL REPORT

2000–2008

Grant Number: DOE Grant DE-FG02-02ER25515

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RESUMÉ

This material is the Final Technical Report for DOE Grant DE-FG-02-02ER25515. The principal investigator was Dr. Ronald E. Mickens of the Physics Department at Clark Atlanta University. The particular items stated in this Report are a concise summary of the research and related activities conducted under funding received from the above stated DOE grant. The full, detailed, and specific items, citations, etc., for essentially all research activities were given in the 2007 Progress Report to DOE. This report was submitted on March 21, 2008 to Ms. Teresa Beachley for transmission to Dr. George R. Seweryniak, DOE/Office of Advanced Scientific Computing Research. The current Final Technical Report provides the final reporting activity under DOE Grant DE-FG-02-02ER25515. Copies of this report are also distributed to the various relevant grant associated offices at Clark Atlanta University; in particular, copies will be provided to the CAU Grants Administration Office.

The DOE grant supported the PI in a number of research related activities. First, funds for release-time allowed the PI to conduct his investigations during the academic year. Likewise, additional funds for summer salary provided the support needed for a continuous effort of two months of uninterrupted work. Second, student support funds allowed the PI to train students in the methods of scientific research and also made possible an enhanced learning environment for the students to actively engage in "real" research work at levels appropriate to their academic preparation and interests. Third, it is important to point out that the PI's research productivity was excellent. More than 40 publications appeared in peer-reviewed journals and proceedings; several books/edited volumes were written; and the PI presented his research results at a large number of professional meetings, research conferences/workshops, and universities. Of interest and significance is that the citation rate for PI related research was approximately 100/year. Over the duration of the DOE grant, several hundred papers were published by researchers other than the PI.

As PI, my general view is that my research efforts involving the formulation of the nonstandard finite difference (NSFD) methodology has been immensely successful. An increasing number of other international based researchers are using these techniques, extending its range of applicability, and providing additional mathematical justification for its validity. I will continue my research on NSFD schemes.

A. NSFD Methodology and Impact of Research Methodology

The general methodology and philosophical basis of the nonstandard finite difference (NSFD) discretization of differential equations, for the purposes of obtaining numerical solutions, is given in various places in the research literature. A good, general introduction to the NSFD methodology and its applications is given in:

- R. E. Mickens, "Dynamic consistency: A fundamental principal for constructing NSFD schemes for differential equations," *Journal of Difference Equations and Applications* **11** (2005), 645–653.
- R. E. Mickens (editor), *Advances in the Applications of NSFD Schemes* (World Scientific, Singapore, 2005).
- R. E. Mickens, "Calculation of denominator functions for NSFD schemes for differential equations satisfying a positivity condition," *Numerical Methods for Partial Differential Equations* **23** (2007), 672–691.

In brief, the general NSFD scheme methodology is based on three basic principles:

i) the use of a **modified form** for the **discretization of derivatives**, where the concept of a denominator function is introduced;

ii) the **nonlocal discrete representation** of both linear and nonlinear functions of the dependent variables and their derivatives;

iii) the application of the principal of **dynamic consistency**.

The above indicated publications provide the full details and rationalizations for these three principles.

Impact of Research

Based on search of the published literature, private communications, and my requested review evaluations of manuscripts for peer-reviewed journals, I can conclude that the general NSFD scheme methodology has generated great interest in a certain community of researchers who either want to calculate numerical solutions for differential equations or who wish to understand at a deep level the discretization of continuous systems.

My formal and informal networks indicate that over 100 citations are made to my

NSFD scheme work each year and that papers are being published by an international based group of researchers. In addition to my review articles, at least two others, not by me have been published on NSFD methods. Further, (approximately) five dissertations and theses have been done on such schemes. Further, more than several hundred publications have been published on this topic in the following areas:

- NSFD theory and methodology
- nonlinear heat transfer
- dynamic systems (ODE's)
- advection, reaction, diffusion, wave systems (PDE's)
- population models, disease dynamics, biosciences
- computational electromagnetics
- non-smooth mechanics
- simulation of robotic systems.

In summary, I think that it is clear that the general NSFD methodology is becoming incorporated into the research agendas of an ever increasing number of scientists, engineers, mathematicians, and mathematical modelers.

B. Technical Achievements and Applications

The major technical achievements all involve general and fundamental issues related to the construction of NSFD schemes for particular, yet still broad classes of both ODE's and PDE's. The four most significant accomplishments are:

1) an enhanced, deeper understanding of both the physical and mathematical foundations of the NSFD methodology;
2) a precise definition of the concept of "dynamic consistency" and the role that it can play in constructing NSFD discretizations;
3) the discovery/creation of a method for determining denominator functions, which appear in the discretizations of derivatives, for the case of coupled, nonlinear ODE's, satisfying a positivity condition;
4) the comprehension of the powerful role played by symmetry principles and the associated conservation laws for restricting the possible NSFD functional forms for terms

in both single and systems of ODE's and PDE's.

Using the above stated "understandings," we have applied the NSFD methodology to a broad range of particular differential equations. In most instances, our major purpose was to increase understanding of the discretization process using NSFD schemes and, in turn, to use these results to clarify, improve, and extend the NSFD methodology. The following topical areas cover the particular types of differential equations that were investigated:

- parabolic PDE's having nonlinear diffusion, and/or reaction, and/or advection
- the asymptotics of discrete Airy equations
- ODE models of HIV transmission and control
- discrete-time models for periodic diseases (with or without vaccination)
- the damped wave equation (phase-lagging heat transport)
- coupled, nonlinear oscillators
- ODE models in the bio-sciences
- the Volterra integro-differential equation.

C. Dissemination Activities

The research findings of the PI have been widely disseminated through a broad range of scientific publication activities: peer-reviewed publications, abstracts, review articles, and books. Below I only list the total numbers of PI generated papers and abstracts, but give explicit citations to the review articles and books based on support from the DOE grant.

Abstracts

These abstracts give summaries of presentations made at professional meetings and research based conferences/workshops. During 2000 to 2008, they total to 43 items. The details of the full citations have been given in previous yearly Progress Reports to DOE.

Full Journal Publications

The total number of peer-reviewed journal and peer-reviewed conference/workshop proceedings during 2000 to 2008 is 59. In general, all these publications have been fully cited in previous yearly Progress Reports to DOE.

Review Articles by R. E. Mickens on NSFD Schemes

1) R. E. Mickens, "Asymptotic Solutions to a Discrete Airy Equation," *Abstracts of Papers Presented to the American Mathematical Society* **22**, 95 (2001). Abstract 962-39-1430.

2) R. E. Mickens, "Willie Hobb Moore: A Life in Science and Service," Conference Abstracts, XXVII Day of Scientific Lectures and 23rd Annual Meeting of the National Society of Black Physicists (North Carolina A and T State University; Greensboro, NC; March 15–18, 2000), pp. 17.

3) R. E. Mickens, "Analysis of a Nonstandard Finite Difference Scheme for the Korteweg-de-Vries Equation," *Book of Abstracts, The Third IMACS International Conference on Nonlinear Evolution Equations and Wave Phenomena: Computation and Theory* (The University of Georgia; Athens, GA; April 7–10, 2003); pp. 97.

4) K. Oyedeji, S. A. Rucker, and R. E. Mickens, "Numerical Analysis of a Linear Oscillator Having 'Volleyball Aerodynamics Drag' Damping," pp. 67.

5) R. E. Mickens, "A Combustion Model Exhibiting Metastability," Abstract 1023–L5–33, pp. 294.

6) K. Oyedeji, S. A. Rucker and R. E. Mickens, "Numerical and Asymptotic Solutions for the Nonlinear Oscillator $\ddot{y} + t^2 y/(1+t^2) = 0$," pps. 50–51.

7) Ronald Mickens, Kale Oyedeji, and Anthony Afuwape, "A Third-Order Differential Equation Modeling Stellar Pulsation," *Bulletin of the American Physical Society* **52** (#15), 19 (2007).

8) R. E. Mickens, "SIR Models with Square-Root Dynamics," Abstract 1035-39-234 (pp. 120).

Books

During the DOE grant support period the following research related books were published:

1) R. E. Mickens (editor), *Applications of Nonstandard Finite Difference Schemes* (World Scientific, Singapore, 2000).

2) R. E. Mickens, *Mathematical Methods for the Natural and Engineering Sciences* (Series on Advances in Mathematics for Applied Sciences, World Scientific, Singapore, 2004).

3) R. E. Mickens (editor), *Advances in the Applications of Nonstandard Finite Difference Schemes* (World Scientific, Singapore, 2005).

Edited volumes 1) and 3) presented up to date (at that point in time) advances in the methodology and applications of nonstandard finite difference (NSFD) schemes.

A dated, but excellent general introduction to NSFD schemes is

4) R. E. Mickens, *Nonstandard Finite Difference Models of Differential Equations* (World Scientific, Singapore, 1994).

Invited Presentations

During the grant period 2000–2008, approximately 43 seminars and professional presentations were given on NSFD schemes and their applications. These talks took place at various conferences/workshops and universities.

D. Research Related Professional Activities

Below is a summary of professional activities related to research carried out under the DOE grant. We only present major items for the period 2000–2008.

Journal Editorial Boards

I serve on the following peer-reviewed, research journals editorial boards:

- *Journal of Difference Equations and Applications*
- *International Journal of Evolution Equations*
- *Computing in Science and Engineering*

Organizer/Chair of Special Sessions at Meetings/Workshops

1) **Co-Chair**: AMS Special Session on "Discrete Dynamics and Difference Equations," Joint Mathematics Meeting; Baltimore, MD; January 18, 2003.
2) **Chair**: Session DEA-V, "Differential Equations and Applications," 4th International Conference on Dynamic Systems and Application; Atlanta, GA; May 23, 2003.
3) **Co-Chair**: Session VIB-60, "Dynamics and Control of Time-Varying and Time-Delay Systems and Structures II;" 19th Biannual Conference on Mechanical Vibration and Noise; Chicago, IL; September 4, 2003.

4) **Co-Chair and Co-Organizer**: Special Sessions on "Mathematical and Computational Biology," AIMS 5th International Conference on Dynamical Systems and Differential Equations; Pomona, CA; June 18–19, 2004.
5) **Members**: International Scientific Committee, 5th WSEAS International Conference on Mathematics and Computers in Biology and Chemistry; Venice, Italy; November 15–17, 2004.
6) **Member**, Organizing Committee, Joint Summer Research Conference in the Mathematical Sciences: "Competitive Mathematical Models of Disease Dynamics: Emerging Paradigms and Challenges," Snowbird Resort; Snowbird, Utah; July 17–21, 2005.
7) **Organizer**, Focus Sessions A32 on "Novel Computational Algorithms: From Materials to the Universe," 2005 March Meeting of the American Physical Society; Los Angeles, CA; March 21–22, 2005.
8) **Organizer and Chair**, Minisymposium MS58: "Biological Applications of Nonstandard Finite Difference Schemes," 2005 SIAM Annual Meeting; New Orleans, LA; July 14, 2005.
9) **Member**, Scientific Committee, 2006 International Conference on Computational and Mathematical Methods in Science and Engineering; Madrid, Spain; September 20–24, 2006.
10) **Chair**, Session H14: "Novel (Computational) Techniques," American Physical Society April 2006 Meeting, Hyatt Regency Hotel; Dallas, TX: April 23, 2006.
11) **Organizer and Chair**: Session DD, "Nonlinear Waves and Continuum Mechanics Phenomena," 74th Annual Meeting of the Southeastern Section of the APS; Nashville, TN; November 8, 2007.
12) **Chair**: Session on "Mathematical Biology," 6th International Conference on Differential Equations and Dynamical Systems; Baltimore, MD; May 24, 2008.

Manuscript Reviews

During the funding period of the DOE Grant, I provided evaluations of research and book manuscripts for more than twenty peer-reviewed research journals and book publishers; these include

- *Journal of Computational and Applied Mathematics*
- *Applied Numerical Mathematics*
- *Journal of Difference Equations and Applications*
- *Journal of Mathematics and Computers in Simulation*
- *Proceedings of the Royal Society*
- *Numerical Methods for Partial Differential Equations*
- *Nonlinear Dynamics*
- *International Journal of Nonlinear Mechanics*
- *Physics Letters A*

The subject matter of these manuscripts covered general finite difference techniques for the numerical integration of differential equations, including the application of NSFD schemes.

E. Unresolved Research Issues

While the general NSFD methodology has been very successful, there exists a current set of issues that have not been fully resolved at the present time. The following is a listing of four such topics.

• Differential equations having the dependent variable appear to some fractional power exist as models of various physical phenomena. The case of interest is where this power is positive, but bounded by one in value. If an expression containing such a term appears in a differential equation for which positivity holds, then the question arises as to how it should be discretely modeled. Some of our preliminary work suggests that for rational-valued powers, NSFD schemes do exist for these situations.

• We have essentially solved the problem of constructing NSFD schemes for systems of ODE's satisfying a conservation law and for which a condition of positivity holds for the dependent variables. The question now arises as to what should be done for the case where positivity holds, but no conservation law exists. For example, many phenomena in the biosciences may be modeled in this way. While we have no current answer to this issue, one possibility is to model discretely similar terms, occurring in different equations, exactly the same way. Also, it may happen that nontrivial, nonlinear combinations of the equations may provide a function of the dependent variables that is conserved. For this case, this restriction may give hints as to the proper NSFD scheme to be used for the original system of ODE's.

• Oscillatory systems are quite common in the natural sciences. For some systems the dependent variables are non-negative, while for others the variables can be of either sign. The systems of interest here are those for which the oscillations take place in the appropriate phase-space in the neighborhood of a linear center fixed-point. It is well known that this situation is unstable with regard to perturbations. Consequently, the discretization may change the nature of this fixed-point to either a stable or unstable node. There is also the difficulty arising from the fact that associated with these problems are time scales related to the characteristic oscillation periods. The two fundamental issues for oscillatory systems are how to discretely model both the linear and nonlinear terms, and how to construct the appropriate set of denominator functions. Also, it seems clear that whatever discretizations are required, they will differ for the two cases where the dependent variables are non-negative and where they can be of either sign. However, some recent work has provided insight into how the denominator functions can be calculated.

• Many physical and biosciences systems can be understood in terms of "cross-diffusion" (CD), i.e., the modeling nonlinear, coupled PDE's have diffusion coefficients depending on all the dependent variables. Since these mixed-diffusion coefficients can be of either mathematical sign, stability issues immediately arise for discretizations of these equations. Further, when the dependent variables satisfy a positivity condition, it becomes very difficult to properly incorporate this into the scheme. Previous, but, preliminary work by the PI on this topic was not very productive. We were able to satisfy the positivity condition, but with a loss in the accuracy of the numerical results. Our research continues on this issue.

• Current NSFD schemes for PDE's are currently semi-implicit, i.e., the independent variables always appear linearly at the advance discrete-time level and at one discrete-space grid location. This means that the discretized dependent variables can be solved to give (mathematically) expressions for the dependent variables at the previous discrete-time level. An important issue is how to construct dynamical consistent NSFD schemes that are fully implicit, but still linear in all the discretized independent variables at the advanced level. Valid schemes of this type would have immediate impact on the numerics of parabolic PDE's. In particular, such NSFD schemes would have enhanced values for the magnitudes of the time-space step-sizes relative to current explicit schemes.