STABILITY AND CONVERGENCE FOR NONLINEAR PARTIAL DIFFERENTIAL EQUATIONS

by Oday Mohammed Waheeb

A thesis

submitted in partial fulfillment of the requirements for the degree of Master of Science in Mathematics Boise State University

December 2012

© 2012 Oday Mohammed Waheeb ALL RIGHTS RESERVED

BOISE STATE UNIVERSITY GRADUATE COLLEGE

DEFENSE COMMITTEE AND FINAL READING APPROVALS

of the thesis submitted by

Oday Mohammed Waheeb

Thesis Title: Stability and Convergence for Nonlinear Partial Differential Equations

Date of Final Oral Examination: 16 October 2012

The following individuals read and discussed the thesis submitted by student Oday Mohammed Waheeb, and they evaluated his presentation and response to questions during the final oral examination. They found that the student passed the final oral examination.

Barbara Zubik-Kowal, Ph.D.	Chair, Supervisory Committee
Mary J. Smith, Ph.D.	Member, Supervisory Committee
Uwe Kaiser, Ph.D.	Member, Supervisory Committee

The final reading approval of the thesis was granted by Barbara Zubik-Kowal, Ph.D., Chair of the Supervisory Committee. The thesis was approved for the Graduate College by John R. Pelton, Ph.D., Dean of the Graduate College.

DEDICATION

بسْم الله الرَّحْمَن الرَّحِيم

اقْرَأْ بِاسْمِ رَبِّكَ الَّذِي خَلَقَ (١) خَلَقَ الْإِنْسَانَ مِنْ عَلَقٍ (٢) اقْرَأْ وَرَبُّكَ الْأَكْرَمُ (٣) الَّذِي عَلَّمَ بِالْقَلَم (٤) عَلَّمَ الْإِنْسَانَ مَا لَمْ يَعْلَم

صدق الله العظيم

اهدي رسالة الماجستير هذه الى روح والدتي رحمها الله والى والدي العزيز (محمد و هيب) اطال الله عمره والى اخوتي عطيل ولبيد واختي اروى. والى ولدي الملاكين مريم ومحمد حفظهما الله. واخيرا وليس اخرا اهديه الى زوجتي الغالية التي ساندتني وشجعتني في كل الخطوات (ود سعد).

> عدي محمد و هيب بويزي ـ و لاية ايداهو ـ الو لايات المتحدة الامريكية ديسمبر ٢٠١٢

> > Oday Mohammed Waheeb Boise-Idaho-USA December 2012

ACKNOWLEDGMENTS

I am greatly indebted to my thesis supervisor Dr. Barbara Zubik-Kowal for kindly providing guidance. Her comments have been a great help at all times. I would also like to express my gratitude to Dr. Mary Smith and Dr. Uwe Kaiser for their helpful comments.

ABSTRACT

If used cautiously, numerical methods can be powerful tools to produce solutions to partial differential equations with or without known analytic solutions. The resulting numerical solutions may, with luck, produce stable and accurate solutions to the problem in question, or may produce solutions with no resemblance to the problem in question at all. More such numerical computations give no hope of solving this troublesome feature and one needs to resort to investing time in a theoretical approach. This thesis is devoted not solely to computations, but also to a theoretical analysis of the numerical methods used to generate computationally the approximate solutions. After deriving theoretical results for a wide class of problems, I use them to validate that my numerical computations produce reliable solutions.

The fundamentals of this work are based on mathematical analysis with which the application of analysis to PDEs in a numerical and computational framework was possible.

TABLE OF CONTENTS

A	BSTRACT	v
LI	IST OF FIGURES	vii
1	INTRODUCTION	1
2	NUMERICAL SOLUTIONS TO NONLINEAR PARTIAL DIFFER-	
	ENTIAL EQUATIONS	4
3	STABILITY ANALYSIS FOR NONLINEAR PARTIAL DIFFER-	
	ENTIAL EQUATIONS	8
4	CONVERGENCE ANALYSIS FOR NONLINEAR PARTIAL DIF-	
	FERENTIAL EQUATIONS	16
5	NUMERICAL COMPUTATIONS	22
6	CONCLUDING REMARKS	37
R	EFERENCES	39

LIST OF FIGURES

5.1	Numerical solutions to (5.1).	23
5.2	(A) Numerical solution to (5.1), (5.2), (5.3) computed with $\Delta x = 0.05$	
	and $\Delta t = \frac{1}{2} \Delta x^2$; (B) numerical error (5.4); (C) maximum error (5.5);	
	and (D) maximum error (5.6)	24
5.3	Numerical error (5.4) with decreasing stepsizes $\triangle x$	25
5.4	Solutions and errors for the Fitzhugh-Nagumo equation (1.4) solved	
	with the step-sizes $\triangle t = 0.005$ and $\triangle x = 0.1$: (A) numerical solution	
	$V^{(i)}_{\Delta x}(t_j)$; (B) numerical error (5.4); (C) exact solution $u(x,t)$; (D)	
	maximum error (5.5) .	27
5.5	Numerical errors for the Fitzhugh-Nagumo equation (1.4) : (A) (5.4)	
	with $\triangle x = 0.2$, (B) (5.4) with $\triangle x = 0.02$, (C) (5.5) with $\triangle x = 0.2$,	
	(D) (5.5) with $\Delta x = 0.02$. The time step-size $\Delta t = 0.005$ was applied	
	for all the subplots	28
5.6	Numerical solutions $V^{(i)}_{\Delta x}(t_j)$ to the Kolmogorov-Petrovskii-Piskunov	
	equation (1.5) for the indicated temporal grid-points t_j and all spacial	
	grid-points x_i	30
5.7	Numerical solutions $V^{(i)}_{\Delta x}(t_j)$ to the Kolmogorov-Petrovskii-Piskunov	
	equation (1.5) for the indicated spacial grid-points x_i and all time grid-	
	points t_j	31

- 5.9 Numerical solutions $V_{\Delta x}^{(i)}(t_j)$ to the Fisher-Kolmogorov equation (1.6) for the indicated temporal grid-points t_j and all spacial grid-points x_i . 34

CHAPTER 1

INTRODUCTION

Vast parts of real-world physical systems are described by nonlinear partial differential equations. Such equations arise in various fields of applications, for example, fluid mechanics, gas dynamics, combustion theory, relativity, elasticity, thermodynamics, biology, ecology, neurology, and many others.

For this thesis, we study numerical solutions for a general class of nonlinear parabolic differential equations. We discretize the partial differential equations in the spatial variable and obtain systems of ordinary differential equations, which we then integrate in time and compute numerical solutions. In order to validate our computations, we analyze the stability of the numerical method and convergence of the numerical solutions of the semi-discrete systems derived for nonlinear partial differential equations. The analysis is provided for the general class of nonlinear parabolic differential equations. We also present our results of numerical experiments with examples of partial differential equations that belong to the general class. We use our theoretical results to validate that our numerical computations produce reliable results.

Specifically, we devote our study to nonlinear partial differential equations of evolution, which are written in the form

$$\frac{\partial u}{\partial t}(x,t) = f\left(x,t,u(x,t),\frac{\partial^2 u}{\partial x^2}(x,t)\right). \tag{1.1}$$

Using appropriate definitions for the function f from (1.1), we can obtain a huge variety of nonlinear partial differential equations. Here $x \in [x_a, x_b]$ and $t \in [t_0, T]$ represent the space and time variables, respectively. The equation (1.1) is supplemented by the boundary conditions

$$u(x_a, t) = a(t),$$

 $u(x_b, t) = b(t), \quad t \in [t_0, T],$
(1.2)

and the initial condition

$$u(x, t_0) = u_0(x), \quad x \in [x_a, x_b].$$
 (1.3)

Here, $x_a < x_b$ and $t_0 < T$ are arbitrary constants and a, b, and u_0 are functions of t and x, accordingly.

If we define

$$f(x,t,p,q) = Dq - p(1-p)(\alpha - p),$$

where D and α are constants such that D > 0 and $0 \le \alpha \le 1$, then (1.1) generates the Fitzhugh-Nagumo equation

$$\frac{\partial u}{\partial t}(x,t) = D \frac{\partial^2 u}{\partial x^2}(x,t) - u(x,t) \left(1 - u(x,t)\right) \left(\alpha - u(x,t)\right),\tag{1.4}$$

which arises in population genetics. This equation models the transmission of nerve impulses. More details about (1.4) are provided in [10], [13], [14], [6], and [3].

If the function f is defined by

$$f(x, t, p, q) = Dq + \alpha p + \beta p^m,$$

where α , β , and m are all different than 1, then (1.1) generates the Kolmogorov-Petrovskii-Piskunov equation

$$\frac{\partial u}{\partial t}(x,t) = D \frac{\partial^2 u}{\partial x^2}(x,t) + \alpha u(x,t) + \beta \left(u(x,t)\right)^m.$$
(1.5)

This equation arises in heat and mass transfer, combustion theory, biology, and ecology. More details about (1.5) are provided in [11], [14], and [2].

If the function f is defined by

$$f(x, t, p, q) = q + p(1 - p^{r}),$$

where r > 0, then (1.1) generates the Fisher-Kolmogorov equation

$$\frac{\partial u}{\partial t}(x,t) = \frac{\partial^2 u}{\partial x^2}(x,t) + u(x,t) \Big(1 - \big(u(x,t)\big)^r\Big),\tag{1.6}$$

with applications in biology [12].

More equations (also linear) can be generated from (1.1) by defining the function f in infinitely many ways.

The goal of the thesis is to analyze stability and convergence of numerical solutions to equations written in the general form (1.1) with a general function f, which can be used to generate more examples (not only (1.4), (1.5), and (1.6)). The analysis is presented in Chapters 3 and 4. The goal of presenting numerical computations for the above particular examples is realized in Chapter 5 where numerical solutions to (1.4), (1.5), and (1.6) are illustrated graphically. The reliability of these graphical results (used for illustration only) is validated by the analysis and theorems proved in the previous Chapters 3 and 4. Finally, Chapter 6 includes concluding remarks.

CHAPTER 2

NUMERICAL SOLUTIONS TO NONLINEAR PARTIAL DIFFERENTIAL EQUATIONS

In many cases, exact solutions of nonlinear partial differential equations are unknown and numerical solutions provide valuable information in the study of the physical processes. In this chapter, we investigate numerical solutions constructed for nonlinear partial differential equations.

In order to solve (1.1) numerically, we first consider the numerical method of lines and discretize the spatial domain $[x_a, x_b]$. We consider discrete sets included in the continuum set $[x_a, x_b]$ and, on each discrete set, we replace the differential operator with respect to x by a finite difference operator. This process is also called *semi-discretization* as, at this stage, the time variable stays in the continuum set $[t_0, T]$.

In order to discretize (1.1) in the spatial domain, we introduce the grid-points

$$x_i = x_a + i \Delta x, \quad i = 0, 1, \dots, N+1,$$
 (2.1)

where $\Delta x = \frac{x_b - x_a}{N+1}$ is called a *spatial step-size* and $x_{N+1} = x_b$. Here, N + 1 is the number of subintervals $[x_i, x_{i+1}] \subset [x_a, x_b]$. We will consider the following family of meshes

$$\left\{ \{x_i\}_{i=0}^{N+1} \subset [x_a, x_b] \quad : \quad \Delta x \in (0, 1) \right\}$$

and, in order to analyze convergence of numerical solutions, we will also consider the meshes for $\Delta x \to 0$.

We will consider exact and numerical solutions on lines determined by the spatial grid-points (2.1). For each Δx , let

$$X_p = \{x_i : i = 0, 1, \dots, N+1\}, \quad R_p = X_p \times [t_0, T],$$

u be the exact solution to problem (1.1)-(1.3), $u_p : R_p \to \mathbb{R}$ be the projection of the exact solution u to the lines R_p , and $v_{\triangle x} : R_p \to \mathbb{R}$ be a numerical solution computed on the lines. For an index i = 1, 2, ..., N and the step-size $\triangle x$, we define an operator $\phi_{\triangle x}^{(i)} : \mathcal{C}([t_0, T], \mathbb{R}^{N+2}) \times [t_0, T] \to \mathbb{R}$ in the following way

$$\phi_{\Delta x}^{(i)}(w,t) = \frac{1}{\Delta x^2} \Big(w_{i+1}(t) - 2w_i(t) + w_{i-1}(t) \Big),$$

where $w \in \mathcal{C}([t_0, T], \mathbb{R}^{N+2})$ and $t \in [t_0, T]$.

In order to construct semi-discrete systems for (1.1), we define a vector function $V_{\Delta x} \in \mathcal{C}([t_0, T], \mathbb{R}^{N+2})$ in the following way

$$V_{\Delta x}(t) = \begin{bmatrix} V_{\Delta x}^{(0)}(t) \\ V_{\Delta x}^{(1)}(t) \\ \vdots \\ V_{\Delta x}^{(N)}(t) \\ V_{\Delta x}^{(N)}(t) \\ V_{\Delta x}^{(N+1)}(t) \end{bmatrix}, \qquad V_{\Delta x}^{(i)}(t) = v_{\Delta x}(x_i, t), \qquad i = 0, 1, \dots, N, N+1,$$

where

$$V_{\Delta x}^{(0)}(t) = a(t), \quad V_{\Delta x}^{(N+1)}(t) = b(t).$$
 (2.2)

For the general problem (1.1)-(1.3), we consider the semi-discrete system

$$\begin{cases} \frac{d}{dt} V_{\Delta x}^{(i)}(t) = f\left(x_i, t, V_{\Delta x}^{(i)}(t), \phi_{\Delta x}^{(i)}\left(V_{\Delta x}, t\right)\right), \\ V_{\Delta x}^{(i)}(t_0) = u_0(x_i), \end{cases}$$
(2.3)

where $t \in [t_0, T]$ and i = 1, 2, ..., N. The problem of solving (1.1)-(1.3) is now transformed into the problem of solving (2.3).

The purpose of the thesis is to analyze if

$$\lim_{\Delta x \to 0} v_{\Delta x}(x_i, t) = u_p(x_i, t),$$

for all i = 1, 2, ..., N and $t \in [t_0, T]$. It is worth pointing out that (2.3) is a family of initial-value problems with a system of N nonlinear ordinary differential equations, where N depends on the parameter Δx and taking smaller Δx results in larger systems.

In order to solve (2.3) for each Δx , we transform (2.3) into the form

$$\begin{cases} y'(t) = F(t, y(t)) \\ y(t_0) = y_0, \end{cases}$$
(2.4)

where F depends on $\triangle x$ and

$$y(t) = \begin{bmatrix} y_0(t) \\ y_1(t) \\ \vdots \\ y_N(t) \\ y_{N+1}(t) \end{bmatrix}, \quad F(t, y(t)) = \begin{bmatrix} F_0(t, y(t)) \\ F_1(t, y(t)) \\ \vdots \\ F_N(t, y(t)) \\ F_{N+1}(t, y(t)) \end{bmatrix}, \quad y_0 = \begin{bmatrix} u_0(x_0) \\ u_0(x_1) \\ \vdots \\ u_0(x_N) \\ u_0(x_{N+1}) \end{bmatrix}.$$

For this transformation, we define

$$F_i(t, y(t)) \stackrel{\text{def}}{=} f\left(x_i, t, y_i(t), \phi_{\Delta x}^{(i)}(y, t)\right),$$
$$y \stackrel{\text{def}}{=} V_{\Delta x},$$

and apply numerical methods for ordinary differential equations, e.g. Runge-Kutta methods (see [1], [4], [5], [16], and [17]), to solve the resulting system in t and compute numerical approximations to $v_{\Delta x}(x_i, t_n)$, where $t_n \in [t_0, T]$ are temporal grid-points. The numerical solutions to the problems (1.4), (1.5), and (1.6) are presented in Chapter 5.

Finite difference operators are used, e.g., by Iserles [8], where the stability and convergence of the finite difference method is thoroughly presented for *linear* partial differential equations. In this thesis, we present a stability and convergence analysis of the method applied to more challenging problems, namely, the *nonlinear* partial differential equations written in the form (1.1).

Nonlinear partial differential equations and finite difference methods are also investigated by Strikwerda [18], Hundsdorfer and Verwer [7], and LeVeque [9] but the stability and convergence analysis presented in this work for (1.1) is not considered in these references.

CHAPTER 3

STABILITY ANALYSIS FOR NONLINEAR PARTIAL DIFFERENTIAL EQUATIONS

In this chapter, we investigate stability of the method (2.3) and prove the following stability theorem.

Theorem 3.0.1. Let $x_a < x_b$, $t_0 < T$ be real constants and assume that the function $f : [x_a, x_b] \times [t_0, T] \times \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ is continuous, satisfies the Lipschitz condition

$$|f(x,t,p,q) - f(x,t,\bar{p},q)| \le L_p |p - \bar{p}|,$$
(3.1)

and

$$\frac{\partial f}{\partial q}(x,t,p,q) \ge 0, \tag{3.2}$$

for $x \in [x_a, x_b]$, $t \in [t_0, T]$, $p, \bar{p}, q \in \mathbb{R}$. Moreover, suppose that the functions $V_{\triangle x}, W_{\triangle x} \in \mathcal{C}([t_0, T], \mathbb{R}^{N+2})$ satisfy the following conditions

- $V_{\triangle x}$ are solutions of (2.3) and satisfy (2.2)
- $W_{\triangle x}$ satisfy (2.2) and the inequalities

$$\left| \frac{d}{dt} W_{\Delta x}^{(i)}(t) - f\left(x_i, t, W_{\Delta x}^{(i)}(t), \phi_{\Delta x}^{(i)}\left(W_{\Delta x}, t\right)\right) \right| \le \eta(\Delta x)$$

$$\left| W_{\Delta x}^{(i)}(t_0) - u_0(x_i) \right| \le \lambda(\Delta x),$$
(3.3)

for
$$i = 1, 2, ..., N$$
 and $t \in [t_0, T]$ with $\eta(\Delta x), \ \lambda(\Delta x) > 0$ such that $\lim_{\Delta x \to 0} \eta(\Delta x) = 0$
0 and $\lim_{\Delta x \to 0} \lambda(\Delta x) = 0$.

Then there exist $\xi(\Delta x) > 0$ such that

$$\left|V_{\Delta x}^{(i)}(t) - W_{\Delta x}^{(i)}(t)\right| \le \xi(\Delta x),\tag{3.4}$$

for i = 1, 2, ..., N, $t \in [t_0, T]$, and $\lim_{\Delta x \to 0} \xi(\Delta x) = 0$.

In the next part of the thesis, we will need the following lemma.

Lemma 3.0.2. The operator $\phi_{\Delta x}^{(i)} : \mathcal{C}([t_0, T], \mathbb{R}^{N+2}) \times [t_0, T] \to \mathbb{R}, i = 1, 2, ..., N$, is linear with respect to the functional argument.

Proof of Lemma 3.0.2. Let $w, \tilde{w} \in \mathcal{C}([t_0, T], \mathbb{R}^{N+2}), t \in [t_0, T]$, and $\alpha, \beta \in \mathbb{R}$. Note that, according to the notation introduced in Chapter 2, w, \tilde{w} are vector functions with zero as the index for their first components. Then

$$\begin{split} \phi_{\Delta x}^{(i)}(\alpha w + \beta \tilde{w}, t) &= \frac{1}{\Delta x^2} \Big(\Big(\alpha w_{i+1}(t) + \beta \tilde{w}_{i+1}(t) \Big) - 2 \Big(\alpha w_i(t) + \beta \tilde{w}_i(t) \Big) \\ &+ \Big(\alpha w_{i-1}(t) + \beta \tilde{w}_{i-1}(t) \Big) \Big) \\ &= \frac{1}{\Delta x^2} \Big(\alpha \Big(w_{i+1}(t) - 2w_i(t) + w_{i-1}(t) \Big) \\ &+ \beta \Big(\tilde{w}_{i+1}(t) - 2\tilde{w}_i(t) + \tilde{w}_{i-1}(t) \Big) \Big) \\ &= \alpha \frac{1}{\Delta x^2} \Big(w_{i+1}(t) - 2w_i(t) + w_{i-1}(t) \Big) \\ &+ \beta \frac{1}{\Delta x^2} \Big(\tilde{w}_{i+1}(t) - 2\tilde{w}_i(t) + \tilde{w}_{i-1}(t) \Big) \\ &= \alpha \phi_{\Delta x}^{(i)}(w, t) + \beta \phi_{\Delta x}^{(i)}(\tilde{w}, t), \end{split}$$

for i = 1, 2, ..., N, which finishes the proof of the lemma.

In the proof of the stability result stated in Theorem 3.0.1, we will also apply the following lemma.

Lemma 3.0.3. Suppose that $\mathcal{F} : [\alpha, \beta] \to \mathbb{R}$ is such that its derivative \mathcal{F}' is integrable on $[\alpha, \beta]$. Then

$$\mathcal{F}(\beta) = \mathcal{F}(\alpha) + (\beta - \alpha) \int_0^1 \mathcal{F}'(\alpha + s(\beta - \alpha)) ds.$$

Proof of Lemma 3.0.3. We apply the Fundamental Theorem of Calculus [15] and obtain

$$\mathcal{F}(\beta) = \mathcal{F}(\alpha) + \int_{\alpha}^{\beta} \mathcal{F}'(t) dt.$$
(3.5)

We now use the substitution

$$t = \alpha + s(\beta - \alpha),$$

which gives $dt = (\beta - \alpha)ds$ and

$$\int_{\alpha}^{\beta} \mathcal{F}'(t) dt = (\beta - \alpha) \int_{0}^{1} \mathcal{F}'(\alpha + s(\beta - \alpha)) ds.$$

This together with (3.5) proves the lemma.

We now apply both auxiliary Lemmas 3.0.2 and 3.0.3 and prove the stability theorem.

Proof of Theorem 3.0.1. Let $\Gamma_{\Delta x} = V_{\Delta x} - W_{\Delta x}$. Then

$$\frac{d}{dt}\Gamma_{\Delta x}^{(i)}(t) = \frac{d}{dt}V_{\Delta x}^{(i)}(t) - \frac{d}{dt}W_{\Delta x}^{(i)}(t)
= f\left(x_i, t, V_{\Delta x}^{(i)}(t), \phi_{\Delta x}^{(i)}(V_{\Delta x}, t)\right) - f\left(x_i, t, V_{\Delta x}^{(i)}(t), \phi_{\Delta x}^{(i)}(W_{\Delta x}, t)\right)
+ f\left(x_i, t, V_{\Delta x}^{(i)}(t), \phi_{\Delta x}^{(i)}(W_{\Delta x}, t)\right) - f\left(x_i, t, W_{\Delta x}^{(i)}(t), \phi_{\Delta x}^{(i)}(W_{\Delta x}, t)\right)
+ f\left(x_i, t, W_{\Delta x}^{(i)}(t), \phi_{\Delta x}^{(i)}(W_{\Delta x}, t)\right) - \frac{d}{dt}W_{\Delta x}^{(i)}(t).$$

Let

$$\Theta_f^{(i)}(t) = \int_0^1 \frac{\partial f}{\partial q} \left(x_i, t, V_{\Delta x}^{(i)}(t), \phi_{\Delta x}^{(i)}(W_{\Delta x}, t) + s \left(\phi_{\Delta x}^{(i)}(V_{\Delta x}, t) - \phi_{\Delta x}^{(i)}(W_{\Delta x}, t) \right) \right) ds.$$

Then, by Lemmas 3.0.2 and 3.0.3, we obtain

$$f\left(x_{i}, t, V_{\Delta x}^{(i)}(t), \phi_{\Delta x}^{(i)}(V_{\Delta x}, t)\right) - f\left(x_{i}, t, V_{\Delta x}^{(i)}(t), \phi_{\Delta x}^{(i)}(W_{\Delta x}, t)\right)$$
$$= \Theta_{f}^{(i)}(t) \left(\phi_{\Delta x}^{(i)}(V_{\Delta x}, t) - \phi_{\Delta x}^{(i)}(W_{\Delta x}, t)\right)$$
$$= \Theta_{f}^{(i)}(t) \phi_{\Delta x}^{(i)}(\Gamma_{\Delta x}, t).$$

From this, the Lipschitz condition (3.1), the triangle inequality, and (3.3) we obtain

$$\begin{aligned} \left| \frac{d}{dt} \Gamma_{\Delta x}^{(i)}(t) - \Theta_{f}^{(i)}(t) \phi_{\Delta x}^{(i)}(\Gamma_{\Delta x}, t) \right| \\ &= \left| f \left(x_{i}, t, V_{\Delta x}^{(i)}(t), \phi_{\Delta x}^{(i)}(W_{\Delta x}, t) \right) - f \left(x_{i}, t, W_{\Delta x}^{(i)}(t), \phi_{\Delta x}^{(i)}(W_{\Delta x}, t) \right) \right. \\ &+ f \left(x_{i}, t, W_{\Delta x}^{(i)}(t), \phi_{\Delta x}^{(i)}(W_{\Delta x}, t) \right) - \frac{d}{dt} W_{\Delta x}^{(i)}(t) \right| \\ &\leq \left| f \left(x_{i}, t, V_{\Delta x}^{(i)}(t), \phi_{\Delta x}^{(i)}(W_{\Delta x}, t) \right) - f \left(x_{i}, t, W_{\Delta x}^{(i)}(t), \phi_{\Delta x}^{(i)}(W_{\Delta x}, t) \right) \right| \\ &+ \left| \frac{d}{dt} W_{\Delta x}^{(i)}(t) - f \left(x_{i}, t, W_{\Delta x}^{(i)}(t), \phi_{\Delta x}^{(i)}(W_{\Delta x}, t) \right) \right| \\ &\leq L_{p} \left| \Gamma_{\Delta x}^{(i)}(t) \right| + \eta(\Delta x). \end{aligned}$$

We now define

$$\Psi(t) = \sup \Big\{ \big| \Gamma_{\Delta x}^{(i)}(\tau) \big| : t_0 \le \tau \le t, \quad i = 1, 2, \dots, N \Big\},\$$

for $t \in [t_0, T]$. The supremum exists because $|\Gamma_{\Delta x}^{(i)}(\tau)|$ is a continuous function on the compact (closed and bounded) interval $[t_0, t]$ and, therefore, $|\Gamma_{\Delta x}^{(i)}(\tau)|$ is bounded. Moreover, since $\Gamma_{\Delta x}^{(i)}(\tau)$ is continuous, $\Psi \in \mathcal{C}([t_0, T], \mathbb{R}_+)$, where $\mathbb{R}_+ = [0, \infty)$. Since $V_{\Delta x}^{(i)}(t_0) = u_0(x_i)$ and $|u_0(x_i) - W_{\Delta x}^{(i)}(t_0)| \leq \lambda(\Delta x)$, we obtain $\Psi(t_0) \leq \lambda(\Delta x)$. We will show that

$$\Psi(t) \le \gamma(t),\tag{3.6}$$

for $t \in [t_0, T]$, where $\gamma(t)$ is the solution to the initial-value problem

$$\begin{cases} \gamma'(t) = L_p \gamma(t) + \eta(\Delta x) \\ \gamma(t_0) = \lambda(\Delta x). \end{cases}$$
(3.7)

There exists $\tilde{\varepsilon} > 0$ such that for all $0 < \varepsilon < \tilde{\varepsilon}$ the solution $\tilde{\gamma}_{\varepsilon}(t)$ of

$$\begin{cases} \tilde{\gamma}_{\varepsilon}'(t) = L_p \tilde{\gamma}_{\varepsilon}(t) + \eta(\Delta x) + \varepsilon \\ \tilde{\gamma}_{\varepsilon}(t_0) = \lambda(\Delta x) + \varepsilon. \end{cases}$$

satisfies the property

$$\lim_{\varepsilon \to 0} \tilde{\gamma}_{\varepsilon}(t) = \gamma(t)$$

uniformly with respect to $t \in [t_0, T]$. Let $0 < \varepsilon < \tilde{\varepsilon}$. We will show that

$$\Psi(t) < \tilde{\gamma}_{\varepsilon}(t), \tag{3.8}$$

for $t \in [t_0, T]$. By contradiction, suppose it is false. Then, since

$$\Psi(t_0) \le \lambda(\triangle x) < \lambda(\triangle x) + \varepsilon = \tilde{\gamma}_{\varepsilon}(t_0)$$

and $\Psi, \tilde{\gamma}_{\varepsilon} \in \mathcal{C}([t_0, T], \mathbb{R}_+)$, there exists $t_1 \in (t_0, T]$ such that

$$\Psi(t_1) = \tilde{\gamma}_{\varepsilon}(t_1)$$

and

$$\Psi(\tau) < \tilde{\gamma}_{\varepsilon}(\tau),$$

for all $\tau \in [t_0, t_1)$. Since $\tilde{\gamma}'_{\varepsilon}$ is positive, $\tilde{\gamma}_{\varepsilon}$ is increasing and we get

$$\Psi(\tau) < \tilde{\gamma}_{\varepsilon}(\tau) \le \tilde{\gamma}_{\varepsilon}(t_1) = \Psi(t_1)$$

for all $\tau \in (t_0, t_1)$. From this strict inequality and by the definition of Ψ , there exists an index $i \in \{1, 2, ..., N\}$ such that

$$\Psi(t_1) = |\Gamma_{\Delta x}^{(i)}(t_1)|.$$

Therefore, there are two cases, either

Case I :
$$\Psi(t_1) = \Gamma^{(i)}_{\triangle x}(t_1)$$

or

Case II :
$$\Psi(t_1) = -\Gamma^{(i)}_{\wedge r}(t_1).$$

We will show the proof for Case I. The proof for Case II is similar. Suppose Case I and that $i \in \{1, 2, ..., N\}$. For h < 0, we obtain

$$\Psi(t_1+h) \ge \Gamma^{(i)}_{\wedge x}(t_1+h)$$

$$\frac{\Psi(t_1+h)-\Psi(t_1)}{h} \le \frac{\Gamma_{\Delta x}^{(i)}(t_1+h)-\Gamma_{\Delta x}^{(i)}(t_1)}{h}.$$

We now take $h \to 0^-$ and get $D_-\Psi(t_1) \leq \frac{d}{dt}\Gamma^{(i)}_{\Delta x}(t_1)$. Then

$$D_{-}\Psi(t_{1}) \leq \frac{d}{dt}\Gamma_{\Delta x}^{(i)}(t_{1}) \leq \Theta_{f}^{(i)}(t_{1})\phi_{\Delta x}^{(i)}(\Gamma_{\Delta x},t_{1}) + L_{p}\Gamma_{\Delta x}^{(i)}(t_{1}) + \eta(\Delta x)$$

$$= \frac{1}{\Delta x^{2}}\Theta_{f}^{(i)}(t_{1})\left(\Gamma_{\Delta x}^{(i+1)}(t_{1}) - 2\Gamma_{\Delta x}^{(i)}(t_{1}) + \Gamma_{\Delta x}^{(i-1)}(t_{1})\right)$$

$$+ L_{p}\Gamma_{\Delta x}^{(i)}(t_{1}) + \eta(\Delta x)$$

$$= \Gamma_{\Delta x}^{(i)}(t_{1})\left(L_{p} - \frac{2}{\Delta x^{2}}\Theta_{f}^{(i)}(t_{1})\right)$$

$$+ \frac{1}{\Delta x^{2}}\Theta_{f}^{(i)}(t_{1})\left(\Gamma_{\Delta x}^{(i+1)}(t_{1}) + \Gamma_{\Delta x}^{(i-1)}(t_{1})\right) + \eta(\Delta x).$$

From (3.2), we get $\Theta_f^{(i)}(t_1) \ge 0$, which implies further that

$$D_{-}\Psi(t_{1}) \leq \Gamma_{\Delta x}^{(i)}(t_{1})\left(L_{p}-\frac{2}{\Delta x^{2}}\Theta_{f}^{(i)}(t_{1})\right)+\frac{1}{\Delta x^{2}}\Theta_{f}^{(i)}(t_{1})\left(\Psi(t_{1})+\Psi(t_{1})\right)$$
$$+\eta(\Delta x)$$
$$= \Psi(t_{1})\left(L_{p}-\frac{2}{\Delta x^{2}}\Theta_{f}^{(i)}(t_{1})\right)+\frac{2}{\Delta x^{2}}\Theta_{f}^{(i)}(t_{1})\Psi(t_{1})+\eta(\Delta x)$$
$$= L_{p}\Psi(t_{1})+\eta(\Delta x)=L_{p}\tilde{\gamma}_{\varepsilon}(t_{1})+\eta(\Delta x)$$
$$< L_{p}\tilde{\gamma}_{\varepsilon}(t_{1})+\eta(\Delta x)+\varepsilon=\tilde{\gamma}_{\varepsilon}^{\prime}(t_{1})$$

and

$$D_{-}\Psi(t_1) < \tilde{\gamma}'_{\varepsilon}(t_1). \tag{3.9}$$

On the other hand, take h < 0 such that the value |h| is small enough to satisfy $t_0 \le t_1 + h < t_1$. Then

$$\Psi(t_1+h) < \tilde{\gamma}_{\varepsilon}(t_1+h)$$

and since

$$\Psi(t_1+h) - \Psi(t_1) < \tilde{\gamma}_{\varepsilon}(t_1+h) - \tilde{\gamma}_{\varepsilon}(t_1),$$

we get

$$\frac{\Psi(t_1+h)-\Psi(t_1)}{h} > \frac{\tilde{\gamma}_{\varepsilon}(t_1+h)-\tilde{\gamma}_{\varepsilon}(t_1)}{h}$$

and taking $h \to 0^-$ we obtain

$$D_{-}\Psi(t_{1}) \ge D_{-}\tilde{\gamma}_{\varepsilon}(t_{1}) = \tilde{\gamma}_{\varepsilon}'(t_{1}). \tag{3.10}$$

The equality in (3.10) is true because $\tilde{\gamma}_{\varepsilon}$ is differentiable. The relations (3.10) contradict (3.9) and show the inequality (3.8) for all $t \in [t_0, T]$ in Case I with $i \in \{1, 2, ..., N\}$. The proof is similar in Case II. We now take $\varepsilon \to 0$ in (3.8) and get (3.6). Finally, since γ solves (3.7), we get an analytic solution for γ :

$$\gamma(t) = \exp\left(L_p(t-t_0)\right)\lambda(\triangle x) + \frac{1}{L_p}\left(\exp\left(L_p(t-t_0)\right) - 1\right)\eta(\triangle x)$$

so by (3.6),

$$\Psi(t) \leq \exp\left(L_p(t-t_0)\right)\lambda(\Delta x) + \frac{1}{L_p}\left(\exp\left(L_p(t-t_0)\right) - 1\right)\eta(\Delta x)$$

$$\leq \exp\left(L_p(T-t_0)\right)\lambda(\Delta x) + \frac{1}{L_p}\left(\exp\left(L_p(T-t_0)\right) - 1\right)\eta(\Delta x)$$

and (3.4) is satisfied with

$$\xi(\Delta x) = \exp\left(L_p(T - t_0)\right)\lambda(\Delta x) + \frac{1}{L_p}\left(\exp\left(L_p(T - t_0)\right) - 1\right)\eta(\Delta x).$$
(3.11)

Moreover, by the properties of λ and η we obtain $\lim_{\Delta x \to 0} \xi(\Delta x) = 0$, which finishes the proof.

CHAPTER 4

CONVERGENCE ANALYSIS FOR NONLINEAR PARTIAL DIFFERENTIAL EQUATIONS

This chapter deals with nonlinear problems written in the general forms (1.1) and (2.3). The purpose of the analysis presented in this chapter is to answer the question whether the solutions $V_{\Delta x}$ of the general scheme (2.3) converge to the solution u of (1.1)-(1.3). The following theorem states a property about their convergence.

Theorem 4.0.4. Let u be a solution of (1.1)-(1.3) and $V_{\Delta x}$ be a solution of (2.3). Moreover, suppose that u is of class $C^4([x_a, x_b] \times [t_0, T], \mathbb{R})$ and the function $f \in C([x_a, x_b] \times [t_0, T] \times \mathbb{R} \times \mathbb{R}, \mathbb{R})$ satisfies the Lipschitz condition

$$\left| f(x,t,p,q) - f(x,t,\bar{p},\bar{q}) \right| \le L_p |p - \bar{p}| + L_q |q - \bar{q}|, \tag{4.1}$$

and the condition

$$\frac{\partial f}{\partial q}(x,t,p,q) \ge 0, \tag{4.2}$$

for $x \in [x_a, x_b]$, $t \in [t_0, T]$, $p, \bar{p}, q, \bar{q} \in \mathbb{R}$, where $x_a < x_b$, $t_0 < T$ are real constants. Then there exists $\mu(\Delta x) > 0$ such that

$$|u(x_i, t) - V_{\Delta x}^{(i)}(t)| \le \mu(\Delta x), \tag{4.3}$$

for
$$i = 1, 2, ..., N$$
, $t \in [t_0, T]$, and $\lim_{\Delta x \to 0} \mu(\Delta x) = 0$.

In the proof of Theorem 4.0.4, we will need the following lemma.

Lemma 4.0.5. Suppose that $u \in C^4([x_a, x_b] \times [t_0, T], \mathbb{R})$ and $u(x_a, t) = a(t), u(x_b, t) = b(t)$. Let $u_{\triangle x} : [t_0, T] \to \mathbb{R}^{N+2}$ be defined by

$$u_{\Delta x}^{(i)}(t) = u(x_i, t),$$
 (4.4)

for i = 0, 1, ..., N, N + 1 and $t \in [t_0, T]$. Then there exists a positive constant C > 0such that

$$\left|\frac{\partial^2 u}{\partial x^2}(x_i, t) - \phi_{\Delta x}^{(i)}(u_{\Delta x}, t)\right| \le C \Delta x^2 \tag{4.5}$$

for i = 1, 2, ..., N and $t \in [t_0, T]$.

Proof of Lemma 4.0.5. Let i = 2, 3, ..., N-1. Using Taylor's expansion at (x_i, t) we have

$$u(x_{i} + \Delta x, t) = u(x_{i}, t) + \Delta x \frac{\partial u(x_{i}, t)}{\partial x} + \frac{\Delta x^{2}}{2!} \frac{\partial^{2} u(x_{i}, t)}{\partial x^{2}} + \frac{\Delta x^{3}}{3!} \frac{\partial^{3} u(x_{i}, t)}{\partial x^{3}} + \frac{\Delta x^{4}}{4!} \frac{\partial^{4} u(\theta_{i}, t)}{\partial x^{4}}$$

$$(4.6)$$

and

$$u(x_{i} - \Delta x, t) = u(x_{i}, t) - \Delta x \frac{\partial u(x_{i}, t)}{\partial x} + \frac{\Delta x^{2}}{2!} \frac{\partial^{2} u(x_{i}, t)}{\partial x^{2}} - \frac{\Delta x^{3}}{3!} \frac{\partial^{3} u(x_{i}, t)}{\partial x^{3}} + \frac{\Delta x^{4}}{4!} \frac{\partial^{4} u(\lambda_{i}, t)}{\partial x^{4}},$$

$$(4.7)$$

where θ_i and λ_i are some points between $x_i - \Delta x$ and $x_i + \Delta x$. Adding both sides of (4.6) and (4.7) and subtracting $2u(x_i, t)$, we obtain

$$u(x_i + \Delta x, t) - 2u(x_i, t) + u(x_i - \Delta x, t) =$$
$$\Delta x^2 \frac{\partial^2 u(x_i, t)}{\partial x^2} + \frac{\Delta x^4}{4!} \left[\frac{\partial^4 u(\theta_i, t)}{\partial x^4} + \frac{\partial^4 u(\lambda_i, t)}{\partial x^4} \right]$$

Then, dividing by Δx^2 and subtracting $\frac{\partial^2 u(x_i, t)}{\partial x^2}$ from both sides we get

$$\left| \frac{u(x_i + \Delta x, t) - 2u(x_i, t) + u(x_i - \Delta x, t)}{\Delta x^2} - \frac{\partial^2 u(x_i, t)}{\partial x^2} \right|$$

$$= \frac{\Delta x^2}{4!} \left| \frac{\partial^4 u(\theta_i, t)}{\partial x^4} + \frac{\partial^4 u(\lambda_i, t)}{\partial x^4} \right|$$

$$\leq \frac{\Delta x^2}{4!} \cdot 2\tilde{C} = C \Delta x^2,$$
(4.8)

where the constant \tilde{C} is defined by

$$\tilde{C} = \max\left\{ \left| \frac{\partial^4 u}{\partial x^4}(x,t) \right| : (x,t) \in [x_a, x_b] \times [t_0, T] \right\}$$
(4.9)

and $C = \tilde{C}/12$. Since $\frac{\partial^4 u}{\partial x^4}$ is continuous on the compact set $[x_a, x_b] \times [t_0, T]$, it is bounded and the maximum in (4.9) exists, [15], and \tilde{C} is well defined. Since $u(x_a, t) = a(t)$ and $u(x_b, t) = b(t)$, using a property similar to (4.8) at the boundaries $x = x_a$ and $x = x_b$ corresponding to i = 1 and i = N, we can derive the following inequalities

$$\frac{u(x_1 + \Delta x, t) - 2u(x_1, t) + a(t)}{\Delta x^2} - \frac{\partial^2 u(x_1, t)}{\partial x^2} \le \frac{\Delta x^2}{4!} \cdot 2\tilde{C} = C\Delta x^2$$
(4.10)

and

$$\frac{b(t) - 2u(x_N, t) + u(x_N - \Delta x, t)}{\Delta x^2} - \frac{\partial^2 u(x_N, t)}{\partial x^2} \le \frac{\Delta x^2}{4!} \cdot 2\tilde{C} = C\Delta x^2 \qquad (4.11)$$

for i = 1 and i = N, respectively. Now (4.8), (4.10), and (4.11) imply (4.5), which finishes the proof.

Proof of Theorem 4.0.4. We define $u_{\Delta x}^{(i)} \in \mathcal{C}^4([t_0, T], \mathbb{R})$ for $i = 0, 1, \ldots, N, N+1$ by (4.4). Then, since u is a solution of (1.1)-(1.3), we get

$$\begin{aligned} \frac{\partial u}{\partial t}(x_i,t) &= f\left(x_i,t,u(x_i,t),\frac{\partial^2 u}{\partial x^2}(x_i,t)\right) - f\left(x_i,t,u(x_i,t),\phi_{\Delta x}^{(i)}(u_{\Delta x},t)\right) \\ &+ f\left(x_i,t,u(x_i,t),\phi_{\Delta x}^{(i)}(u_{\Delta x},t)\right). \end{aligned}$$

From this and the Lipschitz condition (4.1) and by Lemma 4.0.5 we obtain

$$\left| \frac{\partial u}{\partial t}(x_i, t) - f\left(x_i, t, u(x_i, t), \phi_{\Delta x}^{(i)}(u_{\Delta x}, t)\right) \right|$$

= $\left| f\left(x_i, t, u(x_i, t), \frac{\partial^2 u}{\partial x^2}(x_i, t)\right) - f\left(x_i, t, u(x_i, t), \phi_{\Delta x}^{(i)}(u_{\Delta x}, t)\right) \right|$
 $\leq L_q \left| \frac{\partial^2 u}{\partial x^2}(x_i, t) - \phi_{\Delta x}^{(i)}(u_{\Delta x}, t) \right| \leq L_q C \Delta x^2,$

for some positive constant C. Therefore, since

$$\frac{d}{dt}u_{\Delta x}^{(i)}(t) = \frac{\partial u}{\partial t}(x_i, t),$$

and (4.4), we obtain

$$\begin{aligned} & \left| \frac{d}{dt} u_{\Delta x}^{(i)}(t) - f\left(x_i, t, u(x_i, t), \phi_{\Delta x}^{(i)}(u_{\Delta x}, t)\right) \right| \\ &= \left| \frac{d}{dt} u_{\Delta x}^{(i)}(t) - f\left(x_i, t, u_{\Delta x}^{(i)}(t), \phi_{\Delta x}^{(i)}(u_{\Delta x}, t)\right) \right| \le \eta(\Delta x), \end{aligned}$$

with

$$\eta(\Delta x) = L_q C \Delta x^2, \tag{4.12}$$

and $u_{\Delta x}$ satisfies the first inequality in (3.3). From (1.3) and (4.4) we obtain $u_{\Delta x}^{(i)}(t_0) = u_0(x_i)$ and conclude that $u_{\Delta x}$ also satisfies the second inequality in (3.3) with

$$\lambda(\triangle x) \equiv 0. \tag{4.13}$$

We now apply Theorem 3.0.1 and from (3.4) obtain

$$\left|V_{\Delta x}^{(i)}(t) - u_{\Delta x}^{(i)}(t)\right| \le \xi(\Delta x),$$

for i = 1, 2, ..., N, $t \in [t_0, T]$, with $\lim_{\Delta x \to 0} \xi(\Delta x) = 0$. Therefore, from (4.4), we get (4.3) with $\mu(\Delta x) = \xi(\Delta x)$ and the proof is finished.

Note that the error estimation (4.3) is given with $\mu(\triangle x) = \xi(\triangle x)$, where $\xi(\triangle x)$ is defined by (3.11). Therefore,

$$|u(x_i,t) - V_{\Delta x}^{(i)}(t)| \le \exp\left(L_p(T-t_0)\right)\lambda(\Delta x) + \frac{1}{L_p}\left(\exp\left(L_p(T-t_0)\right) - 1\right)\eta(\Delta x)$$

with $\eta(\Delta x)$ and $\lambda(\Delta x)$ defined by (4.12) and (4.13), respectively. From this we obtain

$$|u(x_i, t) - V_{\Delta x}^{(i)}(t)| \le \frac{1}{L_p} \Big(\exp \left(L_p(T - t_0) \right) - 1 \Big) L_q C \Delta x^2$$

and the following corollary.

Corollary 4.0.6. Suppose that the assumptions of Theorem 4.0.4 are satisfied. Then there exists a positive constant C such that

$$|u(x_i,t) - V_{\Delta x}^{(i)}(t)| \le C \Big(\exp\left(L_p(T-t_0)\right) - 1 \Big) \Delta x^2,$$

for $i = 1, 2, ..., N, t \in [t_0, T]$.

In the next chapter, we present numerical examples with partial differential equations (1.1). The results of the numerical experiments are validated by the theoretical results proved in Chapters 3 and 4.

CHAPTER 5

NUMERICAL COMPUTATIONS

This chapter is devoted to numerical examples and computations. The numerical results presented in this chapter are validated by the theoretical results obtained in the previous chapters.

We consider four examples with problems written in the form (1.1)-(1.3). We transform the problems into the form (2.3) with different step-sizes Δx . Next, we transform (2.3) into the form (2.4) and apply Runge-Kutta methods to integrate the resulting systems of ODEs in time using the time step-sizes Δt .

Since the general form (1.1) includes also linear partial differential equations, to demonstrate the efficiency of the numerical approach for both cases, linear and nonlinear, we choose a linear partial differential equation for our first example. For the next numerical examples, we test the method with nonlinear PDEs.

Example 1

For this example, we investigate the linear equation

$$\frac{\partial u}{\partial t}(x,t) = D \frac{\partial^2 u}{\partial x^2}(x,t) + \nu(x,t)u(x,t) + \mu(x,t)$$
(5.1)

for $x \in [0, L]$ and $t \ge 0$. Here, D is a diffusion coefficient and $\nu(x, t)$, $\mu(x, t)$ are

given functions. The equation (5.1) is supplemented with the boundary conditions (1.2) with $x_a = 0$ and $x_b = L$ and the initial condition (1.3) with $t_0 = 0$. Figure 5.1 illustrates numerical solutions $V_{\Delta x}^{(i)}(t_j)$ obtained with different functions $\nu(x,t)$, $\mu(x,t)$ and different initial and boundary conditions.



Figure 5.1: Numerical solutions to (5.1).

The numerical solution to (5.1), (1.2), (1.3) with

$$\nu(x,t) = 2(t-c) + (2-c)^2 - 3, \quad \mu(x,t) = (x-c)\exp\left(-(t-c)^2 - (x-c)^2\right),$$

c = 2.5, D = 0.5 and L = 5 with the initial function

$$u_0(x) = c(x-c) \exp\left(-c^2 - (x-c)^2\right)$$
(5.2)

and the boundary functions

$$a(t) = c(t-c) \exp\left(-c^2 - (t-c)^2\right), \quad b(t) = -a(t), \tag{5.3}$$

is presented in Figure 5.2(A).



Figure 5.2: (A) Numerical solution to (5.1), (5.2), (5.3) computed with $\Delta x = 0.05$ and $\Delta t = \frac{1}{2} \Delta x^2$; (B) numerical error (5.4); (C) maximum error (5.5); and (D) maximum error (5.6).

The exact solution of the problem is given by the formula

$$u(x,t) = (c-x)(t-c)\exp\left(-(x-c)^2 - (t-c)^2\right)$$

and we can compute the errors of numerical solutions. The errors are presented in Figures 5.2(B), (C), (D) and 5.3.



Figure 5.3: Numerical error (5.4) with decreasing stepsizes Δx .

Figures 5.2(B) and 5.3 present the error

$$E(x_i, t_j) = \left| u(x_i, t_j) - V_{\Delta x}^{(i)}(t_j) \right|,$$
(5.4)

where x_i and t_j are spatial and temporal grid-points, Figure 5.2(C) presents the

maximum error

$$E^{(t)}(x_i) = \max\left\{ \left| u(x_i, t_j) - V_{\Delta x}^{(i)}(t_j) \right| : t_j \in [0, T] \right\},\tag{5.5}$$

with T = 5 and for all spatial grid-points x_i , and Figure 5.2(D) presents the maximum error

$$E^{(x)}(t_j) = \max\left\{ \left| u(x_i, t_j) - V^{(i)}_{\Delta x}(t_j) \right| : x_i \in [0, L] \right\},\tag{5.6}$$

for all temporal grid-points t_j . Figure 5.3 compares the errors (5.4) for different step-sizes $\Delta x = 5/10, 5/14, 5/20, 5/50$ in (A),(B),(C),(D), respectively. The chosen time step-sizes Δt are significantly smaller and the error of the integration in time is negligible.

In the next three examples, we investigate partial differential equations (1.1) with nonlinear functions f(x, t, p, q).

Example 2

For this example, we solve the nonlinear Fitzhugh-Nagumo equation (1.4) supplemented by the boundary conditions (1.2) with $x_a = -L$ and $x_b = L$ and the initial condition (1.3) with $t_0 = 0$. The boundary functions are defined by the formulas

$$a(t) = \left(1 + \exp\left(\frac{-L}{\sqrt{2D}} + \left(\alpha - \frac{1}{2}\right)t\right)\right)^{-1},$$

$$b(t) = \left(1 + \exp\left(\frac{L}{\sqrt{2D}} + \left(\alpha - \frac{1}{2}\right)t\right)\right)^{-1}$$
(5.7)

and the initial function is defined by

$$u_0(x) = \frac{1}{1 + \exp\left(\frac{x}{\sqrt{2D}}\right)}.$$
(5.8)



Figure 5.4: Solutions and errors for the Fitzhugh-Nagumo equation (1.4) solved with the step-sizes $\Delta t = 0.005$ and $\Delta x = 0.1$: (A) numerical solution $V_{\Delta x}^{(i)}(t_j)$; (B) numerical error (5.4); (C) exact solution u(x,t); (D) maximum error (5.5).

The numerical solution $V_{\Delta x}^{(i)}(t_j)$ to the Fitzhugh-Nagumo equation (1.4) with D = 0.03 and $\alpha = 0.139$ is presented in Figure 5.4(A). This solution was computed with the step-sizes $\Delta x = 0.1$ and $\Delta t = 0.005$. For comparison, we also present (in Figure 5.4(C)) the exact solution to (1.4), (1.2), (1.3) with a(t), b(t), and $u_0(x)$ defined by (5.7) and (5.8), respectively.

The exact solution is written in the form

$$u(x,t) = \left(1 + \exp\left(\frac{x}{\sqrt{2D}} + \left(\alpha - \frac{1}{2}\right)t\right)\right)^{-1}$$

and we can use it to compute the errors of the numerical solutions. The errors obtained after computations with $\Delta x = 0.1$ and $\Delta t = 0.005$ are presented in Figure 5.4(B) and (D). The error (5.4) is presented in Figure 5.4(B) and the maximum error (5.5) is presented in Figure 5.4(D).



Figure 5.5: Numerical errors for the Fitzhugh-Nagumo equation (1.4): (A) (5.4) with $\Delta x = 0.2$, (B) (5.4) with $\Delta x = 0.02$, (C) (5.5) with $\Delta x = 0.2$, (D) (5.5) with $\Delta x = 0.02$. The time step-size $\Delta t = 0.005$ was applied for all the subplots.

Figure 5.5 (A) and (C) illustrates the errors (5.4) and (5.5), respectively. These errors were obtained with $\Delta x = 0.2$ and $\Delta t = 0.005$. Similarly, the errors obtained with $\Delta x = 0.02$ and $\Delta t = 0.005$ are presented in Figure 5.5 (B) and (D). The subplots in Figure 5.5 show that the errors decrease with decreasing Δx , thus confirming the order of the finite difference operator used for the spatial derivative.

From the proofs of Theorems 3.0.1 and 4.0.4, we observe that if the assumptions of Theorem 4.0.4 are satisfied then, from Corollary 4.0.6, we obtain the following error estimation

$$u(x_i, t_j) = V^{(i)}_{\Delta x}(t_j) + \mathcal{O}(\Delta x^2).$$
(5.9)

The estimation (5.9) is illustrated by the numerical experiments. Figure 5.5 (A) and (C) show that, for $\Delta x = 2 \cdot 10^{-1}$, the errors are less than 10^{-2} , thus satisfying (5.9). Figure 5.5 (B) and (D) also illustrate (5.9) and show that the errors for $\Delta x = 2 \cdot 10^{-2}$ are less than 10^{-4} .

The errors presented in Figures 5.2(B)(C)(D) were obtained with $\Delta x = 0.05$ and the plots show that they are less than $2.5 \cdot 10^{-3}$, which illustrates the estimation (5.9). Furthermore, the error from Figures 5.3(A) was obtained with $\Delta x = 1/2$ and is less than $2.5 \cdot 10^{-1}$ illustrating (5.9). The error from Figures 5.3(B) was obtained with $\Delta x = 5/14$ and is less than 10^{-1} , the error from Figures 5.3(C) was obtained with $\Delta x = 5/20$ and is less than $5 \cdot 10^{-2}$, the error from Figures 5.3(D) was obtained with $\Delta x = 5/50$ and is less than 10^{-2} , and parts (B), (C), and (D) also illustrate the estimation (5.9).

Numerical experiments for the next examples agree with (5.9) as well.

Example 3

We solve the Kolmogorov-Petrovskii-Piskunov equation (1.5) supplemented by the boundary conditions (1.2) with

$$a(t) = \left(\gamma + \exp\left(\lambda t - \mu L/\sqrt{D}\right)\right)^{2/(1-m)}$$

$$b(t) = \left(\gamma + \exp\left(\lambda t + \mu L/\sqrt{D}\right)\right)^{2/(1-m)}$$
(5.10)

where



Figure 5.6: Numerical solutions $V_{\Delta x}^{(i)}(t_j)$ to the Kolmogorov-Petrovskii-Piskunov equation (1.5) for the indicated temporal grid-points t_j and all spacial grid-points x_i .

$$\lambda = \frac{\alpha(1-m)(m+3)}{2(m+1)}, \quad \mu = \sqrt{\frac{\alpha(1-m)^2}{2(m+1)}}, \quad \gamma = \sqrt{\frac{-\beta}{\alpha}}$$

and the initial condition (1.3) with

$$u_0(x) = \left(\gamma + \exp\left(\mu x / \sqrt{D}\right)\right)^{2/(1-m)}$$
(5.11)

for $x \in [-L, L]$. Figures 5.6, 5.7, and 5.8 (A) illustrate the numerical solution $V_{\Delta x}^{(i)}(t_j)$ to (1.5) with $\alpha = 1, \beta = -1, m = 2, D = 0.1$, and L = 10. The solution $V_{\Delta x}^{(i)}(t_j)$ was computed with $\Delta x = 0.2$ and $\Delta t = 0.02$. Figure 5.6 presents $V_{\Delta x}^{(i)}(t_j)$ at the temporal



Figure 5.7: Numerical solutions $V_{\Delta x}^{(i)}(t_j)$ to the Kolmogorov-Petrovskii-Piskunov equation (1.5) for the indicated spacial grid-points x_i and all time grid-points t_j .

grid-points $t_j = 0.98, 2.98, 4.98, 6.98, 8.98$, and for all spacial grid-points x_i showing the evolution of $u(\cdot, t_j)$ in space. Figure 5.7 presents the numerical solution $V_{\Delta x}^{(i)}(t_j)$ at the spacial grid-points $x_i = -1.8, -0.2, 1.4, 3, 4.6$ showing the evolution of $u(x_i, \cdot)$ in time. Figure 5.8(A) presents $V_{\Delta x}^{(i)}(t_j)$ for all spacial and temporal grid-points.



Figure 5.8: Solutions and errors for the Kolmogorov-Petrovskii-Piskunov equation (1.5) solved with $\Delta x = 0.2$ and $\Delta t = 0.02$: (A) numerical solution $V_{\Delta x}^{(i)}(t_j)$; (B) numerical error (5.4); (C) exact solution u(x,t); (D) maximum error (5.5).

The exact solution to (1.5), (1.2), (1.3) with the boundary functions (5.10) and the initial function (5.11) is written in the form

$$u(x,t) = \left(\gamma + \exp\left(\lambda t + \mu x/\sqrt{D}\right)\right)^{2/(1-m)}$$
(5.12)

and, for comparison with the numerical solution $V_{\Delta x}^{(i)}(t_j)$, the exact solution u(x,t) is presented in Figure 5.8 (C). From parts (A) and (C), we conclude that the numerical solution properly expresses all features of the exact solution.

Furthermore, we use the formula (5.12) to compute the numerical errors and compare them with the error estimation (5.9) derived from Theorems 3.0.1 and 4.0.4. The errors (5.4) and (5.5) are presented in Figure 5.8 (B) and (D), respectively. They were obtained with $\Delta x = 0.2$ and illustrate the estimation (5.9).

Example 4

For this example, we solve the Fisher-Kolmogorov equation (1.6) supplemented by the boundary conditions (1.2) with

$$a(t) = \frac{1}{\left(1 + \alpha e^{\beta(x_a - ct)}\right)^s}, \quad b(t) = \frac{1}{\left(1 + \alpha e^{\beta(x_b - ct)}\right)^s}, \tag{5.13}$$

where, as suggested in [12], $\alpha = \sqrt{2} - 1$ and

$$s = \frac{2}{q}, \quad \beta = \frac{q}{(2(q+2))^{1/2}}, \quad c = \frac{q+4}{(2(q+2))^{1/2}}.$$

The initial function for (1.3) is written in the form

$$u_0(x) = \frac{1}{\left(1 + \alpha e^{\beta x}\right)^s}.$$
 (5.14)

The numerical solution $V_{\Delta x}^{(i)}(t_j)$ to this problem with $x_a = -5$, $x_b = 10$, and q = 1 is presented in Figure 5.9 (A) for $t_j = 0.245$, 0.745, 1.245, 1.745, 2.245, and all spacial grid-points x_i . The exact solution u(x, t) is written in the form

$$u(x,t) = \frac{1}{\left(1 + \alpha e^{\beta(x-ct)}\right)^s}$$

and we use it to compute numerical errors.

Figures 5.10 and 5.11 present the errors (5.4) and (5.5) for different spacial stepsizes Δx . Parts (A) and (B) of Figure 5.10 present errors obtained with $\Delta x = 0.25$. The errors are less than $3 \cdot 10^{-3}$, which agrees with the error estimation (5.9). The errors presented in Parts (C) and (D) were obtained with $\Delta x = 0.2$ and are less than $2 \cdot 10^{-3}$, again in agreement with (5.9).



Figure 5.9: Numerical solutions $V_{\Delta x}^{(i)}(t_j)$ to the Fisher-Kolmogorov equation (1.6) for the indicated temporal grid-points t_j and all spacial grid-points x_i .

The errors presented in Figure 5.11 were obtained with $\Delta x = 1/6$ (Parts (A) and (C)) and $\Delta x = 1/8$ (Parts (B) and (D)). From Figure 5.11, we observe that the errors obtained with $\Delta x = 1/6$ are less than $6 \cdot 10^{-4}$, which is in agreement with (5.9), and the errors obtained with $\Delta x = 1/8$ are less than $2 \cdot 10^{-4}$, which is also in agreement with the error estimation (5.9).



Figure 5.10: Numerical errors (5.4) and maximum errors (5.5) obtained with $\Delta x = 0.25$, in (A) and (B), and with $\Delta x = 0.2$ in (C) and (D).



Figure 5.11: Numerical errors (5.4) and maximum errors (5.5) obtained with $\Delta x = 1/6$, in (A) and (B), and with $\Delta x = 1/8$ in (C) and (D).

CHAPTER 6

CONCLUDING REMARKS

In this work, we have investigated nonlinear partial differential equations written in the general form (1.1). In this form, the function f(x, t, p, q) can be defined in many different ways generating a wide class of nonlinear problems. We consider the semi-discrete scheme (2.3) for this general class of problems and address the questions about its stability and convergence. We state and prove Stability and Convergence Theorems for the general scheme (2.3) and provide an error estimation for its numerical errors.

We have investigated four examples with four problems written in the form (1.1). Since the general form (1.1) includes also linear problems, one of our examples is with a linear equation. The other three examples are nonlinear equations: the Fitzhugh-Nagumo equation, the Kolmogorov-Petrovskii-Piskunov equation, and the Fisher-Kolmogorov equation. Our numerical experiments with four partial differential equations are validated by the stability and convergence results as well as the estimation for the numerical errors, thus confirming their reliability.

The analysis of the stability and convergence properties of the numerical scheme (2.3) derived for (1.1) can be utilized for constructions of numerical schemes for yet more general nonlinear partial differential equations written in the form

$$\frac{\partial u}{\partial t}(x,t) = f\left(x,t,u(x,t),\frac{\partial^2 u}{\partial x^2}(x,t),u_{(x,t)}\right),\tag{6.1}$$

where the last argument $u_{(x,t)}$ differs from the first four arguments. This difference is significant as the arguments $x, t, u(x,t), \frac{\partial^2 u}{\partial x^2}(x,t)$ are real values while the last argument $u_{(x,t)}$ is a function defined in the following way

$$u_{(x,t)}(y,s) = u(x+y,t+s),$$

where $s \leq 0$ and y belongs to a certain spatial subdomain. Therefore, $u_{(x,t)}$ is called a functional argument.

The functional argument $u_{(x,t)}$ in (6.1) allows to generate a more general (than (1.1)) class of problems, where the partial differential equations depend not only on the values of the solution at the present state u(x,t) (third argument in (6.1) and (1.1)) but also on its values at some previous state or stages. More details about such problems and numerical methods for solving them are provided by Zubik-Kowal [19], [20], [21], and [22].

The stability and convergence analysis presented in this work provides confidence that our computationally obtained numerical solutions can be trusted and are reliable.

REFERENCES

- [1] J. C. Butcher, Numerical methods for ordinary differential equations. Second edition. John Wiley & Sons, Ltd., Chichester, 2008.
- [2] A. Fasano, M.A. Herrero, M.R. Rodrigo, Slow and fast invasion waves in a model of acid-mediated tumour growth, *Math. Biosci.* 220 (2009) 45-56.
- [3] J. Guckenheimer, C. Kuehn, Homoclinic orbits of the Fitzhugh-Nagumo equation: The singular limit, discrete and continuous dynamical systems Series S, 2, no. 4 (2009) 851–872.
- [4] E. Hairer, S. P. Nrsett, G. Wanner, Solving ordinary differential equations. I. Nonstiff problems. Second edition. Springer Series in Computational Mathematics, 8. Springer-Verlag, Berlin, 1993.
- [5] E. Hairer, G. Wanner, Solving ordinary differential equations. II. Stiff and differential-algebraic problems. Second edition. Springer Series in Computational Mathematics, 14. Springer-Verlag, Berlin, 1996.
- S.P. Hastings, Some mathematical problems from neurobiology, Am. Math. Mon., 82 (1975) 881–895.
- [7] W. Hundsdorfer, J. Verwer, Numerical solution of time-dependent advectiondiffusion-reaction equations. Springer Series in Computational Mathematics, 33.
 Springer-Verlag, Berlin, 2003.
- [8] A. Iserles, A first course in the numerical analysis of differential equations. Cambridge Texts in Applied Mathematics, Cambridge University Press, Cambridge, 1996.
- [9] R. J. LeVeque, Finite difference methods for ordinary and partial differential equations. Steady-state and time-dependent problems. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2007.
- [10] H.P. McKean, Nagumo's equation, Adv. in Math., 4:209–223, 1970.
- [11] H.P. McKean. Application of Brownian motion to the equation of Kolmogorov-Petrovskii-Piskunov. Comm. Pure Appl. Math., 28:323–331, 1975.

- [12] J.G. Murray, Mathematical Biology, I: An Introduction, third ed., Springer, New York, 2002.
- [13] J.G. Murray, Mathematical Biology, II: Spatial Models and Biomedical Applications, third ed., Springer, New York, 2003.
- [14] A.D. Polyanin, V.F. Zaitsev, Handbook of Nonlinear Partial Differential Equations, Chapman & Hall/CRC, Boca Raton, FL, 2004.
- [15] W. Rudin, *Principles of Mathematical Analysis*, McGraw-Hill, New York, 1976.
- [16] L. F. Shampine, Numerical solution of ordinary differential equations. Chapman & Hall, New York, 1994.
- [17] L. F. Shampine, I. Gladwell, S. Thompson, Solving ODEs with MATLAB. Cambridge University Press, Cambridge, 2003.
- [18] J.C. Strikwerda, Finite difference schemes and partial differential equations. Second edition. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2004.
- [19] B. Zubik-Kowal, The method of lines for parabolic differential-functional equations, IMA Jour. Num. Anal., 17 (1997), 103–123.
- [20] B. Zubik-Kowal, Chebyshev pseudospectral method and waveform relaxation for differential and differential-functional parabolic equations, *Appl. Numer. Math.*, 34(2-3), (2000), 309–328.
- [21] B. Zubik-Kowal, Error bounds for spatial discretization and waveform relaxation applied to parabolic functional-differential equations, J. Math. Anal. Appl. 293 (2004), 496-510.
- [22] B. Zubik-Kowal, Solutions for the cell cycle in cell lines derived from human tumors, Comput. Math. Methods Med., 7(4) (2006), 215–228