FINITE ELEMENTS AND PRACTICAL ERROR ANALYSIS OF HUXLEY AND EFK EQUATIONS

Champike Attanayake

A Dissertation

Submitted to the Graduate College of Bowling Green
State University in partial fulfillment of
the requirements for the degree of

DOCTOR OF PHILOSOPHY

December 2008

Committee:

Tong Sun, Advisor

Hassan Rajaei,
Graduate Faculty Representative

So-Hsiang Chou

Steven M. Seubert

ABSTRACT

Tong Sun, Advisor

In this dissertation, long time error estimates are obtained using non-traditional methods for the Hodgkin-Huxley equation

$$u_t - u_{xx} = u(1-u)(u-a) \quad \text{for} \quad 0 < a < 1/2,$$

and the extended Fisher-Kolmogorov equation

$$u_t + \gamma\Delta^2 u - \Delta u = u - u^3.$$

Traditional methods for analyzing exact error propagation depends on the stability of the numerical method employed. Whereas, in this dissertation the analysis of the exact error propagation uses evolving attractors and only depends on the stability of the dynamical system. The use of the smoothing indicator yields *a posteriori* estimates on the numerical error instead of *a priori* estimates.

This dissertation is dedicated to my loving parents.

ACKNOWLEDGMENTS

This thesis arose (in part) out of research that has been done since I came to Bowling Green State University. In the first place I would like to record my gratitude to Dr. Tong Sun for his supervision, advice and guidance from the early stage of this research as well as giving me extraordinary experiences throughout the work. His truly scientific ideas and passions for mathematics, which exceptionally inspired and enriched my growth as a student and encouraged a researcher I want to be. I am indebted to him more than he knows. I gratefully acknowledge Professor So-Hsiang Chou for his valuable advice and for using his precious time to read this thesis and gave his critical comments about it. Many thanks go in particular to Dr. Steven M. Seubert and Dr. Hassan Rajaei for their constructive comments on this thesis. I am thankful that in the midst of all their activity, they accepted to be members of the reading committee. I also want to thank the faculty of the Department of Mathematics and Statistics for excellent instruction and help throughout my graduate studies at Bowling Green.

Table of Contents

CHAPTER 1

Introduction

The ever increasing activity in the area of mathematics and those applied sciences concerned with parabolic equations marks the important role of modeling physical phenomena in such diverse fields as physics, chemistry, biology, computer science, engineering, finance and sociology. Numerical analysis of parabolic problems has become a central tool in such studies, because of the many barriers that exist for mathematical analysis. In these situations, when little is known about the true solution, determining the accuracy of a numerical solution becomes critical.

At the same time, it is crucial to understand that all numerical solutions are subject to some form of a deviation from the exact solution of the differential equation. So it is important to understand how to express and how to analyze such approximations in order to draw reliable conclusions using them. The ability to draw valid conclusions relies on the ability to deal with error properly. In view of which, very little is known about the reliability of results unless probable size of the error in the numerical results can be estimated or controlled.

However, the same difficulties that occur in the mathematical analysis also give rise to some difficult problems in accurate analytical estimation of the error in the numerical scheme. Stability of the numerical scheme is one such issue. Numerical stability usually depends on controlling the error propagation of the numerical scheme.

Particularly when dealing with long time error, careful analysis of error propagation is required. Traditionally error analyzes of evolution equations are based on the stability of the numerical scheme. Under typical conditions, in order for the numerical solution to converge to the real solution, it is necessary and sufficient to have numerical stability (See Theorem 5.4 on p. 91, [22]). Determining the stability of numerical schemes used to analyze complicated non-linear equations is typically difficult and tedious. In view of which there often is a huge gap between the theory of the error analysis and implementation of particular numerical methods.

This fact can be illustrated by examining a traditional error splitting technique in a way that it is applied in many publications. Let $u(t_{n+1}|u(t_n))$ denote the exact solution at time t_{n+1} having exact initial condition $u(t_n)$. Similarly, let $u_N(t_{n+1}|u_N(t_n))$ denote the corresponding numerical solution with numerical initial condition $u_N(t_n)$. Traditional methods estimate the error over the time interval $[t_n, t_{n+1}]$ by applying the triangular inequality as follows:

$$
\begin{aligned}
&|u(t_{n+1}|u(t_n)) - u_N(t_{n+1}|u_N(t_n))| \\
&\leq |u(t_{n+1}|u(t_n)) - u_N(t_{n+1}|u(t_n))| + |u_N(t_{n+1}|u(t_n)) - u_N(t_{n+1}|u_N(t_n))|,
\end{aligned}
$$

where $u_N(t_{n+1}|u(t_n))$, is the numerical solution with exact initial condition $u(t_n)$. Figure (a) indicates an estimate of the error when split using this traditional method. The first difference on the right hand side of above is the local error, and can be estimated using the smoothing properties of the numerical scheme. The second difference above is the error at time t_{n+1} propagated by the numerical scheme over the time interval.

An alternate error splitting method, that we are going to use, can be found in Estep and Stuart [7], and Sun and Ewing [26]. This method estimates the error over the time interval

$[t_n, t_{n+1}]$ by applying the triangular inequality as follows:

$$\begin{aligned} &|u(t_{n+1}|u(t_n)) - u_N(t_{n+1}|u_N(t_n))| \\ &\le |u(t_{n+1}|u(t_n)) - u(t_{n+1}|u_N(t_n))| + |u(t_{n+1}|u_N(t_n)) - u_N(t_{n+1}|u_N(t_n))|, \end{aligned}$$

where $u(t_{n+1}|u_N(t_n))$, is the exact solution with numerical initial condition $u(t_n)$.
Figure (b) indicates an estimate of the error when split using this alternate method. Now, the second difference above is the actual local error. Because both terms have numerical initial values, estimates of the actual error can be obtained using the smoothing properties of the numerical schemes [26]. That is, the smoothing indicator can be used to estimate the actual local error. In traditional methods, it is difficult to compute an indicator in order to determine whether the numerical scheme is stable, because the splitting term $u_N(t_{n+1}|u(t_n))$ is not computable. However, it is easy to compute an indicator for a computational numerical scheme using its smoothing properties [27].
The first difference above is the error at time t_{n+1}, and is propagated by the dynamical system. This error can be estimated using the contraction properties of the solution to the dynamical system and evolving attractors, a concept which was first introduced by Sun and Ewing [26]. Evolving attractors are collection of sets which depend on time. It is this more general notion of evolving attractor which facilitate effective long time error analysis, unattainable by the use of the attractors alone, in the nonlinear problems [26].
In this dissertation, we obtain long-term estimates when finite element methods are applied to the Hodgkin-Huxley equation,

$$u_t - u_{xx} = u(1-u)(u-a), \quad \text{on } \mathbb{R} \times [0, \infty),$$

an equation widely regarded as one of the greatest achievements of 20th century biophysics. Then we generalis these results to a fourth order parabolic equation, the extended Fisher

Kolmogorov (EFK) equation,

$$
\begin{aligned}
u_t + \gamma\Delta^2 u - \Delta u &= u - u^3, \quad \text{in } \Omega \times ([0,\infty), \\
u &= 0, \quad \text{on } \partial\Omega \times ([0,\infty).
\end{aligned}
$$

This type of equations occurs mainly in the application of pattern formulation in bi-stable systems [5].

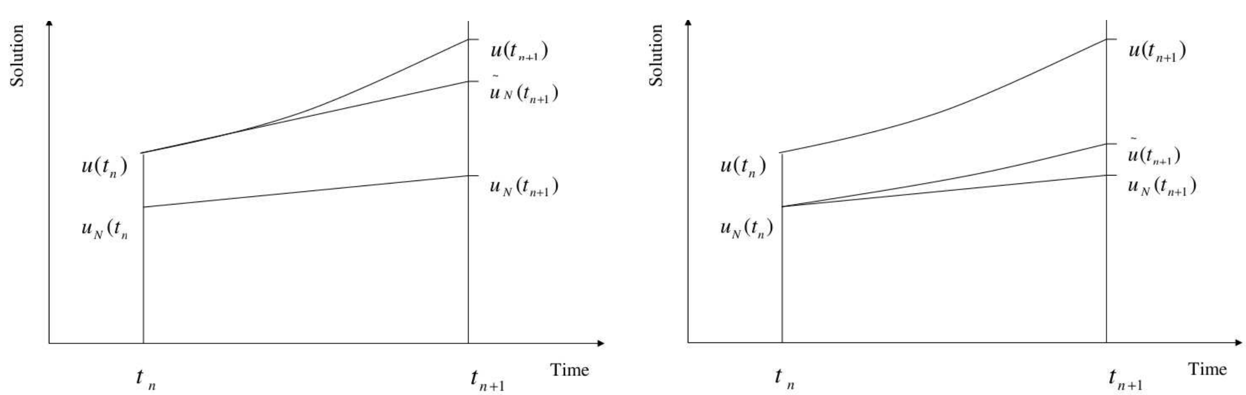
In Chapter 2, we show that the solutions of the Hodgkin-Huxley equation contract to a traveling wave solution of the form $\phi(x - vt)$, where v is a constant.

In Chapter 3, we describe the long time error estimates of the Hodgkin-Huxley equation, using evolving attractors and the smoothing indicator.

In Chapter 4, we estimate errors for the numerical solutions of semi-discrete and completely discrete EFK equations.

In Chapter 5, we obtain long time error estimates for the EFK equation in polygonal domains, using evolving attractors and the smoothing indicator.

In Chapter 6, we summarize the results and show the value of the present research.



(a) Numerical Stability (b) Numerical Smoothing

Figure 1.1: Error Splitting.

CHAPTER 2

Contractive Solutions of Hodgkin-Huxley Equations

In this chapter we deduce the contraction properties of solutions to Hodgkin-Huxley equations, which in Chapter 3 we use to obtain estimates for exact error propagation. Contraction is a local property in terms of time, which shows how solutions evolve in a finite time interval. It has been shown by Evans [9] and Sattinger [24] that solutions of many parabolic equations converge to a traveling wave. This convergence is a global property in terms of time. However, using techniques developed in these two papers, we can show contraction property of solutions to Hodgkin-Huxley equations.

In section 2.1, we introduce Hodgkin-Huxley equations. Then in section 2.2 we define, what it mean for the solutions of Hodgkin-Huxley equations to have a contraction property. After showing existence of the solution in section 2.3, in section 2.4 we study contraction properties of the linearized version of the Hodgkin-Huxley equation. Then in section 2.5, we use the contraction of the linearized solution to show the contraction of solutions of Hodgkin-Huxley equations. Finally in section 2.6 we provide some computational results.

2.1 The Hodgkin-Huxley Equations

The theory of a cable consisting of a resistive core surrounded by a membrane offering capacitance and variable resistance to ionic current is important in neurology. The Hodgkin-Huxley equation is one of the few equations that realistically model the propagation of nerve impulses [14]. This equation is a PDE system in four variables. A simplified equation that retains some of its crucial features is Huxley's equation namely,

$$W_t = \Delta W + g(W), \tag{2.1}$$

where $g(W) = W(1-W)(W-a)$ with $0 < a < 1/2$. Note that this equation has a linear diffusion term and a nonlinear reaction term.

2.2 The Contraction Property

Propagation of waves, described by nonlinear parabolic equations, were first considered in a paper by A. N Kolmogorov, I. G. Petrovski and N. S. Piskunov. These mathematical investigations arose in connection with a model for the propagation of dominant genes, a topic also considered by R. A. Fisher. In systems with more than one stationary homogeneous solution, a typical solution is given by a traveling wave front. These solutions move with constant speed without changing their shape and are of the form $u(x,t) = \phi(y)$ with $y = x - vt$, where v is the speed of the traveling wave. Wave solutions of above type arise in numerous problems of physical interest; such as propagation of nerve impulses, propagation of favorable genes, shock waves, and propagation of flams.

Homogeneous solutions to Huxley's equations have monotone traveling wave solutions. Most importantly according to Sattinger [24], if Huxley's equation has the initial data of the form

$$u(x,0) = \phi(x) + \epsilon u_0(x),$$

then for sufficiently small ϵ, there exist constants $K, \omega > 0$ such that,

$$\|u(y,t) - \phi_\epsilon(y,t)\| \le Ke^{-\omega t}, \quad t \ge 0,$$

where $\phi_\epsilon = \phi(y+\epsilon)$. Based on the above stability property of solutions, we can define the contraction property of solutions to the Huxley's equations as follows: There exist constants s, T_0 and $\theta_s \in (0,1)$ such that

$$\|u(y,t+s) - \phi_\epsilon(y,t+s)\| \le \theta_s \|u(y,t) - \phi(y,t)\|,$$

for all $t > T_0$.

Purpose of Chapter 2 is to show that solutions to Huxley's equations are contractive. In the next chapter we define the evolving attractor as a collection of all translates of the wave profile $\phi(y)$. Using this attractor and the smoothing indicator, we can estimate long time error of the numerical solutions to the Huxley's equations.

2.3 Existence of Solutions

Huxley's equation $W_t = \Delta W + g(W)$ in the 1-dimensional case takes the form

$$-v\frac{\partial \phi}{\partial y} - \frac{\partial^2 \phi}{\partial y^2} = g(\phi), \tag{2.2}$$

where $W(x,t) = \phi(x - vt) = \phi(y)$ is a traveling wave propagating at a constant velocity v. The existence and uniqueness of the solution to (2.2) can be obtained by standard phase plane arguments. we deduce in Section 2.5 contraction of solutions $W(x,t)$ to Huxley's equation, using stability properties of the solutions to the linear equation approximating the equation (2.1) about ϕ. Therefore, if $\phi(y)$ is a solution to (2.2) with $y = x - vt$, let

$U(y,t) = W(y+vt,t)$, where W is a solution to (2.1). Thus on the moving frame

$$\frac{\partial U}{\partial t} - v\frac{\partial U}{\partial y} - \frac{\partial^2 U}{\partial y^2} = g(U). \tag{2.3}$$

On the other hand, linearization of (2.3) about ϕ leads to the equation

$$\frac{\partial \tilde{U}}{\partial t}(y,t) - v\frac{\partial \tilde{U}}{\partial y}(y,t) - \frac{\partial^2 \tilde{U}}{\partial y^2}(y,t) = \frac{\partial g}{\partial \phi}(\phi(y))\tilde{U}(y,t). \tag{2.4}$$

Note that if ϕ is a solution of (2.2), so is $\phi_\epsilon = \phi(\epsilon + y)$. Furthermore, $\tilde{U}(y,t) = \frac{d\phi}{dy}(y)$ is a solution of the linear system (2.4). Formally, (2.1) can be integrated using the fundamental solution of the heat equation

$$F(x,y,t) = \exp\left[\frac{-(x-y)^2}{4}\right]/\sqrt{4\pi t}.$$

This gives

$$W(x,t) = \int_{-\infty}^{\infty} F(x,y,t)W(y,0)dy + \int_0^t \int_{-\infty}^{\infty} F(x,y,t-s)g(W(y,s))dyds, \tag{2.5}$$

for $0 \le t \le T$ and all x. For bounded continuous initial conditions $W(\cdot,0)$, an iterative procedure based on Picards iterative procedure for ODEs shows the existence of a unique bounded solution $W(x,t)$ to (2.5) for $0 \le t \le T$. Since (2.3) is related by a change of coordinates, we have that if $U(\cdot,0)$ is bounded and continuous, a bounded $U(x,t)$ for $0 \le t \le T$ and all x with initial value $U(\cdot,0)$ satisfies

$$U(x,t) = \int_{-\infty}^{\infty} F(x+vt,y,t)U(y,0)dy + \int_0^t \int_{-\infty}^{\infty} F(x+vt,y,t-s)g(U(y-vs,s))dyds. \tag{2.6}$$

In an identical fashion there corresponds to (2.4) the system of integral equation

$$\tilde{U}(x,t) = \int_{-\infty}^{\infty} F(x+vt,y,t)U(y,0)dy + \int_0^t \int_{-\infty}^{\infty} F(x+vt,y,t-s)\frac{\partial g}{\partial \phi}(\phi(y-vs))\tilde{U}(y-vs,s)dyds. \tag{2.7}$$

2.4 Contraction of Solutions Linearized Problem

In this section we study the related linearized system of (2.3). By use of the spectral theory of linear operators, contraction of the system under small perturbations of the initial conditions is shown to depend on the solution to certain ordinary differential equations derived from (2.1) and ϕ. Of importance in neurology are the resting states and the traveling waves. The resting states correspond to $g(W) = W(1-W)(W-a) = 0$ in (2.1), which occur at $W = 0$, $W = a$ and $W = 1$, and the traveling wave corresponds traveling solution to (2.1), which has the form $\phi(x - vt)$. As a matter of fact, Huxley found the traveling solution with the traveling front to be

$$\phi(y) = \frac{1}{1 + e^{\frac{-y}{\sqrt{2}}}}, \quad y = x - vt, \quad v = \sqrt{2}(a - \frac{1}{2}).$$

Because $\phi(y) \to 0$ and $\phi(y) \to 1$ as $y \to \infty$ and $y \to -\infty$ receptively, $W = 0$ and $W = 1$ are stable stationary points and $W = a$ is an unstable point. So after long period of time, any initial solution of the Huxley's equation tend to move closer to the stable stationary points 0 and 1. In other words they converge into a traveling front with above asymptotic properties. Next, we want to normalize Huxley's equation so that the traveling velocity $v = 1$. To this end, set

$$\tilde{x} = vx \qquad \tilde{t} = v^2 t \qquad \tilde{W}(\tilde{x},\tilde{t}) = W\left(\frac{\tilde{x}}{v}, \frac{\tilde{t}}{v^2}\right),$$

and with $\tilde{g}(\tilde{W}) = v^{-2}g(W)$ we obtain a system equivalent to (2.1),

$$\frac{\partial \tilde{W}}{\partial t} = \Delta \tilde{W} + \tilde{g}(\tilde{W})$$

with a solution

$$\tilde{W}(\tilde{x},\tilde{t}) = \tilde{\phi}(\tilde{x}-\tilde{t}) = \phi\left(\frac{\tilde{x}}{v} - \frac{\tilde{t}}{v^2}\right).$$

We will therefore assume that $v = 1$. Under the coordinate change $y = x - t$ with $U(y,t) = W(y+t,t)$ we obtain the system

$$\frac{\partial U}{\partial t} = \frac{\partial^2 U}{\partial y^2} + \frac{\partial U}{\partial y} + g(U) \tag{2.8}$$

with $U(y,t) = \phi(y)$ as a standing solution. Now in this new coordinates the linearization of (2.8) about $U = \phi_\epsilon$ is given by

$$\frac{\partial \tilde{U}}{\partial t} = \frac{\partial^2 \tilde{U}}{\partial y^2} + \frac{\partial \tilde{U}}{\partial y} + \frac{\partial g}{\partial \phi_\epsilon}(\phi_\epsilon(y))\tilde{U}. \tag{2.9}$$

Note that, the function $U(y,t) = (d\phi_\epsilon/dy)(y)$ is a solution of (2.9). Furthermore, we define operator L,

$$L\psi \;\; = \;\; \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial \psi}{\partial y} + \frac{\partial g}{\partial \phi_\epsilon}(\phi_\epsilon(y))\psi, \tag{2.10}$$

Now, for a fixed $t > 0$, let Y be the space of functions $u(x,t)$, defined for $0 < t < T$ for all x. Define the function G form Y into Y by

$$\begin{aligned}(Gu)(x,t) &= \int_{-\infty}^{\infty} F(x+t,t)u(y,t)dy \\ &+ \int_0^t \int_{-\infty}^{\infty} F(x+t,y,t-s)\left(\frac{\partial g}{\partial u}(\phi(y-s))u(y-s,s)\right) dyds,\end{aligned} \tag{2.11}$$

where $F(x,y,t)$ is the fundamental solution of the heat equation. Given $\psi \in L^2$, if we set $u_0(x,t) = \psi(x)$ for $0 \leq t \leq T$ and all x, then $\lim_{m\to\infty}(G^m u_0)(x,t) = u(x,t)$ exists with uniform convergence for $0 \leq t \leq T$ and all x. Moreover, u is the unique solution to $Gu = u$ with $u(\cdot,0) = \psi$. For $t \geq 0$ and $\psi \in X$, we denote $\Lambda_t\psi$ with the function $\psi = u(\cdot,0)$, where u is the unique solution to $Gu = u$. We note that from [9], there exists a semigroup operator

$\Lambda_t = e^{tL}$ on X with infinitesimal generator L, where X is a space of continuous bounded functions.

It has been shown in Sattinger [24] and Evans [9] that the operator L has an isolated simple eigenvalue at the origin with the remainder of the spectrum in the parabolic region $\{y^2 + a + x < 0\}$, $(0 < a < 1/2)$ in the left half plane. Then using the fact that $\Lambda_t \left(\frac{d\phi_\epsilon}{dy}\right) = \frac{d\phi_\epsilon}{dy}$ for $t \geq 0$, we can define a projection operator S from the space of continues bounded functions, onto the space of multiples of $\frac{d\phi_\epsilon}{dy}$, by $S\psi = (\psi, \gamma^*)\frac{d\phi_\epsilon}{dy}$, where $\gamma^* \in \mathrm{Null}(\Lambda_t^* - I)$ and $(\cdot, \cdot)$ is the L^2 inner product (see [9]).

For such an operator S, from Theorem 5 of [9], we can find a small circle C about 1, such that

$$\frac{1}{2\pi i}\int_C (zI - \Lambda_t)^{-1} dz = S. \tag{2.12}$$

Theorem 2.1 *There exist constants K and ω such that,*

$$\left\| \tilde{V}(t) - h\left(\frac{d\phi_\epsilon}{dy}\right) \right\|_{L^p} \leq K e^{-\omega t} \|\tilde{V}(0)\|_{L^p}, \quad p = 2, \infty,$$

for all $t > 0$, where $\tilde{V}(t)$ is the solution of the linearized equation (2.9) with initial condition $\tilde{V}(0)$, $k = 1/(\gamma^*, \frac{d\phi_\epsilon}{dy})$ and $h = (\tilde{V}(0), k e^y \frac{d\phi_\epsilon}{dy})$.

Proof. From the proof of Theorem 1, of Evans [9], if $\tilde{V}(0)$ is the initial condition of the linearized equation (2.9), then there exist constants K and ω such that,

$$\|(\Lambda_t - S)\tilde{V}(0)\|_{L^p} \leq K e^{-\omega t} \|\tilde{V}(0)\|_{L^p}$$

for all $t > 0$ and $p = 2, \infty$. Now, let $\tilde{V}(t)$ be the solution of linearized equation (2.9) with the initial condition $\tilde{V}(0)$. Since $\tilde{V}(t) = \Lambda_t \tilde{V}(0)$ and $h\frac{d\phi_\epsilon}{dy} = S\tilde{V}(0)$, we have that,

$$\left\| \tilde{V}(t) - h\left(\frac{d\phi_\epsilon}{dy}\right) \right\|_{L^p} \leq K e^{-\omega t} \|\tilde{V}(0)\|_{L^p}, \quad p = 2, \infty,$$

for all $t > 0$. $\blacksquare$

Remark: It follows from the proceeding theorem that, there exist constants K and ω such that

$$\left\| \tilde{V}(t+s) - h\frac{d\phi_\epsilon}{dy}(t+s) \right\|_{L^p} \le Ke^{-\omega s}\|U(t) - \phi_\epsilon(t)\|_{L^p}$$

for all $s > 0$ and $t > 0$, where $U(t)$ is the solution to Huxley's equation (2.1) and $\tilde{V}(r) = U(r) - \phi_\epsilon(r)$. In particular for all $s > (\log K)/\omega$ we have that,

$$\left\| \tilde{V}(t+s) - h\frac{d\phi_\epsilon}{dy}(t+s) \right\|_{L^p} \le \theta_s\|U(t) - \phi_\epsilon(t)\|_{L^p},$$

where $\theta_s = Ke^{-\omega s} < 1$ and $p = 2, \infty$.

2.5 Contraction of Solutions to Huxley's Equation

Now we are in a position to prove the contraction property of the second order parabolic equations. If U is the solution of original nonlinear Huxley's equation. Let

$$\rho(t) = \|U(\cdot,t) - \phi_\epsilon(t) - \tilde{V}(\cdot,t)\|_\infty.$$

Note that, if the initial condition of the linearized form is $\tilde{V}(0) = U(0) - \phi_\epsilon(0)$ then $\rho(0) = 0$. This property going to be very useful in the proof of the next theorem. To show the relation between the linear and nonlinear solutions to the Huxley's equation, we state and prove the Lemma 1 of Evans [8], for the case of the Huxley's equation.

Lemma 2.2 *If $\|\tilde{V}(\cdot,t)\|_\infty$ of (2.9) is bounded by M for all $t \ge 0$, then*

$$\rho(t) \le \rho(0)e^{Lt} + \frac{M^2 Q}{L}(e^{Lt} - 1), \quad t \ge 0,$$

where L and Q are upper bounds for $\left|\frac{\partial g(U)}{\partial U}\right|$ and $\left|\frac{\partial^2 g(U)}{\partial U^2}\right|$ respectively.

Follwing proof is due to Evans [8].

Proof. Recall that U has the representation (2.6)

$$U(x,t) = \int_{-\infty}^{\infty} F(x+vt,y,t)U(y,0)dy + \int_0^t \int_{-\infty}^{\infty} F(x+vt,y,t-s)g(U(y-vs))dyds.$$

Similarly ϕ_ϵ has the representation

$$\phi_\epsilon(x) = \int_{-\infty}^{\infty} F(x+vt,y,t)\phi_\epsilon(y)dy + \int_0^t \int_{-\infty}^{\infty} F(x+vt,y,t-s)g(\phi_\epsilon(y-vs))dyds$$

and $\tilde{V}$ has the representation (2.7)

$$\tilde{V}(x,t) = \int_{-\infty}^{\infty} F(x+vt,y,t)\tilde{V}(y,0)dy + \int_0^t \int_{-\infty}^{\infty} F(x+vt,y,t-s)\frac{\partial g}{\partial \phi_\epsilon}(\phi_\epsilon(y-vs))\tilde{V}(y-vs,s)dyds.$$

Using, the fact that $\int_{-\infty}^{\infty} F(x,y,t)dy = 1$ for $t > 0$ and all x, and the representation of ϕ_ϵ, we have that

$$|U(x,t) - \phi_\epsilon(x) - \tilde{V}(x,t)| \le \|U(\cdot,0) - \phi_\epsilon - \tilde{V}(\cdot,0)\|_\infty + \int_0^t H(s)ds,$$

where $H(s)$ is the least upper bound for all y of

$$\left| g(U(y-vs,s)) - g(\phi_\epsilon(y-vs)) - \frac{\partial g}{\partial \phi_\epsilon}(\phi_\epsilon(y-vs))\tilde{V}(y-vs,s) \right|.$$

Now letting $V = U - \phi_\epsilon$, by the mean value theorem and Taylor's expansion, we have

$$\begin{aligned} \left| g(\phi_\epsilon + V) - g(\phi_\epsilon) - \frac{\partial g}{\partial \phi_\epsilon}\tilde{V} \right| &\le \left| g(\phi_\epsilon + V) - g(\phi_\epsilon + \tilde{V}) + g(\phi_\epsilon + \tilde{V}) - g(\phi_\epsilon) - \frac{\partial g}{\partial \phi_\epsilon}\tilde{V} \right| \\ &\le L\|V - \tilde{V}\|_\infty + Q\|\tilde{V}\|_\infty^2. \end{aligned} \tag{2.13}$$

If $\|\tilde{V}\|_\infty$ is bounded by M for $t > 0$, the above gives $\rho(t) \le \rho(0) + \int_0^t (L\rho(s) + QM^2)ds$ and by standard methods $\rho(t)$ is dominated by $\rho(0)e^{Lt} + (M^2Q/L)(e^{Lt} - 1)$, the solution to

$dy/dt = Ly + QM^2$ with $y(0) = \rho(0)$.■

Note that, $L \in (1/4, 1/3)$ and $Q \in (1/3, 1/2)$.

Now we prove the main theorem of this section.

Theorem 2.3 *Let $U(t) = U(y,t)$ be a solution to Huxley's equation with initial data $U(y,0) = \phi(y) + \epsilon U_0(y)$, for all ϵ such that $U(y,t)$ converge to ϕ_ϵ, where ϕ is the traveling wave solution and U_0 is a continuous bounded function. Then, there exist numbers s, T_0, δ and $\theta_s \in (0,1)$ such that,*

$$\|U(s+t) - \phi_\delta(s+t)\|_\infty \le \theta_s \|U(t) - \phi_\epsilon(t)\|_\infty$$

for all $t > T_0$.

Proof. We know that $\phi(y)$, converge to 0 and 1 exponentially as y goes to $-\infty$ and ∞, respectively. So we use the interval $\Omega = [-A, A]$ with sufficiently large A as our domain, for this estimation. From the remark after the Theorem 2.1, there exists a number s such that

$$\left\| \tilde{V}(t+s) - h\frac{d\phi_\epsilon}{dy}(t+s) \right\|_\infty \le \theta_s \|U(t) - \phi_\epsilon(t)\|_\infty$$

for all $t > 0$. Then for this s, we can choose T_0 so that for a fixed $t > T_0$, we have

$$\|U(t) - \phi_\epsilon(t)\|_\infty \left(1 + \frac{PN_\infty}{\theta_s}\right)^2 \frac{Q}{L} e^{sL} \le 1, \tag{2.14}$$

$$4RP^2 \|U(t) - \phi_\epsilon(t)\|_\infty \le \theta_s, \tag{2.15}$$

where N_∞, R and P are the upper bounds of $\|d\phi_\epsilon/dy\|_\infty$, $\|d^2\phi_\epsilon/dy^2\|_\infty$ and $\|ke^y \frac{d\phi_\epsilon}{dy}\|_{L^1(\Omega)}$, and Q, L are constants defined in the previous Lemma. So from (2.14) we can have,

$$\|U(t) - \phi_\epsilon(t)\|_\infty \left(1 + \frac{PN_\infty}{\theta_s}\right)^2 \frac{Q}{L} \theta_s (e^{sL} - 1) \le 1. \tag{2.16}$$

Then if we choose initial condition $\tilde{V}(t) = (U(t) - \phi_\epsilon(t))$ because $\phi(y) = 1/(1+e^{-vy})$, by definition of h in Theorem 2.1 we have,

$$\begin{aligned} h &= \left(U(t) - \phi_\epsilon(t), k e^y \frac{d\phi_\epsilon}{dy} \right) \\ &\leq \|U(t) - \phi_\epsilon(t)\|_\infty \left\| k e^y \frac{d\phi_\epsilon}{dy} \right\|_{L^1(\Omega)} \\ &\leq P\|U(t) - \phi_\epsilon(t)\|_\infty. \end{aligned} \tag{2.17}$$

Then from Theorem 2.1 and (2.17) we have that,

$$\begin{aligned} \|\tilde{V}(t+s)\|_\infty &\leq \left\| \tilde{V} - h\frac{d\phi_\epsilon}{ds} \right\|_\infty + \left\| h\frac{d\phi_\epsilon}{ds} \right\|_\infty \\ &\leq \theta_s \|U(t) - \phi_\epsilon(t)\|_\infty + |h| N_\infty \\ &\leq \theta_s \|U(t) - \phi_\epsilon(t)\|_\infty \left(1 + \frac{PN_\infty}{\theta_s} \right) \qquad (2.18) \\ &= M. \qquad (2.19) \end{aligned}$$

Now, from Lemma 2.2 and, (2.16) and (2.19),

$$\begin{aligned} \left\| \left(U - \phi_\epsilon - \frac{\tilde{V}}{4} \right)(t+s) \right\|_\infty &\leq \frac{M^2}{4^2}\frac{Q}{L}(e^{sL} - 1) \\ &= \theta_s^2 \|U(t) - \phi_\epsilon(t)\|_\infty^2 \left(1 + \frac{PN_\infty}{\theta_s} \right)^2 \frac{Q}{16L}(e^{sL} - 1) \\ &\leq \frac{\theta_s}{16}\|U(t) - \phi_\epsilon(t)\|_\infty. \end{aligned} \tag{2.20}$$

Again from Theorem 2.1,

$$\frac{1}{4}\left\| \tilde{V}(t+s) - h\frac{d\phi_\epsilon}{dy}(t+s) \right\|_\infty \leq \frac{1}{4}\theta_s \left\| U(t) - \phi_\epsilon(t) \right\|_\infty. \tag{2.21}$$

From (2.15) and (2.17),

$$\begin{aligned} Rh^2 &\leq RP^2\|U(t)-\phi_\epsilon(t)\|_\infty^2 \\ &\leq \frac{1}{4}\theta_s\|U(t)-\phi_\epsilon(t)\|_\infty \end{aligned} \tag{2.22}$$

Then since R is an upper bound for $d^2\phi_\epsilon/dy^2$ using (2.20), (2.21) and (2.22), we have that,

$$\begin{aligned} \left\|U(t+s)-\phi_{h/4}(t+s)\right\|_\infty &\leq \left\|U-\phi_\epsilon-\frac{\tilde{V}}{4}\right\|_\infty + \frac{1}{4}\left\|\tilde{V}-h\frac{d\phi_\epsilon}{dy}\right\|_\infty + \left\|\phi_{h/4}-\phi_\epsilon-\frac{h}{4}\frac{d\phi_\epsilon}{dy}\right\|_\infty \\ &\leq \frac{1}{16}\theta_s\|U(t)-\phi_\epsilon(t)\|_\infty + \frac{1}{4}\theta_s\|U(t)-\phi_\epsilon(t)\|_\infty + \frac{Rh^2}{16} \\ &\leq \theta_s\|U(t)-\phi_\epsilon(t)\|_\infty. \end{aligned}$$

When $\delta = h/4$ gives the required result. ∎

Now we can prove the same result for the L^2 norm in the finite domain $\Omega = [-A, A]$. First we prove the similar result to Lemma 2.2. So let

$$\rho(t) = \|U(\cdot,t)-\phi_\epsilon(t)-\tilde{V}(\cdot,t)\|,$$

and if the initial condition of the linearized form is $\tilde{V}(0) = U(0)-\phi_\epsilon(0)$ then $\rho(0) = 0$.

Lemma 2.4 *If $\|\tilde{V}(\cdot,t)\|$ of (2.9) is bounded by M for all $t \geq 0$, then*

$$\rho(t) \leq \rho(0)e^{Lt} + \frac{M^2Q}{L}(e^{P_\Omega Lt}-1), \quad t \geq 0,$$

where L and Q are upper bounds for $\left|\frac{\partial g(U)}{\partial U}\right|$ and $\left|\frac{\partial^2 g(U)}{\partial U^2}\right|$ respectively.

Proof. Recall that U has the representation (2.6)

$$U(x,t) = \int_{-\infty}^{\infty} F(x+vt,y,t)U(y,0)dy + \int_0^t\int_{-\infty}^{\infty} F(x+vt,y,t-s)g(U(y-vs))dyds.$$

Similarly ϕ_ϵ has the representation

$$\phi_\epsilon(x) = \int_{-\infty}^{\infty} F(x+vt,y,t)\phi_\epsilon(y)dy + \int_0^t \int_{-\infty}^{\infty} F(x+vt,y,t-s)g(\phi_\epsilon(y-vs))dyds$$

and $\tilde{V}$ has the representation (2.7)

$$\tilde{V}(x,t) = \int_{-\infty}^{\infty} F(x+vt,y,t)\tilde{V}(y,0)dy + \int_0^t \int_{-\infty}^{\infty} F(x+vt,y,t-s)\frac{\partial g}{\partial \phi_\epsilon}(\phi_\epsilon(y-vs))\tilde{V}(y-vs,s)dyds.$$

Using, the fact that $\int_{-\infty}^{\infty} F(x,y,t)dy = 1$, and $\|F(x,y,t)\|_\infty \leq 1$ for all x and $t > 0$, we have that

$$\begin{aligned}
&\int_{-\infty}^{\infty} F(x+vt,y,t)(U(y,0) - \phi_\epsilon(y) - \tilde{V}(y,0))dy \\
&\leq \|F(x+vt,y,t)\|\|U(y,0) - \phi_\epsilon(y) - \tilde{V}(y,0)\| \\
&\qquad \leq \|F(x+vt,y,t)\|_\infty \|F(x+vt,y,t)\|_{L^1}\|U(y,0) - \phi_\epsilon(y) - \tilde{V}(y,0)\| \\
&\qquad \leq \|U(y,0) - \phi_\epsilon(y) - \tilde{V}(y,0)\|,
\end{aligned}$$

and similarly

$$\begin{aligned}
&\int_0^t \int_{-\infty}^{\infty} F(x+vt,y,t-s)\left(g(U) - g(\phi_\epsilon) - \frac{\partial g}{\partial \phi_\epsilon}\tilde{V}\right)dyds \\
&\qquad \leq \int_0^t \|F(x+vt,y,t-s)\| \left\| g(U) - g(\phi_\epsilon) - \frac{\partial g}{\partial \phi_\epsilon}\tilde{V} \right\| ds \\
&\qquad \leq \int_0^t \left\| g(U) - g(\phi_\epsilon) - \frac{\partial g}{\partial \phi_\epsilon}\tilde{V} \right\| ds.
\end{aligned}$$

Thus,

$$|U(x,t) - \phi_\epsilon(x) - \tilde{V}(x,t)| \leq \|U(\cdot,0) - \phi_\epsilon - \tilde{V}(\cdot,0)\| + \int_0^t H(s)ds \tag{2.23}$$

for all x, where

$$H(s) = \left\| g(U(y-vs,s)) - g(\phi_\epsilon(y-vs)) - \frac{\partial g}{\partial \phi_\epsilon}(\phi_\epsilon(y-vs))\tilde{V}(y-vs,s) \right\|.$$

Moreover, For finite domain $\Omega = [-A, A]$, there exists a constant P_Ω depends on Ω such that,

$$\|U(x,t) - \phi_\epsilon(x) - \tilde{V}(x,t)\| \leq P_\Omega \|U(x,t) - \phi_\epsilon(x) - \tilde{V}(x,t)\|_\infty. \tag{2.24}$$

Now letting $V = U - \phi_\epsilon$, by the mean value theorem, we have

$$\begin{aligned} \left\| g(\phi_\epsilon + V) - g(\phi_\epsilon) - \frac{\partial g}{\partial \phi_\epsilon}\tilde{V} \right\| &\leq \left\| g(\phi_\epsilon + V) - g(\phi_\epsilon + \tilde{V}) + g(\phi_\epsilon + \tilde{V}) - g(\phi_\epsilon) - \frac{\partial g}{\partial \phi_\epsilon}\tilde{V} \right\| \\ &\leq L\|V - \tilde{V}\| + Q\|\tilde{V}\|^2. \end{aligned} \tag{2.25}$$

If $\|\tilde{V}\|$ is bounded by M for $t > 0$, then (2.23), (2.24) and (2.25) gives $\rho(t) \leq P_\Omega \rho(0) + P_\Omega \int_0^t (L\rho(s) + QM^2) ds$ and by standard methods $\rho(t)$ is dominated by $P_\Omega \rho(0) e^{P_\Omega Lt} + (M^2 Q/L)(e^{Lt} - 1)$, the solution to $dy/dt = Ly + QM^2$ with $y(0) = \rho(0)$.■

Theorem 2.5 *Let $U(t) = U(y,t)$ be a solution to Huxley's equation with initial data $U(y,0) = \phi(y) + \epsilon U_0(y)$, for all ϵ such that $U(y,t)$ converge to ϕ_ϵ, where ϕ is the traveling wave solution and U_0 is a continuous bounded function. Then, there exist numbers s, T_0, δ and $\theta_s \in (0,1)$ such that,*

$$\|U(s+t) - \phi_\delta(s+t)\| \leq \theta_s \|U(t) - \phi_\epsilon(t)\|$$

for all $t > T_0$.

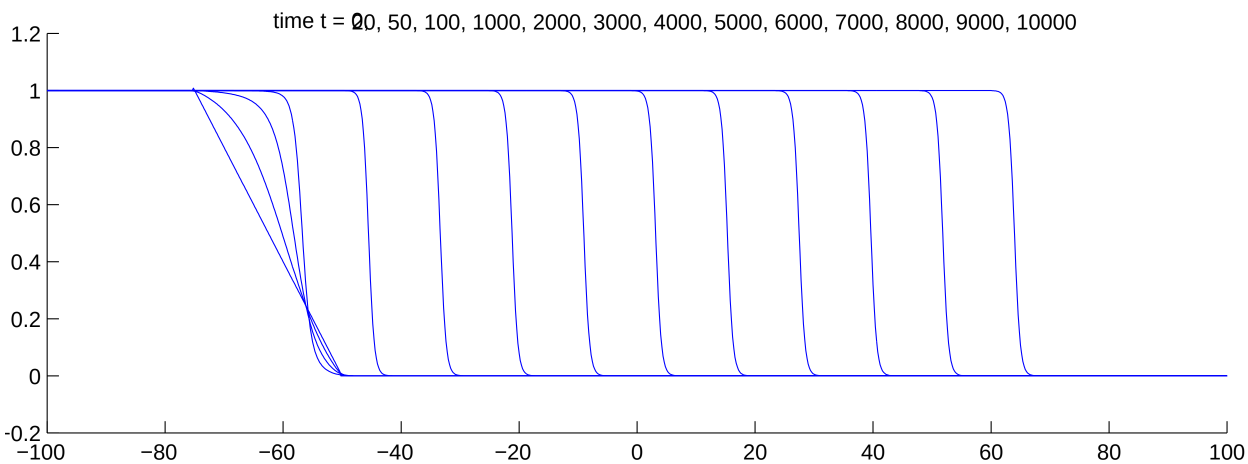
Proof. The Proof follows from the same argument replacing L^∞ norm with L^2 norm in the Theorem 2.3, we can get the required result. ■

2.6 Computational Result

Consider Huxley's equation on the following form

$$
\begin{aligned}
U_t &= U_{xx} + U(1-U)(U-0.25) \\
U(x,0) &= \begin{cases} 1, & \text{if } -100 < x < -75 \\ -0.04x - 2, & \text{if } -75 < x < -50 \\ 0, & \text{if } -50 < x < 100. \end{cases}
\end{aligned}
$$

Then convergence of the solution is shown in the following figure.



(c)

Figure 2.1: Convergence to the Traveling Wave.

CHAPTER 3

Long-Time Error Estimate for the Second Order Problem

This chapter sets the stage towards the development of long-time error analysis for the numerical solution of the EFK equation. We begin with the error estimation for the numerical solution of the Huxley's equation, which can be viewed as the second order counterpart of the fourth order EFK equation. To establish the estimates for the numerical error propagation and actual error defined in Chapter 1, we use the concepts of the smoothing indicator initiated by Sun([26], [27]) and the evolving attractor defined in Chapter 2.

We start with general notation in Section 2.1. Then in Section 2.2 we describe briefly the finite element method and some properties of the solutions of the Huxley's equations. Next the smoothing indicator is determined in Section 2.3. The moving attractor is introduced in Section 2.4 and finally the error estimates are presented in Section 2.5.

3.1 General Notations

Here and throughout, we use the standard Banach spaces $L_p = L_p(\Omega)$, $1 \leq p \leq \infty$ and standard Sobolev space $H^m = H^m(\Omega), m = 1, 2, \ldots$. The norm for elements in $L_p(\Omega)$ are

$$\begin{aligned} \|u\|_{L_p} &= \left(\int_\Omega |u|^p d\Omega \right)^{1/p} \\ \|u\|_{L_\infty} &= \sup_{x\in\Omega} |u(x)|. \\ \|u\|_{W^r_\infty} &= \sup_{|\alpha|\leq r} \|D^\alpha u\|_\infty. \end{aligned}$$

For $p = 2$, we use the simplified notation $\|u\| = \|u\|_{L^2}$ and $\|u\|_\infty = \|u\|_{L^\infty}$. The inner product $L_2(\Omega)$ is denoted by

$$(u, v) = \int uv d\Omega.$$

The norm for the elements in $H^m(\Omega)$ is

$$\|u\|_m = \left(\sum_{|\alpha|\leq m} \|D^\alpha u\|^m \right)^{1/m}.$$

We will also use the standard Sobolev space with the homogeneous boundary condition

$$H^1_0(\Omega) = \left\{ u \in H^1(\Omega); \forall x \in \partial\Omega, u(x) = 0 \right\}.$$

For the convenience of error propagation analysis in the following sections, we use the notation

$$u(p, t, v)$$

to stand for the value of the solution of PDE at time $t + p$ with initial time t, initial value $v \in L^2(\Omega)$, and time increment p.

3.2 Finite Element Methods

We define a class of initial boundary value problem to which Huxley's and FK equations belong:

$$\frac{\partial u}{\partial t} = \Delta u + f(u), \qquad \text{in } \Omega \tag{3.1}$$

in a convex polygonal domain $\Omega \in \mathbb{R}^2$, subject to the boundary conditions

$$u = 0 \qquad \text{on } \partial\Omega$$

or

$$\frac{\partial u}{\partial n} = 0 \qquad \text{on } \partial\Omega$$

for $t \in [t_0, \infty)$ and the initial condition

$$u(t_0) = u_0.$$

The equation (3.1) is Huxley's equation when $f(u) = u(1-u)(u-a)$.

For the global existence of a solution, we consider the concept of an invariant region [25]. With this, the possibility of any finite time blow-up can be excluded. It has been shown that for any initial value $u_0 \in H_0^1$, there exists $u(t)$ in $[t_0, \infty)$, for all t. (See [25], Chapter 14 for a more general results and their proof). Since both Huxley's equation and FK equation satisfy one-sided Lipschtiz condition

$$(\Delta u + f(u) - \Delta v - f(v), u - v) \leq m\|u - v\|^2, \tag{3.2}$$

for all $u, v \in H_0^1(\Omega)$. By Theorem 3.3 of [27] we can see that for any initial value $u(t_0) = u_0$ and $v(t_0) = u_0$ in $H_0^1(\Omega)$ the corresponding solutions $u(t)$ and $v(t)$ satisfy,

$$\|u(t) - v(t)\| \leq e^{m(t-t_0)}\|u_0 - v_0\|. \tag{3.3}$$

We next consider a weak formulation of the above IBVP: Find $u(t) \in C^1([t_0, \infty), H_0^1(\Omega))$, such that

$$\left(\frac{\partial u}{\partial t}, v\right) + (\nabla u, \nabla v) = (f(u), v) \tag{3.4}$$

for all $v \in H_0^1(\Omega)$. Let $\mathcal{T}_h$ be a quasi-uniform triangulation of Ω, where h is the maximum mesh size of $\mathcal{T}_h$,

$$h = \max\{\text{diam}(T), \quad T \in \mathcal{T}_h\}.$$

Let $V_{h,p}$ be the finite element space consisting of continuous piecewise polynomials of order p:

$$V_{h,p} = \left\{q \in H_0^1(\Omega) : q|_T \in \mathcal{P}_p(T)\right\}$$

where $\mathcal{P}_p(T)$ is the set of all the polynomials in T up to order p. When it is clear that the order is p from the context, we use V_h for $V_{h,p}$.

After these preparations we now turn to the initial-boundary value problem (3.1) for the heat equation. It is convenient to proceed in two steps with the definition and analysis of the approximation solution. As the first step we shall approximate $u(x,t)$ by means of a function $u_h(x,t)$ which for each fixed t, belongs to a finite dimensional linear space V_h of functions of x of the type considered above. This function will be the solution of h-dependent finite system of ordinary differential equations in time and is referred to as a semidiscrete solution. The specially discrete problem is based on a variational formulation (3.4). In the second step, we discretize this system in the time variable to produce a fully discrete scheme for the approximated solution of (3.1). For simplicity, we use a fixed time step size τ for the discretization of time.

For the numerical solution for the fully discrete scheme, we use the notation $u_N(t)$, and in error propagation we write the numerical solution as $u_N(p,t,v)$. Similarly the semi-discrete solution is written in the form $u_h(p,t,v)$, mimicking those notations we introduces in Section 2.

For the discrete space, we introduce the discrete Laplacian operator $\Delta_h : H_0^1(\Omega) \to V_h$

defined by

$$(\Delta_h u, v) = -(\nabla u, \nabla v) \qquad \forall v \in V_h$$

and the L^2 projection operator $P_h : L^2(\Omega) \to V_h$ by

$$(P_h u, v) = (u, v) \qquad \forall v \in V_h.$$

Then we can prove following short time stability property for the semi-discrete solution.

Lemma 3.1 *For the initial values u_0 and $v_0 \in H_0^1$ the corresponding semi-discrete solutions $u_h(t)$ and $v_h(t)$ satisfy*

$$\|u_h - v_h\| \leq e^{m(t-t_0)} \|u_0 - v_0\|. \tag{3.5}$$

Proof of (a). Theorem 4.1 of [27]. ■

3.3 Smoothing Indicator

The numerical error is uniformly bounded if the numerical method is stable. According to [11] the concept of stability is continuous dependence of the solution on initial data in the infinite interval in time. The stability of the solutions for the differential equations is also discussed in [19], [21], [31]. In general, we expect the numerical solution to approximate the exact solution for the differential equation with certain accuracy. That is, the solutions of the discretized problem to converge to the solution of the original problem, as mesh size decreases to zero. However, this question of convergence is usually very hard to investigate. The concept of stability helps us to discuss the question of convergence. As a matter of fact, they are closely related. From Lax-Richtmyer Theorem, we know that given a well posed initial value problem and a consistent difference method, stability is necessary and sufficient for convergence. In the literature the definition of the stability is given as "for a stable difference scheme small errors in the initial conditions cause the small error in the solution." Though it is easier to show stability than convergence, showing stability is still a difficult problem, especially for nonlinear parabolic problems. Moreover, for complex nonlinear systems treated by combination of numerical techniques such as linearization, partially implicit schemes, local time stepping etc., it is difficult, sometimes impossible to carry out stability analysis. So we adapt a methodology suggested by Sun and Ewing [26] to do our long-time error analysis. Their techniques were specially designed to overcome difficulties in nonlinear problems. The next theorem is crucial for the estimation of the actual error, and consequently for the definition of the smoothing indicator.

Theorem 3.2 *For any initial value $\bar{u} \in V_h$, if*

$$\begin{aligned} \bar{v} &= \Delta_h \bar{u} + P_h f(\bar{u}), \\ \bar{w} &= \Delta_h \bar{v} + P_h(f'(\bar{u})\bar{v}), \end{aligned}$$

and there is a constant $\bar{C}$ such that $\|\bar{u}\|_1 \leq \bar{C}$, $\|\bar{v}\| \leq \bar{C}$, $\|\bar{w}\| \leq \bar{C}$, then the corresponding semi-discrete solution $u_h(p,t,\bar{u})$ satisfies

$$\begin{aligned} &(a) \qquad \left\| \frac{\partial^2}{\partial p^2} u_h(p,t,v) \right\| \leq C_0 + C_1\|\bar{u}\| + C_2\|\bar{v}\| + C_3\|\bar{w}\| \\ &(b) \qquad \left\| \frac{\partial^2}{\partial p^2} u_h(p,t,v) \right\|_\infty \leq C_0 + C_1\|\bar{u}\| + C_2\|\bar{v}\| + C_3\|\bar{w}\| \end{aligned}$$

for sufficiently small p and some constants C_0, C_1, C_2 and C_3.

Proof of (a): Same as the proof of the Theorem 4.2 in [27].

Proof of (b): Let $v_h = \frac{du_h}{dp}$ and $w_h = \frac{d^2u_h}{dp^2}$. Since the weak solution is also a strong solution, it is easy to see that u_h, v_h and w_h satisfy that

$$\frac{\partial u_h}{\partial p} = \Delta_h u_h + f(u_h) \tag{3.6}$$

$$\frac{\partial v_h}{\partial p} = \Delta_h v_h + f'(u_h)v_h \tag{3.7}$$

$$\frac{\partial w_h}{\partial p} = \Delta_h w_h + f'(u_h)w_h + f''(u_h)v_h^2. \tag{3.8}$$

Since

$$\begin{aligned} f(u_h) &= u_h(1-u_h)(u_h-a) \\ f'(u_h) &= (1-2u_h)(u_h-a)-a(u_h-u_h^2) \\ f''(u_h) &= 2(a-u_h)-2a(1-2u_h), \end{aligned}$$

using the bounds of of u_h, v_h and w_h we have

$$\frac{d}{dp}(1+\|u_h\|_\infty+\|v_h\|_\infty+\|w_h\|_\infty) \leq C(1+\|u_h\|_\infty+\|v_h\|_\infty+\|w_h\|_\infty).$$

Then by the Gronwall lemma we have

$$(1+\|u_h(t+p)\|_\infty+\|v_h(t+p)\|_\infty+\|w_h(t+p)\|_\infty) \leq e^{Cp}(1+\|u_h(t)\|_\infty+\|v_h(t)\|_\infty+\|w_h(t)\|_\infty).$$

A special case of the last inequality is

$$\left\| \frac{\partial^2}{\partial p^2} u_h(p,t,v) \right\|_\infty \leq C_0 + C_1\|\bar{u}\| + C_2\|\bar{v}\| + C_3\|\bar{w}\|. \qquad \blacksquare$$

Now to monitor the stability and smoothing behavior of the numerical scheme, we define smoothing indicator as proposed in [26] and [27]. Suppose that a time step size τ of a fully discrete scheme is less than the sufficiently small p given in the previous theorem.

Definition 3.3 *For each node t_i of the time stepping, $t_i = t_0 + i\tau$, and the value of the numerical solution at t_i, $\bar{u} = u_N(t_i)$, let*

$$\begin{aligned} \bar{v} &= \Delta_h \bar{u} + P_h f(\bar{u}), \\ \bar{w} &= \Delta_h \bar{v} + P_h(f'(\bar{u})\bar{v}). \end{aligned}$$

Depending on the necessity for

1. L_2 *norm* $S_i^2 = (\|\bar{u}\|_1, \|\bar{v}\|, \|\bar{w}\|, \|\Delta_h \bar{u}\|)$

2. L_∞ *norm* $S_i^2 = (\|\bar{u}\|_1, \|\bar{v}\|_\infty, \|\bar{w}\|_\infty, \|\Delta_h \bar{u}\|)$

We call the S_i^q *the smoothing indicator.*

3.4 Moving Attractor

In this section we recall the concept of the moving attractor initially introduced in [26] and [27]. It is a compact subset of phase space that attracts all the trajectories. As such we can expect the set of solutions that lie in the attractor to cover all the possible dynamical behaviors of the system [23]. We also need an invariant condition, which guarantees that the absorbing set does not decrease as $t \to \infty$. For many problems such as those in [6],[30], the concept of moving attractor is more general than that of the global and exponential attractor.

If $\mathcal{M}$ is a one-parameter family of sets in L^2, $\mathcal{M} = \{M_t \subset L^2 | t > T\}$, we say that $\mathcal{M}$ is positively invariant under the dynamical system if for any $v \in M_t$ and $p > 0$, $u(p, t, v) \in M_{t+p}$. Now we define the moving attractor as in [27].

Definition 3.4 *A positively invariant one parameter family of sets* $\mathcal{M}$ *in* L^2 *is called a moving attractor, if there exists real number* $\theta_s \in (0, 1)$ *depending on* s*, and a one parameter family of open sets* $\mathcal{U} = \{U_t \subset L_2 | t > T\}$*, positively invariant under the dynamical system, with* $M_t \subset U_t$ *for all* $t > T$*, such that for any* $v \in U_t$

$$d(u(s,t,v), M_{t+s}) \leq \theta_s d(v, M_t),$$

where $d(u, M) = \inf_{w \in M} \|u - w\|$. $\mathcal{U}$ *is called a basin of the moving attractor.*

Now, let

$$M_t = \{\phi(x + vt + c) | c \in \mathbb{R}, \phi \text{ a wave profile of Huxley's equation}\}.$$

Then if $\phi(x+vt+c)$ is initial value of the Huxley's equation, we know that $\phi(x+v(t+s)+c)$ is solution to Huxley's equation after time s. In other words if $\phi(x+vt+c) \in M_t$ then $\phi(x+v(t+s)+c) \in M_{t+s}$. Therefore, the sets

$$\mathcal{M} = \{M_t | t > T_0\}$$

positively invariant under the Huxley's equation. Similarly,

$$\mathcal{U} = \{U_t | t > T_0\},$$

where

$$U_t = \{u(x,t) | \text{solutions to Huxley's equation with initial conditions } \phi(x) + \epsilon u_0(x)\},$$

also positively invariant under the Huxley's equation and $M_t \subset U_t$. Then, from the contraction property that we introduced in the last chapter we know that, there exist $s > 0$ and $\theta_s \in (0,1)$, for any $v \in U_t$ such that

$$\|u(s,t,v) - \phi_\epsilon(t+s)\| \leq \theta_s \|v - \phi_\epsilon(t)\|.$$

Thus

$$d(u(s,t,v), M_{t+s}) \leq \theta_s d(v, M_t).$$

Hence

$$\begin{aligned} \mathcal{M} &= \{M_t | t > T_0\} \\ &= \{\phi(x+vt+c) | c \in \mathbb{R}, t > T_0\} \end{aligned}$$

is a moving attractor for the Huxley's equation.

3.5 Error Estimation

Now we state the error estimation theorems.

Theorem 3.5 *Assume that*

1. $u_N(t)$ *is a numerical solution of equation (3.1), computed by the finite element method and the discretization in time is consistent with the differential equation with a local error of order* $q = 2$ *or* $q = 3$.

2. *A one-sided Lipschtiz condition is satisfied in* $H_0^1(\Omega)$

$$(\Delta u + f(u) - \Delta v - f(v), u - v) \leq m\|u - v\|^2$$

for some m.

3. *There is a moving attractor* $\mathcal{M}$ *such that*

$$d(u(s, t, v), M_{t+s}) \leq \theta_s d(v, M_t)$$

for all $t \geq t_0$.

4. *The time step size* τ *is chosen so that* s *is a multiple of* τ*:* $s = k\tau$ *for a positive integer* k.

5. *The smoothing indicator remains bounded.*

Then we have the following global error estimate:

$$d\left(\mathcal{M}, u_N(ns, t_0, u_N(t_0))\right) \leq C\frac{se^{m^+s}\tau^{q-1}S_M^q + e^{m^+s}h^2 S_H^2}{1 + \theta_s} + \theta_s^n d(M_{t_0}, u_N(t_0)),$$

where $m^+ = \max\{0, m\}$, *and*

$$\begin{aligned} S_M^q &= C_M + \sum_{j=0}^{q} C_j \max_i S_{ij}^q \\ S_H^2 &= \max_i \|\Delta_h u_N(t_i)\| . \end{aligned}$$

Here S_{ij}^q *denotes the jth node component of* S_j^q.

Proof. Theorem 6.1 of [27]

Even though we can define moving attractor for L_∞, it is still a challenge to find short term error estimates and Lipschitz conditions for the problem defined in an infinite domain.

CHAPTER 4

Finite Element Methods for the EFK Equation

Extended Fisher Kolmogorov equation occurs in a variety of applications such as pattern formulation in bistable systems [5], propagation of domain walls in liquid crystals [32], travelling waves in reaction diffusion systems and mezoscopic model of a phase transition in a binary system near the Lipschitz point [13]. In particular, in the phase transition near critical points (Lipschitz points), the higher order gradient terms in the free energy functional can no longer be neglected and the fourth order derivative becomes important [4].

In this chapter we study the standard Galerkin finite element method for the approximation of the solutions of extended Fisher-Kolmogorov equation,

$$\begin{aligned} u_t + \gamma\Delta^2 u - \Delta u &= f(u) \qquad \text{in } \Omega \text{ for } t > 0, \\ u(\cdot, 0) &= v \quad \text{in } \Omega. \end{aligned}$$

with Dirichlet boundary conditions

$$u = \Delta u = 0 \quad \text{on } \partial\Omega \text{ for } t > 0,$$

or with Neumann boundary conditions

$$\frac{\partial u}{\partial n} = \frac{\partial \Delta u}{\partial n} = 0 \quad \text{on } \partial\Omega \text{ for } t > 0$$

where Ω is a convex polygonal domain in $\mathbb{R}^2$ with boundary $\partial\Omega$. As for the computational studies there is not much literature on the numerical approximations of the EFK equation. Moreover error estimates in the paper [4] have bounds containing the factor $\exp \frac{T}{\gamma}$, which is less useful when γ is small. We shall establish in this chapter short error analysis and the long term error estimates in the next chapter. Our error estimates only depend on the γ^{-1}. In the future, special efforts will be made to establish error estimates free of the term γ.
In Section one we define finite element method for the EFK equation. In Section two we proceed to discretized the problem in the spacial variable and approximate the solution in the finite element space, as a finite dimensional system of ordinary differential equations. Then in Section three we define fully discrete scheme by discretizing in time using finite difference approximations. Error estimates are derived for both the spatially and complete discrete solutions.

4.1 Finite Element Method

We construct the finite dimensional space $V_h \in H^2(\Omega)$ of continuous bilinear polynomials. Let K_h be quasi-uniform decomposition of the domain Ω into disjoint triangles such that no vertex of any triangle lies on the interior of a side of another triangle. Let h denote the maximal length of a side of a triangle. We also knows that $V_h \in H_0^2(\Omega)$, if and only if $V_h \in C^1(\Omega)$. Thus we work with polynomials of degree five on each triangle. Therefore let K be a triangle with vertices's a^i $i = 1, 2, 3$ and let a^{ij} be the mid point on the side $a^i a^j$ $i, j = 1, 2, 3$, $i < j$. A function $v \in P_5(K)$ is uniquely determined by the following degrees of freedom

$$\begin{aligned} D^\alpha v(a^i), \quad i &= 1,2,3, \quad |\alpha| \leq 2 \\ \frac{\partial v}{\partial n}(a^{ij}), \quad i,j &= 1,2,3, \quad i<j, \end{aligned}$$

where $\frac{\partial}{\partial n}$ denotes differentiation in the outward normal direction to the boundary of K. This space is often known as the space of Argyris triangular elements and it belongs to C^1 finite element class. The following approximation property holds (chapter 6 of [2]). When $H_0^r \hookrightarrow H_0^m$ for all $v \in H_0^r$ there is a positive constant c, so that

$$\inf_{\chi \in S_h} \|v-\chi\|_m \leq ch^{r-m}\|v\|_r, \quad 3 \leq r \leq 6 \quad m=0,1,2. \tag{4.1}$$

4.1.1 Semi-Discrete Schemes

In this section we study the spatially semidiscrete problem. The problem can be formulated as: Find $u_h \in V_h$, such that,

$$\begin{aligned} (u_{h,t},\chi) + \gamma(\Delta u_h, \Delta\chi) + (\nabla u_h, \chi) &= (f,\chi), \quad \forall \chi \in V_h, \quad t \in [0,\infty) \\ (u_h(.,0),\chi) &= (v,\chi), \quad \forall \chi \in V_h. \end{aligned} \tag{4.2}$$

Now let the basis function in V_h be denoted by ψ, $i = 1,2,\ldots,m$ and express u_h as

$$u_h(x,t) = \sum_{j=1}^{m} a_j(t)\psi_j(x), \quad (x,t) \in \Omega \times [0,\infty) \tag{4.3}$$

where a_j are nodal values. For $j = 1,2,\ldots,m$ taking $v = \psi_j$ in (4.2) with (4.3), we see that

$$\begin{aligned} \sum_{j=1}^{m} a_i'(t)(\psi_i,\psi_j) + \sum_{j=1}^{m} a_i(t)\gamma(\Delta\psi_i,\Delta\psi_j) + \sum_{j=1}^{m} a_i(t)(\nabla\psi_i,\nabla\psi_j) &= (f,\psi_j) \\ \sum_{j=1}^{m}(\psi_i,\psi_j)a_i(0) &= (v,\psi_j). \end{aligned} \tag{4.4}$$

In the matrix form, this is

$$\begin{aligned}
\mathbf{a}'(t) + \mathbf{M}^{-1}(\gamma\mathbf{A} + \mathbf{B})\mathbf{a}(t) &= \mathbf{M}^{-1}\mathbf{f}, \\
\mathbf{M}\mathbf{a}(0) &= \mathbf{v},
\end{aligned}$$

where the $m \times m$ matrices **A, B** and **M** and the vectors **a, v, f** are

$$\begin{aligned}
\mathbf{A} &= (a_{ij}) = (\Delta\psi_i, \Delta\psi_j), \\
\mathbf{B} &= (b_{ij}) = (\nabla\psi_i, \nabla\psi_j), \\
\mathbf{M} &= (m_{ij}) = (\psi_i, \psi_j), \\
\mathbf{a} &= (a_j), \\
\mathbf{f} &= (f_j) = (f, \psi_j), \\
\mathbf{v} &= (v - j) = (v, \psi_j).
\end{aligned}$$

In the standard finite element method the matrix with elements $m_{ij} = (\psi_i, \psi_j)$ is the mass matrix $\mathbf{M}$, and the matrix with the elements $a_{ij} = (\nabla\psi_i, \nabla\psi_j)$ and $a_{ij} = (\Delta\psi_i, \Delta\psi_j)$ is the stiffness matrices $\mathbf{A}$ and $\mathbf{B}$. The mass matrix $\mathbf{M}$ is positive definite and hence invertible. So we can write (4.4) as a system of ordinary differential equations:

$$\mathbf{a}'(t) + \mathbf{M}^{-1}\left(\mathbf{A} + \gamma\mathbf{B}\right)\mathbf{a}(t) = \mathbf{M}^{-1}\mathbf{f}.$$

Now we prove the L_2 error estimate between the solution of the semidiscrete and continuous problem. Define the Ritz or elliptic projection $R_h : H_0^2 \to S_h$ as the orthogonal projection with respect to bilinear form $A(u, v) = \gamma(\Delta u, \Delta v) + (\nabla u, \nabla v)$, so that for $v \in H_0^2$,

$$A(R_h v, \chi) = A(v, \chi) \quad \text{for all } \chi \in S_h.$$

Then we split the error

$$u_h - u = \theta + \rho,$$

where $\theta = u_h - R_h u$ and $\rho = R_h u - u$. Then for all χ in S_h

$$\begin{aligned} A(R_h u - u, R_h u - u) &\leq \gamma(\Delta(R_h u - u), \Delta(R_h u - u)) + (\nabla(R_h u - u), \nabla(R_h u - u)) \\ &= \gamma(\Delta(R_h u - u), \Delta(\chi - u)) + (\nabla(R_h u - u), \nabla(\chi - u)) \\ &\leq \gamma c\|R_h u - u\|_2 \|\chi - u\|_2 + c\|R_h u - u\|_1 \|\chi - u\|_1. \end{aligned}$$

Thus by approximation property (4.1) with $m = 2$ and $m = 1$

$$\begin{aligned} A(R_h u - u, R_h u - u) &\leq \gamma c\|R_h u - u\|_2 \inf_{\chi \in S_h} \|\chi - u\|_2 + c\|R_h u - u\|_1 \inf_{\chi \in S_h} \|\chi - u\|_1 \\ &\leq \gamma c\|R_h u - u\|_2 h^{r-2}\|u\|_r + c\|R_h u - u\|_1 h^{r-1}\|u\|_r, \quad 3 \leq r \leq 6. \end{aligned}$$

That is

$$\gamma\|R_h u - u\|_2^2 + \|R_h u - u\|_1^2 \leq \gamma c h^{r-2}\|R_h u - u\|_2 \|u\|_r + c h^{r-1}\|R_h u - u\|_1 \|u\|_r. \tag{4.5}$$

Now when $\gamma < 1$, for small enough h, there is constant c independent of γ such that

$$\begin{aligned} \gamma^2\|R_h u - u\|_2^2 + \|R_h u - u\|_1^2 &\leq c h^{r-2}\|u\|_r \left(\gamma\|R_h u - u\|_2 + \|R_h u - u\|_1\right), \\ \frac{1}{2}\left(\gamma\|R_h u - u\|_2 + \|R_h u - u\|_1\right)^2 &\leq c h^{r-2}\|u\|_r \left(\gamma\|R_h u - u\|_2 + \|R_h u - u\|_1\right), \\ \left(\gamma\|R_h u - u\|_2 + \|R_h u - u\|_1\right) &\leq c h^{r-2}\|u\|_r. \end{aligned} \tag{4.6}$$

Thus

$$\gamma\|\rho\|_2 = \gamma\|R_h u - u\|_2 \leq c h^{r-2}\|u\|_r, \quad 3 \leq r \leq 6. \tag{4.7}$$

When $\gamma > 1$, from the boundedness of $A(.,.)$ from (4.5) we have

$$\gamma\|R_h u - u\|_2^2 \le \gamma\|R_h u - u\|_2^2 + \|R_h u - u\|_1^2 \le \gamma c h^{r-2}\|R_h u - u\|_2\|u\|_r$$

Thus

$$\|\rho\|_2 = \|R_h u - u\| \le c h^{r-2}\|u\|_r \quad 3 \le r \le 6,$$

which is similar to inequality as (4.7). For the L_2 error analysis we use the Aubin-Nitsche duality argument. Let ψ be a solutions of

$$\begin{aligned} \gamma\Delta^2\psi - \Delta\psi &= \varphi \quad \text{in } \Omega, \\ \psi = \Delta\psi &= 0 \quad \text{on } \partial\Omega. \end{aligned}$$

For any $\psi_h \in S_h$ we have

$$\begin{aligned} (R_h u - u, \varphi) &= \gamma(\Delta(R_h u - u), \Delta\psi) + (\nabla(R_h u - u), \nabla\psi) \\ &= \gamma(\Delta(R_h u - u), \Delta(\psi - \psi_h)) + (\nabla(R_h u - u), \nabla(\psi - \psi_h)) \\ &\le c\gamma\|R_h u - u\|_2\|\psi - \psi_h\|_2 + c\|R_h u - u\|_1\|\psi - \psi_h\|_1. \end{aligned}$$

Hence by (4.1) for $r = 4$

$$\begin{aligned} (R_h u - u, \varphi) &\le c\gamma\|R_h u - u\|_2 \inf_{\psi_h \in V_h}\|\psi - \psi_h\|_2 + c\|R_h u - u\|_1 \inf_{\psi_h \in V_h}\|\psi - \psi_h\|_1 \\ &\le c\gamma\|R_h u - u\|_2 h^2\|\psi\|_4 + c\|R_h u - u\|_1 h^3\|\psi\|_4. \end{aligned} \tag{4.8}$$

When $\gamma < 1$, multiply above inequality by γ and together with (4.6) and the elliptic regularity

$$
\begin{aligned}
\gamma(R_h u - u, \varphi) &\leq c\gamma^2 \|R_h u - u\|_2 h^2 \|\psi\|_4 + c\gamma \|R_h u - u\| h^3 \|\psi\|_4 \\
&\leq ch^2 \|\varphi\| (\gamma \|R_h u - u\|_2 + \|R_h u - u\|_1) \\
&\leq ch^2 \|\varphi\| ch^{r-2} \|u\|_r .
\end{aligned}
$$

So when $\varphi = R_h u - u$ we have

$$\gamma \|\rho\| = \gamma \|R_h u - u\| \leq ch^r \|u\|_r \qquad 3 \leq r \leq 6. \tag{4.9}$$

For $\gamma > 1$ from (4.8)

$$
\begin{aligned}
(R_h u - u, \varphi) &\leq c\gamma \|R_h u - u\|_2 h^2 \|\psi\|_4 \\
&\leq c\gamma h^{r-2} \|u\|_r h^2 \|\psi\|_4 \\
&\leq ch^r \|u\|_r \|\varphi\| .
\end{aligned}
$$

Again when $\varphi = R_h u - u$ we have

$$\|\rho\| = \|R_h u - u\| \leq ch^r \|u\|_r , \qquad 3 \leq r \leq 6. \tag{4.10}$$

Moreover, in order to estimate θ, note that

$$
\begin{aligned}
&(\theta_t, \chi) + (\nabla \theta, \nabla \chi) + \gamma(\Delta \theta, \Delta \chi) \\
&= (u_{h,t}, \chi) + (\nabla u_h, \nabla \chi) + \gamma(\Delta u_h, \Delta \chi) - (R_h u_t, \chi) - (\nabla R_h u, \nabla \chi) - \gamma(\Delta R_h u, \Delta \chi) \qquad (4.11) \\
&= (f, \chi) - (R_h u_t, \chi) - (\nabla u, \nabla \chi) - \gamma(\Delta u, \Delta \chi) \\
&= (u_t, \chi) - (R_h u_t, \chi) \\
&= (u_t - R_h u_t, \chi),
\end{aligned}
$$

or

$$(\theta_t, \chi) + \gamma(\Delta\theta, \Delta\chi) + (\nabla\theta, \nabla\chi) = -(\rho_t, \chi).$$

When $\chi = \theta$

$$\frac{1}{2}\frac{d}{dt}\|\theta\|^2 + \|\nabla\theta\|^2 + \gamma\|\Delta\theta\|^2 = -(\rho_t, \theta) \leq c\|\rho_t\|\|\theta\|.$$

Thus

$$\begin{aligned}
\frac{1}{2}\frac{d}{dt}\|\theta\|^2 &\leq c\|\rho_t\|\|\theta\| \\
(\theta^2)^{\frac{1}{2}}\frac{d}{dt}\left(\|\theta\|^2\right)^{\frac{1}{2}} &\leq c\|\rho_t\|\|\theta\|.
\end{aligned}$$

After integrating and multiplying by γ

$$\gamma\|\theta(t)\| \leq \gamma\|\theta(0)\| + \gamma\int_0^t \|\rho_t\| ds. \tag{4.12}$$

For $\gamma < 1$, since $\gamma\|\rho\| \leq ch^r\|u\|_r$, we have

$$\begin{aligned}
\gamma\|\theta(0)\| &\leq \|v_h - R_h v\| \\
&\leq \gamma\|v_h - v\| + \gamma\|R_h v - v\| \\
&\leq \gamma\|v_h - v\| + ch^r\|v\|_r.
\end{aligned}$$

And we already know that

$$\gamma\|\rho_t\| = \gamma\|R_h u_t - u_t\| \leq ch^r\|u_t\|_r.$$

Then together with (4.9) and (4.12)

$$\begin{aligned}
\gamma\|\rho(t)\| &\leq ch^r\left(\|v\|_r + \int_0^t \|u_t\|_r ds\right) \\
\gamma\|\theta(t)\| &\leq \gamma\|v_h - v\| + ch^r\|v\|_r + ch^r\int_0^t \|u_t\|_r ds.
\end{aligned}$$

Hence the semi-discrete error when $\gamma < 1$ is

$$\gamma\|u_h(t) - u(t)\| \leq \|v_h - v\| + ch^r \left(\|v\|_r + ch^r \int_0^t \|u_t\|_r ds \right), \quad \text{for } 3 \leq r \leq 6.$$

Similarly for $\gamma > 1$ we have

$$\|u_h(t) - u(t)\| \leq \|v_h - v\| + ch^r \left(\|v\|_r + ch^r \int_0^t \|u_t\|_r ds \right), \quad \text{for } 3 \leq r \leq 6.$$

4.1.2 Completely Discrete Schemes

In complete discrete approximation of the solution of EFK equation we discretize the problem in both spatial and time variables. The time discretization is accomplished by a finite difference approximation of the time derivative. Let k be the time step and U^n be the approximations in V_h of $u(t)$, at $t = t_n = nk$. Set $w^n = w(t_n)$ for generic function w of time. The backward Euler method is defined by replacing the time derivative of the semidiscrete version (4.2) by

$$\bar{\partial}U^n = \frac{U^n - U^{n-1}}{k}.$$

That is: Find $U^n \in S_h$, $n \geq 1$, such that

$$\begin{aligned} (\bar{\partial}U^n, \chi) + \gamma(\Delta U^n, \Delta\chi) + (\nabla U^n, \nabla\chi) &= (f(U^n), \chi) \quad \forall \chi \in S_h \\ (U^0, \chi) &= (c, \chi). \end{aligned} \tag{4.13}$$

As in (4.2), (4.13) can be expressed in the matrix form

$$\begin{aligned} (\mathbf{M} + k(\gamma\mathbf{A} + \mathbf{B}))\, \mathbf{a}^n &= \mathbf{B}\mathbf{a}^{n-1} + k\mathbf{f} \\ \mathbf{M}\mathbf{a}^n &= \mathbf{v} \end{aligned}$$

where

$$U^n = \sum_{j=1}^{m} a_j^n \psi_j^n$$

and

$$\mathbf{a}^n = (a_1^n, a_2^n, \ldots, a_m^n)^T .$$

As in the semi-discrete scheme, we split the error and define

$$\begin{aligned} U^n - u(t_n) &= (U^n - R_h u(t_n)) + (R_h u(t_n) - u(t_n)) \\ &= \theta^n + \rho^n. \end{aligned}$$

Similar to (4.9) and (4.10) we can write

$$\begin{aligned} \gamma\rho^n &\leq ch^r \|u(t^n)\|_r, \quad \text{for } \gamma < 1, \\ \rho^n &\leq ch^r \|u(t^n)\|_r, \quad \text{for } \gamma \geq 1. \end{aligned}$$

In analogy with (4.11) we have

$$(\bar{\partial}\theta^n, \chi) + \gamma(\Delta\theta^n, \Delta\chi) + (\nabla\theta^n, \nabla\chi) = -(\omega^n, \chi), \quad \forall \chi \in V_h, \quad n > 0, \tag{4.14}$$

where

$$\begin{aligned} \omega^n &= R_h \bar{\partial} u(t_n) - u_t(t_n) \\ &= (R_h - I)\bar{\partial} u(t_n) + (\bar{\partial} u(t_n) - u_t(t_n)), \end{aligned}$$

and define

$$\begin{aligned} \omega_1^n &= R_h \bar{\partial} u(t_n) - \bar{\partial} u(t_n), \\ \omega_2^n &= \bar{\partial} u(t_n) - u_t(t_n). \end{aligned}$$

Letting $\chi = \theta^n$ on (4.14), we have

$$(\bar{\partial}\theta^n, \theta^n) = \left(\frac{\theta^n - \theta^{n-1}}{k}, \theta^n\right) \leq \|\omega^n\| \|\theta^n\|.$$

That is

$$\begin{aligned} \|\theta^n\|^2 - (\theta^{n-1}, \theta^n) &\leq k\|\omega^n\| \|\theta^n\| \\ \|\theta^n\| &\leq \|\theta^{n-1}\| + k\|\omega^n\|. \end{aligned}$$

Using above inequality repeatedly

$$\begin{aligned} \|\theta^n\| &\leq \|\theta^0\| + k\sum_{j=1}^{n} \|\omega^j\| \\ &\leq \|\theta^0\| + k\sum_{j=1}^{n} \|\omega_1^j\| + k\sum_{j=1}^{n} \|\omega_2^j\|, \end{aligned}$$

here it is clear that $\theta^0 = \theta(0)$. Then

$$\omega_1^j = (R_h - I)k^{-1}\int_{t_{j-1}}^{t_j} u_t ds = k^{-1}\int_{t_{j-1}}^{t_j} (R_h - I)u_t ds,$$

and using boundedness of ρ^n, we can obtain

$$\begin{aligned} \gamma k\sum_{j=1}^{n} \|\omega_1^j\| &\leq \sum_{j=1}^{n}\int_{t_{j-1}}^{t_j} ch^r\|u_t\|_r ds = ch^r\int_0^{t_n} \|u_t\|_r ds \quad \text{for } \gamma < 1, \\ k\sum_{j=1}^{n} \|\omega_1^j\| &\leq \sum_{j=1}^{n}\int_{t_{j-1}}^{t_j} ch^r\|u_t\|_r ds = ch^r\int_0^{t_n} \|u_t\|_r ds \quad \text{for } \gamma \geq 1. \end{aligned}$$

Moreover

$$k\omega_2^j = u(t_j) - u(t_{j-1}) - ku_t(t_j) = -\int_{t_{j-1}}^{t_j} (s - t_{j-1})u_{tt}(s)ds,$$

so that

$$k\sum_{j=1}^{n}\|\omega_2^j\| \le \sum_{j=1}^{n}\left\|\int_{t_{j-1}}^{t_j}(s-t_{j-1})u_{tt}(s)ds\right\| \le k\int_0^{t_n}\|u_{tt}\|ds.$$

Together, for $\gamma < 1$ we can estimate,

$$\begin{aligned}\gamma\|U^n-u(t_n)\| &\le \gamma\theta(0)+\gamma k\sum_{j=1}^{k}\|\omega_1^j\|+\gamma k\sum_{j=1}^{k}\|\omega_2^j\|+\gamma\rho^n \\ &\le \gamma\|v_h-v\|+ch^r\int_0^{t_n}\|u_t\|_r ds+\gamma k\int_0^{t_n}\|u_{tt}\|ds+ch^r\left(\|v\|_r+\int_0^{t_n}\|u_t\|_r ds\right).\end{aligned}$$

Hence when $\gamma < 1$ the complete discrete error with backward Euler method, if $\gamma\|v_h - v\| \le Ch^r\|v\|_r$ is

$$\gamma\|U^n-u(t_n)\| \le Ch^r\left(\|v\|_r+\int_0^{t_n}\|u_t\|_r ds\right)+k\int_0^{t_n}\|u_{tt}\|ds,$$

and similarly for $\gamma \ge 1$ we have

$$\|U^n-u(t_n)\| \le Ch^r\left(\|v\|_r+\int_0^{t_n}\|u_t\|_r ds\right)+k\int_0^{t_n}\|u_{tt}\|ds.$$

Note that backward Euler method is of order $O(h^r+k)$. It is only first order in k. We therefore now turn to the backward difference method. We can obtain second order accuracy in the discretization in time if we approximate the time derivative in the differential equation by a second order backward difference quotient. Let

$$\bar{D}U^n = \bar{\partial}U^n+\frac{1}{2}k\bar{\partial}^2U^n = \frac{1}{k}\left(\frac{3}{2}U^n-2U^{n-1}+\frac{1}{2}U^{n-2}\right).$$

Then we define the discrete problem in two steps, when $n \geq 2$ and $n = 1$. That is, find $U^n \in V_h$ such that

$$\begin{aligned} (\bar{D}U^n, \chi) + \gamma(\Delta U^n, \Delta\chi) + (\nabla U^n, \nabla\chi) &= (f, \chi), \quad \forall\chi \in V_h, n \geq 2, \\ (\bar{\partial}U^1, \chi) + \gamma(\Delta U^1, \Delta\chi) + (\nabla U^n, \nabla\chi) &= (f, \chi), \quad \forall\chi \in V_h, n = 1, \\ (U^n, \chi) &= (v, \chi). \end{aligned} \tag{4.15}$$

The linear system for (4.15) is

$$\left(\frac{3}{2}\mathbf{M} + k(\gamma\mathbf{A} + \mathbf{B})\right)\mathbf{a}^n = 2\mathbf{M}\mathbf{a}^{n-1} - \frac{1}{2}\mathbf{M}\mathbf{a}^{n-2} + k\mathbf{f}^n \quad n \geq 2.$$

Writing again $U^n - u^n = \theta^n + \rho^n$ we only need to bound θ^n. As before we can show that θ^n satisfies

$$\begin{aligned} (\bar{D}\theta^n, \chi) + \gamma(\Delta\theta^n, \Delta\chi) + (\nabla\theta^n, \nabla\chi) &= -(\omega^n, \chi), \quad \text{for } n \geq 2, \\ (\bar{\partial}\theta^1, \chi) + \gamma(\Delta\theta^1, \Delta\chi) + (\nabla\theta^1, \nabla\chi) &= -(\omega^1, \chi), \end{aligned}$$

where

$$\begin{aligned} \omega^n &= \bar{D}R_h u^n - u_t^n = (R_h - I)\bar{D}u^n + (\bar{D}u^n - u_t^n) = \omega_1^n + \omega_2^n, \quad n \geq 1, \\ \omega^1 &= (R_h - I)\bar{\partial}u^1 + (\bar{\partial}u^1 - u_t^1) = \omega_1^1 + \omega_2^1. \end{aligned}$$

It is shown in [29] page 19, that

$$\|\theta^n\| \leq \|\theta^0\| + 2k\sum_{j=2}^{n}\|\omega^j\| + \frac{5}{2}k\|\omega^1\|, \quad \text{for } n \geq 1.$$

Now we can bound ω_1^j and ω_2^j. Using Taylor expansion as before we can find

$$\begin{aligned} k\|\omega_1^j\| &\leq Ch^r k\|\bar{D}u^j\|_r \leq Ch^r \int_{t_{j-2}}^{t_j} \|u_t\|_r ds, \\ k\|\omega_2^j\| &\leq Ck^2 \int_{t_{j-2}}^{t_j} \|u_{ttt}\| ds. \end{aligned}$$

As for the backward Euler method we have

$$k\|\omega_1^1\| + k\|\omega_2^1\| \leq Ch^r \int_0^k \|u_t\|_r ds + k \int_0^k \|u_{tt}\| ds,$$

then together for $\gamma < 1$ we can estimate the complete discrete error, if $\|v_h - v\| \leq ch^r\|v\|_r$ as

$$\begin{aligned} \gamma\|U^n - u^n\| \leq Ch^r &\left(\|v\|_r + \int_r^{t_n} \|u_t\|_r ds\right) \\ &+ Ck \int_0^k \|u_{tt}\| ds + Ck^2 \int_0^{t_n} \|u_{ttt}\| ds, \quad \text{for } n \geq 0,\, 3 \leq r \leq 6. \end{aligned}$$

Similarly for $\gamma \geq 1$, we have

$$\begin{aligned} \|U^n - u^n\| \leq Ch^r &\left(\|v\|_r + \int_r^{t_n} \|u_t\|_r ds\right) \\ &+ Ck \int_0^k \|u_{tt}\| ds + Ck^2 \int_0^{t_n} \|u_{ttt}\| ds, \quad \text{for } n \geq 0,\, 3 \leq r \leq 6. \end{aligned}$$

Therefore we have $O(h^r + k^2)$ error estimate.

CHAPTER 5

Long Time Error Analysis

In this chapter we study the *a priori* error estimates, considering the exact error propagation. In the first section we establish global existence and some bounds for the solution and its first and second derivatives. In the second section we introduce the concept of smoothing indicator. In the last section we estimate the total error by considering contribution of the error from local and propagation errors.

5.1 Existence, Uniqueness, and Stability

In order to study the long time error, we need the global existence, uniqueness and stability of the EFK equation. We start with the weak formulation of the EFK equation: Find $u(.,t) \in H_0^2(\Omega)$, $t \in (0,T]$, such that

$$\begin{aligned} (u_t,\chi) + \gamma(\Delta u, \Delta\chi) + (\nabla u, \nabla\chi) &= (f(u),\chi), \qquad (5.1)\\ u(0) &= u_0, \end{aligned}$$

for all $\chi \in H_0^2$, where $f(u) = u - u^3$. For the convenience of the error propagation analysis we use the notation of a dynamical system for the solution of equation (5.1). That is, $u(p,t,v)$ stands for the value of the solution of equation (5.1) at the time $t+p$ with initial time

t, initial value v of $H_0^2(\Omega)$, and time increment p. With this relation it is also clear that $u(p+r,t,v) = u(p,t+r,u(r,t,v))$, which is well known semigroup property.

The global existence and uniqueness result is established in [4] by Danumjaya and Panni. We include this result for convenience.

Theorem 5.1 *Let $u_0 \in H_0^2(\Omega)$. For any $T > 0$, there exists a unique $u = u(x,t)$ in $\Omega \times [0,T)$ with $u \in L^\infty(0,T;H_0^2(\Omega))$ and $u_t \in L^\infty(0,T;L_0^2(\Omega))$, such that u satisfies the initial condition $u(0) = u_0$ and equation (5.1).*

Then we show local stability of the boundary value problem, which will be useful later in this chapter.

Theorem 5.2 *Let $\tilde{\mathcal{B}}$ be a bounded subset of $H_0^2(\Omega)$. If the EFK equations*

$$\begin{aligned} u_t + \gamma\Delta^2 u - \Delta u &= f(u), \qquad & u(t_0) &= u_0, \\ v_t + \gamma\Delta^2 v - \Delta v &= f(v), \qquad & v(t_0) &= v_0, \end{aligned}$$

are satisfied for all u and v in $\tilde{\mathcal{B}}$ then

$$\|u(t) - v(t)\| \leq \exp(m(t-t_0))\|u_0 - v_0\|.$$

Proof: Consider the Lyapunov functional $\mathcal{L}(u)$ as

$$\mathcal{L}(u) = \int_\Omega \left\{ \frac{\gamma}{2}|\Delta u|^2 + \frac{1}{2}|\nabla u|^2 + F(u) \right\} dx \tag{5.2}$$

where $F(u) = \frac{1}{4}(u^2-1)^2$, and note that $F' = -f$. Differentiate the Lyapunov functional with respect to t, we get

$$\frac{d}{dt}\mathcal{L}(u) = \gamma(\Delta u, \Delta u_t) + (\nabla u, \nabla u_t) + (F'(u), u_t).$$

Setting $\chi = u_t$ in (5.1), we obtain

$$\gamma(\Delta u, \Delta u_t) + (\nabla u, \nabla u_t) - (f(u), u_t) = -\|u_t\|^2.$$

From above two equations, we find that

$$\frac{d}{dt}\mathcal{L}(u) = -\|u_t\|^2 \leq 0,$$

and hence $\mathcal{L}(u) \leq \mathcal{L}(u_0)$. Using the definition of $\mathcal{L}(.)$ with elliptic regularity $\gamma\|\Delta u\|_2 + \|u\|_2 \leq \|f(u)\|$, it follows that

$$\begin{aligned}
\int_\Omega \left(\frac{\gamma}{2}|\Delta u|^2 + \frac{1}{2}|\nabla u|^2 + F(u)\right) d\Omega &\leq \int_\Omega \left(\frac{\gamma}{2}|\Delta u_0|^2 + \frac{1}{2}|\nabla u_0|^2 + F(u_0)\right) d\Omega \\
&\leq \frac{1}{2}\|f(u_0)\|^2 + \int_\Omega F(u_0) d\Omega \\
&\leq C_{u_0}.
\end{aligned}$$

Thus $\|u\|_1^2 \leq C_{u_0}$. Since Ω is bounded convex domain in $\mathbb{R}^2$, by Sobolev embedding theorem $\|u\|_{L^p} \leq C\|u\|_1 \leq C_{u_0}$. Now because $u, v \in \tilde{\mathcal{B}} \subset H_0^1(\Omega)$,

$$(u_t - v_t, u - v) + \gamma\|\Delta(u - v)\|^2 + \|\nabla(u - v)\|^2 = (f(u) - f(v), u - v).$$

Also we have

$$\begin{aligned}
\frac{1}{2}\frac{d}{dt}\|u - v\|^2 &\leq (f(u) - f(v), u - v) \\
&= (u - u^3 - (v - v^3), u - v) \\
&= C\|u - v\|^2.
\end{aligned}$$

That is

$$\frac{d}{dt}\|u - v\| \leq C\|u - v\|,$$

where C is a constant depend only on u_0 and v_0. This implies

$$e^{-mt}\|u(t)-v(t)\| \le e^{-mt_0}\|u(t_0)-v(t_0)\|,$$

and the required result. ■

5.2 Stability and Smoothing Indicator

In the proof of the error analysis of discretized space, we split the error between a solution of the weak formulation (5.1) and numerical schemes (semi-discrete and complete discrete). In each of them, how well we can control the local error over the time period of length p , which depends on the numerical solution of the previous step. So it is crucial to monitor the stability and the smoothing behavior of the numerical scheme. To this end we define stability-smoothing indicator as proposed in [26], which is computed from numerical scheme. For the numerical solution of the complete discrete form we use the notation $u_N(t)$. However in error analysis we will write the numerical solution as $u_N(p,t,v)$ mimicking the notation we used in the previous section. In $u_N(p,t,v)$, t is the initial time, v is the initial value at time t, and p is the time increment. It is easy to see the semi-group property $u_N(p+r,t,v) = u_N(p,t+r,u_N(r,t,v))$ holds. Similarly, we use the notation $u_h(p,t,v)$ for semi-discrete solution with initial time t, initial value v and time increment p. Again for the semi-discrete solution we can verify semi-group property $u_h(p+r,t,v) = u_h(p,t+r,u_h(r,t,v))$. For the proofs of the next two theorems and definition, we need to introduce discrete Laplace operator $\Delta_h : H_0^1(\Omega) \to V_h$ defined by $(\Delta_h u, v) = -(\nabla u, \nabla v)$, $\forall v \in V_h$, and discrete bi-harmonic operator $\Delta_h^2 : H_0^2(\Omega) \to V_h$ defined by $(\Delta_h^2 u, v) = -(\Delta u, \Delta v)$, $\forall v \in V_h$, where V_h is finite element space. Moreover the L_2 projection operator $P_h : L^2(\Omega) \to V_h$ defined by $(P_h u, v) = (u, v)$, for all $v \in V_h$.

Now let $v_h = \frac{du_h}{dp}$, $w_h = \frac{d^2u_h}{dp^2}$. From (5.1) it is easy to verify that u_h, v_h and w_h satisfy

$$\begin{aligned}
\left(\frac{\partial u_h}{\partial p}, z_0\right) + \gamma(\Delta u_h, \Delta z_0) + (\nabla u_h, \nabla z_0) &= (f(u_h), z_0), && (5.3)\\
\left(\frac{\partial v_h}{\partial p}, z_1\right) + \gamma(\Delta v_h, \Delta z_1) + (\nabla v_h, \nabla z_1) &= (f'(u_h)v_h, z_1), && (5.4)\\
\left(\frac{\partial w_h}{\partial p}, z_2\right) + \gamma(\Delta w_h, \Delta z_2) + (\nabla w_h, \nabla z_2) &= (f'(u_h)w_h + f''(u_h)v_h^2, z_2), && (5.5)
\end{aligned}$$

for all z_0, z_1 and z_2 in V_h. Furthermore, for any initial value $\bar{u}$ of (5.3) we can define initial values of (5.4) and (5.5) as

$$\begin{aligned}
\bar{v} &= -\Delta^2\bar{u} + \Delta\bar{u} + f(\bar{u}),\\
\bar{w} &= -\Delta^2\bar{v} + \Delta\bar{v} + f'(\bar{u})\bar{v}.
\end{aligned}$$

Theorem 5.3 *Let u_h be a solution of (5.3). Then there exists positive constant $C_{\bar{u}}$ depends only on $\bar{u}$ such that*

1. $\gamma\|u_h\|_2 \le C_{\bar{u}}$.

2. $\|u_h\|_1 \le C_{\bar{u}}$.

3. $\|u_h\|_{L^p} \le C_{\bar{u}}$.

Proof: Define the Lyapunov functional $\mathcal{L}(\chi)$ such that

$$\mathcal{L}(\chi) = \int_\Omega \left(\frac{\gamma}{2}|\Delta\chi|^2 + \frac{1}{2}|\nabla\chi|^2 + F(\chi)\right) d\Omega,$$

where $F(\chi) = \frac{1}{4}(\chi^2 - 1)^2 \ge 0$ and $F' = -f$. Setting $z_0 = \frac{du_h}{dp} = v_h$ on (5.3) we have

$$\|v_h\|^2 + \gamma(\Delta u_h, \Delta v_h) + (\nabla u_h, \nabla v_h) = (f(u_h), v_h),$$

and

$$\frac{d}{dp}\mathcal{L}(u_h) = \gamma(\Delta u_h, \Delta v_h) + (\nabla u_h, \nabla v_h) + (F'(u_h), v_h) = -\|v_h\|^2.$$

That is

$$\frac{d}{dp}\mathcal{L}(u_h) = -\|v_h\|^2 \leq 0.$$

Thus $\mathcal{L}(u_h) \leq \mathcal{L}(\bar{u})$. Then

$$\begin{aligned}
\int_\Omega \left(\frac{\gamma}{2}|\Delta u_h|^2 + \frac{1}{2}|\nabla u_h|^2 + F(u_h)\right) d\Omega &\leq \int_\Omega \left(\frac{\gamma}{2}|\Delta \bar{u}|^2 + \frac{1}{2}|\nabla \bar{u}|^2 + F(\bar{u})\right) d\Omega \\
&\leq \frac{1}{2}\|f(\bar{u})\|^2 + \int_\Omega F(\bar{u}) d\Omega \\
&\leq C_{\bar{u}}.
\end{aligned}$$

Since $F(u_h) \geq 0$, using Poincaré inequality, we arrive at

$$\gamma\|u_h\|_2 \leq C_{\bar{u}}, \tag{5.6}$$

$$\|u_h\|_1 \leq C_{\bar{u}}. \tag{5.7}$$

Since $\Omega \subset \mathbb{R}^2$, Sobolev embedding theorem gives us $\|u_h\|_{L^p} \leq C\|u_h\|_1 \leq C_{\bar{u}}$. ■

Note: Integrating both sides of $\frac{d}{dp}\mathcal{L}u_h + \|v_h\|^2 = 0$ and using the fact that $\mathcal{L}(\bar{u}) > \mathcal{L}(u_h)$, we have

$$\begin{aligned}
\int_t^{t+p} \|v_h(s)\|^2 ds &= \mathcal{L}(\bar{u}) - \mathcal{L}(u_h) \\
&\leq \mathcal{L}(\bar{u}) \\
&\leq C_{\bar{u}}. \qquad (5.8)
\end{aligned}$$

Next theorem is crucial for the estimation of the error, resulting from the discretization of time.

Theorem 5.4 *For any initial value $\bar{u} \in V_h$, if*

$$\begin{aligned}\bar{v} &= -\Delta_h^2 \bar{u} + \Delta_h \bar{u} + P_h f(\bar{u}), \\ \bar{w} &= -\Delta_h^2 \bar{v} + \Delta_h \bar{v} + P_h f'(\bar{u}) \bar{v},\end{aligned}$$

and there is a constant $\bar{C}$ such that $\|\bar{u}\|_2 \leq \bar{C}$, $\|\bar{v}\| \leq \bar{C}$, $\|\bar{w}\| \leq \bar{C}$, then the corresponding semi-discrete solution $u_h(p, t, \bar{u})$ satisfies

$$\left\| \frac{\partial^2}{\partial p^2} u_h(p, t, v) \right\| \leq C_0 + C_1 \|\bar{u}\| + C_2 \|\bar{v}\| + C_3 \|\bar{w}\|,$$

for sufficiently small p and some constants C_0, C_1, C_2 and C_3.

Proof: Since Ω is in $\mathbb{R}^2$ and u_h is in $H_0^2(\Omega) \subset H_0^1(\Omega)$, by Sobolov inequality we have $\|u_h\|_{L^p} \leq C\|u_h\|_1$, for $1 \leq p < \infty$. And Holder's inequality for $\frac{1}{r} = \frac{1}{p} + \frac{1}{q}$ is given by $\left(\int_\Omega |ab|^r d\Omega\right)^{1/r} \leq \|a\|_{L^p} \|b\|_{L^q}$. We start by showing bounds for $\|f'(u_h) v_h\|$ and $|\left(f'(u_h) w_h + f''(u_h) u_h^2, w_h\right)|$, where $f(u) = u - u^3$.

$$\begin{aligned}\|f'(u_h) v_h\|^2 &= \|(1 - 3u_h^2) v_h\|^2 \\ &\leq \|v_h\|^2 + 9\|u_h^2 v_h\|^2 \\ &\leq \|v_h\|^2 + 9\|u_h^2\|_{L^4}^2 \|v_h\|_{L^4}^2 \\ &\leq \|v_h\|^2 + 9\|u_h\|_{L^8}^4 \|v_h\|_{L^4}^2 \\ &\leq C\|v_h\|_1^2 + C\|u_h\|_1^4 \|v_h\|_1^2.\end{aligned}$$

That is from from previous theorem,

$$\|f'(u_h) v_h\|^2 \leq C\left(1 + \|u_h\|_1^4\right) \|v_h\|_1^2 \leq C_{\bar{u}} \|v_h\|_1^2. \tag{5.9}$$

Similarly because $(u_h^2 w_h, w_h) = \|u_h w_h\| > 0$

$$
\begin{aligned}
\big(f'(u_h)w_h + f''(u_h)v_h^2, w_h\big) &= \big((1-3u_h^2)w_h + (-6u_h)v_h^2, w_h\big) \\
&= \big(1-3u_h^2)w_h, w_h\big) - \big(6u_h v_h^2, w_h\big) \\
&= (w_h, w_h) - 3(u_h^2 w_h, w_h) - 6(u_h v_h^2, w_h) \\
&\leq \|w_h\|^2 + 6|(u_h v_h^2, w_h)| \\
&\leq \|w_h\|^2 + 3\|u_h v_h^2\|^2 + 3\|w_h\|^2.
\end{aligned}
$$

Then by Holder's and Sobolov inequality and Theorem 5.3, as before

$$
\begin{aligned}
|\,\big(f'(u_h)w_h + f''(u_h)u_h^2, w_h\big)\,| &\leq C\|w_h\|^2 + C\|u_h\|_{L^4}^2\|v_h\|_{L^8}^4 \\
&\leq C\|w_h\|^2 + C\|u_h\|_1^2\|v_h\|_1^4. \qquad (5.10) \\
&\leq C_{\bar{u}}(\|w_h\|^2 + \|v_h\|_1^4). \qquad (5.11)
\end{aligned}
$$

Now choosing $z_1 = w_h$ on (5.4), we obtain

$$
\begin{aligned}
\|w_h\|^2 + \frac{\gamma}{2}\frac{d}{dp}\|\Delta v_h\|^2 + \frac{1}{2}\frac{d}{dp}\|\nabla v_h\|^2 &= (f'(u_h)v_h, w_h) \\
&\leq \frac{1}{2}\|f'(u_h)v_h\|^2 + \frac{1}{2}\|w_h\|^2 \\
&\leq C_{\bar{u}}\|v_h\|_1^2 + \frac{1}{2}\|w_h\|^2,
\end{aligned}
$$

and hence

$$
\|w_h\|^2 + \gamma\frac{d}{dp}\|\Delta v_h\|^2 + \frac{d}{dp}\|\nabla v_h\|^2 \leq C_{\bar{u}}\|v_h\|_1^2.
$$

Integrating both sides with respect to t, then (5.9) and elliptic regularity $\gamma\|\Delta_h \bar{v}\|^2 + \|\nabla_h \bar{v}\|^2 \leq$

$\|P_h f(\bar{u})\bar{v}\|^2$ yield

$$\begin{aligned}
\int_t^{t+p} \|w_h\|^2 ds + \gamma\|\Delta v_h\|^2 + \|\nabla v_h\|^2 &\leq C_{\bar{u}} \int_t^{t+p} \|v_h\|_1^2 ds + \gamma\|\Delta_h \bar{v}\|^2 + \|\nabla_h \bar{v}\|^2 \\
&\leq C_{\bar{u}} \int_t^{t+p} \|v_h\|_1^2 ds + \|P_h f(\bar{u})\bar{v}\|^2 \\
&\leq C_{\bar{u}} \int_t^{t+p} \|v_h\|_1^2 ds + C_{\bar{u}}\|\bar{v}\|_1^2. \qquad (5.12)
\end{aligned}$$

We now evaluate $\|\bar{v}\|_1$ and $\int_t^p \|v_h\|_1^2 ds$. A use of (5.4) gives us,

$$\begin{aligned}
\gamma\|\Delta\bar{v}\|^2 + \|\nabla\bar{v}\|^2 &= -(\bar{w}, \bar{v}) + (f'(\bar{u})\bar{v}, \bar{v}) \\
&\leq C\|\bar{w}\|\|\bar{v}\| + \big((1-3\bar{u}^2)\bar{v}, \bar{v}\big) \\
&\leq C\|\bar{w}\|\|\bar{v}\| + \|\bar{v}\|^2 - 9\|\bar{u}\bar{v}\|^2 \\
&\leq C\left(\|\bar{w}\| + \|\bar{v}\|^2\right)\|\bar{v}\|_1.
\end{aligned}$$

Thus

$$\|\bar{v}\|_1 \leq C\|\bar{w}\| + \|\bar{v}\|. \qquad (5.13)$$

Again choosing $z_1 = v_h$ of (5.4), Similarly,

$$\begin{aligned}
(w_h, v_h) + \gamma\|\Delta v_h\|^2 + \|\nabla v_h\|^2 &= (f'(u_h)v_h, v_h) \\
\frac{1}{2}\frac{d}{dp}\|v_h\|^2 + \gamma\|\Delta v_h\|^2 + \|\nabla v_h\|^2 &= \big((1-3u_h^2)v_h, v_h\big) \\
&\leq \|v_h\|^2.
\end{aligned}$$

So then integrating both sides with respect to t and from (5.8) we obtain

$$\int_t^{t+p} \|v_h\|_1^2 ds \leq 2\int_t^{t+p} \|v_h\|^2 ds + \|\bar{v}\|^2 \leq C_{\bar{u}} + \|\bar{v}\|^2. \qquad (5.14)$$

Together with inequalities (5.12), (5.13) and (5.14) we can write,

$$\begin{aligned}\int_t^{t+p} \|w_h\|^2 ds &\leq C_{\bar{u}} \left(\|\bar{w}\|^2 + \|\bar{v}\|^2 + \int_t^{t+p} \|v_h\|_1^2 ds \right) \\ &\leq C_{\bar{u}} + 2\|\bar{v}\|^2 + \|\bar{w}\|^2. \end{aligned} \tag{5.15}$$

Similarly from (5.12),

$$\|v_h\|_1^2 \leq C_{\bar{u}} + \|\bar{v}\|^2 + \|\bar{w}\|^2. \tag{5.16}$$

Finally setting $z_2 = w_h$ on (5.5), we have

$$\frac{1}{2}\frac{d}{dp}\|w_h\|^2 + \gamma\|\Delta w_h\|^2 + \|\nabla w_h\|^2 = \left(f'(u_h)w_h + f''(u_h)v_h^2, w_h\right).$$

Thus from (5.11) and (5.16),

$$\begin{aligned}\frac{1}{2}\frac{d}{dp}\|w_h\|^2 &\leq C_{\bar{u}}(\|w_h\|^2 + \|v_h\|_1^4) \\ &\leq C_{\bar{u}}(\|w_h\|^2 + C_{\bar{u}}\left(C_{\bar{u}} + 2\|\bar{v}\|^2 + \|\bar{w}\|^2\right)\|v_h\|_1^2).\end{aligned}$$

Now integrating both sides of the above inequality with (5.15),

$$\begin{aligned}\|w_h\|^2 &\leq 8\int_t^{t+p} \|w_h\|^2 ds + \|\bar{w}\| + C_{\|\bar{u}\|}\left(C_{\|\bar{u}\|} + 2\|\bar{v}\|^2 + \|\bar{w}\|^2\right)\int_t^{t+p} \|v_h\|_1^2 ds \\ &\leq C_{\|\bar{u}\|} + 9\|\bar{w}\|^2 + 2\|\bar{v}\|^2 + C_{\|\bar{u}\|}\left(C_{\|\bar{u}\|} + 2\|\bar{v}\|^2 + \|\bar{w}\|^2\right)\left(C_{\|\bar{u}\|} + \|\bar{v}\|^2\right).\end{aligned}$$

Hence we have the required inequality

$$\|w_h\| \leq C_0 + C_1\|\bar{u}\| + C_2\|\bar{v}\| + C_3\|\bar{w}\|. \qquad \blacksquare$$

Based on above theorem we define the following stability and moving indicator.

Definition 5.5 *For each t_i of the $t_i = t_0 + i\tau$ and the value of the numerical solution at t_i,*

$\bar{u} = u_N(t_i),$ *let*

$$\begin{aligned}\bar{v} &= \Delta_h \bar{u} - \gamma \Delta_h^2 \bar{u} + P_h \dot{f}(\bar{u}), \\ \bar{w} &= \Delta_h \bar{v} - \gamma \Delta_h^2 \bar{v} + P_h \ddot{f}(\bar{u}) \bar{v},\end{aligned}$$

and let

$$S_i^2 = \left(\|\bar{u}\|_2, \|\bar{v}\|, \|\bar{w}\|, \|\gamma \Delta_h^2 \bar{u} + \Delta_h \bar{u}\| \right).$$

We call the sequence $\{S_i | i \geq 0\}$ *the stability and smoothing indicator.*

5.3 The Error Estimation Theorem

Theorem 5.6 *Assume that*

1. $u_N(t)$ *is numerical solution of equation (5.1), computed with a finite element method described in chapter 3 and the discretization in time is consistent to the differential equation with a local error of order* $q = 2$ *or* 3.

2. *There is a moving attractor* $\mathcal{M}$ *for equation (5.1)*

$$d(u(s,t,v), M_{t+s}) \leq \theta_s d(v, M_t)$$

   for all $t > t_0$.

3. *The time step size* τ *chosen so that* s *is a multiple of* $\tau : s = k\tau$ *for a positive integer* k.

4. *Stability-smoothing indicator remains bounded.*

Then we have following global error estimate. For any node of the form $t_0 + ns$ *from* t_0 *to* ∞*, when* $\gamma < 1$

$$d\left(\mathcal{M}, u_N(ns, t_0, u_N(t_0))\right) \leq C\frac{se^{m^+s}\tau^{q-1}S_M^q + e^{m^+s}h^2S_H^2 + C_{\|u_N(t_0)\|_4}}{\gamma(1+\theta_s)} + \theta_s^n d(M_{t_0}, u_N(t_0)),$$

when $\gamma \geq 1$*,*

$$d\left(\mathcal{M}, u_N(ns, t_0, u_N(t_0))\right) \leq C\frac{se^{m^+s}\tau^{q-1}S_M^q + e^{m^+s}h^2S_H^2}{1+\theta_s} + \theta_s^n d(M_{t_0}, u_N(t_0)),$$

where $m^+ = \max\{0, m\}$*, and*

$$\begin{aligned} S_M^q &= C_M + \sum_{j=0}^{q} C_j \max_i S_{ij}^q, \\ S_H^2 &= \max_i \left\|\Delta_h^2 u_N(t_i) - \Delta_h u_N(t_i)\right\|. \end{aligned}$$

Here S_{ij}^q *denotes the jth node component of* S_j^q*.*

Proof. First we consider the case where $\gamma < 1$. For any node $t \leq t_0$ and the value of the numerical solution $u_N(t)$ at t, we consider a function w in $H_0^2(\Omega) \cap H^4(\Omega)$ given by

$$\gamma(\Delta w, \Delta v) + (\nabla w, \nabla v) = \gamma(\Delta_h^2 u_N(t), v) - (\Delta_h u_N(t), v) \tag{5.17}$$

$$= \left(\gamma\Delta_h^2 u_N(t) - \Delta_h u_N(t), v\right), \tag{5.18}$$

for all $v \in H_0^2(\Omega)$. From the regularity of the solution, we knows that

$$\gamma\|w\|_4 + \|w\|_2 \leq \|\gamma\Delta_h^2 u_N(t) - \Delta_h u_N(t)\| \leq S_H^2.$$

If v is restricted in V_h in (5.17) we can obtain

$$\gamma\left(\Delta u_N(t), \Delta v\right) + (\nabla u_N(t), \nabla v) = \gamma\left(\Delta^2 w, v\right) - (\Delta w, v) \qquad \forall v \in V_h,$$

by Greens theorem. Since

$$\gamma\left(\Delta w,\Delta v\right)+\left(\nabla w,\nabla v\right)=\gamma\left(\Delta^{2}w,v\right)-\left(\Delta w,v\right)\qquad\forall v\in H_{0}^{2}(\Omega).$$

We realize that $u_N(t)$ is the Galerkin finite element approximation of the solution w, of above equation. Moreover we have proved in chapter 3 that

$$\gamma\|w-u_N(t)\|\leq ch^{r}\|w\|_{r}. \tag{5.19}$$

We now split the error between the numerical solution of time $t+s$ and the attractor in to five parts

$$\begin{aligned}
d\left(M_{t+s},u_N(s,t,u_N(t))\right) &\leq d(M_{t+s},u(s,t,u_N(t))) && (5.20)\\
&+ \|u(s,t,u_N(t))-u(s,t,w)\| && (5.21)\\
&+ \|u(s,t,w)-u_h(s,t,w)\| && (5.22)\\
&+ \|u_h(s,t,w)-u_h(s,t,u_N(t))\| && (5.23)\\
&+ \|u_h(s,t,u_N(t))-u_N(s,t,u_N(t))\|. && (5.24)
\end{aligned}$$

Since $\mathcal{M}$ is a moving attractor, the distance in (5.20) can estimated by

$$d(M_{t+s},u(s,t,u_N(t)))\leq\theta_{s}d(M_{t},u_N(t)). \tag{5.25}$$

Due to the inequality in theorem 5.2 and (5.19), the difference in (5.21) satisfy

$$\|u(s,t,u_N(t))-u(s,t,w)\|\leq e^{ms}\|u_N(t)-w\|\leq\frac{C}{\gamma}e^{ms}h^{2}\|w\|_{2}. \tag{5.26}$$

For the difference in (5.22), we observe that semi discrete solution (chapter 3), both having

H^2 smooth initial value w, bounded by

$$\|u(s,t,w) - u_h(s,t,w)\| \leq \frac{C}{\gamma} h^2 \|w\|_2. \tag{5.27}$$

Again from the inequality in theorem 5.2 for the semi discrete problem we have, for the difference in (5.23)

$$\|u_h(s,t,w) - u_h(s,t,u_N(t))\| \leq e^{ms}\|w - u_N(t)\| \leq \frac{C}{\gamma} e^{ms} h^2 \|w\|_2. \tag{5.28}$$

The difference in (5.24) is the error in approximating the ODE from time t to $t+s$. Since the local error of the time discretization is of order $q = 2$ or $q = 3$ for each $t_i \in [t, t+s)$, we have

$$\|u_N(\tau, t_i, u_N(t_i) - u_h(\tau, t_i, u_N(t_i)))\| \leq C\tau^q \max_{p\in[0,\tau]} \left\| \frac{\partial^q}{\partial p^q} u_h(p, t_i, u(t_i)) \right\|. \tag{5.29}$$

Based on the stability-smoothing indicator we know that,

$$\max_{p\in[0,\tau]} \left\| \frac{\partial^q}{\partial p^q} u_h(p, t_i, u(t_i)) \right\| \leq S_M^q.$$

Therefore,

$$\begin{aligned}
&\|u_h(\tau, t_i, u_h(t_i) - u_N(\tau, t_i, u_N(t_i)))\| \\
&\leq |u_h(\tau, t_i, u_h(t_i) - u_h(\tau, t_i, u_N(t_i)))\| + \|u_h(\tau, t_i, u_N(t_i) - u_N(\tau, t_i, u_N(t_i)))\| \\
&\leq e^{m\tau}\|u_h(t_i) - u_N(t_i)\| + C\tau^q S_M^q.
\end{aligned} \tag{5.30}$$

Recall that $s = k\tau$ and identify each node $t_i \in [t, t+s]$ with $t + j\tau$ for some $t \geq 0$. By using (5.30) repeatedly, we obtain

$$
\begin{aligned}
&\|u_h(s,t,u_N(t)) - u_N(s,t,u_N(t))\| \\
&= \|u_h(k\tau,t,u_N(t)) - u_N(k\tau,t,u_N(t))\| \\
&\leq \|u_h(\tau,t+k\tau-\tau,u_N(k\tau-\tau,t,u_N(t))) - u_h(\tau,t+k\tau-\tau,u_N(t+k\tau-\tau))\| \\
&+ \|u_h(\tau,t+k\tau-\tau,u_N(t+k\tau-\tau)) - u_N(\tau,t+k\tau-\tau,u_N(t+k\tau-\tau))\| \\
&\leq e^{m\tau}\|u_h((k-1)\tau,t,u_N(t)) - u_N((k-1)\tau,t,u_N(t))\| + C\tau^q S_M^q \\
&\leq \cdots \leq e^{jm\tau}\|u_h((k-j)\tau,t,u_N(t)) - u_N((k-j)\tau,t,u_N(t))\| \\
&+ (1+e^{m\tau}+\cdots+e^{(j-1)m\tau})C\tau^q S_M^q \\
&\leq \cdots \leq (1+e^{m\tau}+\cdots+e^{(k-1)m\tau})C\tau^q S_M^q.
\end{aligned}
$$

if $m \leq 0$,

$$\tau\left(1+e^{m\tau}+\cdots+e^{(k-1)m\tau}\right) \leq k\tau = s.$$

if $m > 0$, by the simple inequality $1 \leq (e^x-1)/x \leq e^x$ for $x > 0$, we know

$$\tau(1+e^{m\tau}+\cdots+e^(k-1)m\tau) = \tau\frac{e^{ms}-1}{e^{m\tau-1}} \leq \frac{e^{ms}-1}{m} = s\frac{e^{ms}-1}{ms} \leq se^{ms}.$$

In either case, we have

$$\|u_h(s,t,u_N(t)) - u_N(s,t,u_N(t))\| \leq C\tau^{q-1}se^{m^+s}S_M^q. \tag{5.31}$$

Now combining the terms (5.20)and (5.21) to (5.24) with (5.25), (5.26),(5.27), (5.28) and (5.31) we get

$$d(M_{t+s},u_N(s,t,u_N(t))) \leq \theta_s d(M_t,u_N(t)) + C(se^{m^+s}\tau^{q-1}S_M^q + \frac{1}{\gamma}e^{m^+s}h^2S_H^2)$$

Now be repeatedly using above inequality,

$$
\begin{aligned}
&d(M_{t_0+ns}, u_N(ns, t_0, u_N(t_0))) \\
&\le d(M_{t_0+(n-1)s+s}, u(s, t_0+(n-1)s, u_N((n-1)s, t_0, u_N(t_0)))) \\
&\quad + \|u(s, t_0+(n-1)s, u_N((n-1)s, t_0, u_N(t_0))) \\
&\qquad - u(s, t_0+(n-1)s, u_N((n-1)s, t_0, u_N(t_0)))\| \\
&\quad + \|u(s, t_0+(n-1)s, u_N((n-1)s, t_0, u_N(t_0))) \\
&\qquad - u_N(s, t_0+(n-1)s, u_N((n-1), t_0, u_N(t_0)))\| \\
&\le \theta_s d(M_{t_0+(n-1)s}, u_N((n-1)s, t_0, u_N(t_0))) + C(se^{m^+s}\tau^{q-1}S_M^q + \gamma^{-1}e^{m^+s}h^2S_H^2) \\
&\le \ldots \le C(1+\theta_s+\ldots+\theta_s^{n-1})(se^{m^+s}\tau^{q-1}S_M^q + \gamma^{-1}e^{m^+s}h^2S_H^2) + \theta_s^n d(M_{t_0}, u_N(t_0)) \\
&\le C\frac{se^{m^+s}\tau^{q-1}S_M^q + \gamma^{-1}e^{m^+s}h^2S_H^2 + C_{\|u_N(t_0)\|_4}}{1+\theta_s} + \theta_s^n d(M_{t_0}, u_N(t_0)).
\end{aligned}
$$

Similarly we can prove for the $\gamma > 1$. ∎

CHAPTER 6

Concluding Remarks

In this chapter, summaries of the main results are presented.

In this dissertation, new results are presented for the long time error estimations for the Hodgkin and Huxley's equation and Extended Fisher-Kolmogorov (EFK) equation. Huxley's equation is a second order parabolic equation and the EFK equation is a fourth order parabolic equation, which has a parameter γ with the fourth order term. We estimate the error using nontraditional but more practical error splitting technique, considering exact error propagation instead of classical numerical error propagation.

Our analysis for the Huxley's equation shows that its solutions are contracted to a traveling wave form locally. Using this local contraction property we show that the exsistance of the evolving attractor, and it is in the form

$$M_t = \{\phi(x - vt - c) | c \in \mathbb{R}\},$$

where $\phi(x - vt)$ is the traveling wave solution of the Hodgken-Huxley equation at time t. This result is very important and it provides an essential foundation for the long time error estimates. This estimate on exact error propagation is actually what makes long time error estimation possible.

This preliminary result allows us to develop a non-traditional method to solve Huxley's equation. Instead of using the stability of the numerical scheme, we compute a smoothing indicator, which allows us to estimate the numerical error. Moreover, with the help of this evolving attractor, we can show that the global error of a numerical solution is uniformly bounded in time.

To solve the EFK equation, we first discretize it in space, with the Agyris finite elements. Using error estimates for the semi-discrete problem, we are able to obtain the estimate for the local error. This local error is proven to be of order $h^2 + \Delta t$. Then we discretize the time, using backward Euler and multi strip methods to find the complete discrete solution. Furthermore, we also compute a smoothing indicator and long time time error estimates for the EFK equation. We note that of all the error bounds for the EFK equation contain a factor, γ^{-1}, which is less useful when γ is small. However, they are better than the existing bounds which grow in a low polynomial order of γ^{-1} [4].

There are several advantages of using exact error propagation and numerical smoothing. Since error propagation is estimated by using evolution equation instead of scheme, we can apply any contraction properties of the dynamical system. The smoothing indicator gives essentially an upper bound of the second time derivative. Knowing this, we can choose the size of the next time step. So the indicator also serves as a tool for adaptive step sizing. Moreover, because the computation of the smoothing indicator at each t_n does not depend on the time discretization, error estimates can be computet regardless of scheme complications.

The main result of the present research is the theoretical foundation for long-time error estimates using exact error propagation and numerical smoothing. Future research in this area may involve study of contraction properties of other PDEs, smoothing indicator for the mixed finite elements, finite volume and other finite element methods, stronger and weaker norm estimates, and applications to hyperbolic problems.

The author believes that present research will help to solve various computational problems more effectively.

BIBLIOGRAPHY

[1] Z. Chen, *Finite Element Methods and Their Applications*, Springer, 2005.

[2] P. G. Ciarlet, *The Finite Element Method for Elliptic Problems*, SIAM, 2002.

[3] J. B. Conway, *A Course in Functional Analysis*, Springer, 2000.

[4] P. Danumjaya and A. K. Pani, *Numerical Methods for the Extended Fisher-Kolmogorov (EFK) Equation,* Int. J. Numer. Anal. Mod. **33** (2006), 186-210.

[5] G. T. W. Dee Van Sarloos, *Bistable Systems with Propagation Fronts Leading to Pattern Formulation,* Phy. Rev. Lett. **60** (1988), 2641-2644.

[6] A. Eden, C. Foias, B. Nicolaenko, and R. Temam, *Exponential Attractors for Dissipative Evolution Equations,* John Wiley & Sons Ltd., 1994.

[7] D. Estep and A. Stuart, *The Rate of Error Growth in the Hamiltonian Conserving Integrators*, Springer, 2005.

[8] J. W. Evans, *Nerve Axon Equation, I: Linear Approximation,* Indiana Univ. Math. J. **21** (1972), 577-593.

[9] J. W. Evans, *Nerve Axon Equation, III: Stability of the Nerve Impulse,* Indiana Univ. Math. J. **22** (1972), 577-593.

[10] B. Garrett and R. Gian-Carlo, *Ordinary Differential Equations*, John Wiley & Sons Ltd., 1989.

[11] J. K. Hale, *Ordinary Differential Equations*, Robert E. Krieger Publishing Company, 1982.

[12] J. Z. Hearon, *Applications of Results from Linear Kinetics to the Hodgkin-Huxley Equations,* Biophys. J. **4** (1964), 65-75.

[13] R. M. Hornreich, *Critical Behavior at the Onset of K-space Instability at the λ-line,* Phy. Rev. Lett. **35** (1975), 1678-1681.

[14] A. L. Hodgkin and A. F. Huxley, *A Quantitative Description of Membrane Current and its Applications to Conduction and Excitation in Nerve,* J. Physiol. **117** (1952), 500-544.

[15] R. B. Kellogg and J. E. Osborn, *A Regularity Result for the Stokes Problem in a Convex Polygon,* J. Funct. Anal. **21** (1976), 367-431.

[16] O. A. Ladyzhenskaya, *The Mathematical Theory of Viscous Incompressible Flow*, Gordon and Breach, 1969.

[17] S. Larsson, *Numerical Analysis of Semi-Linear Parabolic Problems,* The Graduate Student's Guide to Numerical Analysis, SSCM, Springer **26** (1999), 83-117.

[18] L. Perko, *Differential Equations and Dynamical Systems*, Springer, 1991.

[19] A. Pazy, *Semigroups of Linear Operators and Applications to Partial Differential Equations*, Springer, 1993.

[20] W. Rall and G. N. Shepherd, *Theoretical Reconstruction of Field Potential and Dendrodendritic Synaptic Interactions in Olfactory Bulb,* J. Neurophysiol. **31** (1968), 848-915.

[21] M. Renardy and R. C. Rogers, *An Introduction to Partial Differential Equations*, Springer, 2002.

[22] R. D. Richtmyer and R. F. Morton, *Differential Methods for Initial Value Problems*, Interscience, NY., 1967.

[23] J. C. Robinson, *Infinite Dimensional Dynamical Systems*, Cambridge Text in Applied Mathematics, 2001.

[24] D. H. Sattinger, *On the Stability of Waves of Nonlinear Parabolic Systems,* Advances in Math. **22** (1976), 312-355.

[25] J. Smoller, *Shock Waves and Reaction-Diffusion Equations*, Springer, 1993.

[26] T. Sun and R. E. Ewing, *Long-Time Error Estimation and a Stability-Smoothing Indicator,* Dyn. Contin. Discrete and Impuls. Systems **9** (2002), 115-129.

[27] T. Sun and D. Fillipova, *Long-Time Error Estimation on Semi-Linear Parabolic Equations,* J. Comput. Appl. Math. **185** (2006), 1-18.

[28] R. Thomas, *Numerical Partial Differential Equations,* Springer, 1995.

[29] V. Thomée, *Galerkin Finite Element Methods for Parabolic Problems,* Springer, 2006.

[30] V. C. Vladimir and M. I. Vishik, *Attractors for Equations of Mathematical Physics,* Amer. Math. Soc., 2001.

[31] J. Wolka, *Partial Differential Equations,* Cambridge University Press, 1989.

[32] G. Zhu, *Experiments on Director Waves in Nematic Liquid Crystals,* Phys. Rev. Lett. **49** (1982), 1332-1335.