NUMERICAL SOLUTION OF THE FISHER'S EQUATION WITH DISCONTINOUS GALERKIN METHOD

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ABSTRACT

NUMERICAL SOLUTION OF THE FISHER'S EQUATION WITH DISCONTINOUS GALERKIN METHOD

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In this thesis, the Fisher's equation is discretized in space with the symmetric interior point discontinuous Galerkin (SDIPG). As time integrator Kahan's method is used, which is n efficient linearly implicit time integrator for PDE with quadratic nonlinearities like the Fisher's equation. Numerical results for the SIPG method, Kahan's method and mid-point method confirm the theoretically predicted convergence orders in space and time. Travelling waves with steep fronts are numerically well resolved in reaction dominated regimes.

Keywords: Diffusion reaction equation, Fisher's equation, Discontinuous Galerkin method, Kahan's method

ÖZ

FISHER DENKLEMİNİN KESİNTİLİ GALERKİN YÖNTEMİYLE NÜMERİK ÇÖZÜMÜ

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Tez Yöneticisi : Prof. Dr. Bülent Karasözen

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Bu tezde, Fisher Denklemi uzayda sürekli olmayan simetrik iç nokta kesintili Galerkin yöntemi (SIPG) kullanılarak ayrıklaştırılmıştır. Zaman ayrıklaştırılması için de Fisher denklemi gibi ikinci dereceden doğrusal olmayan terimleri difarensiyel denklemlerin çözümünde uygun Kahan yöntemi kullanılmıştır. Kahan ve orta nokta yöntemi kullanılarak elde edilen sayısal sonuçlar da teorik olan beklenen yaklaşım oranlarını doğrulamıştır. Reaksiyon kısmı ağır basan denklemlerde, dik cepheli hareket halindeki dalgalar sayısal açıdan düzgün sonuçlar vermistir.

Anahtar Kelimeler : Difüzyon reaksiyon denklemi, Fisher denklemi, Süreksiz Galerkin yöntemi, Kahan yöntemi

To My Family

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CHAPTER 1

INTRODUCTION

In many branches of science such as biology and chemistry, non-linear reaction diffusion equations are used as a standard model to describe the evolution of natural phenomena such as a mutant gene dispersion, flame propagation or pattern formation. These equations are semi-linear reaction-diffusion partial differential equations (PDEs) of the following form:

$$\frac{\partial u}{\partial t} = \epsilon \Delta u + r(u) \tag{1.1}$$

where the first part linear diffusion part, the second part $r(u)$, is the non-linear reaction part. In many models, u denote the concentration of the molecules such as genes or chemicals, ϵ is the diffusion constant, Δ the Laplace operator.

One of the most popular reaction-diffusion equations is the Fisher'sa equation or Fisher-Kolmogorov equation which was introduced by Fisher in the [6]in 1937 as a model of propagation of genes :

$$u_t = \epsilon u_{xx} + \rho u(1 - \frac{u}{K}) \qquad \forall x \in (0, L) \qquad and \qquad t \in (0, \tau) \tag{1.2}$$

where ϵ is the diffusion constant, ρ is the growth rate and K is the carrying capacity of the habitat. $u(x, t)$is considered as the mutant population in the space x and at the time t. It is also used as the logistic population growth models, chemical wave propagation models and neutron population models in nuclear reactors.

The Fisher's equation (1.2) can be reduced to non-dimensional form with the scaling factors

$$\widetilde{t} = \rho t, \qquad \widetilde{x} = \frac{x}{L}, \qquad \widetilde{u} = \frac{u}{K}.$$

$$u_t = u_{xx} + u(1 - u), \tag{1.3}$$

where u is the ratio of mutant population to the carrying capacity.

The boundary conditions are generally in form of [12]:

$$\lim_{x\to-\infty} u(x,t) = 1 \qquad and \qquad \lim_{x\to\infty} u(x,t) = 0, \tag{1.4}$$

or

$$\lim_{x\to-\infty} u(x,t) = 0 \qquad and \qquad \lim_{x\to\infty} u(x,t) = 0. \tag{1.5}$$

The boundary conditions (1.4) are referred to as nonlocal conditions, while conditions (1.5) are called local conditions [12].

The Fisher equation (1.3) exhibits traveling wave solutions of the form $u(x-ct) = u(x,t)$, where c is the speed of the wave solution. Kolmogorov showed that the travelling wave solutions $u(x-ct)$ are descending monotonically with $c_{min} = 2$ when $t \to \infty$ in [10]. Since the traveling wave solutions have the fixed shapes with the fixed speed, the aim in this thesis to construct numerically stable wave solutions to resolve the sharp travelling wave fronts.

Many studies were devoted to find travelling wave solutions of Fisher's equation analytically and numerically The earliest one is the Larson's study [11] to find analytical solutions of Fisher's equation. He discovered that the stability of wave dispersion as $t \to \infty$ is highly correlated with the initial data. He showed that it was too difficult to find an analytical solution of the non-dimensionless Fisher's equation (1.3) due to complex non-linear reaction part.

The first numerical study was conducted by the Gazdag and Canosa in [7] with using pseudo-spectral method. Later, Finite Difference methods [13], Finite Element methods [15], Sinc Collacation method [1] and Modified Cubic B-spline method [14] are applied to solve the Fisher's equation numerically. In recent years, Galerkin methods [22], B-spline Galerkin methods [5] and Wavelet Galerkin methods [16], Local discontinuous Galerkin method [12] are also applied.

In this study, we use the interior point discontinuous Galerkin method for space discretization and Kahan's method for time discretization.

In this thesis, the discontinuous Galerkin (DG) methods are chosen as a finite element method for the Fisher equation since DG Methods have the efficient properties that is a combination of good properties of both Finite Volume methods and continuous Galerkin methods. The DG method also damps out the non-physical oscillations, whereas the standard continuous finite elements can not do.

The DG methods are firstly defined by Reed and Hill in 1973 to study [17] neutron transportation for a first-order hyperbolic case. Later on, similar studies such as [2] for the Navier-Stokes equations. Cockburn and Shu developed some model to the time-dependent hyperbolic equations[4]. Operator splitting methods are applied to biological diffusion-reaction equations for modeling pattern formation of embryos. In this thesis,the Fisher's equation is used with the interior point discontinuous Galerkin method [18]. We use the MATLAB programs for the DG discretization in space [23] developed for semi-linear convection-reaction-diffusion equations.

In this thesis, we use the Kahan's reflexive formula as a time integrator to solve the

system of ordinary differential equation (ODEs) arising from semi-discretization of Fisher's equation by DG method. Kahan's method was introduced by William Kahan [9] for solving the Riccati and Lotka-Volterra equations. Serna applied Kahan's method to Hamiltionian systems [21] and showed that it preserves the symplectic for of the Lotka-Volterra equations. Kahan's method was applied in a general form to the Korteweg De-Vries equation in [24]. In [20] it was applied to the Lotka-Volterra equations and concluded that this method is preferable to the other methods since it keeps the solutions in a closed curve near the fixed points of the equations. Celledoni et all. proved in the study [3] that Kahan method is in the family of Runge Kutta methods. In other words, midpoint and trapezoidal methods are strongly connected to Kahan's method with respect to numerical stability and conservation properties. The most important feature of Kahan's method is that it is a linearly implicit method for differential equations with quadratic non-linear terms like Fisher's equation. Kahan's method requires only one Newton iteration at each time step in contrast to the mid-point rule or trapezoidal method.

The thesis organized as follows. In Chapter 2 we briefly describe the interior point discontinuous Galerkin method. Time discretization methods are introduced in Chapter 3 and applied to Fisher's equation. In Chapter 4, some numerical test examples are presented to compare the convergence rates of the DG discretization space and of the time integrators. Numerical results for different demonstrate the accuracy of the DG discretization space combined with the Kahan's method as an effective time integrator. The thesis ends with some conclusions in Chapter 5.

CHAPTER 2

DISCONTINUOUS GALERKIN METHOD

The Diffusion-Reaction equations are hard to solve with the conventional methods such as Least Squares or Standard Finite Element Methods due to some variations of the physical attributes of the nature. Therefore,it is needed to construct some other method to eliminate these inconsistencies generated by changing variables. The Discontinuous Galerkin (DG) Finite Element Method is one of the additional method which was firstly served with Reed and Hill [17] in 1973 in their steady-state neutron transportation case with 1st order hyperbolic equations.After this study,several studies on DG FEM are presented for both Elliptic and Parabolic equations such as Navier-Stokes equations case in the Bassi study [2].The notable usage is presented by Cockburn and Shu in the study [4] with constructing some framework for the solutions of the nonlinear time dependent hyperbolic conservative laws.

The DG Method is one of the favorite methods in the numerical solutions of various equations defining the structures of the chemical reaction processes, nuclear reactors etc. since it combines the positive parts of both Finite Volume Method which can be used only with lower degree polynomials and the continuous Finite Element Methods which gives the higher regularities due to the continuity. The DG method also provides good approximate solutions having effective properties such as flexibility, stability and consistency. Firstly, the flexibility property of the DG method can make the unstructured meshes and their hanging nodes usable on the inter-element boundaries on which the functions are discontinuous, so the non-physical oscillations can be reduced. Secondly, since the jump values of the solutions on the interior boundaries must be penalized by the DG method, the stability generated by the adapted polynomials obtained by p-refinement process, can pass one element from the another element without any extra effort on adaptivity. Thirdly, the consistency is provided by the Galerkin Orthogonality property of the FEM. In spite of these advantages, there are weak points of the DG FEM such as higher degree of freedoms or ill-conditioned matrices which gets larger linearly with the order of the basis functions.

In this chapter, the construction of the interior penalty Galerkin methods, a special DG methods, on a simple Poisson equation. After, SIPG semi-discretization of the Fisher's equation (1.2) is given.

2.1 Interior Penalty Galerkin Method

In this section, we present the application of the interior penalty Galerkin (IPG) method [19] to the general Poisson equation

$$\begin{aligned} -\epsilon\Delta u &= f \quad \text{in } \Omega, \\ u &= g_D \quad \text{on } \partial\Omega^D, \\ \epsilon\nabla u\cdot\mathbf{n} &= g_N \quad \text{on } \partial\Omega^N, \end{aligned} \tag{2.1}$$

with $\partial\Omega = \partial\Omega^D \cup \partial\Omega^N$ and $\partial\Omega^D \cap \partial\Omega^N = \emptyset$.

We first give some basic definitions used in the construction of IPG methods. The spaces $L^p(\Omega)$ are defined on the polygonal domain in $\mathbb{R}^d$, for $1 < p < \infty$,by

$$L^p(\Omega) = \{w \text{ Lebesgue measurable } : \ \|w\|^2_{L^p(\Omega)} < \infty\},$$

with the norms

$$\begin{aligned} \|w\|_{L^p(\Omega)} &= \left(\int_\Omega |w(x)|^p dx\right)^{1/p} \quad , \quad 1 \le p < \infty, \\ \|w\|_{L^\infty(\Omega)} &= esssup\{|w(x)| : x \in \Omega\} \quad , \quad p = \infty. \end{aligned}$$

The $L^2(\Omega)$ space which is a Hilbert space given with the usual L^2-inner product

$$(u,w)_\Omega = \int_\Omega u(x)w(x)dx \ , \ \|w\|_{L^2(\Omega)} = \sqrt{(w,w)_\Omega}.$$

Let $\mathcal{D}(\Omega)$ denotes the subspace of the space C^∞ having compact support in Ω. For any multi-index $\gamma = (\gamma_1, \ldots, \gamma_d) \in \mathbb{N}^d$ with $|\gamma| = \sum_{i=1}^d \gamma_i$, the distributional derivative $D^\gamma w$ is defined by

$$D^\alpha w(\psi) = (-1)^{|\gamma|}\int_\Omega w(x)\frac{\partial^{|\gamma|}\psi}{\partial x_1^{\gamma_1}\cdots\partial x_d^{\gamma_d}} \ , \quad \forall\psi \in \mathcal{D}(\Omega).$$

Then, the Sobolev space $W^{(s,p)}$ is introduced as

$$W^{(s,p)}(\Omega) = \{w \in L^p(\Omega) : D^\gamma w \in L^p(\Omega) \ , \ \forall\, 0 \le |\gamma| \le s\}.$$

Our main interest along this thesis is the Sobolev space given as $H^s(\Omega) = W^{(s,2)}(\Omega)$ for an integer s with the associated Sobolev norm

$$\|w\|_{H^s(\Omega)} = \left(\sum_{0\le|\gamma|\le s} \|D^\gamma w\|^2_{L^2(\Omega)}\right)^{1/2},$$

and the associated Sobolev seminorm

$$|w|_{H^s(\Omega)} = \|\nabla^s w\|_{L^2(\Omega)} = \left(\sum_{|\gamma|=s} \|D^\gamma w\|^2_{L^2(\Omega)}\right)^{1/2}.$$

The Sobolev spaces with vanishing functions on the domain boundary are defined by

$$H_0^s(\Omega) = \{w \in H^s(\Omega) : w|_{\partial\Omega} = 0\},$$

and we have for $s = 1$

$$H^1(\Omega) = \{w \in L^2(\Omega) : \nabla w \in (L^2(\Omega))^d\},$$

For a partition of triangles $\mathcal{T}_h$ of Ω the broken Sobolev spaces are defined by

$$H^s(\mathcal{T}_h) = \{w \in L^2(\Omega) : w|_E \in H^s(E)\ ,\ \forall E \in \mathcal{T}_h\},$$

with the associated broken Sobolev norm

$$\|w\|_{H^s(\mathcal{T}_h)} = \left(\sum_{E\in\mathcal{T}_h} \|w\|^2_{H^s(E)}\right)^{1/2},$$

and the associated broken gradient semi–norm

$$|w|_{H^0(\mathcal{T}_h)} = \left(\sum_{E\in\mathcal{T}_h} \|\nabla w\|^2_{L^2(E)}\right)^{1/2}.$$

Let $\{\mathcal{T}_h\}$ be a family of shape regular meshes with triangular elements, i.e., there exists a constant c_0 such that

$$\max_{E\in\mathcal{T}_h} \frac{h_E^2}{|E|} \leq c_0$$

where h_E is the diameter and $|E|$ is the area of E, and also the elements $E_i \in \mathcal{T}_h$ satisfies $\overline{\Omega} = \cup\overline{E}$ and $E_i \cap E_j = \emptyset$ for E_i, $E_j \in \mathcal{T}_h$. We split the set of all edges E_h into the set of interior edges E_h^0, the set of Dirichlet boundary edges E_h^D and the set of Neumann boundary edges E_h^N, so that $E_h = E_h^\partial \cup E_h^0$ with $E_h^\partial = E_h^D \cup E_h^N$. Then, set the finite dimensional solution and test function space by

$$V_h = \left\{u \in L^2(\Omega) : u|_E \in \mathbb{P}^q(E),\ \forall E \in \mathcal{T}_h\right\} \not\subset H_0^1(\Omega),$$

where $\mathbb{P}^q(E)$ denotes the set of all polynomials on $E \in \mathcal{T}_h$ of degree at most q. Note that the space of solution and test functions are chosen to be the same since the boundary conditions in DG methods are imposed weakly. In contrast to continuous finite element method, discontinuous Galerkin methods are suitable to use non–conforming spaces in which case the functions in $V_h \not\in\subset H_0^1$ are allowed to be discontinuous along the inter-element boundaries.

Because of the discontinuity of the functions in V_h along the inter element boundaries, there are two different traces from the neighboring elements sharing that edge. Accordingly, let us first give some notations before the construction of IPG methods. Let the edge e be a common edge for two elements E_i and E_j ($i < j$), (see Figure 2.1). Then for a scalar function u, there are two common traces of u along e, denoted by

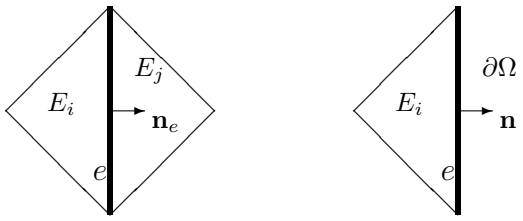

Figure 2.1: Left: two neighbour elements sharing an edge, Right: an element adjacent to boundary of the domain

$u_{|_{E_i}}$ from inside E_i and $u_{|_{E_j}}$ from inside E_j. Then, the jump and average of u across the edge e are defined as

$$[u] = u_{|_{E_i}}\mathbf{n}_e - u_{|_{E_j}}\mathbf{n}_e, \quad \{u\} = \frac{1}{2}(u_{|_{E_i}} + u_{|_{E_j}}),$$

where $\mathbf{n}_e$ is the unit normal to the edge e oriented from E_i to E_j. Similarly, we set the jump and average values of a vector field ∇u on e

$$[\nabla u] = \nabla u_{|_{E_i}} \cdot \mathbf{n}_e - \nabla u_{|_{E_j}} \cdot \mathbf{n}_e, \quad \{\nabla u\} = \frac{1}{2}(\nabla u_{|_{E_i}} + \nabla u_{|_{E_j}}),$$

Observe that $[u]$ is a vector for a scalar function u, while, $[\nabla u]$ is scalar for a vector field ∇u. On the other hand, for a boundary edge $e \subset E_i \cap \partial\Omega$, we set

$$[u] = u_{|_{E_i}}\mathbf{n}, \quad \{u\} = u_{|_{E_i}}, \quad [\nabla u] = \nabla u_{|_{E_i}} \cdot \mathbf{n}, \quad \{\nabla u\} = \nabla_{|_{E_i}}$$

where $\mathbf{n}$ is the unit outward normal to the boundary at e.

When we multiply the continuous equation (2.1) by a test function $v \in V_h$, integrate over Ω and split the integrals, we obtain

$$-\sum_{E\in\mathcal{T}_h}\int_E \epsilon\Delta u v dx = \sum_{E\in\mathcal{T}_h}\int_E f v dx.$$

Applying the divergence theorem on every element integral gives

$$\sum_{E\in\mathcal{T}_h}\int_E \epsilon\nabla u\cdot\nabla v dx - \sum_{E\in\mathcal{T}_h}\int_{\partial E}\epsilon(\nabla u\cdot\mathbf{n})v ds = \sum_{E\in\mathcal{T}_h}\int_K f v dx + \sum_{e\in E_h^N}\int_e g_N v ds$$

Using the jump definitions ($v \in V_h$ are element-wise discontinuous), we get

$$\sum_{E\in\mathcal{T}_h}\int_E \epsilon\nabla u\cdot\nabla v dx - \sum_{e\in E_h^0\cup E_h^D}\int_e [\epsilon v\nabla u] ds = \sum_{E\in\mathcal{T}_h}\int_E f v dx + \sum_{e\in E_h^N}\int_e g_N v ds$$

It can be easily verified that $[\epsilon v\nabla u] = \{\epsilon\nabla u\}\cdot[v] + [\epsilon\nabla u]\cdot\{v\}$. Also, using the fact that $[\nabla u] = 0$ (u is assumed to be smooth enough so that ∇u is continuous), we get

$$\sum_{E\in\mathcal{T}_h}\int_E \epsilon\nabla u\cdot\nabla v dx - \sum_{e\in E_h^0\cup E_h^D}\int_e \{\epsilon\nabla u\}\cdot[v] ds = \sum_{E\in\mathcal{T}_h}\int_E f v dx + \sum_{e\in E_h^N}\int_e g_N v ds$$

However, the left hand side is not coercive, even not symmetric. To handle this and to penalize the solutions, using the fact that $[u] = 0$ along the interior edges (u is assumed to be continuous), we reach at

$$\sum_{E\in\mathcal{T}_h}\int_E \epsilon\nabla u\cdot\nabla v dx - \sum_{e\in E_h^0\cup E_h^D}\int_e \{\epsilon\nabla u\}\cdot[v]ds - \sum_{e\in E_h^0}\int_e \{\epsilon\nabla v\}\cdot[u]ds$$

$$+\sum_{e\in E_h^0}\frac{\sigma}{h_e}\int_e [u]\cdot[v]ds = \sum_{E\in\mathcal{T}_h}\int_K fvdx + \sum_{e\in E_h^N}\int_e g_N v ds$$

where h_e denotes the length of the edge e and σ is called the penalty parameter. It should be sufficiently large to ensure the stability of the DG discretization with a lower bound depending only on the polynomial degree such that for 1D problems $\sigma = \frac{5}{2}(q+1)^2$ and $\sigma = 3q(q+1)$ for 2D problems.

Finally, by keeping unknown on the left hand side and imposing Dirichlet boundary condition on the right hand side, we add to the both sides the edge integrals on the Dirichlet boundary edges

$$\sum_{E\in\mathcal{T}_h}\int_E \epsilon\nabla u\cdot\nabla v dx - \sum_{e\in E_h^0\cup E_h^D}\int_e \{\epsilon\nabla u\}\cdot[v]ds + \mathcal{K}\sum_{e\in E_h^0\cup E_h^D}\int_e \{\epsilon\nabla v\}\cdot[u]ds$$

$$+\sum_{e\in E_h^0\cup E_h^D}\frac{\sigma}{h_e}\int_e [u]\cdot[v]ds = \sum_{E\in\mathcal{T}_h}\int_E fvdx + \sum_{e\in E_h^D}\int_e g_D\left(\frac{\sigma}{h_e}v - \epsilon\nabla v\cdot\mathbf{n}\right)ds$$

$$+\sum_{e\in E_h^N}\int_e g_N v ds.$$

which gives the IPG formulation. In this formulation, the parameter κ determines the type of the IPG method. It takes the values on $\mathcal{K}\in\{-1,0,1\}$ giving that

- $\mathcal{K} = -1$: symmetric interior penalty Galerkin (SIPG) method
- $\mathcal{K} = 0$: incomplete interior penalty Galerkin (IIPG) method
- $\mathcal{K} = 1$: non–symmetric interior penalty Galerkin (NIPG) method

In this thesis, symmetric interior penalty Galerkin (SIPG) method is considered.

2.2 SIPG Discretization of Fisher's Equation

In this section, we describe the DG discretization based on SIPG method applied to the diffusion part of the Fisher's equation (1.2) with Dirichlet boundary conditions. Using the definitions and notations from the previous section, the solution of (1.2) reads as: for each $t\in(0,T]$ find $u_h(t)\in V_h$ such that

$$(\partial_t u_h, \upsilon_h)_\Omega + a_h(u_h, \upsilon_h) + b_h(u_h, \upsilon_h)_\Omega = I_h(\upsilon_h), \quad \forall \upsilon_h \in V_h \tag{2.2}$$

where $b_h(u,v)_\Omega = (\rho u^2/K, v)$ and the bilinear form is a_h is given by

$$\begin{aligned} a_h(u,\upsilon) &= \sum_{E\in\mathcal{T}_h}\int_E (\epsilon\nabla u\cdot\nabla\upsilon - \rho u)dx - \sum_{e\in E_h^0\cup E_h^D}\int_e \{\epsilon\nabla u\}\cdot[\upsilon]ds \\ &\quad - \sum_{e\in E_h^0\cup E_h^D}\int_e \{\epsilon\nabla\upsilon\}\cdot[u]ds + \sum_{e\in E_h^0\cup E_h^D}\frac{\sigma\epsilon}{h_e}\int_e [u]\cdot[\upsilon]ds \\ b_h(u,\upsilon)_\Omega &= \sum_{E\in\mathcal{T}_h}\int_E \frac{\rho}{K}u^2\upsilon dx \\ I_h(\upsilon) &= \sum_{e\in E_h^D}\int_e \left(\frac{\sigma\epsilon}{h_e}\upsilon - \epsilon\nabla\upsilon\cdot\mathbf{n}\right) g_D ds \end{aligned}$$

2.2.1 Semi–Discrete System in Matrix–Vector Form

The approximate solution of the semi–problem (2.2) has the form

$$u_h(t) = \sum_{m=1}^{N}\sum_{j=1}^{n_q} U_j^m(t)\psi_j^m \tag{2.3}$$

where ψ_j^m are the basis functions of V_h and U_j^m are the unknown coefficients, n_q is local dimension with $n_q = q+1$ for 1D problems, $n_q = \frac{(q+1)(q+2)}{2}$ for 2D problems, and N is the number of intervals for 1D problems or the number of triangular elements for 2D problems. In DG methods, the basis functions ψ_j^m's are chosen in such a way that each piecewise basis polynomial has only one triangle as a support, i.e., on a specific triangle E_e, $e \in \{1,2,\ldots,N\}$, the basis polynomials ψ_j^e are zero outside E_e. This construction makes the stiffness matrix in DG methods block structure, each of which related to a triangle. The product $dof := N * n_q$ gives the degree of freedom in DG methods. Inserting the approximate solution u_h in (2.2) and choosing the test functions as $\upsilon_h = \psi_j^m$, $j = 1,2,\ldots,n_q$, $m = 1,2,\ldots,N$, the semi–discrete system (2.2) in matrix vector form is given by

$$MU_t + A\mathbf{U} + r(\mathbf{U}) = L, \tag{2.4}$$

where $\mathbf{U} \in \mathbb{R}^{dof}$ is the vector of unknown coefficients U_j^m's, $M \in \mathbb{R}^{dof\times dof}$ is the mass matrix, $A \in \mathbb{R}^{dof\times dof}$ is the stiffness matrix corresponding to the bilinear form $a_h(u_h,\upsilon_h)$, $r \in \mathbb{R}^{dof}$ is the vector function of U related to the non-linear form $r_h(u_h,\upsilon_h)$ and $L \in \mathbb{R}^{dof}$ is the load vector related to the linear term $I_h(\upsilon_h)$. The

explicit definitions are given by

$$M = \begin{bmatrix} M_{11} & M_{12} & \cdots & M_{1,N} \\ M_{21} & M_{22} & & \vdots \\ \vdots & & \ddots & \\ M_{N,1} & \cdots & & M_{N,N} \end{bmatrix}, \quad A = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1,N} \\ A_{21} & A_{22} & & \vdots \\ \vdots & & \ddots & \\ A_{N,1} & \cdots & & A_{N,N} \end{bmatrix}$$

$$\mathbf{U} = \begin{bmatrix} \mathbf{U}_1 \\ \mathbf{U}_2 \\ \vdots \\ \mathbf{U}_N \end{bmatrix}, \quad r(\mathbf{U}) = \begin{bmatrix} \mathbf{r}_1 \\ \mathbf{r}_2 \\ \vdots \\ \mathbf{r}_N \end{bmatrix}, \quad \mathbf{L} = \begin{bmatrix} \mathbf{L}_1 \\ \mathbf{L}_2 \\ \vdots \\ \mathbf{L}_N \end{bmatrix}$$

where all the block matrices have dimension n_q:

$$M_{ji} = \begin{bmatrix} (\phi_1^i, \phi_1^j) & (\phi_2^i, \phi_1^j) & \cdots & (\phi_{n_q}^i, \phi_1^j) \\ (\phi_1^i, \phi_2^j) & (\phi_2^i, \phi_2^j) & & \vdots \\ \vdots & & \ddots & \\ (\phi_1^i, \phi_{n_q}^j) & \cdots & & (\phi_{n_q}^i, \phi_{n_q}^j) \end{bmatrix},$$

$$A_{ji} = \begin{bmatrix} a_h(\kappa; \phi_1^i, \phi_1^j) & a_h(\kappa; \phi_2^i, \phi_1^j) & \cdots & a_h(\kappa; \phi_{n_q}^i, \phi_1^j) \\ a_h(\kappa; \phi_1^i, \phi_2^j) & a_h(\kappa; \phi_2^i, \phi_2^j) & & \vdots \\ \vdots & & \ddots & \\ a_h(\kappa; \phi_1^i, \phi_{n_q}^j) & \cdots & & a_h(\kappa; \phi_{n_q}^i, \phi_{n_q}^j) \end{bmatrix},$$

$$\mathbf{U}_i = \begin{bmatrix} U_1^i \\ U_2^i \\ \vdots \\ U_{n_q}^i \end{bmatrix}, \quad \mathbf{r}_i = \begin{bmatrix} r_h(u_h, \phi_1^i) \\ r_h(u_h, \phi_2^i) \\ \vdots \\ r_h(u_h, \phi_{n_q}^i) \end{bmatrix}, \quad \mathbf{L}_i = \begin{bmatrix} I_h(\phi_1^i) \\ I_h(\phi_2^i) \\ \vdots \\ I_h(\phi_{n_q}^i) \end{bmatrix}.$$

Under the coercivity condition for the bilinear form $a_h(u, v)$ and monotonicity of the nonlinear reaction term, there exist a unique solution of (2.4).

CHAPTER 3

TIME DISCRETIZATION

In this Chapter the fully discrete form of Fisher's equation in space by dG method and in time by the linearly implicit Kahan's method presented. Kahan's method [9] was applied for the Riccati and Lotka-Volterra equations, as symplectic integrator for Hamiltonian systems [21], to the Korteweg De-Vries equation [24]. Kahan's method was applied In [20] to the Lotka-Volterra equations and it was shown that the local stability of fixed points are preserved. It was applied to various biological models with quadratic nonlinearities in [8].

3.1 Kahan's Method

For time integration we use the "unconventional" method of Kahan's [9] for ordinary differential equations (ODEs) with quadratic terms like the semi-discretized form of the Fisher equation (2.4). We consider the following system of ODEs with quadratic vector fields

$$\frac{dU}{dt} = BU + Q(U) + q \tag{3.1}$$

where Q and B are quadratic and the linear forms, respectively, and q is the constant term. Kahan's method, then, is given as

$$\frac{U_{n+1} - U_n}{\Delta t} = Q(U_n, U_{n+1}) + B\frac{U_{n+1} + U_n}{2} + q \tag{3.2}$$

where $Q(U_n, U_{n+1})$ is symmetric bilinear form:

$$Q(U_n, U_{n+1}) = \frac{1}{2}[Q(U_n + U_{n+1}) - Q(U_n) - Q(U_{n+1})] \tag{3.3}$$

More specifically, the linear terms are approximated as the average of the approximate solutions

$$U^i = \frac{U_n^i + U_{n+1}^i}{2},$$

the quadratic terms by [8, 9, 3]

$$U^{ij} = \frac{U_n^i U_{n+1}^j + U_n^j U_{n+1}^i}{2}$$

The right hand side of (3.2) depends linearly on U_{n+1}. Therefore, Kahan's method is a linearly implicit method since U_{n+1} can be computed by solving a linear system of equations at each time step. The system of nonlinear equations are solved iteratively by Newton's method in other implicit methods like, the implicit mid-point method and implicit Runge Kutta methods.

Kahan's method is second order and symmetric, yielding a time reversible birational map $\phi : U_n \longrightarrow U_{n+1}$ for the discrete solution of the ODE system [8]. (3.1)

$$\dot{U} = f(U).$$

where $f(U)$ is a quadratic vector field.

$$\phi : \quad U_{n+1} = U_n + \Delta t \left(I - \frac{\Delta t}{2} f'(U_n) \right)^{-1} f(U_n) + g_d(t),$$

$$\phi^{-1} : \quad U_n = U_{n-1} - \Delta t \left(I + \frac{\Delta t}{2} f'(U_{n+1}) \right)^{-1} f(U_{n+1}) + g_d(t),$$

where I denotes the identity matrix and $f'(U)$ the Jacobian.

It was shown in [3] that Kahan's Method belongs to the following family of Runge-Kutta methods

$$\frac{U_{n+1} - U_n}{\Delta t} = af(U_n) + (1 - 2a) f(\frac{U_n + U_{n+1}}{2}) + af(U_{n+1}) \tag{3.4}$$

- If $a = -\frac{1}{2}$: Kahan's method.
- If $a = 0$: the midpoint method.
- If $a = \frac{1}{2}$: the trapezoidal method.
- If $a = \frac{1}{6}$: the Simpson method.

3.2 Time Discretization of Fisher's Equation

In this section, the fully discrete formulation of Fisher's equation in matrix–vector notation is given by using the Kahan's method through the semi–discrete formulation (2.4).

The semi-discrete form of the Fisher's equation (1.2) by SIPG method is given as the following system of ODE'a

$$MU_t + AU + r(U) = f(t), \tag{3.5}$$

where M and A are mass and stiffness matrices, respectively, $r(U)$ the semi-discrete quadratic nonlinearity and $f(T9$ contains the semi-discrete non-homogeneuous terms of the boundary conditions.

Let consider the uniform partition $0 = t_0 < t_1 < \ldots < t_J = T$ of the time interval $[0, T]$ with the uniform time step-size $\Delta t = t_k - t_{k-1}$, $k = 1, 2, \ldots, J$. Denote by $U_n \approx U(t_n)$ the coefficient vector of the approximate solution at $t = t_n$. For $t = 0$, let $u_h(0) \in V_h$ be the projection (orthogonal L^2-projection) of the initial condition u_0 onto V_h, and let U_0 be the corresponding coefficient vector satisfying (2.3). Then, the Kahan's method applied to the semi linear system (3.5) reads as: for $n = 0, 1, \ldots, J - 1$, solve

$$M\frac{U_{n+1} - U_n}{\Delta t} + \frac{1}{2}A(U_{n+1} + U_n) + r(U_{n+1}, U_n) = f(t_n), \tag{3.6}$$

which is the fully discretized system that we will solve for U_{n+1}. In (3.6), $r(U_{n+1}, U_n)$ refers to the form related to the quadratic nonlinearity, and it is given by

$$r(U_{n+1}, U_n) = \begin{bmatrix} \mathbf{r}_1 \\ \mathbf{r}_2 \\ \vdots \\ \mathbf{r}_N \end{bmatrix}, \quad \mathbf{r}_i = \begin{bmatrix} \mathbf{r}_{i,1} \\ \mathbf{r}_{i,2} \\ \vdots \\ \mathbf{r}_{i,nq} \end{bmatrix}, \quad \mathbf{r}_{i,j} = \int_{E_i} u_{h,n} u_{h,n+1} \phi_j^i dx$$

where $u_{h,n} \approx u(x, t_n)$ is the approximate solution at the discrete time $t = t_n$ satisfying the linear expansion (2.3). Note that the the for $r(U_{n+1}, U_n)$ is linear in the argument. As a result the system (3.6) is linear system for U_{n+1}, and can be solved in an efficient way. In the computational point of view, the known approximation $u_{h,n}$ behaves as a variable (non-constant) linear reaction coefficient for the unknown $u_{h,n+1}$.

Algorithm 1 Kahan's Method

Given U_0
for $n = 0, 1, 2, \ldots, J - 1$ **do**
  Compute the reaction matrix R which takes U_n as the variable reaction coefficient
  Solve the linear system (3.6) by setting $r(U_{n+1}, U_n) = RU_{n+1}$
end for

CHAPTER 4

NUMERICAL RESULTS

In this chapter, we demonstrate the effectiveness of Kahan's method by several numerical test examples. The dimensionless analysis of Fisher equation (1.2) shows for the case of $D = 1$ and $\rho = 1$, 1the minimal speed of the self similar traveling wave is $c > 2$ [12]. Similarly, in [10] it was shown that travelling waves exits for $c > 0$ which are decreasing monotonically. At the minimum wave speed $c = 2$ travelling waves propagate into shock-like waves [12]. For reaction dominated, i.e. larger ratios of ρ/ϵ, the velocity is preserved, but the maximal gradient is multiplied by a factor ρ which introduces stiffness in the equation. In the following examples, we investigate for different values of the diffusion ϵ and reaction ρ parameters, how accurately the travelling waves are resolved in time and space. We give also the convergence rates in space for the SIPG discretization, in time for Kahan's method and the mid-point method.

4.1 Example 1

We consider the Fisher equation in [12, 14] on $t \in [0, 1]$ and with the diffusion coefficient $\epsilon = 1$.

with the Dirichlet boundary conditions

$$\lim_{x\to-\infty} u(x,t) = 1, \qquad \lim_{x\to\infty} u(x,t) = 0,$$

and the initial condition

$$u(x,0) = \frac{1}{\left[1 + \exp\left(\sqrt{\frac{\rho}{6}}\, x\right)\right]^2}.$$

The exact solution is given by

$$u(x,t) = \frac{1}{\left[1 + \exp\left(\left(\sqrt{\frac{\rho}{6}}\right) x - \left(\frac{5\rho}{6}\right) t\right)\right]^2}.$$

In the following, we compare numerical numerical errors, convergence orders in time for Kahan's method with the midpoint method by taking the step size in space as $\Delta x =$

0.01 at the final time $T = 0.1$ by taking $x \in [-30, 30]$ as the truncated computational domain. We observe from the Tables 4.1-4.4 that the convergence rate of the midpoint method is about two as expected. Convergence rate of Kahan's method is about one which is due to the linearly implicit nature of the method. We can conclude that Kahan's method has the same order as the implicit Euler method but it requires only one solution of a linear system of equations at each time step.

Table 4.1: Kahan's method $\rho = 10$

Δt	L_2 error	L_2 convergence rate	L_∞ error	L_∞ convergence rate
1.00e-2	1.24e-1	-	2.28e-1	-
5.00e-3	5.96e-2	1.06	1.09e-1	1.06
2.50e-3	2.92e-2	1.03	5.36e-2	1.03
1.25e-3	1.44e-2	1.02	2.65e-2	1.02

Table 4.2: Midpoint method $\rho = 10$

Δt	L_2 error	L_2 convergence rate	L_∞ error	L_∞ convergence rate
1.00e-2	2.28e-3	-	4.41e-3	-
5.00e-3	5.64e-4	2.02	1.09e-3	2.02
2.50e-3	1.36e-4	2.06	2.57e-4	2.08
1.25e-3	2.86e-5	2.24	4.97e-5	2.37

Table 4.3: Kahan's method $\rho = 100$

Δt	L_2 error	L_2 convergence rate	L_∞ error	L_∞ convergence rate
5.00e-3	1.59e-1	-	8.83e-1	-
2.50e-3	6.30e-2	1.34	3.63e-1	1.28
1.25e-3	2.82e-2	1.16	1.64e-1	1.15
6.25e-4	1.34e-2	1.08	7.76e-2	1.08

Table 4.4: Midpoint method $\rho = 100$

Δt	L_2 error	L_2 convergence rate	L_∞ error	L_∞ convergence rate
5.00e-3	1.07e-2	-	6.53e-2	-
2.50e-3	2.56e-3	2.06	1.56e-2	2.06
1.25e-3	6.24e-4	2.04	3.79e-3	2.04
6.25e-4	1.46e-4	2.10	8.62e-4	2.13

In the following tables, we compare numerical numerical errors, convergence orders in space for linear DG polynomials integrated in time by Kahan's method and by the midpoint method for the time steps $\Delta t = 5 * 10^{-5}$ inn the computational domain $x \in [-30, 30]$ final time $T = 0.1$.

Table 4.5: Kahan's method $\rho = 10$

Δt	L_2 error	L_2 convergence rate	L_∞ error	L_∞ convergence rate
2.00	2.54e-2	-	1.02e-1	-
1.00	4.94e-3	2.36	1.62e-2	2.66
0.50	1.11e-3	2.15	3.70e-3	2.13
0.25	2.71e-4	2.03	9.15e-4	2.02

Table 4.6: Midpoint method $\rho = 10$

Δt	L_2 error	L_2 convergence rate	L_∞ error	L_∞ convergence rate
2.00	2.54e-2	-	1.02e-1	-
1.00	4.94e-3	2.36	1.62e-2	2.66
0.50	1.11e-3	2.16	3.69e-3	2.13
0.25	2.70e-4	2.04	9.02e-4	2.03

The convergence rates of the SIPG method with linear polynomials in the Tables 4.5-4.6, are two as expected for both time discretizations.

The plots of the numerical solutions computed by Kahan's method, mid-point method and exact solutions for increasing values of the reaction coefficients ρ in Figs. 4.1-4.3. We observe that the sharp fronts for larger values of the reaction coefficient ρ can be resolved accurately by taking smaller meshes in space and time.

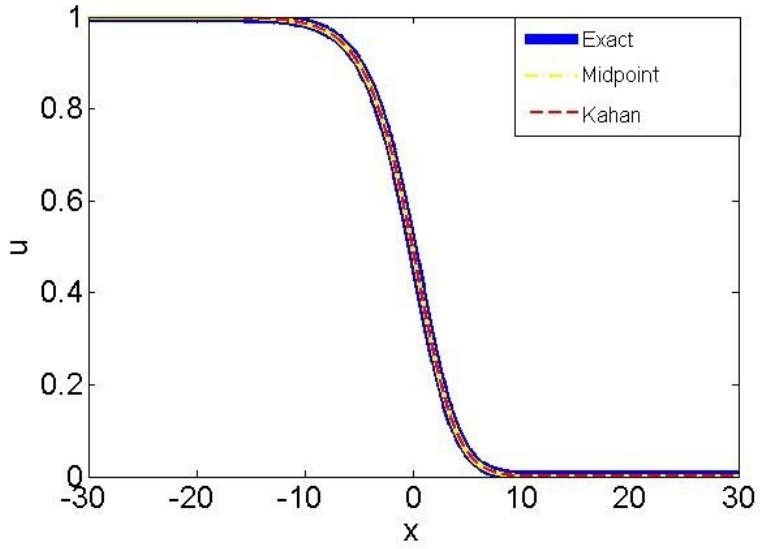

Figure 4.1: Comparison of solutions for $\Delta t = \Delta x = 0.01$, $\rho = 1$

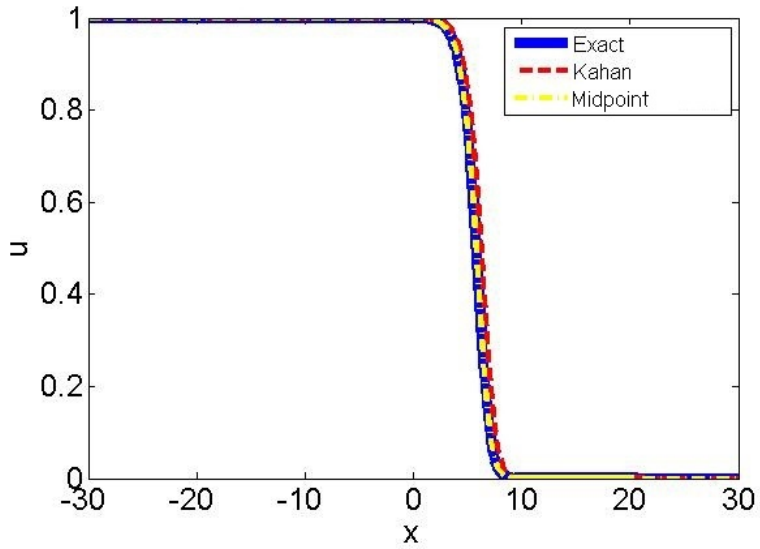

Figure 4.2: Example 1: Comparison of solutions for $\Delta t = \Delta x = 0.01$, and $\rho = 10$

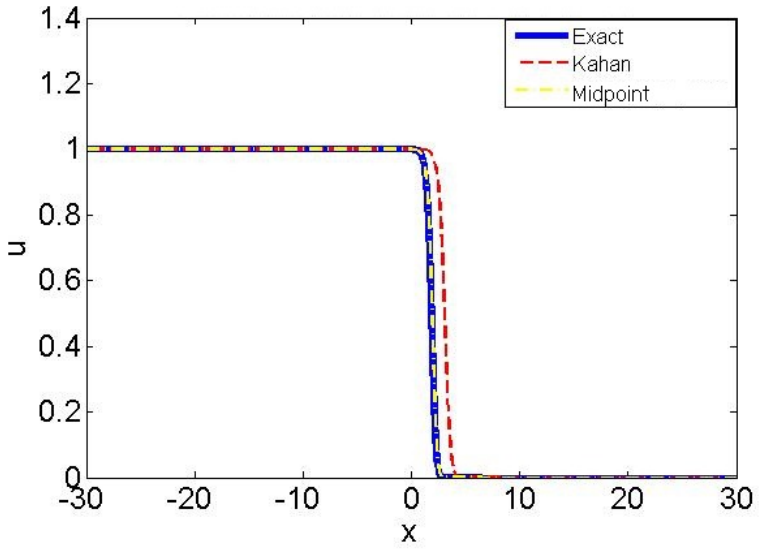

Figure 4.3: Example 1: Comparison of solutions for $\Delta t = 0.005,\ \Delta x = 0.01$, and $\rho = 100$

4.2 Example 2

We consider the modified Fisher equation in [14]

$$\frac{\partial u}{\partial t} = \epsilon \frac{\partial^2 u}{\partial x^2} + \rho_1 u - \rho_2 u^2, \tag{4.1}$$

with the Dirichlet boundary conditions

$$\lim_{x \to -\infty} u(x,t) = 0.5, \qquad \lim_{x \to \infty} u(x,t) = 0, \tag{4.2}$$

.

The exact solution is given

$$u(x,t) = -\frac{1}{4}\frac{-\rho_1}{\rho_2}\left[\operatorname{sech}^2(-\sqrt{\frac{\rho_1}{24}}x) - 2\tanh(-\sqrt{\frac{\rho_1}{24}}x) - 2\right]. \tag{4.3}$$

In the Tables 4.7-4.8, convergence rates for Kahan's method and mid-point method are given, by taking $\epsilon = 10,\ \rho_1 = 0.5,\ \rho_2 = 1$. Numerical solutions re computed in the computational domain $x \in [-30, 30]$ at the final time $t \in [0, 5]$ with the step length $\Delta x = 0.1$. In Fig. 4.4, numerical solutions obtained by Kahan's method and exact solutions are plotted which are in good agreement.

Table 4.7: Kahan's method

Δt	L_2 error	L_2 convergence rate	L_∞ error	L_∞ convergence rate
1.00e-1	4.83e-2	-	3.56e-2	-
5.00e-2	2.38e-2	1.02	1.76e-2	1.02
2.50e-2	1.18e-2	1.01	8.73e-3	1.01
1.25e-2	5.88e-3	1.01	4.35e-3	1.00

Table 4.8: Midpoint method

Δt	L_2 error	L_2 convergence rate	L_∞ error	L_∞ convergence rate
1.00e-1	4.03e-4	-	2.98e-4	-
5.00e-2	1.02e-4	1.99	7.53e-5	1.98
2.50e-2	2.64e-5	1.94	1.98e-5	1.93
1.25e-2	8.11e-6	1.71	6.08e-6	1.70

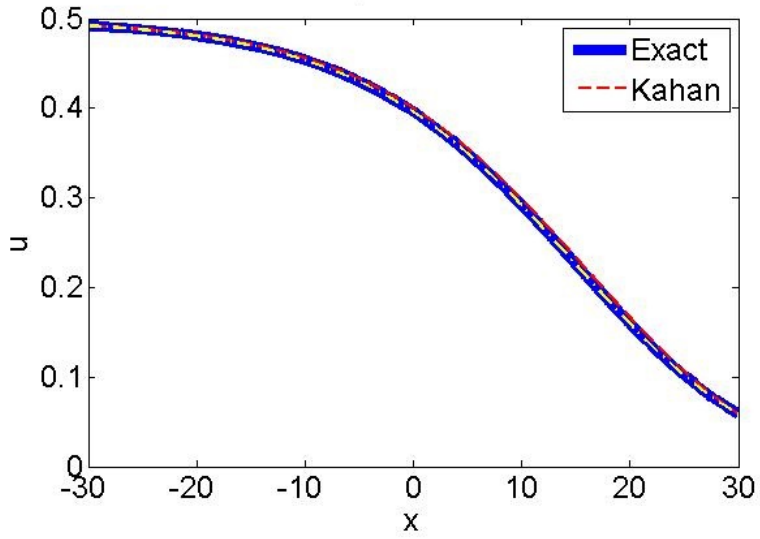

Figure 4.4: Example 2: Kahan's method

4.3 Example 3

We consider as example the Fisher equation in [14]

with the initial condition

$$u_0(x) = sech^2(10x)$$

with the homogeneous Dirichlet boundary conditions

$$\lim_{x\to-\infty} u(x) = \lim_{x\to\infty} u(x) = 0$$

with $\epsilon = 0.1$ and $\rho = 1$ in the time interval $t \in [0, 0.2]$ and in the computational domain $x \in [-4, 4]$ with spatial step is as $\Delta x = 0.05$ and time step is taken as $\Delta t = 0.005$. The plots in Figs. 4.5-4.6 reveal that the numerical results of mid-point method and Kahan'a method's are very close.

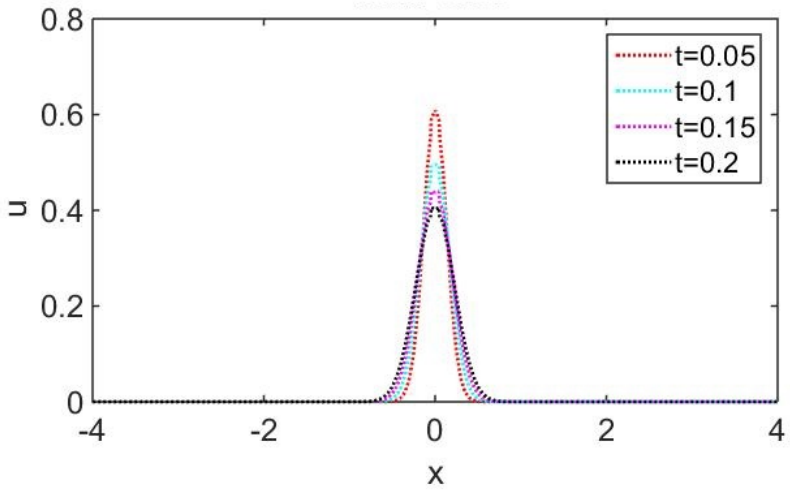

Figure 4.5: Example 3: Midpoint method

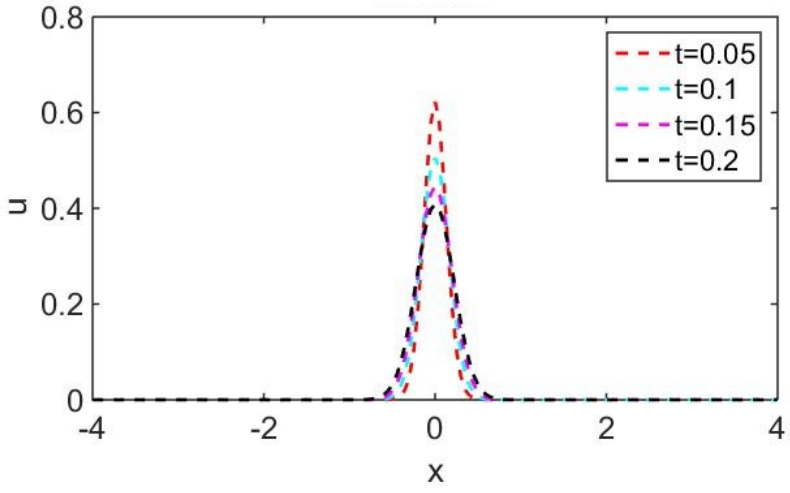

Figure 4.6: Example 3: Kahan's method

CHAPTER 5

CONCLUSION

In this thesis, the the travelling wave solutions of the one dimensional Fisher's equation is studies. Numerical convergence results confirm the second order accuracy of the SIPG discretization in space. The predicted orders of convergence of the two time integrators used in this thesis, namely Kahan's method and mid-point method were also validated by the numerical results. Due its special structure Kahan's method requires less computation time than the mid-point method for semi-linear PDEs with quadratic nonlinear terms like the Fisher's equation. In all numerical experiments, travelling waves with steep fronts are well resolved in the reaction dominated regimes due to the less diffusive nature of the SIPG method.

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