A numerical study of the cable equation in mathematical neuroscience

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Preface

This master thesis, written at the Department of Mathematical Sciences and Technology, Norwegian University of Life Sciences, marks the end of my masters degree in Applied Mathematics.

It has been five exiting years with many different and interesting subjects ranging from complex analysis in mathematics to quantum mechanics in physics.

I would like to thank my two supervisors John Wyller and Gaute Einevoll for the support, not only during the work of the master thesis, but during my entire masters degree. Their passion for their field have been of great inspiration. I would like to express a special thanks to my main supervisor John Wyller. During our weakly meetings he has always supported and motivated me and shown a great interest in my work.

At the end I would like to thank my parents who have always been there for me and encouraged me throughout the studies. A special thanks to my partner Thomas who has had to cope up with my endless talk about the studies for the last five years.

Ås, May 2012

Hilde Larsen

Abstract

The aim of this thesis is to compare different numerical methods for solving the cable equation for electrical signal propagation along dendrites with diameter varying in space.

We solve the model with four different methods: a finite difference scheme, finite element method, separation of variables combined with a finite difference scheme and separation of variables combined with the finite element method. The different methods gives quite different solution even if the solutions main properties are the same. Separation of variables combined with the finite element method offers a solution of much lower value than the other methods. This can be a result of an overestimate of the eigenvalue of the problem. The finite element method and the method of separation of variables combined with a finite difference scheme gives almost the exact same solutions, a fact that was to expect during the derivations. The finite difference scheme is the easiest method to use even if it is important for the schemes consistency how the derivatives was replaced by finite differences. Finite difference method is the method that give the less complicated programming in Matlab as well.

The solutions for different diameter geometry are as expected from the mathematical analysis done in advance. The solutions stays symmetric about the mid point in space if the diameter and the initial condition have the same symmetry. The peak of the solutions for non-symmetric diameters move towards increasing space variable for a decreasing diameter and towards decreasing space variable for an increasing diameter.

Introduction

Electricity transfer and electric activity in the human body has been a topic of investigation for centuries. An understanding of the brain, not only physically but mathematically as well, is an important aspect of the understanding of the human body. It is the brain that controls and make the different parts of the body and mind interact properly with each other. The understanding of the brain involves how the neurons communicate with each other, and how a neuron respond to an incoming signal.

William Thomas (later Lord Kelvin) started in the early 1850s to work on a mathematical theory describing the signal decay of a underwater cable across the Atlantic ocean [1]. His finished work was called the telegrapher's equation and is the origin of the cable equation.

The cable equation in neuroscience describes how the membrane potential of a neuron vary in both time and space along a given length of a dendrite or axon with a given diameter. The diameter can be modelled by any geometric shape, but a constant diameter or a linear variable diameter are the most common used. For that reason the focus of this paper is the modelling of the membrane potential in a part of a dendrite with a sigmoidal decaying diameter profile.

The cable equation with a linear variable diameter has been solved analytically in [2]. If a sigmoidal diameter profile is assumed, the cable equation, which is a linear partial differential equation, cannot be solved analytically. A numerical method has to be applied in order to find a solution. The purpose of this thesis will therefore be to give an overview of some numerical methods for solving partial differential equations, discuss which solution method is the best if both the accuracy and amount of work is taken into consideration. An other interesting aspect of the model is how we could expect the solution to behave for different diameter geometries.

This paper is organized in the following manner: Chapter 1 gives a short introduction to relevant theory in neuroscience. In chapter 2 the cable equation is derived, and chapter 3 completes the model by including initial and boundary conditions and specifying the diameter function. Chapter 3 also

includes a scaling of the model. Chapter 4 discusses some properties of the model, followed by chapter 5 where several numerical solutions methods are introduced and applied. An error analysis of the numerical methods are given in chapter 6. The numerical results are presented in chapter 7. Chapter 8 contains the concluding remark. In the appendix details about the scaling, derivation of the numerical methods, error analysis and proof of result 1, 2 and 3 from section 5.3.1 can be found. Some theory about Sturm-Liouville problems is included, as well as the Matlab programs used to solve the model.

Contents

Chapter 1

Neurophysical background

1.1 Structure of the brain

The human brain [3] is basically a lump of tissue. It can be divided into three main parts, rhombencephalo (hindbrain), which is connected to the spinal cord, mesencephalo (midbrain) and prosencephalo (forebrain).

The forebrain includes what is called the cerebrum. Cerebrum is a major part of the brain and is divided into two almost identically hemispheres, connected to each other by corpus callosum (white matter). Each hemisphere is fully equipped with areas for motor and sensory control. The right hemisphere controls the left part of the body and the left hemisphere controls the right part of the body.

Surrounding the cerebrum we find cortex cerebri. Cortex can be divided into different motor and sensory areas. Signal transport in these areas are of great interest.

1.2 Neurons

The brain tissue is mainly made of two types of brain cells, neurogli(glia) and nerve cells (neurons). Glia and neurons have different important roles. While glia play an important role in the development of the brain, make myelin sheeths around axons of neurons and regulates the ionic composition of the extracellular space among other tasks, the neurons take care of the information storing and processing in the brain. For this reason, it is the neurons that are of interest in this paper.

A neuron consists of a cell body, see figure 1.1, usually with one axon and several dendrites emerging from it. The cell body usually emits signals down the axon and receive input from other cells through the dendrites.

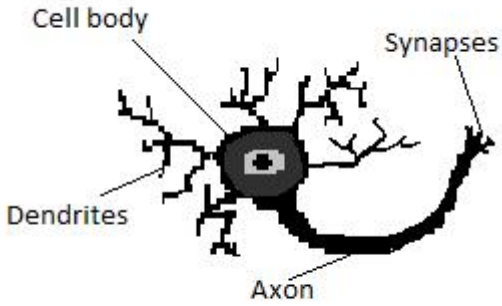

Figure 1.1: Schematic overview of a neuron

Axon, dendrites and the cell body as well have a membrane which acts as an insulator. This membrane makes signals able to travel along the entire length of a dendrite or axon. But the membrane is what can be called semi permeable, which means that it lets selected ions pass through it.

1.3 Communication between neurons

Electrical signals in a neuron are composed of different ion compositions which give rise to a potential difference across the cell membrane. The inside of a cell is dominated by the ions K^+ and A^-, and the outside by Na^+ and Cl^-. In a resting state the membrane potential, called the resting or equilibrium potential has a value of about $-70mV$.

Neurons are connected to each other via synapses. A neuron can initiate an action potential, and then send this signal down an axon, via a synapse to another neuron. At the initiation of an action potential, ion channels in the semi permeable membrane opens in order for K^+ and Na^+ ions to travel in and out of the cell, which give an almost instantaneously large increase in the membrane potential.

A neuron can either be excitatory or inhibitory. An excitatory neuron tends to increase the possibility for other neighbour neurons to initiate an action potential, while an inhibitory neuron tends to decrease this possibility.

Chapter 2

The cable equation

Compartmental modelling is a common used approach when modelling the potential in a network of dendrites. The upcoming derivation is taken from the book of Ermentrout and Terman [4].

Compartmental modelling divides the dendrite into compartments shown in figure 2.1. Assume that the cable is divided unto n equal compartments, which takes on the form of a cylinder, has diameter d_i, length l, and potential V_i relative to the outside. The potential stays constant through each part of a compartment. In addition, the compartments have the same specific membrane capacitance c_M, the same specific membrane resistance r_M and the same longitudinal resistivity r_L. In this paper we look at a dendrite of finite length L which does not branch out or have any synaptic connections.

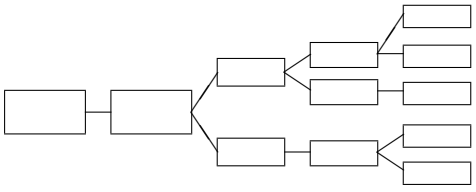

Figure 2.1: Dendrite which branches out modelled by compartmental modelling.

For each compartment there are three currents to consider. First there is a capacitive current per unit area $i_{cap,i}$. The membrane acts as an capacitor, which make ions accumulate at the inside and outside of the surface. But the membrane is what is called semi permeable, which means that it lets selected ions pass through it. This give rise to an ionic current per unit area $i_{ion,i}$. The last current to consider is the longitudinal current per unit area $i_{long,i}$, which is made by ions passing through the compartments in an axial direction.

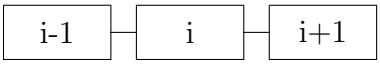

Figure 2.2: Compartment i can only be connected to compartment $i-1$ and $i+1$.

Often a test current, called an electrode current gets injected, but for this paper that current is neglected. The different currents have to balance each other according to the preservation of current principle (Kirchoff's 1.law) [5]

$$i_{cap,i} + i_{ion,i} = i_{long,i} \tag{2.1}$$

From the definition of capacitance, ions accumulating on each side of an insulating surface give rise to a current which can be expressed as

$$i_{cap,i} = c_M \frac{dV_i}{dt}$$

$i_{ion,i}$ can be computed by means of Ohms law

$$i_{ion,i} = \frac{V_i}{r_M}$$

if the resting potential of the neuron is assumed to be $0mV$.

Then we have the longitudinal current. This is the part of the equation that couples two compartments together. In order to find an expression for this current, we first need to find the total resistance between the centres of two nearby compartments. The resistance [5] in a conductor can be found by multiplying the longitudinal resistivity by the length of the conductor and then divide by the cross section area of the conductor. The total resistance between the two centres then become the sum of half the resistance of two nearby compartments. In this derivation the diameter of the highest order compartment (d_j if $j > i$) has been used such that

$$R_{ij} = \frac{4r_L l}{\pi d_j^2}, \qquad \text{for } j > i$$

As figure 2.2 describe, compartment i can only be connected to compartment $i-1$ and compartment $i+1$. By using Ohms law, the total longitudinal

current per unit area of membrane passing through compartment i therefore become

$$i^i_{long} = \frac{1}{4r_L d_i l}\Big(\frac{d^2_{i+1}(V_{i+1} - V_i)}{l} + \frac{d^2_i(V_{i-1} - V_i)}{l}\Big)$$

All the currents have now been specified and equation (2.1) become

$$c_M \frac{dV_i}{dt} = -\frac{V_i}{r_M} + \frac{1}{4r_L d_i l}\Big(\frac{d^2_{i+1}(V_{i+1} - V_i)}{l} - \frac{d^2_i(V_i - V_{i-1})}{l}\Big)$$

The length l of each compartment is assumed to be much smaller than the length of the entire cable. Then assume that

$$\frac{l}{L} \to 0$$

such that the membrane potential can vary smooth over the entire length of the cable and the cable equation that describes the membrane potential becomes

$$\frac{\partial V}{\partial t} = -\frac{V}{\tau_M} + \frac{1}{4r_L c_M d(x)}\frac{\partial}{\partial x}\Big(d(x)^2\frac{\partial V}{\partial x}\Big) \tag{2.2}$$

where $\tau_M = r_M c_M$ is a quantity often called the membrane time constant. It usually falls in the range of $10ms - 100ms$ and give a measure of the time scale for changes in the membrane potential. The membrane time constant is independent of the geometry of the cable.

Chapter 3

The model

3.1 Initial and boundary conditions

There are different types of boundary and initial conditions [6]. First, we have what is called Dirichlet boundary conditions. Such types of boundary conditions define the potential to be constant or equal to zero at the end points,

$$u(0,t) = a \quad u(L,t) = b \quad \text{Dirichlet boundary condition}$$

The next types of boundary conditions called Neumann boundary conditions define the rate of change in potential in space to be constant or equal to zero at the end points,

$$u_x(0,t) = a \quad u_x(L,t) = b \quad \text{Neumann boundary condition}$$

In order for equation (2.2) to have a unique solution, initial and boundary conditions have to be defined. Appropriate choice of boundary conditions can be

$$V(0,t) = V(L,t) = 0, \quad t > 0$$

which means that the potential vanishes at the ends of the cable. The initial condition model the potential along the entire dendrite at the time $t = 0$. This could be an electrode current injected somewhere along the length of the cable. A suitable choice of initial condition could then be to inject a current which make the membrane potential at the point $x = \frac{L}{2}$ equal to $50mV$.

$$V(x,0) = f(x) = \begin{cases} V_0 & x = \frac{L}{2} \\ 0 & \text{otherwise} \end{cases}$$

where $V_0 = 50mV$

3.2 The diameter function

A constant diameter profile is the most common used in modelling of a dendrite. In [2] modelling with a linear non-constant diameter has been preformed. For this reason it is interesting to model the diameter by a non-linear function. In the present work we assume that the diameter function is modelled by means of a sigmoidal function

$$d(x) = \frac{d_{-\infty}}{1 + e^{\frac{x}{\Lambda_d}}} \tag{3.1}$$

where

$$\lim_{x \to -\infty} d(x) = d_{-\infty}$$

and Λ_d is a constant that describes the length of significant changes in the diameter. If Λ_d is small, then the significant change in $d(x)$ will occur on a small distance.

Figure 3.1 shows a plot of a diameter function given by a sigmoidal function.

To summarize, the derivations done in the previous sections, the model for describing the potential across the membrane in a dendrite of variable diameter can be presented by

$$\begin{aligned} \frac{\partial V}{\partial t} &= -\frac{V}{\tau_M} + \frac{1}{4 r_L c_M d(x)} \frac{\partial}{\partial x}\Big(d(x)^2 \frac{\partial V}{\partial x}\Big) \quad \text{for } x \in (0, L),\ t > 0 \\ V(0,t) &= V(L,t) = 0, \quad \tau > 0 \qquad\qquad d(x) = \frac{d_{-\infty}}{1 + e^{\frac{x}{\Lambda_d}}} \\ V(x,0) &= \begin{cases} V_0 & x = \frac{L}{2} \\ 0 & \text{otherwise} \end{cases} \end{aligned} \tag{3.2}$$

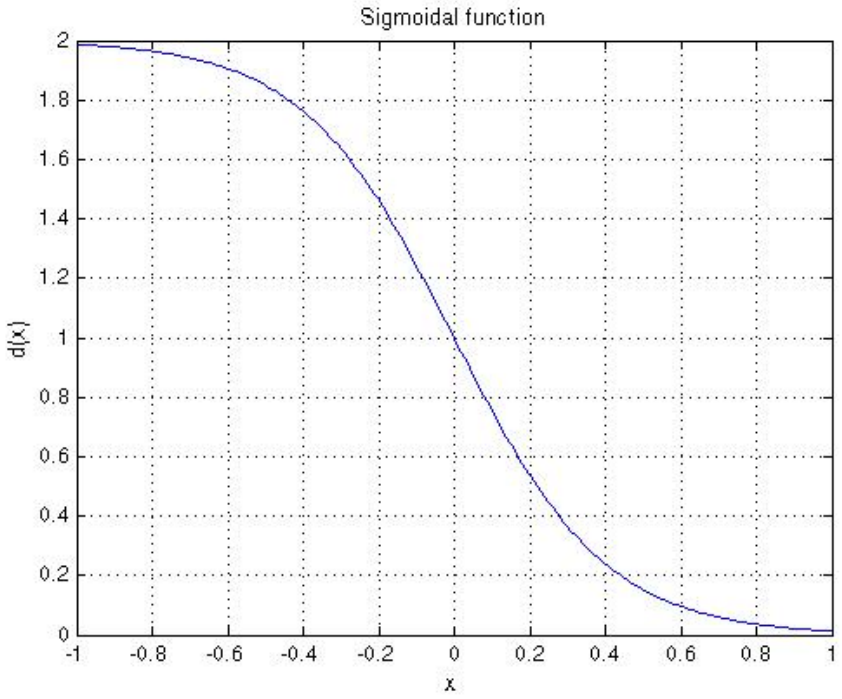

Figure 3.1: Plot of a sigmoidal function

3.3 Scaling

The purpose of scaling is to reduce the number of parameters involved and to transform the actual problem into an equivalent dimensionless problem. In (3.2) the potential V can be expressed as $V(x,t;c_M,r_M,r_L,L)$. If we scale the problem, the number of parameters to assign a value reduces.

Let us introduce the new variables

$$\xi = \frac{x}{L} \qquad \tau = \frac{t}{T} \qquad D(\xi) = \frac{d(x)}{d_0} \tag{3.3}$$

$$V(x,t) = u(\xi,\tau)V_0 e^{-\frac{t}{\tau_M}}, \quad \tau_M = c_M r_M$$

We insert (3.3) into the PDE in problem (3.2) and get

$$\begin{aligned} \frac{\partial u(\xi,\tau)}{\partial \tau} &= \frac{\alpha}{D(\xi)}\frac{\partial}{\partial \xi}\Big(D(\xi)^2\frac{\partial u(\xi,\tau)}{\partial \xi}\Big), \qquad \alpha = \frac{Td_0}{4r_L c_M L^2} \\ u(0,\tau) &= u(1,\tau) = 0\ , \quad \tau > 0 \\ u(\xi,0) &= g(\xi)\ , \quad \xi \in [0,1] \end{aligned} \tag{3.4}$$

See appendix A for details

Now we can see that V, which has the dimension mV, has been transformed from $V(x,t;c_M,r_M,r_L,L)$ to a dimensionless variable $u(\xi,\tau;\alpha)$. The new variables transforms the interval $x \in (0,L)$ into a new dimensionless interval $\xi \in (0,1)$. For simplicity, d_0 can be chosen to be equal to 1.

In equation (3.4) several constants have been combined in a single constant α. For simplicity, and without any loss of generality, α can be chosen to be equal to 1. This makes the characteristic time T equal to

$$T = 4r_L c_M L^2$$

In table 3.1 values for the different parameters used are specified, as well as the value of τ_M, T and suitable values for the diameter at the endpoints of the cable.

r_M	$50k\Omega cm^2$
c_M	$1\mu F/cm^2$
r_L	$0,1k\Omega cm$
L	$0,04cm$
$d(0)$	$0,00037cm$
$d(L)$	$0,00006cm$
T	$0,00064ms$
τ_M	$50ms$

Table 3.1: Values of different parameters used in model (3.2)

The scaled version of problem (3.2) can then be given by

$$\begin{aligned} \frac{\partial u(\xi,\tau)}{\partial \tau} &= \frac{1}{D(\xi)}\frac{\partial}{\partial \xi}\Big(D(\xi)^2\frac{\partial u(\xi,\tau)}{\partial \xi}\Big), \quad \text{for } \xi \in (0,1),\ \tau > 0 \\ u(0,\tau) &= u(1,\tau) = 0\ , \quad \tau > 0 \qquad\qquad D(\xi) = \frac{d_{-\infty}}{1+e^{\frac{\xi L}{\Lambda_d}}} \\ u(\xi,0) &= g(\xi) = \begin{cases} 1 & \xi = \frac{1}{2} \\ 0 & \text{otherwise} \end{cases} \end{aligned} \tag{3.5}$$

Chapter 4

Stationary states and symmetry of the solution

4.1 Stationary states

A stationary state of a differential equation arises when the derivative in time is equal to zero. This means that the solution is independent of time and $V(x,t)$ reduces to $V(x)$.

In the stationary state, equation (3.2) reduces to

$$\frac{d}{dx}\big(d^2(x)\frac{dV(x)}{dx}\big) = V(x)\frac{4r_L d(x)}{r_M}$$

Multiply each side by $V(x)$ and integrate over $x \in (0, L)$. By means of integration by parts and because of the boundary condition introduced earlier, the left side becomes

$$\int_0^L V(x)\frac{d}{dx}\big(d^2(x)\frac{dV(x)}{dx}\big)dx = -\int_0^L \big(\frac{dV(x)}{dx}\big)d^2(x)dx$$

At the end we are left with

$$\int_0^L V^2(x)\frac{4r_L d(x)}{r_M} + \big(\frac{dV(x)}{dx}\big)^2 d^2(x)dx = 0 \tag{4.1}$$

We now prove that $V(x) = 0$ for all $0 \leq x \leq L$

The integrand cannot be negative because all the constants, the diameter function and the squared terms are all greater than or equal to zero. Let us

then assume that the integrand is strictly positive at some point $x_0 \in (0, L)$. Because both $V(x)$ and its derivative are continuous on the interval $x \in (0, L)$, then so is the entire integrand. By the definition of continuity [8], and the assumption that the integrand is strictly positive at x_0, the integrand has to be positive in a small interval about $x = x_0$.This means that the integral has to be greater than zero, which contradicts (4.1). Then the only option left is for the integrand to be equal to zero. This only occur when $V(x)$ is equal to zero as well. $V(x) = 0$ will therefore be the only possible solution in the case where the potential is assumed to be constant in time and when the potential is assumed to vanish at the end points.

4.2 Symmetry of the solution

An interesting aspect regarding the model is how the diameter affects the solution. Figures describing the solutions for different diameter geometry can be found in section 7.2. The figures show a symmetry of the solution about $\xi = \frac{1}{2}$ when the diameter is symmetric. It is therefore interesting to investigate this further from a mathematical point of view.

Consider the problem found in (3.5). Introduce the new variable

$$\eta \in (-\frac{1}{2}, \frac{1}{2})$$

We then want to show that

$$u(\frac{1}{2} + \eta, \tau) = u(\frac{1}{2} - \eta, \tau)$$

if we require symmetry of the initial condition and the diameter function as below

$$\begin{aligned} u(\frac{1}{2} + \eta, 0) = u(\frac{1}{2} - \eta, 0), \qquad & -\frac{1}{2} \leq \eta \leq \frac{1}{2} \\ D(\frac{1}{2} + \eta) = D(\frac{1}{2} - \eta), \qquad & -\frac{1}{2} \leq \eta \leq \frac{1}{2} \end{aligned}$$

First assume that there are functions $v(\eta, \tau)$ and $\tilde{D}(\eta)$ such that

$$v(\eta, \tau) = u(\frac{1}{2} + \eta, \tau) \qquad \tilde{D}(\eta) = D(\frac{1}{2} + \eta)$$

Notice that $\frac{\partial \eta}{\partial \xi} = 1$ and insert the above relations into equation (3.5). We are then left with the following partial differential problem

$$\begin{aligned} \frac{\partial}{\partial \tau} v(\eta, \tau) &= \frac{1}{\tilde{D}(\eta)} \frac{\partial}{\partial \eta} \big(\tilde{D}^2(\eta) \frac{\partial}{\partial \eta} v(\eta, \tau) \big) \\ v(\eta, 0) &= u(\frac{1}{2} + \eta, 0) = u(\frac{1}{2} - \eta, 0) = v(-\eta, 0) \\ v(-\frac{1}{2}, \tau) &= u(0, \tau) = 0 \\ v(\frac{1}{2}, \tau) &= u(1, \tau) = 0 \end{aligned} \tag{4.2}$$

Now the original model has been moved $\frac{1}{2}$ units to the left on the spatial axis, and we want to prove that

$$v(\eta, \tau) = v(-\eta, \tau)$$

The next step is then to introduce the function

$$w(\eta, \tau) = v(-\eta, \tau)$$

This relation can then be inserted into equation (4.2), take notice of the fact that $\frac{\partial \eta}{\partial \xi} = -1$, and the partial differential problem governing $w(\eta, \tau)$ become

$$\begin{aligned} \frac{\partial}{\partial \tau} w(\eta, \tau) &= \frac{1}{\tilde{D}(-\eta)} \frac{\partial}{\partial \eta} \big(\tilde{D}^2(-\eta) \frac{\partial}{\partial \eta} w(\eta, \tau) \big) \\ V(\eta, 0) &= v(-\eta, 0) = v(\eta, 0) \\ V(-\frac{1}{2}, \tau) &= v(\frac{1}{2}, \tau) = 0 \\ V(\frac{1}{2}, \tau) &= v(-\frac{1}{2}, \tau) = 0 \end{aligned} \tag{4.3}$$

Hence w and v are solutions of the same initial value problem. The energy method [9] now implies uniqueness of solution to this problem. Therefore $w(\eta, \tau) = v(\eta, \tau)$ from which it follows that we have spatially symmetry of the solution $u(\frac{1}{2} - \eta, \tau) = u(\frac{1}{2} + \eta, \tau)$.

Chapter 5

Solution methods

5.1 Method 1: Finite difference scheme

Complicated differential equations can usually not be solved analytically. To be able to construct solutions to such problems, numerical methods have to be applied.

The finite difference method is a numerical method that enables us to find an approximated solution to a differential equation. The method replaces the derivatives of the equation by finite differences, and the solutions get approximated at discrete points, also called grid points.

The first step when approximating a solution by means of the finite difference method is to discretize the problem. For this paper, the solution is dependent of a temporal and a spatial variable.

Let us define ξ at discrete points called ξ_i for $i = 0, 1, 2, \ldots, N$. The distance between two spatial points, called the step size in space, become $\Delta\xi = \frac{\xi_N - \xi_0}{N}$, and ξ_i gets defined as $\xi_i = i\Delta\xi$.

Define $\Delta\tau$ as the step size in the time domain. τ then gets defined at discrete points $\tau_j = j\Delta\tau$, for $j \geq 0$. The set of all points (ξ, τ) and the set of all grid points (interior and boundary points) are defined as below

Definition 1

$$\begin{aligned} R &= \left\{(\xi,\tau) \in \mathrm{R}^2 \mid 0 < \xi < 1, \quad 0 < \tau\right\} \\ C &= C_1 \cup C_2 \cup C_3 \\ C_1 &= \left\{(\xi,\tau) \in \mathrm{R}^2 \mid \xi = 0,\, \tau > 0\right\} \\ C_2 &= \left\{(\xi,\tau) \in \mathrm{R}^2 \mid \xi = 1,\, \tau > 0\right\} \\ C_3 &= \left\{(\xi,\tau) \in \mathrm{R}^2 \mid \tau = 0,\, 1 \leq \xi \leq 1\right\} \end{aligned}$$

Definition 2

$$\begin{aligned} R_\Delta &= \{(\xi_i, \tau_j) \in \mathrm{R}^2 \mid i = 1, 2, ..., N-1, \quad j = 1, 2, ...\} \\ C_\Delta &= C_{\Delta 1} \cup C_{\Delta 2} \cup C_{\Delta 3} \\ C_{\Delta 1} &= \{(\xi_i, \tau_j) \in \mathrm{R}^2 \mid \xi_0,\ j = 1, 2, \dots\} \\ C_{\Delta 2} &= \{(\xi_i, \tau_j) \in \mathrm{R}^2 \mid \xi_N,\ j = 1, 2, \dots\} \\ C_{\Delta 1} &= \{(\xi_i, \tau_j) \in \mathrm{R}^2 \mid \tau_0,\ i = 0, 1, 2, \dots, N\} \end{aligned}$$

We can now introduce U_i^j, which represents the approximated value of the solution u at the point (ξ_i, τ_j) on $R_\Delta \cup C_\Delta$. Our goal is to approximate this solution by means of finite differences.

Now that we have discretized the $\xi\tau$-plane, it is time to replace the derivatives with finite differences. By means of Taylor series expansion [10], the derivative in time can be approximated by

$$\frac{\partial u}{\partial \tau}(\xi, \tau) \approx \frac{U_i^{j+1} - U_i^j}{\Delta \tau} \qquad \text{(forward difference approximation)} \quad (5.1)$$

The term involving the derivatives in space gets a bit more complicated. The outer derivative cannot simply be calculated by means of the product rule, because the derivative (the steepness) of the diameter function may have an impact on the consistency of the problem. The steepness can be hard to detect if the step size $\Delta\xi$ is not small enough. In order to avoid this problem the derivatives have to be replaced by finite differences in a manner that preserves the properties of the problem. As a result of this we get

$$\frac{\partial}{\partial \xi}\Big(D(\xi_i)^2 \frac{\partial u(\xi_i, \tau_j)}{\partial \xi}\Big) \approx \frac{D^2_{i+\frac{1}{2}} \frac{U^j_{i+1} - U^j_i}{\Delta\xi} - D^2_{i-\frac{1}{2}} \frac{U^j_i - U^j_{i-1}}{\Delta\xi}}{\Delta\xi}$$

See C.1 for details. Now we can replace the derivatives of equation (3.5) by the finite differences above, and the explicit scheme for the interior points of the domain become

$$U_i^{j+1} = U_{i+1}^j \Big(s \frac{D^2_{i+\frac{1}{2}}}{D_i}\Big) + U_i^j \Big(1 - s \frac{D^2_{i+\frac{1}{2}}}{D_i} - s \frac{D^2_{i-\frac{1}{2}}}{D_i}\Big) + U_{i-1}^j \Big(s \frac{D^2_{i-\frac{1}{2}}}{D_i}\Big) \quad (5.2)$$

on R_Δ where $s = \frac{\Delta\tau}{\Delta\xi^2}$

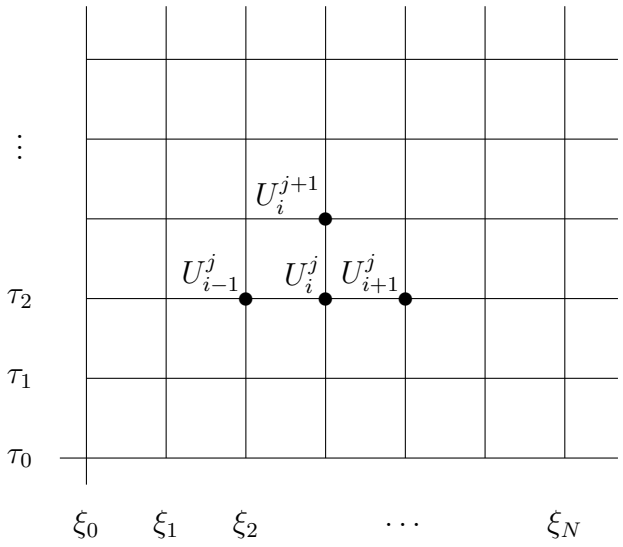

Figure 5.1: Discretization of the $\xi\tau$-plane

Figure 5.1 gives a description of the explicit scheme. To find an approximated value of the solution at the next time step, the approximated value of the solution at the present time step at the previous, present and next space step have to be evaluated.

A formula for the interior grid points has now been defined and we need to specify the properties of the initial and boundary points of the scheme. The discretized form of the boundary conditions become

$$u(0,\tau) = 0 \quad \Rightarrow \quad U_0^j = 0, \qquad u(1,\tau) = 0 \quad \Rightarrow \quad U_N^j = 0, \qquad j > 0$$

and the discretized form of the initial condition becomes

$$U_i^0 = \begin{cases} 1 & \xi_i = \frac{1}{2} \\ 0 & \text{otherwise} \end{cases}, \qquad 0 \geq i \geq N$$

To summarize, the finite explicit scheme corresponding to problem (3.5) is

$$
\begin{aligned}
U_i^{j+1} &= U_{i+1}^j\Big(s\frac{D^2_{i+\frac{1}{2}}}{D_i}\Big) + U_i^j\Big(1 - s\frac{D^2_{i+\frac{1}{2}}}{D_i} - s\frac{D^2_{i-\frac{1}{2}}}{D_i}\Big) + U_{i-1}^j\Big(s\frac{D^2_{i-\frac{1}{2}}}{D_i}\Big) \\
&\text{on } R_\Delta, \qquad s = \frac{\Delta\tau}{\Delta\xi^2} \qquad (5.3) \\
U_0^j = U_N^j &= 0, \qquad j > 0 \\
U_i^0 &= \begin{cases} 1 & \xi_i = \frac{1}{2} \\ 0 & \text{otherwise} \end{cases}, \qquad 0 \geq i \geq N
\end{aligned}
$$

5.2 Method 2: Finite element method

Another numerical method for solving a differential equation is the finite element method [11].

The method begins with deriving a variational formulation. Introduce the space V_0 defined in the following way:

Definition 3

$$
\begin{aligned}
V_0 = H_0^1(I) &= \{v(\xi) \mid v(\xi), v'(\xi) \in L_2(I), v(\xi)|_{\partial I} = 0\} \\
L_2(I) &= \{v(\xi) \mid \int_I |v(\xi)|^2 dx < \infty\} \\
I &= (0,1)
\end{aligned}
$$

Multiply each side of the differential equation in (3.5) by the test function $v(\xi) \in V_0$ and integrate with respect to ξ over I. By means of integration by parts the variational formulation becomes

Find $u(\xi,\tau) \in V_0$ such that

$$
\int_0^1 D(\xi)\frac{\partial u(\xi,\tau)}{\partial \tau}v(\xi)d\xi = -\int_0^1 D^2(\xi)\frac{\partial u(\xi,\tau)}{\partial \xi}\frac{dv(\xi)}{d\xi}d\xi, \quad v \in V_0
$$

The problem regarding the continuous variational formulation is that the space V_0 are of infinite dimension. We therefore have to discretize the interval for the space variable into N subintervals, where V_h become the space of all continuous piecewise linear functions corresponding to the discretization. In

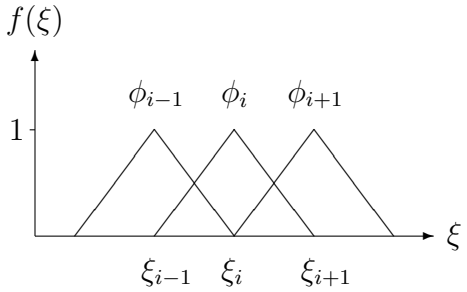

Figure 5.2: The graph of $\phi_i(\xi)$, also called a hat-function

this paper N equal subintervals have been used and the distance between two neighbour points are denoted by $\Delta\xi$.

Define $\phi_i(\xi)$ like

$$\phi_i(\xi) = \begin{cases} \frac{\xi - \xi_{i-1}}{\Delta\xi} & \text{if } \xi_{i-1} \leq \xi \leq \xi_i \\ \frac{\xi_{i+1} - \xi}{\Delta\xi} & \text{if } \xi_i \leq \xi \leq \xi_{i+1} \\ 0 & \text{otherwise} \end{cases} \tag{5.4}$$

Figure 5.2 visualize the function. Introduce $V_{h,0}$, a subspace of V_h, where the boundary conditions as in V_0 has been included

Definition 4

$$V_{h,0} = \{v(\xi) \in V_h, v(\xi)|_{\partial I} = 0\} \tag{5.5}$$

which means that

$$V_{h,0} = \text{span}\{\phi_1, \cdots, \phi_{N-1}\}$$

After making this change of space, the variational formulation for the finite element approximation $u_h(\xi, \tau)$ become

Find $u_h(\xi, \tau) \in V_{h,0}$ such that

$$\int_0^1 D(\xi)\frac{\partial u_h(\xi,\tau)}{\partial \tau}v(\xi)d\xi = -\int_0^1 D^2(\xi)\frac{\partial u_h(\xi,\tau)}{\partial \xi}\frac{dv(\xi)}{d\xi}d\xi, \quad v \in V_0$$

$v(\xi)$ can be replaces by $\phi_i(\xi)$ because the set of $\phi_i(\xi)$ for $i = 1, \ldots, N-1$ represents a basis for $V_{h,0}$. Because the finite element approximation $u_h(\xi, \tau)$

is a part of the same space it can be expressed as a linear combination of the basis functions

$$u_h(\xi,\tau) = \sum_{j=1}^{N-1} \mu_j(\tau)\phi_j(\xi)$$

The variational formulation now reads

$$\sum_{j=1}^{N-1} \frac{d\mu_j(\tau)}{d\tau} \int_0^1 D(\xi)\phi_j(\xi)\phi_i(\xi)d\xi = -\sum_{j=1}^{N-1} \mu_j(\tau) \int_0^1 D(\xi)^2 \frac{d\phi_j(\xi)}{d\xi}\frac{d\phi_j(\xi)}{d\xi}d\xi$$

If we define the matrices A and B and the vector $\vec{\mu_j}(\tau)$ like

$$\begin{aligned} A = [A_{ij}] \Rightarrow A_{ij} &= \int_0^1 D(\xi)^2 \phi_i'(\xi)\phi_j'(\xi)d\xi \\ B = [B_{ij}] \Rightarrow B_{ij} &= \int_0^1 D(\xi)\phi_i(\xi)\phi_j(\xi)d\xi \\ \vec{\mu}(\tau) &= \begin{bmatrix} \mu_1(\tau) \\ \mu_2(\tau) \\ \mu_3(\tau) \\ \vdots \\ \mu_{N-1}(\tau) \end{bmatrix} \end{aligned}$$

the following system of ordinary differentials equation for $\mu_j(\tau)$ appears

$$B\frac{d\vec{\mu}(\tau)}{d\tau} + A\vec{\mu}(\tau) = \vec{0} \tag{5.6}$$

$$A = \begin{bmatrix} b_1 & -c_1 & 0 & \cdots & \cdots & \cdots & 0 \\ -a_2 & b_2 & -c_2 & 0 & & & \vdots \\ 0 & -a_3 & b_3 & -c_3 & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & & & \ddots & \ddots & \ddots & -c_{N-2} \\ 0 & \cdots & \cdots & \cdots & 0 & -a_{N-1} & b_{N-1} \end{bmatrix} \tag{5.7}$$

with

$$\begin{aligned} a_i &= D^2_{i-\frac{1}{2}} \\ b_i &= a_i + c_i \\ c_i &= D^2_{i+\frac{1}{2}} \end{aligned}$$

$$B = \Delta\xi^2 \begin{bmatrix} D_1 & 0 & \dots & \dots & 0 \\ 0 & D_2 & 0 & & \vdots \\ \vdots & 0 & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \ddots & 0 \\ \vdots & \dots & \dots & 0 & D_{N-1} \end{bmatrix} \tag{5.8}$$

In the process of deriving (5.7) and (5.8) we have exploited the properties of the basis functions $\phi_i(\xi)$: For $\mid i-j \mid \leq 1$, we have A_{ij} and B_{ij} different from zero. The coefficients a_i, b_i and c_i are approximated by means of the mid point rule and the trapezoidal rule. The next step is then to solve the differential equation (5.6). This is done by means of a finite difference scheme. First we discretize the temporal variable by introducing the time step $\Delta\tau = \frac{1}{M}$, where M is an integer. $\vec{\mu}^l$ then get defined as the approximated solution for $\vec{\mu}(\tau_l)$ evaluated at the time τ_l for $l = 0, 1, 2, \dots, M$.

Then replace the derivative by the following forward difference approximation

$$\frac{d\vec{\mu}(\tau)}{d\tau} \approx \frac{\vec{\mu}^{l+1} - \vec{\mu}^l}{\Delta\tau}$$

The finite explicit difference scheme corresponding to the differential equation (5.6) then become

$$\vec{\mu}^{l+1} = \big(1 - \Delta\tau\frac{A}{B}\big)\vec{\mu}^l$$

In order to complete the difference scheme, an initial condition has to be defined. When $\tau = 0$, the solution of $u(\xi, \tau)$ take on the form of the initial condition $g(\xi)$. This means that

$$\sum_{j=1}^{N-1} \mu_j^0 \phi_j(\xi) = g(\xi)$$

Now assume that we only evaluate the solution at the points ξ_i in space. Because $\phi_j(\xi_i)$ is equal to 1 for all $j = i$ and zero otherwise, the initial condition (when the solution only get evaluated at the points ξ_i) takes on the values of the initial vector $\vec{g}$, meaning that $\mu_j^0 = g(\xi_j)$.

5.3 Separation of variables

In this section we have used the separation of variable technique [12] on the problem (3.5). We proceed as follows: Let us assume that the solution $u(\xi, \tau)$ can be presented as the product of two functions, one function only dependent on ξ, and the other on τ as below

$$u(\xi, \tau) = X(\xi)T(\tau) \tag{5.9}$$

If we in equation (3.5) replace $u(\xi, \tau)$ by (5.9), see appendix C.3 for details, then we are left with two ordinary differential equations

$$\frac{dT(\tau)}{d\tau}\frac{1}{T(\tau)} = -\lambda, \qquad \frac{1}{D(\xi)}\frac{1}{X(\xi)}\frac{d}{d\xi}\Big(D(\xi)^2\frac{dX(\xi)}{d\xi}\Big) = -\lambda \tag{5.10}$$

$$X(0) = X(1) = 0$$

The ODE involving the spatial variable can be recognized as a regular Sturm-Liouville problem with eigenvalues λ and eigenfunctions $X(\xi)$. Sturm-Liouville theory are presented in appendix B. We have the following result regarding λ:

Result 1 *The eigenvalues of the spatial differential equation have to be strictly positive, e.i.* $\lambda > 0$

See appendix D.1 for the detailed proof. In addition we notice the following property of the eigenfunctions corresponding to different eigenvalues

Result 2 *Two eigenfunction* X_i *and* X_j *are orthogonal with respect to the inner product* $(X_i, X_j)_D = \int_0^1 X_i X_j D(\xi) d\xi$ *, i.e* $(X_i, X_j)_D = 0$ *for* $\lambda_i \neq \lambda_j$.

See appendix D.3 for details.

5.3.1 Method 3a: Separation of variables and finite difference scheme

In order to solve the spatial differential equation in (5.10) a numerical code based on a finite difference scheme is designed. By means of this scheme we get a generalized eigenvalue problem

$$A\vec{v} = \tilde{\lambda}B\vec{v} \tag{5.11}$$

where $\vec{v}$ denote the eigenvectors and $\tilde{\lambda}$ the eigenvalues. The matrices A and B are defined as matrix (5.7) and matrix (5.8) in section 5.2, and the eigenvector as

$$\vec{v} = \begin{bmatrix} X_1 \\ X_2 \\ X_3 \\ \vdots \\ X_{N-1} \end{bmatrix}$$

It is important that the eigenvalue problem made by means of the finite difference scheme preserves the properties of the continuous ODE. Therefore we have the following result proved in appendix D.2

Result 3 *The approximated value of λ has to be strictly positive, e.i. $\tilde{\lambda} > 0$*

The proof that the eigenvectors of equation (5.11) are mutually orthogonal can be found in appendix D.3. Result 3 and the fact that the eigenvectors are mutually orthogonal implies that the finite difference scheme (5.11) has the same properties as the spatial differential equation in (5.10).

After solving the above eigenvalue problem we are left with $N-1$ eigenvalues $\tilde{\lambda}_k$ and $N-1$ eigenvectors $\vec{v}_k$.

The next step on our way to find an approximated solution for $u(\xi, \tau)$ is then to combine the spatial and temporal solution. The analytical solution of the temporal differential equation is given as

$$T(\tau) = Ce^{-\lambda\tau} \tag{5.12}$$

where C is a constant. To construct the approximated solution U we have to multiply each eigenvector by the corresponding temporal part, i.e

$$\vec{U}_k(\tau) = c_k e^{-\tilde{\lambda}_k \tau} \vec{v}_k, \quad k = 1, 2, ..., N-1$$

where c_k are constants. The superposition principle yields

$$\vec{U}(\tau) = \sum_{k=1}^{N-1} c_k e^{-\tilde{\lambda}_k \tau} \vec{v}_k$$

as approximated solution to the original problem.

The constant c_k have been computed in appendix C.5 by means of the initial vector

$$\vec{g} = \begin{bmatrix} g(\xi_1) \\ g(\xi_2) \\ g(\xi_3) \\ \vdots \\ g_{\xi_{N-1}} \end{bmatrix}$$

and the expression for the approximated solution becomes

$$\vec{U}(\tau) = \sum_{k=1}^{N-1} \frac{\vec{v}_k^t B \vec{g}}{\vec{v}_k^t B \vec{v}_k} e^{-\tilde{\lambda}_k \tau} \vec{v}_k, \quad \tau > 0 \tag{5.13}$$

5.3.2 Method 3b: Separation of variables and finite element method

The spatial differential equation in (5.10) can also be solved by means of the finite element method. In order to do this, we first have to derive a variational formulation. Let V_0 be the space defined in definition 3 in section 5.2. Now multiply each side of the differential equation by $v(\xi)$ and integrate over the entire interval for ξ. By means of integration by parts and the fact that $v(\xi)$ vanishes at the endpoints, we are left with the following continuous variational formulation

Find $X(\xi) \in V_0$ such that

$$\int_0^1 D(\xi)^2 X'(\xi) v'(\xi) d\xi = \lambda \int_0^1 D(\xi) X(\xi) v(\xi) d\xi \quad \forall v \in V_0$$

In order for $X(\xi)$ to be in a space of finite dimension a change of space from V_0 to $V_{h,0}$ like in section 5.2 is made. The variational formulation for the finite element approximation $X_h(\xi)$ then become

Find $X_h(\xi) \in V_{h,0}$ such that

$$\int_0^1 D(\xi)^2 X_h'(\xi) v'(\xi) d\xi = \tilde{\lambda} \int_0^1 D(\xi) X_h(\xi) v(\xi) d\xi \quad \forall v \in V_{h,0} \qquad (5.14)$$

where $\tilde{\lambda}$ represent the approximated value of λ.

For the same reasons as in section 5.2, $v(\xi)$ can be replaced by $\phi_i(\xi)$ and the finite element approximation $X_h(\xi)$ can be expressed as

$$X_h(\xi) = \sum_{j=1}^{N-1} \mu_j \phi_j(\xi)$$

where μ_j are constants. In order to find the finite element approximation we need to determine these constants. Equation (5.14) becomes equivalent to

$$\sum_{j=1}^{N-1} \mu_j \int_0^1 D(\xi)^2 \phi_j'(\xi) \phi_i'(\xi) d\xi = \tilde{\lambda} \sum_{j=1}^{N-1} \mu_j \int_0^1 D(\xi) \phi_j(\xi) \phi_i(\xi) d\xi, \quad i = 1, 2, \ldots, N-1$$

This system of equations can be seen as an eigenvalue problem

$$A\vec{\mu} = \tilde{\lambda} B \vec{\mu}$$

where matrix A and B are defined as in (5.7) and (5.8) in section 5.2, and the vector $\vec{\mu}$ by

$$\vec{\mu} = \begin{bmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \\ \vdots \\ \mu_{N-1} \end{bmatrix}$$

The above eigenvalue problem is exactly the same as the one derived in section 5.3.1

The next step it then to combine the spatial and temporal solution. The

analytical solution of the temporal differential equation is given by equation (5.12). Combining the temporal and spatial solution, using the superposition principle, the approximated solution for $u(\xi, \tau)$ becomes

$$u_h(\xi, \tau) = \sum_{k=1}^{N-1} \sum_{j=1}^{N-1} c_k e^{-\tilde{\lambda}_k \tau} \mu_j^{(k)} \phi_j(\xi) \tag{5.15}$$

where $\tilde{\lambda}_k$ represents the approximated value for the eigenvalue λ and $\mu_j^{(k)}$ denote the j'th component of the k'th eigenvector. An equation for calculating the constants c_k has been derived in the appendix C.6.

Chapter 6

Error analysis

6.1 Truncation error for the finite difference scheme

In order to measure the error that arises when the derivatives in a partial differential equation are replaced by finite differences, the truncation error can be used. Because Δ defines the set of all grid points (ξ_i, τ_j), the truncation error Φ is defined as

$$\Phi_i^j = L(u) - L_\Delta(u)$$

where L, a differential operator, and L_Δ, a finite difference operator associated with L, are given by

$$L(u) = \frac{\partial u(\xi_i, \tau_j)}{\partial \tau} - \frac{1}{D(\xi_i)} \frac{\partial}{\partial \xi} \Big(D(\xi_i)^2 \frac{\partial u(\xi_i, \tau_j)}{\partial \xi} \Big) \tag{6.1}$$

$$L_\Delta(u) = \frac{u_i^{j+1} - u_i^j}{\Delta \tau} - \frac{1}{D_i} \Big(\frac{D^2_{i+\frac{1}{2}}(u_{i+1}^j - u_i^j) - D^2_{i-\frac{1}{2}}(u_i^j - u_{i-1}^j)}{\Delta \xi^2} \Big)$$

By replacing the derivatives in $L(u)$ with expressions found by means of Taylor series expansion the truncation error reduces to

$$\Phi_i^j = C\Delta\tau + G\Delta\xi + H\Delta\xi^2$$

where C, G and H are given as.

$$
\begin{aligned}
C &= -\frac{1}{2}\frac{\partial^2 u(\xi_i,\bar{\tau}_j)}{\partial\tau^2} \\
G &= \frac{1}{D_i}\frac{1}{3!8}\Big(D^2_{i+\frac{1}{2}}\big(\frac{\partial^3 u(\bar{\bar{\xi}}_{i+\frac{1}{2}},\tau_j)}{\partial\xi^3}+\frac{\partial^3 u(\bar{\xi}_{i+\frac{1}{2}},\tau_j)}{\partial\xi^3}\big)-D^2_{i-\frac{1}{2}}\big(\frac{\partial^3 u(\bar{\bar{\xi}}_{i-\frac{1}{2}},\tau_j)}{\partial\xi^3}+\frac{\partial^3 u(\bar{\xi}_{i-\frac{1}{2}},\tau_j)}{\partial\xi^3}\big)\Big) \\
H &= \frac{1}{D_i}\frac{1}{3!8}\Big(\frac{\partial^3 \gamma(\bar{\bar{\xi}}_i,\tau_j)}{\partial\xi^3}+\frac{\partial^3 \gamma(\bar{\xi}_i,\tau_j)}{\partial\xi^3}\Big)
\end{aligned}
$$

Details regarding the derivation can be found in appendix E.1. Now it is evident that the truncation error goes to zero as $\Delta\tau$ and $\Delta\xi$ goes to 0.

If we in the derivation of the explicit difference scheme use the product rule on the term involving the derivative in space like below

$$\frac{1}{D(\xi)}\frac{\partial}{\partial\xi}(D(\xi)^2\frac{\partial u(\xi,\tau)}{\partial\xi}) = 2D'(\xi)\frac{\partial u(\xi,\tau)}{\partial\xi}+D(\xi)\frac{\partial^2 u(\xi,\tau)}{\partial\xi^2} \tag{6.2}$$

the finite difference operator associated with L would be

$$L_\Delta(u) = \frac{u_i^{j+1}-u_i^j}{\Delta\tau}-\Big(2D'_i\frac{(u^j_{i+1}-u^j_i)}{\Delta\xi}+D_i\frac{(u^j_{i+1}-2u^j_i+u^j_{i-1})}{\Delta\xi^2}\Big) \tag{6.3}$$

If we assume $L(u)$ to be as in equation (6.1) and $L_\Delta(u)$ as in (6.3), the truncation error becomes

$$
\begin{aligned}
\Phi_i^j = \quad & C\Delta\tau+G\Delta\xi-H\Delta\xi^2+2D'(\xi)\frac{(u^j_{i+1}-u^j_i)}{\Delta\xi} \\
& +D_i\frac{(u^j_{i+1}-2u^j_i+u^j_{i-1})}{\Delta\xi^2}-\frac{1}{D_i}\Big(\frac{D^2_{i+\frac{1}{2}}(u^j_{i+1}-u^j_i)-D^2_{i-\frac{1}{2}}(u^j_i-u^j_{i-1})}{\Delta\xi^2}\Big)
\end{aligned}
$$

where C, G and H are defined above. No matter how we rearrange this equation, the truncation error will not go to zero as $\Delta\xi$ and $\Delta\tau$ go to zero. An explicit scheme based on the assumption that the relation in equation (6.2) is true will therefore not be consistent with the partial differential equation in problem (3.5).

As stated in the derivation of the finite difference scheme, the steepness of the diameter function can give some problems. Assume the differential operator L to be defined by

$$L = \frac{\partial u(\xi_i, \tau_j)}{\partial \tau} - \Big(2D'(\xi_i)\frac{\partial u(\xi_i, \tau_j)}{\partial \xi} + D(\xi_i)\frac{\partial^2 u(\xi_i, \tau_j)}{\partial \xi^2}\Big)$$

and L_Δ like in (6.3). The truncation error for this case then become

$$\Phi_i^j = D'_i\frac{\partial^2 u}{\partial \xi^2}(\bar{\xi}_i, \tau_j)\Delta\xi - \frac{1}{2}\frac{\partial^2 u}{\partial \tau^2}(\xi_i, \bar{\tau}_j)\Delta\tau - D_i\frac{1}{12}\frac{\partial^4 u}{\partial \xi^4}(\bar{\bar{\xi}}_i, \tau_j)\Delta\xi^2$$

The two last terms will in this case tend to zero as $\Delta\xi$ and $\Delta\tau$ goes to zero. The first term on the other hand may grow large because of the steepness of the diameter function, even if $\Delta\xi$ goes to zero.

In section 5.3.1 we have introduced the eigenvalue λ. If the difference scheme given in equation (6.3), which is based on the wrong assumption in equation (6.2), is assumed to be correct, then spurious eigenvalues occur. In table 6.1 corresponding correct and spurious values of the approximated eigenvalues $\tilde{\lambda}_k$ have been listed. The absolute values of the eigenvalues of both set form a decreasing sequence, but in the set of spurious eigenvalues some negative values occasionally occur. This contradicts result 3 in section 5.3.1, which mean that the scheme corresponding to the spurious eigenvalues is not consistent with the partial differential equation (3.5).

Right scheme	Wrong scheme
0,0999	6,1478
0,0709	4,2410
0,0522	-1,8556
0,0390	2,9916
0,0292	2,0852
0,0205	1,2648
0,0126	-0,9489
0,0019	0,4371
0,0061	-0,3107

Table 6.1: Eigenvalues corresponding to the correct finite difference scheme and to a finite difference scheme based on the wrong calculation of the derivative in space. N has been set equal to 10 in both cases.

6.2 Convergence and stability of the finite difference scheme

The truncation error describes how well a finite difference scheme approximates the corresponding differential equation. It does not say anything about how well U_i^j approximate the exact solution $u(\xi, \tau)$. In order to find out whether or not U_i^j is a good approximation for $u(\xi, \tau)$, we have to find out if the approximated solution converges [13] against the exact solution. This means that

$$\lim_{\Delta\xi\to 0, \Delta\tau\to 0} u_i^j - U_i^j = 0 \qquad \text{on} \qquad R_\Delta \cup C_\Delta$$

First, define the error as the difference between the exact and the approximated solution

$$e_i^j = u_i^j - U_i^j$$

The truncation error given by equation (E.1) can be written as

$$u_i^{j+1} = u_{i+1}^j(s\frac{D^2_{i+\frac{1}{2}}}{D_i}) + u_i^j(1 - s\frac{D^2_{i+\frac{1}{2}}}{D_i} - s\frac{D^2_{i-\frac{1}{2}}}{D_i}) + u_{i-1}^j(s\frac{D^2_{i-\frac{1}{2}}}{D_i}) - \Phi_i^j\Delta\tau \quad (6.4)$$

where $s = \frac{\Delta\tau}{\Delta\xi^2}$. Now subtract the difference equation (5.2) from (6.4), and we get the following difference equation for the error

$$e_i^{j+1} = e_{i+1}^j(s\frac{D^2_{i+\frac{1}{2}}}{D_i}) + e_i^j(1 - s\frac{D^2_{i+\frac{1}{2}}}{D_i} - s\frac{D^2_{i-\frac{1}{2}}}{D_i}) + e_{i-1}^j(s\frac{D^2_{i-\frac{1}{2}}}{D_i}) - \Phi_i^j\Delta\tau$$

If we assume

$$0 < s \leq \frac{D_i}{D^2_{i+\frac{1}{2}} + D^2_{i-\frac{1}{2}}}$$

then the triangle inequality can be used and we get the following equation

$$\begin{aligned} \mid e_i^{j+1} \mid &\leq \mid e_{i+1}^j \mid (s\frac{D_{i+\frac{1}{2}}^2}{D_i}) \\ &+ \mid e_i^j \mid (1 - s\frac{D_{i+\frac{1}{2}}^2}{D_i} - s\frac{D_{i-\frac{1}{2}}^2}{D_i}) \\ &+ \mid e_{i-1}^j \mid (s\frac{D_{i-\frac{1}{2}}^2}{D_i}) + \mid \Phi_i^j \mid \Delta\tau \end{aligned} \tag{6.5}$$

Define

$$E_j = max_i \mid e_i^j \mid \qquad \hat{\Phi} = max \mid \Phi_i^j \mid$$

Take the maximum over $0 \leq i \leq N$, and equation (6.5) reduces to

$$E_{j+1} \leq E_j + \Delta\tau\hat{\Phi}$$

After applying the above inequality repeatedly, and by using the fact that $E_0 = 0$ and $j\Delta\tau \leq K$, the inequality reduces to

$$E_j \leq K\hat{\Phi}$$

When $\Delta\xi$ and $\Delta\tau$ goes to zero, so does the truncation error, and hence $\hat{\Phi}$. This means that E_j goes to zero as well. Because E_j is defined as the maximum of the error, the difference between the exact and approximated solution has to go to zero as $\Delta\xi$ and $\Delta\tau$ goes to zero. This means we have convergence.

Above we have assumed

$$0 < s \leq s_i$$

where

$$s_i = \frac{D_i}{D_{i+\frac{1}{2}}^2 + D_{i-\frac{1}{2}}^2} \tag{6.6}$$

In order to have convergence at every point, s has to be less than or equal to the minimum value of s_i. Because $s = \frac{\Delta\tau}{\Delta\xi^2}$, this give us a stability condition

for the finite difference scheme, which means that the scheme is stable under the condition

$$\frac{\Delta\tau}{\Delta\xi^2} \leq min\Big[\frac{D_i}{D^2_{i+\frac{1}{2}} + D^2_{i-\frac{1}{2}}}\Big]$$

Stability can also be proved by means of Lax equivalence theorem [14]

Theorem 6.2.1 (Lax Equivalence Theorem) *Let U_i^j be a consistent approximation to a well-posed linear initial-value problem. U_i^j is then convergent if and only if it is stable.*

6.3 Error estimate for $\tilde{\lambda}$

Theorem 6.3.1 (Convergence of $\tilde{\lambda}$) *Let λ_i be an eigenvalue and $X_i(\xi)$ the eigenfunction of the Sturm-Liouville problem*

$$\begin{aligned} \frac{d}{d\xi}\big(D(\xi)^2\frac{dX_i(\xi)}{d\xi}\big) &= \lambda_i D(\xi) X_i(\xi) \\ X_i(0) = X_i(1) &= 0 \end{aligned} \tag{6.7}$$

and let $\tilde{\lambda}_i$ be the eigenvalue of the generalized eigenvalue problem

$$A\vec{\mu}_i = \tilde{\lambda}_i B\vec{\mu}_i$$

obtained by discretization of the problem (6.7). We then get that

$$\mid \lambda_i - \tilde{\lambda}_i \mid \rightarrow 0 \qquad as \qquad \Delta\xi \rightarrow 0 \tag{6.8}$$

In order to prove Theorem 6.3.1 we derive the Rayleigh coefficient [15]

$$\lambda_i = \frac{\int_0^1 \big(\frac{dX_i(\xi)}{d\xi}\big)^2 D(\xi)^2 d\xi}{\int_0^1 X_i(\xi)^2 D(\xi) d\xi} \tag{6.9}$$

from equation (6.7) by multiplying by the eigenfunction $X_i(\xi)$ and integrate over the interval $\xi \in (0,1)$. Next we derive the Rayleigh coefficient of the corresponding discretized problem, which can be give by

$$\tilde{\lambda}_i = \frac{\vec{\mu}_i^t A\vec{\mu}_i}{\vec{\mu}_i^t B\vec{\mu}_i} \tag{6.10}$$

The integrals of the numerator and denominator in equation (6.9) can be approximated by

$$\begin{aligned}\int_0^1 \big(\frac{dX_i(\xi)}{d\xi}\big)^2 D(\xi)^2 d\xi &= \int_0^1 \pi\Big(\big(\frac{dX_i(\xi)}{d\xi}\big)^2 D(\xi)^2\Big) d\xi + O((\Delta\xi)^2) \\ \int_0^1 X_i(\xi)^2 D(\xi) d\xi &= \int_0^1 \pi\Big(X_i(\xi)^2 D(\xi)\Big) d\xi + O((\Delta\xi)^2)\end{aligned}$$

where $\pi(f)$ denotes the linear interpolant of $f : C^2, \xi \in [0,1]$ given by the mid-point rule and the trapezoidal rule [16]. Further we can proceed as follows

$$\begin{aligned}&\int_0^1 \pi\Big(\big(\frac{dX_i(\xi)}{d\xi}\big)^2 D(\xi)^2\Big) d\xi \\ =\ &\int_0^1 \pi\Big(D(\xi)^2 \sum_{j=1}^{N-1} \mu_j^i \frac{d\phi_j(\xi)}{d\xi} \sum_{k=1}^{N-1} \mu_k^i \frac{d\phi_k(\xi)}{d\xi}\Big) d\xi \qquad (6.11) \\ =\ &\sum_{j=1}^{N-1}\sum_{k=1}^{N-1} \mu_j^i \mu_k^i \int_0^1 \pi\Big(D(\xi)^2 \frac{d\phi_j(\xi)}{d\xi}\frac{d\phi_k(\xi)}{d\xi}\Big) d\xi\end{aligned}$$

and

$$\begin{aligned}&\int_0^1 \pi\Big(X_i(\xi)^2 D(\xi)\Big) d\xi \\ =\ &\int_0^1 \pi\Big(D(\xi) \sum_{j=1}^{N-1} \mu_j^i \phi_j(\xi) \sum_{k=1}^{N-1} \mu_k^i \phi_k(\xi)\Big) d\xi \qquad (6.12) \\ =\ &\sum_{j=1}^{N-1}\sum_{k=1}^{N-1} \mu_j^i \mu_k^i \int_0^1 \pi\Big(D(\xi)\phi_j(\xi)\phi_k(\xi)\Big) d\xi\end{aligned}$$

The last integrals of equation (6.11) and (6.12) can be approximated as in appendix C.2, which means that

$$\begin{aligned}\int_0^1 \big(\frac{dX_i(\xi)}{d\xi}\big)^2 D(\xi)^2 d\xi &= \vec{\mu}_i^t A \vec{\mu}_i + O((\Delta\xi)^2) \\ \int_0^1 X_i^2 D(\xi) d\xi &= \vec{\mu}_i^t B \vec{\mu}_i + O((\Delta\xi)^2)\end{aligned}$$

Hence we get $\lambda_i = \tilde{\lambda}_i + O((\Delta\xi)^2)$ from which it follows that$\tilde{\lambda}_i \to \lambda_i$ as $\Delta\xi$ goes to zero.

Chapter 7

Numerical results

7.1 Comparison of solutions

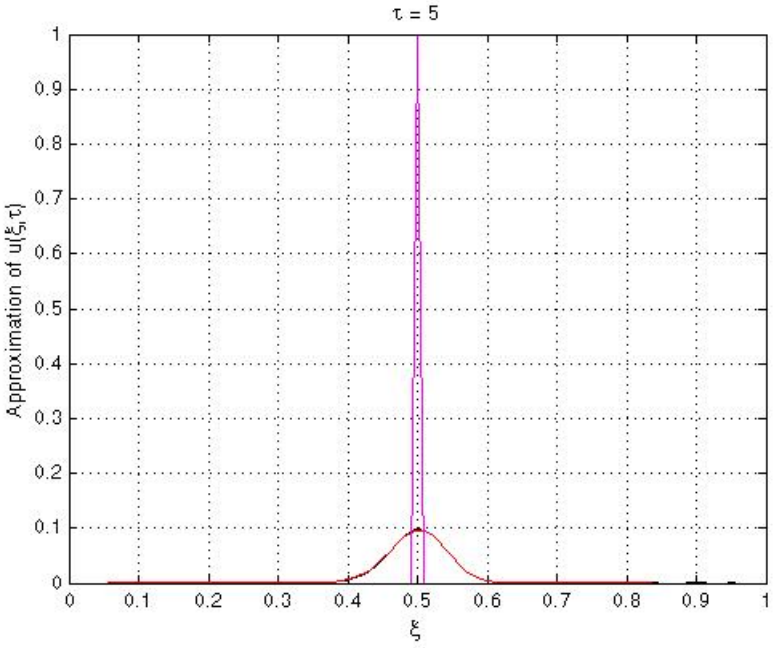

Figure 7.1: Snapshot of the numerical solutions of the model (3.5) for the time $\tau = 5$. Purple line: initial potential. Red line: finite difference scheme. Green line: Finite element method. Blue line: Separation of variables combined with finite difference scheme. Black line: Separation of variables combined with finite element method.

Figure 7.1, 7.2 and 7.3 show snapshots of the approximated solutions of model (3.5) for three different times: $\tau = 5$, $\tau = 50$ and $\tau = 100$ respectively.

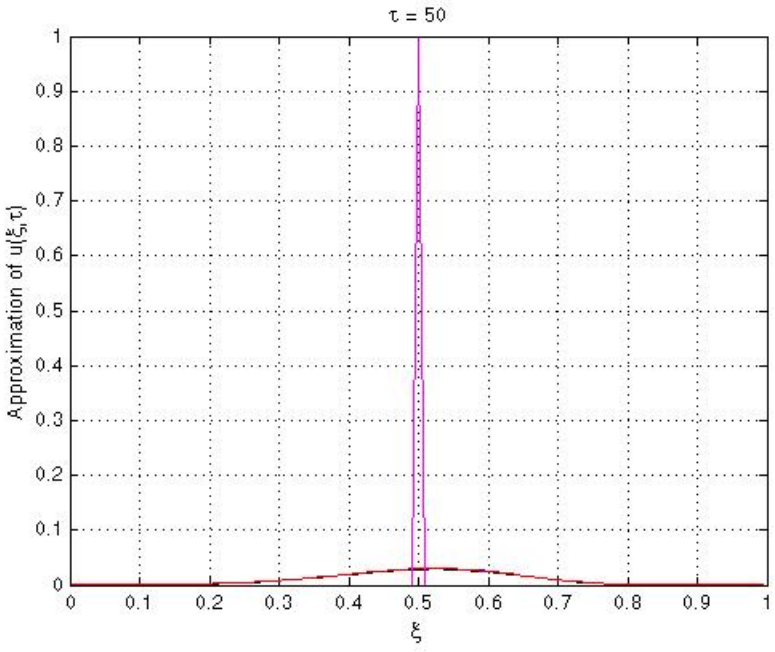

Figure 7.2: Snapshot of the numerical solutions of the model (3.5)for the time $\tau = 50$. The coloured lines represent the same solutions as in figure 7.1

By means of the relation

$$\tau = \frac{t}{T}$$

in section 3.3 this gives the following times: $\tau = 5 \Rightarrow t = 0,0032ms$, $\tau = 50 \Rightarrow t = 0,032ms$ and $\tau = 100 \Rightarrow t = 0,064ms$. Figure 7.4, 7.5 and 7.6 take a closer look at the points where the difference between the solutions are most significant.

The initial data used are the function

$$g(\xi) = \begin{cases} 1 & \xi = \frac{1}{2} \\ 0 & \text{otherwise} \end{cases}$$

and the input data are $\tau = 0,01$ and $N = 100$ which gives $\Delta\xi = 0,01$.

One can see that the solutions tends to 0 as the time increases. This property is expected because as the time increases the membrane potential will always approach the resting potential. The peak of the solutions move toward increasing ξ as the time increases.

The solution of the finite element method ($u_{FEM}(\xi, \tau)$, green line, located behind the blue line) given in section 5.2 and the solution of the finite difference method combined with separation of variables ($u_{sep.FDS}(\xi, \tau)$, blue line)

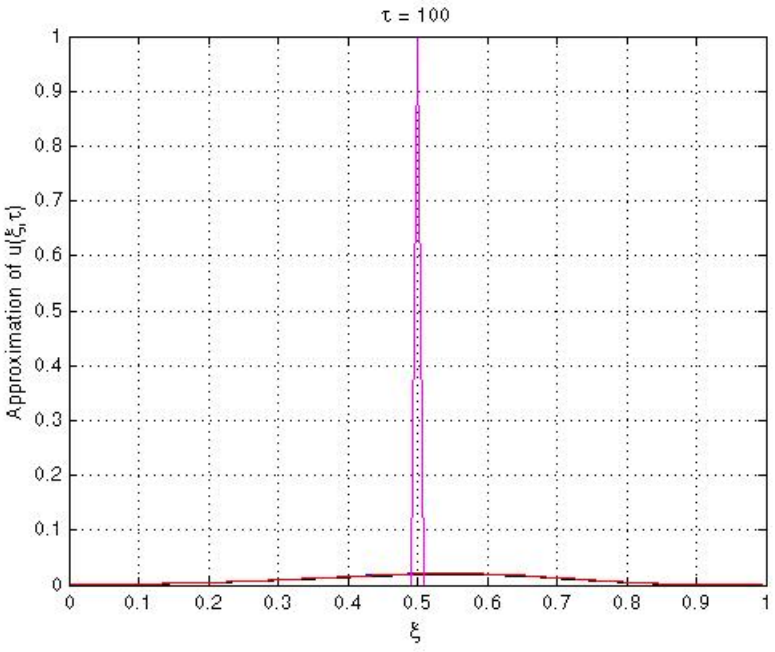

Figure 7.3: Snapshot of the numerical solutions of the model (3.5) for the time $\tau = 100$. The coloured lines represent the same solutions as in figure 7.1.

given by (5.13) gives almost exactly the same solutions

$$u_{FEM}(\xi, \tau) \approx u_{sep.FDS}(\xi, \tau) \qquad \text{for all } \xi \text{ and } \tau$$

The solution of the finite element method combined with separation of variables ($u_{sep.FEM}$ black line) given by (5.15) has in general a much lower value, about 6%, which seems to increase with time, lower than u_{FEM} and $u_{sep.FDS}$. The finite difference solutions (u_{FDS}, red line) given by (5.3) also has a lower value, but is located closer to the first two solutions.

7.2 Solutions for different diameter geometry

Different diameter geometry can model different parts of a dendrite and the change in geometry affects the signal. In figure 7.7, figure 7.8 and figure 7.9 solutions for different diameter geometry have been plotted for different times. The red line and the blue line represents constant diameter. Red line represents the thinnest diameter and the blue line represents the thickest diameter. All the other solutions where variable diameter have been used are located between these two solutions.

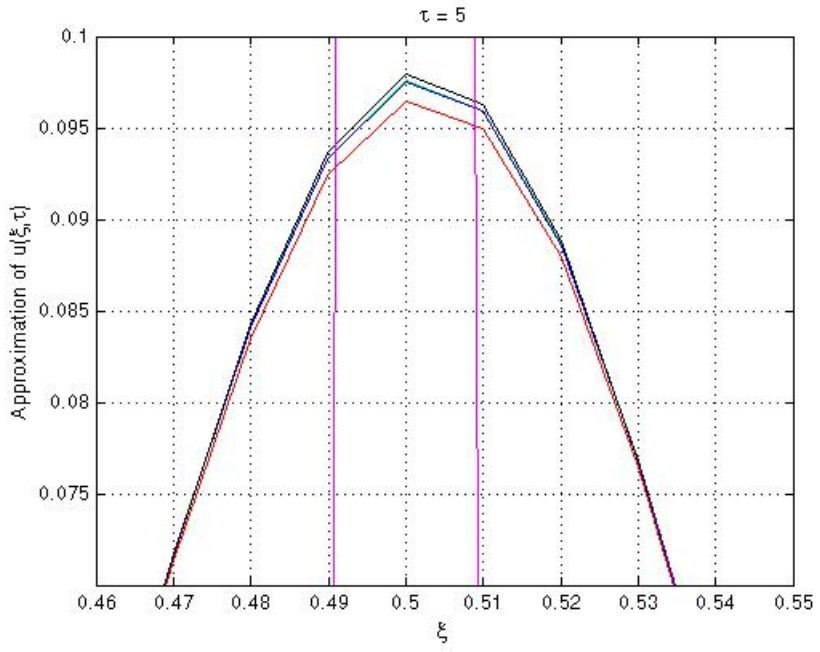

Figure 7.4: Magnified plot of the numerical solutions for the time $\tau = 5$. The coloured lines represents the same solutions as in figure 7.1.

One can see that as the time increases, the solutions modelled by a constant diameter (and therefore a symmetric diameter) tends to decrease and stay symmetric about $\xi = \frac{1}{2}$ consistent with the symmetry analysis done in section 4.2.

In the case of a diameter function modelled by means of the sigmoidal function (3.1) a spatial asymmetry is developed: If the diameter increases with increasing space variable, then the peak of the solutions moves to the left as the time increases. One can also show that if the diameter is a decreasing function of space, the peak of the solution moves to the right.

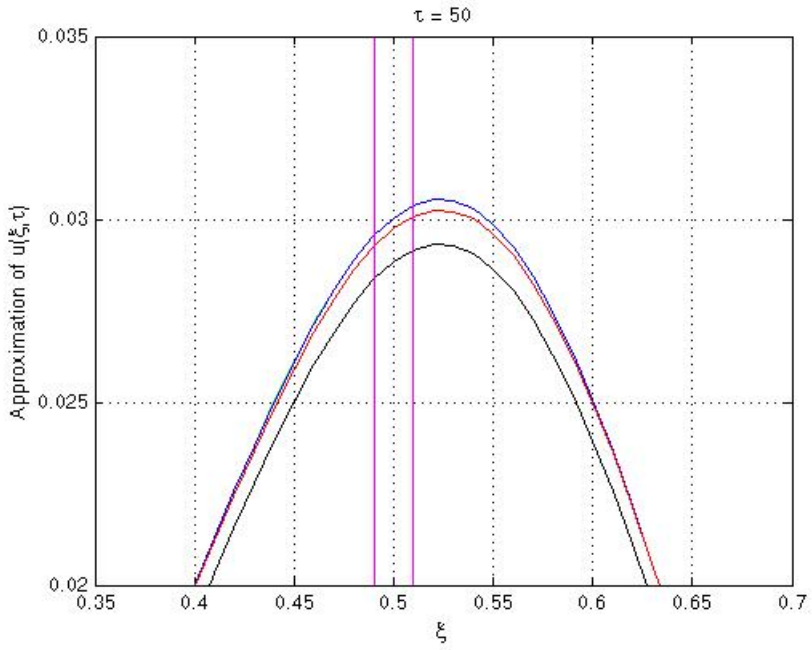

Figure 7.5: Magnified plot of the numerical solutions for the time $\tau = 50$. The coloured lines represents the same solutions as in figure 7.1.

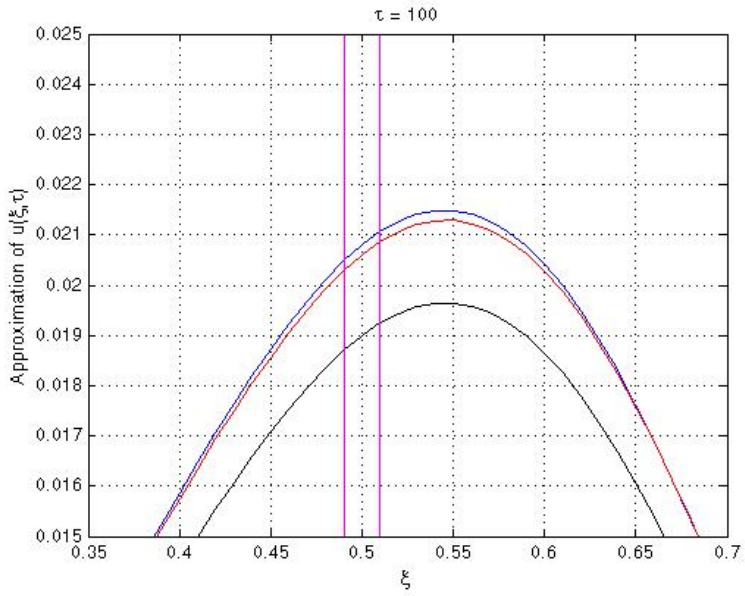

Figure 7.6: Magnified plot of the numerical solutions for the time $\tau = 100$. The coloured lines represents the same solutions as in figure 7.1.

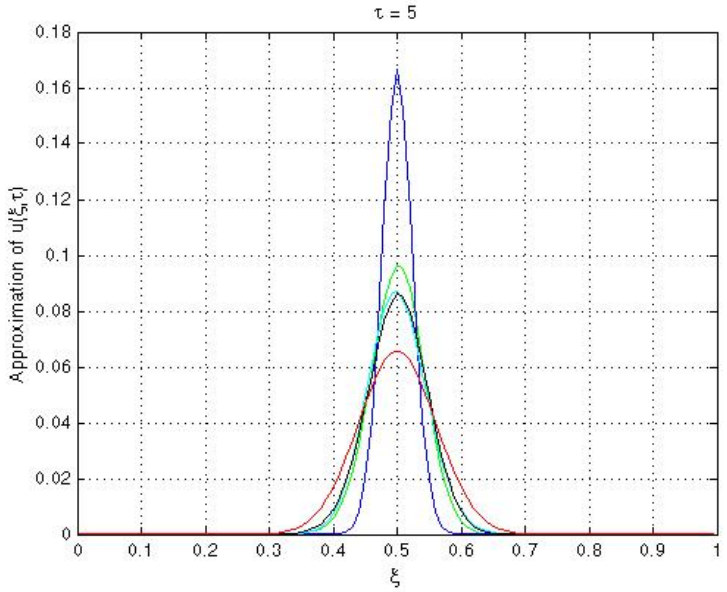

Figure 7.7: Finite difference solution for different diameter geometry for the time $\tau = 5$. Red line: $D(\xi) = 0,00037$. Blue line: $D(\xi) = 0,00006$. Green line: $D(\xi) = \frac{0,00074}{1+e^{2,43\xi}}$. Black line: $D(\xi) = 0,00037 - 0,00031\xi$. Light blue line: $D(\xi) = 0,00006 + 0,00031\xi$.

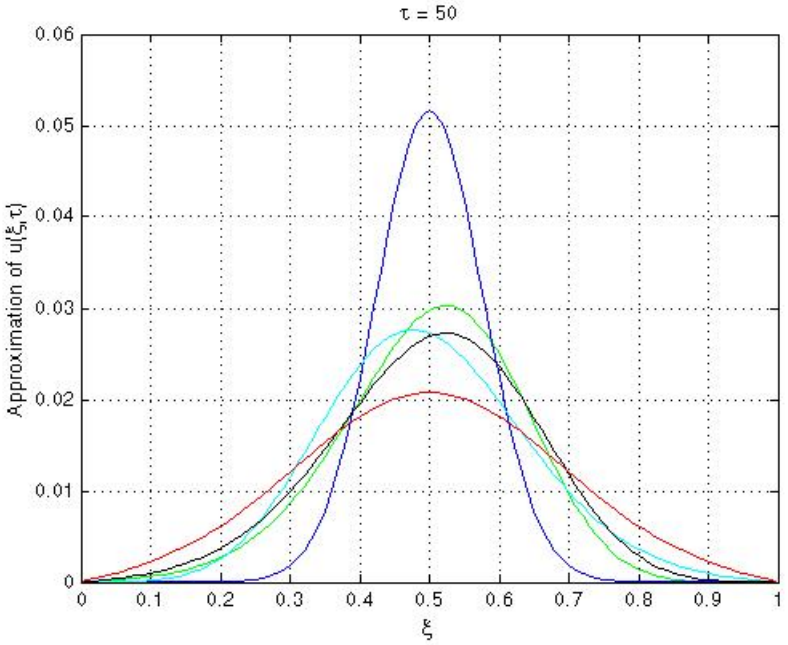

Figure 7.8: Finite difference solution for different diameter geometry for the time $\tau = 50$. The coloured lines represent the same diameters as in figure 7.7

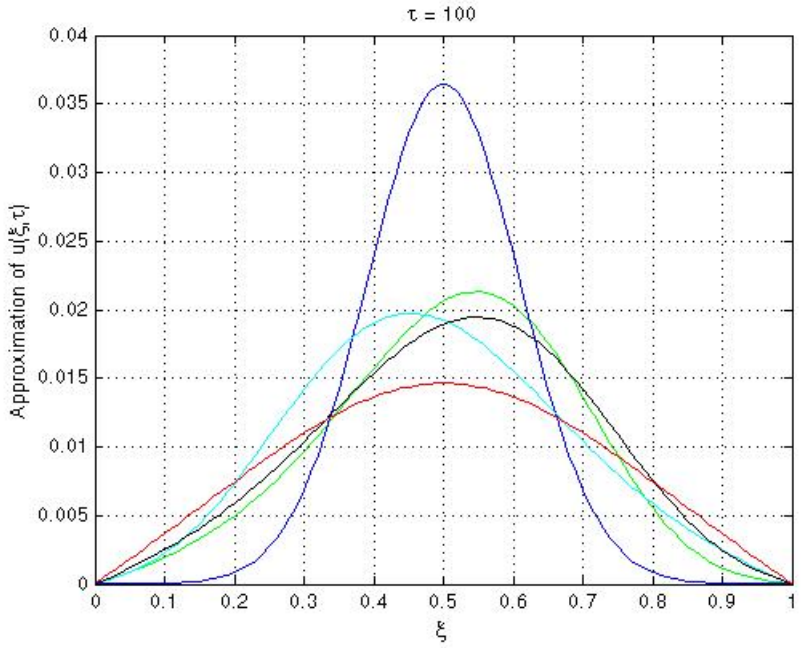

Figure 7.9: Finite difference solution for different diameter geometry for the time $\tau = 100$. The coloured lines represent the same diameters as in figure 7.7

Chapter 8

Conclusion

In the present thesis we have investigated different numerical methods for solving the linear cable equation where the cable diameter is assumed to be modelled by means of a sigmoidal functions. The equation models the propagation of voltage distributed along one single dendrite in a neuron.

The model has been solved in four different ways. The first two methods used were a finite difference scheme and the finite element method. For the last two methods, separation of variables transformed the model into two ordinary differential equations, and then the spatial equation was solved numerically by means of a finite difference scheme and the finite element method.

In the derivation of the finite difference method for both the cable equation and the Sturm-Liouville problem obtained by means of separation of variables technique one has to use a symmetric center difference approximation to obtain consistent schemes.

The derivation of the finite difference scheme certainly needed less work and the programming in Matlab for this method was the easiest one. The other methods had to be done with much more work.

The finite element method and the separation of variables combined with a finite difference scheme offered almost exact similar solutions. From the derivations done in section 5.2 and section 5.3.1 one can see that the two methods both end up with the same coefficient matrices A and B for the discretized problem. The method of separation of variables combined with the finite element method involved the same matrix A and B, but the method gave in general a significant lower value of the solution. The difference was about 6% and seemed to increase with time. It is the eigenvalue of the problem that controls the decay of the solution and it is therefore reasonable to assume that the eigenvalue approximated for this method, which has an approximation error of order $\Delta\xi^2$, may be overestimated. The solution derived

from separation of variables combined with a finite difference scheme lies somewhere in between the other solutions.

All the different solutions revealed qualitatively the same properties. As the time increased, the signal decreased. This is a property that would be expected because the membrane potential will always approach the resting potential, $0mV$ for this model. For the decaying sigmoidal diameter used, the peak of the signal moved towards increasing space variable as the time increased.

The analysis of the stationary state of the model gave a result that was to expect from a neurophysical point of view. If the membrane potential is assumed to be clamped to zero at the ends of the cable and do not change in time, then the potential stay the same.

If we used the finite difference scheme and changed the diameter, then the results showed that the solution, under the assumption that the initial condition were symmetric, would stay symmetric about the mid point in space if the diameter was symmetric about the same point. This result agrees with the analysis done in section 4.

As a future work it would be interesting to give a more exact analysis of the error of each solution method in order to determine the method that gives most realistic solution. It would also be interesting to compare the results from this thesis with the results from the program Neuron. Neuron is based on a finite difference scheme, the Crank Nicolson scheme.

Appendix A

Scaling

We consider the new variables introduced in Chapter 3.3. The derivatives in time and space become

$$\begin{aligned}
\frac{\partial V(x,t)}{\partial t} &= \frac{\partial}{\partial \tau}\left(V_0 u(\xi,\tau)e^{-\frac{\tau T}{\tau_M}}\right)\frac{d\tau}{dt} \\
&= V_0 e^{-\frac{\tau T}{\tau_M}}\left(\frac{1}{T}\frac{\partial u(\xi,\tau)}{\partial \tau} - \frac{1}{\tau_M}u(\xi,\tau)\right) \\
\frac{\partial V(x,t)}{\partial x} &= \frac{\partial}{\partial \xi}\left(V_0 u(\xi,\tau)e^{-\frac{\tau T}{\tau_M}}\right)\frac{\partial \xi}{\partial x} \\
&= V_0 e^{-\frac{\tau T}{\tau_M}}\frac{\partial u(\xi,\tau)}{\partial \xi}\frac{1}{L}
\end{aligned}$$

We insert the derivatives and the new variables into equation (3.5) and get

$$\begin{aligned}
& c_M V_0 e^{-\frac{\tau T}{\tau_M}}\left(\frac{1}{T}\frac{\partial u(\xi,\tau)}{\partial \tau} - \frac{1}{\tau_M}u(\xi,\tau)\right) \\
= \; & -\frac{V_0 u(\xi,\tau)e^{-\frac{t}{\tau_M}}}{r_M} + \frac{1}{4r_L d_0 D(\xi)}\frac{\partial}{\partial \xi}\left(d_0^2 D(\xi)^2 V_0 e^{-\frac{\tau T}{\tau_M}}\frac{\partial u(\xi,\tau)}{\partial \xi}\frac{1}{L}\right)\frac{d\xi}{dx}
\end{aligned}$$

With some rearrangements the equation becomes

$$
\begin{aligned}
& V_0 e^{-\frac{\tau T}{\tau_M}} \Big(\frac{1}{T} \frac{\partial u(\xi,\tau)}{\partial \tau} - \frac{u(\xi,\tau)}{\tau_M} \Big) \\
= \; & V_0 e^{-\frac{\tau T}{\tau_M}} \Big(- \frac{u(\xi,\tau)}{\tau_M} + \frac{d_0}{4 r_L c_M L^2 D(\xi)} \frac{\partial}{\partial \xi} (D(\xi)^2 \frac{\partial u(\xi,\tau)}{\partial \xi}) \Big)
\end{aligned}
$$

and at the end the equation assumes the form

$$
\frac{\partial u(\xi,\tau)}{\partial \tau} = \frac{\alpha}{D(\xi)} \frac{\partial}{\partial \xi} \Big(D(\xi)^2 \frac{\partial u(\xi,\tau)}{\partial \xi} \Big), \qquad \alpha = \frac{T d_0}{4 r_L c_M L^2}
$$

In order to complete the scaling, boundary and initial conditions have to be scaled as well. The two boundary conditions become

$$
\begin{aligned}
V(0,t) &= 0 \quad \Rightarrow \quad u(0,\tau) V_0 e^{-\frac{\tau T}{\tau_M}} = 0 \quad \Rightarrow \quad u(0,\tau) = 0 \\
V(L,t) &= 0 \quad \Rightarrow \quad u(1,\tau) V_0 e^{-\frac{\tau T}{\tau_M}} = 0 \quad \Rightarrow \quad u(1,\tau) = 0
\end{aligned}
$$

and the initial condition can be scaled in the following way

$$
\begin{aligned}
V(\xi,0) = f(x) \quad & \Rightarrow \quad u(\xi,0) V_0 e^{-\frac{0T}{\tau_M}} = f(x) \\
& \Rightarrow \quad u(\xi,0) = \frac{f(x)}{V_0} = g(\xi)
\end{aligned} \tag{A.1}
$$

Appendix B

Sturm Liouville theory

After preforming the method of separation of variable, the ODE depending on the variable ξ become a regular Sturm-Liouville problem.

A Sturm-Liouville problem [12] is an ODE of the form

$$[p(x)y'(x)]' + [q(x) + \lambda r(x)]y(x) = 0, \qquad a < x < b \tag{B.1}$$

with the boundary conditions

$$c_1 y(a) + c_2 y'(a) = 0, \qquad d_1 y(b) + d_2 y'(b) = 0 \tag{B.2}$$

where either c_1 or c_2 has to be different from zero, and either d_1 or d_2 has to be different from zero.

A Sturm-Liouville problem can either be regular or singular. For the regularity conditions we have that $p(x)$, $p'(x)$, $q(x)$ and $r(x)$ have to be continuous on the interval $a \leq x \leq b$. In addition $p(x)$ and $r(x)$ have to be greater than zero on the same interval.

In order for a Sturm-Liouville problem to be singular, the ODE can either be defined on an infinite interval, or defined on a finite interval where one or more of the regularity properties fails.

A non-trivial solution of (B.1) with boundary conditions (B.2) is called an eigenfunction, while the corresponding value λ is called an eigenvalue.

Theorem B.0.1 *The eigenvalues of a regular Sturm-Liouville problem are all real and form an increasing sequence* $\lambda_1 < \lambda_2 < \lambda_3 < \cdots$ *where* $\lambda \to \infty$ *as* $j \to \infty$

To each eigenvalue of a regular Sturm-Liouville problem there exists only one linear independent eigenfunction, and the eigenfunctions are orthogonal with respect to the weight function $r(x)$. The last part of the statement above can be true for a singular problem as well, assumed that the following condition is fulfilled

$$\lim_{x\to b}[p(x)(y_1(x)y_2'(x)-y_2(x)y_1'(x))]-\lim_{x\to a}[p(x)(y_1(x)y_2'(x)-y_2(x)y_1'(x))]=0$$

where y_1 and y_2 are eigenvalues corresponding to the distinct eigenvalues λ_1 and λ_2 respectively.

The statements above can be summarized in theorem B.0.2 found in [12]

Theorem B.0.2

1. *Each eigenvalue of a regular Sturm-Liouville problem has just one linearly independent eigenfunction corresponding to it.*

2. *Eigenfunctions corresponding to different eigenvalues of a regular Sturm-Liouville problem are orthogonal with respect to the weight function $r(x)$.*

The Sturm-Liouville problem for this paper become

$$\frac{d}{d\xi}\Big(D(\xi)^2\frac{dX(\xi)}{d\xi}\Big)+\lambda X(\xi)D(\xi)=0 \tag{B.3}$$

with the boundary conditions $X(0)=X(1)=0$.
The problem is regular since $D(\xi)$ is strictly positive and smooth.

Appendix C

Derivation of numerical solutions

C.1 Derivation of the finite difference scheme

Let us introduce the variable

$$\gamma(\xi_i, \tau_j) = D^2(\xi_i)\frac{\partial u(\xi_i, \tau_j)}{\partial \xi}$$

By means of a centred difference approximation, the derivative of γ with respect to ξ around the point ξ_i can be approximated by

$$\frac{\partial \gamma}{\partial \xi} \approx \frac{\gamma^j_{i+\frac{1}{2}} - \gamma^j_{i-\frac{1}{2}}}{\Delta \xi}$$

where γ^j_i present the approximated value of $\gamma(\xi_i, \tau_j)$. Then we have to approximate the quantities $\gamma^j_{i+\frac{1}{2}}$ and $\gamma^j_{i-\frac{1}{2}}$. This is done again by using a centred difference approximation, but this time around the points $\xi_{i+\frac{1}{2}}$ and $\xi_{i-\frac{1}{2}}$. The quantities become

$$\gamma^j_{i+\frac{1}{2}} = D^2_{i+\frac{1}{2}}\frac{U^j_{i+1} - U^j_i}{\Delta \xi} \qquad \gamma_{i-\frac{1}{2}} = D^2_{i-\frac{1}{2}}\frac{U^j_i - U^j_{i-1}}{\Delta \xi}$$

This means that $\frac{\partial \gamma}{\partial \xi}$ can be approximated by

$$\frac{\partial \gamma}{\partial \xi} \approx \frac{D^2_{i+\frac{1}{2}}\frac{U^j_{i+1} - U^j_i}{\Delta \xi} - D^2_{i-\frac{1}{2}}\frac{U^j_i - U^j_{i-1}}{\Delta \xi}}{\Delta \xi} \tag{C.1}$$

C.2 Approximation of the integrals in matrix A and B section 5.2

The mid-point rule [11] has been used to approximate the integrals in matrix A. The rule states that

$$\int_a^b f(x)dx \approx f(m)(b-a), \quad m = \frac{a+b}{2} \quad a \leq x \leq b$$

A_{ij} is zero for $\mid i-j \mid > 1$, and therefore we only need to approximate $A_{i,i-1}$, $A_{i,i+1}$ and $A_{i,i}$. The derivative of $\phi_i(\xi)$ become

$$\phi_i'(\xi) = \begin{cases} \frac{1}{\Delta\xi} & \text{if } \xi_{i-1} \leq \xi \leq \xi_i \\ -\frac{1}{\Delta\xi} & \text{if } \xi_i \leq \xi \leq \xi_{i+1} \\ 0 & otherwise \end{cases} \tag{C.2}$$

Because $\phi_i(\xi)$ and $\phi_{i-1}(\xi)$ only overlap at the interval $\xi \in [\xi_{i-1}, \xi_i]$, $A_{i,i-1}$ become

$$\begin{aligned} A_{i,i-1} &= \int_0^1 D^2(\xi)\phi_i'(\xi)\phi_{i-1}'(\xi)d\xi \\ &= \int_{\xi_{i-1}}^{\xi_i} -D^2(\xi)\frac{1}{\Delta\xi^2}d\xi \\ &\approx -\frac{1}{\Delta\xi}D^2(\xi_{i-\frac{1}{2}}), \quad (m = \xi_{i-\frac{1}{2}}, \quad \xi_i - \xi_{i-1} = \Delta\xi) \end{aligned}$$

$\phi_i(\xi)$ and $\phi_{i+1}(\xi)$ overlap only at the interval $\xi \in [\xi_i, \xi_{i+1}]$, and $A_{i,i+1}$ become

$$\begin{aligned} A_{i,i+1} &= \int_0^1 D^2(\xi)\phi_i'(\xi)\phi_{i+1}'(\xi)d\xi \\ &= \int_{\xi_i}^{\xi_{i+1}} -D^2(\xi)\frac{1}{\Delta\xi^2}d\xi \\ &\approx -\frac{1}{\Delta\xi}D^2(\xi_{i+\frac{1}{2}}), \quad (m = \xi_{i+\frac{1}{2}}, \quad \xi_{i+1} - \xi_i = \Delta\xi) \end{aligned}$$

For $A_{i,i}$ we got that $(\phi_i'(\xi))^2 = \frac{1}{\Delta\xi^2}$ for $\xi \in [\xi_{i-1}, \xi_{i+1}]$, and the integral can be approximated in the following way

$$\begin{aligned} A_{i,i} &= \int_0^1 D^2(\xi)(\phi_i'(\xi))^2 d\xi \\ &= \int_{\xi_{i-1}}^{\xi_i} D^2(\xi)\frac{1}{\Delta\xi^2} + \int_{\xi_i}^{\xi_{i+1}} D^2(\xi)\frac{1}{\Delta\xi^2} \\ &\approx \frac{1}{\Delta\xi}\big(D^2(\xi_{i-\frac{1}{2}}) + D^2(\xi_{i+\frac{1}{2}})\big) \end{aligned}$$

When approximating the integral in matrix B the trapezoidal rule have been used [11]. The rule states that

$$\int_a^b f(x)dx \approx \frac{f(a)+f(b)}{2}(b-a), \quad a \le x \le b$$

We do only need to look at $B_{i,i-1}$, $B_{i,i+1}$ and $B_{i,i}$. Taking into consideration that the basis functions overlap at the same place described above, $B_{i,i-1}$ and $B_{i,i+1}$ reduces to zero as below

$$\begin{aligned} B_{i,i-1} &= \int_0^1 D(\xi)\phi_i(\xi)\phi_{i-1}(\xi)d\xi \\ &= \int_{\xi_{i-1}}^{\xi_i} D(\xi)\frac{(\xi_i-\xi)(\xi-\xi_{i-1})}{\Delta\xi^2}d\xi \\ &\approx \frac{D(\xi_i)(\xi_i-\xi_i)(\xi_i-\xi_{i-1}) + D(\xi_{i-1})(\xi_i-\xi_{i-1})(\xi_{i-1}-\xi_{i-1})}{2\Delta\xi^2} \\ &= 0 \end{aligned}$$

$$\begin{aligned} B_{i,i+1} &= \int_0^1 D(\xi)\phi_i(\xi)\phi_{i+1}(\xi)d\xi \\ &= \int_{\xi_i}^{\xi_{i+1}} D(\xi)\frac{(\xi_{i+1}-\xi)(\xi-\xi_i)}{\Delta\xi^2}d\xi \\ &\approx \frac{D(\xi_{i+1})(\xi_{i+1}-\xi_{i+1})(\xi_{i+1}-\xi_i) + D(\xi_i)(\xi_{i+1}-\xi_i)(\xi_i-\xi_i)}{2\Delta\xi^2} \\ &= 0 \end{aligned}$$

For $B_{i,i}$ we get the following

$$\begin{aligned} B_{i,i} &= \int_0^1 D(\xi)\phi_i(\xi)^2 d\xi \\ &= \int_{\xi_{i-1}}^{\xi_i} D(\xi)\frac{(\xi-\xi_{i-1})^2}{\Delta\xi^2}d\xi + \int_{\xi_i}^{\xi_{i+1}} D(\xi)\frac{(\xi_{i+1}-\xi)^2}{\Delta\xi^2} \\ &\approx \big(\frac{D(\xi_i)(\xi_i-\xi_{i-1})^2 + D(\xi_{i-1})(\xi_{i-1}-\xi_{i-1})^2}{2\Delta\xi^2}\big)(\xi_i-\xi_{i-1}) \\ &+ \big(\frac{D(\xi_{i+1})(\xi_{i+1}-\xi_{i+1})^2 + D(\xi_i)(\xi_{i+1}-\xi_i)^2}{2\Delta\xi^2}\big)(\xi_{i+1}-\xi_i) \\ &= D(\xi_i)\Delta\xi \end{aligned}$$

C.3 The method of separation of variables

For the method of separation of variables assume

$$u(\xi,\tau) = X(\xi)T(\tau)$$

The derivatives become

$$\frac{\partial u(\xi,\tau)}{\partial\tau} = X(\xi)\frac{dT(\tau)}{d\tau}, \qquad \frac{\partial u(\xi,\tau)}{\partial\xi} = T(\tau)\frac{dX(\xi)}{d\xi} \tag{C.3}$$

This can then be put into equation (3.5)

$$X(\xi)\frac{dT(\tau)}{d\tau} = \frac{1}{D(\xi)}\frac{\partial}{\partial\xi}\Big(D(\xi)^2T(\xi)\frac{dX(\xi)}{d\xi}\Big)$$

Divide each side by $X(\xi)T(\tau)$ and we get two equations we can assume to be equal to a constant denoted by $-\lambda$, because the two equation does not depend on the same variable. The two equations that remains to solve are then

$$\frac{dT(\tau)}{d\tau}\frac{1}{T(\tau)} = -\lambda, \qquad \frac{1}{D(\xi)}\frac{1}{X(\xi)}\frac{d}{d\xi}\Big(D(\xi)^2\frac{dX(\xi)}{d\xi}\Big) = -\lambda$$

C.4 Derivation of the spatial eigenvalue problem in section 5.3.1

In order to design a numerical code for the Sturm-Liouville problem based on a finite difference scheme we proceed as follows:

We assume that the spatial variable can be defined only at discrete points ξ_i, where $i = 0, 1, 2, \ldots, N$. Then the step size get defined as $\Delta\xi = \frac{1}{N}$ and the approximation of X at the point ξ_i can be denoted by X_i.

Because of the same reason explained in section C.1, the derivative cannot simply be calculated by means of the product rule. In order to solve this problem, the same approach as i section C.1 has been used.

Assume

$$\gamma(\xi_i) = D(\xi_i)^2\frac{dX(\xi_i)}{d\xi})$$

By means of Taylor series expansion [10], the derivative of γ can be approximated by the centered difference approximation around the point ξ_i

$$\frac{d\gamma}{d\xi} \approx \frac{\gamma_{i+\frac{1}{2}} - \gamma_{i-\frac{1}{2}}}{\Delta\xi}$$

The quantities $\gamma_{i+\frac{1}{2}}$ and $\gamma_{i-\frac{1}{2}}$ can then be approximated by

$$\gamma_{i+\frac{1}{2}} = D^2_{i+\frac{1}{2}}\frac{X_{i+1} - X_i}{\Delta\xi} \qquad \gamma_{i-\frac{1}{2}} = D^2_{i-\frac{1}{2}}\frac{X_i - X_{i-1}}{\Delta\xi}$$

and $\frac{d\gamma(\xi_i)}{d\xi}$ then become

$$\frac{d\gamma(\xi_i)}{d\xi} \approx \frac{D^2_{i+\frac{1}{2}}\frac{X_{i+1}-X_i}{\Delta\xi} - D^2_{i-\frac{1}{2}}\frac{X_i-X_{i-1}}{\Delta\xi}}{\Delta\xi}$$

The approximations of the derivatives can then be put into (B.3)

$$\frac{D^2_{i+\frac{1}{2}}\frac{X_{i+1}-X_i}{\Delta\xi} - D^2_{i-\frac{1}{2}}\frac{X_i-X_{i-1}}{\Delta\xi}}{\Delta\xi} + \tilde{\lambda}X_iD_i = 0$$

By some rearrangements we get the following difference scheme

$$-X_{i-1}(D^2_{i-\frac{1}{2}}) + X_i(D^2_{i+\frac{1}{2}} + D^2_{i-\frac{1}{2}}) - X_{i+1}(D^2_{i+\frac{1}{2}}) = \tilde{\lambda}X_iD_i\Delta\xi^2$$

for $i = 1, 2, \ldots, N-1$, with the boundary conditions $X_0 = X_N = 0$. $\tilde{\lambda}$ denote the approximation of the exact eigenvalue λ

This scheme can then be seen as an eigenvalue problem with $N-1$ eigenvalues $\tilde{\lambda}_i$ and $N-1$ eigenvectors $\vec{v}_i$.

C.5 The constant c_k in section 5.3.1

Define the initial vector as

$$\vec{g} = \begin{bmatrix} g(\xi_1) \\ g(\xi_2) \\ g(\xi_3) \\ \vdots \\ g(\xi_{N-1}) \end{bmatrix} \tag{C.4}$$

If we now impose the initial condition for $\tau = 0$ we get

$$\sum_{k=1}^{N-1} c_k\vec{v}_k = \vec{g}$$

Multiply each side by the product $\vec{v}_l^tB$. As stated in result 2, two eigenvectors of the Sturm-Liouville problem are orthogonal with respect to the weight B, which means that the product $\vec{v}_l^tB\vec{v}_k$ become zero for all $k \neq l$. We are then left with

$$c_k\vec{v}_k^tB\vec{v}_k = \vec{v}_k^tB\vec{g}$$

which give the following expression for the constant c_k

$$c_k = \frac{\vec{v}_k^tB\vec{g}}{\vec{v}_k^tB\vec{v}_k}$$

C.6 The constant c_k in section 5.3.2

Assume τ to be zero and $g(\xi)$ to be the initial condition. We then get the equation

$$\sum_{k=1}^{N-1} c_k \sum_{j=1}^{N-1} \mu_j^{(k)} \phi_j(\xi) = g(\xi)$$

Then evaluate the function $\phi_j(\xi)$ and $g(\xi)$ only at the nodal points ξ_i. $\phi_j(\xi_i)$ then take on the value 1 when $j = i$ and zero otherwise. This means that the above equation reduces to

$$g(\xi_i) = \sum_{k=1}^{N-1} c_k \mu_i^{(k)}$$

Because i goes from 1 to $N-1$, we get a system of $N-1$ equation which can be written on compact matrix form as

$$\vec{g} = \Omega \vec{c}$$

where $\vec{g}$ is define as in equation (C.4) and

$$\Omega = \begin{bmatrix} \vec{\mu}^{(1)} & \vec{\mu}^{(2)} & \cdots & \vec{\mu}^{(N-1)} \end{bmatrix} \qquad c = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_{N-1} \end{bmatrix}$$

Appendix D

Proof of result 1, 2 and 3

D.1 Result 1: $\lambda > 0$

From theorem B.0.1 we get that the eigenvalues of a Sturm-Liouville problem forms an increasing sequence. Here we prove explicitly that the eigenvalues λ corresponding to (B.3) are strictly positive.
Let us consider (B.3). First we multiply each term by $X(\xi)$ and then integrate over $\xi \in (0, 1)$.

$$\int_0^1 \frac{d}{d\xi}\Big(D(\xi)^2 \frac{dX(\xi)}{d\xi}\Big) X(\xi) d\xi = -\int_0^1 \lambda X(\xi)^2 D(\xi) d\xi$$

By means of integration by part the equation can be written as

$$\Big[D(\xi)^2 \frac{dX(\xi)}{d\xi} X(\xi)\Big]_0^1 - \int_0^1 (\frac{dX(\xi)}{d\xi})^2 D(\xi)^2 d\xi = -\lambda \int_0^1 X(\xi)^2 D(\xi) d\xi$$

Because of the boundary conditions $X(0) = X(1) = 0$, the first term on the left side of the equation become zero, and we obtain the Rayleigh coefficient

$$\lambda = \frac{\int_0^1 (\frac{dX(\xi)}{d\xi})^2 D(\xi)^2 d\xi}{\int_0^1 X(\xi)^2 D(\xi) d\xi} \tag{D.1}$$

$D(\xi)$ is smooth and the eigenfunctions $X(\xi)$ are non-trivial solutions of the Sturm-Liouville problem (B.3), hence, by (D.1) we get $\lambda > 0$

D.2 Result 2: $\tilde{\lambda} > 0$

From calculations done in the previous section, we know that λ has to be greater than zero. This property has to preserved for the finite difference scheme as well. In (5.11), where $\vec{v} \neq 0$, A is a symmetric diagonal matrix, ($c_i = a_{i+1}$), and thus $A = A^t$. B is a symmetric diagonal matrix as well, and the same relation applies for this matrix.

Let us consider (5.11). We want to find an expression for $\tilde{\lambda}$. First we left-multiply by $\vec{v}^t$ and then rearrange to get the Rayleigh coefficient

$$\tilde{\lambda} = \frac{\vec{v}^t A \vec{v}}{\vec{v}^t B \vec{v}}$$

In order for $\tilde{\lambda}$ to be greater than zero, the denominator has to be greater than zero. Let β_i be the eigenvalues of B, which are all real and strictly positive, and let x_i be the corresponding eigenvectors so that $B\vec{x} = \beta\vec{x}$. From the spectral theorem [18] we have the following implication

$$\begin{aligned} B^t = B \quad &\Rightarrow \quad \vec{v} \in \mathbb{R}^{N-1}, \quad \vec{v} = \sum_{i=1}^{N-1} \mu_i \vec{x_i} \\ &\Rightarrow \quad \vec{x_i}^t \vec{x_j} = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases} \end{aligned}$$

This leads to

$$\begin{aligned} \vec{v}^t B \vec{v} &= \big(\sum_{i=1}^{N-1} \mu_i \vec{x_i}\big)^t B \big(\sum_{j=1}^{N-1} \mu_j \vec{x_j}\big) \\ &= \sum_{i,j=1}^{N-1} \mu_i \mu_j \vec{x}_i^t B \vec{x}_j \\ &= \sum_{i,j=1}^{N-1} \mu_i \mu_j \vec{x}_i^t \beta_j \vec{x}_j \\ &= \sum_{i=1}^{N-1} \beta_i \mu_i^2 > 0 \end{aligned}$$

A similar proof has to be made for the numerator $\vec{v}^t A \vec{v}$. From the spectral theorem we get the implication

$$A^t = A \;\Rightarrow\; \vec{v} \in \mathbb{R}^{N-1}, \quad \vec{v} = \sum_{i=1}^{N-1} \gamma_i \vec{y_i}$$
$$\Rightarrow\; \vec{y_i}^t \vec{y_j} = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases}$$

where $\vec{y_i}$ denotes the eigenvector corresponding to the eigenvalue α_i for the eigenvalue problem, $A\vec{y} = \alpha\vec{y}$. With the same calculations made for the matrix B, the following relation is true:

$$\vec{v}^t A \vec{v} = \sum_{i=1}^{N-1} \alpha_i \gamma_i^2$$

Since A is symmetric, α is real. Moreover $A - \alpha I$ for $\alpha < 0$ is a strictly diagonal dominant matrix. Hence, by Corollary 1 in [19], $A - \alpha I$ for $\alpha < 0$ is invertible, from which it follows that all the eigenvalues of A are positive.

If $\alpha_i = 0$ is a root of the characteristic polynomial $det(A - \alpha I)$ of multiplicity less than or equal to $N - 2$, then $\vec{v}^t A \vec{v} > 0$.

D.3 Result 3: Orthogonal eigenvectors

Another way to verify that (5.11) has the same properties as the corresponding Sturm-Liouville problem is to check whether the eigenfunctions are orthogonal with respect to the weight matrix B Assume $\lambda \neq \mu$ are two eigenvalues with two corresponding eigenvectors $\vec{v}, \vec{w}$. We then get the two equations

$$A\vec{v} = \lambda B\vec{v} \qquad A\vec{w} = \mu B\vec{w}$$

From this we get the identity

$$\begin{aligned} \lambda(B\vec{v})^t\vec{w} &= \lambda\vec{v}^t B^t \vec{w} \\ &= \lambda\vec{v}^t B\vec{w} \\ &= \vec{v}^t A\vec{w} \\ &= \mu\vec{v}^t B\vec{w} = \mu(B\vec{v})^t\vec{w} \end{aligned}$$

Since $\lambda \neq \mu$, the inner product on each side has to be zero, which means that any two eigenvectors have to be orthogonal with respect to the weight matrix B.

Appendix E

Truncation error

E.1 Finite difference scheme

The truncation error for the finite difference scheme is defined as

$$\begin{aligned}\Phi_i^j &= \Big[\frac{\partial u(\xi_i,\tau_j)}{\partial \tau} - \frac{1}{D(\xi_i)}\frac{\partial}{\partial \xi}\Big(D(\xi_i)^2\frac{\partial u(\xi_i,\tau_j)}{\partial \xi}\Big)\Big] \\ &\quad -\Big[\frac{u_i^{j+1}-u_i^j}{\Delta\tau} - \frac{1}{D_i}\Big(\frac{D^2_{i+\frac{1}{2}}(u_{i+1}^j-u_i^j) - D^2_{i-\frac{1}{2}}(u_i^j-u_{i-1}^j)}{\Delta\xi^2}\Big)\Big]\end{aligned} \tag{E.1}$$

By means of Taylor series expansion [10] the derivative in time can be replaced by

$$\frac{\partial u(\xi_i,\tau_j)}{\partial \tau} = \frac{u_i^{j+1}-u_i^j}{\Delta\tau} - \frac{1}{2}\frac{\partial^2 u(\xi_i,\bar{\tau}_j)}{\partial \tau^2}\Delta\tau, \qquad \tau_i < \bar{\tau}_i < \tau_{i+1} \tag{E.2}$$

For the derivative in space we define the variable

$$\gamma(\xi_i,\tau_j) = D(\xi_i)^2\frac{\partial u(\xi_i,\tau_j)}{\partial \xi}$$

We approximate the derivative of γ, as in section C.1, but this time the truncation error of the Taylor series expansion is included. This gives us the expression

$$\frac{\partial \gamma}{\partial \xi} = \frac{\gamma^j_{i+\frac{1}{2}} - \gamma^j_{i-\frac{1}{2}}}{\Delta\xi} - \frac{1}{3!8}\Big(\frac{\partial^3\gamma(\bar{\xi}_i,\tau_j)}{\partial\xi^3} + \frac{\partial^3\gamma(\bar{\bar{\xi}}_i,\tau_j)}{\partial\xi^3}\Big)(\Delta\xi)^2$$

where $\xi_i < \bar{\xi}_i < \xi_{i+\frac{1}{2}}$ and $\xi_{i-\frac{1}{2}} < \bar{\bar{\xi}}_i < \xi_i$

Next, we need to find expressions for $\gamma^j_{i+\frac{1}{2}}$ and $\gamma^j_{i-\frac{1}{2}}$. This is also done in the same way as in section C.1, but the truncation errors are included here as well, i.e.

$$\begin{aligned}
\gamma^j_{i+\frac{1}{2}} &= D^2_{i+\frac{1}{2}}\Big(\frac{u^j_{i+1}-u^j_i}{\Delta\xi} - \frac{1}{3!8}\big(\frac{\partial^3 u(\bar{\xi}_{i+\frac{1}{2}},\tau_j)}{\partial\xi^3} + \frac{\partial^3 u(\bar{\bar{\xi}}_{i+\frac{1}{2}},\tau_j)}{\partial\xi^3}\big)(\Delta\xi)^2\Big)\\
\gamma^j_{i-\frac{1}{2}} &= D^2_{i-\frac{1}{2}}\Big(\frac{u^j_{i}-u^j_{i-1}}{\Delta\xi} - \frac{1}{3!8}\big(\frac{\partial^3 u(\bar{\xi}_{i-\frac{1}{2}},\tau_j)}{\partial\xi^3} + \frac{\partial^3 u(\bar{\bar{\xi}}_{i-\frac{1}{2}},\tau_j)}{\partial\xi^3}\big)(\Delta\xi)^2\Big)
\end{aligned}$$

where

$$\begin{aligned}
\xi_{i+\frac{1}{2}} < \bar{\xi}_{i+\frac{1}{2}} < \xi_{i+1}, \quad \xi_i < \bar{\bar{\xi}}_{i+\frac{1}{2}} < \xi_{i+\frac{1}{2}}\\
\xi_{i-\frac{1}{2}} < \bar{\xi}_{i-\frac{1}{2}} < \xi_{i}, \quad \xi_{i-1} < \bar{\bar{\xi}}_{i-\frac{1}{2}} < \xi_{i-\frac{1}{2}}
\end{aligned}$$

The expression for $\frac{d\gamma}{d\xi}$ then become

$$\begin{aligned}
\frac{\partial\gamma}{\partial\xi} &= D^2_{i+\frac{1}{2}}\Big(\frac{u^j_{i+1}-u^j_i}{\Delta\xi^2} - \frac{1}{3!8}\big(\frac{\partial^3 u(\bar{\xi}_{i+\frac{1}{2}},\tau_j)}{\partial\xi^3} + \frac{\partial^3 u(\bar{\bar{\xi}}_{i+\frac{1}{2}},\tau_j)}{\partial\xi^3}\big)\Delta\xi\Big)\\
&- D^2_{i-\frac{1}{2}}\Big(\frac{u^j_{i}-u^j_{i-1}}{\Delta\xi^2} - \frac{1}{3!8}\big(\frac{\partial^3 u(\bar{\xi}_{i-\frac{1}{2}},\tau_j)}{\partial\xi^3} + \frac{\partial^3 u(\bar{\bar{\xi}}_{i-\frac{1}{2}},\tau_j)}{\partial\xi^3}\big)\Delta\xi\Big)\\
&- \frac{1}{3!8}\Big(\frac{\partial^3\gamma(\bar{\xi}_i,\tau_j)}{\partial\xi^3} + \frac{\partial^3\gamma(\bar{\bar{\xi}}_i,\tau_j)}{\partial\xi^3}\Big)(\Delta\xi)^2
\end{aligned}$$

When the derivatives in the truncation error Φ^j_i are replaced by the expressions found for the derivatives, the terms involving the finite differences disappear, and we are left with the truncation error

$$\Phi^j_i = C\Delta\tau + G\Delta\xi + H\Delta\xi^2 \tag{E.3}$$

where C, G and H are defined as in section 6.1.

Appendix F

Matlab programs

Matlab script for solution method 1, finite difference scheme.

```
N = 100;
M = 100000;

deltaxi = 1/N;
deltatau = 0.01;

xi = 0:deltaxi:1;
xihalv = deltaxi/2:deltaxi:1-deltaxi/2;
tau = 0:deltatau:M*deltatau;

s = deltatau/((deltaxi)^2);

D = 0.00074./(1+exp(2.43.*xi));
Dhalv = 0.00074./(1+exp(2.43.*xihalv));

U = zeros(M+1,N+1);

U(:,1) = 0;
U(:,N+1) = 0;
U(1,(N/2)+1) = 1;

for j = 1:M
    for i = 2:N
                U(j+1,i) = U(j,i+1).*(s.*D(i).^2./D(i))
                + U(j,i).*(1-s.*(D(i).^2./D(i))
                -s.*(D(i-1).^2./D(i))) + U(j,i-1)
```

```
                .*(s.*D(i-1).^2./D(i));
    end
end



figure(1)
plot(xi,U(501,:),'r')
hold on
xlabel('\xi')
ylabel('Approximation of u(\xi,\tau)')
title('\tau = 5')
plot(xi,U(1,:),'m')
grid on

figure(2)
plot(xi,U(5001,:),'r')
hold on
xlabel('\xi')
ylabel('Approximation of u(\xi,\tau)')
title('\tau = 50')
plot(xi,U(1,:),'m')
grid on

figure(3)
plot(xi,U(10001,:),'r')
hold on
xlabel('\xi')
ylabel('Approximation of u(\xi,\tau)')
title('\tau = 100')
plot(xi,U(1,:),'m')
grid on
```

Matlab script for solution method 2, finite element method

```
N = 100;
M = 100000;

deltaxi = 1/N;
deltatau = 0.01;

tau = 0:deltatau:M*deltatau;

xi = 0:deltaxi:1;
xihalv = deltaxi/2:deltaxi:1-deltaxi/2;

my = zeros(M+1,N-1);

my(1,(N/2)) = 1;

D = 0.00074./(1+exp(2.43.*xi));
Dhalv = 0.00074./(1+exp(2.43.*xihalv));

Dvec = D(2:N);
B = (deltaxi.^2).*diag(Dvec);

ACvec = -(Dhalv(2:N-1)).^2;
Bvec = (Dhalv(2:N)).^2+(Dhalv(1:N-1)).^2;

A = diag(ACvec,-1)+diag(ACvec,1)+ diag(Bvec);

K = (B + deltatau.*A)\B;

for l = 1:M
    my(l+1,:) = K*(my(l,:))';
end

Phi = eye(N-1);

U = zeros(M+1,N+1);

U(:,1) = 0;
U(:,N+1) = 0;
```

```
U(1:M+1,2:N) = my;

figure(1)
plot(xi,U(501,:),'g')
hold on

figure(2)
plot(xi,U(5001,:),'g')
hold on

figure(3)
plot(xi,U(10001,:),'g')
hold on
```

Matlab script for solution method 3a, separation of variables and finite difference scheme

```
N = 100;
M = 100000;

deltatau = 0.01;
deltaxi = 1/N;

tau = 0:deltatau:M*deltatau;

xi = 0:deltaxi:1;
xihalv = deltaxi/2:deltaxi:1-deltaxi/2;

D = 0.00074./(1+exp(2.43.*xi));
Dhalv = 0.00074./(1+exp(2.43.*xihalv));

Dvec = D(2:N);
B = (deltaxi.^2).*diag(Dvec);

ACvec = -(Dhalv(2:N-1)).^2;
Bvec = (Dhalv(2:N)).^2+(Dhalv(1:N-1)).^2;

A = diag(ACvec,-1)+diag(ACvec,1)+ diag(Bvec);

E = B\A;

[eigvec,lambda] = eig(E);

lambdak = diag(lambda);

U = zeros(M+1,N+1);
U(:,1) = 0;
U(:,N+1) = 0;
U(1,(N/2)+1) = 1;
g = U(1,2:N);

for l = 2:M+1
      U(l,2:N) = ((eigvec(:,1))'*B*g')/((eigvec(:,1))'
       *(B*eigvec(:,1)))*exp(-lambdak(1).*tau(l))
```

```
    .*eigvec(:,1);
    for k = 2:N-1
        U(l,2:N) =U(l,2:N) + ((g*(B*eigvec(:,k)))/
        ((eigvec(:,k))'*(B*eigvec(:,k)))
        .*exp(-lambdak(k).*tau(l))*eigvec(:,k))';
    end
end




figure(1)
plot(xi,U(501,:))
hold on


figure(2)
plot(xi,U(5001,:))
hold on


figure(3)
plot(xi,U(10001,:))
hold on
```

Matlab script for solution method 3b, separation of variables and finite element method

```
N = 100;
M = 100000;

deltatau = 0.01;
deltaxi = 1/N;

xi = 0:deltaxi:1;
tau = 0:deltatau:M*deltatau;

D = 0.00074./(1+exp(2.43.*xi));

acvec = ((D(3:N).^(2))+(D(2:N-1).^2))./2;
bvec = (D(3:N+1).^2)+(D(1:N-1).^2);

A = diag(-acvec,-1)+diag(-acvec,1)+diag(bvec);

dvec = D(2:N);
B = (deltaxi).^2.*diag(dvec);

C = B\A;

[eigvect,lambdat] = eig(C);

g = zeros(1,N-1);
g((N/2)+1) = 1;

Umat = [eigvect g'];

radred = rref(Umat);

ck = radred(:,N);

U = zeros(M+1,N+1);

U(1,(N/2)+1) = 1;
U(:,1) = 0;
U(:,N+1) = 0;
```

```
Emat = zeros(M,N-1);

for i = 2:M+1
    for k = 1:N-1
        Emat(i,k) = ck(k).*exp(-lambdat(k,k).*tau(i));
    end
end


for l = 2:M+1
   for j = 2:N-1
       U(l,j) = sum(Emat(l,:).*eigvect(j,:));
   end
end


figure(1)
plot(xi,U(501,:),'k')
hold on

figure(2)
plot(xi,U(5001,:),'k')
hold on

figure(3)
plot(xi,U(10001,:),'k')
hold on
```

List of Figures

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