Finite Volume Approximations of Hyperbolic Conservation Law Arising in Neuronal Variability

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Submitted by

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CERTIFICATE

I hereby certify that the work which is being presented in the thesis entitled " **Finite Volume Approximations of Hyperbolic Conservation Law Arising in Neuronal Variability***" in partial fulfillment of the requirements for the award of degree of Master of Science, School of Mathematics and Computer Applications, Thapar University, Patiala is an authentic record of my own work carried out under the supervision of Dr. Paramjeet Singh.*

The matter presented in this thesis has not been submitted for the award of any other degree of this or any other university.

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ABSTRACT

Partial differential equations form the basic tool of many mathematical model in the natural science, engineering, economics, finance and many other fields. A transport equation is general hyperbolic partial differential equation that describe the transport phenomena such as heat transfer, mass transfer, etc. Several biological phenomena can be modeled by the first order hyperbolic partial differential equation which contain negative and positive shift or point-wise delay and advance. In this thesis, we investigate the mathematical and numerical analysis of hyperbolic model for Neuroscience.

Chapter 1 starts with an introduction to classification of partial differential equation, analysis of numerical method (FDM, FVM, FEM) and the brief discussion on hyperbolic conservation law.

In Chapter 2, we discuss the finite volume approximation of hyperbolic conservation law. Initially we derive the general finite volume method for advection equation. Further with the help of general finite volume method, we discuss the Upwind, Lax-Friedrichs and Godunov scheme.
Finally, in Chapter 3, we study the transport equation with negative or positive shift and discuss the Stein's Model. The distribution of firing intervals is written in the term of a transport equation having point-wise delay and advance. Then we construct finite volume approximation based on Godunov scheme for the numerical analysis of neuronal model.

Contents

Chapter 1

Introduction

1.1 Numerical Analysis

Numerical analysis is the branch of mathematics which develops and studies algorithms for the problems of continuous mathematics and the subject can be viewed as: (i) the construction of methods for the solution of specific computational problems, (ii) the provision and investigation of algorithms for fundamental mathematical calculations that are common to many applications, and (iii) the theoretical work on questions that are crucial to the success of algorithms. Its fields of research include function approximation, data fitting and smoothing, optimization, numerical linear algebra (matrix computation), ordinary differential equations, partial differential equations, functional differential equations, computational aspects of dynamical systems, computational neuroscience and many more.

1.2 Partial Differential Equations

Differential equations are the most common and important mathematical models in science and engineering. Many phenomena in nature may be described mathematically by functions of independent variables and parameters. In particular given by a function of position and time.
Partial differential equations (PDE) form the basis of many mathematical models in the natural sciences, engineering, economics, finance, image processing and other fields. Partial differential equation that describes transport phenomena such as heat transfer, mass transfer, fluid dynamics (momentum transfer), etc. All the transfer processes express a certain conservation principle. Gases and liquids surround us, flow inside our bodies, and have a profound influence on the environment in which we live. Fluid flows produce winds, rains, floods, and hurricanes. Convection and diffusion are responsible for temperature fluctuations and transport of pollutants in air, water or soil. Setting up a differential equation model and by choosing appropriate numerical methods, these physical problems can be solved. This help us in deeper exploration of the concepts with the

help of adequate software and programming. It is nowadays referred to as scientific computing and its purpose is to perform simulation of processes in science and engineering [1].
A general formulation of a system of partial differential equation (PDEs) is:

$$\frac{\partial u}{\partial t} = f(t,x,y,z,u,\frac{\partial u}{\partial x},\frac{\partial u}{\partial y},\frac{\partial u}{\partial z},\frac{\partial^2 u}{\partial x^2},\frac{\partial^2 u}{\partial y^2},\frac{\partial^2 u}{\partial z^2},\frac{\partial^2 u}{\partial x \partial y}.....) \tag{1.2.1}$$

The independent variables t,x,y,z, are defined in some region, which may be bounded or unbounded and the variables u is called the dependent variable. It is also a solution of (1.2.1) if they satisfy the PDEs for all t,x,y,z in the region. Among the dependent variables t is used to denote time and x,y,z denote the space variables. If time is among the independent variables, the PDE is called a time-dependent or evolution problem, if not then problem is called an equilibrium or a steady-state problem.
The solution of a PDE is called a field, a function which depends on time and space or just space. The field is scalar-valued if the PDE (1.2.1) is scalar and vector-valued if (1.2.1) is a system of PDEs.

1.2.1 Classification of PDEs

Consider a general scalar linear second order PDE with constant coefficients

$$a\frac{\partial^2 u}{\partial x^2} + 2b\frac{\partial^2 u}{\partial x \partial y} + c\frac{\partial^2 u}{\partial y^2} + d_1\frac{\partial u}{\partial x} + d_2\frac{\partial u}{\partial y} + eu = f(x,y) \tag{1.2.2}$$

Assuming that at least one of a,b,c is $\neq 0$, is classified as following:
hyperbolic if

$$b^2 - ac > 0$$

parabolic if

$$b^2 - ac = 0$$

elliptic if

$$b^2 - ac < 0.$$

If $a = b = c = 0$ but $d_1 \neq 0, d_2 \neq 0$, then equation is said to be hyperbolic partial differential equation of first order.
The following are general cases of partial differential equations of second-order.

Parabolic PDE :

Parabolic PDE in 1-dimension (heat equation) is

$$\frac{\partial u}{\partial t} = c\frac{\partial^2 u}{\partial x^2}, \quad 0 \leq x \leq L, \quad 0 \leq t \leq t_{end} \tag{1.2.3}$$

where c is a positive constant.

Initial condition: $u(x,0) = u_0(x)$, a known function of x

Boundary conditions: $u(0,t) = \alpha(t)$, $u(L,t) = \beta(t)$.

$\alpha(t)$ and $\beta(t)$ are known function of t.

Elliptic PDE :

Elliptic PDE in 2-D (Poisson's equation on the unit square) :

$$\frac{\partial^2 u}{\partial x^2} + c\frac{\partial^2 u}{\partial y^2} = f(x,y) \quad \{(x,y) \in \Omega : 0 \leq x,y \leq 1,) \tag{1.2.4}$$

Boundary condition:$u = 0$, on $\partial\Omega$, the boundary of Ω

The important special case when $f(x,y) = 0$ in (1.2.4) is called Laplace's equation.

Hyperbolic PDE

Hyperbolic in 1-D (wave equation)

$$\frac{\partial^2 u}{\partial t^2} = c\frac{\partial^2 u}{\partial x^2}, \quad 0 \leq x \leq L, \quad 0 \leq t \leq t_{end} \tag{1.2.5}$$

where c is a constant.

Initial condition:

$$u(x,0) = u_0(x), \ \frac{\partial u}{\partial t}(x,0) = \nu_0(x).$$

Boundary conditions:

$$u(0,t) = \alpha(t), u(L,t) = \beta(t)$$

Hyperbolic first order PDE in 1-D (advection equation)

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0, \quad 0 \leq x \leq L, \quad 0 \leq t \leq t_{end}$$

where a is a constant.

Initial condition:$u(x,0) = u_0(x)$, a known function of x

Boundary condition: $u(0,t) = \alpha(t)$.

1.2.2 Importance of Hyperbolic Partial Differential Equations

Hyperbolic partial differential equations arise in many physical problems, typically whenever wave motion is observed. Acoustic waves, electromagnetic waves, seismic waves, shock waves, and many other types of waves can be modeled by hyperbolic equations. Hyperbolic PDEs occur as mathematical models of conservation laws and are found in, e.g., transport process and wave propagation problems. Information travels with finite speed in contrast to parabolic PDEs where an initial value immediately effects the solution in all other space points.

A fundamental property of hyperbolic PDEs is that geometric features like steep fronts, discontinuities in the solution (in the weak sense), are propagated with time. For linear problems jumps come from initial data, while in nonlinear cases discontinuities can develop in the solution even from smooth initial data. Therefore, for hyperbolic PDEs, we are not only interested in the order of accuracy of a method but also in the treatment of discontinuities. Important concepts in the description of the conservation properties dissipation (loss of energy) and dispersion (distorted phase relations due to variable wave speed).

1.3 Introduction to Numerical Methods

In scientific computing the numerical methods used to solve mathematical models should be robust, i.e., they should be reliable and give accurate values for a large range of parameter values. Sometimes, however, a method may fail and give unexpected results. Then it is important to know how to investigate why an erroneous result has occurred and how it can be remedied.

1.3.1 Properties of Numerical Methods

Two basic concepts in numerical analysis are **stability and accuracy**. When choosing a method for solving a differential equation problem it is necessary to have some knowledge about how to analyze the result if the method with respect to these concepts. The solution method should have certain properties. In most cases, it is not possible to analyze the complete solution method. The most important properties are summarized below.

Consistency

Consistency implies that the solution of the partial differential equation, if it is smooth, is an approximate solution of the finite difference scheme.
As the gird spacing tends to zero, the discretization should become exact. The difference between the discretized equation and the exact equation is called the truncation error. It is usually estimated by replacing all the nodal values in the discrete approximation by a Taylors series expansion about a single point. Consistency is certainly necessary for convergence, but a scheme may be consistent but not convergent [2, 3, 4].

Convergence

The most basic property that a scheme must have in order to be useful is that its solutions approximate the solution of the corresponding partial differential equation and that the approximation improves as the grid spacings, h and k, tend to zero. We call such a scheme a **convergent scheme**.

A numerical method is said to converge if the solution of the discretized equations tends to the exact solution of the differential equation as the grid spacing tends to zero. For linear initial value problems, the Lax Equivalence Theorem states that the stability is the necessary and sufficient condition for convergence.
Obviously, a consistent scheme is useless unless the solution method converges. For non-linear problems which are strongly influenced by boundary conditions, the stability and convergence of a method are difficult to demonstrate. Therefore convergence is usually checked using numerical experiments, i.e., repeating the process on series of successively refined grids. If the method is stable and if all approximations used in the discretization process are consistent, we usually find that the solution does converge to a grid-independent solution For sufficiently small grid sizes, the rate of convergence is governed by the order of principal truncation error component. This allows us to calculate the error in the solution [5, 6, 7].

Stability

A numerical solution is said to be stable if it does not magnify the errors that appear in the course of numerical solution process. For temporal problems, stability guarantees that the method produces a bounded solution whenever the solution of the exact equation is bounded. For iterative methods, a stable method is one that does not diverge.
Stability can be difficult to investigate, particularly when boundary conditions and non-linearities are present. For this reason, it is very common to investigate the stability of a numerical method for a linear problems with constant coefficients without boundary conditions. The experience shows that the results obtained by this way can often be applied to more complex problems except few problems. The most widely used approach is to study stability of numerical schemes by the **Von Neumanns Method**. However, when solving complicated, non-linear and coupled equations with complicated boundary conditions, there are few stability results, therefore we have to rely on experience and intuition. Many solution schemes require that the time step be smaller than a certain limit or that under relaxation be used.

Conservation

If the partial differential equations to be solved are conservation laws, the numerical scheme should also obey these laws. This means that, at steady state and in the absence of sources, the amount of a conserved quantity leaving a closed volume is equal to the amount entering that volume. If the strong conservation form of equation and a finite volume are used, this is guaranteed for each individual control volume and for the solution domain as a whole.
Other discretization methods can be made conservative if care is taken in the choice of approxima-

tions. The treatment of sources or sink terms should be consistent so that the total source or sink in the domain is equal to the net flux of the conserved quantity through the boundaries. This is an important property of the solution method, since it imposes a constraint on the solution error. If the conservation of mass, momentum and energy are insured, the error can only improperly distribute these quantities over the solution domain. Non-conservative schemes can produce artificial sources and sinks, changing the balance both locally and globally.
However, non-conservative schemes can be consistent and stable and therefore lead to correct solutions in the limit of very fine grids. The errors due to non-conservation are in most cases appreciable only on relatively coarse grids. The problem is that it is difficult to know on which grid these errors are small enough. Therefore conservation schemes are preferred.

Boundedness

Numerical solutions must lie within proper bounds. Physically non-negative quantities (like density, kinetic energy) must always have positive value; other quantities, such as concentration, must have the value between 0 and 100. In the absence of sources, some equations (example: Heat equation) require that the minimum and maximum values of the variable be found on the boundaries of the domain. These conditions should be inherited by the numerical approximation.
Boundedness is difficult to guarantee. Only some first-order schemes guarantee this property. All higher order schemes produce unbounded solutions when the grids are too coarse. Hence a solution with undershoots and overshoots is an indication that the errors in the solution are large and the grids needs some refinement. The problem is that schemes prone to producing unbounded solutions may have stability and convergence. Therefore these methods should be avoided.

Accuracy

Numerical solutions of physical problems are only approximate solutions. In addition to the errors that might be introduced in the course of the development of the solution algorithm, in programming or setting up the boundary conditions, numerical solutions always have three kinds of systematic errors:
Modeling errors:
These errors are arising due to the difference between the actual flow and the exact solution of the mathematical model.
Discretization errors:
These errors are due to the difference between the exact solution of the conservation equations and the exact solution of the algebraic system of equations which is obtained by discretizing these equations.

Iteration errors:

Iteration errors are defined as the difference between the iterative and exact solutions of the algebraic equations systems. These are also called convergence.

It is important for us to be aware of the existence of these errors, and even more to try to distinguish one error from another. Various may cancel each other, so that sometimes a solution obtained on a coarse grid may agree better with the experiment than a solution on a finer grid, in which, by definition should be more accurate. Modeling errors depends on the assumptions made in deriving the transport equations for the variables. They may be considered negligible when laminar flows are investigated, since the Navier-Stokes equations represent a sufficiently accurate model of the flow. However, for turbulent flows, combustion, etc., the modeling errors may be very large. These errors are also introduced by simplifying the geometry of the solution domain, by simplifying boundary conditions. These errors can be evaluated only by comparing solutions with the accurate experimental data or data obtained by accurate models.

It is essential to control and estimate the convergence and discretization errors before the models of physical phenomena can be judged. The discretization error decreases as the grid is refined. However, on a given grid, methods of same order may produce solution errors which differ by as much as an order of magnitude. This is because the order only tells us the rate at which the error decreases as the mesh spacing is reduced but it gives no information about the error on a single grid. Errors due to iterative solution and round-off are easier to control.

1.3.2 Finite Difference methods

Finite difference method [8] is the oldest method for numerical solution of partial differential equations which is introduced by Euler in the 18^{th} century. Because of the simplicity and easy to use for simple geometries, it is the most popular method for solving partial differential equations. The starting point is the conservation equation in differential form. The given region or domain is divided into a network of rectangles called grid. The points of intersection of these lines are called grid points or mess points. At each grid point, the differential equation is approximated by replacing the partial derivatives by their corresponding difference approximations.

This results in algebraic equations for each grid point, in which the variable value at that point and a certain number of neighbour points appears as unknown. In other words, by knowing the value of the variable at neighbouring points the unknown value of that variable at a particular point can be calculated. In principle, the finite difference method can be applied to any grid type. However, in practice finite difference method is best suitable for only structured grids.

Taylor series expansion or polynomial fitting is used to obtain approximations to the coordinates. When necessary, these methods are also used to obtain variable values at locations other than grid points (interpolation). On structured grids, the finite difference method is very simple and effec-

tive. It is especially easy to obtain higher order schemes on regular grids.
The disadvantage of finite difference methods is that the conservation is not enforced unless special care is taken. Also, the restriction to simple geometries is a significant disadvantage in complex flows. The first step in obtaining a numerical solution is to discretize the geometric domain (i.e. a numerical grid must be defined). Here the grid is usually structured (i.e the grid are equally spaced).
Each grid point is uniquely identified by set of indices (i, j), which define the intersection of grid line. The neighbour points are implicitly defined by increasing or lowering one of the indices by unity. Thus each grid point has one unknown variable associated with it and must provide one algebraic equation. The algebraic equation thus obtained is a relation between the variable values at that point and at some of the neighbouring points. It is obtained by replacing each term of the partial differential equation at the particular point by a finite difference approximation. Also, the numbers of equations and unknowns must be equal. However, at boundary where variable values are known, no equation is needed. When the boundary conditions involve derivatives (as in Neumann conditions), the boundary condition must be discretized to provide the required equation.

1.3.3 Finite Element methods

The finite element is similar to finite difference in several ways. This method is based on the use of functionals. The domain or region is broken into a set of discrete volumes or finite number of subregions called elements that are generally unstructured and over for each element the variational formulation is constructed for the given differential equations using simple functions for approximations. Then the individual elements are assembled and the algebraic systems of equations are formed by a piecewise application of the variational method. To get the better accuracy, it would be sufficient to use finer mesh and there is no need for increase in the number of functional.
The distinguishing feature of finite element method is that the equations are multiplied by a weight function before they are integrated over the entire domain. In the simplest finite element methods, the solution is approximated by a linear shape function with in each element in a way that guarantees continuity of the solution across element boundaries. Such a function can be constructed from its values at the corners of the elements. The weight function is usually of the same form. This approximation is then substituted into the weighted integral of the conservation law and the equations to be solved are derived by required the derivative of the integral with respect to each nodal value to be zero; this corresponds to selecting the best solution within the set of allowed functions (the function with minimum residual) and this results in a set of non-linear algebraic equations. Following are the basic steps involved in the finite element method:
Discretization : The discretization of the given differential equation is obtained by dividing the given domain D into a finite number of elements. The points at which those finite elements inter-

sects are called nodes. The nodes and elements both are numbered by a suitable indices.

Derivation of finite element equations: For any given differential equation, a variational formulation is constructed for each element. Then the element equations are obtained by substituting a typical dependent variable, say

$$u = \sum_{i=1}^{n} u_i \psi_i$$

into the variational formulation. After choosing the variable ψ and the interpolation functions, the element matrices can be computed.

Assembly: After the calculation of element matrices, the next step is to assemble those element equations so that the final solution is continuous. When this assembly is done, the entire system of equations takes the matrix form

$$Au' = F'$$

where A is assemblage property matrix, u' and F' are column vectors containing unknowns and external forces.

Boundary conditions: Apply the boundary conditions for that problem to the above system of equations.

Solution of the equations: Finally the system is solved by any available standard technique, for example Gauss elimination An important advantage of finite element methods is the ability to deal with arbitrary geometries; there is an extensive literature devoted to the construction of grids for finite element methods. The grids are easily refined, each element is simply subdivided. Finite element methods are relatively easy to analyze mathematically and can be shown to have optimality properties for certain types of equations. The principal drawback is that, for unstructured grids, the matrices of the linearized equations are not as well structured as those for regular grids making it more difficult to find efficient solution methods.

1.3.4 Finite Volume Method

Discontinuities [3] lead to computational difficulties, and our main object is the accurate approximation of such solutions. Classical finite difference methods, in which derivatives are approximated by finite differences, can be expected to break down near discontinuities in the solution where the differential equation does not hold. In finite volume methods, which are based on the integral form of conservation laws instead of the differential equation. Rather than point-wise approximations at mesh points, we divide the domain into grid cells and approximate the total integral of unknown function over each grid cell, or actually the cell average of unknown function, which is the integral divided by the volume of the grid. These values are modified in every time step by the flux through the edges of the grid cells, and the primary problem is to determine good numerical

flux functions that approximate the true fluxes reasonably well, based on the approximate cell averages available from the data. We will discuss the class of high-resolution finite volume methods that have been proved to be very effective for computing the solutions of discontinuous problems.

Conclusion : A finite difference method (FDM) discretization is based on the differential form of the PDE to be solved. Each derivative is replaced with an approximate difference formula. The computational domain is usually divided into cells or the grids, and the solution will be obtained at each grid point. The FDM is easiest to understand when the physical grid is Cartesian, but through the use of curvilinear transforms the method can be extended to domains that are not easily represented Cartesian co-ordinates. The discretization results in a system of equation of the variable at grid points, and once a solution is found, then we have a discrete representation of the solution of the given problem.

A finite volume method (FVM) is based upon an integral form of the PDE to be solved (for example conservation of mass, momentum, or energy). The PDE is written in a form which can be solved for a given finite volume (or cell). The computational domain is discretized into finite volumes and then for every volume the resulting governing equations are solved. The resulting system of equations usually involves fluxes of the conserved variable, and thus the calculation of fluxes is very important in FVM. The basic advantage of this method over FDM is that FVM does not require the use of structured grids, and the effort to convert the given mesh in to structured numerical grid internally is completely avoided. As with FDM, the resulting approximate solution is a discrete, but the variables are typically placed at cell centers rather than at nodal points. This is not always true, as there are also face-centered finite volume methods.

A finite element method (FEM) discretization is based upon a piecewise representation of the solution in terms of specified basis functions. The computational domain is divided into smaller domains which are known as finite elements and the solution in each element is constructed from the basis functions. The actual equations that are solved are typically obtained by restating the conservation equation in weak form: the field variables are written in terms of the basis functions, the equation is multiplied by appropriate test functions, and then integrated over an element. Since the FEM solution is in terms of specific basis functions, a great deal more is known about the solution than for either FDM or FVM. The choice of basis functions is very important and boundary conditions may be more difficult to formulate. Then a system of equations is obtained for nodal values and can be solved to find a solution.

1.4 Conservation Law

Any physical law stating that a quantity or property does not change and after an interaction or process is called a conservation law. For example, homogeneous hyperbolic equation are called conservation law. In one space dimension its takes the form

$$\frac{\partial u(x,t)}{\partial t} + \frac{\partial f(u(x,t))}{\partial x} = 0 \tag{1.4.1}$$

where $u : R \times R \to R^n$ is $n-$dimensional vector of conserved quantity or state variables, such as mass, momentum and energy in a fluid dynamic problem. Also u_j is the density function of the j^{th} variable with the interpretation that

$$\int_{x_1}^{x_2} u_j dx$$

is the total quantity of this state variable in the interval $[x_1, x_2]$ at time t. In fact these state variables are conserved means that $\int_{-\infty}^{\infty} u_j dx$ should be constant with respect to time.

1.4.1 The Derivation of Conservation Law

Now we will see how conservation law arise from physical principles. So we will begin deriving the equation for conservation of mass in a one dimensional gas dynamic problem.
For example flow in a tube where properties of the gas such as density and velocity are assumed to be constant across each cross section of the tube. Let x represent the distance along the tube and $\rho(x,t)$ represent the density of the gas at the point x and time t. Then the total mass of guess in any section $[x_1, x_2]$ is

$$\int_{x_1}^{x_2} \rho(x,t) dx.$$

If we assume that the walls of the tube are tight so that mass is neither created nor destroyed, then the mass in this section can change only due to the gas flowing across the end points. Let $v(x,t)$ be the velocity of the gas at the point x and time t. Then the rate of flow or flux of gas at this point is given by
mass flux at $(x,t) = \rho(x,t)v(x,t)$.
The the rate of change of mass in $[x_1, x_2]$ is given by the difference in fluxes at x_1, and x_2 .i.e

$$\frac{d}{dt}\int_{x_1}^{x_2} \rho(x,t) dx = \rho(x_1,t)v(x_1,t) - \rho(x_2,t)v(x_2,t). \tag{1.4.2}$$

This is one of the **integral form of conservation law**. Another form is obtained by integrating this in time t_1 to t_2 giving an expression for the mass in $[x_1, x_2]$ at time $t_2 > t_1$ i.e

$$\int_{x_1}^{x_2} \rho(x,t_2) dx - \int_{x_1}^{x_2} \rho(x,t_1) dx = \int_{t_1}^{t_2} \rho(x_1,t)v(x_1,t) dt - \int_{t_1}^{t_2} \rho(x_2,t)v(x_2,t) dt \tag{1.4.3}$$

To derive the differential form of the conservation law, we must now assume that $\rho(x,t)$ and $v(x,t)$ are differentiable function. Then using

$$\rho(x,t_2)-\rho(x,t_1)=\int_{t_1}^{t_2}\frac{\partial}{\partial t}\rho(x,t)dt \tag{1.4.4}$$

and

$$\rho(x_2,t)v(x_2,t)-\rho(x_1,t)v(x_1,t)=\int_{x_1}^{x_2}\frac{\partial}{\partial x}\rho(x,t)v(x,t)dx \tag{1.4.5}$$

which implies that

$$\int_{t_1}^{t_2}\int_{x_1}^{x_2}\left\{\frac{\partial}{\partial t}\rho(x,t)+\frac{\partial}{\partial x}\rho(x,t)v(x,t)\right\}dxdt=0 \tag{1.4.6}$$

This must hold for any section $[x_1,x_2]$ and over any interval $[t_1,t_2]$. Now (1.4.6) is only hold when integrand must be identically zero, i.e,

$$\rho_t+(\rho v)_x=0.$$

This is the desired **differential form of the conservation law** for the conservation of mass.

1.4.2 Scalar Conservation Law

A scalar conservation law in one space dimension is a first-order partial differential equation of the form

$$u_t+f(u)_x=0.$$

Here $u=u(t,x)$ is the conserved quantity, f is the flux. Equation of this type describes a transport phenomenon and hyperbolic in nature. Integrating the above equation over the interval $[a,b]$, we obtain:

$$\int_a^b\frac{d}{dt}u(t,x)dx=\int_a^b u(t,x)dx=-\int_a^b f(u(t,x))_{xdx}=f(u(t,a))-f(u(t,b)) \tag{1.4.7}$$

In other words, the quantity u is neither created nor destroyed: the total amount of u contained inside any given interval $[a,b]$ can change only due to the flow of u across boundary points. if total mass of the substance is not conserved , then conservation law include source term.

1.4.3 Examples of Scalar Conservation Law

Linear advection equation:

$$\rho_t+(\rho a)_x=\rho_t+a\rho_x=0$$

where a is a constant and $\rho(x,t)$ is density of the fluid. (a) Traffic Flow : Let unknown $\rho(t,x)$ be the density of cars on a highway, and $u(x,t)$ be the velocity at the point x at time t. Since cars are conserved,

$$\rho_t+(\rho u)x=0$$

(b) Burgers equation:

$$u_t + (\frac{u^2}{2})_x = 0$$

with appropriate initial-boundary conditions. This equation occurs in various areas of applied mathematics, such as modeling of gas dynamics and traffic flow.

1.5 Some Definitions

A. Domain of dependence: Let (X,T) be some fixed point in space-time domain. We know that the solution $q(X,T)$ depends on the data q_0 at m particular points.

$$X - \lambda^p T$$

for $p = 1,2,\cdots,m$ These set of points

$$D(X,T) = [X - \lambda_p T; p = 1,2\cdots,m].$$

In other words region bounded by the curve is called domain of dependence.

B. Weak Solution: Solution which are initially smooth become a discontinuity with a finite time is called weak solution. Let $f : \Re^n \to \Re^n$ be a smooth vector field. A measurable function $u = u(t,x)$, defined on an open set $\Omega \subseteq \Re \times \Re$ and with values in $\Re^n$, is a weak solution of the system of conservation laws

$$u_t + f(u)_x = 0$$

C. The Riemann Problem: The Riemann problem is a conservation law together with piecewise constant data having a single discontinuity

$$u_t + f(u)_x = 0$$

$$u(x,0) = \begin{cases} u_L, x < 0 \\ u_R, x > 0 \end{cases}$$

Case(1)

$$u_L > u_R.$$

In this case there is unique weak solution.

$$u(x,t) = \begin{cases} u_L, x < st \\ u_R, x > st \end{cases}$$

where

$$s = \frac{u_L + u_R}{2}$$

is a shock speed at which the discontinuity travels.

Case(2):

In this case infinitely many weak solutions in which discontinuity propagates with speed s.

D. CFL Condition: CFL Condition is a necessary condition for an explicit finite difference scheme for a hyperbolic PDE that of each mesh point the domain of dependence of the PDE must lie within the discrete domain of dependence.

Chapter 2

Finite Volume Approximations of Hyperbolic Equations

In this chapter, firstly we will study the solutions to the Riemann Problem, which gives the equations with some special initial data consisting of a piecewise constant function with single jump discontinuity. Then we discuss the finite volume approximations of hyperbolic conservation law.
Linear hyperbolic systems of the form

$$u_t + Au_x = 0 \tag{2.0.1}$$

if $A \in \Re^{m\times m}$ is diagonalizable with real eigen-values.
We can write

$$A = R\Lambda R^{-1} \tag{2.0.2}$$

Let R be the matrix of right eigen vectors.
By introducing a new variable

$$w = R^{-1}u,$$

we can reduce the system (2.0.1) to

$$w_t + \Lambda w_x = 0 \tag{2.0.3}$$

which is a set of m decoupled advection equation. Here A is a constant.

2.1 Solution of Cauchy Problem

Consider the Cauchy Problem for the constant-coefficient system (2.0.1) in which the data is given

$$u(x,0) = u^0(x), \text{ for } -\infty < x < \infty.$$

From this data we can compute data

$$w^0(x) \equiv R^{-1}u(x)$$

the p^{th} equation of the (2.0.3) is the advection equation is:

$$w_t^p + \lambda^p w_x^p = 0 \tag{2.1.1}$$

with solution

$$w^p(x,t) = w^p(x - \lambda^p t, 0) = w_0^p(x - \lambda^p, t)$$

We can combine these into the vectors $w(x,t)$ and then

$$u(x,t) = Rw(x,t) \tag{2.1.2}$$

gives the original equation of the solution.

2.2 Superposition of Waves and Characteristics Variable

We can write (2.1.1) as

$$u(x,t) = \sum_{p=1}^{m} w^p(x,t) r^p \tag{2.2.1}$$

The vector $u(x,t)$ is a linear combination of the right eigen vectors $r^1, r^2, \cdots, r^m$ at each point in space-time and hence as a superposition of waves propagating at different velocities λ^p.
$w^p(x,t)$ for $p = 1, 2, \cdots, m$ be the strength of each wave.
In equation (2.1.1) show that the eigen coefficient at speed λ^p as time.
i.e

$$w^p(x,t) \equiv w^0 p(x_0)$$

all along the curve

$$X(t) = x_0 + \lambda^p t.$$

These curves are called characteristics of the p^{th} family or p-characteristics. These are straight line in case of constant-coefficient.
The coefficient $w^p(x,t)$ of the eigen vector r^p in the eigen vector expansion (2.2.1) of $u(x,t)$ is constant along any p-characteristics. The function $w^p(x,t)$ are called characteristic variables.

2.3 Discontinous Solution

If the initial data $u^0(x)$ is not smooth or is even discontinuous, at some point x_0, then one or more of the characteristic variable $w^p(x,0)$ will also have discontinuity at this point.
Conversely, if the initial data is smooth in the neighborhood of all points $x^- - \lambda^p t^-$, then the solution $u(x,t)$ must be smooth in a neighborhood of point (x^-, t^-). This means that discontinuity can propagate along characteristics for a linear system.

2.4 Riemann Problem for a Linear System

Riemann Problem consists of the hyperbolic equation together with special initial data that is piecewise with a single jump discontinuity.

$$u^0(x) = \begin{cases} u_l, \ x < 0 \\ u_r, \ x > 0. \end{cases} \tag{2.4.1}$$

For a scalar advection equation

$$u_t + a^- u_x = 0$$

eigen value is $\lambda^1 = a^-$.
We choose eigen vector $r^1 = 1$. Solution to the Riemann problem consists of discontinuity $u_r - u_l$ propagating at speed a^-, along the characterstic and the solution is $u(x,t) = u^0(x - a^- t)$.
If we decompose u_l and u_r as

$$u_l = \sum_{p=1}^{m} w_l^p r^p$$

$$u_r = \sum_{p=1}^{m} w_r^p r^p.$$

The p^{th} advection has Riemann data

$$w_0^p(x) = \begin{cases} w_l^p, \ x < 0 \\ w_r^p, \ x > 0 \end{cases} \tag{2.4.2}$$

and discontinuity propagates with speed λ^p.

$$w^p(x,t) = \begin{cases} w_l^p, \ x - \lambda^p t < 0 \\ w_r^p, \ x - \lambda^p t > 0. \end{cases}$$

Let $P(x,t)$ be the maximum value of p for which $x - \lambda^p t > 0$. Then

$$u(x,t) = \sum_{p=1}^{P(x,t)} w_r^p r^p + \sum_{p=P(x,t)+1}^{m} w_l^p r^p \tag{2.4.3}$$

Rewriting above equation gives

$$u(x,t) = \sum_{p:\lambda^p < x/t} w_r^p r^p + \sum_{p:\lambda^p > x/t} w_l^p r^p$$

the determination of $u(x,t)$ at a given point (X,T) is given by

$$u(X,T) = w_r^1 r^1 + w_l^2 r^2 + w_l^3 r^3.$$

For the case of linear system, solving Riemann problem consists of taking initial data (u_l, u_r) and decomposing the jump $u_r - u_l$ into A.

$$u_r - u_l = \alpha^1 r^1 + \cdots + \alpha^m r^m.$$

Solving the linear system of equations, we obtain

$$R\alpha = u_r + u_l$$

for the vector α, and $\alpha = R^{-1}(u_r + u_l)$ α has component

$$\alpha^p = l^p(u_r + u_l)$$

where l^p be the left eigen-vector and

$$\alpha^p = w_r^p - w_l^p.$$

Since $\alpha^p r^p$ is jump in u across p^{th} have in the solution to the Riemann problem .
We introduce the notation

$$W^p = \alpha^p r^p$$

The wave in two different forms are given by

$$u(x,t) = u_l + \sum_{p:\lambda^p < x/t} W^p$$

$$u(x,t) = u_r + \sum_{p:\lambda^p > x/t} W^p.$$

This can also be written as

$$u(x,t) = u_l + \sum_{p=1}^{m} H(x - \lambda^p t) W^p$$

where $H(x)$ is a Heaviside function

$$H(x) = \begin{cases} 0, & x < 0 \\ 1, & x > 0. \end{cases}$$

2.5 Finite Volume Methods

In this section, we begin to study finite volume methods for the solution of conservation laws. The fundamental concepts will be introduced, and then we will focus on first-order accurate methods for linear equations, in particular the upwind method for advection equations.

Finite volume methods are closely related to finite difference methods, and a finite volume method can often be interpreted directly as a finite difference approximation to the differential equation. However, finite volume methods are derived on the basis of the integral form of the conservation law, and this formulation have many advantages.

2.6 General Formulation for Conservation Laws

In one space dimension, a finite volume method is based on subdividing the spatial domain into intervals (the finite volumes, also called grid cells) and keeping track of an approximation to the integral of q over each of these volumes. In each time step we update these values using approximations to the flux through the endpoints of the intervals. Denote thei^{th} grid cell by

$$c_i = (x_{i-1/2}, x_{i+1/2})$$

Q_i^n will approximate the average value over the i^{th} interval at time t_n.

$$Q_i^n \approx \frac{1}{\Delta x}\int_{x_{i-1/2}}^{x_{i+1/2}} (q(x,t_n)dx = \frac{1}{\Delta x}\int_{c_i}(q(x,t_n))dx \tag{2.6.1}$$

where $\Delta x = x_{i+1/2} - x_{i-1/2}$ is the length of cell. If $q(x,t)$ is a smooth function, then the integral in (2.6.1) agrees with the value of q at the midpoint of the interval $O(\Delta x^2)$.
The integral form of the conservation law is

$$\frac{d}{dt}\int_{c_i}(q(x,t))dx = f(q(x_{i-1/2},t)) - f(q(x_{i+1/2},t))$$

where Q_i^n be the cell average at time t_n. We want to approximate Q_i^{n+1}, the cell averages at the next time t_{n+1} after a time step of length

$$\Delta t = t_{n+1} - t_n.$$

Integrating above equation in time from t_n to t_{n+1}.

$$\int_{c_i}(q(x,t_{n+1}))dx - \int_{c_i}(q(x,t_n)dx = \int_{t_n}^{t_{n+1}} f(q(x_{i-1/2},t))dt - \int_{t_n}^{t_{n+1}} f(q(x_{i+1/2},t))dt.$$

Dividing both sides by Δx and multiply byΔt to obtain

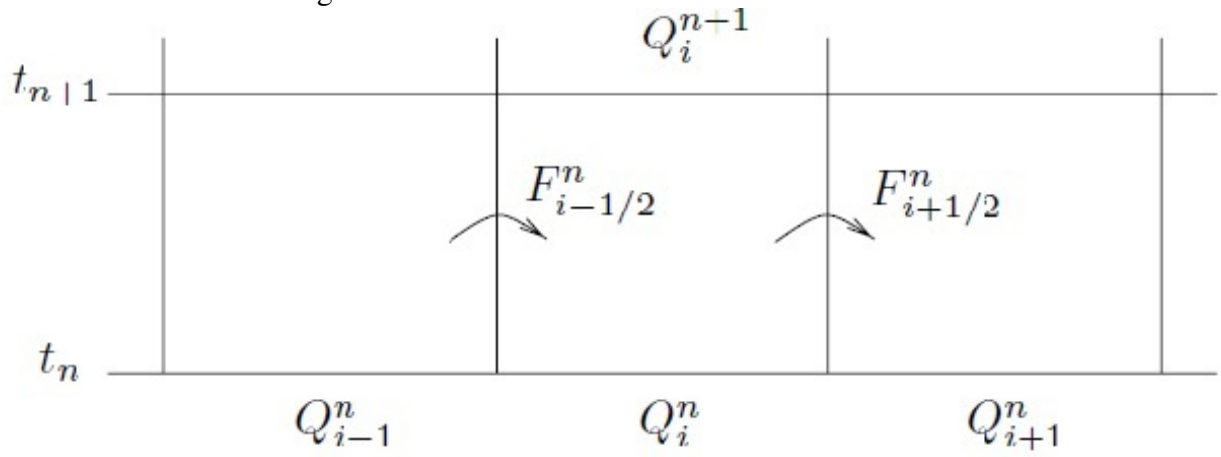
$$\frac{\Delta t}{\Delta x}\int_{c_i}(q(x,t_{n+1})dx = \frac{\Delta t}{\Delta x}\int_{c_i}(q(x,t_n) - \frac{\Delta t}{\Delta x}[\int_{t_n}^{t_{n+1}} f(q(x_{i+1/2},t))dt - \int_{t_n}^{t_{n+1}} f(q(x_{i-1/2},t))dt$$

$$Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x}(F_{i+1/2}^n - F_{i-1/2}^n) \tag{2.6.2}$$

where $F_{i-1/2}^n$ is some approximation to the average flux along $x = x_{i-1/2}$.

$$F_{i-1/2}^n \approx \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} (f(q(x_{i-1/2},t))dt$$

Figure 2.1: Formulation of a finite volume method



If we can approximate this average flux based on the values Q_n, then we will have a fully discrete method. See Figure (2.1) for a schematic of this process.
For a hyperbolic problem information propagates with finite speed, so it is reasonable to first suppose that we can obtain $F_{i-1/2}^n$ based only on the values Q_{i-1}^n and Q_i^n . We use formula

$$F_{i-1/2}^n = \Im(Q_{i-1}^n, Q_i^n).$$

where $\Im$ is numerical flux function, then equation (2.6.2) becomes

$$Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x}[\Im(Q_i^n, Q_{i+1}^n) - \Im(Q_{i-1}^n, Q_i^n)]. \tag{2.6.3}$$

The specific method obtained depends on how we choose the formula F, but in general any method of this type is an explicit method with a three-point stencil, meaning that value Q_i^{n+1} will depend on the three values Q_{i-1}^n,Q_i^n and Q_{i+1}^n at the previous time level. Note that if we sum $\Delta x Q_i^{n+1}$ over any set of cells, we obtain

$$\Delta x \sum_{i=1}^{j} Q_i^{n+1} = \Delta x \sum_{i=1}^{n} -\frac{\Delta t}{\Delta x}(F_{j+1/2}^n - F_{j-1/2}^n)$$

The method (2.6.3) can be viewed as a direct finite difference approximation to the conservation law

$$q_t + f(q)_x = 0,$$

as after rearranging it gives

$$\frac{Q_i^{n+1} - Q_i^n}{\Delta t} + \frac{F_{i+1/2}^n - F_{i-1/2}^n}{\Delta x} = 0. \tag{2.6.4}$$

2.7 A Numerical Flux for the Diffusion Equation

The above derivation was presented for a conservation law in which the flux $f(q)$ depends only on the state q. For example if the flux depends explicitly on x or if it depends on derivatives of the solution such as q_x. Consider diffusion equation

$$q_t = \beta q_{xx}$$

where the flux is $f(q_x, x) = -\beta(x) q_x$.
Given two cell averages Q_{i-1} and Q_i, the numerical flux $\Im(Q_{i-1}, Q_i)$ at the cell interface between can very naturally be defined as

$$\Im(Q_{i-1}, Q_i) = -\beta_{i-1/2} \frac{(Q_i - Q_{i-1})}{\Delta x}$$

where $\beta_{i-1/2} \approx \beta(x_{i-1/2})$.
Using above equation in (2.6.3) gives a standard finite difference discretization of the diffusion equation,

$$Q_i^{n+1} = Q_i^n + \frac{\Delta t}{\Delta x^2}[\beta_{i+1/2}(Q_{i+1}^n - Q_i) - \beta_{i-1/2}(Q_i^n - Q_{i-1}^n)]$$

If $\beta \equiv$ constant, then this takes the simpler form

$$Q_i^{n+1} = Q_i^n + \frac{\Delta t}{\Delta x^2}\beta(Q_{i-1}^n - 2Q_i^n + Q_{i+1}^n)$$

and we recognize the centered approximation to q_{xx}. For parabolic equations, explicit methods of this type are generally not used, since they are only stable.
Crank Nicolson method is given by

$$Q_i^{n+1} = Q_i^n + \frac{\Delta t}{2(\Delta x^2)}[\beta_{i+1/2}(Q_{i+1}^n - Q_i^n) - \beta_{i-1/2}(Q_i^n - Q_{i-1}^n) + \beta_{i+1/2}(Q_{i+1}^{n+1} - Q_i^{n+1})$$

$$-\beta_{i-1/2}(Q_i^{n+1} - Q_{i-1}^{n+1}).$$

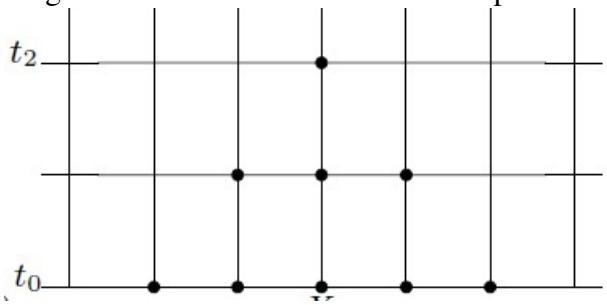
This can also be viewed as finite volume method with flux

$$F_{i-1/2}^n = -\frac{1}{2\Delta x}[\beta_{i-1/2}(Q_i^n - Q_{i-1}^n) + \beta_{i-1/2}(Q_i^{n+1} - Q_{i-1}^{n+1})].$$

2.8 CFL Condition

The CFL condition named after Courant, Friedrichs, and Lewy. This is a necessary condition that must be satisfied by any Finite Volume or Finite Difference Method, if we expect it to be stable and converge to the true solution of the differential equation as the grid is refined.

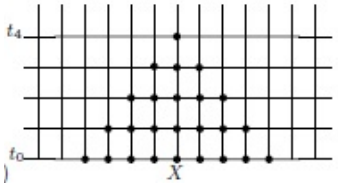
Figure 2.2: Numerical Domain of Dependence



It states that a numerical method can be convergent only if numerical domain of dependence contains the true domain of dependence of the PDE, at least in the limit as Δt and Δx go to zero.
Let $D(X,T)$ be the domain of dependence.

In Fig.(2.2), we see that Q_i^2 depends on Q_{i-1}^1, Q_i^1, Q_{i+1}^1 and hence on $Q_{i-2}^0,\cdots,Q_{i+2}^0$. Only initial data in the interval $X-2\Delta x^a \leq x \leq X+2\Delta x^a$, where Δx^a is the mesh length.
If we refine the grid by a factor of 2 in both space and time but continue to focus on the same physical point (X,T).
Let $\Delta x^b = \frac{\Delta x^a}{2}$

Figure 2.3: Numerical Domain of Dependence on a finer grid with mesh spacing $\Delta x^b = \frac{\Delta x^b}{2}$



In Fig (2.3) the numerical approximation at this point depends on initial data at more points in the interval $X-4\Delta x^b \leq x \leq X+4\Delta x^b$.
If we continue to refine the grid with the ratio $\frac{\Delta t}{\Delta x} \equiv r$, fixed then the numerical domain of dependence of a general point (X,T) is $\frac{X-T}{r} \leq x \leq \frac{X+T}{r}$.
For advection equation

$$q_t + \bar{u} q_x = 0$$

$D(X,T)$ is single point $X-\bar{u}t$, since $q(X,T) = q^0(X-\bar{u}t)$
then the CFL condition requires

$$X - \frac{T}{r} \leq X - \bar{u}T \leq X + \frac{T}{r}.$$

Hence

$$\upsilon = |\frac{\bar{u}\Delta t}{\Delta x}| \leq 1$$

where υ is called CFL number or more frequency Courant number.
For hyperbolic system of equations there are generally a set of m wave speeds $\lambda^1, \lambda^2, \cdots, \lambda^m$. In this case we define the Courant number by

$$\upsilon = \frac{\Delta t}{\Delta x} \max |\lambda^p|.$$

2.8.1 Unstable Flux

Average flux at $x_{i-1/2}$ is given by

$$F^n_{i-1/2} = \Im(Q^n_{i-1}, Q^n_i) = \frac{1}{2}[f(Q^n_{i-1}) + f(Q^n_i)].$$

This method is generally unstable for hyperbolic problems and cannot be used. Even if the time step is small enough that the CFL condition is satisfied.

2.9 Lax-Friedrichs Method

In this finite volume approximation, we approximate both the derivatives by second-order approximation. This Method has the following form:

$$Q^{n+1}_i = \frac{1}{2}(Q^n_{i-1} + Q^n_{i+1}) - \frac{\Delta t}{2\Delta x}(f(Q^n_{i+1}) - f(Q^n_{i-1})) \tag{2.9.1}$$

In equation (2.9.1) Q^n_i is replaced by $\frac{1}{2}(Q^n_{i-1} + Q^n_{i+1})$.
For a linear hyperbolic equation this method is stable provided $\upsilon \leq 1$.
In the form of numerical flux

$$\Im(Q^n_{i-1}, Q^n_i) = \frac{1}{2}[f(Qi-1^n) + f(Q^n_i)] - \frac{\Delta x}{2\Delta t}(Q^n_i - Q^n_{i-1})$$

2.10 The Richtmyer Two Step Lax-Wendroof Method

In this method, second-order accuracy can be achieved by using a better approximation to the integral in

$$F^n_{i-1/2} \approx \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} f(q(x_{i-1/2}, t) dt$$

at $t_{n+1/2}$

$$t_{n+1/2} = t_n + \frac{1}{2}\Delta t$$

The Richtmyer Two Step Lax-Wendroof Method is of this form with

$$F^n_{i-1/2} = f(Q^{n+1/2}_{i-1/2})$$

where

$$Q_{i-1/2}^{n+1/2} = \frac{1}{2}(Q_{i-1}^n + Q_{i+1}^n) - \frac{\Delta t}{2\Delta x}[f(Q_i^n) - f(Q_{i-1}^n].$$

2.11 Upwind Method

Upwind method is a one-sided method with Q_i^{n+1} determined based on values only to the left or only to the right. For a system of equations there may be waves traveling in both directions, we can still use information from both sides, but typically uses characteristic decomposition to select which information to use from each side.

2.11.1 Upwind Method for Advection Equation

Advection equation is given by

$$q_t + \bar{u}q_x = 0.$$

Numerical flux is given by

$$\Im_{i-1}^n = \bar{u}Q_{i-1}^n$$

First-order upwind method for advection equation is given by

$$Q_i^{n+1} = Q_i^n - \frac{\bar{u}\Delta t}{\Delta x}(Q_i^n - Q_{i-1}^n).$$

The above equation can also be written as

$$\frac{(Q_i^{n+1} - Q_i^n)}{\Delta t} + \bar{u}\frac{(Q_i^n - Q_{i-1}^n)}{\Delta x} = 0$$

whereas unstable centered method from Lax-Freidrichs as following:

$$Q_i^{n+1} = Q_i^n - \frac{\Delta t}{2\Delta x}(f(Q_{i+1}^n) - f(Q_{i-1}^n))$$

By applying to the advection equation yields

$$\frac{Q_i^{n+1} - Q_i^n}{\Delta t} + \bar{u}\frac{(Q_{i+1}^n - Q_{i-1}^n)}{2\Delta x} = 0.$$

The upwind method uses a one-sided approximation to the derivative q_x in place of the centered approximation. Another interpretation of the upwind method is shown in Figure (2.4-2.5). If we think of the Q_i^n as being values at grid points, $Q_i^n \approx q(x_i, t_n)$ as is standard in a finite difference method, then since $q(x,t)$ is constant along characteristics we expect

$$Q_i^{n+1} \approx q(x_i, t_{n+1}) = q(x_i - \bar{u}\Delta t, t_n.)$$

Figure 2.4: If Q_i^n gives the value at a grid point, and we can trace the characteristic back and interpolate

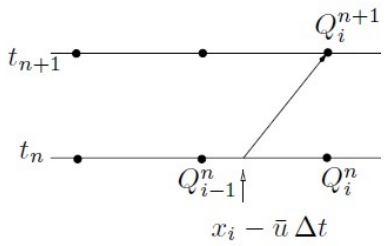
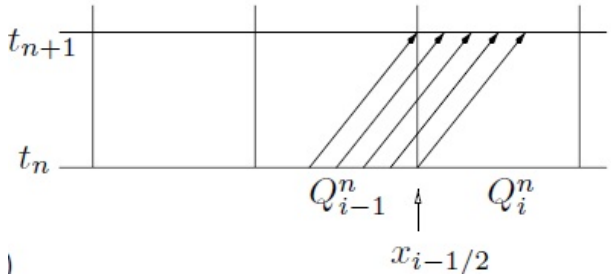


Figure 2.5: If Q_i^n gives the cell average, then the flux at the interface is determined by the cell value on the upwind side



If we approximate the value on the right by a linear interpolation between the grid values Q_{i-1}^n and Q_i^n we obtain the method

$$Q_i^{n+1} = \frac{\bar{u}\Delta t}{\Delta x} Q_{i-1}^n + (1 - \bar{u}\frac{\Delta t}{\Delta x}) Q_i^n.$$

This is the simply upwind method.

We must have

$$0 \leq \bar{u}\frac{\Delta t}{\Delta x} \leq 1,$$

this equation can be satisfied in order for the upwind method to be stable and also follows from CFL Condition.

$$W_{i-1/2} \equiv Q_i^n - Q_{i-1}^n$$

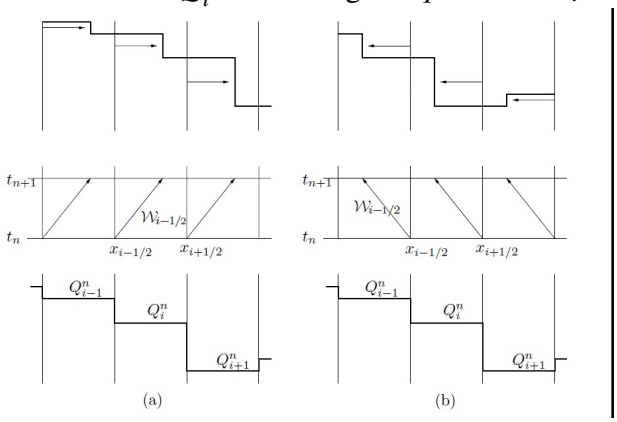
can be viewed as a wave that is moving into cell C_i at velocity $\bar{u}$. The cell average is modified by this fraction $-W_{i-1/2}$

$$Q_i^{n+1} = Q_i^n + \bar{u}\frac{\Delta t}{\Delta x}(-W_{i-1/2}).$$

The above equation is also in the upwind method discussed before.

In the above discussion we have assumed that $\bar{u} > 0$. On the other hand if $\bar{u} < 0$ then the upwind

Figure 2.6: The value Q_i^n cell average of q over the C_i at time t_n



direction is to the right and so the numerical flux at $x_{i-1/2}$ is given by

$$F_{i-1/2}^n = \bar{u} Q_i^n$$

then the upwind method has the form

$$Q_i^{n+1} = Q_i^n - \bar{u}\frac{\Delta t}{\Delta x}(Q_{i+1}^n - Qi^n).$$

The above can also be written in the wave propagation form

$$Q_i^{n+1} = Q_i^n - \bar{u}\frac{\Delta t}{\Delta x} W_{i+1/2}$$

with $W_{i+1/2} = Q_{i+1}^n - Q_i^n$ over $\bar{u} < 0$
The method is stable provided that

$$-1 \leq \bar{u}\frac{\Delta t}{\Delta x} \leq 0,$$

the two formulas for upwind can be combined into a single upwind formula that is valid for $\bar{u}$ of either sign.

$$F_{i-1/2}^n = \bar{u}^- Q_i^n + \bar{u}^+ Q_{i+1}^n \tag{2.11.1}$$

$$\text{where } \bar{u}^+ = \max(\bar{u}, 0); \quad \bar{u}^- = \min(\bar{u}^-, 0).$$

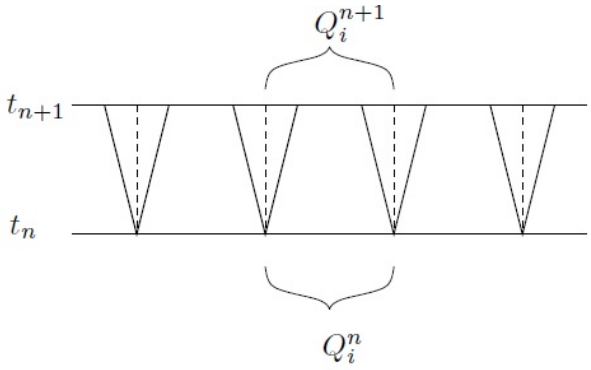
The wave propagation versions of the upwind method is the following

$$Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x}(\bar{u}^+ W_{i-1/2} + \bar{u}^- W_{i-1/2}). \tag{2.11.2}$$

2.12 Godunov's Method for Linear System

In this section, we develop the basic ideas of the upwind method for the advection equation and can be derived as a special case of the following approach, which can also be applied to systems of

Figure 2.7: The Riemann problem is solved over the grid cell to determine Q_i^{n+1}



equations. This is based on a REA algorithm (Reconstruct-Evolve-Average).
Algorithm:(REA)
(1): Reconstruct is a piecewise constant function $\tilde{q}^n(x,t_n)$ that takes the value Q_i^n in the i^{th} grid cell.

$$\tilde{q}^n(x,t_n) = Q_i^n \quad \forall x \in C$$

(2): Evolve the hyperbolic equation with initial data to obtain $\tilde{q}^n(x,t_{n+1})$ at time Δt. (3): Average this function over each grid cell to obtain new cell average.

$$Q_i^{n+1} = \frac{1}{\Delta x}\int_{C_i} \tilde{q}^n(x,t_{n+1})dx$$

$$C\Delta t \leq \frac{\Delta x}{2}$$

where C is a sound speed and Δt is the time step. After rearranging the above equation, we get

$$\frac{C\Delta t}{\Delta x} \leq \frac{1}{2}.$$

2.12.1 Numerical Flux Function for the Godunov's Method

Numerical flux at $x_{i-1/2}$ over the time step

$$F_{i-1/2}^n \approx \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} f(q(x_{i-1},t))dt.$$

In general the function $q(x_{i-1/2},t)$ varies with t and we can compute this integral exactly if we replace $q(x,t)$ by the function $\tilde{q}(x,t)$

2.12.2 Example

Let $\tilde{q}^n(x_{i-1/2},t)$ is constant over time interval $t_n < t < t_{n+1}$. Then the numerical flux is

$$F_{i-1/2}^n = \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} f(q(Q_{i-1}^n, Q_i^n))dt = f(q(Q_{i-1}^n, Q_i^n))$$

Godunov's method for a general system of conservation laws

(1): Solve the Riemann Problem at $x_{i-1/2}$ to obtain $q(Q^n_{i-1}, Q^n_i)$

(2): Define flux $F^n_{i-1/2} = \Im(Q^n_{i-1}, Q^n_i)$.

Chapter 3

Hyperbolic Conservation Law Arising in Neuronal Variability

3.1 Introduction

Hyperbolic equation (Transport equation) containing point-wise delay or advance can be found in mathematical models from other sciences like biology, engineering, physical and humanity sciences. These equation also implemented to simulate the observed behavior of a physical process. Moreover mathematical model of petroleum reservoirs consist a set of transport equation that describe the flow of fluid along with suitable boundary and initial condition.
This chapter is devoted to the study of a neuronal model which arises in neuronal variability which is a transport equation having point-wise delay and advance. Here we used the term negative and positive shift in transport equation for point-wise delay and advance, respectively. Detailed discussion about such type of models can be found in [9, 10] and about their numerical approximation can be found in [11, 12, 13, 14, 15, 16].

3.2 Motivation From Neuroscience

Neuroscience is the scientific study of a nervous system. A biological neuron model (also known as a spiking neuron model) is a mathematical description of the properties of neurons, which is designed to accurately describe and predict biological processes. This is in the contrast to the artificial neuron, which aims for computational effectiveness, although these goals sometimes overlap. The Computational neuroscience is an approach to understand the information content of signals by modeling the neurons system at many different scales. In the case of modelling a biological neuron, physical analogues are used in place of abstractions such as weight and transfer function. The input to a neuron is often described by an ion current through the cell membrane that occurs when neurotransmitters cause an activation of ion channels in the cell. This is described by a physical time-dependent current $I(t)$.
Neurons are highly specialized for generating electrical signals in response to chemical and other

inputs and transmitting them to other cells. The dendrites that receive inputs from other neurons and the axons that carries the neuronal output to other cells. The electrical signal of relevance to the nervous system is the difference in electrical potential between the interior of a neuron and the surrounding extracellular medium. Under resting conditions, the potential inside the cell membrane of a neuron is about -60 mV relative to that of the surrounding bath which is conventionally defined to be 0 mV, and the cell is said to be polarized. Current in the form of positively charged ions flowing out of the cell (or negatively charged ions flowing into the cell) through open channels makes the membrane potential more negative, a process called hyperpolarization. Current flowing into the cell changes the membrane potential to less negative or even positive values which is called depolarization. An elementary introduction to neurons and synapses can be found in the book by Thompson [17]. A standard textbook on neuroscience covering a wealth of experimental results is Principles of Neural Science by Kandel and Schwartz [18]. Details of spiking neuron models also can be found in texts by Wilson (1999), Dayan et al. (2001), and Gerstner et al. (2002) [19, 20, 21].

A neuron operates by receiving signals from other neurons through connections, called synapses. The combination of these signals, in excess of a certain threshold or activation level, will result in the neuron firing, that is sending a signal on to other neurons connected to it. Some signals act as excitations and others as inhibitions to a neuron firing. The behavior of the neuron is modeled by a membrane potential Vm and a threshold r. Whenever the membrane potential reaches a threshold, an action potential or spike is produced. The duration of the spike is 1 ms. After each spike, membrane potential is reset to a hyperpolarization. When a neuron fires, an electrical impulse is created which is the result of a change in potential to about 90 to 100 mv. Once a neuron fires, it must rest for several milliseconds before it can fire again. During the recovery period, which is called the refractory period, the neuron is less excitable in the sense that a larger depolarization is needed to produce a spike. When the neuron has not discharged for a long time its membrane potential is at the resting value U_R. The firing threshold thus remains constant.

A considerable progress has been made in understanding the basis of the initiation and transmission of neuronal impulses in quantitative terms during the mid of last century. A number of theories [22, 23, 24] have been determinate; that is, a given applied voltage pattern or pattern of presynaptic neuronal firings is assumed to determine the subsequent behavior of the neuron exactly but in complex neuronal systems the most striking observations is the variability in firing intervals when external stimuli are held constant. It is generally assumed that the variability results from the fact that neurons possess large numbers of synapses and several types of inputs, so that excitatory impulses occur effectively at random. It has been shown experimentally at cholinergic [25] and non-cholinergic neuromuscular junctions [26] and at some cholinergic [27] and central nervous system synapses [28] that, in the absence of neural inputs, excitatory quanta of transmitter are released at random and that the resulting depolarization decays roughly exponentially. Finally,

excitatory an d inhibitory presynaptic neuronal firings have been shown to produce individual depolarizations which sum and decay roughly exponentially [22].

3.3 Conservation Law in Neuronal model

The integrate-and-fire neuron model describes the state of a neuron in terms of its membrane potential, which is determined by the synaptic inputs and the injected current that the neuron receives. Integrate-and-fire equation was proposed in 1907 as a simple model for neuron activity by Lapicque [**?**]. In this model, when an input current is applied, the membrane voltage increases with time until it reaches a constant threshold, at which point a delta function spike occurs and the voltage is reset to its resting potential, after which the model continues to run. The firing frequency of the model thus increases linearly without bound as input current increases. There is a refractory period which limits the firing frequency of a neuron by preventing it from firing during that period. A remaining shortcoming of this model was that it implements no time-dependent memory. If the model receives a below-threshold signal at some time, it will retain that voltage boost forever until it fires again. This characteristic is clearly not in line with observed neuronal behavior.

In 1952, A. L. Hodgkin and A. Huxley [23] introduced Hodgkin Huxley Model to explain the ionic mechanisms underlying the initiation and propagation of action potentials in the squid giant axon. This was the most successful and widely used models of neurons. The FitzHugh Nagumo model [29], named after Richard FitzHugh who suggested the system in 1961 and J. Nagumo et al. who created the equivalent circuit the following year, describes a prototype of an excitable system (e.g., a neuron) [30]. In 1981, Morris and Lecar combined Hodgkin-Huxley and FitzHughNagumo into a voltage-gated calcium channel model with a delayed rectifier potassium channel. This model is known as Morris Lecar Model [31]. Building upon the FitzHugh Nagumo model, Hindmarsh and Rose proposed in 1984 a model of neuronal activity described by three coupled first-order differential equations which is known as Hindmarsh Rose Model [32].

Richard B. Stein studied the neuronal behavior around 1960 and presented a description of spontaneous neuronal activity which was published in Biophysical Journal in 1965. This is a simplified determinate model, together with the assumption that excitatory impulses of unit size do occur at random intervals [9]. Based on theories and predictions, the following assumptions of a simple neuronal model were observed by Stein:

1. Excitatory impulses occur randomly with frequency pe per second.
2. After each neuronal firing there is a refractory period of duration t_0, during which the impulse have no effect and the membrane depolarization Vt is reset to be zero.
3. At times $t > t_0$, each impulse produces unit depolarization.
4. If the depolarization reaches a threshold of r units, the neuron fires.

5. For subthreshold levels, the depolarization decays exponentially between impulses with the time constant τ_0.

For many neurons, inhibition play a very important role. Stein included the role of inhibition. The size of the potential change resulting from an impulse is a function of the potential difference between the equilibrium potential for the impulse and the membrane potential V_t. For excitatory impulses the equilibrium potential is typically five to ten times greater than the threshold depolarization so the assumption of constant-size impulses is a good one. However, for inhibitory impulses the equilibrium potential may be higher or lower than the resting potential and the size of an inhibitory impulse will not be constant [33].

To include the inhibition in neuronal model, it is observed that both excitatory and inhibitory impulse occur randomly with a frequency p_e and p_i per second respectively and at times $t > t_0$, an excitatory impulse produces unit depolarization while an inhibitory impulse produces v_0 unit repolarization. Let V_t equal the depolarization at time t and $p(v,t)$ equal the probability that $V_t \leq v$ at time t. From assumption (5) we have

$$\frac{dV_i}{dt} = -V_i/\tau_0$$

except for random points of discontinuity when impulse occur.

Assumption (3) above implies that for a short time interval δt , the probability of an excitatory impulse occurring is $p_i\delta t$ and the probability of an inhibitory impulse is $p_i\delta t$. The change of $p(v,t)$ with time is given by

$$\begin{aligned} p(v,t+\delta t) - p(v,t) &= [1(p_e+p_i)\delta t][p(v+\delta v,t) - p(v,t)] \\ & \quad p_e\delta t[p(v,t) - p(v-1,t)] + p_i\delta t[p(v+v_0,t) - p(v,t)]. \end{aligned} \tag{3.3.1}$$

Dividing equation (3.3.1) by δt and taking the limit as $\delta t \to 0$, we have

$$\begin{aligned} \frac{\partial p}{\partial t}(v,t) - (v/\tau_0)\frac{\partial p}{\partial v}(v,t) &= p_e[p(v-1,t) - p(v,t)] \\ & \quad +p_i[p(v+v_0,t) - p(v,t)]. \end{aligned} \tag{3.3.2}$$

Now we add the intensity of incoming current and we write the above equation with general coefficients as following

$$p_t + [-v + I(t)]p_v = a(v,t)[p(v-\alpha,t) - p(v,t)] + b(v,t)[p(v+\beta,t) - p(v,t)] \tag{3.3.3}$$

where $I(t)$ is the given intensity of incoming current and $I(t)$ will be given by the sum of periodic input signal or a constant current, i.e.,

$$I(t) = I_0(1 + m\cos(\Omega t)).$$

where $\Omega = 2\pi/T$, T being the signal period.
Rewrite the equation 3.3.3 as following

$$p_t + [(-v + I(t))p]_v = -p(v,t) + a(v,t)[p(v-\alpha,t) - p(v,t)] + b(v,t)[p(v+\beta,t) - p(v,t)] \quad (3.3.4)$$

Or

$$p_t + f(p)_v = S(p,v), \quad (v,t) \in (R \times R_+), \quad p(v,0) = p_0(v), v \in \mathbb{R}.$$

Where $p = p(v,t)$ is unknown function, f is the flux function and $S = S(p,v)$ is the source term which has the form

$$S(p,v) = -p(v,t) + a(v,t)[p(v-\alpha,t) - p(v,t)] + b(v,t)[p(v+\beta,t) - p(v,t)]$$

which is a first-order partial differential difference equation (transport equation with point-wise delay as well as advance). Appropriate initial-boundary conditions are included as following

$$p(0,v) = p^0(v) \geq 0, \int p^0(v)dv = 1.$$

For boundary conditions, we use localization properties, i.e. $p = 0$ on both the boundaries and outside as well.

3.4 Finite Volume Approximation

In this section we define the well-balanced Godunov type finite volume scheme firstly for homogeneous equation

$$p_t + [(-v + I(t))p]_v = 0.$$

Integrate this equation on the rectangle $[v_{j-\frac{1}{2}}, v_{j+\frac{1}{2}}] \times [t_n, t_{n+1}]$, we get

$$p_j^{n+1} = p_j^n - \frac{\Delta t}{\Delta v}[v_j - I(t^n)][F^n_{j+\frac{1}{2}} - F^n_{j-\frac{1}{2}}]$$

where

$$F^n_{j+\frac{1}{2}} = \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} [-v_{j+\frac{1}{2}} + I(t)]p(v_{j+\frac{1}{2}}, t)dt.$$

Assume that at time $t = t_n$, the cell averages p_j^n are known.
Now define $p(v,t_n) = p_j^n; \quad v_{j-\frac{1}{2}} \leq v \leq v_{j+\frac{1}{2}}$.
Then finding an approximation for the flux $F_{j+1/2}$, amounts to solving the Riemann problem

$$p_t + [(-v + I(t))p]_v = 0; \quad t \in [t_n, t_{n+1}]$$

$$p(v,t_n) = \begin{cases} p_j^n, & \text{if } v < v_{j+\frac{1}{2}} \\ p_{j+1}^n, & \text{if } v > v_{j+\frac{1}{2}} \end{cases}.$$

To compute the flux $F_{j+\frac{1}{2}}$, we need to know the solution along the interface

$$v = v_{j+\frac{1}{2}},\ t_n \le t \le t_{n+1}.$$

We introduce the shock speed at the cell interface $s = \frac{f(p^n_{j+1})-f(p^n_j)}{p^n_{j+1}-p^n_j}$ according to the Rankine-Hugoniot jump condition.Under the condition that $f(p)$ is convex, using method of characteristic. We have, for $t_n \le t \le t_n + \Delta t$

$$p(v_{j+1/2},t) = \begin{cases} p^n_j & \text{if } f'(p^n_j) > 0 \text{ and } f'(p^n_{j+1}) > 0 \\ p^n_{j+1} & \text{if } f'(p^n_j) < 0 \text{ and } f'(p^n_{j+1}) < 0 \\ p^n_j & \text{if } f'(p^n_j) \ge 0 \text{ and } f'(p^n_{j+1}) \le 0 \text{ and } s > 0 \\ p^n_{j+1} & \text{if } f'(p^n_j) \ge 0 \text{ and } f'(p^n_{j+1}) \le 0 \text{ and } s < 0 \\ \hat{u} & \text{if } f'(p^n_j) \le 0 \text{ and } f'(p^n_{j+1}) \ge 0 \end{cases}$$

where $\hat{u}$ is sonic point such that $f'(\hat{u}) = 0$.

The Godunovs method is now obtained by simply using the solution to the Riemann problem in at each interface $v_{j+1/2}$ to computes the numerical fluxes$F_{j1/2}, F_{j+1/2}$ yielding

$$F_{j+1/2} = \begin{cases} f(p^n_j) & \text{if } f'(p^n_j) > 0 \text{ and } f'(p^n_{j+1}) > 0 \\ f(p_{j+1})^n & \text{if } f'(p^n_j) < 0 \text{ and } f'(p^n_{j+1}) < 0; \\ f(p^n_j) & \text{if } f'(p^n_j) \ge 0 \text{ and } f'(p^n_{j+1}) \le 0 \text{ and } s > 0 \\ f(p^n_{j+1}) & \text{if } f'(p^n_j) \ge 0 \text{ and } f'(p^n_{j+1}) \le 0 \text{ and } s < 0 \\ f(\hat{u}) & \text{if } f'(p^n_j) \le 0 \text{ and } f'(p^n_{j+1}) \ge 0\ . \end{cases}$$

The right side is approximated by a linear interpolation. Initial-boundary conditions are given by

$$\begin{aligned} &P^0_j = P^0(v_j), \quad \forall\ j = -J+1, ..., J-1 \\ &P^n_{-J} = 0,\ n = 0,1,2\ldots \\ &P^n_J = 0,\ n = 0,1,2\ldots. \end{aligned}$$

3.5 Computational Results and Discussion

Some test cases are considered and solved using the methods presented in this chapter.

Numerical Examples: We take Gaussian initial data

$p_0(v) = \dfrac{1}{\sigma\sqrt{2\pi}} \exp\left[-\dfrac{(v-\mu)^2}{2\sigma^2}\right]$, and perform some numerical computations. We take the domain $[-4,4]$. For this choice of domain, we take $\alpha = 3$ and $\beta = 3$. The value of intensity is taken as $I(t) = 1 + \cos(2\pi t)$. Fig. 3.1 shows the solution at time $t = 0.5$. The computed solution is centered

at $v = 1$. In Fig. 3.2, solution is plotted by taking different initial data centered at 0.0, 1.0 and 1.5 (from left to right hand side respectively). Fig. 3.3 shows the approximate solution at different time levels with initial data centered at $v = 1.0$.

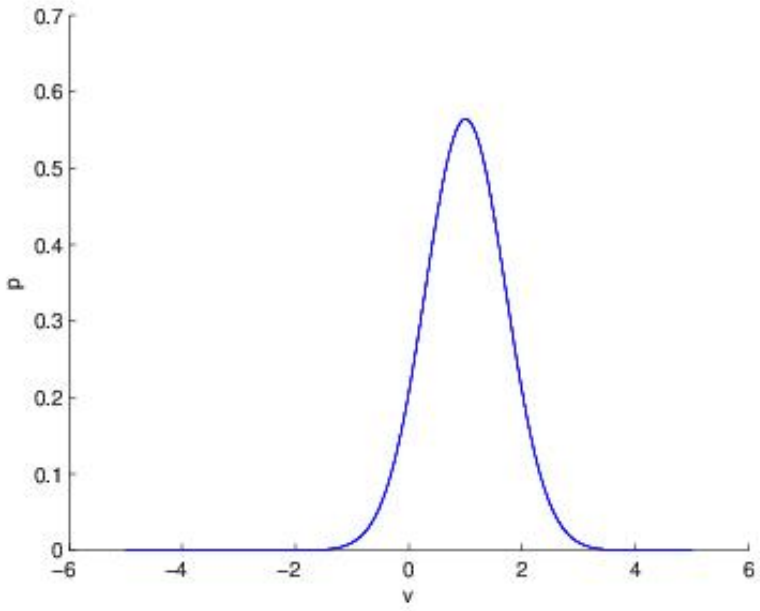


Figure 3.1: The computed solution at time $t = 0.5$

3.6 Conclusions

A transport equation based on neuronal model based is considered in this chapter. Based on the Gudunov's finite volume numerical approximation, a numerical scheme is constructed to find the approximate solution of hyperbolic partial differential equation with delay as well as advance. For numerical computation we take initial data as Gaussian. We have shown the behavior of solution in plotted figures. This study demonstrates that the model preserve the conservation principle and the total probability is concentrated near the reset value of the potential.

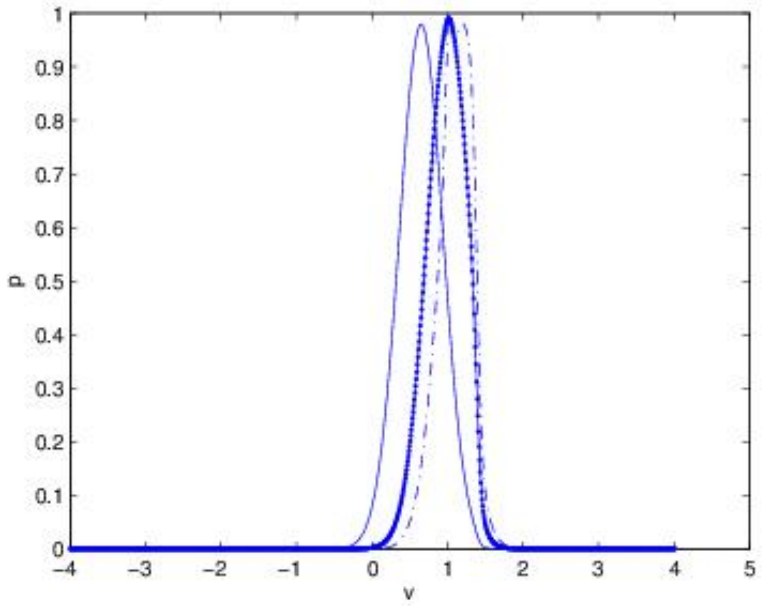


Figure 3.2: The computed solution for different initial values

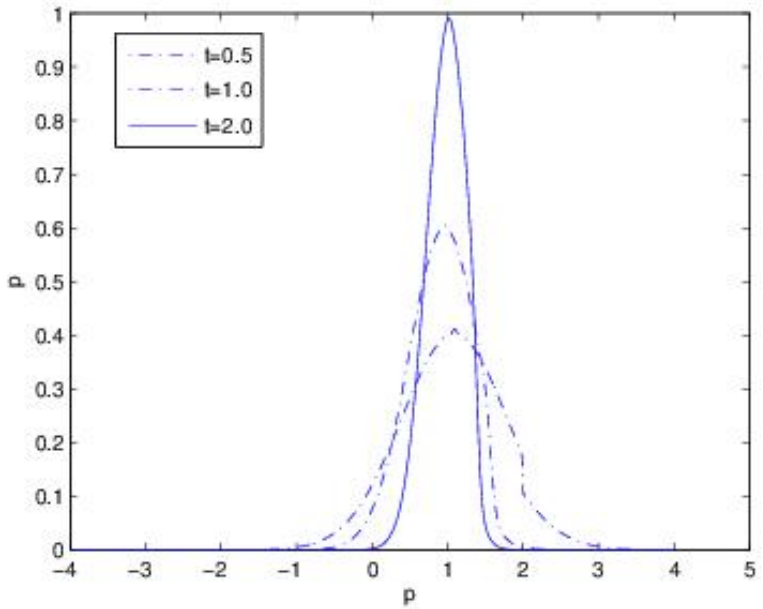


Figure 3.3: The computed solution at different time levels

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