ANALYTICAL AND NUMERICAL TREATMENT OF PARTIAL DIFFERENTIAL EQUATIONS

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by

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To My Family ...

ABSTRACT

ANALYTICAL AND NUMERICAL TREATMENT OF PARTIAL DIFFERENTIAL EQUATIONS IN PHYSICS

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In this thesis a technique which classifies partial differential equations with respect to their structural properties has first been studied. One of the important results reached is that this classification technique also classifies the physical processes indirectly. In the light of this technique several important partial differential equations having different structures are considered and are investigated using analytical and numerical methods. From the comparison of the solutions obtained by both methods, it is understood that these methods produce almost identical results.

Keywords: Partial Differential Equations, Classification Technique, Analytical Method, Numerical Method

ÖZET

FİZİKTEKİ KISMİ DİFERANSİYEL DENKLEMLERİN ANALİTİK VE NÜMERİK İNCELENMESİ

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Temmuz 2002, 65 sayfa

Bu tezde öncelikle kısmi diferansiyel denklemleri yapısal özelliklerine göre ayıran bir tekniğe bakılmıştır. Varılan sonuçlardan en önemlisi, bu teknikle fiziksel olayların da dolaylı olarak sınıflandırıldığını görmek olmuştur. Bu sınıflandırma ışığında fizikte sık sık karşılaşılan farklı yapılara haiz önemli birkaç kısmi diferansiyel denklem ele alınarak, analitik ve de nümerik metodlarla incelenmiştir. Her iki metodla elde edilen çözümler karşılaştırıldığında, bu metodların hemen hemen eşdeğer sonuçlar ürettiği anlaşılmıştır.

Anahtar sözcükler: Kısmi Diferansiyel Denklemler, Sınıflandırma Tekniği, Analitik Metod, Nümerik Metod

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CHAPTER 1

INTRODUCTION

In the study of many physical problems the main purpose is to investigate a vector field or a scalar field. The ultimate goal of such a study is to be able to predict the behaviour of this field throughout all space and for all time provided the initial local behaviour of the field is given. Usually the local behaviour of a field is specified with the aid of a relation which must hold at each point of space and time, and which interrelates, at any given point the rates of change of the field in different directions. Such a relation is referred to as a partial differential equation. Thus the problem of determining the future behaviour of the field throughout all space and for all time is then equivalent to solving this partial differential equation.

Some examples of the applications of partial differential equations are on vibrations of solids, flow of fluids, wave equations modelling the propagation of sound, light and water waves, the Schroedinger equation predicting the properties of atomic and molecular systems in quantum mechanics, the diffusion equation describing the spread of heat, Maxwell's equations governing electrodynamical phenomena and Newton's equations describing mechanical systems. Thus it is clear that partial differential equations are of vital importance in the following areas of science: acoustics, aerodynamics, elasticity, electrodynamics, fluid dynamics, geophysics, heat transfer, meteorology, oceanography, optics, quantum mechanics and plasma physics.

As it is well-known, the partial differential equations which are encountered in physics are mostly of the second order. Some very well-known examples are

Laplace's equation, Poisson's equation, the wave equation, the heat diffusion equation, the Klein-Gordon equation and the Schroedinger equation.

General techniques of solving these partial differential equations may be classified as follows:

a) Reduction to ordinary differential equations by:

1. Separation of variables

2. Transform methods

3. Method of characteristics

4. Similarity transformations

b) The Green function method

c) Numerical methods

Chapter two is essentially a review of a classification technique of linear second-order partial differential equations that are in two variables. This technique is presented in elementary steps without consulting to a general theory. It involves the transformation of a partial differential equation into a canonical form. The classification based upon this technique shows that there are three distinct structural forms of partial differential equations. These are called hyperbolic, parabolic and elliptical equations. Hyperbolic equations describe vibrating systems and wave motion, parabolic equations describe heat flow and diffusion processes and elliptical equations describe steady-state phenomena. As it is known the nature of the boundary and initial conditions that are imposed on a partial differential equation depend on its structure. Therefore the classification technique mentioned above, is a consequence of a structural characterization of partial differential equations.

Following the order of the classification given in chapter two, several important linear partial differential equations which are often dealt with in various branches of physics are investigated in chapter three. Analytical methods of solving them are studied and for some pre-specified initial and boundary conditions their special solutions are obtained.

Finally in chapter four, the emphasis is given to the importance of numerical methods in solving partial differential equations. In particular, attention is focused on the finite-difference method. Using this method, the numerical solutions of the same equations we dealt with in chapter three, are obtained and are compared with their analytical counterparts. Lastly a discussion is presented.

CHAPTER 2

STRUCTURAL CHARACTERIZATION OF PARTIAL DIFFERENTIAL EQUATIONS

An ordinary differential equation is classified according to its order and whether it is linear or nonlinear [1]. However the classification of partial differential equations is more complicated. This is because besides the important concepts like order and linearity, the structure of a partial differential equation is equally important as well. In fact the structure of a partial differential equation determines the type of boundary and initial conditions which are to be imposed on it. Moreover the classification of partial differential equations according to their structural characteristics is in the physical sense equivalent to the classification of the physical phenomena that these equations describe [2].

2.1 Classification of Second-Order Linear Partial Differential Equations In Two Variables

In this section a review of the classification technique mentioned above is presented. This technique is briefly discussed in elementary steps without reference to a general theory. A linear second-order partial differential equation has the general form

$$aU_{xx} + 2bU_{xy} + cU_{yy} + dU_x + eU_y + fU = g \tag{2.1}$$

where a, b, c, d, e and f are linear coefficients. The purpose of this analysis is to transform equation(2.1) into a canonical form in terms of the new variables [3]

$$\xi = \xi(x,y) \qquad \eta = \eta(x,y) \tag{2.2}$$

Let $U = U(\xi,\eta)$ be the function into which U(x,y) is transformed. Now applying the chain rule we get

$$\begin{aligned}
U_x &= U_\xi \xi_x + U_\eta \eta_x \\
U_y &= U_\xi \xi_y + U_\eta \eta_y \\
U_{xx} &= U_{\xi\xi}\xi_x^2 + 2U_{\xi\eta}\xi_x\eta_x + U_{\eta\eta}\eta_x^2 + U_\xi \xi_{xx} + U_\eta \eta_{xx} \\
U_{xy} &= U_{\xi\xi}\xi_x\xi_y + U_{\xi\eta}(\xi_x\eta_y + \xi_y\eta_x) + U_{\eta\eta}\eta_x\eta_y \\
&+ U_\xi \xi_{xy} + U_\eta \eta_{xy} \\
U_{yy} &= U_{\xi\xi}\xi_y^2 + 2U_{\xi\eta}\xi_y\eta_y + U_{\eta\eta}\eta_y^2 \\
&+ U_\xi \xi_{yy} + U_\eta \eta_{yy}
\end{aligned} \tag{2.3}$$

Inserting equation(2.3) into equation(2.1) we obtain

$$AU_{\xi\xi} + 2BU_{\xi\eta} + CU_{\eta\eta} + DU_\xi + EU_\eta + FU = G \tag{2.4}$$

where

$$\begin{aligned}
G = g \qquad &, \qquad F = f \\
E &= d\eta_x + e\eta_y + a\eta_{xx} + 2b\eta_{xy} + c\eta_{yy} \\
D &= d\xi_x + e\xi_y + a\xi_{xx} + 2b\xi_{xy} + c\xi_{yy} \\
A &= a\xi_x^2 + 2b\xi_x\xi_y + c\xi_y^2 \\
B &= a\xi_x\eta_x + b(\xi_x\eta_y + \xi_y\eta_x) + c\xi_y\eta_y
\end{aligned} \tag{2.5}$$

$$C = a\eta_x^2 + 2b\eta_x\eta_y + c\eta_y^2$$

From the relations given in equation(2.5) we can note that

$$B^2 - AC = (b^2 - ac)J^2 \tag{2.6}$$

where J is the Jacobian of the transformation given by equation(2.2):

$$J = \begin{vmatrix} \xi_x & \xi_y \\ \eta_x & \eta_y \end{vmatrix} = \xi_x\eta_y - \xi_y\eta_x \neq 0 \tag{2.7}$$

Since $J^2 > 0$ then from equation(2.6) the sign of $B^2 - AC$ must be the same as the sign of $b^2 - ac$. Thus we conclude that the sign of the discriminant $b^2 - ac$ of the quadratic form $Q = aX^2 + 2bXY + cY^2$ is an invariant under the transformation from the coordinates (x,y) to (ξ,η). The choices of the functions ξ,η are made according to the invariance of the sign of the discriminant. Thus we have the following cases where the names are suggested by the quadratic form [3]

$$\begin{aligned} b^2 - ac &> 0 \quad \text{Hyperbolic type} \\ b^2 - ac &= 0 \quad \text{Parabolic type} \\ b^2 - ac &< 0 \quad \text{Elliptic type} \end{aligned} \tag{2.8}$$

and in this way the linear, second-order partial differential equations are divided into three distinct classes. Physically speaking, each class governs different phenomena.

(i)Hyperbolic Case: From equation(2.5) one can choose real ξ and η in such a way as to satisfy:

$$A = C = 0 \tag{2.9}$$

Thus equation(2.4) together with equation(2.9) gives the canonical form

$$U_{\xi\eta} + \frac{D}{2B}U_{\xi} + \frac{E}{2B}U_{\eta} + \frac{F}{2B}U = \frac{G}{2B} \tag{2.10}$$

Now using equation(2.5) and equation(2.9) the canonical coordinates can be chosen as

$$\begin{aligned} \xi_x + \lambda_1 \xi_y &= 0 \\ \eta_x + \lambda_2 \eta_y &= 0 \end{aligned} \tag{2.11}$$

where λ_1 and λ_2 are the roots of the quadratic equation

$$a\lambda^2 - 2b\lambda + c = 0 \tag{2.12}$$

i.e.

$$\lambda_{1,2} = \frac{1}{a}(b \pm \sqrt{b^2 - ac}) \tag{2.13}$$

(ii) Parabolic Case: $b^2 - ac = 0$ leads to the result $\lambda_1 = \lambda_2 = \frac{b}{a}$ in equation(2.13). Now C can be set equal to zero ;i.e.

$$C = 0 \tag{2.14}$$

Also from equation(2.11) and equation(2.13) we have

$$\begin{aligned} \xi_x &= -\frac{b}{a}\xi_y \\ \eta_x &= -\frac{b}{a}\eta_y \end{aligned} \tag{2.15}$$

Therefore with equation(2.15), B in equation(2.5) becomes

$$\begin{aligned} B &= a\xi_x(-\frac{b}{a})\eta_y + b[\xi_x\eta_y + \xi_y(-\frac{b}{a}\eta_y)] + c\xi_y\eta_y \\ &= -\frac{1}{a}(b^2 - ac)\xi_x\eta_y = 0 \end{aligned} \tag{2.16}$$

Consequently from equation(2.4) the canonical form in parabolic case is given by

$$U_{\xi\xi} + \frac{D}{A}U_\xi + \frac{E}{A}U_\eta + \frac{F}{A}U = \frac{G}{A} \tag{2.17}$$

(iii)Elliptical Case: From equation(2.13) we note that λ_1 and λ_2 are complex and

$$\lambda_2 = \lambda_1^* \tag{2.18}$$

because $b^2 - ac < 0$. Thus from equation(2.11), equation(2.18) implies that

$$\eta = \xi^* \tag{2.19}$$

Also setting $A = C = 0$, the canonical form, from equation(2.4) reads

$$U_{\xi\xi} + \frac{D}{2B}U_\xi + \frac{E}{2B}U_\eta + \frac{F}{2B}U = \frac{G}{2B} \tag{2.20}$$

CHAPTER 3

ANALYTICAL TREATMENT OF PARTIAL DIFFERENTIAL EQUATIONS

In this chapter following the classification discussed in chapter two, several partial differential equations possessing different structural properties are analytically treated. The partial differential equations which are in question are of utmost importance in physics because they describe a broad spectrum of physical phenomena including wave motion, heat flow mechanisms and steady-state problems [4]. Methods of solving these partial differential equations are illustrated and moreover their special solutions for some specified initial and boundary conditions are provided.

3.1 One Dimensional Wave Equation- String Problem

In this section we analyze the one dimensional wave equation [1] as an example of partial differential equations of hyperbolic type. This kind of partial differential equations deal with propagation problems so that a variety of engineering systems such as vibrations of rods and beams, motion of fluid waves, transmission of sound and electrical signals can all be characterized by this kind of partial differential equations. As a physical application of this equation, we consider the string problem [5]. Let us take a string that is tightly stretched between two fixed points on the x-axis as in figure(3.1).

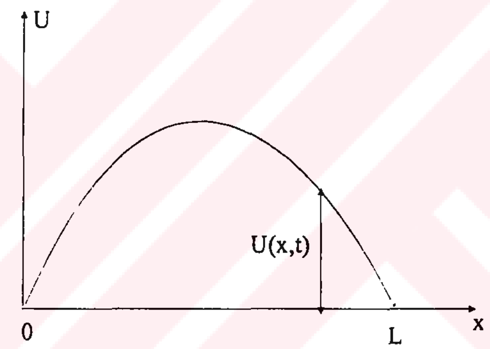

Figure 3.1: A string attached between two points.

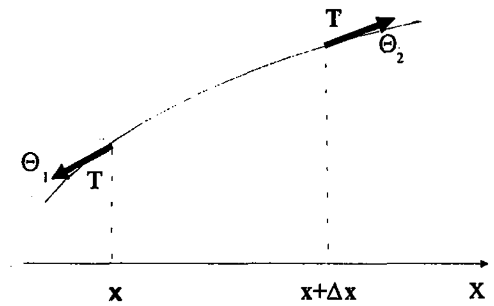

Figure 3.2: A small segment of a vibrating string.

We assume that the string is made of a homogeneous material, and its vibrations take place in a plane as in figure(3.1). Our task is to determine which equation governs the motion of the string under various initial and boundary conditions and find a function U(x,t) which gives the deflection of the string at any point x and at any time t. To describe mathematically the vibrations of this string, we consider a small segment of length Δx and apply Newton's second law as shown in figure(3.2).

The total force acting on this piece of string is equal to the mass of the piece of the string multiplied by its acceleration

$$F = \rho \Delta x \frac{\partial^2 U}{\partial t^2} \tag{3.1}$$

where ρ is the density of the string which is constant. The forces which maybe acting on the string are; any external force such as gravity $F_{ext}(x,t) = -mg$, frictional force against the string $-\beta U_t$ if the string is vibrating in a medium that offers resistance to the string's velocity and restoring force $-\gamma U$ which is directed opposite to the displacement of the string. Since we assume that the string moves only in the u-x plane, there is also a net tangential force due to the tension T on the string. This net force due to the tension is

$$F = T\sin\theta_2 - T\sin\theta_1 \tag{3.2}$$

since we assume that the angles θ_1 and θ_2 are small we can write

$$\sin\theta \approx \tan\theta \tag{3.3}$$

so we get

$$F = T(\tan\theta_2 - \tan\theta_1) \tag{3.4}$$

we see that each term in the above equation is the slope of the string at $x + \Delta x$

and at x respectively. We can thus write

$$F = T[U_x(x+\Delta x,t) - U_x(x,t)] \tag{3.5}$$

Combining all the forces acting on the string, we get

$$\begin{aligned} \rho \Delta x U_{tt} &= T[U_x(x+\Delta x,t) - U_x(x,t)] + \Delta x F(x,t) \\ &- \Delta x \beta U_t(x,t) - \Delta x \gamma U(x,t) \end{aligned} \tag{3.6}$$

where the external force, restoring force and the frictional force are multiplied by Δx to get the total force acting on a segment of the string. Dividing each side by Δx and letting Δx go to zero, we obtain

$$U_{tt} = \alpha^2 U_{xx} + \frac{F(x,t)}{\rho} - \frac{\beta}{\rho} U_t - \frac{\gamma}{\rho} U \tag{3.7}$$

where

$$\alpha^2 = \frac{T}{\rho} \tag{3.8}$$

which has the dimension of velocity squared. We now assume that there is no external force, no resistive force of the medium and no restoring force. Thus equation(3.7) becomes

$$U_{tt} = \alpha^2 U_{xx} \tag{3.9}$$

which is the wave equation.

Here U_{tt} represents the vertical acceleration of the string and U_{xx} is the force (tension) on the string.

Now we will examine the following initial-boundary value problem as a specific example of the wave equation.

$$U_{tt} = c^2 U_{xx} \qquad 0 < x < l \ , \ \ t > 0 \tag{3.10}$$

$$U(0,t) = U(l,t) = 0 \qquad t > 0 \tag{3.11}$$

$$U(x,0) = f(x), \qquad U_t(x,0) = g(x) \qquad 0 \le x \le l \tag{3.12}$$

the solution of the equation(3.10) can be obtained by the method of separation of variables. Letting

$$U(x,t) = X(x).T(t) \tag{3.13}$$

gives

$$\frac{T''}{T} = c^2 \frac{X''}{X} \tag{3.14}$$

The left side of this equation is a function of t only and the right side is a function of x only, so both sides must be equal to a constant

$$\frac{T''}{T} = c^2 \frac{X''}{X} = -k^2 \tag{3.15}$$

where k is a constant. We thus get two ordinary differential equations which are

$$T'' + k^2 T = 0 \tag{3.16}$$

and

$$X'' + \frac{k^2}{c^2} X = 0 \tag{3.17}$$

The solution for X(x)is

$$X(x) = A\cos(\frac{k}{c}x) + B\sin(\frac{k}{c}x) \tag{3.18}$$

Applying the boundary conditions we get

$$X(x=0)=0=A \qquad \text{and} \qquad X(x=l)=0=B\sin(\frac{k}{c}l) \tag{3.19}$$

which implies $\sin(\frac{k}{c}l)=0$ and $\frac{kl}{c}=n\pi$ where n is an integer. Thus

$$X_n(x)=B_n\sin(\frac{n\pi x}{l}) \tag{3.20}$$

The solution for T(t) is

$$T_n(t)=a_n\cos(\frac{cnt\pi}{l})+b_n\sin(\frac{cnt\pi}{l}) \tag{3.21}$$

The general solution is then given by

$$U(x,t)=\sum_{n=1}^{\infty}[a_n\cos\frac{cnt\pi}{l}+b_n\sin\frac{cnt\pi}{l}]\sin(\frac{n\pi x}{l}) \tag{3.22}$$

Now we apply the initial conditions

$$U(x,0)=f(x) \tag{3.23}$$

and

$$U_t=(x,0)=g(x) \tag{3.24}$$

with

$$f(x)=\sum_{n=1}^{\infty}a_n\sin(\frac{n\pi x}{l}) \tag{3.25}$$

and

$$g(x)=\sum_{n=1}^{\infty}b_n\frac{cn\pi}{l}\sin(\frac{n\pi x}{l}) \tag{3.26}$$

Choosing $l = 1$, $c = 0.25$, $f(x) = 0$ and $g(x) = x(1-x)$ as shown in figure(3.3) we have

$$a_n = 0$$

and

$$b_n = 2\int_0^1 x(1-x)\sin(n\pi x)dx \qquad (3.27)$$

The solution is

$$U(x,t) = \sum_{n=1}^{\infty} \sin(n\pi x)\sin(\frac{n\pi t}{4})[\frac{16}{n^4\pi^4}][1-(-1^n)] \qquad (3.28)$$

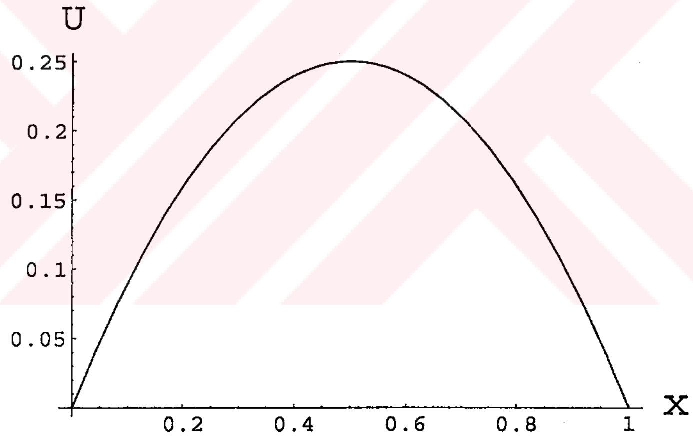

Figure 3.3: A graph of the initial condition for the string problem.

To see how U(x,t) behaves in space and time, we give plots of the solution given above from three different profiles over the domain $0 < x < 1$ for $t = 20$ in figures(3.4.a),(3.4.b) and (3.4.c).

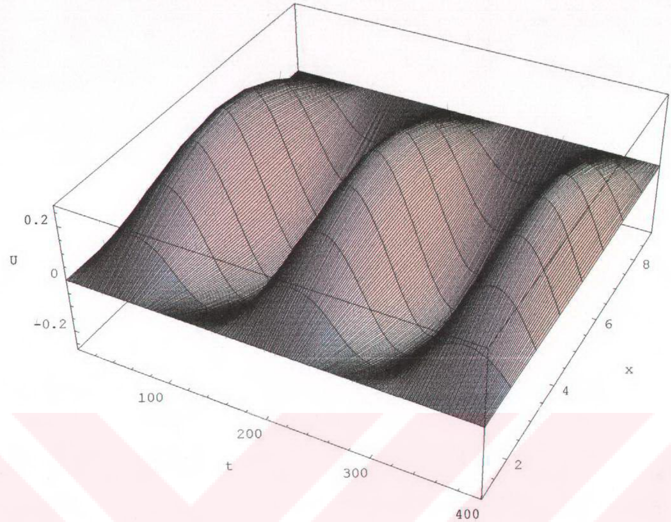

Figure 3.4.a : Graph of the analytic solution of the wave equation.

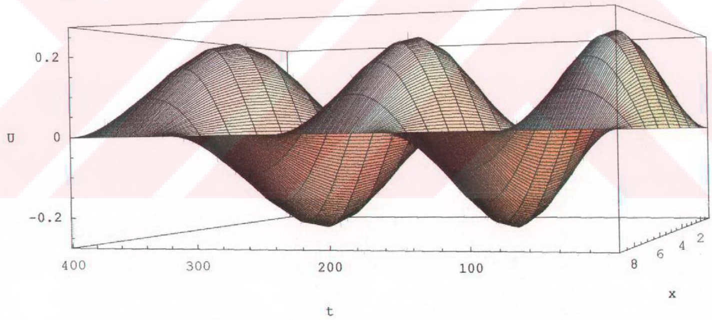

Figure 3.4.b : Graph of the analytic solution of the wave equation.

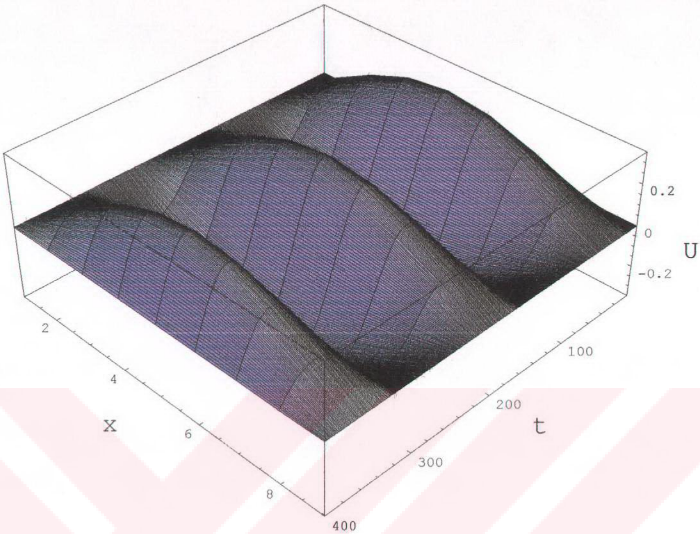

Figure 3.4.c : Graph of the analytic solution of the wave equation.

3.2 One Dimensional Heat Equation-Diffusion Equation

As an example of a partial differential equation of parabolic type we now consider heat equation [1]. When temperatures in an object change with time, we have a problem of unsteady flow of heat, a physical situation that can be represented by a parabolic type of partial differential equation. Let us consider a cylindrical rod of length L and radius R which is made of a uniform heat conducting material. We assume that heat can enter and leave the rod only through its ends, that is, the lateral surface of the rod is completely insulated.

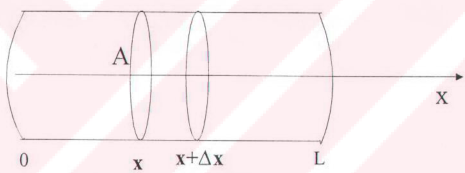

Figure 3.5: A cylindrical heat conducting material.

Let x measure the distance along the rod as in figure(3.5), and let U(x,t) denote the absolute temperature at ant time t at any point x along the rod. We assume that the temperature is uniform across any cross-sectional area A of the rod. Let ρ be the density of the rod which is assumed to be constant. The specific heat c of the rod is defined as the amount of heat that must be supplied to raise the temperature of one unit mass of the rod by one degree. Consider a section of the rod between x and $x + \Delta x$. The mass between these two points is $\rho A \Delta x$. In order to change the temperature of the rod between these two points from zero to U(x,t) degrees, we must supply $U(x,t)c\rho A\Delta x$ units of heat. Thus, between any two points x_0 and x_1 the heat energy contained in the rod at time t is

$$Q(t) = \int_{x_0}^{x_1} U(x,t)c\rho A dx \tag{3.29}$$

By the law of conservation of energy, if there are no heat sources and sinks within the rod the heat energy in any part of the rod can increase or decrease only because of a flow of heat through the boundaries of that part of the rod. Therefore the heat flux $Q_F(x,t)$ is the quantity of heat energy per unit time passing through a unit area in the cross-section. Thus, to find the rate of change of the heat energy between the x_0 and x_1 cross-sections we need only take the difference

$$\frac{dQ}{dt} = AQ_F(x_0,t) - AQ_F(x_1,t) \tag{3.30}$$

where the first term on the right side is the heat energy flowing in and the second is that flowing out. We assume that the heat flux at any point is proportional to the temperature gradient $\frac{\partial U(x,t)}{\partial x}$ at that point. The constant of proportionality is called the thermal conductivity of the rod and is denoted by κ. Since heat flows in the direction of decreasing temperature, we have

$$Q_F(x,t) = -\kappa \frac{\partial U(x,t)}{\partial x} \tag{3.31}$$

where $\kappa > 0$. So we have

$$AQ_F(x_0,t) - AQ_F(x_1,t) = A[\kappa \frac{\partial U(x_1,t)}{\partial x} - \kappa \frac{\partial U(x_0,t)}{\partial x}] = \int_{x_0}^{x_1} \frac{\partial}{\partial x}[\kappa \frac{\partial U(x,t)}{\partial x}]Adx \tag{3.32}$$

Substituting the right side of the equation(3.32) into equation(3.31) and differentiating equation(3.30), we get

$$\int_{x_0}^{x_1} \frac{\partial}{\partial x}[\kappa \frac{\partial U(x,t)}{\partial x}] A dx = \frac{dQ}{dt} = \int_{x_0}^{x_1} c\rho \frac{\partial U(x,t)}{\partial t} A dx \tag{3.33}$$

or

$$\int_{x_0}^{x_1} [c\rho \frac{\partial U(x,t)}{\partial t} - \frac{\partial}{\partial x}(\kappa \frac{\partial U(x,t)}{\partial x})] A dx \tag{3.34}$$

Hence the expression in brackets must be zero for all values of x. Then this leads to

$$c\rho \frac{\partial U(x,t)}{\partial t} = \frac{\partial}{\partial x}(\kappa \frac{\partial U(x,t)}{\partial x}) \tag{3.35}$$

So

$$\frac{\partial U}{\partial t} = \delta \frac{\partial^2 U}{\partial x^2} \tag{3.36}$$

where $\delta = \frac{\kappa}{c\rho}$ and is called the diffusivity of the material. Equation(3.36) is known as the *heat equation.*

As a specific example setting $\delta = 1$, we wish to solve the so called diffusion equation with the given initial and boundary conditions [6]

$$U_t = U_{xx} \tag{3.37}$$

$$U(0,t) = U(L,t) = 0 \qquad t > 0 \tag{3.38}$$

$$U(x,0) = f(x) \qquad 0 < x < L \tag{3.39}$$

The equation can be solved by separation of variables technique. Letting U(x,t)=X(x)T(t) we have from equation(3.37)

$$\frac{X''(x)}{X} = \frac{T'(t)}{T} \tag{3.40}$$

Since the left side is a function of x only and the right side is a function of t only both must be equal to a constant;i.e.

$$\frac{X''(x)}{X} = \frac{T'(t)}{T} = -k^2 \tag{3.41}$$

where k is a constant. This takes us to the following equations:

$$X'' + k^2 X = 0 \tag{3.42}$$

$$T' + k^2 T = 0 \tag{3.43}$$

The solution for X(x)is:

$$X(x) = A\cos kx + B\sin kx \tag{3.44}$$

Now applying the boundary conditions given by equation(3.38) we obtain

$$X(x=0) = 0 = A \tag{3.45}$$

and

$$X(x=L) = 0 = B\sin kL \tag{3.46}$$

so that $\sin kL = 0$ which implies that $kL = n\pi$ and $k = \frac{n\pi}{L}$ where n is an integer. Thus

$$X(x) = B_n \sin\frac{\pi n x}{L} \tag{3.47}$$

On the other hand the solution for T(t)is:

$$T(t) = C\exp(-k^2 t) = C_n \exp(-(\frac{n\pi}{L})^2 t) \tag{3.48}$$

The general solution is then written as

$$U(x,t) = \sum_{n=1}^{\infty} A_n \sin(\frac{n\pi x}{L}) \exp(-(\frac{n\pi}{L})^2 t) \tag{3.49}$$

The initial condition given by equation(3.39) becomes

$$f(x) = \sum_{n=1}^{\infty} A_n \sin(\frac{n\pi x}{L}) \tag{3.50}$$

The coefficients A_n can be calculated by the Fourier transform technique

$$A_n = \frac{2}{L}\int_0^L f(x)\sin(\frac{n\pi x}{L})dx \tag{3.51}$$

taking $L = 1$ and $f(x) = x^3(1-x)$ as shown in figure(3.6) we have

$$A_n = 2\int_0^1 x^3(1-x)\sin(n\pi x)dx = 2[\frac{-24}{(n\pi)^5} + \frac{(24-6n^2\pi^2)}{(n\pi)^5}(-1)^n] \tag{3.52}$$

where the integral is evaluated by the method of integration by parts. A plot of the special solution corresponding to the imposed initial and boundary conditions are shown in Figures:(3.7.a),(3.7.b) and (3.7.c) from three different profiles.

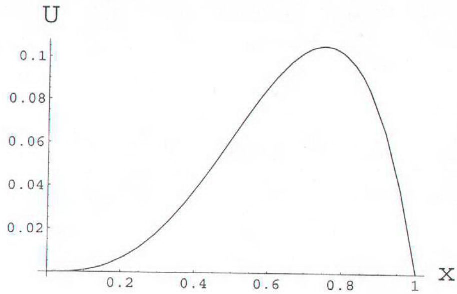

Figure 3.6: A graph of the initial condition for the diffusion equation.

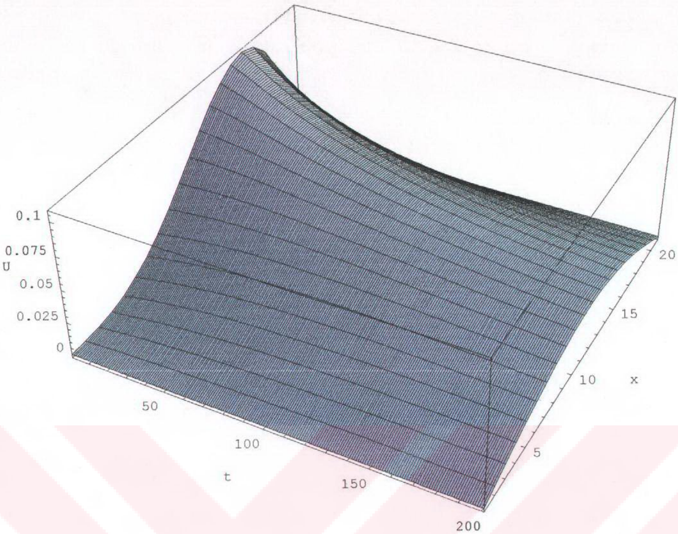

Figure 3.7.a : Analytic solution of the diffusion equation.

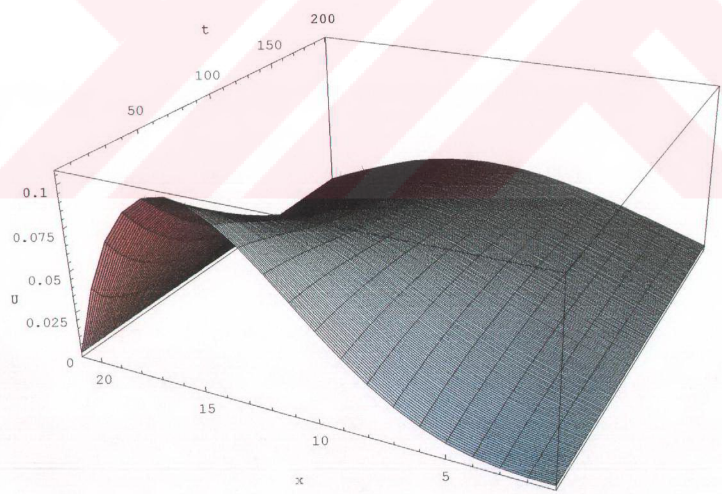

Figure 3.7.b : Analytic solution of the diffusion equation.

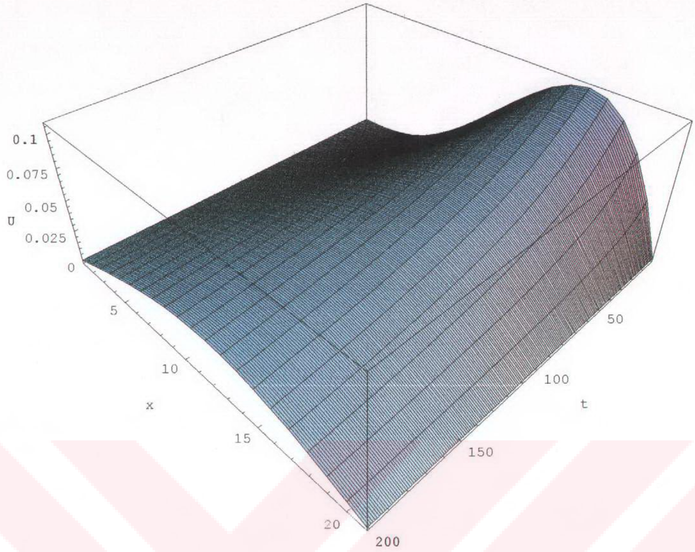

Figure 3.7.c : Analytic solution of the diffusion equation.

3.3 Laplace's Equation

The following problems of physics are described by an elliptic type of a partial differential equation called Laplace's equation; [1] the problem of finding the steady-state temperatures in an isotropic body without sources or sinks of heat, a steady-state potential flow of an incompressible fluid, the potential of an electrostatic field in a region containing no charges, the potential of a gravitational field in a region containing no masses, and so on.

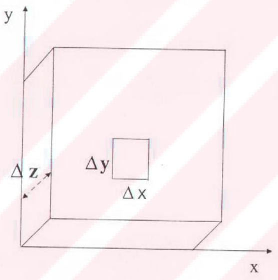

Figure 3.8: A thin rectangular metal plate

In order to derive this equation, we consider an element on the face of a thin rectangular metal plate of thickness Δz as shown in figure(3.8). The plate is insulated everywhere except the edges where the temperature can be set at a prescribed level. The insulation and the thinness of the plate mean that heat transfer is limited to the x and y dimensions. At steady-state the flow of heat into the element over a unit time period must equal to the outflow of heat. This means that

$$\begin{aligned} q(x)\Delta y\Delta z\Delta t \;&+\; q(y)\Delta x\Delta z\Delta t \\ &= q(x+\Delta x)\Delta y\Delta z\Delta t + q(y+\Delta y)\Delta x\Delta z\Delta t \end{aligned} \tag{3.53}$$

where $q(x)$ and $q(y)$ are the heat fluxes at x and y respectively. Dividing by Δz and Δt and collecting terms yield,

$$[q(x) - q(x + \Delta x)]\Delta y + [q(y) - q(y + \Delta y)]\Delta x = 0. \tag{3.54}$$

Multiplying the first term by $\Delta x/\Delta x$ and second term by $\Delta y/\Delta y$ gives

$$\frac{q(x) - q(x + \Delta x)}{\Delta x}\Delta x\Delta y + \frac{q(y) - q(y + \Delta y)}{\Delta y}\Delta y\Delta x = 0 \tag{3.55}$$

Dividing by $\Delta x\Delta y$ and taking the limit results in

$$-\frac{\partial q}{\partial x} - \frac{\partial q}{\partial y} = 0 \tag{3.56}$$

This equation is an expression of the conservation of energy for the plate. The link between flux and temperature is provided by Fourier's law of heat conduction which can be represented as

$$q_i = -k\rho c\frac{\partial U}{\partial i} \tag{3.57}$$

where q_i is the flux in the direction of the i dimension, k is the coefficient of thermal diffusivity, ρ is the density of the material, c is the heat capacity of the material , and U is temperature, which is defined as

$$U = \frac{H}{\rho c V} \tag{3.58}$$

where H is heat and V is volume.

The term in front of the differential in equation(3.57) is treated as a single term

$$k' = k\rho c \tag{3.59}$$

where k' is called the coefficient of thermal conductivity. It is a parameter that reflects how well the material conducts heat. Inspection of equation(3.57) indicates that Fourier's law specifies heat flux which is perpendicular to the i axis is proportional to the gradient or slope of temperature in the i direction. Substituting equation(3.57) into equation(3.56) results in

$$\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} = 0 \tag{3.60}$$

which is the *Laplace's equation.*

Now let us solve Laplace's equation for a specified boundary value problem given as

$$U_{xx} + U_{yy} = 0 \qquad 0 < x < 1 \quad , \quad 0 < y < 1 \tag{3.61}$$

$$U(0, y) = U(1, y) = 0 \tag{3.62}$$

$$U(x, 0) = f(x) \qquad U(x, 1) = 0 \tag{3.63}$$

To solve the partial differential equation we apply the method of separation of variables

$$U(x, y) = X(x)Y(y) \tag{3.64}$$

we get

$$\frac{X''}{X} = -\frac{Y''}{Y} \tag{3.65}$$

The left side of this equation is a function of x only and the right side is a function of y only, so each must be equal to a constant

$$\frac{X''}{X} = -\frac{Y''}{Y} = -\lambda^2 \tag{3.66}$$

where λ is a constant. The solution for X(x) is

$$X(x) = A\cos(\lambda x) + B\sin(\lambda x) \tag{3.67}$$

Applying the boundary conditions

$$X(x=0) = 0 = A \qquad \text{and} \qquad X(x=1) = 0 = B\sin(\lambda x) \tag{3.68}$$

gives $\lambda = n\pi$ where n is an integer. Then

$$X_n(x) = B_n \sin(n\pi x) \tag{3.69}$$

The solution for Y(y)is

$$Y(y) = C\cosh(\lambda y) + D\sinh(\lambda y) \tag{3.70}$$

or

$$Y_n(y) = C_n \cosh(n\pi y) + D_n \sinh(n\pi y) \tag{3.71}$$

We can write

$$Y_n(y) = E_n \sinh[n\pi(y - y_0)] \tag{3.72}$$

Use of the boundary condition $U(x,1) = 0$ implies that

$$E_n \sinh[n\pi(1 - y_0)] = 0 \tag{3.73}$$

which gives $y_0 = 1$. Therefore the solution becomes

$$U(x,y) = \sum_{n=1}^{\infty} = b_n \sin(n\pi x)\sinh n\pi(y-1) \tag{3.74}$$

The last boundary condition is expressed as

$$U(x,0) = \sum_{n=1}^{\infty} = b_n \sin(n\pi x)\sinh(-n\pi) = f(x) \tag{3.75}$$

giving

$$b_n = \frac{-2}{\sinh(n\pi)} \int_0^1 f(x)\sin(n\pi x)dx \tag{3.76}$$

We again take $f(x) = x^3(1-x)$ as shown in the figure(3.9) so that

$$b_n = \frac{-2}{\sinh(n\pi)}[\frac{-24}{(n\pi)^5} + \frac{24 - 6n^2\pi^2(-1)^n}{(n\pi)^5}] \tag{3.77}$$

A plot of the solution given by equation(3.74) is shown in figures(3.10.a), (3.10.b) and (3.10.c) from three different profiles.

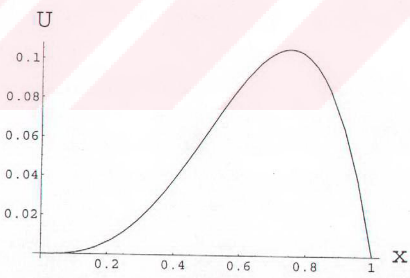

Figure 3.9: The graph of the boundary condition for Laplace's Equation.

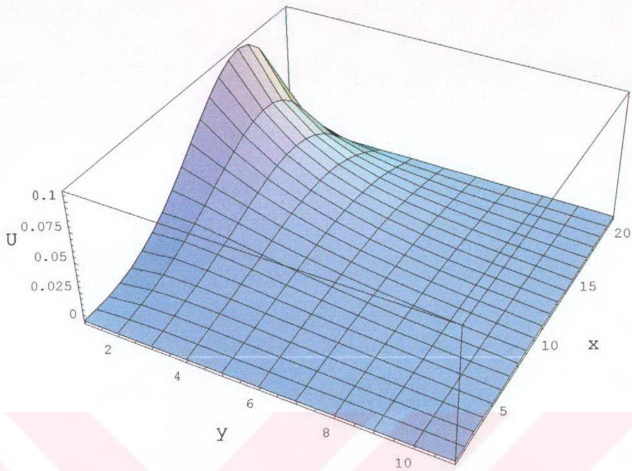

Figure 3.10.a : Analytical solution of Laplace ' s equation.

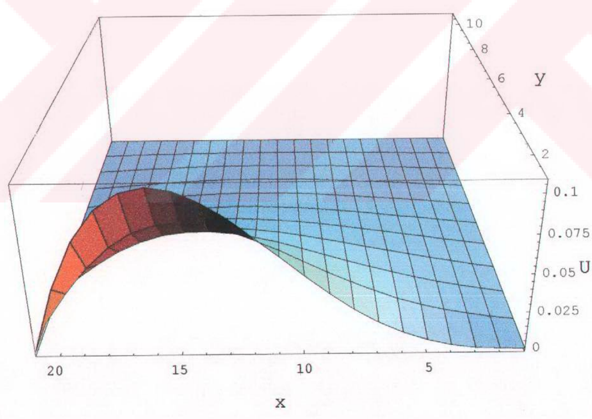

Figure 3.10.b : Analytical solution of Laplace ' s equation.

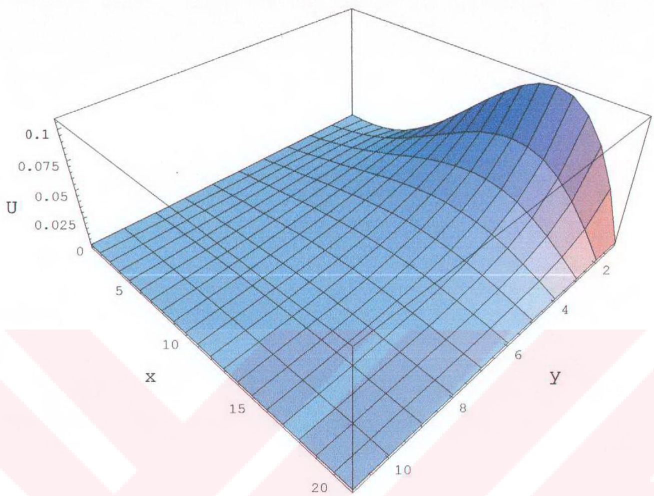

Figure 3.10.c : Analytical solution of Laplace's equation.

CHAPTER 4

NUMERICAL TREATMENT OF PARTIAL DIFFERENTIAL EQUATIONS

4.1 The Finite-Difference Method

In the previous chapter we have studied the analytical solutions of some of the physically important partial differential equations that are of different structure. Now in this chapter we wish to investigate the numerical solutions of the same equations. As we all know, most of the real-world problems are too complicated to handle analytically and therefore with the aid of a suitable method they are solved numerically [7]. The use of a numerical method generally means that a continuous problem is replaced by a discrete problem which can be solved on a computer in finitely many steps [14].

In this section, we briefly study a basic numerical method to solve partial differential equations which is known as the finite-difference method [9]. In this method, the main point is to replace the partial derivatives in the continuous equation by their difference-quotient approximations. Hence in this way a continuous partial differential equation is converted into a difference equation. As an example let us consider the following initial value problem

$$y' = f(t, y) \quad , \quad 0 < t < 1 \tag{4.1}$$

with $y(0) = y_0$. Here $y' = \frac{dy}{dt}$.

In order to solve equation(4.1) numerically, the first step is to discretize the continuous interval $0 \leq t \leq 1$ by defining a finite number of discrete points $t_n = n\Delta t$ where $n = 0, 1, .., N$, Δt is the time step size and $\Delta t = \frac{1}{N}$. At each point t_n a value Y_n is determined which is a reasonably good approximation to the exact value $y(t_n)$ of the solution. From calculus it is known that $y'(t_n)$ can be approximated by a forward difference quotient

$$y'(t_n) \approx \frac{y(t_{n+1}) - y(t_n)}{\Delta t} \tag{4.2}$$

provided that Δt is small enough. Consequently the continuous differential equation is approximated by

$$Y_{n+1} = Y_n + \Delta t f(t_n, Y_n) \tag{4.3}$$

where $n = 0, 1, 2, ..., N$. Now given $Y_0 = y_0$, the difference equation(4.3) given above provides a numerical algorithm to calculate the approximations $Y_1, Y_2, ...$ recursively.

4.2 The Wave Equation-The String Problem

As an example we consider the wave equation which is expressed as [9]

$$U_{tt} = c^2 U_{xx} \quad , \quad 0 < x < 1 \ , \ t > 0 \tag{4.4}$$

$$U(0,t) = U(1,t) = 0 \qquad , \quad t > 0 \tag{4.5}$$

$$U(x,0) = f(x) \quad , \quad U_t(x,0) = g(x) \quad , \quad 0 \leq x \leq 1 \tag{4.6}$$

It should be noted that we have already examined this problem analytically in the previous chapter and now we want to solve it numerically. Here in this and the following sections, our purpose is to illustrate the use of finite-difference method and also to compare the numerical solutions with their analytical counterparts.

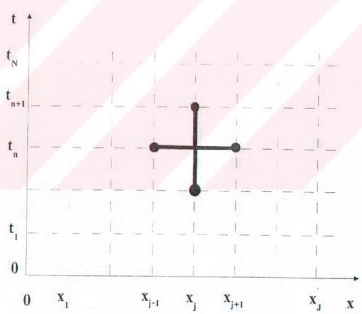

Figure 4.1: Lattice for the wave equation.

Choosing the lattice as given in figure(4.1), the equation(4.4) can be approximated as the following difference equation

$$U_j^{n+1} = 2U_j^n - U_j^{n-1} + (\frac{c\Delta t}{\Delta x})^2 (U_{j-1}^n - 2U_j^n + U_{j+1}^n) \tag{4.7}$$

From equation(4.7) it is apparent that the value of U_j^{n+1} at the time level $n+1$ can be computed only if its values from the previous two time levels are known. The value of U_j^n at $t_0 = 0$ is provided by the initial condition; that is

$$U_j^0 = f(x_j) \qquad \text{with} \qquad j = 0, 1, 2, ..., J \tag{4.8}$$

The value of U_j^n at $t = t_1$ can be computed using the initial velocity condition given by $U_t(x, 0) = g(x)$. The finite-difference approximation of this condition can be written as

$$U_j^1 = U_j^0 + \Delta t g(x_j) \tag{4.9}$$

To avoid numerical instability, the following stability condition

$$c \leq \frac{\Delta x}{\Delta t} \tag{4.10}$$

must be satisfied. Here c is the speed of the waves propagated in the system and equation(4.10) is known as the Courant-Friedrichs-Lax condition.

Using the computer program given in Appendix:A, the equation(4.9) is first solved for U_j^1 at the first time level and then the equation(4.7) is numerically integrated in the rest of the integration period.

Hence in this manner, the future values of U_j^n are determined. With $c = 0,25$, $N = 400$ and $J = 8$, a plot of U_j^n is depicted in Figures:4.2(a-b-c) from three different profiles.

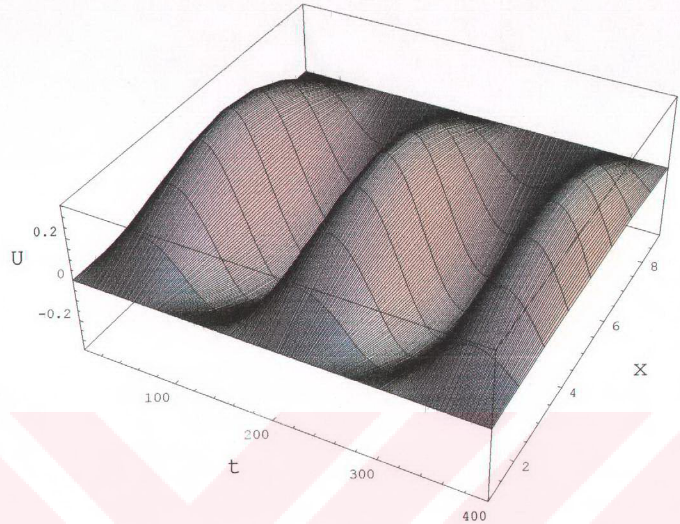

Figure 4.2.a : Numerical solution of the wave equation.

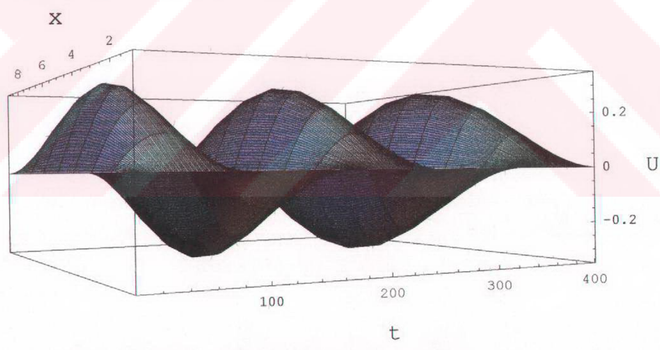

Figure 4.2.b : Numerical solution of the wave equation.

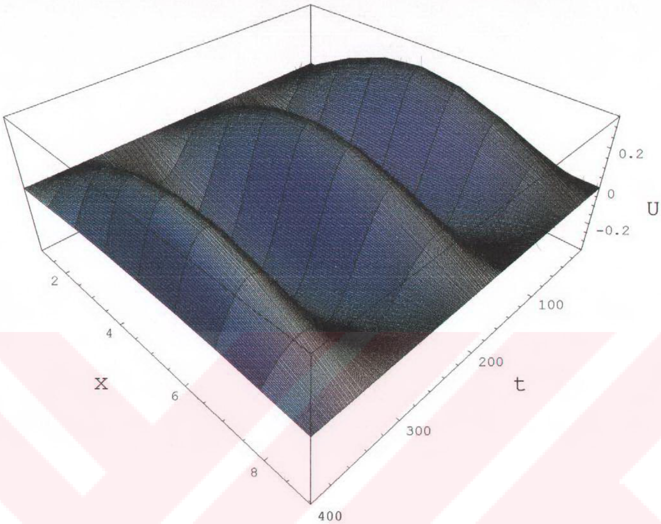

Figure 4.2.c : Numerical solution of the wave equation.

4.3 Heat Diffusion Equation

We now wish to solve numerically the following one-dimensional heat diffusion equation [9].

$$U_t = U_{xx} \quad , \quad 0 < x < 1 \ , \quad t > 0 \tag{4.11}$$

$$U(0,t) = U(1,t) = 0 \quad , \quad t > 0 \tag{4.12}$$

$$U(x,0) = f(x) \quad , \quad 0 < x < 1 \tag{4.13}$$

We must recall that this initial-boundary value problem has already been treated analytically in chapter three.

The first step is to replace the continuous space-time domain by a discrete domain defined on the lattice points shown in figure 4.3. where $x_j = j\Delta x$, $t_n = n\Delta t$ with $j = 0, 1, ..., J$ and $n = 0, 1, ..., N$.

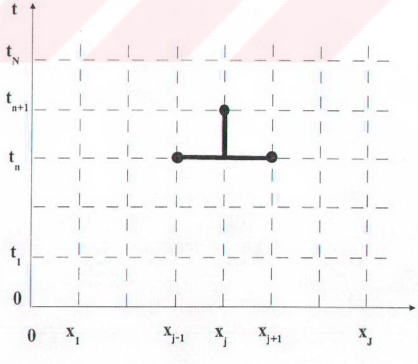

Figure 4.3: Lattice for the diffusion equation.

Here Δx is the step size along x-axis. The integer J is the number of subintervals in $0 \leq x \leq 1$ and N is the number of time steps to be taken. Now the main idea is to look for an approximation which we call U_j^n to the exact value $U(x_j, t_n)$ of the solution at each point (x_j, t_n) of the lattice. To achieve this goal, we replace the partial derivatives in equation(4.11) by their finite-difference quotients; that is

$$U_t(x_j, t_n) \approx \frac{U(x_j, t_{n+1}) - U(x_j, t_n)}{\Delta t} \tag{4.14}$$

and

$$U_{xx}(x_j, t_n) \approx \frac{U(x_{j-1}, t_n) - 2U(x_j, t_n) + U(x_{j+1}, t_n)}{(\Delta x)^2} \tag{4.15}$$

Hence in this way the following difference equation for $U(x_j, t_n)$ can be derived

$$U_j^{n+1} = U_j^n + \frac{\Delta t}{(\Delta x)^2}(U_{j-1}^n - 2U_j^n + U_{j+1}^n) \tag{4.16}$$

The initial and boundary conditions are given by

$$U_j^0 = f(x_j) = x_j^3(1 - x_j) \qquad \text{with} \quad j = 0, 1, ..., N \tag{4.17}$$

$$U_0^n = 0 \quad , \quad U_j^n = 0 \qquad \text{with} \quad n = 1, 2, ..., N \tag{4.18}$$

We must also remember that to ensure the stability of the numerical solution, we must have the following stability condition

$$\frac{\Delta t}{(\Delta x)^2} \leq \frac{1}{2} \tag{4.19}$$

to be satisfied [9].

Using the computer program given in Appendix:B, the difference equation can be applied at all the interior lattice points. The algorithm is such that the iterative scheme starts with the initial temperature values and computes the temperature values at the next time step. The iteration proceeds until a desired time level is reached.

In our computations we take $\Delta x = 0,05$ and $\Delta y = 0,0004$. The evolution of the approximate temperature values in time on the lattice is displayed in Figures:4.4(a-b-c) from three different profiles.

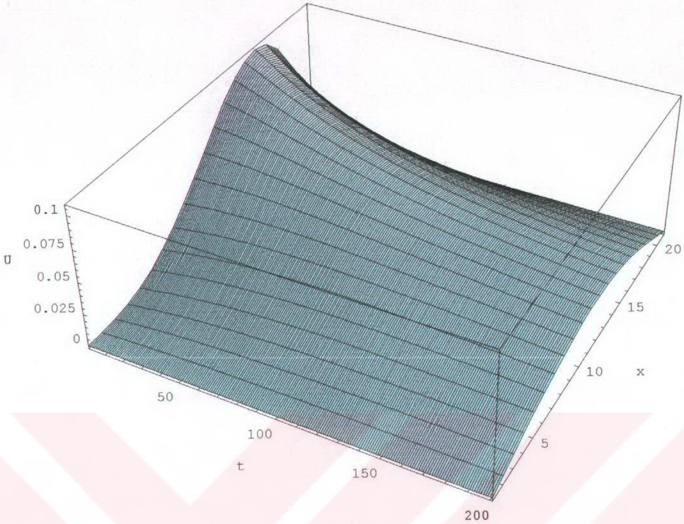

Figure : 4.4.a : Numerical solution for the diffusion equation.

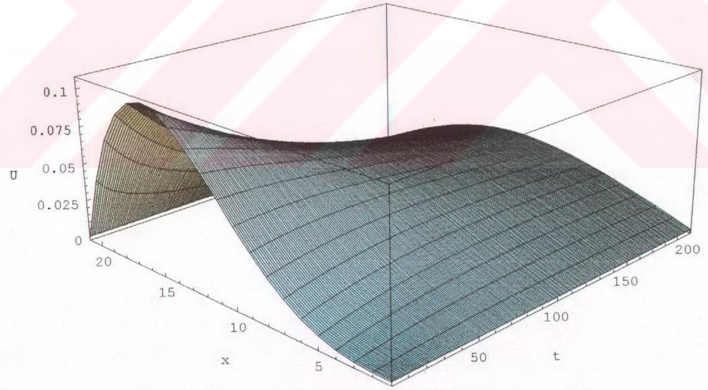

Figure : 4.4.b : Numerical solution for the diffusion equation.

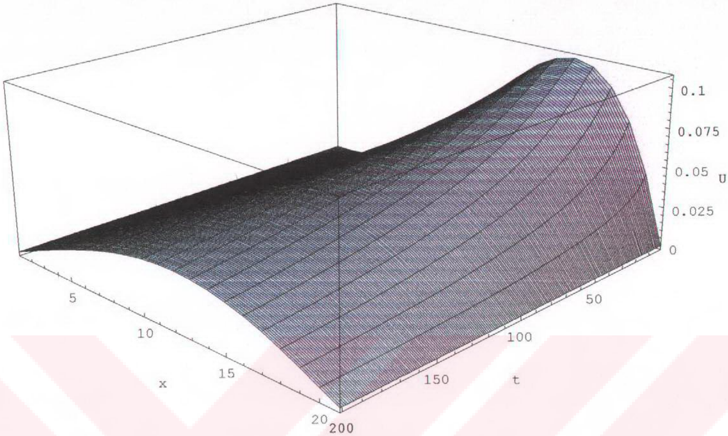

Figure : 4.4.c : Numerical solution for the diffusion equation .

4.4 Laplace's Equation

Lastly in this section we wish to study Laplace's equation [4] again. But as we mentioned in preceding sections our present purpose is to analyze this boundary value problem numerically. In particular this equation is solved in the unit square with given values on the boundary of the square using the finite-difference method. As it is known this kind of a boundary value problem is a typical example of a Dirichlet problem. The problem we want to focus our attention at is given as

$$U_{xx} + U_{yy} = 0 \quad , \quad 0 < x < 1 \quad , \quad 0 < y < 1 \tag{4.20}$$

$$U(0, y) = U(1, y) = 0 \quad , \quad 0 < y < 1 \tag{4.21}$$

$$U(x, 0) = f(x) \quad , \quad U(x, 1) = 0 \quad , \quad 0 \leq x \leq 1 \tag{4.22}$$

The equations(4.20)-(4.22) which do not involve the time as an independent variable are said to describe the so-called steady state phenomena.

The unit square in the xy-plane, which is in fact the domain of the solution, can be discretized by defining the lattice points as

$$x_i = i\Delta x \quad , \quad y_j = j\Delta y \quad , \quad i = 0, 1, \ldots I \quad , \quad j = 0, 1, \ldots. J \tag{4.23}$$

where $\Delta x = \frac{1}{I}$ and $\Delta y = \frac{1}{J}$ are the step sizes in the x and y directions respectively(See Figure:4.5). Now it can be shown that equation(4.20) can be approximated by the following difference equation

$$U_{i,j} = \frac{\Delta y^2}{2(\Delta x^2 + \Delta y^2)}(U_{i-1,j} + U_{i+1,j}) + \frac{\Delta x^2}{2(\Delta x^2 + \Delta y^2})(U_{i,j-1} + U_{i,j+1}) \tag{4.24}$$

The boundary conditions(4.21)-(4.22) provide the values of $U_{i,j}$ at the lattice

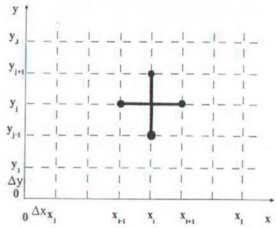

Figure 4.5: Lattice for the Laplace's equation.

points on the boundary of the square. Our task is then to find the values of $U_{i,j}$ at the $(I-1)*(J-1)$ interior lattice points. To do this we apply the finite-difference equation(4.24) to each interior lattice point simultaneously. This results in $(I-1)*(J-1)$ number of linear algebraic equations for $(I-1)*(J-1)$ number of unknowns $U_{i,j}$. Hence in this way the boundary value problem reduces to a linear algebra problem. Choosing $f(x) = x^3(1-x)$ as shown in Figure:4.6 and $\Delta x = 0.05$,$\Delta y = 0.1$ and using the algorithm presented in Appendix:C, we obtain all the values of $U_{i,j}$ at the interior lattice points. A graph of these values of $U_{i,j}$ over the discretized unit square from three different profiles is shown in Figures:4.7(a-b-c).

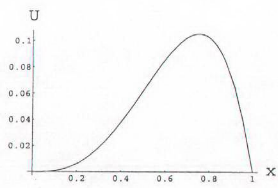

Figure 4.6: A graph of the boundary condition $f(x)$ for Laplace's Equation.

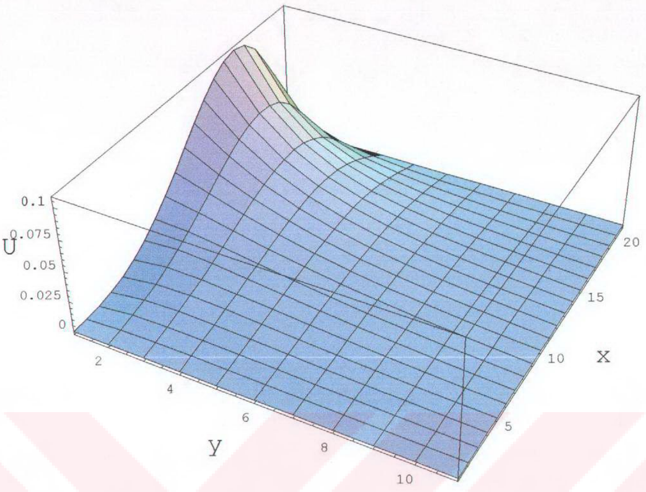

Figure 4.7.a : Numerical solution for Laplace ' s equation.

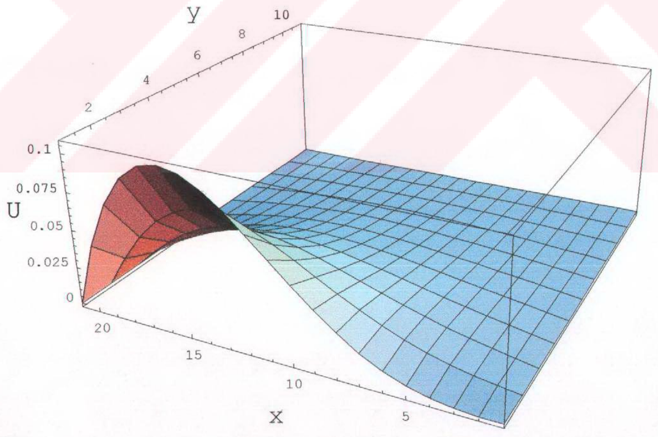

Figure 4.7.b : Numerical solution for Laplace ' s equation.

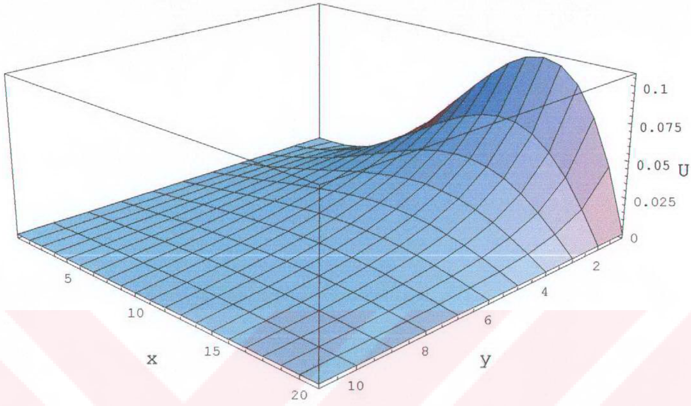

Figure 4.7.c : Numerical solution for Laplace ' s equation.

4.5 Discussion

In the present thesis a brief review of some important partial differential equations in physics is made. The strategy of the review was such that we looked first at a classification technique. This technique classifies partial differential equations according to their structural forms. This way of classifying the equations means that the physical phenomena governed by these equations are in fact indirectly being classified. Therefore in the light of this substantial point we selected several partial differential equations of physical significance and studied them analytically in chapter three. Generally speaking, this type of an approach illustrates the use and application of some of the frequently encountered analytical solution methods. In addition to the general solutions of these equations, we also obtained their special solutions for some of the specified initial boundary value problems.

Next in chapter four we studied the same equations using the finite-difference method. The main point behind this numerical treatment was to see which of the two approaches is more advantageous. To be able to give an answer to this, we compared the analytical and numerical solutions of the equations we considered in chapters three and four as given by the figures:3.4.(a-b-c), 3.7.(a-b-c), 3.10.(a-b-c), 4.2.(a-b-c), 4.4.(a-b-c), 4.7.(a-b-c). Also for each equation we plotted the variation of the differences between the analytical solutions and the numerical solutions as shown in figures:4.8.(a-b-c). The non-dimensionalized and scaled amplitudes of the analytical and numerical solutions (see figures:3.4.(a-b-c), 3.7.(a-b-c), 3.10.(a-b-c), 4.2.(a-b-c), 4.4.(a-b-c), 4.7.(a-b-c)) are larger than the amplitudes of the differences between the analytical and numerical solutions (see figures:4.8.(a-b-c)) by an order of magnitude 10^3. This tells us that the truncation errors in the numerical solutions are almost negligible. Also as for the time-dependent equations, numerical instability has not shown itself at all.

From this analysis it is clearly seen that both approaches produce almost identical solutions.

As a conclusion we may state that a major advantage offered by the analytical approach is that the analytical solution allows us to find the solution at any point in the domain of solution and not just the lattice points. Another advantage is that the analytical solution enables us to see how physical variables, initial and boundary conditions affect the solution [10].

However an important advantage of the numerical approach is that almost all nonlinear real-world problems which do not have analytical solutions must be treated by numerical methods. In fact, most realistic models in physics, chemistry, biology and so forth, are nonlinear in nature [7].

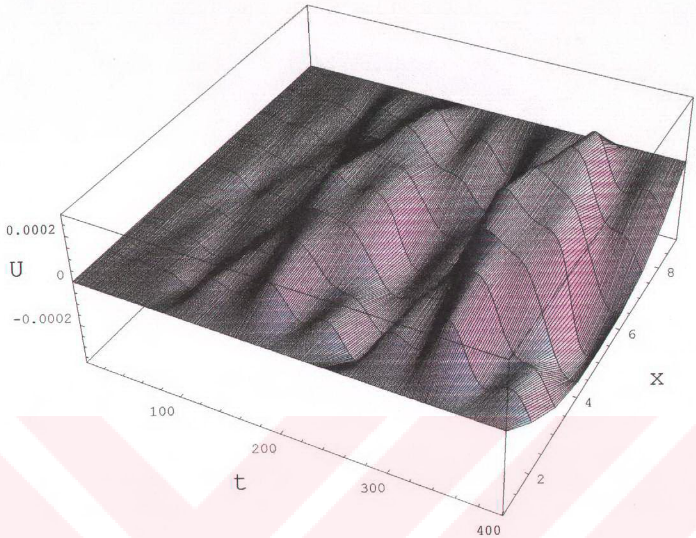

Figure 4.8.a : The graph of the difference between the analytic and the numerical solutions of the string problem.

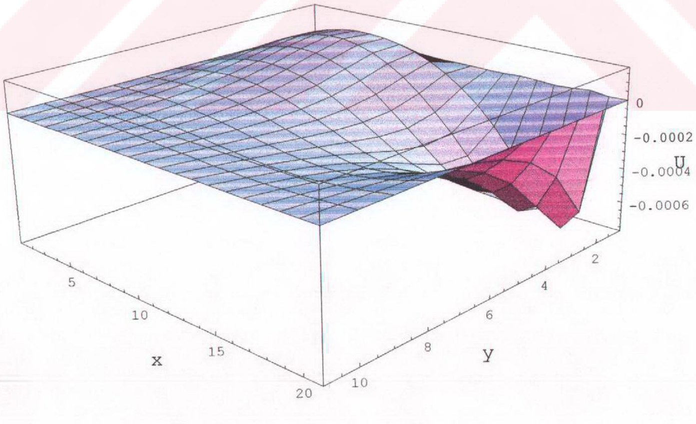

Figure 4.8.b : The graph of the difference between the analytic and the numerical solutions of Laplace ' s equation.

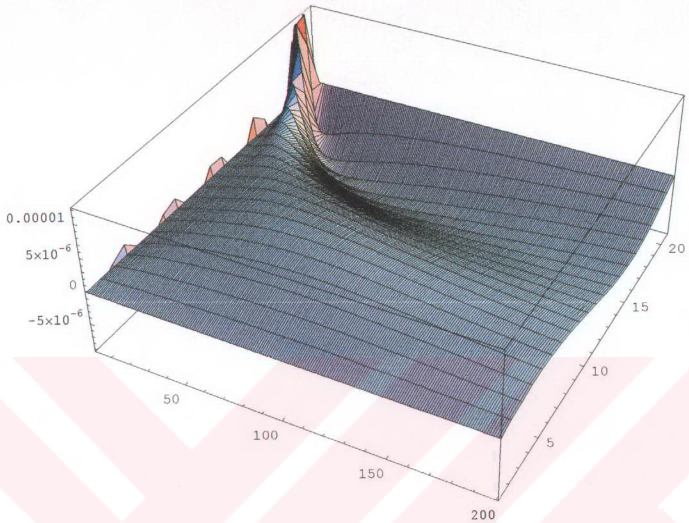

Figure 4.8.c : The graph of the difference between the analytic and the numerical solutions of the heat diffusion problem.

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APPENDIX A

MATHEMATICA PROGRAM FOR WAVE EQUATION

```
f[x_] := 0;              (*initial condition*)
g[x_] := (1 - x) * x;    (*initial velocity condition*)
c = 0.25;
FD[J_, N_, k_] := Module[{h}, h = 0.125;
  r = h / (k);
  Print["The Stability Condition:  ", r]; (*the Stability condition*)
  f2[x_] := 0.0;
  U = Array[f2[0.0], {J + 1, N + 1}];
  Do[U[[j, 1]] = 0.0, {j, 1, J + 1}];
  Do[U[[j, 2]] = k * g[h * (j - 1)], {j, 1, J + 1}];
  Do[U[[1, n]] = 0.0, {n, 1, N + 1}];   (*boundary condition*)
  Do[U[[J + 1, n]] = 0.0, {n, 1, N + 1}];  (*boundary condition*)
  Do[Do[U[[j, n + 1]] =
      2 * U[[j, n]] - U[[j, n - 1]] + ((c * k) / h) ^2 * (U[[j - 1, n]] - 2 * U[[j, n]]
          + U[[j + 1, n]]), {j, 2, J}], {n, 2, N}];
  U]

unum = Table[FD[8, 400, 0.05]];
```

APPENDIX B

MATHEMATICA PROGRAM FOR DIFFUSION EQUATION

```
funct[x_] := (1 - x)*x^3  (*initial condition*)
FD[J_, N_] := Module[{h, k},
 h = 0.05; k = 0.0004;
 r= k/(h*h);
 Print["The Stability Condition:  ",r];    (*the Stability condition*)
 f2[x_] := 0.0;
 U = Array[f2[0.0], {J + 1, N + 1}];
 Do[U[[j, 1]] = funct[h*(j - 1)], {j, 1, J + 1}];
 Do[U[[1, n]] = 0.0, {n, 1, N + 1}];
 Do[U[[J + 1, n]] = 0.0, {n, 1, N + 1}];
 Do[Do[U[[j, n + 1]] = U[[j, n]] + k/(h*h)*(U[[j - 1, n]]
 - 2*U[[j, n]] + U[[j + 1, n]]), {j, 2, J}], {n, 1, N}] U]
num=ListPlot3D[FD[20, 200],AxesLabel->{"t","x","U   "}]
```

APPENDIX C

MATHEMATICA PROGRAM FOR LAPLACE'S EQUATION

```
funct[x_] := (1 - x) * x^3
FD[I_, J_] := Module[{h, k, U}, h = 0.05; k = 0.1;
   r = 0.5 * k^2 / ((h^2) + (k^2));
   s = 0.5 * h^2 / ((h^2) + (k^2));
   f2[x_] := 0.0;
   U = Table[0, {i, 1, I + 1}, {j, 1, J + 1}];
   Do[U[[i, 1]] = funct[h * (i - 1)], {i, 1, I + 1}];
   Do[U[[i, J + 1]] = 0.0, {i, 1, I + 1}];
   Do[U[[1, j]] = 0.0, {j, 1, J + 1}];
   Do[U[[I + 1, j]] = 0.0, {j, 1, J + 1}];
   Do[Do[Do[U[[i, j]] = r * (U[[i - 1, j]] + U[[i + 1, j]]) +
         s * (U[[i, j - 1]] + U[[i, j + 1]]),
      {i, 2, I}], {j, 2, J}], {n, 1, 200}];
   U]
 fdif = FD[20, 10];
  ab =
   ListPlot3D[fdif, PlotRange → All, AxesLabel → {"y", "x", "U"}]
```