DOKUZ EYLÜL UNIVERSITY
GRADUATE SCHOOL OF NATURAL AND APPLIED SCIENCES

MATHEMATICAL MODELING AND SIMULATION OF DIFFUSION PROCESSES

by
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İZMİR

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We have read the thesis entitled **"MATHEMATICAL MODELING AND SIMULATION OF DIFFUSION PROCESSES"** completed by **BARIŞ ÇİÇEK** under supervision of **PROF. DR. VALERY YAKHNO** we certify that in our opinion it is fully adequate, in scope and in quality, as a thesis for the degree of Master of Science.

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MATHEMATICAL MODELING AND SIMULATION OF DIFFUSION PROCESSES

ABSTRACT

Modeling and simulating diffusion processes are studied in this thesis. The explicit formulae for solutions of initial value problems and initial boundary value problems are obtained. Using these formulae the simulations of the diffusion processes have been done. The pulse point sources are used for computational applications. These sources have real physical sources and they are described by generalized functions (the Dirac delta function).

Fourier series expansion method is applied for the construction of explicit formulae for initial boundary value problems of the diffusion equation in one, two and three dimensional cases with Dirichlet, Neumann and Mixed (Robin) boundary conditions.

Green's function method is used for finding explicit formulae of initial value problems and initial boundary value problems with Dirichlet boundary condition.

Theory of partial differential equations and ordinary differential equations, theory of generalized functions and modern computer tools (symbolic calculation, graph packages at etc.) are actively used in this thesis.

Keywords: Diffusion processes, simulation, symbolic calculation.

DİFUZYON İŞLEMİNİN MODELLEMESİ VE SİMÜLASYONU

ÖZ

Bu tezde difüzyon işleminin matematiksel modellemesi ve simülasyonu çalışıldı. Başlangıç sınır değer ve sınır değer problemlerinin çözümleri elde edildi. Bu çözümler kullanılarak simülasyonlar yapıldı. Hesaplamalar için noktasal kaynaklar kullanıldı. Bu kaynaklar reel fiziksel kaynaklardır ve genelleştirilmiş fonksiyonlar (Dirac delta fonksiyonu) olarak tanımlandılar.

Fourier serileri methodu kullanılarak bir, iki ve üç boyutlu uzaylarda Dirichlet, Neumann ve Mixed sınır koşulları ile başlangıç ve sınır değer problemlerinin çözümleri oluşturuldu.

Başlangıç değer ve Dirichlet sınır koşullu başlangıç sınır değer problemlerinin çözümleri için Green fonksiyon metodu kullanıldı.

Kısmi diferansiyel denklemler ve adi diferansiyel denklemler teorileri, genelleştirilmiş fonksiyon teorisi ve bilgisayar araçları (sembolik hesaplama, grafik paketleri vs) tezde aktif olarak kullanıldı.

Anahtar sözcükler: Difüzyon işlemi, simülasyon, sembolik hesaplama.

CONTENTS

Page

CHAPTER ONE
INTRODUCTION

1.1 Goal and Methods

The main object of the thesis is the diffusion processes. Diffusion equation is a mathematical model of the diffusion processes. This equation is the partial differential equation. We will consider two types of problems for this diffusion equation: Initial value problems (IVPs) and Initial boundary value problems (IBVPs). We consider these problems in one dimensional (1-D), two dimensional (2-D) and three dimensional (3-D) spaces.

The main aim of the study is

- obtain explicit formulae for solutions of IVPs and IBVPs.
- adjust these formulae for the case of pulse point sources described by the Dirac delta function.
- using obtained formulae and modern computer tools to simulate diffusion processes on a string, in a rectangle and in a homogeneous parallelepiped and for unbounded space.
- obtain 1-D, 2-D and 3-D graphs and animated movies of processes of the diffusion propagations.
- analyze the obtained simulation results.

The theory and methods of partial differential equations, symbolic computation, Mathematica, graphic facilities are actively used in the thesis.

1.2 Statements of the IBVP for the Heat-Diffusion Equation

Let $D \in \mathbf{R^3}$ be a bounded domain, $x \in D$, $t \geq 0$. Consider the following system

$$\frac{1}{c^2}\frac{\partial u(x,t)}{\partial t} = \Delta_x u(x,t) + f(x,t)\ , x \in D, \quad t \geq 0\ , \tag{1.2.1}$$

$$u(x,0) = \phi(x)\ , \tag{1.2.2}$$

$$\big(\alpha_1 u(x,t) + \alpha_2 \frac{\partial u(x,t)}{\partial n}\big)\big|_{\partial D} = 0\ , \tag{1.2.3}$$

where ∂D is the boundary of the bounded domain D, $f(x,t)$ is a given scalar function which depends on x, t, and $\phi(x)$ is a given scalar function of x. Problem (1.2.1)-(1.2.3) is called the **initial boundary value problem for the heat-diffusion equation**. And for different α_1 and α_2 values we have different boundary value problems. The initial boundary value problem (1.2.1)-(1.2.3) will be studied for the following boundary conditions Cohen (2002):

1. Dirichlet boundary condition : $\alpha_1 \neq 0\ , \quad \alpha_2 = 0\ ,$
2. Neumann boundary condition : $\alpha_1 = 0\ , \quad \alpha_2 \neq 0\ ,$
3. Mixed (or Robin) boundary condition : $\alpha_1 \neq 0\ , \quad \alpha_2 \neq 0\ .$

1.3 Pulse Point Heat Source

If a source of the heat propagation is acting in a moment, in order to model this physical situation we will use pulse point sources. The mathematical model represent this pulse point sources is the Dirac delta function which was originally introduced by Paul Dirac, a well known physicist of the first half of the C20.

The function $f(x,t)$ in the equation (1.2.1) is the internal source in the domain and the equation (1.2.2) is the initial condition.

In our study we use the Dirac delta function in the following cases of the heat-diffusion equation in a bounded domain D. And these functions are written only for 3-D domain,

1. $\phi(x) = 0\ ,\ f = \delta(x - x_0)\delta(y - y_0)\delta(z - z_0)\delta(t - t_0)\ ,$
2. $\phi(x) = \delta(x - x_0)\delta(y - y_0)\delta(z - z_0)\ ,\ f = 0\ ,$

where $\delta(\cdot)$ is the Dirac delta function.

Here (x_1, x_2, x_3) is the location of the source and t_0 is the time when the source acts.

CHAPTER TWO
IBVP FOR HEAT-DIFFUSION EQUATION WITH DIRICHLET BOUNDARY CONDITION

In this section IBVP for 1D, 2D and 3D heat(diffusion) equation with Dirichlet Boundary condition in a homogeneous strip, rectangle and parallelepiped will be studied. The formulas will be generated and using these formulas simulations will be found. Sources are taken as pulse point source and here we substituted Dirac delta function.

2.1 IBVP for a Homogeneous 1D Heat-Diffusion Equation with Dirichlet Boundary Condition

Let $x \in (0,\ell)$, $t \in (0,T)$, where ℓ and T are given positive numbers. Let us consider the IBVP for the diffusion equation on a string :

$$\frac{1}{c^2}\frac{\partial u(x,t)}{\partial t} = \frac{\partial^2 u(x,t)}{\partial x^2}\ , x \in (0,\ell), \quad t \in (0,T)\ , \tag{2.1.1}$$

$$u(x,0) = \phi(x)\ , \tag{2.1.2}$$

$$u(0,t) = u(\ell,t) = 0\ , \tag{2.1.3}$$

where $c > 0$ is a given number. Here $\phi(x)$ is a given smooth function for $x \in [0,\ell]$. IBVP consists of finding $u(x,t)$ satisfying (2.1.1), (2.1.2), (2.1.3).
We will use the separation of variables :

$$u(x,t) = T(t)X(x)\ . \tag{2.1.4}$$

Substituting (2.1.4) into (2.1.1) we find

$$\frac{1}{c^2}T'(t)X(x) = T(t)X''(x)\ .$$

Dividing both sides of the last equation by $T(t)X(x)$, we have

$$\frac{1}{c^2}\frac{T'(t)}{T(t)} = \frac{X''(x)}{X(x)}\ .$$

Let us fix t and let $x \in (0,\ell)$. Since t and x are independent variables then the last equality takes place if and only if the left hand side and the right hand side of this equation are equal to the same constant which we denote as $-\lambda$.

$$\frac{1}{c^2}\frac{T'(t)}{T(t)} = \frac{X''(x)}{X(x)} = -\lambda \; .$$

As a result of it we get the following equations :

$$X''(x) + \lambda X(x) = 0, \quad x \in (0,\ell) \; , \tag{2.1.5}$$

$$T'(t) + c^2\lambda T(t) = 0, \quad t \in (0,T) \; . \tag{2.1.6}$$

Substituting (2.1.4) into (2.1.3) we obtain

$$X(0) = 0 \quad \& \quad X(\ell) = 0 \; . \tag{2.1.7}$$

That is, $X(x)$ has to be a solution of the following eigenvalue-eigenfunction problem (Sturm-Liouville problem) :

$$X''(x) + \lambda X(x) = 0, \; x \in (0,\ell) \; , \tag{2.1.8}$$

$$X(0) = 0 \quad \& \quad X(\ell) = 0 \; . \tag{2.1.9}$$

The solution of the eigenvalue-eigenfunction problem (2.1.7)-(2.1.8) of the form

$$\lambda_i = \left(\frac{i\pi}{\ell}\right)^2 \; , \tag{2.1.10}$$

$$X_i(x) = \sqrt{\frac{2}{\ell}}\sin\sqrt{\lambda_i}x, \quad i = 1,2,... \tag{2.1.11}$$

We can construct the Fourier series by using the following remark.

Remark 2.1.1. *The system of eigenfunctions $\{X_i\}_{i=1,2,...}$ is a complete orthonormal basis. And we can write each function $\phi(x)$ in the form of Fourier series expansion which is convergent :*

$$\phi(x) = \sum_{i=1}^{\infty} \phi_i X_i(x) \; ,$$

where

$$\phi_i = \int_0^{\ell} \phi(x)X_i(x)dx \; .$$

Remark 2.1.2. *(Fourier Series Expansion of $\delta(x)$ function) We can generalize the idea of Fourier expansion of a classical function for the Dirac delta function*

$\delta(x-x_0)$, where (x_0) is a fixed point in $x \in (0,\ell)$. It may be written in the form of the Fourier Series expansion as follows :

$$\delta(x-x_0) = \sum_{i=1}^{\infty} \delta_i X_i(x) \ , \tag{2.1.12}$$

where

$$\delta_i = \int_0^{\ell} \delta(x-x_0) X_i(x) dx = X_i(x_0) \ .$$

Let us consider the equation (2.1.6) for $\lambda = \lambda_i$ for $i = 1, 2, \ldots$. This equation may be written in the form

$$T_i'(t) + c^2 \lambda_i T_i(t) = 0, \quad i = 1, 2, \ldots \ . \tag{2.1.13}$$

A general solution of (2.1.13) is given by

$$T_i(t) = A_i \ e^{-c^2 \lambda_i t}, \quad i = 1, 2, \ldots \ , \tag{2.1.14}$$

where A_i are arbitrary constant for $i = 1, 2, \ldots$. Let us consider the function $u(x,t)$ defined by

$$u(x,t) = \sum_{i=1}^{\infty} A_i \ e^{-c^2 \lambda_i t} X_i(x) \ , \tag{2.1.15}$$

where A_i are arbitrary constants for $i = 1, 2, \ldots$. This function satisfies (2.1.1)-(2.1.3). The main goal consists in finding A_i for which the initial data (2.1.2) holds. Using the orthonormal functions $X_i(x)$, we can write $\phi(x)$ in the form of the Fourier series expansion as follows :

$$\phi(x) = \sum_{i=1}^{\infty} \phi_i X_i(x) \ , \tag{2.1.16}$$

where

$$\phi_i = \int_0^{\ell} \phi(x) X_i(x) dx \ .$$

Using the initial conditions (2.1.2) and (2.1.15), (2.1.16) we can find A_i by

$$A_i = \phi_i \ ,$$

Substituting found values of A_i into (2.1.15), we have

$$u(x,t) = \sum_{i=1}^{\infty} \phi_i \, e^{-c^2\lambda_i t} X_i(x) \ , \tag{2.1.17}$$

where

$$\phi_i = \int_0^{\ell} \phi(x) X_i(x) dx \ ,$$

$$X_i(x) = \sqrt{\frac{2}{\ell}} \sin \sqrt{\lambda_i} x \ ,$$

$$\lambda_i = \left(\frac{i\pi}{\ell}\right)^2 \ , \quad i = 1, 2, \dots \ .$$

This function $u(x,t)$ satisfies (2.1.1)-(2.1.3). Therefore this function is a solution of the problem (2.1.1)-(2.1.3).

2.2 IBVP for a Non-Homogeneous 1D Heat-Diffusion Equation with Dirichlet Boundary Condition

Let $x \in (0,\ell)$, $t \in (0,T)$, where ℓ and T are given positive numbers. Let us consider the IBVP for the diffusion equation on a string :

$$\begin{aligned} \frac{1}{c^2}\frac{\partial u(x,t)}{\partial t} &= \frac{\partial^2 u(x,t)}{\partial x^2} \\ &\quad + F(x,t) \ , \quad x \in (0,\ell), t \in (0,T) \ , && (2.2.1) \\ u(x,0) &= \phi(x) \ , && (2.2.2) \\ u(0,t) &= u(\ell,t) = 0 \ , && (2.2.3) \end{aligned}$$

where $c > 0$ is a given positive number; $\phi(x)$ is a given smooth functions for $x \in [0,\ell]$, $F(x,t)$ is a given smooth function for $(x,t) \in ([0,\ell] \times [0,t])$. IBVP consists of finding $u(x,t)$ satisfying (2.2.1)-(2.2.3).

Consider the system of eigenfunctions which is a solution of eigenvalue-eigenfunction problem for the Laplace operator in a parallelepiped with the Dirichlet Boundary Condition. These are functions $X_i(x)_{i=1,2,\dots}$ satisfying (2.1.8) and (2.1.9). Using this system of functions, we will find the solution in the form :

$$u(x,t) = \sum_{i=1}^{\infty} T_i(t) X_i(x) \ , \tag{2.2.4}$$

where $T_i(t)$ are unknown Fourier coefficients of $u(x,t)$. We have

$$F(x,t) = \sum_{i=1}^{\infty} F_i(t) X_i(x) , \tag{2.2.5}$$

where

$$F_i(t) = \int_0^{\ell} F(x,t) X_i(x) dx , \quad i = 1, 2, \ldots . \tag{2.2.6}$$

Substituting (2.2.5) and (2.2.4) into (2.2.1) we will get

$$\sum_{i=1}^{\infty} \left\{ \frac{1}{c^2} T_i'(t) X_i(x) - T_i(t) X_i''(x) - F_i(t) X_i(x) \right\} = 0 .$$

And using (2.1.8) we get

$$\sum_{i=1}^{\infty} \left\{ \frac{1}{c^2} T_i'(t) X_i(x) + \lambda_i T_i(t) X_i(x) - F_i(t) X_i(x) \right\} = 0 .$$

Hence

$$\sum_{i=1}^{\infty} \left\{ \frac{1}{c^2} T_i'(t) + \lambda_i T_i(t) - F_i(t) \right\} X_i(x) = 0 .$$

Since the function system $\{X_i\}_{i=1,2,\ldots}$ are normalized orthogonal system, the previous equation implies a first order ordinary differential equation as follows

$$\frac{1}{c^2} T_i'(t) + \lambda_i T_i(t) - F_i(t) = 0, \ t \in (0, T) .$$

And using (2.2.2) and (2.1.16) we get

$$T_i(0) = \phi_i .$$

So we have the following system for $T_i(t)$, $i = 1, 2, \ldots$

$$\frac{1}{c^2} T_i'(t) + \lambda_i T_i(t) - F_i(t) = 0, \quad t > 0 , \tag{2.2.7}$$

$$T_i(0) = \phi_i . \tag{2.2.8}$$

Remark 2.2.1. *The function*

$$u(x,t) = \sum_{i=1}^{\infty} T_i(t) X_i(x) ,$$

is a solution for (2.2.1)-(2.2.3) if and only if $T_i(t)$ satisfy (2.2.7), (2.2.8) for

$i = 1, 2, ...$ *which is given by*

$$T_i(t) = \phi_i e^{-c^2\lambda_i t} + c^2 \int_0^t F_i(\tau) e^{-c^2\lambda_i(t-\tau)} d\tau \ , \qquad (2.2.9)$$

(See Appendix A.1). Thus

$$u(x,t) = \sum_{i=1}^{\infty} T_i(t) X_i(x) \ , \qquad (2.2.10)$$

is the solution of the problem (2.2.1)-(2.2.3), where $T_i(t)$ is defined in (2.2.9) and $X_i(x)$ is defined in (2.1.11) for $i = 1, 2, ...$

2.3 IBVP for a Homogeneous 2D Heat-Diffusion Equation with Dirichlet Boundary Condition

Let $(x, y) \in \mathbb{R}^2$, $t \in \mathbb{R}$, $D = \{(x, y) \in \mathbb{R}^2 : 0 \leq x \leq b_1, 0 \leq y \leq b_2\}$ be a homogeneous rectangle. Let us consider the IBVP for the diffusion equation in the rectangle D :

$$\frac{1}{c^2}\frac{\partial u(x,y,t)}{\partial t} = \Delta_{x,y}u(x,y,t) \, , (x,y) \in D, \quad t \geq 0 \, , \tag{2.3.1}$$

$$u(x,y,0) = \phi(x,y) \, , \tag{2.3.2}$$

$$u(x,y,t)|_{\partial D} = 0 \, , \tag{2.3.3}$$

where ∂D is the boundary of D. Here $\phi(x, y)$ is given function in $D \cup \partial D$, c is a positive constant. IBVP consists of finding $u(x, y, t)$ satisfying (2.3.1), (2.3.2), (2.3.3).

We will use the separation of variables :

$$u(x,y,t) = T(t)V(x,y) \, . \tag{2.3.4}$$

Substituting (2.3.4) into (2.3.1) we find

$$\frac{1}{c^2}T'(t)V(x,y) = T(t)\Delta_{x,y}V(x,y) \, .$$

Dividing both sides of the last equation by $T(t)V(x, y)$, we have

$$\frac{1}{c^2}\frac{T'(t)}{T(t)} = \frac{\Delta_{x,y}V(x,y)}{V(x,y)} \, .$$

Let us fix t and let (x, y) vary in the rectangle D. Since t and (x, y) are independent variables then the last equality takes place if and only if the left hand side and the right hand side of this equation are equal to the same constant which we denote as $-\lambda$.

$$\frac{1}{c^2}\frac{T'(t)}{T(t)} = \frac{\Delta_{x,y}V(x,y)}{V(x,y)} = -\lambda \, .$$

As a result of it we get the following equations :

$$\Delta_{x,y}V(x,y) + \lambda V(x,y) = 0, \quad (x,y) \in D \, , \tag{2.3.5}$$

$$T'(t) + c^2\lambda T(t) = 0, \quad t > 0 \, . \tag{2.3.6}$$

Substituting (2.3.4) into (2.3.3) we obtain

$$V(x,y)|_{\partial D} = 0 \ . \tag{2.3.7}$$

This means that $V(x,y)$ has to be a solution of the following eigenvalue-eigenfunction problem (Stum-Liouville problem) :

$$\Delta_{x,y} V(x,y) + \lambda V(x,y) = 0 \ , \quad (x,y) \in D \ , \tag{2.3.8}$$

$$V(x,y)|_{\partial D} = 0 \ . \tag{2.3.9}$$

For the solution of the eigenvalue-eigenfunction problem we will use the method of separation of variables. Setting

$$V(x,y) = X(x)Y(y) \ , \tag{2.3.10}$$

and substituting (2.3.10) into (2.3.8) and dividing both sides of the equation (2.3.8) by $X(x)Y(y)$, we have

$$\frac{X''(x)}{X(x)} + \frac{Y''(y)}{Y(y)} + \lambda = 0 \ .$$

Thus

$$\frac{Y''(y)}{Y(y)} + \lambda = -\frac{X''(x)}{X(x)} \ .$$

The left hand side of the last equation depends on variable y, right hand side depends on x. Since the variables x, y are independent variables, the last equation holds if and only if the both sides of this equation are equal to the same constant which we denote as α

$$\frac{Y''(y)}{Y(y)} + \lambda = -\frac{X''(x)}{X(x)} = \alpha \ .$$

or equivalently

$$\frac{Y''(y)}{Y(y)} + \lambda = \alpha \ .$$

Hence

$$\lambda - \alpha = -\frac{Y''(y)}{Y(y)} = \beta \ .$$

where α, β are constants such that

$$\lambda = \alpha + \beta \ .$$

Also substituting (2.3.10) into (2.3.9) we have three Strum-Liouville equations for the ordinary differential equations :

$$X''(x) + \alpha X(x) = 0, \quad X(0) = X(b_1) = 0 \ , \tag{2.3.11}$$

$$Y''(y) + \beta Y(y) = 0, \quad Y(0) = Y(b_2) = 0 \ , \tag{2.3.12}$$

The solutions of these eigenvalue-eigenfunction problem (2.3.11), (2.3.12) are given by

$$\alpha_i = (\frac{i\pi}{b_1})^2, \quad X_i(x) = \sqrt{\frac{2}{b_1}} \sin \sqrt{\alpha_i} x \ , \quad i = 1, 2, ... \ ;$$

$$\beta_j = (\frac{j\pi}{b_2})^2, \quad Y_j(y) = \sqrt{\frac{2}{b_2}} \sin \sqrt{\beta_j} y \ , \quad j = 1, 2, ... \ ;$$

(see Appendix A1 for detailed explanation) As a result of this we get the solution of eigenvalue-eigenfunction problem (2.3.8), (2.3.9) as follows :

$$\lambda_{ij} = \left(\frac{i\pi}{b_1}\right)^2 + \left(\frac{j\pi}{b_2}\right)^2 \ , \tag{2.3.13}$$

$$V_{ij} = \sqrt{\frac{4}{b_1 b_2}} \sin \sqrt{\alpha_i} x \sin \sqrt{\beta_j} y \ , \quad i, j = 1, 2, ... \tag{2.3.14}$$

Remark 2.3.1. *The system of eigenfunctions* $\{V_{ij}\}_{i,j=1,2,...}$ *is a complete orthonormal basis,* $D = \{(x, y) \in \mathbb{R}^2 : 0 \le x \le b_1, 0 \le y \le b_2\}$*. This means that each function* $\phi(x, y)$ *may be written in the form of Fourier series expansion which is convergent:*

$$\phi(x, y) = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \phi_{ij} V_{ij}(x, y) \ ,$$

where

$$\phi_{ij} = \int_0^{b_1} \int_0^{b_2} \phi(x, y) V_{ij}(x, y) dy dx \ .$$

Remark 2.3.2. *(Fourier Series Expansion of* $\delta(x, y)$ *function) We can generalize the idea of Fourier expansion of a classical function for the Dirac delta function* $\delta(x - x_0, y - y_0)$*, where* (x_0, y_0) *is a fixed point in* D*. It may be written in the form of the Fourier Series expansion as follows :*

$$\delta(x - x_0, y - y_0) = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \delta_{ij} V_{ij}(x, y) \ , \tag{2.3.15}$$

where

$$\delta_{ij} = \int_0^{b_1} \int_0^{b_2} \delta(x - x_0, y - y_0) V_{ij}(x, y) dy dx$$
$$= V_{ij}(x_0, y_0) \ .$$

Let us consider the equation (2.3.6) for $\lambda = \lambda_{ij}$ for $i, j = 1, 2, ...$ This equation may be written in the form

$$T'_{ij}(t) + c^2 \lambda_{ij} T(t) = 0, \quad i, j = 1, 2, ... \ . \tag{2.3.16}$$

A general solution of (2.3.16) is given by

$$T_{ij}(t) = A_{ij} \ e^{-c^2 \lambda_{ij} t} \ , \quad i, j = 1, 2, ... \ , \tag{2.3.17}$$

where A_{ij} are arbitrary constant for $i, j = 1, 2, ...$ Let us consider the function $u(x, y, t)$ defined by

$$u(x, y, t) = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} A_{ij} \ e^{-c^2 \lambda_{ij} t} V_{ij}(x, y) \ , \tag{2.3.18}$$

where A_{ij} are arbitrary constants for $i, j = 1, 2, ...$ This function satisfies (2.3.1)-(2.3.3). The main goal consists in finding A_{ij} for which the initial data (2.3.2) is hold. Using the orthonormal functions $V_{ij}(x, y)$, we can write $\phi(x, y)$ in the form of the Fourier series expansion as follows :

$$\phi(x, y) = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \sum_{k=1}^{\infty} \phi_{ij} V_{ij}(x, y) \ , \tag{2.3.19}$$

where

$$\phi_{ij} = \int_0^{b_1} \int_0^{b_2} \phi(x, y) V_{ij}(x, y) dy dx \ ,$$

Using the initial conditions (2.3.2) and (2.3.18),(2.3.19) we can find A_{ij} by

$$A_{ij} = \phi_{ij} \ ,$$

Substituting found values of A_{ij} into (2.3.18), we have

$$u(x, y, t) = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \phi_{ij} \ e^{-c^2 \lambda_{ij} t} V_{ij}(x, y) \ , \tag{2.3.20}$$

where

$$\phi_{ij} = \int_0^{b_1}\int_0^{b_2} \phi(x,y)V_{ij}(x,y)dydx ,$$

$$V_{ij} = X_i(x)Y_j(y) = \sqrt{\frac{4}{b_1b_2}}\sin\sqrt{\alpha_i}x ,$$

$$\lambda_{ij} = \alpha_i\beta j = \left(\frac{i\pi}{b_1}\right)^2 + \left(\frac{j\pi}{b_2}\right)^2 , \quad i,j = 1,2,\dots .$$

This function $u(x,y,t)$ satisfies (2.3.1)-(2.3.3). Therefore this function is a solution of the problem (2.3.1)-(2.3.3).

2.4 IBVP for a Non-Homogeneous 2D Heat-Diffusion Equation with Dirichlet Boundary Condition

Let $(x,y) \in \mathbb{R}^2,\ \ t \in \mathbb{R}, D = \{(x,y) \in \mathbb{R}^2 : 0 \le x \le b_1, 0 \le y \le b_2\}$ be a homogeneous rectangle. Let us consider the IBVP for the heat-diffusion equation in the rectangle D :

$$\begin{aligned} \frac{1}{c^2}\frac{\partial u(x,y,t)}{\partial t} &= \Delta_{x,y}u(x,y,t) \\ &\quad + F(x,y,t) , \quad (x,y) \in D, \quad t \ge 0 , \qquad (2.4.1) \\ u(x,y,0) &= \phi(x,y) , \qquad (2.4.2) \\ u(x,y,t)|_{\partial D} &= 0 , \qquad (2.4.3) \end{aligned}$$

where ∂D is the boundary of D. Here $F(x,y,t)$, $\phi(x,y)$ are given functions, c is a positive constant. IBVP consist of finding $u(x,y,t)$ satisfying (2.4.1)-(2.4.3).

Consider the system of eigenfunctions which is a solution of eigenvalue-eigenfunction problem for the Laplace operator in a rectangle with the Dirichlet Boundary Condition. These are functions $V_{ij}(x,y)_{i,j=1,2,\dots}$ satisfying (2.3.8) and (2.3.9). Using this system of functions, we will find the solution in the form :

$$u(x,y,t) = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty} T_{ij}(t)V_{ij}(x,y) , \qquad (2.4.4)$$

where $T_{ij}(t)$ are unknown Fourier coefficients of $u(x,y,t)$. We have

$$F(x,y,t) = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty} F_{ij}(t)V_{ij}(x,y) , \qquad (2.4.5)$$

where

$$F_{ij}(t) = \int_0^{b_1} \int_0^{b_2} F(x,y,t) V_{ij}(x,y) dy dx \ , \quad i,j = 1,2,... \tag{2.4.6}$$

Substituting (2.4.5) and (2.4.4) into (2.4.1) we will get

$$\sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \left\{ \frac{1}{c^2} T'_{ij}(t) V_{ij}(x,y) - T_{ij}(t) \Delta_{x,y} V_{ij}(x,y) - F_{ij}(t) V_{ij}(x,y) \right\} = 0 \ .$$

And using (2.3.8) we get

$$\sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \left\{ \frac{1}{c^2} T'_{ij}(t) V_{ij}(x,y) + \lambda_{ij} T_{ij}(t) V_{ij}(x,y) - F_{ij}(t) V_{ij}(x,y) \right\} = 0 \ .$$

Hence

$$\sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \left\{ \frac{1}{c^2} T'_{ij}(t) + \lambda_{ij} T_{ij}(t) - F_{ij}(t) \right\} V_{ij}(x,y) = 0 \ .$$

Since the function system $\{V_{ij}\}_{i,j=1,2,...}$ are normalized orthogonal system, the previous equation implies a first order ordinary differential equation as follows

$$\frac{1}{c^2} T'_{ij}(t) + \lambda_{ij} T_{ij}(t) - F_{ij}(t) = 0, \quad t > 0 \ .$$

And using (2.4.2) and (2.3.19) we get

$$T_{ij}(0) = \phi_{ij} \ .$$

So we have the following system for $T_{ij}(t)$, $i,j = 1,2,...$

$$\frac{1}{c^2} T'_{ij}(t) + \lambda_{ij} T_{ij}(t) - F_{ij}(t) = 0, \quad t > 0 \ , \tag{2.4.7}$$

$$T_{ij}(0) = \phi_{ij} \ . \tag{2.4.8}$$

Remark 2.4.1. *The function*

$$u(x,y,t) = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} T_{ij}(t) V_{ij}(x,y) \ ,$$

is a solution for (2.4.1)-(2.4.3) if and only if $T_{ij}(t)$ satisfy (2.4.7), (2.4.8) for $i,j = 1,2,...$ which is given by

$$T_{ij}(t) = \phi_{ij} e^{-c^2 \lambda_{ij} t} + c^2 \int_0^t F_{ij}(\tau) e^{-c^2 \lambda_{ij}(t-\tau)} d\tau \ , \tag{2.4.9}$$

(See Appendix A.1). Thus

$$u(x, y, t) = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} T_{ij}(t) V_{ij}(x, y) \ , \tag{2.4.10}$$

is the solution of the problem (2.4.1)-(2.4.3), where $T_{ij}(t)$ is defined in (2.4.9) and $V_{ij}(x, y)$ is defined in (2.3.14) for $i, j = 1, 2, ...$

2.5 IBVP for a Homogeneous 3D Heat-Diffusion Equation with Dirichlet Boundary Condition

Let $(x,y,z)\in\mathbb{R}^3$, $t\in\mathbb{R}$, $D=\{(x,y,z)\in\mathbb{R}^3 : 0\le x\le b_1, 0\le y\le b_2, 0\le z\le b_3\}$ be a homogeneous parallelepiped. Let us consider the IBVP for the diffusion equation in the parallelepiped D :

$$\begin{aligned}
\frac{1}{c^2}\frac{\partial u(x,y,z,t)}{\partial t} &= \Delta_{x,y,z}u(x,y,z,t)\ ,(x,y,z)\in D,\quad t\ge 0\ , && (2.5.1)\\
u(x,y,z,0) &= \phi(x,y,z)\ , && (2.5.2)\\
u(x,y,z,t)|_{\partial D} &= 0\ , && (2.5.3)
\end{aligned}$$

where ∂D is the boundary of D. Here $\phi(x,y,z)$ is given function in $D\cup\partial D$, c is a positive constant. IBVP consists of finding $u(x,y,z,t)$ satisfying (2.5.1), (2.5.2), (2.5.3).
We will use the separation of variables :

$$u(x,y,z,t)=T(t)V(x,y,z)\ . \tag{2.5.4}$$

Substituting (2.5.4) into (2.5.1) we find

$$\frac{1}{c^2}T'(t)V(x,y,z)=T(t)\Delta_{x,y,z}V(x,y,z)\ .$$

Dividing both sides of the last equation by $T(t)V(x,y,z)$, we have

$$\frac{1}{c^2}\frac{T'(t)}{T(t)}=\frac{\Delta_{x,y,z}V(x,y,z)}{V(x,y,z)}\ .$$

Let us fix t and let (x,y,z) vary in the parallelepiped D. Since t and (x,y,z) are independent variables then the last equality takes place if and only if the left hand side and the right hand side of this equation are equal to the same constant which we denote as $-\lambda$.

$$\frac{1}{c^2}\frac{T'(t)}{T(t)}=\frac{\Delta_{x,y,z}V(x,y,z)}{V(x,y,z)}=-\lambda\ .$$

As a result of it we get the following equations :

$$\Delta_{x,y,z}V(x,y,z)+\lambda V(x,y,z)=0,\quad (x,y,z)\in D\ , \tag{2.5.5}$$

$$T'(t)+c^2\lambda T(t)=0,\quad t>0\ . \tag{2.5.6}$$

Substituting (2.5.4) into (2.5.3) we obtain

$$V(x,y,z)|_{\partial D} = 0 \; . \tag{2.5.7}$$

This means that $V(x,y,z)$ has to be a solution of the following eigenvalue-eigenfunction problem (Stum-Liouville problem) :

$$\Delta_{x,y,z}V(x,y,z) + \lambda V(x,y,z) = 0, \quad (x,y,z) \in D \; , \tag{2.5.8}$$

$$V(x,y,z)|_{\partial D} = 0 \; . \tag{2.5.9}$$

For the solution of the eigenvalue-eigenfunction problem we will use the method of separation of variables. Setting

$$V(x,y,z) = X(x)Y(y)Z(z) \; , \tag{2.5.10}$$

and substituting (2.5.10) into (2.5.8) and dividing both sides of the equation (2.5.8) by $X(x)Y(y)Z(z)$, we have

$$\frac{X''(x)}{X(x)} + \frac{Y''(y)}{Y(y)} + \frac{Z''(z)}{Z(z)} + \lambda = 0 \; .$$

Thus

$$\frac{Y''(y)}{Y(y)} + \frac{Z''(z)}{Z(z)} + \lambda = -\frac{X''(x)}{X(x)} \; .$$

The left hand side of the last equation depends on variables y, z, right hand side depends on x only. Since the variables x, y, z are independent variables, the last equation holds if and only if the both sides of this equation are equal to the same constant which we denote as α

$$\frac{Y''(y)}{Y(y)} + \frac{Z''(z)}{Z(z)} + \lambda = -\frac{X''(x)}{X(x)} = \alpha \; .$$

Hence

$$\frac{Y''(y)}{Y(y)} + \frac{Z''(z)}{Z(z)} + \lambda = \alpha \; .$$

Repeating the same argument to the last equation we find

$$\frac{Z''(z)}{Z(z)} + \lambda - \alpha = -\frac{Y''(y)}{Y(y)} \; ,$$

$$\frac{Z''(z)}{Z(z)} + \lambda - \alpha = -\frac{Y''(y)}{Y(y)} = \beta \; ,$$

where α, β, γ are constants such that

$$\lambda - \alpha - \beta = -\frac{Z''(z)}{Z(z)} = \gamma \ ,$$

$$\lambda = \alpha + \beta + \gamma \ .$$

Also substituting (2.5.10) into (2.5.9) we have three Strum-Liouville equations for the ordinary differential equations :

$$X''(x) + \alpha X(x) = 0, \quad X(0) = X(b_1) = 0 \ , \tag{2.5.11}$$

$$Y''(y) + \beta Y(y) = 0, \quad Y(0) = Y(b_2) = 0 \ , \tag{2.5.12}$$

$$Z''(z) + \gamma Z(z) = 0, \quad Z(0) = Z(b_3) = 0 \ . \tag{2.5.13}$$

The solutions of these eigenvalue-eigenfunction problem (2.5.11), (2.5.12), (2.5.13) are given by

$$\alpha_i = (\frac{i\pi}{b_1})^2, \quad X_i(x) = \sqrt{\frac{2}{b_1}} \sin \sqrt{\alpha_i} x \ , \quad i = 1, 2, ... \ ;$$

$$\beta_j = (\frac{j\pi}{b_2})^2, \quad Y_j(y) = \sqrt{\frac{2}{b_2}} \sin \sqrt{\beta_j} y \ , \quad j = 1, 2, ... \ ;$$

$$\gamma_k = (\frac{k\pi}{b_3})^2, \quad Z_k(z) = \sqrt{\frac{2}{b_3}} \sin \sqrt{\gamma_k} z \ , \quad k = 1, 2, ... \ ;$$

(see Appendix A1 for detailed explanation) As a result of this we get the solution of eigenvalue-eigenfunction problem (2.5.8), (2.5.9) as follows :

$$\lambda_{ijk} = \left(\frac{i\pi}{b_1}\right)^2 + \left(\frac{j\pi}{b_2}\right)^2 + \left(\frac{k\pi}{b_3}\right)^2 \ , \tag{2.5.14}$$

$$V_{ijk} = \sqrt{\frac{8}{b_1 b_2 b_3}} \sin \sqrt{\alpha_i} x \sin \sqrt{\beta_j} y \sin \sqrt{\gamma_k} z, \quad i, j, k = 1, 2, ... \tag{2.5.15}$$

Remark 2.5.1. *The system of eigenfunctions* $\{V_{ijk}\}_{i,j,k=1,2,...}$ *is a complete orthonormal basis in the space* L_2, $D = \{(x, y, z) \in \mathbb{R}^3 : 0 \le x \le b_1, 0 \le y \le b_2, 0 \le z \le b_3\}$. *This means that each function* $\phi(x, y, z)$ *from* $L_2(D)$ *may be written in the form of Fourier series expansion which is convergent in* $L_2(D)$ *:*

$$\phi(x, y, z) = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \sum_{k=1}^{\infty} \phi_{ijk} V_{ijk}(x, y, z) \ ,$$

where

$$\phi_{ijk} = \int_0^{b_1}\int_0^{b_2}\int_0^{b_3} \phi(x,y,z)V_{ijk}(x,y,z)dzdydx \ .$$

Remark 2.5.2. *(Fourier Series Expansion of $\delta(x,y,z)$ function) We can generalize the idea of Fourier expansion of a classical function for the Dirac delta function $\delta(x-x_0, y-y_0, z-z_0)$, where (x_0, y_0, z_0) is a fixed point in D. It may be written in the form of the Fourier Series expansion as follows :*

$$\delta(x-x_0, y-y_0, z-z_0) = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\sum_{k=1}^{\infty} \delta_{ijk}V_{ijk}(x,y,z) \ , \tag{2.5.16}$$

where

$$\begin{aligned}\delta_{ijk} &= \int_0^{b_1}\int_0^{b_2}\int_0^{b_3} \delta(x-x_0, y-y_0, z-z_0)V_{ijk}(x,y,z)dzdydx \\ &= V_{ijk}(x_0, y_0, z_0) \ .\end{aligned}$$

Let us consider the equation (2.5.6) for $\lambda = \lambda_{ijk}$ for $i,j,k = 1,2,....$ This equation may be written in the form

$$T'_{ijk}(t) + c^2\lambda_{ijk}T(t) = 0, \quad i,j,k = 1,2,... \tag{2.5.17}$$

A general solution of (2.5.17) is given by

$$T_{ijk}(t) = A_{ijk}\ e^{-c^2\lambda_{ijk}t}, \quad i,j,k = 1,2,...\ , \tag{2.5.18}$$

where A_{ijk} are arbitrary constant for $i,j,k = 1,2,....$ Let us consider the function $u(x,y,z,t)$ defined by

$$u(x,y,z,t) = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\sum_{k=1}^{\infty} A_{ijk}\ e^{-c^2\lambda_{ijk}t}V_{ijk}(x,y,z) \ , \tag{2.5.19}$$

where A_{ijk} are arbitrary constants for $i,j,k = 1,2,....$ This function satisfies (2.5.1)-(2.5.3). The main goal consists in finding A_{ijk} for which the initial data (2.5.2) is hold. Using the orthonormal functions $V_{ijk}(x,y,z)$, we can write $\phi(x,y,z)$ in the form of the Fourier series expansion as follows :

$$\phi(x,y,z) = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\sum_{k=1}^{\infty} \phi_{ijk}V_{ijk}(x,y,z) \ , \tag{2.5.20}$$

where

$$\phi_{ijk} = \int_0^{b_1}\int_0^{b_2}\int_0^{b_3} \phi(x,y,z)V_{ijk}(x,y,z)dzdydx \ .$$

Using the initial conditions (2.5.2) and (2.5.19),(2.5.20) we can find A_{ijk} by

$$A_{ijk} = \phi_{ijk} \ ,$$

Substituting found values of A_{ijk} into (2.5.19), we have

$$u(x,y,z,t) = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\sum_{k=1}^{\infty} \phi_{ijk}\ e^{-c^2\lambda_{ijk}t} V_{ijk}(x,y,z) \ , \tag{2.5.21}$$

where

$$\phi_{ijk} = \int_0^{b_1}\int_0^{b_2}\int_0^{b_3} \phi(x,y,z)V_{ijk}(x,y,z)dzdydx \ ,$$

$$V_{ijk} = X_i(x)Y_j(y)Z_k(z) = \sqrt{\frac{8}{b_1b_2b_3}}\sin\sqrt{\alpha_i}x\sin\sqrt{\beta_j}y\sin\sqrt{\gamma_k}z \ ,$$

$$\lambda_{ijk} = \alpha_i\beta j\gamma k = \left(\frac{i\pi}{b_1}\right)^2 + \left(\frac{j\pi}{b_2}\right)^2 + \left(\frac{k\pi}{b_3}\right)^2 \ , \quad i,j,k = 1,2,\dots \ .$$

This function $u(x,y,z,t)$ satisfies (2.5.1)-(2.5.3). Therefore this function is a solution of the problem (2.5.1)-(2.5.3).

2.6 IBVP for a Non-Homogeneous 3D Heat-Diffusion Equation with Dirichlet Boundary Condition

Let $(x,y,z) \in \mathbb{R}^3$, $t \in \mathbb{R}$, $D = \{(x,y,z) \in \mathbb{R}^3 : 0 \le x \le b_1, 0 \le y \le b_2, 0 \le z \le b_3\}$ be a homogeneous parallelepiped. Let us consider the IBVP for the heat-diffusion equation in the parallelepiped D :

$$\begin{aligned}
\frac{1}{c^2}\frac{\partial u(x,y,z,t)}{\partial t} &= \Delta_{x,y,z}u(x,y,z,t) \\
&\quad + F(x,y,z,t) \ , \quad (x,y,z) \in D, \quad t \ge 0 \ , && (2.6.1) \\
u(x,y,z,0) &= \phi(x,y,z) \ , && (2.6.2) \\
u(x,y,z,t)|_{\partial D} &= 0 \ , && (2.6.3)
\end{aligned}$$

where ∂D is the boundary of D. Here $F(x,y,z,t)$, $\phi(x,y,z)$ are given functions, c is a positive constant. IBVP consist of finding $u(x,y,z,t)$ satisfying (2.6.1)-(2.6.3).

Consider the system of eigenfunctions which is a solution of eigenvalue-eigenfunction problem for the Laplace operator in a parallelepiped with the Dirichlet Boundary Condition. These are functions $V_{ijk}(x,y,z)_{i,j,k=1,2,...}$ satisfying (2.5.8) and (2.5.9). Using this system of functions, we will find the solution in the form :

$$u(x,y,z,t)=\sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\sum_{k=1}^{\infty}T_{ijk}(t)V_{ijk}(x,y,z)\ , \qquad (2.6.4)$$

where $T_{ijk}(t)$ are unknown Fourier coefficients of $u(x,y,z,t)$. We have

$$F(x,y,z,t)=\sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\sum_{k=1}^{\infty}F_{ijk}(t)V_{ijk}(x,y,z)\ , \qquad (2.6.5)$$

where

$$F_{ijk}(t)=\int_0^{b_1}\int_0^{b_2}\int_0^{b_3}F(x,y,z,t)V_{ijk}(x,y,z)dzdydx\ ,\quad i,j,k=1,2,... \qquad (2.6.6)$$

Substituting (2.6.5) and (2.6.4) into (2.6.1) we will get

$$\sum_{i,j,k=1}^{\infty}\left\{\frac{1}{c^2}T'_{ijk}(t)V_{ijk}(x,y,z)-T_{ijk}(t)\Delta_{x,y,z}V_{ijk}(x,y,z)-F_{ijk}(t)V_{ijk}(x,y,z)\right\}=0\ .$$

And using (2.5.8) we get

$$\sum_{i,j,k=1}^{\infty}\left\{\frac{1}{c^2}T'_{ijk}(t)V_{ijk}(x,y,z)+\lambda_{ijk}T_{ijk}(t)V_{ijk}(x,y,z)-F_{ijk}(t)V_{ijk}(x,y,z)\right\}=0\ .$$

Hence

$$\sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\sum_{k=1}^{\infty}\left\{\frac{1}{c^2}T'_{ijk}(t)+\lambda_{ijk}T_{ijk}(t)-F_{ijk}(t)\right\}V_{ijk}(x,y,z)=0\ .$$

Since the function system $\{V_{ijk}\}_{i,j,k=1,2,...}$ are normalized orthogonal system, the previous equation implies a first order ordinary differential equation as follows

$$\frac{1}{c^2}T'_{ijk}(t)+\lambda_{ijk}T_{ijk}(t)-F_{ijk}(t)=0,\quad t>0\ .$$

And using (2.6.2) and (2.5.20) we get

$$T_{ijk}(0)=\phi_{ijk}\ .$$

So we have the following system for $T_{ijk}(t)$, $i, j, k = 1, 2, ...$

$$\frac{1}{c^2}T'_{ijk}(t) + \lambda_{ijk}T_{ijk}(t) - F_{ijk}(t) = 0, \quad t > 0 \ , \tag{2.6.7}$$

$$T_{ijk}(0) = \phi_{ijk} \ . \tag{2.6.8}$$

Remark 2.6.1. *The function*

$$u(x, y, z, t) = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\sum_{k=1}^{\infty} T_{ijk}(t)V_{ijk}(x, y, z) \ ,$$

is a solution for (2.6.1)-(2.6.3) if and only if $T_{ijk}(t)$ satisfy (2.6.7), (2.6.8) for $i, j, k = 1, 2, ...$ which is given by

$$T_{ijk}(t) = \phi_{ijk}e^{-c^2\lambda_{ijk}t} + c^2\int_0^t F_{ijk}(\tau)e^{-c^2\lambda_{ijk}(t-\tau)}d\tau \ , \tag{2.6.9}$$

(See Appendix A.1).

Thus

$$u(x, y, z, t) = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\sum_{k=1}^{\infty} T_{ijk}(t)V_{ijk}(x, y, z) \ , \tag{2.6.10}$$

is the solution of the problem (2.6.1)-(2.6.3), where $T_{ijk}(t)$ is defined in (2.6.9) and $V_{ijk}(x, y, z)$ is defined in (2.5.15) for $i, j, k = 1, 2, ...$

2.7 Examples of simulations for Heat-Diffusion equation with Dirichlet B.C. (1-D, 2-D, 3-D cases)

This section contains some examples of modeling and simulations of a diffusion process in 1-D, 2-D and 3-D bounded domains with Dirichlet boundary condition. IBVP for heat equation with the Dirichlet boundary condition on a string, in a rectangle and in a parallelepiped will be simulated by using mathematical tools. We took a pulse point source concentrated in different points in these domains: in the center, near the boundary, on the corner.

2.7.1 1-D Heat-Diffusion equation

In this case we have a string on $[0, 4]$.

Example 2.7.1. The mathematical model of the diffusion process is given by (2.1.1)-(2.1.3), where

$$\phi(x) = \delta(x - x_0), \quad x_0 \in [0, \ell],$$

and $\delta(x)$ is Dirac delta function. Using the formula for $\phi(x)$ and the properties of Dirac delta function the solution of (2.1.1)-(2.1.3) is given by the formula:

$$u(x,t) = \sum_{i=1}^{\infty} \phi_i \, e^{-c^2 \lambda_i t} X_i(x), \ t \geq 0 \ , \tag{2.7.1}$$

where

$$\phi_i = \int_0^\ell \phi(x) X_i(x) dx = \int_0^\ell \delta(x - x_0) X_i(x) dx = X_i(x_0) \ ,$$

λ_i and $X_i(x)$ are defined in (2.1.10), (2.1.11) for $i = 1, 2, 3, \ldots$.

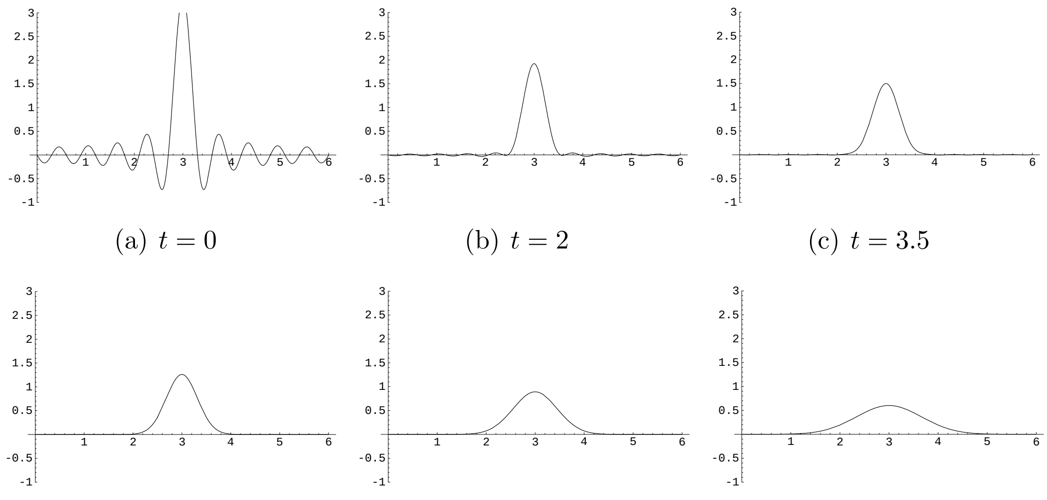
For the given data of Example 2.7.1, we used mathematica codes in order to find the solution and to animate when $x_0 = 2$, $c = 0.1$. Using (2.7.1) into the finite series form we get

$$u(x,t) = \sum_{i=1}^{n} \phi_i \, e^{-c^2 \lambda_i t} X_i(x), \ t \geq 0 \ , \tag{2.7.2}$$

where $n = 20$.

2.7.1.1 Results of the simulation by Formula 2.7.2 :

Using the formula (2.7.2) for $n = 20$ and the Mathematica codes we simulated our problem and the source is located in the center of the domain. Now we will give some pictures for different times



(a) $t = 0$ (b) $t = 2$ (c) $t = 3.5$

(d) $t = 5.0$ (e) $t = 10$ (f) $t = 22$

Figure 2.1: Example 2.7.1: The source in the center of the bounded domain for 1D homogeneous problem.

We can see in the pictures that our solution makes a big pick in the first picture and then this pick is getting smaller and smaller when the time increasing.At the same time it extends to the domain up to boundaries. Our problem has a bounded domain, we are concerning about IBVP so we may get some reflections near the boundaries of the domain but in the nature of heat-diffusion equation we can not see this reflections very well.

Example 2.7.2. Let us consider the problem (2.2.1)-(2.2.3). The functions $\phi(x)$ and $F(x,t)$ are given by

$$\phi(x) = 0 \ ,$$

$$F(x,t) = \delta(x - x_0)\delta(t) \ , x_0 \in [0, \ell] \ .$$

Using formulas for $\phi(x)$ and $F(x,t)$ and the properties of the Dirac delta function we can construct the solution of the problem (2.2.1)-(2.2.3).

Substituting the given data into the equation (2.2.6) we have

$$F_i(t) = \int_0^\ell F(x,t) X_i(x) dx = \int_0^\ell \delta(x - x_0)\delta(t) X_i(x) dx = \delta(t) X_i(x_0) \ ,$$

and using (2.2.9) and (2.2.10) for $n = 20$ we have

$$u(x,t) = \sum_{i=1}^{n} \left\{ \phi_i e^{-c^2\lambda_i t} + c^2 \int_0^t F_i(\tau) e^{-c^2\lambda_i (t-\tau)} d\tau \right\} X_i(x) \ ,$$

since $\phi(x) = 0$ we have $\phi_i = 0$ and using $F_i(t) = \delta(t) X_i(x_0)$ we get

$$u(x,t) = c^2 \sum_{i=1}^{n} \{ \int_0^t \delta(\tau) X_i(x_0) e^{-c^2\lambda_i (t-\tau)} d\tau \} X_i(x) \ ,$$

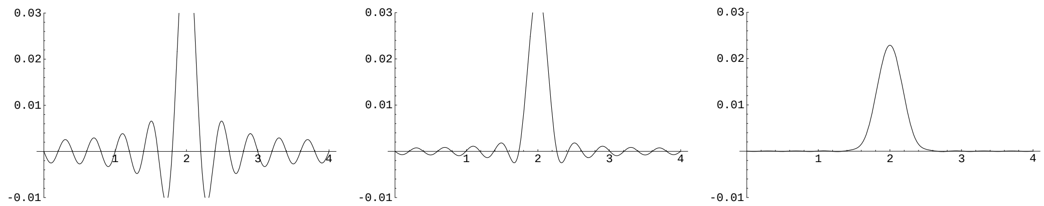
and using the definitions of Dirac delta function we get the solution as in the form

$$u(x,t) = c^2 \sum_{i=1}^{n} e^{-c^2\lambda_i t} X_i(x_0) X_i(x) \ , \tag{2.7.3}$$

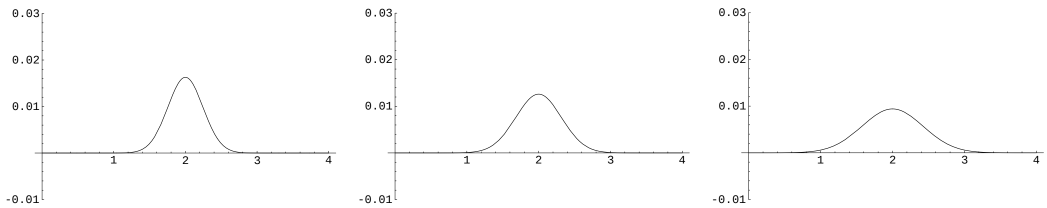
and λ_i and $X_i(x)$ are defined in (2.1.10), (2.1.11) for $i = 1, 2, 3, ...$.

2.7.1.2 Results of the simulation by Formula 2.7.3 :

For this example we consider $x_0 = 2$, $c = 0.1$ and $n = 20$. And the simulations will be in the form



(a) $t = 0$ (b) $t = 0.5$ (c) $t = 1.5$



(d) $t = 3.0$ (e) $t = 5$ (f) $t = 9$

Figure 2.2: Example 2.7.1.1: The source in the center of the bounded domain for non-homogeneous problem .

We can see that if we multiply equation (2.7.2) with c^2 we get directly equation (2.7.3). In the non-homogeneous problem we have extra c^2 and it only makes change the range of the solution. For $c = 1$ the homogeneous and the non-homogeneous problems have the same solutions.

2.7.2 2-D Heat-Diffusion equation

In this case we have a rectangle $D = ([0,6] \times [0,12])$.

Example 2.7.3. The mathematical model the diffusion process is given by (2.3.1)-(2.3.3), where

$$\phi(x,y) = \delta(x-x_0)\delta(y-y_0), \quad (x_0,y_0) \in D,$$

where $\delta(x)$ and $\delta(y)$ are Dirac delta functions. Using the formula for $\phi(x,y)$ and the properties of Dirac delta function the solution of (2.3.1)-(2.3.3) is given by the formula:

$$u(x,y,t) = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty} \phi_{ij}\, e^{-c^2\lambda_{ij}t} V_{ij}(x,y),\ t \geq 0\ , \tag{2.7.4}$$

where

$$\phi_{ij} = \int_0^{b_1}\int_0^{b_2} \phi(x,y)V_{ij}(x,y)dxdy = \int_0^{b_1}\int_0^{b_2} \delta(x-x_0)\delta(y-y_0)V_{ij}(x,y)dxdy\ ,$$

or equivalently

$$\phi_{ij} = V_{ij}(x_0,y_0)\ ,$$

λ_{ij} and $V_{ij}(x,y)$ are defined in (2.3.13), (2.3.14) for $i,j = 1,2,3,...$.

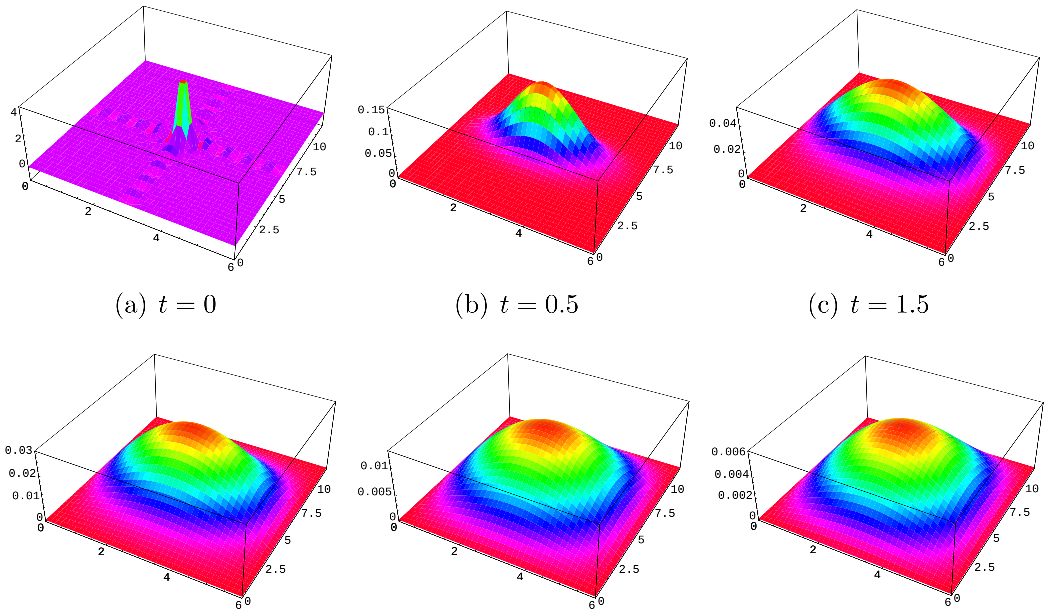
For the given data of Example 2.7.2, we used mathematica codes in order to find the solution and to animate when $x_0 = 3$, $y_0 = 6$, $c = 1$. Using (2.7.4) into the finite series form we get

$$u(x,y,t) = \sum_{i=1}^{n}\sum_{j=1}^{n} \phi_{ij}\, e^{-c^2\lambda_{ij}t} V_{ij}(x,y),\ t \geq 0\ , \tag{2.7.5}$$

where $n = 20$.

2.7.2.1 Results of the simulation by Formula 2.7.5 :

Using the formula (2.7.5) for $n = 20$ and the Mathematica codes we simulated our problem and the source is located in the center of the domain. Now we will give some pictures for different times



(a) $t = 0$ (b) $t = 0.5$ (c) $t = 1.5$

(d) $t = 2.5$ (e) $t = 4.5$ (f) $t = 6.5$

Figure 2.3: Example 2.7.2: The source in the center of the bounded domain for 2D homogeneous problem.

For 2-D case; we can see in the pictures that our solution makes a big pick in the first picture and then this pick is getting smaller and smaller when the time increasing. Our problem has a bounded domain, we are concerning about IBVP so we may get some reflections near the boundaries of the domain but in the nature of heat-diffusion equation we can not see very well this reflections.

Example 2.7.4. Let us consider the problem (2.4.1)-(2.4.3). The functions $\phi(x, y)$ and $F(x, y, t)$ are given by

$$\phi(x, y) = 0 \ ,$$

$$F(x, y, t) = \delta(x - x_0)\delta(y - y_0)\delta(t) \ , (x_0, y_0) \in D \ .$$

Using formulas for $\phi(x, y)$ and $F(x, y, t)$ and the properties of the Dirac delta function we can construct the solution of the problem (2.4.1)-(2.4.3).

Substituting the given data into the equation (2.4.6) we have

$$F_{ij}(t) = \int_0^{b_1} \int_0^{b_2} F(x, y, t) V_{ij}(x, y) dx dy$$

$$= \int_0^{b_1} \int_0^{b_2} \delta(x - x_0)\delta(y - y_0)\delta(t) V_{ij}(x, y) dx dy \ ,$$

or equivalently

$$F_{ij}(t) = \delta(t) V_{ij}(x_0, y_0) \ ,$$

and using (2.4.9) and (2.4.10) for $n = 20$ we have

$$u(x, y, t) = \sum_{i=1}^{n} \sum_{j=1}^{n} \left\{ \phi_{ij} e^{-c^2 \lambda_{ij} t} + c^2 \int_0^t F_{ij}(\tau) e^{-c^2 \lambda_{ij}(t-\tau)} d\tau \right\} V_{ij}(x, y) \ ,$$

since $\phi(x, y) = 0$ we have $\phi_{ij} = 0$ and using $F_{ij}(t) = \delta(t) V_{ij}(x_0, y_0)$ we get

$$u(x, y, t) = c^2 \sum_{i=1}^{n} \sum_{j=1}^{n} \{ \int_0^t \delta(\tau) V_{ij}(x_0, y_0) e^{-c^2 \lambda_{ij}(t-\tau)} d\tau \} V_{ij}(x, y) \ ,$$

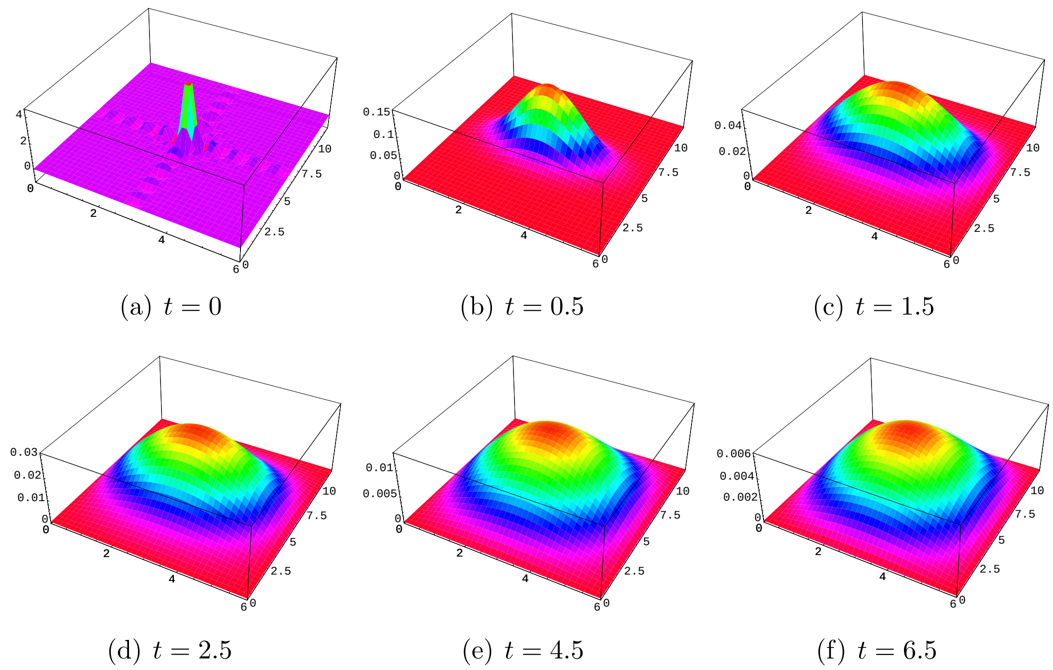
and using the definitions of Dirac delta function we get the solution as in the form

$$u(x, t) = c^2 \sum_{i=1}^{n} \sum_{j=1}^{n} e^{-c^2 \lambda_{ij} t} V_{ij}(x_0, y_0) V_{ij}(x, y) \ , \tag{2.7.6}$$

and λ_{ij} and $V_{ij}(x, y)$ are defined in (2.3.13), (2.3.14) for $i, j = 1, 2, 3, ...$.

2.7.2.2 Results of the simulation by Formula 2.7.6 :

For this example we consider $x_0 = 3$, $y_0 = 6$, $c = 1$ and $n = 20$. And the simulations will be in the form



(a) $t = 0$ (b) $t = 0.5$ (c) $t = 1.5$

(d) $t = 2.5$ (e) $t = 4.5$ (f) $t = 6.5$

Figure 2.4: Example 2.7.2.1: The source in the center of the bounded domain for 2-D non-homogeneous problem .

We can see that if we multiply equation (2.7.5) with c^2 we get directly equation (2.7.6). In the non-homogeneous problem we have extra c^2 and it only changes the range of the solution. For $c = 1$ the homogeneous and the non-homogeneous problems have the same solutions.

2.7.3 3-D Heat-Diffusion equation

In this case we have a parallelepiped $D = ([0,6] \times [0,12] \times [0,3])$.

Example 2.7.5. The mathematical model of heat equation is given by (2.5.1)-(2.5.3), where

$$\phi(x,y,z) = \delta(x-x_0)\delta(y-y_0)\delta(z-z_0), \quad (x_0,y_0,z_0) \in D,$$

where $\delta(x)$, $\delta(y)$ and $\delta(z)$ are Dirac delta functions. Using the formula for $\phi(x,y,z)$ and the properties of Dirac delta function the solution of (2.5.1)-(2.5.3) is given by the formula:

$$u(x,y,z,t) = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\sum_{k=1}^{\infty} \phi_{ijk}\, e^{-c^2\lambda_{ijk}t} V_{ijk}(x,y,z), \ t \geq 0 \ , \tag{2.7.7}$$

where

$$\phi_{ijk} = \int_0^{b_1}\int_0^{b_2}\int_0^{b_3} \phi(x,y,z)V_{ijk}(x,y,z)dxdydz$$

$$= \int_0^{b_1}\int_0^{b_2}\int_0^{b_3} \delta(x-x_0)\delta(y-y_0)\delta(z-z_0)V_{ijk}(x,y,z)dxdydz = V_{ijk}(x_0,y_0,z_0) \ ,$$

λ_{ijk} and $V_{ijk}(x,y,z)$ are defined in (2.5.14), (2.5.15) for $i,j,k = 1,2,3,\ldots$.

For the given data of Example 2.7.3, we used mathematica codes in order to find the solution and to animate when $x_0 = 3$, $y_0 = 6$, $z_0 = 2$ $c = 1$. Using (2.7.7) into the finite series form we get

$$u(x,y,z,t) = \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n} \phi_{ijk}\, e^{-c^2\lambda_{ijk}t} V_{ijk}(x,y,z), \ t \geq 0 \ , \tag{2.7.8}$$

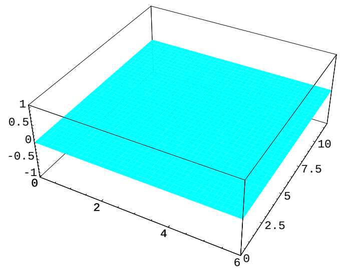
where $n = 20$.

2.7.3.1 Commands in Mathematica for Example 2.7.3 :

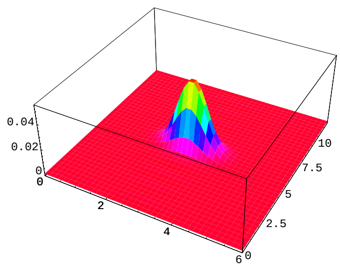
```
<< Graphics‘Animation‘
bx = 6; by = 12; bz = 3; (dimension of the parallelepiped)
x0 = 3; y0 = 6; z0 = 2; (the position of the source where
it is located)
n:=20; (number of terms in the sum)
sc:=1; (the speed of propagation)

(eigenvalues)
a[kk_] = (kk*Pi/bx)^2; b[kk_] = (kk*Pi/by)^2;
c[kk_] = (kk*Pi/bz)^2;

(computing the eigenfunctions and Fourier coefficients)
For[i = 1, i <= n, i++,
 For[j = 1, j <= n, j++,
  For[k = 1, k <= n, k++,
       Lambda[i, j, k] = a[i] + b[j] + c[k];
       V[i, j, k] = Sqrt[8/(bx*by*bz)]*Sin[Sqrt[a[i]]*x]
*Sin[Sqrt[b[j]]*y]*Sin[Sqrt[c[k]]*z];
Apsi[i, j, k] =ReplaceAll[ReplaceAll[ReplaceAll[V[i, j, k]
, x -> x0], y -> y0], z -> z0];
T[i, j, k] = Apsi[i, j, k]*e^((sc^2)*(-Lambda[i, j, k]*t))
];];]

(computing the sum)
son := Sum[Sum[Sum[T[i, j, k]*V[i, j, k], {i, 1, n}]
, {j, 1, n}], {k, 1, n}]

fixing parameter z=1
son2 = ReplaceAll[son, z -> 1];

(animating the picture w.r.t time variable with step size 0.25)
Animate[Plot3D[son2, {x, 0, 6}, {y, 0, 12}, ColorFunction
 -> (Hue[1 - #] &),PlotRange -> All, AspectRatio -> Automatic,
Mesh -> False,PlotPoints -> 40], {t, 0, 34, 0.5}]
```

2.7.3.2 Results of the simulation by Formula 2.7.8 :

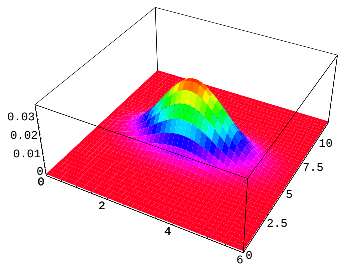
Using the formula (2.7.8) for $n = 20$ and the Mathematica codes we simulated our problem and the source is located in the center of the domain. Now we will give some pictures for different times



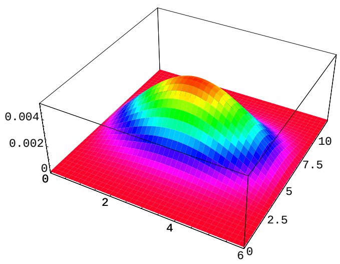
(a) $t = 0$



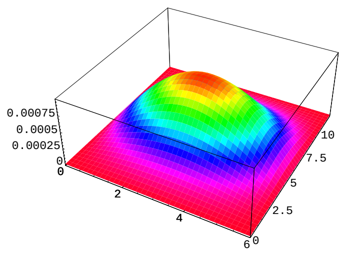
(b) $t = 0.1$



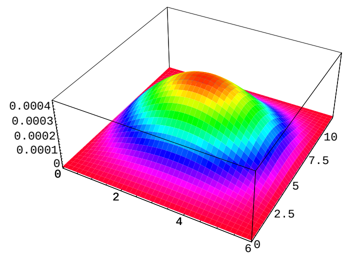
(c) $t = 0.5$



(d) $t = 1.5$



(e) $t = 2.5$



(f) $t = 3.0$

Figure 2.5: Example 2.7.3: The source in the center of the bounded domain for 3D homogeneous problem.

We can see in the pictures that our solution makes a big pick in the first picture and then this pick is getting smaller and smaller when the time increasing. Our problem has a bounded domain, we are concerning about IBVP so we may get some reflections near the boundaries of the domain but in the nature of heat-diffusion equation we can not see very well this reflections.

Example 2.7.6. Let us consider the problem (2.6.1)-(2.6.3). The functions $\phi(x,y,z)$ and $F(x,y,z,t)$ are given by

$$\phi(x,y,z)=0\ ,$$

$$F(x,y,z,t)=\delta(x-x_0)\delta(y-y_0)\delta(z-z_0)\delta(t)\ ,(x_0,y_0,z_0)\in D\ .$$

Using formulas for $\phi(x,y,z)$ and $F(x,y,z,t)$ and the properties of the Dirac delta function we can construct the solution of the problem (2.6.1)-(2.6.3).

Substituting the given data into the equation (2.6.6) we have

$$F_{ijk}(t)=\int_0^{b_1}\int_0^{b_2}\int_0^{b_3}F(x,y,z,t)V_{ijk}(x,y,z)dxdydz$$

$$=\int_0^{b_1}\int_0^{b_2}\int_0^{b_3}\delta(x-x_0)\delta(y-y_0)\delta(z-z_0)\delta(t)V_{ijk}(x,y,z)dxdydz$$

$$=\delta(t)V_{ijk}(x_0,y_0,z_0)\ ,$$

and using (2.6.9) and (2.6.10) for $n=20$ we have

$$u(x,y,z,t)=\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n}\left\{\phi_{ijk}e^{-c^2\lambda_{ijk}t}+c^2\int_0^t F_{ijk}(\tau)e^{-c^2\lambda_{ijk}(t-\tau)}d\tau\right\}V_{ijk}(x,y,z)\ ,$$

since $\phi(x,y,z)=0$ we have $\phi_{ijk}=0$ and using $F_{ijk}(t)=\delta(t)V_{ijk}(x_0,y_0,z_0)$ we get

$$u(x,y,z,t)=c^2\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n}\{\int_0^t\delta(\tau)V_{ijk}(x_0,y_0,z_0)e^{-c^2\lambda_{ijk}(t-\tau)}d\tau\}V_{ijk}(x,y,z)\ ,$$

and using the definitions of Dirac delta function we get the solution as in the form

$$u(x,y,z,t)=c^2\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n}e^{-c^2\lambda_{ijk}t}V_{ijk}(x_0,y_0,z_0)V_{ijk}(x,y,z)\ , \tag{2.7.9}$$

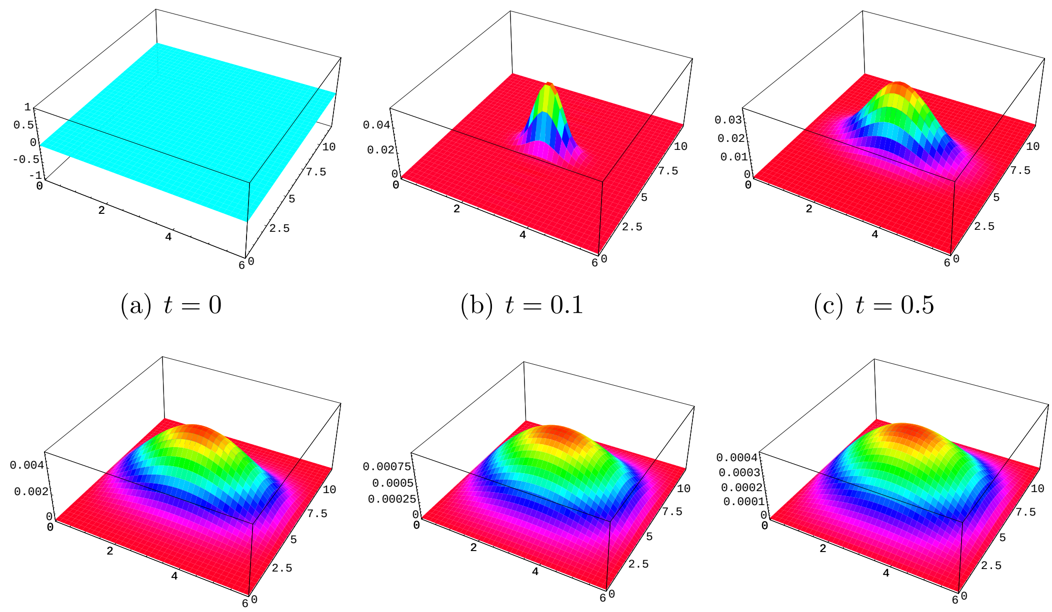
and λ_{ijk} and $V_{ijk}(x,y,z)$ are defined in (2.5.14), (2.5.15) for $i,j,k=1,2,3,...$.

2.7.3.3 Commands in Mathematica for Example 2.7.3.2 :

```
<< Graphics`Animation`
bx = 6; by = 12; bz = 3; (dimension of the parallelepiped)
x0 = 3; y0 = 6; z0 = 2; (the position of the source where
it is located)
n:=20; (number of terms in the sum)
sc:=1; (the speed of propagation)

(eigenvalues)
a[kk_] = (kk*Pi/bx)^2; b[kk_] = (kk*Pi/by)^2;
c[kk_] = (kk*Pi/bz)^2;

(computing the eigenfunctions and Fourier coefficients)
For[i = 1, i <= n, i++,
 For[j = 1, j <= n, j++,
  For[k = 1, k <= n, k++,
       Lambda[i, j, k] = a[i] + b[j] + c[k];
       V[i, j, k] = Sqrt[8/(bx*by*bz)]*Sin[Sqrt[a[i]]*x]
*Sin[Sqrt[b[j]]*y]*Sin[Sqrt[c[k]]*z];
PV[i, j, k] =ReplaceAll[ReplaceAll[ReplaceAll[V[i, j, k]
, x -> x0], y -> y0], z -> z0];
T[i, j, k] = sc^2*e^((sc^2)*(-Lambda[i, j, k]*t))*PV[i,j,k]
];];]

(computing the sum)
son := Sum[Sum[Sum[T[i, j, k]*V[i, j, k], {i, 1, n}]
, {j, 1, n}], {k, 1, n}]

fixing parameter z=1
son2 = ReplaceAll[son, z -> 1];

(animating the picture w.r.t time variable with step size 0.25)
Animate[Plot3D[son2, {x, 0, 6}, {y, 0, 12}, ColorFunction
 -> (Hue[1 - #] &),PlotRange -> All, AspectRatio -> Automatic,
Mesh -> False,PlotPoints -> 40], {t, 0, 34, 0.5}]
```

2.7.3.4 Results of the simulation by Formula 2.7.9 :

For this example we consider $x_0 = 3$, $y_0 = 6$, $z_0 = 2$ $c = 1$ and $n = 20$. And the simulations will be in the form



(a) $t = 0$ (b) $t = 0.1$ (c) $t = 0.5$

(d) $t = 1.5$ (e) $t = 2.5$ (f) $t = 3.0$

Figure 2.6: Example 2.7.3.2: The source in the center of the bounded domain for 3-D non-homogeneous problem .

We can see that if we multiply equation (2.7.8) with c^2 we get directly equation (2.7.9). In the non-homogeneous problem we have extra c^2 and it only changes the range of the solution. For $c = 1$ the homogeneous and the non-homogeneous problems have the same solutions.

2.8 Analysis of the chapter 2 study

1. Exact and approximate formulae for the solutions of IBVPs with Dirichlet boundary condition for the diffusion (heat) equations on a string, in a rectangle and in a parallelepiped were obtained.

2. These formulae were adjusted to cases when initial data or inhomogeneous term are the Dirac delta function with a support in a point which is inside the domain D. The pulse point source is modeled by these initial data and in homogeneous term.

3. Obtained formulae for generalized solutions of IBVPs for the heat-diffusion equations were used for modeling and simulations of diffusion processes in bounded domain D arising from the pulse point sources.

4. Results of diffusion processes simulation are presented by 1-D, 2-D and 3-D pictures and animated movies.

5. Obtained formulae and results of the simulation were analyzed.

CHAPTER THREE
IBVP FOR HEAT-DIFFUSION EQUATION WITH NEUMANN BOUNDARY CONDITION

In this section IBVP for 1D, 2D and 3D heat(diffusion) equation with Neumann Boundary condition in a homogeneous strip, rectangle and parallelepiped will be studied. The formulas will be generated and using these formulas simulations will be found. Sources are taken as pulse point sources.

3.1 IBVP for a Homogeneous 1D Heat-Diffusion Equation with Neumann Boundary Condition

Let $x \in (0, \ell)$, $t \in (0, T)$, where ℓ and T are given positive numbers. Let us consider the IBVP for the diffusion equation on a string :

$$
\begin{aligned}
\frac{1}{c^2}\frac{\partial u(x,t)}{\partial t} &= \frac{\partial^2 u(x,t)}{\partial x^2}\ , x \in (0,\ell), \quad t \in (0,T)\ , && (3.1.1)\\
u(x,0) &= \phi(x)\ , && (3.1.2)\\
\frac{\partial u(0,t)}{\partial n} &= \frac{\partial u(\ell,t)}{\partial n} = 0\ , && (3.1.3)
\end{aligned}
$$

Here $\phi(x)$ is a given function, $c > 0$ is a positive constant. IBVP consist of finding $u(x,t)$ satisfying (3.1.1)-(3.1.3). We will use the same method which is applied for the IBVP for heat-diffusion equation in a string with Dirichlet condition. We will use the separation of variables :

$$u(x,t) = T(t)X(x)\ . \tag{3.1.4}$$

Using the same techniques which is done before we get :

$$X''(x) + \lambda X(x) = 0, \quad x \in (0,\ell)\ , \tag{3.1.5}$$

$$T'(t) + c^2\lambda T(t) = 0, \quad t \in (0,T)\ . \tag{3.1.6}$$

Substituting (3.1.4) into (3.1.3) we obtain

$$X'(0) = X'(\ell) = 0\ . \tag{3.1.7}$$

That is, $X(x)$ has to be a solution of the following eigenvalue-eigenfunction problem

$$X''(x) + \lambda X(x) = 0, \quad x \in (0, T) \ , \tag{3.1.8}$$

$$X'(0) = X'(\ell) = 0 \ . \tag{3.1.9}$$

The solution of the eigenvalue-eigenfunction problem (3.1.8), (3.1.9) has the form

$$\lambda_i = \left(\frac{i\pi}{\ell}\right)^2, \quad i = 0, 1, 2, \dots . \tag{3.1.10}$$

$$X_i(x) = \sqrt{\frac{2}{\ell}} \cos \sqrt{\lambda_i} x \quad i = 0, 1, 2, ... \tag{3.1.11}$$

Now we can find the function $T(t)$. Substitute λ_i into (3.1.6) we get

$$T_i'(t) + c^2 \lambda_i T_i(t) = 0, \quad i = 0, 1, 2, ... \tag{3.1.12}$$

Hence (3.1.12) has the following solution

$$T_i(t) = A_i \ e^{-c^2 \lambda_i t}, \quad i = 0, 1, 2, ... \tag{3.1.13}$$

We have $u(x,t) = T_i(t) X_i(x)$ for each $i = 0, 1, 2, ...$ are solutions of (3.1.1)-(3.1.3). Hence

$$u(x,t) = \sum_{i=1}^{\infty} T_i(t) X_i(x) \ . \tag{3.1.14}$$

Using the initial condition (3.1.2) we can find (3.1.1)

$$T_i(0) = \phi_i \ . \tag{3.1.15}$$

So we have for $i = 0, 1, 2, ...$

$$A_i = \phi_i \ , \tag{3.1.16}$$

where

$$\phi_i = \int_0^{\ell} \phi(x) X_i(x) dx \ .$$

So we conclude that we obtain the solution of our problem (3.1.1)-(3.1.3)

$$u(x,t) = \sum_{i=1}^{\infty} T_i(t) X_i(x) \ , \tag{3.1.17}$$

where $T_i(t)$ are defined in (3.1.13) and $X_i(x)$ are defined (3.1.11).

3.2 IBVP for a Non-Homogeneous 1D Heat-Diffusion Equation with Neumann Boundary Condition

Let $x \in (0, \ell)$, $t \in (0, T)$, where ℓ and T are given positive numbers. Let us consider the IBVP for the 1D heat-diffusion equation on a string:

$$\begin{aligned} \frac{1}{c^2}\frac{\partial u(x,t)}{\partial t} &= \frac{\partial^2 u(x,t)}{\partial x^2} + F(x,t)\,, \\ & \quad x \in (0,\ell), \quad t \in (0,T)\,, \qquad (3.2.1) \\ u(x,0) &= \phi(x)\,, \qquad (3.2.2) \\ \frac{\partial u(0,t)}{\partial n} &= \frac{\partial u(\ell,t)}{\partial n} = 0\,, \qquad (3.2.3) \end{aligned}$$

where $c > 0$ is a given positive number; $\phi(x)$ are given functions for $x \in [0, \ell]$, $F(x,t)$ is a given smooth function for $(x,t) \in ((0,\ell) \times (0,t))$. IBVP consists of finding $u(x,t)$ satisfying (3.2.1)-(3.2.3).
Using the same techniques of the chapter two for non-homogeneous problem with the boundary condition $u(x,t)|_{\partial D} = 0$ and the homogeneous problem for the Neumann boundary condition we will get the following results :

$$T_i = \phi_i\, e^{-c^2\lambda_i t} + c^2 \int_0^t F_i(\tau) e^{-c^2\lambda_i (t-\tau)} d\tau, \quad i = 0, 1, 2, ... \qquad (3.2.4)$$

Therefore

$$u(x,t) = \sum_{i=1}^{\infty} T_i(t) X_i(x)\,, \qquad (3.2.5)$$

is the solution of (3.2.1)-(3.2.3), where $T_i(t)$ is defined in (3.2.4) and $X_i(x)$ are defined (3.1.11) for $i = 0, 1, 2, ...$

3.3 IBVP for a Homogeneous 2D Heat-Diffusion Equation with Neumann Boundary Condition

Let $(x, y) \in \mathbb{R}^2,\ \ t \in \mathbb{R}, D = \{(x, y) \in \mathbb{R}^2 : 0 \leq x \leq b_1, 0 \leq y \leq b_2\}$ be a homogeneous rectangle. Let us consider the IBVP for the heat-diffusion equation in the rectangle D :

$$
\begin{aligned}
\frac{1}{c^2}\frac{\partial u(x,y,t)}{\partial t} &= \Delta_{x,y} u(x,y,t)\ , \\
& \quad (x,y) \in D, \quad t \geq 0\ , && (3.3.1) \\
u(x,y,0) &= \phi(x,y)\ , && (3.3.2) \\
\frac{\partial u(x,y,t)}{\partial n}|_{\partial D} &= 0\ , && (3.3.3)
\end{aligned}
$$

where ∂D is the boundary of D. Here $\phi(x, y)$ is a given function, c is a positive constant. IBVP consists of finding $u(x, y, t)$ satisfying (3.3.1)-(3.3.3). We will use the same method which is applied for the IBVP for heat-diffusion equation in a rectangle with Dirichlet condition. We will use the separation of variables :

$$u(x, y, t) = T(t)V(x, y)\ . \tag{3.3.4}$$

Using the same techniques which is done before we get :

$$\Delta_{x,y} V(x, y) + \lambda V(x, y) = 0, \quad (x, y) \in D\ , \tag{3.3.5}$$

$$T'(t) + c^2 \lambda T(t) = 0, \quad t > 0\ . \tag{3.3.6}$$

Substituting (3.3.4) into (3.3.3) we obtain

$$\frac{\partial V(x,y)}{\partial n}|_{\partial D} = 0\ . \tag{3.3.7}$$

This means that $V(x, y)$ has to be a solution of the following eigenvalue-eigenfunction problem (Stum-Liouville problem) :

$$\Delta_{x,y} V(x, y) + \lambda V(x, y) = 0, \quad (x, y) \in D\ , \tag{3.3.8}$$

$$\frac{\partial V(x,y)}{\partial n}|_{\partial D} = 0\ . \tag{3.3.9}$$

For the solution of the eigenvalue-eigenfunction problem we will use the method of separation of variables. Setting

$$V(x,y) = X(x)Y(y)\ . \tag{3.3.10}$$

Substituting (3.3.10) into (3.3.8) we have two eigenvalue-eigenfunction problems:

$$X''(x) + \alpha X(x) = 0, \quad X'(0) = X'(b_1) = 0\ , \tag{3.3.11}$$

$$Y''(y) + \beta Y(y) = 0, \quad Y'(0) = Y'(b_2) = 0\ , -. \tag{3.3.12}$$

We can get the eigenvalues and corresponding to them eigenfunctions for the systems (3.3.11) and (3.3.12) as follows :

$$\alpha_i = (\frac{i\pi}{b_1})^2, \quad X_i(x) = \sqrt{\frac{2}{b_1}} \cos\sqrt{\alpha_i}x, \quad i = 1, 2, ...\ ;$$

$$\beta_j = (\frac{j\pi}{b_2})^2, \quad Y_j(y) = \sqrt{\frac{2}{b_2}} \cos\sqrt{\beta_j}y, \quad j = 1, 2, ...\ ;$$

(see Appendix A.2 for detailed explanation) As a result of this we get the solution of eigenvalue-eigenfunction problem (3.3.8), (3.3.9) as follows :

$$V_{ij} = \sqrt{\frac{4}{b_1 b_2}} \cos\sqrt{\alpha_i}x \cos\sqrt{\beta_j}y, \quad i, j = 1, 2, ... \tag{3.3.13}$$

and corresponding eigenvalues

$$\lambda_{ij} = \left(\frac{i\pi}{b_1}\right)^2 + \left(\frac{j\pi}{b_2}\right)^2\ . \tag{3.3.14}$$

Now we can find the function $T(t)$. Substitute λ_{ij} into (3.3.6) we get

$$T'_{ij}(t) + c^2\lambda_{ij}T_{ij}(t) = 0, \quad i, j = 1, 2, ... \tag{3.3.15}$$

Hence (3.3.15) for $i^2 + j^2 \neq 0$ has the following solution

$$T_{ij} = A_{ij}\ e^{-c^2\lambda_{ij}t}, \quad i, j = 1, 2, ... \tag{3.3.16}$$

Otherwise the solution is

$$T_{00}(t) = A_{00}\ . \tag{3.3.17}$$

We have $u(x,y,t) = T_{ij}V_{ij}(x,y)$ for each $i, j = 1, 2, ...$ are solutions of (3.3.1)-

(3.3.3). Hence by the superposition principle we have the solution

$$u(x,y,t) = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty} T_{ij}(t)V_{ij}(x,y) \ . \tag{3.3.18}$$

Using the initial condition (3.3.2) we can find (3.3.1)

$$T_{ij}(0) = \phi_{ij} \ . \tag{3.3.19}$$

So we have for $i^2 + j^2 \neq 0$; $i, j = 0, 1, 2, ...$

$$A_{ij} = \phi_{ij} \ , \tag{3.3.20}$$

and

$$A_{00} = \phi_{00} \ , \tag{3.3.21}$$

where

$$\phi_{ij} = \int_0^{b_1}\int_0^{b_2} \phi(x,y)V_{ij}(x,y)dydx \ .$$

So we conclude that we obtain the solution of our problem (3.3.1)-(3.3.3)

$$u(x,y,t) = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty} T_{ij}(t)V_{ij}(x,y) \ , \tag{3.3.22}$$

where $T_{ij}(t)$ are defined in (3.3.16), (3.3.17) and $V_{ij}(x,y)$ are defined (3.3.13).

3.4 IBVP for a Non-Homogeneous 2D Heat-Diffusion Equation with Neumann Boundary Condition

Let $(x, y) \in \mathbb{R}^2,\ \ t \in \mathbb{R}, D = \{(x, y) \in \mathbb{R}^2 : 0 \leq x \leq b_1, 0 \leq y \leq b_2\}$ be a homogeneous rectangle. Let us consider the IBVP for the heat-diffusion equation in the rectangle D :

$$\frac{1}{c^2}\frac{\partial u(x,y,t)}{\partial t} = \Delta_{x,y}u(x,y,t) + F(x,y,t)\ , (x,y) \in D, \quad t \geq 0\ , \tag{3.4.1}$$

$$u(x,y,0) = \phi(x,y)\ , \tag{3.4.2}$$

$$\frac{\partial u(x,y,t)}{\partial n}|_{\partial D} = 0\ , \tag{3.4.3}$$

where ∂D is the boundary of D. Here $F(x, y, t)$, $\phi(x, y)$ are given functions in $D \cup \partial D$, c is a positive constant. IBVP consists of finding $u(x, y, t)$ satisfying (3.4.1)-(3.4.3).
Using the same techniques of the chapter two for non-homogeneous problem with the boundary condition $u(x, y, t)|_{\partial D} = 0$ and the homogeneous problem for the Neumann boundary condition we will get the following results :

$$T_{ij} = \phi_{ij}\ e^{-c^2\lambda_{ij}t} + c^2\int_0^t F_{ij}(\tau)e^{-c^2\lambda_{ij}(t-\tau)}d\tau, \quad i,j = 1,2,... \tag{3.4.4}$$

$$i^2 + j^2 \neq 0;\ i,j = 0,1,2,...$$

$$T_{00}(t) = \phi_{00} + c^2\int_0^t F_{00}(\tau)d\tau\ . \tag{3.4.5}$$

Therefore

$$u(x,y,t) = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty} T_{ij}(t)V_{ij}(x,y)\ , \tag{3.4.6}$$

is the solution of (3.4.1)-(3.4.3), where $T_{ij}(t)$ is defined in (3.4.6) and $V_{ij}(x, y)$ are defined (3.3.13) for $i, j = 0, 1, 2, ...$

3.5 IBVP for a Homogeneous 3D Heat-Diffusion Equation with Neumann Boundary Condition

Let $(x, y, z) \in \mathbb{R}^3$, $t \in \mathbb{R}$, $D = \{(x, y, z) \in \mathbb{R}^3 : 0 \leq x \leq b_1, 0 \leq y \leq b_2, 0 \leq z \leq b_3\}$ be a homogeneous parallelepiped. Let us consider the IBVP for the heat-diffusion equation in the parallelepiped D :

$$\begin{aligned} \frac{1}{c^2}\frac{\partial u(x,y,z,t)}{\partial t} &= \Delta_{xyz}u(x,y,z,t) \ , (x,y,z) \in D, \quad t \geq 0 \ , && (3.5.1)\\ u(x,y,z,0) &= \phi(x,y,z) \ , && (3.5.2)\\ \frac{\partial u(x,y,z,t)}{\partial n}|_{\partial D} &= 0 \ , && (3.5.3)\end{aligned}$$

where ∂D is the boundary of D. Here $\phi(x, y, z)$ is a given function, c is a positive constant. IBVP consists of finding $u(x, y, z, t)$ satisfying (3.5.1)-(3.5.3). We will use the same method which is applied for the IBVP for heat-diffusion equation in a parallelepiped with Dirichlet condition. We will use separation of variables :

$$u(x, y, z, t) = T(t)V(x, y, z) \ . \tag{3.5.4}$$

Using the same technics which is done before we get :

$$\Delta_{x,y,z}V(x, y, z) + \lambda V(x, y, z) = 0, \quad (x, y, z) \in D \ , \tag{3.5.5}$$

$$T'(t) + c^2\lambda T(t) = 0, \quad t > 0 \ . \tag{3.5.6}$$

Substituting (3.5.4) into (3.5.3) we obtain

$$\frac{\partial V(x, y, z)}{\partial n}|_{\partial D} = 0 \ . \tag{3.5.7}$$

This means that $V(x, y, z)$ has to be a solution of the following eigenvalue-eigenfunction problem (Stum-Liouville problem) :

$$\Delta_{xyz}V(x, y, z) + \lambda V(x, y, z) = 0, \quad (x, y, z) \in D \ , \tag{3.5.8}$$

$$\frac{\partial V(x, y, z)}{\partial n}|_{\partial D} = 0 \ . \tag{3.5.9}$$

For the solution of the eigenvalue-eigenfunction problem we will use the method of separation of variables. Setting

$$V(x, y, z) = X(x)Y(y)Z(z) \ . \tag{3.5.10}$$

Substituting (3.5.10) into (3.5.8) we have three eigenvalue-eigenfunction problems:

$$X''(x) + \alpha X(x) = 0, \quad X'(0) = X'(b_1) = 0 \ , \tag{3.5.11}$$

$$Y''(y) + \beta Y(y) = 0, \quad Y'(0) = Y'(b_2) = 0 \ , \tag{3.5.12}$$

$$Z''(z) + \gamma Z(z) = 0, \quad Z'(0) = Z'(b_3) = 0 \ . \tag{3.5.13}$$

We can get the eigenvalues and corresponding to them eigenfunctions for the systems (3.5.11), (3.5.12), (3.5.13) as follows :

$$\alpha_i = (\frac{i\pi}{b_1})^2, \quad X_i(x) = \sqrt{\frac{2}{b_1}} \cos \sqrt{\alpha_i} x, \quad i = 1, 2, ... \ ;$$

$$\beta_j = (\frac{j\pi}{b_2})^2, \quad Y_j(y) = \sqrt{\frac{2}{b_2}} \cos \sqrt{\beta_j} y, \quad j = 1, 2, ... \ ;$$

$$\gamma_k = (\frac{k\pi}{b_3})^2, \quad Z_k(z) = \sqrt{\frac{2}{b_3}} \cos \sqrt{\gamma_k} z, \quad k = 1, 2, ... \ ;$$

(see Appendix A.2 for detailed explanation) As a result of this we get the solution of eigenvalue-eigenfunction problem (3.5.8), (3.5.9) as follows :

$$V_{ijk} = \sqrt{\frac{8}{b_1 b_2 b_3}} \cos \sqrt{\alpha_i} x \cos \sqrt{\beta_j} y \cos \sqrt{\gamma_k} z, \quad i, j, k = 1, 2, ... \tag{3.5.14}$$

and corresponding eigenvalues

$$\lambda_{ijk} = \left(\frac{i\pi}{b_1}\right)^2 + \left(\frac{j\pi}{b_2}\right)^2 + \left(\frac{k\pi}{b_3}\right)^2 . \tag{3.5.15}$$

Now we can find the function $T(t)$. Substitute λ_{ijk} into (3.5.6) we get

$$T'_{ijk}(t) + c^2 \lambda_{ijk} T_{ijk}(t) = 0, \quad i, j, k = 1, 2, ... \tag{3.5.16}$$

Hence (3.5.16) for $i^2 + j^2 + k^2 \neq 0$ has the following solution

$$T_{ijk} = A_{ijk} \, e^{-c^2 \lambda_{ijk} t}, \quad i, j, k = 1, 2, ... \tag{3.5.17}$$

Otherwise the solution is

$$T_{000}(t) = A_{000} \ . \tag{3.5.18}$$

We have $u(x, y, z, t) = T_{ijk}V_{ijk}(x, y, z)$ for each $i, j, k = 1, 2, ...$ are solutions of (3.5.1)-(3.5.3). Hence by the superposition principle we have the solution

$$u(x, y, z, t) = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\sum_{k=1}^{\infty} T_{ijk}(t)V_{ijk}(x, y, z) \ . \tag{3.5.19}$$

Using the initial condition (3.5.2) we can find (3.5.1)

$$T_{ijk}(0) = \phi_{ijk} \ . \tag{3.5.20}$$

So we have for $i^2 + j^2 + k^2 \neq 0$; $i, j, k = 0, 1, 2, ...$

$$A_{ijk} = \phi_{ijk} \ , \tag{3.5.21}$$

and

$$A_{000} = \phi_{000} \ , \tag{3.5.22}$$

where

$$\phi_{ijk} = \int_0^{b_1}\int_0^{b_2}\int_0^{b_3} \phi(x, y, z)V_{ijk}(x, y, z)dzdydx \ .$$

So we conclude that we obtain the solution of our problem (3.5.1)-(3.5.3)

$$u(x, y, z, t) = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\sum_{k=1}^{\infty} T_{ijk}(t)V_{ijk}(x, y, z) \ , \tag{3.5.23}$$

where $T_{ijk}(t)$ are defined in (3.5.17), (3.5.18) and $V_{ijk}(x, y, z)$ are defined (3.5.14).

3.6 IBVP for a Non-Homogeneous 3D Heat-Diffusion Equation with Neumann Boundary Condition

Let $(x,y,z) \in \mathbb{R}^3,\ \ t \in \mathbb{R}, D = \{(x,y,z) \in \mathbb{R}^3 : 0 \leq x \leq b_1, 0 \leq y \leq b_2, 0 \leq z \leq b_3\}$ be a homogeneous parallelepiped. Let us consider the IBVP for the heat-diffusion equation in the parallelepiped D :

$$\begin{aligned}
\frac{1}{c^2}\frac{\partial u(x,y,z,t)}{\partial t} &= \Delta_{x,y,z}u(x,y,z,t) + F(x,y,z,t)\ , (x,y,z) \in D, \quad t \geq 0\ , && (3.6.1)\\
u(x,y,z,0) &= \phi(x,y,z)\ , && (3.6.2)\\
\frac{\partial u(x,y,z,t)}{\partial n}|_{\partial D} &= 0\ , && (3.6.3)
\end{aligned}$$

where ∂D is the boundary of D. Here $F(x,y,z,t)$, $\phi(x,y,z)$ are given functions in $D \cup \partial D$, c is a positive constant. IBVP consists of finding $u(x,y,z,t)$ satisfying (3.6.1)-(3.6.3).
Using the same techniques of the chapter two for non-homogeneous problem with the boundary condition $u(x,y,z,t)|_{\partial D} = 0$ and the homogeneous problem for the Neumann boundary condition we will get the following results :

$$T_{ijk} = \phi_{ijk}\ e^{-c^2\lambda_{ijk}t} + c^2\int_0^t F_{ijk}(\tau)e^{-c^2\lambda_{ijk}(t-\tau)}d\tau, \quad i,j,k = 1,2,... \qquad (3.6.4)$$

$$i^2 + j^2 + k^2 \neq 0;\ i,j,k = 0,1,2,...$$

$$T_{000}(t) = \phi_{000} + c^2\int_0^t F_{000}(\tau)d\tau\ . \qquad (3.6.5)$$

Therefore

$$u(x,y,z,t) = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\sum_{k=1}^{\infty} T_{ijk}(t)V_{ijk}(x,y,z)\ , \qquad (3.6.6)$$

is the solution of (3.6.1)-(3.6.3), where $T_{ijk}(t)$ is defined in (3.6.6) and $V_{ijk}(x,y,z)$ are defined (3.5.14) for $i,j,k = 0,1,2,...$

3.7 Examples of simulations for Heat-Diffusion equation with Neumann B.C. (1-D, 2-D, 3-D cases)

This section contains some examples of modeling and simulations of diffusion processes in 1-D, 2-D and 3-D bounded domains. IBVP for heat equation with the Neumann boundary condition on a string, in a rectangle and in a parallelepiped will be used for modeling and simultions. We took a pulse point source concentrated in different points in these domains: in the center, near the boundary, in the corner.

3.7.1 1-D Heat-Diffusion equation

In this case we have a string on $[0, 6]$.

Example 3.7.1. Let us consider the problem (3.2.1)-(3.2.3). The functions $\phi(x)$ and $F(x,t)$ are given by

$$\phi(x) = 0 \ ,$$

$$F(x,t) = \delta(x - x_0)\delta(t) \ , x_0 \in [0, \ell] \ ,$$

where $\delta(x)$ is the Dirac delta function. Using formulas for $\phi(x)$ and $F(x,t)$ and the properties of the Dirac delta function the solution of the problem (3.2.1)-(3.2.3) can be found by the following formula

$$u(x,t) = \sum_{i=0}^{\infty} T_i(t) X_i(x) \ , \tag{3.7.1}$$

where

$$T_i(t) = c^2 \int_0^t F_i(\tau) e^{-c^2 \lambda_i (t-\tau)} d\tau \ ,$$

$$i^2 \neq 0 \ , \quad i = 0, 1, 2, ...$$

$$T_0(t) = c^2 \int_0^t \int_0^{\xi} F_0(\tau) d\tau d\xi \ ,$$

and

$$F_i(t) = X_i(x_0)\delta(t) \ ,$$

$$F_0(t) = 0 \ .$$

Hence

$$T_i(t) = c^2 e^{-c^2\lambda_i t} X_i(x_0) \ ,$$

$$i^2 \neq 0 \ , \quad i = 0, 1, 2, ...$$

$$T_0(t) = 0 \ ,$$

and λ_i and $X_i(x)$ are defined in (3.1.10), (3.1.11).

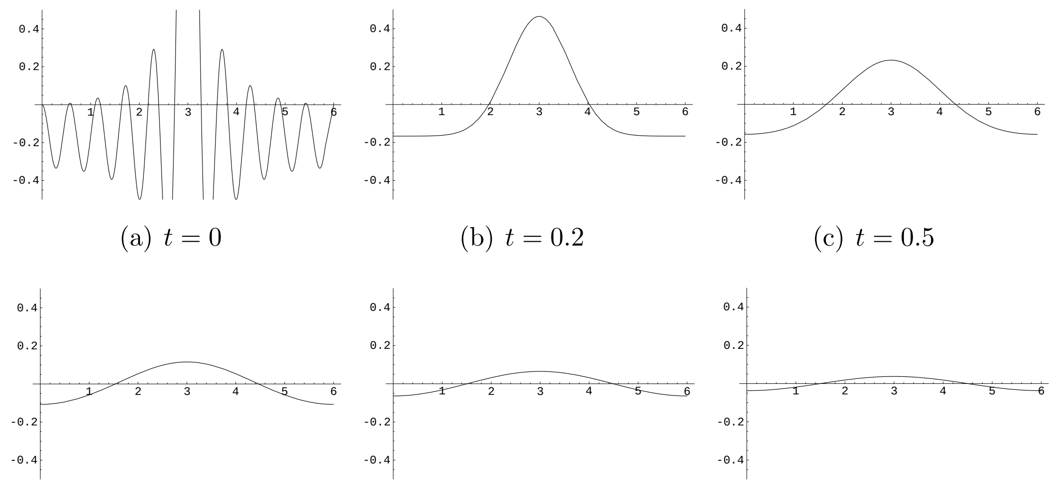
For the given data of Example 3.7.1, we used Mathematica codes in order to find the solution and to animate. The exact solution (3.7.1) is given by the series containing infinite number of terms. We found an approximate solution by means of the formula

$$u(x,t) = c^2 \sum_{i=0}^{n} T_i(t) X_i(x) \ , \tag{3.7.2}$$

where $n = 20$. This number n is chosen by considering the theoretical evaluation of the general term of the series (3.7.2) and the numerical experiments. We will consider each case for the function (3.7.2).

3.7.1.1 Simulations of 1-D Heat-Diffusion equation with Neumann B.C

Using the formula (3.7.2) for $n = 20$ and Mathematica codes we simulated the diffusion processes from the pulse point source which is located in the center of the domain D. The simulations for different times shown in figures below.



(a) $t = 0$ (b) $t = 0.2$ (c) $t = 0.5$

(d) $t = 1.0$ (e) $t = 1.5$ (f) $t = 2.0$

Figure 3.7: Example 3.7.1: The source in the center of the bounded domain for non-homogeneous problem .

In the non-homogeneous problem we have extra c^2 and it only changes the range of the solution. For $c = 1$ the homogeneous and the non-homogeneous problems have the same solutions.

3.7.2 2-D Heat-Diffusion equation

In this case we have a rectangle $D = ([0, 6] \times [0, 12])$.

Example 3.7.2. Let us consider the problem (3.4.1)-(3.4.3). The functions $\phi(x, y)$ and $F(x, y, t)$ are given by

$$\phi(x, y) = 0 \ ,$$

$$F(x, y, t) = \delta(x - x_0)\delta(y - y_0)\delta(t) \ , (x_0, y_0) \in D \ ,$$

where $\delta(x)$ is the Dirac delta function. Using formulas for $\phi(x, y)$ and $F(x, y, t)$ and the properties of the Dirac delta function the solution of the problem (3.4.1)-

(3.4.3) can be found by the following formula

$$u(x,y,t) = \sum_{i=0}^{\infty}\sum_{j=0}^{\infty} T_{ij}(t)V_{ij}(x,y) \ , \tag{3.7.3}$$

where

$$T_{ij}(t) = c^2 \int_0^t F_{ij}(\tau)e^{-c^2\lambda_{ij}(t-\tau)}d\tau \ ,$$

$$i^2 + j^2 \neq 0 \ , \quad i,j = 0,1,2,...$$

$$T_{00}(t) = c^2 \int_0^t \int_0^{\xi} F_{00}(\tau)d\tau d\xi \ ,$$

and

$$F_{ij}(t) = V_{ij}(x_0,y_0)\delta(t) \ ,$$

$$F_{00}(t) = 0 \ .$$

Hence

$$T_{ij}(t) = c^2 e^{-c^2\lambda_{ij}t}V_{ij}(x_0,y_0) \ ,$$

$$i^2 + j^2 \neq 0 \ , \quad i,j = 0,1,2,...$$

$$T_{00}(t) = 0 \ ,$$

and λ_{ij} and $V_{ij}(x,y)$ are defined in (3.3.10), (3.3.11). For this example consider the different positions of (x_0,y_0) (the point in which the pulse point source is concentrated). These positions (x_0,y_0) are given in the following table

	(x_0,y_0)
Case 1	(3,6)
Case 2	(3,11)
Case 3	(1,11)

Table 3.1: Positions of sources in a rectangle D with the Dirichlet B.C.

For the given data of Example 3.7.2, we used Mathematica codes in order to find the solution and to animate for each cases. The exact solution (3.7.3) is given by the series containing infinite number of terms. We found an approximate solution by means of the formula

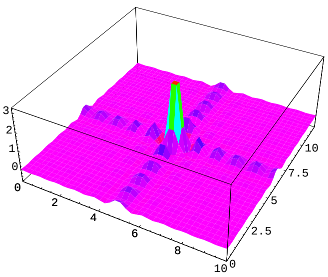
$$u(x,y,t) = c^2 \sum_{i=0}^{n}\sum_{j=0}^{n} T_{ij}(t)V_{ij}(x,y) \ , \tag{3.7.4}$$

where $n = 20$. This number n is chosen by considering the theoretical evaluation of the general term of the series (3.7.4) and the numerical experiments. We will consider each case for the function (3.7.4).

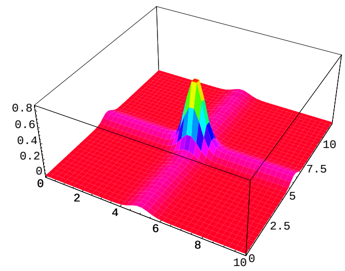
3.7.3 Simulation Examples

3.7.3.1 Simulation for Case1

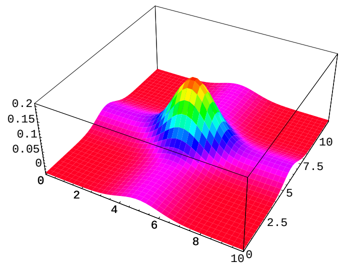
Using the formula (3.7.4) for $n = 20$ and Mathematica codes we simulated the diffusion processes from the pulse point source which is located in the center of the domain D. The simulations for different times shown in figures below.



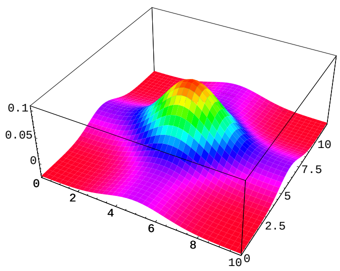
(a) $t = 0$



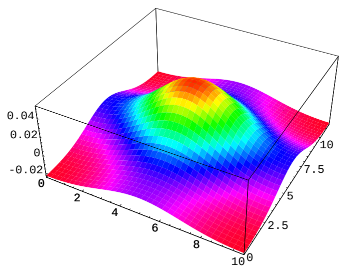
(b) $t = 0.1$



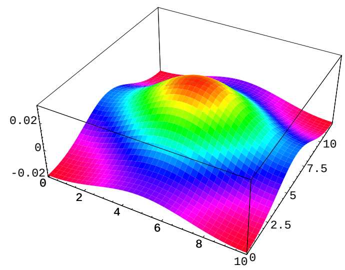
(c) $t = 0.5$



(d) $t = 1.0$



(e) $t = 2.0$



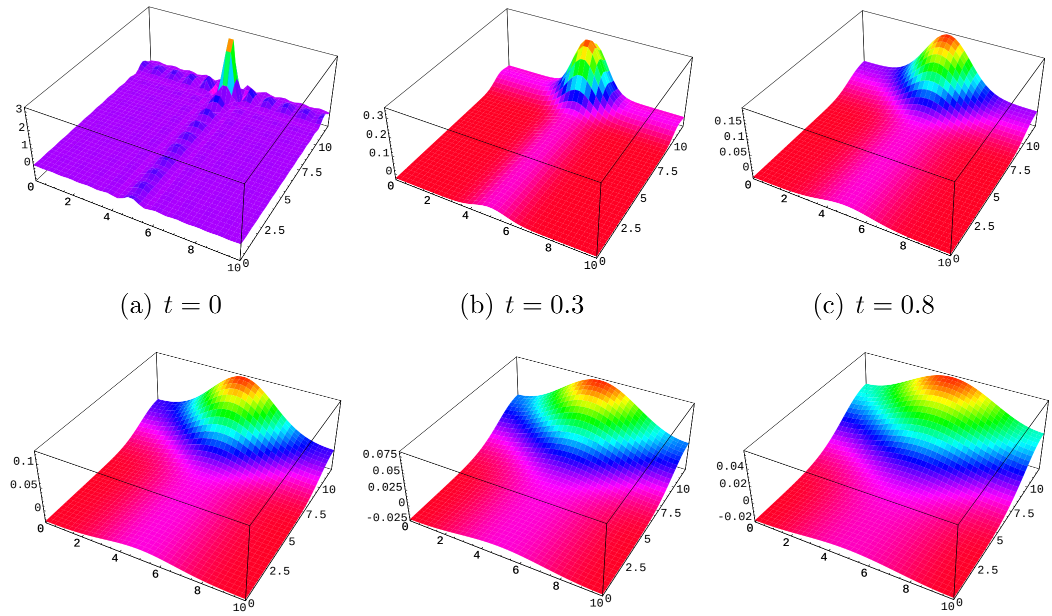
(f) $t = 3.0$

Figure 3.8: Example 3.7.2: The source in the center of the rectangle with Neumann B.C.

In the non-homogeneous problem we have extra c^2 and it only changes the range of the solution. For $c = 1$ the homogeneous and the non-homogeneous problems have the same solutions.

3.7.3.2 Simulation for Case2

The result of the simulation corresponding to Case 2 (the position of the source is near the boundary) is presented on the figure 4.16 (a)-(f).



(a) $t = 0$ (b) $t = 0.3$ (c) $t = 0.8$

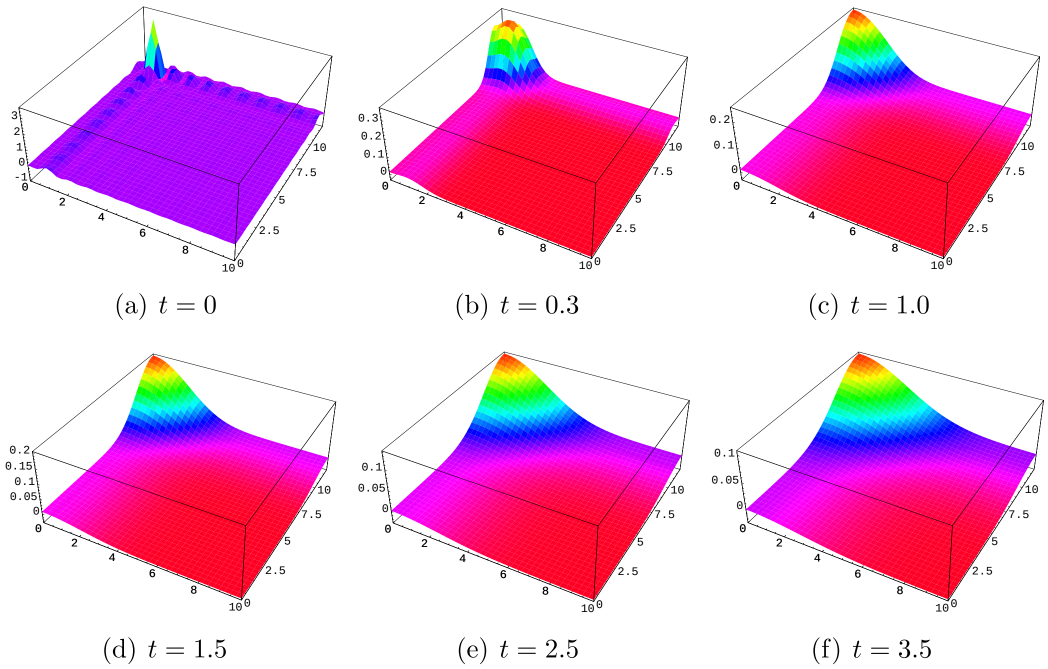
(d) $t = 1.4$ (e) $t = 1.5$ (f) $t = 3.5$

Figure 3.9: Example 3.7.2: Source near the boundary of the rectangle with Neumann B.C.

In the non-homogeneous problem we have extra c^2 and it only changes the range of the solution. For $c = 1$ the homogeneous and the non-homogeneous problems have the same solutions.

3.7.3.3 Simulation for Case3

The result of the simulation corresponding to Case 3 (the position of the source is near the corner) is presented on the figure 4.17 (a)-(f).



(a) $t = 0$ (b) $t = 0.3$ (c) $t = 1.0$

(d) $t = 1.5$ (e) $t = 2.5$ (f) $t = 3.5$

Figure 3.10: Example 3.7.2: Source near the corner of the rectangle with Neumann B.C.

In the non-homogeneous problem we have extra c^2 and it only changes the range of the solution. For $c = 1$ the homogeneous and the non-homogeneous problems have the same solutions.

3.7.4 3-D Heat-Diffusion equation

In this case we have a parallelepiped $D = ([0,6] \times [0,12] \times [0,3])$

Example 3.7.3. Let us consider the problem (3.6.1)-(3.6.3). The functions $\phi(x,y,z)$ and $F(x,y,z,t)$ are given by

$$\phi(x,y,z) = 0 \ ,$$

$$F(x,y,z,t) = \delta(x-x_0)\delta(y-y_0)\delta(z-z_0)\delta(t) \ , (x_0,y_0,z_0) \in D \ ,$$

where $\delta(x)$ is the Dirac delta function. Using formulas for $\phi(x,y,z)$ and $F(x,y,z,t)$ and the properties of the Dirac delta function the solution of the problem (3.6.1)-(3.6.3) can be found by the following formula

$$u(x,y,z,t) = \sum_{i=0}^{\infty}\sum_{j=0}^{\infty}\sum_{k=0}^{\infty} T_{ijk}(t)V_{ijk}(x,y,z) \ , \tag{3.7.5}$$

where

$$T_{ijk}(t) = c^2 \int_0^t F_{ijk}(\tau)e^{-c^2\lambda_{ijk}(t-\tau)}d\tau \ ,$$

$$i^2+j^2+k^2 \neq 0 \ , \quad i,j = 0,1,2,...$$

$$T_{00}(t) = c^2 \int_0^t \int_0^{\xi} F_{00}(\tau)d\tau d\xi \ ,$$

and

$$F_{ijk}(t) = V_{ijk}(x_0,y_0)\delta(t) \ ,$$

$$F_{00}(t) = 0 \ .$$

Hence

$$T_{ijk}(t) = c^2 e^{-c^2\lambda_{ijk}t}V_{ijk}(x_0,y_0) \ ,$$

$$i^2+j^2+k^2 \neq 0 \ , \quad i,j,k = 0,1,2,...$$

$$T_{000}(t) = 0 \ ,$$

and λ_{ijk} and $V_{ijk}(x,y,z)$ are defined in (3.5.10), (3.5.11). For this example consider the different positions of (x_0,y_0,z_0) (the point in which the pulse point source is concentrated). These positions (x_0,y_0,z_0) are given in the following table

For the given data of Example 3.7.4, we used Mathematica codes in order

	(x_0, y_0, z_0)
Case 1	(3,6,2)
Case 2	(3,11,2)
Case 3	(1,11,2)

Table 3.2: Positions of sources in a parallelepiped D with the Dirichlet B.C.

to find the solution and to animate for each cases. The exact solution (3.7.5) is given by the series containing infinite number of terms. We found an approximate solution by means of the formula

$$u(x, y, z, t) = c^2 \sum_{i=0}^{n} \sum_{j=0}^{n} \sum_{k=0}^{n} T_{ijk}(t) V_{ijk}(x, y, z) \ , \tag{3.7.6}$$

where $n = 20$. This number n is chosen by considering the theoretical evaluation of the general term of the series (3.7.6) and the numerical experiments. We will consider each case for the function (3.7.6).

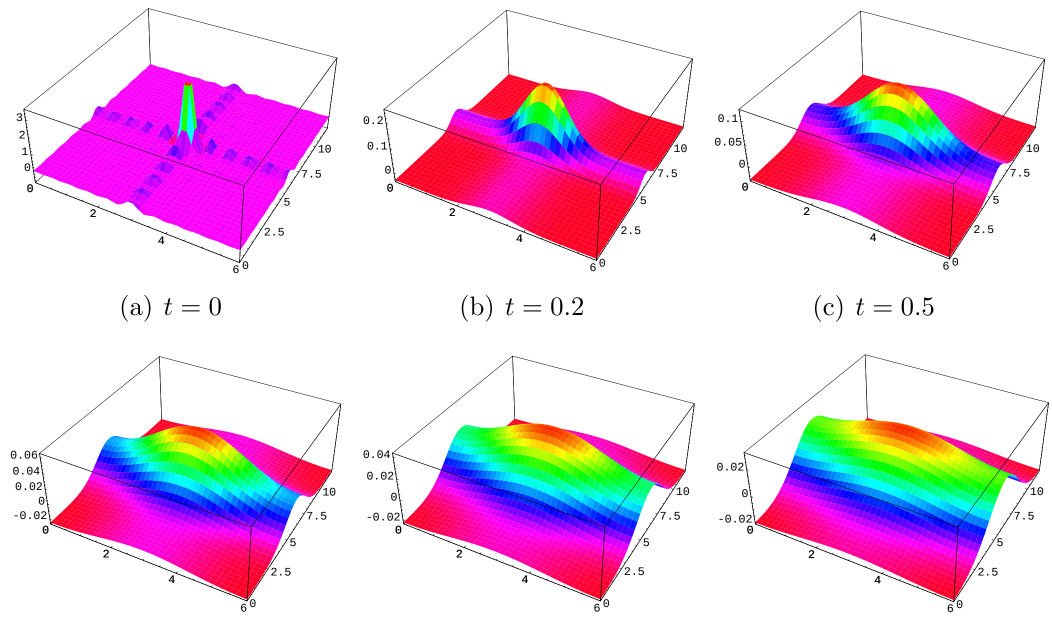
3.7.4.1 Commands in Mathematica for Example 3.7.4 :

```
 << Graphics`Animation`
 bx = 6; by = 12; bz = 3; (dimension of the parallelepiped)
 x0 = 3; y0 = 6; z0 = 2; (the position of the source where
it is located)
 n:=20; (number of terms in the sum)
 sc:=1; (the speed of propagation)

 (eigenvalues)
 a[kk_] = (kk*Pi/bx)^2; b[kk_] = (kk*Pi/by)^2;
 c[kk_] = (kk*Pi/bz)^2;

 (computing the eigenfunctions and Fourier coefficients)
 For[i = 1, i <= n, i++,
  For[j = 1, j <= n, j++,
   For[k = 1, k <= n, k++,
        Lambda[i, j, k] = a[i] + b[j] + c[k];
        V[i, j, k] = Sqrt[8/(bx*by*bz)]*Cos[Sqrt[a[i]]*x]
 *Cos[Sqrt[b[j]]*y]*Cos[Sqrt[c[k]]*z];
 PV[i, j, k] =ReplaceAll[ReplaceAll[ReplaceAll[V[i, j, k]
 , x -> x0], y -> y0], z -> z0];
 If[i==0 && j==0 && k==0,(T[i,j,k]=0),;
(T[i, j, k] = sc^2*PV[i,j,k]*e^((sc^2)*(-Lambda[i, j, k]*t)))
 ];];]

 (computing the sum)
 son := Sum[Sum[Sum[T[i, j, k]*V[i, j, k], {i, 0, n}]
 , {j, 0, n}], {k, 0, n}]

 fixing parameter z=1
 son2 = ReplaceAll[son, z -> 1];

 (animating the picture w.r.t time variable with sitep size 0.25)
 Animate[Plot3D[son2, {x, 0, 6}, {y, 0, 12}, ColorFunction
  -> (Hue[1 - #] &),PlotRange -> All, AspectRatio -> Automatic,
 Mesh -> False,PlotPoints -> 40], {t, 0, 34, 0.5}]
```

3.7.5 Simulation Examples

3.7.5.1 Simulation for Case1

Using the formula (3.7.6) for $n = 20$ and Mathematica codes we simulated the diffusion processes from the pulse point source which is located in the center of the domain D. The simulations for different times shown in figures below.



(a) $t = 0$ (b) $t = 0.2$ (c) $t = 0.5$

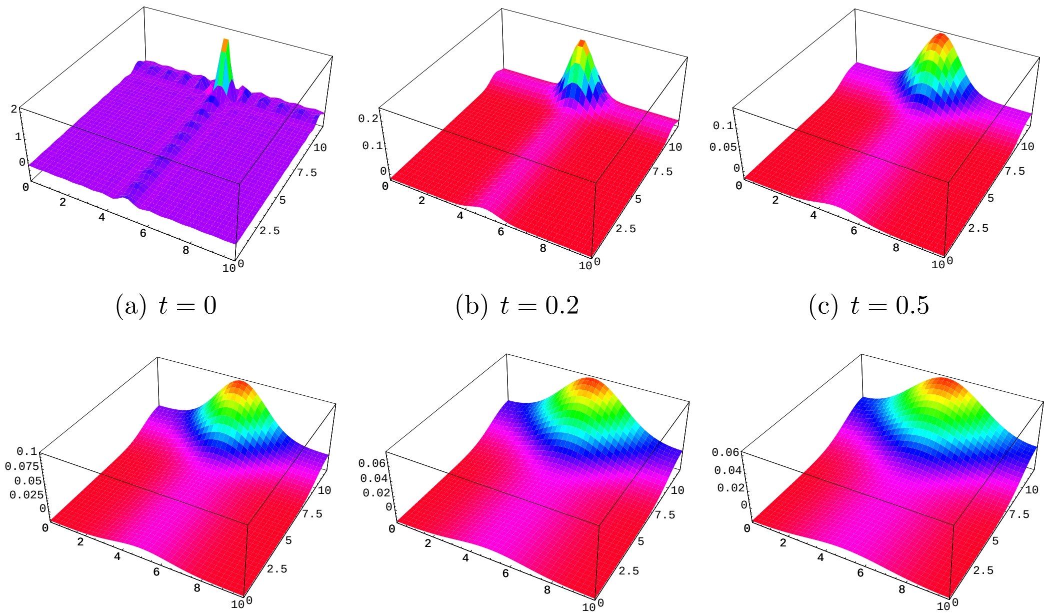
(d) $t = 1.0$ (e) $t = 1.5$ (f) $t = 2.0$

Figure 3.11: Example 3.7.4: The source in the center of the bounded domain for non-homogeneous problem .

In the non-homogeneous problem we have extra c^2 and it only changes the range of the solution. For $c = 1$ the homogeneous and the non-homogeneous problems have the same solutions.

3.7.5.2 Simulation for Case2

The result of the simulation corresponding to Case 2 (the position of the source is near the boundary) is presented on the figure 4.19 (a)-(f).



(a) $t = 0$ (b) $t = 0.2$ (c) $t = 0.5$

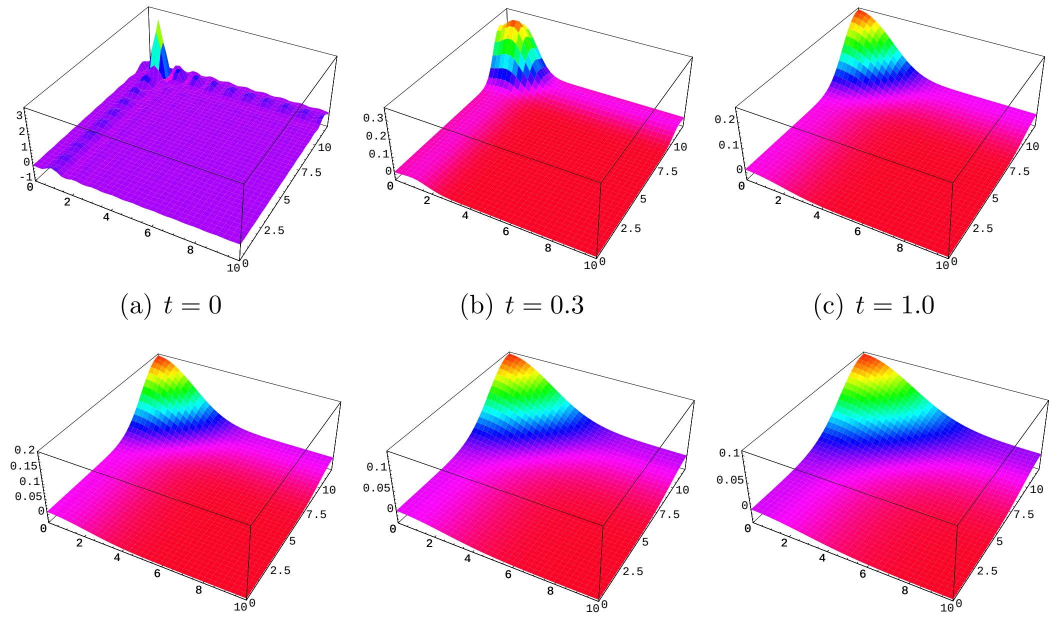
(d) $t = 1.0$ (e) $t = 1.5$ (f) $t = 2.0$

Figure 3.12: Example 3.7.4: Source near the boundary of the bounded domain D .

In the non-homogeneous problem we have extra c^2 and it only changes the range of the solution. For $c = 1$ the homogeneous and the non-homogeneous problems have the same solutions.

3.7.5.3 Simulation for Case3

The result of the simulation corresponding to Case 3 (the position of the source is near the corner) is presented on the figure 4.20 (a)-(f).



(a) $t = 0$ (b) $t = 0.3$ (c) $t = 1.0$

(d) $t = 1.5$ (e) $t = 2.5$ (f) $t = 3.5$

Figure 3.13: Example 3.7.4: Source near the corner of the bounded domain D .

In the non-homogeneous problem we have extra c^2 and it only changes the range of the solution. For $c = 1$ the homogeneous and the non-homogeneous problems have the same solutions.

3.8 Analysis of the chapter3 study

1. Exact and approximate formulae for the solutions of IBVPs with Dirichlet boundary condition for the diffusion (heat) equations on a string, in a rectangle and in a parallelepiped were obtained.

2. These formulae were adjusted to cases when initial data or inhomogeneous term are the Dirac delta function with a support in a point which is inside the domain D. The pulse point source is modeled by these initial data and in homogeneous term.

3. Obtained formulae for generalized solutions of IBVPs for the heat-diffusion equations were used for modeling and simulations of diffusion processes in bounded domain D arising from the pulse point sources.

4. Results of diffusion processes simulation are presented by 1-D, 2-D and 3-D pictures and animated movies.

5. Obtained formulae and results of simulation were analyzed. The different behavior of the boundary due to the Neumann boundary condition was seen.

CHAPTER FOUR
IBVP FOR HEAT-DIFFUSION EQUATION WITH MIXED BOUNDARY CONDITION

In this section IBVP for 1D, 2D and 3D heat(diffusion) equation with Mixed Boundary condition in a homogeneous strip, rectangle and parallelepiped will be studied. The formulas will be generated and using these formulas simulations will be found. Sources are taken as pulse point sources.

4.1 IBVP for a Homogeneous 1D Heat-Diffusion Equation with Mixed Boundary Condition

Let $x \in (0,\ell)$, $t \in (0,T)$,where ℓ and T are given positive numbers. Let us consider the IBVP for the diffusion equation on a string :

$$\frac{1}{c^2}\frac{\partial u(x,t)}{\partial t} = \frac{\partial^2 u(x,t)}{\partial x^2}\ , x \in (0,\ell), \quad t \in (0,T)\ , \tag{4.1.1}$$

$$u(x,0) = \phi(x)\ , \tag{4.1.2}$$

$$\left(\frac{\partial u}{\partial \eta} + \alpha\, u\right)\Big|_{t\in(0,T)} = 0\ , \tag{4.1.3}$$

where $c > 0$ is a given number.Here $\varphi(x)$ is a given smooth function for $x \in [0,\ell]$. IBVP consists of finding $u(x,t)$ satisfying (4.1.1), (4.1.2), (4.1.3).

Using Fourier Series Expansion Method we will find $u(x,t)$ which satisfies (4.1.1)-(4.1.3). We will use the same method which is applied for solving the problem (2.5.1)-(2.5.3) and (3.5.1)-(3.5.3) to solve (4.1.1)-(4.1.3). We will use the separation of variables. Setting

$$u(x,t) = T(t)X(x)\ , \tag{4.1.4}$$

and substituting (4.1.4) into (4.1.1) we find

$$\frac{1}{c^2}\frac{T'(t)}{T(t)} = \frac{X''(x)}{X(x)} = -\lambda\ .$$

So we get the following equations for $T(t)$ and $X(x)$:

$$X''(x) + \lambda X(x) = 0, \quad x \in (0,\ell)\ , \tag{4.1.5}$$

$$T'(t) + c^2 \lambda T(t) = 0, \quad t \in (0, T) \ . \tag{4.1.6}$$

Our aim is to construct Strum-Liouville equations. Substituting (4.1.4) into (4.1.3) we have

$$\left(\frac{\partial u}{\partial \eta} + \alpha \, u \right) = (\nabla u \cdot \overrightarrow{n} + \alpha u) = 0 \ ,$$

and so

$$\big(\nabla X(x) T(t) \cdot \overrightarrow{n} + \alpha X(x) T(t) \big) = 0 \ ,$$

$$T(t) \left(\nabla X(x) \cdot \overrightarrow{n} + \alpha X(x) \right) = 0 \ ,$$

$$\left(\nabla X(x) \cdot \overrightarrow{n} + \alpha X(x) \right) = 0 \ . \tag{4.1.7}$$

Equations (4.1.5), (4.1.7) we will write as an Sturm-Liouville problem

$$X''(x) + \lambda X(x) = 0 \ , \tag{4.1.8}$$

$$\left(\nabla X(x) \cdot \overrightarrow{n} + \alpha X(x) \right) = 0 \ . \tag{4.1.9}$$

We are trying to find eigenvalues and eigenfunctions. Using the separation of variables we find

$$X''(x) + \lambda X(x) = 0, \quad X'(0) - \alpha X(0) = 0, \quad X'(\ell) + \alpha X(\ell) = 0 \ . \tag{4.1.10}$$

Using Appendix A.3 we can get the eigenvalues and correspondingly eigenfunctions for the system (4.1.10) as follows

$$X_i(x) = C_i \sin(\xi_i x + \varphi_i^x), \quad \lambda_i = \xi_i^2, \quad \varphi_i^x = \arctan(\frac{\xi_i}{\alpha}) \ , i = 1, 2, ...$$

where ξ_i for each $i = 1, 2, ...$ is the solution of

$$\cot(x\ell) = \frac{1}{2} \left(\frac{x}{\alpha} - \frac{\alpha}{x} \right) \ ,$$

$\alpha > 0, \ \ell > 0$ fixed and

$$C_i = 2 \sqrt{\frac{\xi_i}{2\ell\xi_i + \sin[2\varphi_i^x] - \sin[2(\ell\xi_i + \varphi_i^x)]}} \ , \quad i = 1, 2, ... \ , \tag{4.1.11}$$

So we get the eigenvalues eigenfunctions of (4.1.8), (4.1.9) as follows

$$X_i(x) = C_i \sin(\xi_i x + \varphi_i^x) \ , \tag{4.1.12}$$

and corresponding eigenvalues

$$\lambda_i = \xi_i^2 \; ; \quad i = 1, 2, ... \; , \tag{4.1.13}$$

where C_i is defined in (4.1.11). We get the solution of the equation (4.1.6) using the equation (4.1.13) from the previous section we get

$$T_i(t) = A_i e^{-c^2 \lambda_i t} \; , \quad i = 1, 2, ... \tag{4.1.14}$$

Hence $u(x,t) = T_i(t)X_i(x)$ are solutions of (4.1.1)-(4.1.3) for each $i = 1, 2, ...$ By the superposition principle we get the solution of the series form

$$u(x,t) = \sum_{i=1}^{\infty} X_i(x) T_i(t) \; . \tag{4.1.15}$$

Now, we can find the Fourier coefficients A_i. By using the orthonormal functions $X_i(x)$, ϕ_i can be written as in the Fourier series form

$$\phi(x) = \sum_{i=1}^{\infty} \phi_i X_i(x) \; , \tag{4.1.16}$$

where

$$\phi_i = \int_0^{\ell} \phi(x) X_i(x) dx \; .$$

Using the initial condition (4.1.2) and (4.1.16) we get

$$A_i = \phi_i \; .$$

Substitution gives

$$u(x,t) = \sum_{i=1}^{\infty} \phi_i \, e^{-c^2 \lambda_i t} X_i(x) \; , \tag{4.1.17}$$

the general solution of (4.1.1)- (4.1.3).

4.2 IBVP for a Non-Homogeneous 1D Heat-Diffusion Equation with Mixed Boundary Condition

Let $x \in (0,\ell)$, $t \in (0,T)$,where ℓ and T are given positive numbers. Let us consider the IBVP for the diffusion equation on a string :

$$\begin{aligned} \frac{1}{c^2}\frac{\partial u(x,t)}{\partial t} &= \frac{\partial^2 u(x,t)}{\partial x^2} + F(x,t) \ , \\ & \quad x \in (0,\ell), \quad t \in (0,T) \ , \qquad (4.2.1) \\ u(x,0) &= \phi(x,y) \ , \qquad (4.2.2) \\ \left(\frac{\partial u}{\partial \eta} + \alpha\, u\right)\Big|_{t\in(0,T)} &= 0 \ , \qquad (4.2.3) \end{aligned}$$

where $c > 0$ is a given positive number; $\varphi(x)$ is a given smooth functions for $x \in [0,\ell]$, $F(x,t)$, is a given smooth function for $(x,t) \in ([0,\ell] \times [0,t])$. IBVP consists of finding $u(x,t)$ satisfying (4.2.1)-(4.2.1).

Using the same techniques from the previous sections for non-homogeneous problem with the Dirichlet and Neumann boundary conditions and homogeneous problem for Mixed boundary condition we will get the following result

$$T_i(t) = \phi_i e^{-c^2\lambda_i t} + c^2 \int_0^t F_i(\tau) e^{-c^2\lambda_i(t-\tau)} d\tau \ , \qquad (4.2.4)$$

and

$$u(x,t) = \sum_{i=1}^{\infty} T_i(t) X_i(x) \ , \qquad (4.2.5)$$

is the solution of (4.2.1)-(4.2.3), where $T_i(t)$ is defined in (4.2.4) and $X_i(x)$ is defined in (4.1.12).

4.3 IBVP for a Homogeneous 2D Heat-Diffusion Equation with Mixed Boundary Condition

Let $(x,y) \in \mathbb{R}^2$, $t \in \mathbb{R}$,$D = \{(x,y) \in \mathbb{R}^2 : 0 \leq x \leq b_1, 0 \leq y \leq b_2\}$ be a homogeneous rectangle. Let us consider the IBVP for the diffusion equation in the rectangle D :

$$\begin{aligned} \frac{1}{c^2}\frac{\partial u(x,y,t)}{\partial t} &= \Delta_{x,y,z}u(x,y,t) \; , (x,y) \in D, \quad t \geq 0 \; , & (4.3.1) \\ u(x,y,0) &= \phi(x,y) \; , & (4.3.2) \\ \left(\frac{\partial u}{\partial \eta} + \alpha\, u\right)\big|_{\partial D} &= 0 \; , & (4.3.3) \end{aligned}$$

where ∂D is the boundary of D. Here $\phi(x,y)$ is given function in $D \cup \partial D$, c is a positive constant.

Using Fourier Series Expansion Method we will find $u(x,y,t)$ which satisfies (4.3.1)-(4.3.3). We will use the same method which is applied for solving the problem (2.5.1)-(2.5.3) and (3.5.1)-(3.5.3) to solve (4.3.1)-(4.3.3). We will use the separation of variables. Setting

$$u(x,y,t) = T(t)V(x,y) \; , \tag{4.3.4}$$

and substituting (4.3.4) into (4.3.1) we find

$$\frac{1}{c^2}\frac{T'(t)}{T(t)} = \frac{\Delta_{x,y}V(x,y)}{V(x,y)} = -\lambda \; .$$

So we get the following equations for $T(t)$ and $V(x,y)$:

$$\Delta_{x,y}V(x,y) + \lambda V(x,y) = 0, \quad (x,y) \in D \; , \tag{4.3.5}$$

$$T'(t) + c^2\lambda T(t) = 0, \quad t > 0 \; . \tag{4.3.6}$$

Our aim is to construct Strum-Liouville equations. Substituting (4.3.4) into (4.3.3) we have

$$\left(\frac{\partial u}{\partial \eta} + \alpha\, u\right)\big|_{\partial D} = \left(\nabla u \cdot \overrightarrow{n} + \alpha u\right)\big|_{\partial D} = 0 \; ,$$

and so

$$\left(\nabla V(x,y)T(t) \cdot \overrightarrow{n} + \alpha V(x,y)T(t)\right)\big|_{\partial D} = 0 \; ,$$

$$T(t)\left(\nabla V(x,y)\cdot\overrightarrow{n}+\alpha V(x,y)\right)\Big|_{\partial D}=0\ ,$$

$$\left(\nabla V(x,y)\cdot\overrightarrow{n}+\alpha V(x,y)\right)\Big|_{\partial D}=0\ . \tag{4.3.7}$$

Equations (4.3.5), (4.3.7) we will write as an Sturm-Liouville problem

$$\Delta_{x,y}V(x,y)+\lambda V(x,y)=0\ , \tag{4.3.8}$$

$$\left(\nabla V(x,y)\cdot\overrightarrow{n}+\alpha V(x,y)\right)\Big|_{\partial D}=0\ . \tag{4.3.9}$$

We are trying to find eigenvalues and eigenfunctions. Using the separation of variables we find

$$V(x,y)=X(x)Y(y)\ . \tag{4.3.10}$$

Substituting (4.3.10) into (4.3.8), (4.3.9) we get

$$X''(x)+\mu X(x)=0,\quad X'(0)-\alpha X(0)=0,\quad X'(b_1)+\alpha X(b_1)=0\ , \tag{4.3.11}$$

$$Y''(y)+\beta Y(y)=0,\quad Y'(0)-\alpha Y(0)=0,\quad Y'(b_2)+\alpha Y(b_2)=0\ . \tag{4.3.12}$$

Using Appendix A.3 we can get the eigenvalues and correspondingly eigenfunctions for the system (4.3.11), (4.3.12) as follows

$$X_i(x)=C_i\sin(\xi_i x+\varphi_i^x),\quad \mu_i=\xi_i^2,\quad \varphi_i^x=\arctan(\frac{\xi_i}{\alpha})\ ,i=1,2,...$$

where ξ_i for each $i=1,2,...$ is the solution of

$$\cot(xb_1)=\frac{1}{2}\left(\frac{x}{\alpha}-\frac{\alpha}{x}\right)\ ,$$

$\alpha>0,\ \ell>0$ fixed and

$$C_i=2\sqrt{\frac{\xi_i}{2b_1\xi_i+\sin[2\varphi_i^x]-\sin[2(b_1\xi_i+\varphi_i^x)]}}\ ,\quad i=1,2,...\ , \tag{4.3.13}$$

$$Y_j(y)=C_j\sin(\eta_j y+\varphi_j^y),\quad \beta_j=\eta_j^2,\quad \varphi_j^y=\arctan(\frac{\eta_j}{\alpha})\ ,j=1,2,...$$

where η_j for each $j=1,2,...$ is the solution of

$$\cot(yb_2)=\frac{1}{2}\left(\frac{y}{\alpha}-\frac{\alpha}{y}\right)\ ,$$

$\alpha > 0,\ \ell > 0$ fixed and

$$C_j = 2\sqrt{\frac{\eta_j}{2b_1\nu_j + \sin[2\varphi_j^y] - \sin[2(b_2\eta_j + \varphi_j^y)]}}\ , \quad j = 1, 2, \dots\ , \tag{4.3.14}$$

So we get the eigenvalues eigenfunctions of (4.3.8), (4.3.9) as follows

$$V_{ij}(x, y) = X_i(x)Y_j(y)\ ,$$

or equivalently

$$V_{ij}(x, y) = C_iC_j \sin(\xi_i x + \varphi_i^x)\sin(\eta_j y + \varphi_j^y)\ , \tag{4.3.15}$$

and corresponding eigenvalues

$$\lambda_{ij} = \xi_i^2 + \eta_j^2\ ; \quad i, j = 1, 2, \dots\ , \tag{4.3.16}$$

where C_i and C_j are defined in (4.3.13) and (4.3.14). We get the solution of the equation (4.3.6) using the equation (4.3.16) from the previous section we get

$$T_{ij}(t) = A_{ij}e^{-c^2\lambda_{ij}t}\ , \quad i, j = 1, 2, \dots \tag{4.3.17}$$

Hence $u(x, y, t) = T_{ij}V_{ij}(x, y)$ are solutions of (4.3.1)-(4.3.3) for each $i, j = 1, 2, \dots$ By the superposition principle we get the solution of the series form

$$u(x, y, t) = \sum_{i,j=1}^{\infty} V_{ij}T_{ij}\ . \tag{4.3.18}$$

Now, we can find the Fourier coefficients A_{ij}. By using the orthonormal functions $V_{ij}(x, y)$, ϕ_{ij} can be written as in the Fourier series form

$$\phi(x, y) = \sum_{i,j=1}^{\infty} \phi_{ij}V_{ij}(x, y)\ , \tag{4.3.19}$$

where

$$\phi_{ij} = \int_0^{b_1}\int_0^{b_2} \phi(x, y)V_{ij}\,dxdy\ .$$

Using the initial condition (4.3.2) and (4.3.19) we get

$$A_{ij} = \phi_{ij}\ .$$

Substitution gives

$$u(x,y,t) = \sum_{i,j=1}^{\infty} \phi_{ij}\, e^{-c^2\lambda_{ij}t} V_{ij}(x,y) \ , \tag{4.3.20}$$

the general solution of (4.3.1)- (4.3.3).

4.4 IBVP for a Non-Homogeneous 2D Heat-Diffusion Equation with Mixed Boundary Condition

Let $(x,y) \in \mathbb{R}^2$, $t \in \mathbb{R}$,$D = \{(x,y) \in \mathbb{R}^2 : 0 \le x \le b_1, 0 \le y \le b_2\}$ be a homogeneous rectangle. Let us consider the IBVP for the diffusion equation in the rectangle D :

$$\begin{aligned} \frac{1}{c^2}\frac{\partial u(x,y,t)}{\partial t} &= \Delta_{x,y} u(x,y,t) + F(x,y,t) \ , \\ &\quad (x,y) \in D, \quad t \ge 0 \ , \qquad (4.4.1) \\ u(x,y,0) &= \phi(x,y) \ , \qquad (4.4.2) \\ \left(\frac{\partial u}{\partial \eta} + \alpha\, u\right)\Big|_{\partial D} &= 0 \ , \qquad (4.4.3) \end{aligned}$$

where ∂D is the boundary of D. Here $F(x,y,t)$ and $\phi(x,y)$ are given functions in $D \cup \partial D$, c is a positive constant. IBVP consists of finding $u(x,y,t)$ satisfying (4.4.1)-(4.4.3).

Using the same techniques from the previous sections for non-homogeneous problem with the Dirichlet and Neumann boundary conditions and homogeneous problem for Mixed boundary condition we will get the following result

$$T_{ij}(t) = \phi_{ij} e^{-c^2\lambda_{ij}t} + c^2 \int_0^t F_{ij}(\tau) e^{-c^2\lambda_{ij}(t-\tau)} d\tau \ , \tag{4.4.4}$$

and

$$u(x,y,t) = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty} T_{ij}(t) V_{ij}(x,y) \ , \tag{4.4.5}$$

is the solution of (4.4.1)-(4.4.3), where $T_{ij}(t)$ is defined in (4.4.4) and $V_{ij}(x,y)$ is defined in (4.3.15).

4.5 IBVP for a Homogeneous 3D Heat-Diffusion Equation with Mixed Boundary Condition

Let $(x,y,z) \in \mathbb{R}^3$, $t \in \mathbb{R}$,$D = \{(x,y,z) \in \mathbb{R}^3 : 0 \le x \le b_1, 0 \le y \le b_2, 0 \le z \le b_3\}$ be a homogeneous parallelepiped. Let us consider the IBVP for the diffusion equation in the parallelepiped D :

$$\begin{aligned} \frac{1}{c^2}\frac{\partial u(x,y,z,t)}{\partial t} &= \Delta_{x,y,z}u(x,y,z,t)\ ,(x,y,z) \in D, \quad t \ge 0\ , && (4.5.1)\\ u(x,y,z,0) &= \phi(x,y,z)\ , && (4.5.2)\\ \left(\frac{\partial u}{\partial \eta} + \alpha\, u\right)\Big|_{\partial D} &= 0\ , && (4.5.3) \end{aligned}$$

where ∂D is the boundary of D. Here $\phi(x,y,z)$ is given function in $D \cup \partial D$, c is a positive constant.

Using Fourier Series Expansion Method we will find $u(x,y,z,t)$ which satisfies (4.5.1)-(4.5.3). We will use the same method which is applied for solving the problem (2.5.1)-(2.5.3) and (3.5.1)-(3.5.3) to solve (4.5.1)-(4.5.3). We will use the separation of variables. Setting

$$u(x,y,z,t) = T(t)V(x,y,z)\ , \qquad (4.5.4)$$

and substituting (4.5.4) into (4.5.1) we find

$$\frac{1}{c^2}\frac{T'(t)}{T(t)} = \frac{\Delta_{x,y,z}V(x,y,z)}{V(x,y,z)} = -\lambda\ .$$

So we get the following equations for $T(t)$ and $V(x,y,z)$:

$$\Delta_{x,y,z}V(x,y,z) + \lambda V(x,y,z) = 0, \quad (x,y,z) \in D\ , \qquad (4.5.5)$$

$$T'(t) + c^2\lambda T(t) = 0, \quad t > 0\ . \qquad (4.5.6)$$

Our aim is to construct Strum-Liouville equations. Substituting (4.5.4) into (4.5.3) we have

$$\left(\frac{\partial u}{\partial \eta} + \alpha\, u\right)\Big|_{\partial D} = (\nabla u \cdot \overrightarrow{n} + \alpha u)\Big|_{\partial D} = 0\ ,$$

and so

$$\big(\nabla V(x,y,z)T(t) \cdot \overrightarrow{n} + \alpha V(x,y,z)T(t)\big)\Big|_{\partial D} = 0\ ,$$

$$T(t)\left(\nabla V(x,y,z)\cdot\overrightarrow{n}+\alpha V(x,y,z)\right)\Big|_{\partial D}=0\ ,$$

$$\left(\nabla V(x,y,z)\cdot\overrightarrow{n}+\alpha V(x,y,z)\right)\Big|_{\partial D}=0\ . \tag{4.5.7}$$

Equations (4.5.5), (4.5.7) we will write as an Sturm-Liouville problem

$$\Delta_{x,y,z}V(x,y,z)+\lambda V(x,y,z)=0\ , \tag{4.5.8}$$

$$\left(\nabla V(x,y,z)\cdot\overrightarrow{n}+\alpha V(x,y,z)\right)\Big|_{\partial D}=0\ . \tag{4.5.9}$$

We are trying to find eigenvalues and eigenfunctions. Using the separation of variables we find

$$V(x,y,z)=X(x)Y(y)Z(z)\ . \tag{4.5.10}$$

Substituting (4.5.10) into (4.5.8), (4.5.9) we get

$$X''(x)+\mu X(x)=0,\quad X'(0)-\alpha X(0)=0,\quad X'(b_1)+\alpha X(b_1)=0\ , \tag{4.5.11}$$

$$Y''(y)+\beta Y(y)=0,\quad Y'(0)-\alpha Y(0)=0,\quad Y'(b_2)+\alpha Y(b_2)=0\ , \tag{4.5.12}$$

$$Z''(z)+\gamma Z(z)=0,\quad Z'(0)-\alpha Z(0)=0,\quad Z'(b_3)+\alpha Z(b_3)=0\ . \tag{4.5.13}$$

Using Appendix A.3 we can get the eigenvalues and correspondingly eigenfunctions for the system (4.5.11), (4.5.12), (4.5.13) as follows

$$X_i(x)=C_i\sin(\xi_i x+\varphi_i^x),\quad \mu_i=\xi_i^2,\quad \varphi_i^x=\arctan(\frac{\xi_i}{\alpha})\ ,i=1,2,...$$

where ξ_i for each $i=1,2,...$ is the solution of

$$\cot(xb_1)=\frac{1}{2}\left(\frac{x}{\alpha}-\frac{\alpha}{x}\right)\ ,$$

$\alpha>0,\ \ell>0$ fixed and

$$C_i=2\sqrt{\frac{\xi_i}{2b_1\xi_i+\sin[2\varphi_i^x]-\sin[2(b_1\xi_i+\varphi_i^x)]}}\ ,\quad i=1,2,...\ , \tag{4.5.14}$$

$$Y_j(y)=C_j\sin(\eta_j y+\varphi_j^y),\quad \beta_j=\eta_j^2,\quad \varphi_j^y=\arctan(\frac{\eta_j}{\alpha})\ ,j=1,2,...$$

where η_j for each $j=1,2,...$ is the solution of

$$\cot(yb_2)=\frac{1}{2}\left(\frac{y}{\alpha}-\frac{\alpha}{y}\right)\ ,$$

$\alpha > 0,\ \ell > 0$ fixed and

$$C_j = 2\sqrt{\frac{\eta_j}{2b_1\nu_j + \sin[2\varphi_j^y] - \sin[2(b_2\eta_j + \varphi_j^y)]}}\ , \quad j = 1, 2, \dots\ , \tag{4.5.15}$$

$$Z_k(z) = C_k \sin(\nu_k z + \varphi_k^z), \quad \gamma_k = \nu_k^2, \quad \varphi_k^z = \arctan(\frac{\nu_i}{\alpha})\ , k = 1, 2, \dots$$

where ν_k for each $k = 1, 2, \dots$ is the solution of

$$\cot(zb_3) = \frac{1}{2}\left(\frac{z}{\alpha} - \frac{\alpha}{z}\right)\ ,$$

$\alpha > 0,\ \ell > 0$ fixed and

$$C_k = 2\sqrt{\frac{\nu_k}{2b_3\nu_k + \sin[2\varphi_k^z] - \sin[2(b_3\nu_k + \varphi_k^z)]}}\ , \quad k = 1, 2, \dots\ , \tag{4.5.16}$$

So we get the eigenvalues eigenfunctions of (4.5.8), (4.5.9) as follows

$$V_{ijk}(x, y, z) = X_i(x)Y_j(y)Z_k(z)\ ,$$

or equivalently

$$V_{ijk}(x, y, z) = C_iC_jC_k \sin(\xi_i x + \varphi_i^x) \sin(\eta_j y + \varphi_j^y) \sin(\nu_k z + \varphi_k^z)\ , \tag{4.5.17}$$

and corresponding eigenvalues

$$\lambda_{ijk} = \xi_i^2 + \eta_j^2 + \nu_k^2\ ; \quad i, j, k = 1, 2, \dots\ , \tag{4.5.18}$$

where C_i, C_j and C_k are defined in (4.5.14), (4.5.15) and (4.5.16). We get the solution of the equation (4.5.6) using the equation (4.5.18) from the previous section we get

$$T_{ijk}(t) = A_{ijk}e^{-c^2\lambda_{ijk}t}\ , \quad i, j, k = 1, 2, \dots \tag{4.5.19}$$

Hence $u_{ijk}(x, y, z, t) = T_{ijk}V_{ijk}(x, y, z)$ are solutions of (4.5.1)-(4.5.3) for each $i, j, k = 1, 2, \dots$ By the superposition principle we get the solution of the series form

$$u(x, y, z, t) = \sum_{i,j,k=1}^{\infty} u_{ijk}\ ,$$

$$u(x,y,z,t) = \sum_{i,j,k=1}^{\infty} V_{ijk} T_{ijk} \; . \tag{4.5.20}$$

Now, we can find the Fourier coefficients A_{ijk}. By using the orthonormal functions $V_{ijk}(x,y,z)$, ϕ_{ijk} can be written as in the Fourier series form

$$\phi(x,y,z) = \sum_{i,j,k=1}^{\infty} \phi_{ijk} V_{ijk}(x,y,z) \; , \tag{4.5.21}$$

where

$$\phi_{ijk} = \int_0^{b_1} \int_0^{b_2} \int_0^{b_3} \phi(x,y,z) V_{ijk} dxdydz \; .$$

Using the initial condition (4.5.2) and (4.5.21) we get

$$A_{ijk} = \phi_{ijk}$$

Substitution gives

$$u(x,y,z,t) = \sum_{i,j,k=1}^{\infty} \phi_{ijk} \, e^{-c^2 \lambda_{ijk} t} V_{ijk}(x,y,z) \; , \tag{4.5.22}$$

the general solution of (4.5.1)- (4.5.3).

4.6 IBVP for a Non-Homogeneous 3D Heat-Diffusion Equation with Mixed Boundary Condition

Let $(x,y,z) \in \mathbb{R}^3$, $t \in \mathbb{R}$,$D = \{(x,y,z) \in \mathbb{R}^3 : 0 \le x \le b_1, 0 \le y \le b_2, 0 \le z \le b_3\}$ be a homogeneous parallelepiped. Let us consider the IBVP for the diffusion equation in the parallelepiped D :

$$\begin{aligned} \frac{1}{c^2} \frac{\partial u(x,y,z,t)}{\partial t} &= \Delta_{x,y,z} u(x,y,z,t) + F(x,y,z,t) \; , \\ & \quad (x,y,z) \in D, \quad t \ge 0 \; , && (4.6.1) \\ u(x,y,z,0) &= \phi(x,y,z) \; , && (4.6.2) \\ \left(\frac{\partial u}{\partial \eta} + \alpha \, u \right) \Big|_{\partial D} &= 0 \; , && (4.6.3) \end{aligned}$$

where ∂D is the boundary of D. Here $F(x,y,z,t)$ and $\phi(x,y,z)$ are given functions in $D \cup \partial D$, c is a positive constant. IBVP consists of finding $u(x,y,z,t)$ satisfying (4.6.1)-(4.6.3).

Using the same techniques from the previous sections for non-homogeneous problem with the Dirichlet and Neumann boundary conditions and homogeneous problem for Mixed boundary condition we will get the following result

$$T_{ijk}(t) = \phi_{ijk} e^{-c^2 \lambda_{ijk} t} + c^2 \int_0^t F_{ijk}(\tau) e^{-c^2 \lambda_{ijk}(t-\tau)} d\tau \ , \tag{4.6.4}$$

and

$$u(x, y, z, t) = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \sum_{k=1}^{\infty} T_{ijk}(t) V_{ijk}(x, y, z) \ , \tag{4.6.5}$$

is the solution of (4.6.1)-(4.6.3), where $T_{ijk}(t)$ is defined in (4.6.4) and $V_{ijk}(x, y, z)$ is defined in (4.5.17).

4.7 Examples of simulations for Heat-Diffusion equation with Mixed B.C. (1-D, 2-D, 3-D cases)

This section contains some examples of modeling and simulations of the diffusion processes in 1-D, 2-D and 3-D bounded domains. IBVP for heat equation with the Mixed boundary condition on a string, in a rectangle and in a parallelepiped will be used for modeling and simulations. We took a pulse point source concentrated in different points in these domains: in the center, near the boundary, in the corner.

4.7.1 1-D Heat-Diffusion equation

In this case we have a string on $[0, 6]$.

Example 4.7.1. Let us consider the problem (4.2.1)-(4.2.3). The functions $\phi(x)$ and $F(x,t)$ are given by

$$\phi(x) = 0 \ ,$$

$$F(x,t) = \delta(x - x_0)\delta(t) \ , x_0 \in [0, \ell] \ ,$$

where $\delta(x)$ is the Dirac delta function. Using formulas for $\phi(x)$ and $F(x,t)$ and the properties of the Dirac delta function the solution of the problem (4.2.1)-(4.2.3) can be found by the following formula

$$u(x,t) = \sum_{i=1}^{\infty} T_i(t) X_i(x) \ , \tag{4.7.1}$$

where

$$T_i(t) = c^2 \int_0^t F_i(\tau) e^{-c^2\lambda_i(t-\tau)} d\tau \ ,$$

$$F_i(t) = X_i(x_0)\delta(t) \ .$$

Hence

$$T_i(t) = c^2 e^{-c^2\lambda_i t} X_i(x_0) \ ,$$

and λ_i and $X_i(x)$ are defined in (4.1.13), (4.1.12).

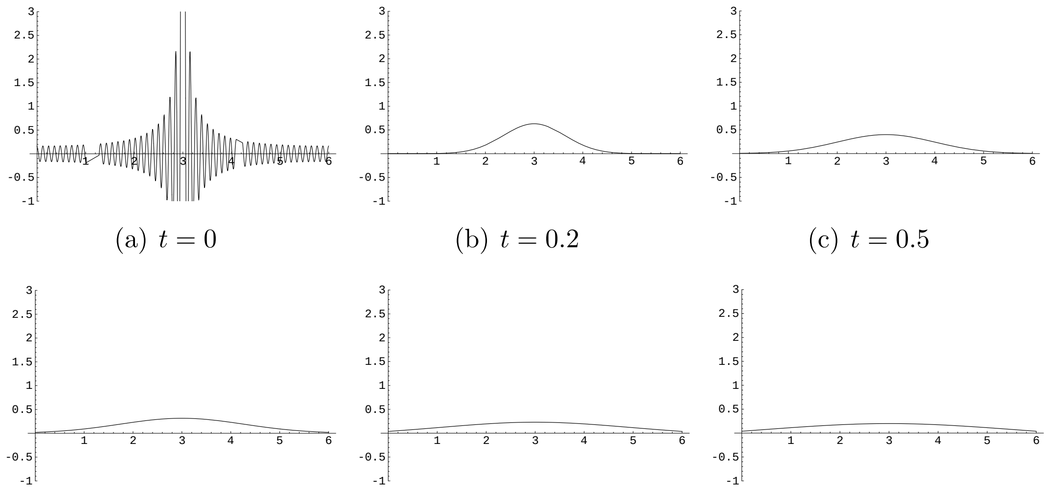
For the given data of Example 4.7.1, we used Mathematica codes in order to find the solution and to animate. The exact solution (4.7.1) is given by the series containing infinite number of terms. We found an approximate solution by means of the formula

$$u(x,t) = c^2 \sum_{i=1}^{n} T_i(t) X_i(x) \; , \tag{4.7.2}$$

where $n = 20$. This number n is chosen by considering the theoretical evaluation of the general term of the series (4.7.2) and the numerical experiments. We will consider each case for the function (4.7.2).

4.7.1.1 Simulations of 1-D Heat-Diffusion equation with Mixed B.C

Using the formula (4.7.2) for $n = 20$ and Mathematica codes we simulated the diffusion processes from the pulse point source which is located in the center of the domain D. The simulations for different times shown in figures below.



(a) $t = 0$ (b) $t = 0.2$ (c) $t = 0.5$

(d) $t = 0.8$ (e) $t = 1.5$ (f) $t = 2.0$

Figure 4.14: Example 4.7.1: The source in the center of the bounded domain with Mixed B.C.

In the non-homogeneous problem we have extra c^2 and it only changes the range of the solution. For $c = 1$ the homogeneous and the non-homogeneous problems have the same solutions.

4.7.2 2-D Heat-Diffusion equation

In this case we have a rectangle $D = ([0,6] \times [0,12])$.

Example 4.7.2. Let us consider the problem (4.4.1)-(4.4.3). The functions $\phi(x,y)$ and $F(x,y,t)$ are given by

$$\phi(x,y) = 0 \ ,$$

$$F(x,y,t) = \delta(x-x_0)\delta(y-y_0)\delta(t) \ , (x_0,y_0) \in D \ ,$$

where $\delta(x)$ is the Dirac delta function. Using formulas for $\phi(x,y)$ and $F(x,y,t)$ and the properties of the Dirac delta function the solution of the problem (4.4.1)-(4.4.3) can be found by the following formula

$$u(x,y,t) = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty} T_{ij}(t)V_{ij}(x,y) \ , \tag{4.7.3}$$

where

$$T_{ij}(t) = c^2 \int_0^t F_{ij}(\tau)e^{-c^2\lambda_{ij}(t-\tau)}d\tau \ ,$$

and

$$F_{ij}(t) = V_{ij}(x_0,y_0)\delta(t) \ .$$

Hence

$$T_{ij}(t) = c^2 e^{-c^2\lambda_{ij}t}V_{ij}(x_0,y_0) \ ,$$

and λ_{ij} and $V_{ij}(x,y)$ are defined in (4.3.16), (4.3.15). For this example consider the different positions of (x_0,y_0) (the point in which the pulse point source is concentrated). These positions (x_0,y_0) are given in the following table

	(x_0,y_0)
Case 1	(3,6)
Case 2	(3,11)
Case 3	(1,11)

Table 4.3: Positions of sources in a rectangle D with the Mixed B.C.

For the given data of Example 4.7.2, we used Mathematica codes in order to find the solution and to animate for each cases. The exact solution (4.7.3) is given by the series containing infinite number of terms. We found an approximate solution by means of the formula

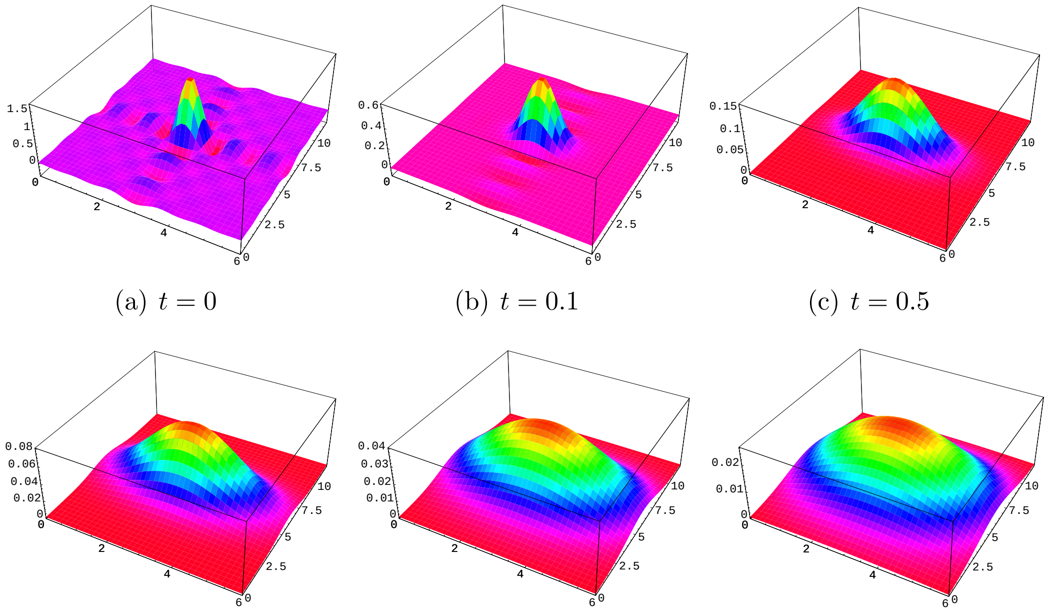
$$u(x, y, t) = c^2 \sum_{i=1}^{n} \sum_{j=1}^{n} T_{ij}(t) V_{ij}(x, y) \ , \tag{4.7.4}$$

where $n = 20$. This number n is chosen by considering the theoretical evaluation of the general term of the series (4.7.4) and the numerical experiments. We will consider each case for the function (4.7.4).

4.7.3 Simulation Examples

4.7.3.1 Simulation for Case1

Using the formula (4.7.4) for $n = 20$ and Mathematica codes we simulated the diffusion processes from the pulse point source which is located in the center of the domain D. The simulations for different times shown in figures below.



(a) $t = 0$ (b) $t = 0.1$ (c) $t = 0.5$

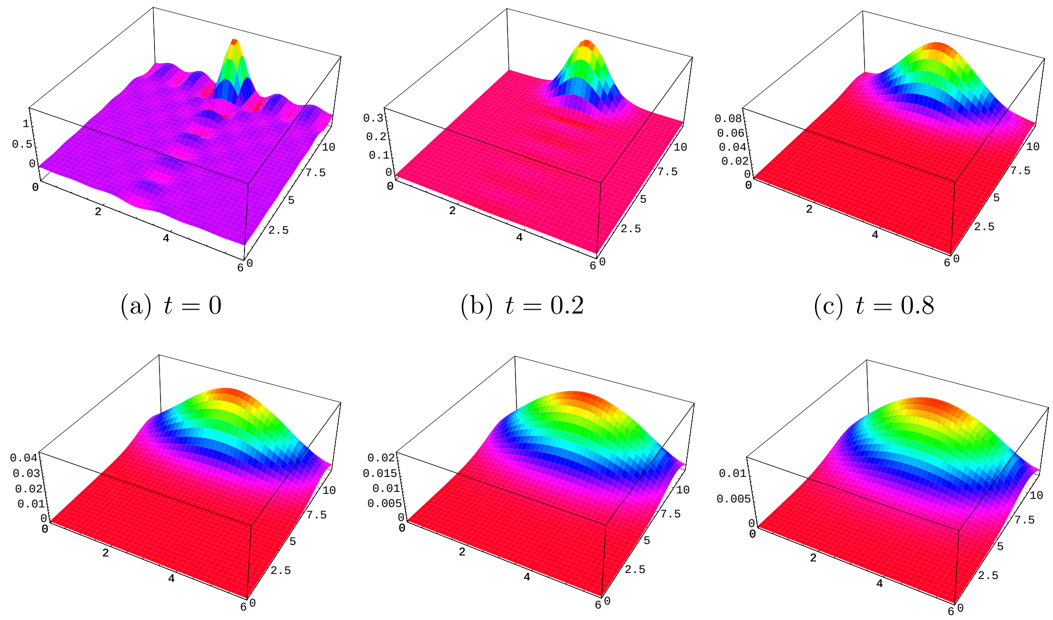
(d) $t = 1.0$ (e) $t = 2.0$ (f) $t = 3.0$

Figure 4.15: Example 4.7.2: The source in the center of the rectangle with Mixed B.C.

In the non-homogeneous problem we have extra c^2 and it only changes the range of the solution. For $c = 1$ the homogeneous and the non-homogeneous problems have the same solutions.

4.7.3.2 Simulation for Case2

The result of the simulation corresponding to Case 2 (the position of the source is near the boundary) is presented on the figure 4.16 (a)-(f).



(a) $t = 0$ (b) $t = 0.2$ (c) $t = 0.8$

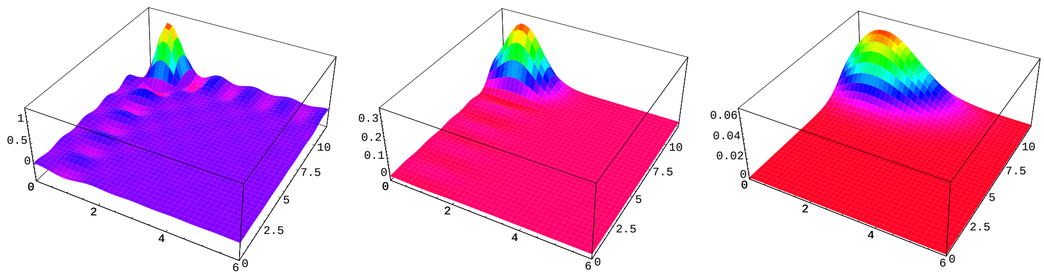
(d) $t = 1.4$ (e) $t = 1.5$ (f) $t = 3.5$

Figure 4.16: Example 4.7.2: Source near the boundary of the rectangle with Mixed B.C.

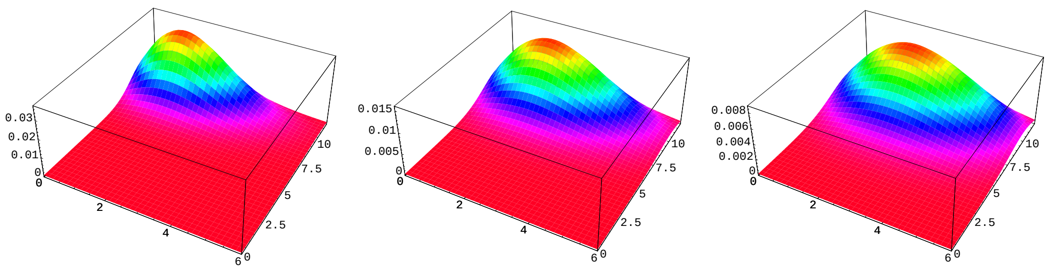
In the non-homogeneous problem we have extra c^2 and it only changes the range of the solution. For $c = 1$ the homogeneous and the non-homogeneous problems have the same solutions.

4.7.3.3 Simulation for Case3

The result of the simulation corresponding to Case 3 (the position of the source is near the corner) is presented on the figure 4.17 (a)-(f).



(a) $t = 0$ (b) $t = 0.2$ (c) $t = 1.0$



(d) $t = 1.5$ (e) $t = 2.5$ (f) $t = 3.5$

Figure 4.17: Example 4.7.2: Source near the corner of the rectangle with Mixed B.C.

In the non-homogeneous problem we have extra c^2 and it only changes the range of the solution. For $c = 1$ the homogeneous and the non-homogeneous problems have the same solutions.

4.7.4 3-D Heat-Diffusion equation

In this case we have a parallelepiped $D = ([0,6] \times [0,12] \times [0,3])$

Example 4.7.3. Let us consider the problem (4.6.1)-(4.6.3). The functions $\phi(x,y,z)$ and $F(x,y,z,t)$ are given by

$$\phi(x,y,z) = 0 \ ,$$

$$F(x,y,z,t) = \delta(x-x_0)\delta(y-y_0)\delta(z-z_0)\delta(t) \ , (x_0,y_0,z_0) \in D \ ,$$

where $\delta(x)$ is the Dirac delta function. Using formulas for $\phi(x,y,z)$ and $F(x,y,z,t)$ and the properties of the Dirac delta function the solution of the problem (4.6.1)-(4.6.3) can be found by the following formula

$$u(x,y,z,t) = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\sum_{k=1}^{\infty} T_{ijk}(t)V_{ijk}(x,y,z) \ , \qquad (4.7.5)$$

where

$$T_{ijk}(t) = c^2 \int_0^t F_{ijk}(\tau)e^{-c^2\lambda_{ijk}(t-\tau)}d\tau \ ,$$

and

$$F_{ijk}(t) = V_{ijk}(x_0,y_0)\delta(t) \ .$$

Hence

$$T_{ijk}(t) = c^2 e^{-c^2\lambda_{ijk}t}V_{ijk}(x_0,y_0) \ ,$$

and λ_{ijk} and $V_{ijk}(x,y,z)$ are defined in (4.5.18), (4.5.17). For this example consider the different positions of (x_0,y_0,z_0) (the point in which the pulse point source is concentrated). These positions (x_0,y_0,z_0) are given in the following table

	(x_0,y_0,z_0)
Case 1	(3,6,2)
Case 2	(3,11,2)
Case 3	(1,11,2)

Table 4.4: Positions of sources in a parallelepiped D with the Mixed B.C.

For the given data of Example 4.7.4, we used Mathematica codes in order to find the solution and to animate for each cases. The exact solution (4.7.5) is given by the series containing infinite number of terms. We found an approximate solution by means of the formula

$$u(x,y,z,t) = c^2 \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} T_{ijk}(t) V_{ijk}(x,y,z) \; , \tag{4.7.6}$$

where $n = 20$. This number n is chosen by considering the theoretical evaluation of the general term of the series (4.7.6) and the numerical experiments. We will consider each case for the function (4.7.6).

4.7.4.1 Commands in Mathematica for Example 4.7.4 :

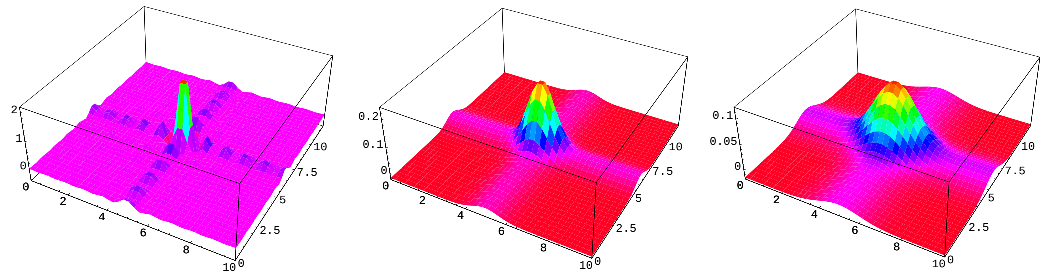
```
 << Graphics‘Animation‘
 bx = 6; by = 12; bz = 3; (dimension of the parallelepiped)
 x0 = 3; y0 = 6; z0 = 2; (the position of the source where
it is located)
 n:=20; (number of terms in the sum)
 sc:=1; (the speed of propagation)
 Alpha := 2;

 For[i = 0, i <= n, i++,
   R[i] = FindRoot[Cot[r[i]*bx] == (1/2)*(r[i]/Alpha - Alpha/r[i]),
     {r[i], 0.001 + i*Pi/bx}];
                       e1[i] = r[i] /. R[i];
 Nrm[i] =(1/Integrate[(Cos[e1[i]*x + ArcCot[-e1[i]/Alpha]])^2,
 {x, 0, bx}])^(1/2);
   X[i] = Nrm[i]*Cos[e1[i]*x + ArcCot[-e1[i]/Alpha]]; ]

 For[j = 0, j <= n, j++,
   R[j] = FindRoot[Cot[r[j]*by] == (1/2)*(r[j]/Alpha - Alpha/r[j]),
     {r[j], 0.001 + j*Pi/by}];
                       e2[j] = r[j] /. R[j];
 Nrm[j] = (1/Integrate[(Cos[e2[j]*y + ArcCot[-e2[j]/Alpha]])^2,
 {y, 0, by}])^(1/2);
   Y[j] = Nrm[j]*Cos[e2[j]*y + ArcCot[-e2[j]/Alpha]];]

 For[k = 0, k <= n, k++,
   R[k] = FindRoot[ Cot[r[k]*bz] == (1/2)*(r[k]/Alpha - Alpha/r[k]),
     {r[k], 0.001 + k*Pi/bz}];
                       e3[k] = r[k] /. R[k];
 Nrm[k] = (1/Integrate[(Cos[e3[k]*z + ArcCot[-e3[k]/Alpha]])^2,
 {z, 0, bz}])^(1/2);
 Z[k] = Nrm[k]*Cos[e3[k]*z + ArcCot[-e3[k]/Alpha]];]
 For[i = 0, i <= n, i++,
    For[j = 0, j <= n, j++,
       For[k = 0, k <= n, k++,
    Lambda[i, j, k] = (e1[i]^2) + (e2[j]^2) + (e3[k]^2);
```

```
    V[i, j, k] = X[i]*Y[j]*Z[k];
    Apsi[i, j, k] =ReplaceAll[ReplaceAll[ReplaceAll[V[i, j, k],
    x -> x0], y -> y0], z -> z0];
  T[i, j, k] = Apsi[i, j, k]*e^((sc^2)*(-Lambda[i, j, k]*t))
  ];];]

son := Sum[Sum[Sum[T[i, j, k]*V[i, j, k], {i, 0, n}]
, {j, 0, n}], {k, 0, n}]

fixing parameter z=1
son2 = ReplaceAll[son, z -> 1];

(animating the picture w.r.t time variable with sitep size 0.25)
Animate[Plot3D[son2, {x, 0, 6}, {y, 0, 12}, ColorFunction
 -> (Hue[1 - #] &),PlotRange -> All, AspectRatio -> Automatic,
Mesh -> False,PlotPoints -> 40], {t, 0, 34, 0.5}]
```

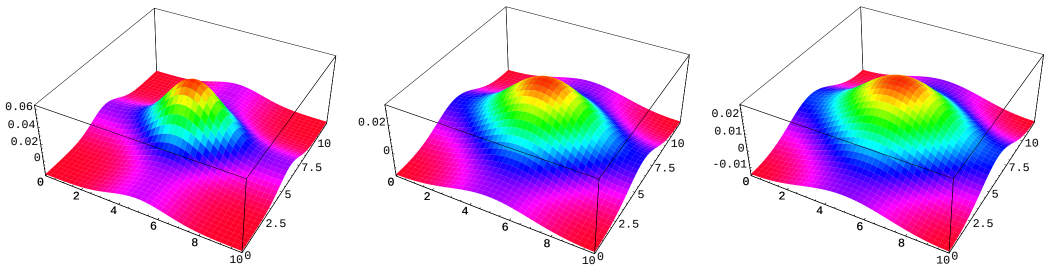
4.7.5 Simulation Examples

4.7.5.1 Simulation for Case1

Using the formula (4.7.6) for $n = 20$ and Mathematica codes we simulated the diffusion processes from the pulse point source which is located in the center of the domain D. The simulations for different times shown in figures below.



(a) $t = 0$ (b) $t = 0.2$ (c) $t = 0.5$



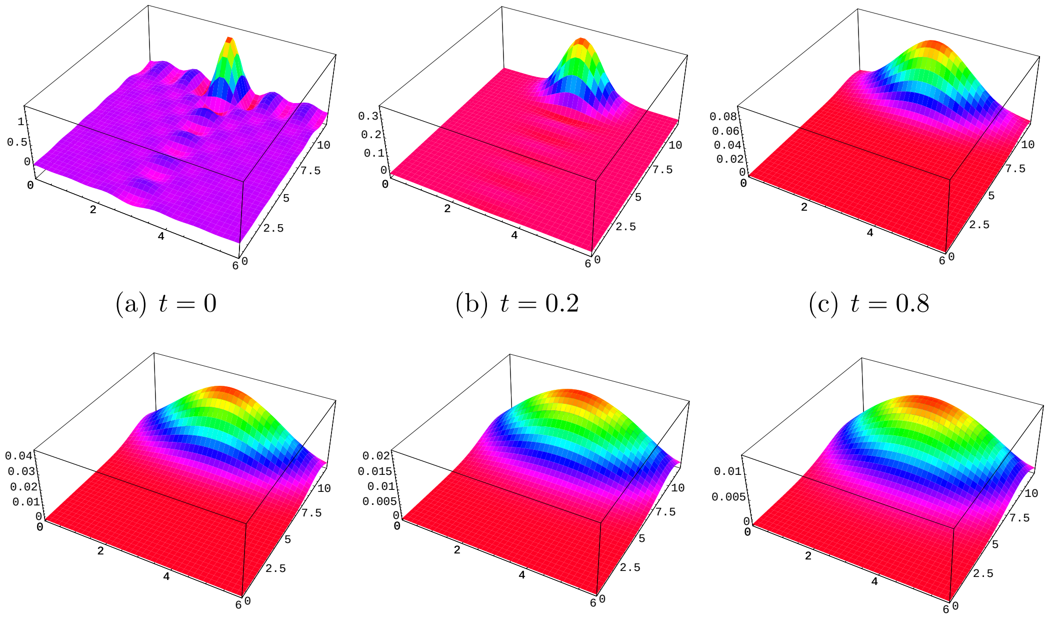
(d) $t = 1.0$ (e) $t = 2.0$ (f) $t = 2.5$

Figure 4.18: Example 4.7.4: The source in the center of the bounded domain for non-homogeneous problem .

In the non-homogeneous problem we have extra c^2 and it only changes the range of the solution. For $c = 1$ the homogeneous and the non-homogeneous problems have the same solutions.

4.7.5.2 Simulation for Case2

The result of the simulation corresponding to Case 2 (the position of the source is near the boundary) is presented on the figure 4.19 (a)-(f).



(a) $t = 0$ (b) $t = 0.2$ (c) $t = 0.8$

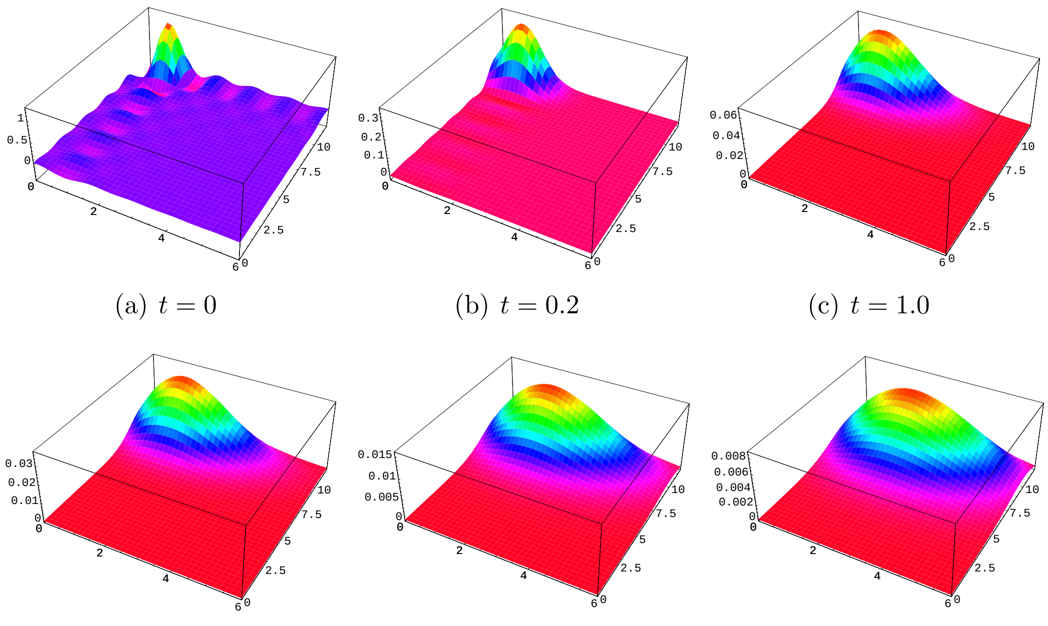
(d) $t = 1.4$ (e) $t = 1.5$ (f) $t = 3.5$

Figure 4.19: Example 4.7.4: Source near the boundary of the bounded domain D .

In the non-homogeneous problem we have extra c^2 and it only changes the range of the solution. For $c = 1$ the homogeneous and the non-homogeneous problems have the same solutions.

4.7.5.3 Simulation for Case3

The result of the simulation corresponding to Case 3 (the position of the source is near the corner) is presented on the figure 4.20 (a)-(f).



(a) $t = 0$ (b) $t = 0.2$ (c) $t = 1.0$

(d) $t = 1.5$ (e) $t = 2.5$ (f) $t = 3.5$

Figure 4.20: Example 4.7.4: Source near the corner of the bounded domain D .

In the non-homogeneous problem we have extra c^2 and it only changes the range of the solution. For $c = 1$ the homogeneous and the non-homogeneous problems have the same solutions.

4.8 Analysis of the chapter4 study

1. Exact and approximate formulae for the solutions of IBVPs with mixed boundary condition for the diffusion (heat) equations on a string, in a rectangle and in a parallelepiped were obtained.

2. These formulae were adjusted to cases when initial data or inhomogeneous term are the Dirac delta function with a support in a point which is inside the domain D. The pulse point source is modeled by these initial data and in homogeneous term.

3. Obtained formulae for generalized solutions of IBVPs for the heat-diffusion equations were used for modeling and simulations of diffusion processes in bounded domain D arising from the pulse point sources.

4. Results of diffusion processes simulation are presented by 1-D, 2-D and 3-D pictures and animated movies.

5. Obtained formulae and results of simulation were analyzed. The behavior of the boundary due to the Mixed boundary condition was seen.

CHAPTER FIVE
GREEN'S FUNCTION OF IBVP FOR HEAT-DIFFUSION EQUATION

In this section IBVP for 1D, 2D and 3D heat(diffusion) equation with Dirichlet Boundary condition in a homogeneous strip, rectangle and parallelepiped will be studied. Green's function method will be used in this section and some important definitions will be given in Appendix. The formulaes will be generated and using these formulaes simulations will be found.

5.1 Generalized IBVP for 1D Heat-Diffusion Equation

Let $x \in \mathbf{R}$, $t \in \mathbf{R}$;

$$L_c = \left(\frac{1}{c^2}\frac{\partial}{\partial t} - \frac{\partial^2}{\partial x^2}\right) \ ,$$

is the heat operator, c is a given positive constant.

Definition 5.1.1. The space $\mathfrak{D}'(U)$ of distributions on U is defined to be the continuous linear dual of $C_c^\infty(U)$; i.e., the space of continuous linear functionals $C_c^\infty(U) \to C$

Definition 5.1.2. (Generalized IBVP for the heat equation) Let

$$L_c u(x,t) = f(x,t), \ t > 0, \ x \in D\,, \tag{5.1.1}$$

$$u(x,+0) = g(x), \ x \in D\,, \tag{5.1.2}$$

$$u(x,t)|_{x \in D} = 0\,, \tag{5.1.3}$$

where $f(x,t) \in \mathfrak{D}'(D \times (0,\infty))$, $g(x) \in \mathfrak{D}'(D)$ are given generalized functions. The problem (5.1.1)-(5.1.3) is called a generalized IBVP for the heat equation with the Dirichlet boundary condition.

Lemma 5.1.1. *Let $u(x,t)$ be a solution of the problem (5.1.1)-(5.1.3) then*

$$v(x,t) = \theta(t)u(x,t) \ ,$$

is a solution of the following problem

$$L_c v(x,t) = F(x,t), \ t > 0, \ x \in D\,, \tag{5.1.4}$$

$$v(x,t)|_{t<0} = 0\,, \tag{5.1.5}$$

$$v(x,t)|_{x\in\partial D} = 0\,, \tag{5.1.6}$$

where

$$F(x,t) = \frac{1}{c^2}\delta(t)u(x,t) + \theta(t)f(x,t)\ ,$$

$\theta(t)$ is the Heaviside function, $\delta(t)$ is the Dirac delta function.

Proof. Substituting $v(x,t)$ into (5.1.4)-(5.1.6), we have

$$v_t(x,t) = \frac{d}{dt}\theta(t)u(x,t) + \theta(t)\frac{\partial}{\partial t}u(x,t)$$

$$= \delta(t)u(x,t) + \theta(t)\frac{\partial}{\partial t}u(x,t)$$

And also
$$\frac{\partial^2}{\partial x^2}v(x,t) = \frac{\partial^2}{\partial x^2}(\theta(t)u(x,t)) = \theta(t)\frac{\partial^2}{\partial x^2}u(x,t)\ .$$

Thus
$$L_c v(x,t) = \frac{1}{c^2}v_t(x,t) - \frac{\partial^2}{\partial x^2}v(x,t)$$

$$= \frac{1}{c^2}\delta(t)u(x,t) + \frac{1}{c^2}\theta(t)\frac{\partial}{\partial t}u(x,t) - \theta(t)\frac{\partial^2}{\partial x^2}u(x,t)$$

$$= \frac{1}{c^2}\delta(t)u(x,t) + \theta(t)\left(\frac{1}{c^2}\frac{\partial}{\partial t}u(x,t) - \frac{\partial^2}{\partial x^2}u(x,t)\right)$$

Using (5.1.1) we have

$$L_c v(x,t) = \frac{1}{c^2}\delta(t)u(x,t) + \theta(t)f(x,t) = F(x,t)\ .$$

And since
$$\theta(t) = \begin{cases} 0 \quad , & t<0 \\ 1 \quad , & t \geq 0 \end{cases}\ ,$$

$$v(x,t)|_{t<0} = (\theta(t)u(x,t))_{t<0} = 0\,.$$

And
$$v(x,t)|_{x\in D} = (\theta(t)u(x,t))_{x\in D} = \theta(t)(u(x,t)_{x\in D}) = 0\,.$$

We showed that $v(x,t)$ satisfies also (5.1.5)-(5.1.6). The Lemma is proved. $\square$

5.2 Green's Function of IBVP for 1D Heat-Diffusion Equation with the Dirichlet Boundary Condition

Definition 5.2.1. Let $\xi \in D$, $\tau \in \mathbf{R}$ be parameters. A generalized function $G(x,t/\xi,\tau) \in \mathfrak{D}'(D \times R)$ is called the Green's function of the IBVP for the Heat-Diffusion operator L_c if

$$L_c G(x,t/\xi,\tau) = \delta(x-\xi, t-\tau),\ (x,t) \in D \times R\,, \tag{5.2.1}$$

$$G(x,t/\xi,\tau)|_{t<\tau} = 0,\ (x,t) \in D \times R\,, \tag{5.2.2}$$

$$G(x,t/\xi,\tau)|_{x\in\partial D} = 0,\ t \in \mathbf{R}\,, \tag{5.2.3}$$

Lemma 5.2.1. *Let $G(x,t/\xi,\tau)$ be Green's function of the IBVP for the Heat-Diffusion operator L_c and $F(x,t) \in \mathfrak{D}'(D\times R)$ is an arbitrary generalized function such as $F(x,t)|_{t<0}$. Then*

$$v(x,t) = \int_{-\infty}^{\infty}\int_0^b G(x,t/\xi,\tau)F(\xi,\tau)d\xi d\tau\,, \tag{5.2.4}$$

is a solution of the generalized IBVP (5.1.4)-(5.1.6).

Proof. Applying L_c to (5.2.4) we get

$$L_c v(x,t) = \int_{-\infty}^{\infty}\int_0^b L_c G(x,t/\xi,\tau)F(\xi,\tau)d\xi d\tau$$

$$= \int_{-\infty}^{\infty}\int_0^b \delta(x-\xi,t-\tau)F(\xi,\tau)d\xi d\tau = F(x,t)\,.$$

And also for $t<0$, we have

$$v(x,t)|_{t<0} = \int_{-\infty}^{\infty}\int_0^b G(x,t/\xi,\tau)|_{t<0}F(\xi,\tau)d\xi d\tau = 0\,,$$

and for $x \in D$

$$v(x,t)|_{x\in D} = \int_{-\infty}^{\infty}\int_0^b G(x,t/\xi,\tau)|_{x\in D}F(\xi,\tau)d\xi d\tau = 0\ .$$

So $v(x,t)$ is the solution of the generalized IBVP (5.1.4)-(5.1.6). $\square$

5.3 Construction of Green's Function by a Fourier Series Expansion

Let ξ be a parameter from D, τ be a parameter from $(0,\infty)$, $D = \{x \in \mathbf{R} : 0 \le x \le b\}$ be a string. Let us consider the IBVP in the string D :

$$L_c G(x,t/\xi,\tau) = \delta(x-\xi, t-\tau),\ (x,t) \in D \times R\,, \tag{5.3.1}$$

$$G(x,t/\xi,\tau)|_{t<\tau} = 0,\ (x,t) \in D \times R\,, \tag{5.3.2}$$

$$G(x,t/\xi,\tau)|_{x\in\partial D} = 0,\ t \in \mathbf{R}\,, \tag{5.3.3}$$

where

$$L_c = \left(\frac{1}{c^2}\frac{\partial}{\partial t} - \Delta_x\right)\ .$$

The solution of (5.3.1)-(5.3.3) can be found by the fourier series expansion method. Using $\bar{t} = t - \tau$, (5.3.1)-(5.3.3) can be written in the form

$$L_c G = \delta(x-\xi, \bar{t}),\ (x,t) \in D \times R\,, \tag{5.3.4}$$

$$G|_{t<\tau} = 0,\ (x,t) \in D \times R\,, \tag{5.3.5}$$

$$G|_{x\in\partial D} = 0,\ t \in \mathbf{R}\,, \tag{5.3.6}$$

Using the reasoning which we applied for the IBVP for a non-homogeneous Heat-Diffusion equation with the Dirichlet boundary condition we can write the solution of (5.3.4)-(5.3.6) as follows

$$G = \sum_{i=1}^{\infty}(c^2\delta_i\int_0^{\bar{t}} e^{-c^2\lambda_i(\bar{t}-\nu)}d\nu)V_i(x)\ , \tag{5.3.7}$$

where

$$\delta_i = \int_0^b \delta(x-\xi)\delta(\bar{t})V_i(\xi)dx = V_i(\xi)\delta(\bar{t})\ . \tag{5.3.8}$$

Using (5.3.8) the equation (5.3.7) can be written as

$$G = \sum_{i=1}^{\infty} c^2\theta(\bar{t})e^{-c^2\lambda_i\bar{t}}V_i(\xi)V_i(x)\ ,$$

where $\theta(\bar{t})$ is the Heaviside function. Replacing $\bar{t} = t - \tau$ we get

$$G = \sum_{i=1}^{\infty} c^2\theta(t-\tau)e^{-c^2\lambda_i(t-\tau)}V_i(\xi)V_i(x)\ .$$

The function is the solution of the generalized problem (5.3.1)-(5.3.3).

5.4 Generalized IBVP for 2D Heat-Diffusion Equation

Let $x = (x_1, x_2) \in \mathbf{R^2}$, $t \in \mathbf{R}$, $\Delta_x = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}$ is the Laplace operator;

$$L_c = \left(\frac{1}{c^2} \frac{\partial}{\partial t} - \Delta_x \right) ,$$

is the heat operator, c is a given positive constant.

Definition 5.4.1. The space $\mathfrak{D}'(U)$ of distributions on U is defined to be the continuous linear dual of $C_c^\infty(U)$; i.e., the space of continuous linear functionals $C_c^\infty(U) \to C$

Definition 5.4.2. (Generalized IBVP for the heat equation) Let

$$L_c u(x,t) = f(x,t),\ t > 0,\ x \in D\,, \tag{5.4.1}$$

$$u(x,+0) = g(x),\ x \in D\,, \tag{5.4.2}$$

$$u(x,t)|_{x \in D} = 0\,, \tag{5.4.3}$$

where $f(x,t) \in \mathfrak{D}'(D \times (0,\infty))$, $g(x) \in \mathfrak{D}'(D)$ are given generalized functions. The problem (5.4.1)-(5.4.3) is called a generalized IBVP for the heat equation with the Dirichlet boundary condition.

Lemma 5.4.1. *Let $u(x,t)$ be a solution of the problem (5.4.1)-(5.4.3) then*

$$v(x,t) = \theta(t) u(x,t) ,$$

is a solution of the following problem

$$L_c v(x,t) = F(x,t),\ t > 0,\ x \in D\,, \tag{5.4.4}$$

$$v(x,t)|_{t<0} = 0\,, \tag{5.4.5}$$

$$v(x,t)|_{x \in \partial D} = 0\,, \tag{5.4.6}$$

where

$$F(x,t) = \frac{1}{c^2} \delta(t) u(x,t) + \theta(t) f(x,t) ,$$

$\theta(t)$ is the Heaviside function, $\delta(t)$ is the Dirac delta function.

Proof. Substituting $v(x,t)$ into (5.4.4)-(5.4.6), we have

$$v_t(x,t) = \frac{d}{dt}\theta(t)u(x,t) + \theta(t)\frac{\partial}{\partial t}u(x,t)$$

$$= \delta(t)u(x,t) + \theta(t)\frac{\partial}{\partial t}u(x,t)$$

And also

$$\Delta_x v(x,t) = \Delta_x(\theta(t)u(x,t)) = \theta(t)\Delta_x u(x,t)\ .$$

Thus

$$L_c v(x,t) = \frac{1}{c^2}v_t(x,t) - \Delta_x v(x,t)$$

$$= \frac{1}{c^2}\delta(t)u(x,t) + \frac{1}{c^2}\theta(t)\frac{\partial}{\partial t}u(x,t) - \theta(t)\Delta_x u(x,t)$$

$$= \frac{1}{c^2}\delta(t)u(x,t) + \theta(t)\left(\frac{1}{c^2}\frac{\partial}{\partial t}u(x,t) - \Delta_x u(x,t)\right)$$

Using (5.4.1) we have

$$L_c v(x,t) = \frac{1}{c^2}\delta(t)u(x,t) + \theta(t)f(x,t) = F(x,t)\ .$$

And since

$$\theta(t) = \begin{cases} 0 \quad , & t < 0 \\ 1 \quad , & t \geq 0 \end{cases}\ ,$$

$$v(x,t)|_{t<0} = (\theta(t)u(x,t))_{t<0} = 0\,.$$

And

$$v(x,t)|_{x\in D} = (\theta(t)u(x,t))_{x\in D} = \theta(t)(u(x,t)_{x\in D}) = 0\,.$$

We showed that $v(x,t)$ satisfies also (5.4.5)-(5.4.6). The Lemma is proved. $\square$

5.5 Green's Function of IBVP for 2D Heat-Diffusion Equation with the Dirichlet Boundary Condition

Definition 5.5.1. Let $\xi \in D$, $\tau \in \mathbf{R}$ be parameters. A generalized function $G(x,t/\xi,\tau) \in \mathfrak{D}'(D \times R)$ is called the Green's function of the IBVP for the Heat-Diffusion operator L_c if

$$L_c G(x,t/\xi,\tau) = \delta(x-\xi, t-\tau),\ (x,t) \in D \times R\,, \tag{5.5.1}$$

$$G(x,t/\xi,\tau)|_{t<\tau} = 0,\ (x,t) \in D \times R\,, \tag{5.5.2}$$

$$G(x,t/\xi,\tau)|_{x\in\partial D} = 0,\ t \in \mathbf{R}\,. \tag{5.5.3}$$

Lemma 5.5.1. *Let $G(x,t/\xi,\tau)$ be Green's function of the IBVP for the Heat-Diffusion operator L_c and $F(x,t) \in \mathfrak{D}'(D\times R)$ is an arbitrary generalized function such as $F(x,t)|_{t<0}$. Then*

$$v(x,t) = \int_{-\infty}^{\infty}\int_0^{b_1}\int_0^{b_2} G(x,t/\xi,\tau)F(\xi,\tau)d\xi d\tau\,, \tag{5.5.4}$$

is a solution of the generalized IBVP (5.4.4)-(5.4.6).

Proof. Applying L_c to (5.5.4) we get

$$L_c v(x,t) = \int_{-\infty}^{\infty}\int_0^{b_1}\int_0^{b_2} L_c G(x,t/\xi,\tau)F(\xi,\tau)d\xi d\tau$$

$$= \int_{-\infty}^{\infty}\int_0^{b_1}\int_0^{b_2} \delta(x-\xi,t-\tau)F(\xi,\tau)d\xi d\tau = F(x,t)\,.$$

And also for $t<0$, we have

$$v(x,t)|_{t<0} = \int_{-\infty}^{\infty}\int_0^{b_1}\int_0^{b_2} G(x,t/\xi,\tau)|_{t<0}F(\xi,\tau)d\xi d\tau = 0\,,$$

and for $x \in D$

$$v(x,t)|_{x\in D} = \int_{-\infty}^{\infty}\int_0^{b_1}\int_0^{b_2} G(x,t/\xi,\tau)|_{x\in D}F(\xi,\tau)d\xi d\tau = 0\,.$$

So $v(x,t)$ is the solution of the generalized IBVP (5.4.4)-(5.4.6). □

5.6 Construction of Green's Function by a Fourier Series Expansion

Let $\xi = (\xi_1, \xi_2)$ be a parameter from D, τ be a parameter from $(0, \infty)$, $D = \{x = (x_1, x_2) \in \mathbf{R^2} : 0 \leq x_1 \leq b_1, 0 \leq x_2 \leq b_2\}$ be a rectangle. Let us consider the IBVP in the rectangle D :

$$L_c G(x, t/\xi, \tau) = \delta(x - \xi, t - \tau),\ (x, t) \in D \times R\,, \tag{5.6.1}$$

$$G(x, t/\xi, \tau)|_{t<\tau} = 0,\ (x, t) \in D \times R\,, \tag{5.6.2}$$

$$G(x, t/\xi, \tau)|_{x \in \partial D} = 0,\ t \in \mathbf{R}\,, \tag{5.6.3}$$

where

$$L_c = \left(\frac{1}{c^2} \frac{\partial}{\partial t} - \Delta_x \right) \,.$$

The solution of (5.6.1)-(5.6.3) can be found by the fourier series expansion method. Using $\bar{t} = t - \tau$, (5.6.1)-(5.6.3) can be written in the form

$$L_c G = \delta(x - \xi, \bar{t}),\ (x, t) \in D \times R\,, \tag{5.6.4}$$

$$G|_{t<\tau} = 0,\ (x, t) \in D \times R\,, \tag{5.6.5}$$

$$G|_{x \in \partial D} = 0,\ t \in \mathbf{R}\,. \tag{5.6.6}$$

Using the reasoning which we applied for the IBVP for a non-homogeneous Heat-Diffusion equation with the Dirichlet boundary condition we can write the solution of (5.6.4)-(5.6.6) as follows

$$G = \sum_{i,j=1}^{\infty} (c^2 \int_0^{\bar{t}} \delta_{ij} e^{-c^2 \lambda_{ij} (\bar{t} - \nu)} d\nu) V_{ij}(\xi_1, \xi_2) \ , \tag{5.6.7}$$

where

$$\delta_{ij} = \int_0^{b_1} \int_0^{b_2} \delta(x - \xi) \delta(\bar{t}) V_{ij}(\xi_1, \xi_2) dx_1 dx_2 = V_{ij}(x_1, x_2) \delta(\bar{t})\,. \tag{5.6.8}$$

Using (5.6.8) the equation (5.6.7) can be written as

$$G = \sum_{i,j=1}^{\infty} c^2 \theta(\bar{t}) e^{-c^2 \lambda_{ij} \bar{t}} V_{ij}(\xi_1, \xi_2) V_{ij}(x_1, x_2) \ ,$$

where $\theta(\bar{t})$ is the Heaviside function. Replacing $\bar{t} = t - \tau$ we get

$$G = \sum_{i,j=1}^{\infty} c^2 \theta(t-\tau) e^{-c^2 \lambda_{ij}(t-\tau)} V_{ij}(\xi_1, \xi_2) V_{ij}(x_1, x_2) \ .$$

The function is the solution of the generalized problem (5.6.1)-(5.6.3).

5.7 Generalized IBVP for 3D Heat-Diffusion Equation

Let $x = (x_1, x_2, x_3) \in \mathbf{R^3}$, $t \in \mathbf{R}$, $\Delta_x = \sum_{i=1}^{3} \frac{\partial^2}{\partial x_i^2}$ is the Laplace operator;

$$L_c = \left(\frac{1}{c^2} \frac{\partial}{\partial t} - \Delta_x \right) \ ,$$

is the heat operator, c is a given positive constant.

Definition 5.7.1. The space $\mathfrak{D}'(U)$ of distributions on U is defined to be the continuous linear dual of $C_c^\infty(U)$; i.e., the space of continuous linear functionals $C_c^\infty(U) \to C$

Definition 5.7.2. (Generalized IBVP for the heat equation) Let

$$L_c u(x,t) = f(x,t),\ t > 0,\ x \in D\,, \tag{5.7.1}$$

$$u(x, +0) = g(x),\ x \in D\,, \tag{5.7.2}$$

$$u(x,t)|_{x \in D} = 0\,, \tag{5.7.3}$$

where $f(x,t) \in \mathfrak{D}'(D \times (0, \infty))$, $g(x) \in \mathfrak{D}'(D)$ are given generalized functions. The problem (5.7.1)-(5.7.3) is called a generalized IBVP for the diffusion equation with the Dirichlet boundary condition.

Lemma 5.7.1. *Let $u(x,t)$ be a solution of the problem (5.7.1)-(5.7.3) then*

$$v(x,t) = \theta(t) u(x,t) \ ,$$

is a solution of the following problem

$$L_c v(x,t) = F(x,t),\ t > 0,\ x \in D\,, \tag{5.7.4}$$

$$v(x,t)|_{t<0} = 0\,, \tag{5.7.5}$$

$$v(x,t)|_{x \in \partial D} = 0\,, \tag{5.7.6}$$

where

$$F(x,t) = \frac{1}{c^2} \delta(t) u(x,t) + \theta(t) f(x,t) \ ,$$

$\theta(t)$ is the Heaviside function, $\delta(t)$ is the Dirac delta function.

Proof. Substituting $v(x,t)$ into (5.7.4)-(5.7.6), we have

$$v_t(x,t) = \frac{d}{dt}\theta(t)u(x,t) + \theta(t)\frac{\partial}{\partial t}u(x,t)$$

$$= \delta(t)u(x,t) + \theta(t)\frac{\partial}{\partial t}u(x,t)$$

And also

$$\Delta_x v(x,t) = \Delta_x(\theta(t)u(x,t)) = \theta(t)\Delta_x u(x,t)\ .$$

Thus

$$L_c v(x,t) = \frac{1}{c^2}v_t(x,t) - \Delta_x v(x,t)$$

$$= \frac{1}{c^2}\delta(t)u(x,t) + \frac{1}{c^2}\theta(t)\frac{\partial}{\partial t}u(x,t) - \theta(t)\Delta_x u(x,t)$$

$$= \frac{1}{c^2}\delta(t)u(x,t) + \theta(t)\left(\frac{1}{c^2}\frac{\partial}{\partial t}u(x,t) - \Delta_x u(x,t)\right)$$

Using (5.7.1) we have

$$L_c v(x,t) = \frac{1}{c^2}\delta(t)u(x,t) + \theta(t)f(x,t) = F(x,t)\ .$$

And since

$$\theta(t) = \begin{cases} 0 & , \quad t < 0 \\ 1 & , \quad t \geq 0 \end{cases} ,$$

$$v(x,t)|_{t<0} = \left(\theta(t)u(x,t)\right)_{t<0} = 0\,.$$

And

$$v(x,t)|_{x\in D} = \left(\theta(t)u(x,t)\right)_{x\in D} = \theta(t)(u(x,t)_{x\in D}) = 0\,.$$

We showed that $v(x,t)$ satisfies also (5.7.5)-(5.7.6). The Lemma is proved. $\square$

5.8 Green's Function of IBVP for 3D Heat-Diffusion Equation with the Dirichlet Boundary Condition

Definition 5.8.1. Let $\xi \in D$, $\tau \in \mathbf{R}$ be parameters. A generalized function $G(x,t/\xi,\tau) \in \mathfrak{D}'(D \times R)$ is called the Green's function of the IBVP for the Heat-Diffusion operator L_c if

$$L_c G(x,t/\xi,\tau) = \delta(x-\xi, t-\tau),\ (x,t) \in D \times R\,, \tag{5.8.1}$$

$$G(x,t/\xi,\tau)|_{t<\tau} = 0,\ (x,t) \in D \times R\,, \tag{5.8.2}$$

$$G(x,t/\xi,\tau)|_{x\in\partial D} = 0,\ t \in \mathbf{R}\,. \tag{5.8.3}$$

Lemma 5.8.1. *Let $G(x,t/\xi,\tau)$ be Green's function of the IBVP for the Heat-Diffusion operator L_c and $F(x,t) \in \mathfrak{D}'(D\times R)$ is an arbitrary generalized function such as $F(x,t)|_{t<0}$. Then*

$$v(x,t) = \int_{-\infty}^{\infty}\int_0^{b_1}\int_0^{b_2}\int_0^{b_3} G(x,t/\xi,\tau)F(\xi,\tau)d\xi d\tau\,, \tag{5.8.4}$$

is a solution of the generalized IBVP (5.7.4)-(5.7.6).

Proof. Applying L_c to (5.8.4) we get

$$L_c v(x,t) = \int_{-\infty}^{\infty}\int_0^{b_1}\int_0^{b_2}\int_0^{b_3} L_c G(x,t/\xi,\tau)F(\xi,\tau)d\xi d\tau$$

$$= \int_{-\infty}^{\infty}\int_0^{b_1}\int_0^{b_2}\int_0^{b_3} \delta(x-\xi,t-\tau)F(\xi,\tau)d\xi d\tau = F(x,t)\,.$$

And also for $t<0$, we have

$$v(x,t)|_{t<0} = \int_{-\infty}^{\infty}\int_0^{b_1}\int_0^{b_2}\int_0^{b_3} G(x,t/\xi,\tau)|_{t<0}F(\xi,\tau)d\xi d\tau = 0\,,$$

and for $x \in D$

$$v(x,t)|_{x\in D} = \int_{-\infty}^{\infty}\int_0^{b_1}\int_0^{b_2}\int_0^{b_3} G(x,t/\xi,\tau)|_{x\in D}F(\xi,\tau)d\xi d\tau = 0\,,$$

So $v(x,t)$ is the solution of the generalized IBVP (5.7.4)-(5.7.6). □

5.9 Construction of Green's Function by a Fourier Series Expansion

Let $\xi = (\xi_1, \xi_2, \xi_3)$ be a parameter from D, τ be a parameter from $(0, \infty)$, $D = \{x = (x_1, x_2, x_3) \in \mathbf{R^3} : 0 \leq x_1 \leq b_1, 0 \leq x_2 \leq b_2, 0 \leq x_3 \leq b_3\}$ be a parallelepiped. Let us consider the IBVP in the parallelepiped D :

$$L_c G(x, t/\xi, \tau) = \delta(x - \xi, t - \tau),\ (x, t) \in D \times R\,, \tag{5.9.1}$$

$$G(x, t/\xi, \tau)|_{t<\tau} = 0,\ (x, t) \in D \times R\,, \tag{5.9.2}$$

$$G(x, t/\xi, \tau)|_{x\in\partial D} = 0,\ t \in \mathbf{R}\,, \tag{5.9.3}$$

where

$$L_c = \left(\frac{1}{c^2}\frac{\partial}{\partial t} - \Delta_x\right)\ .$$

The solution of (5.9.1)-(5.9.3) can be found by the fourier series expansion method. Using $\bar{t} = t - \tau$, (5.9.1)-(5.9.3) can be written in the form

$$L_c G = \delta(x - \xi, \bar{t}),\ (x, t) \in D \times R\,, \tag{5.9.4}$$

$$G|_{t<\tau} = 0,\ (x, t) \in D \times R\,, \tag{5.9.5}$$

$$G|_{x\in\partial D} = 0,\ t \in \mathbf{R}\,. \tag{5.9.6}$$

Using the reasoning which we applied for the IBVP for a non-homogeneous Heat-Diffusion equation with the Dirichlet boundary condition we can write the solution of (5.9.4)-(5.9.6) as follows

$$G = \sum_{i,j,k=1}^{\infty} (c^2 \int_0^{\bar{t}} \delta_{ijk} e^{-c^2\lambda_{ijk}(\bar{t}-\nu)} d\nu) V_{ijk}(\xi_1, \xi_2, \xi_3)\ , \tag{5.9.7}$$

where

$$\delta_{ijk} = \int_0^{b_1}\int_0^{b_2}\int_0^{b_3} \delta(x - \xi)\delta(\bar{t}) V_{ijk}(\xi_1, \xi_2, \xi_3) dx_1 dx_2 dx_3\ ,$$

that is

$$\delta_{ijk} = V_{ijk}(x_1, x_2, x_3)\delta(\bar{t}), \tag{5.9.8}$$

Using (5.9.8) the equation (5.9.7) can be written as

$$G = \sum_{i,j,k=1}^{\infty} c^2\theta(\bar{t}) e^{-c^2\lambda_{ijk}\bar{t}} V_{ijk}(\xi_1, \xi_2, \xi_3) V_{ijk}(x_1, x_2, x_3)\ ,$$

where $\theta(\bar{t})$ is the Heaviside function. Replacing $\bar{t} = t - \tau$ we get

$$G = \sum_{i,j,k=1}^{\infty} c^2 \theta(t-\tau) e^{-c^2 \lambda_{ijk}(t-\tau)} V_{ijk}(\xi_1, \xi_2, \xi_3) V_{ijk}(x_1, x_2, x_3) \ .$$

The function is the solution of the generalized problem (5.9.1)-(5.9.3).

5.9.1 Examples of the simulation using Green's function

5.9.1.1 Commands in Mathematica for 3-D Case:

```
 << Graphics‘Animation‘
 bx = 6; by = 12; bz = 3; (dimension of the parallelepiped)
 x0 = 3; y0 = 6; z0 = 2; (the position of the source where
it is located)
 n:=20; (number of terms in the sum)
 sc:=1; (the speed of propagation)
 tau:=0;

 (eigenvalues)
 a[kk_] = (kk*Pi/bx)^2; b[kk_] = (kk*Pi/by)^2;
 c[kk_] = (kk*Pi/bz)^2;

 (computing the eigenfunctions and Fourier coefficients)
 For[i = 1, i <= n, i++,
  For[j = 1, j <= n, j++,
   For[k = 1, k <= n, k++,
        Lambda[i, j, k] = a[i] + b[j] + c[k];
        V[i, j, k] = Sqrt[8/(bx*by*bz)]*Sin[Sqrt[a[i]]*x]
 *Sin[Sqrt[b[j]]*y]*Sin[Sqrt[c[k]]*z];
 d[i, j, k] =ReplaceAll[ReplaceAll[ReplaceAll[V[i, j, k]
 , x -> x0], y -> y0], z -> z0];
 T[i, j, k] = d[i, j, k]*e^((sc^2)*(-Lambda[i, j, k]*(t-tau)))
 ];];]

 (computing the sum)
```

```
G := Sum[Sum[Sum[T[i, j, k]*V[i, j, k], {i, 1, n}]
, {j, 1, n}], {k, 1, n}]

fixing parameter z=1
G2 = ReplaceAll[son, z -> 1];

(animating the picture w.r.t time variable with sitep size 0.25)
Animate[Plot3D[G2, {x, 0, 6}, {y, 0, 12}, ColorFunction
 -> (Hue[1 - #] &),PlotRange -> All, AspectRatio -> Automatic,
Mesh -> False,PlotPoints -> 40], {t, 0, 34, 0.5}]
```

5.9.1.2 For 1-D Case

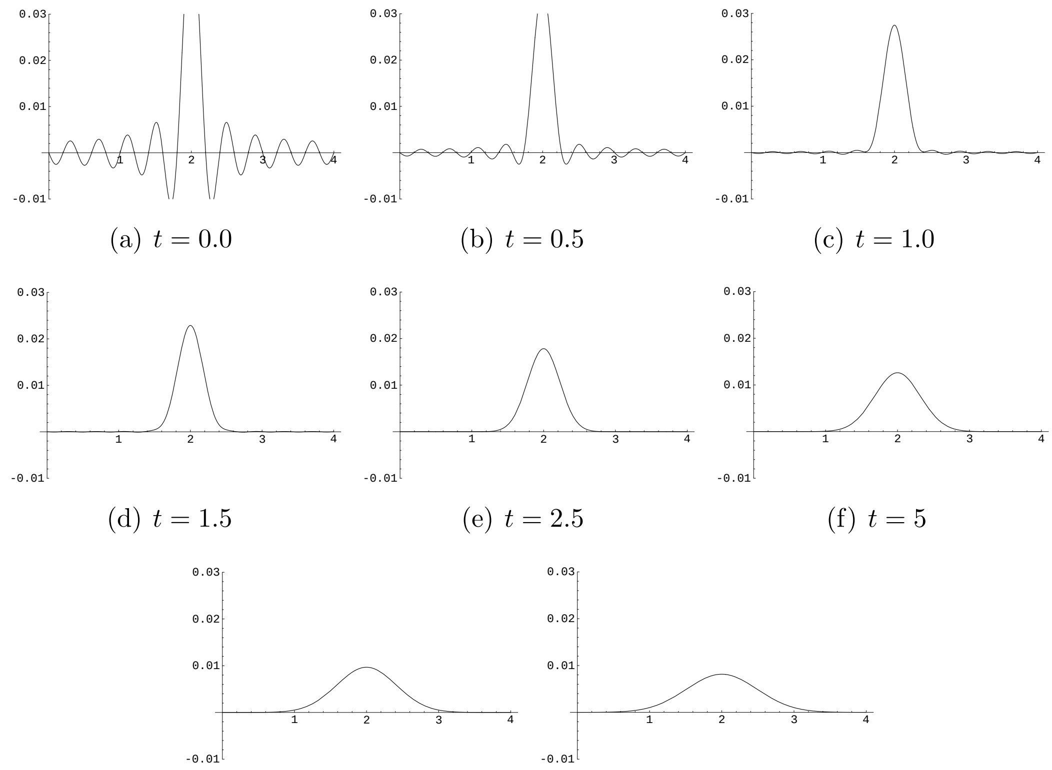
This section deals with modeling and the simulation of diffusion processes by Green's function. We have the formula for the Green's function of the form

$$G = \sum_{i=1}^{\infty} c^2 \theta(t-\tau) e^{-c^2 \lambda_i (t-\tau)} V_i(\xi) V_i(x), \tag{5.9.9}$$

where

$$\theta(t-\tau) = \begin{cases} 0 \quad , & t < \tau \\ 1 \quad , & t \geq \tau \end{cases},$$

ξ is the position of the pulse point source, x is the space variable, τ is the time when the pulse point source starts to act. For $c = 0.1$ we have the following pictures



(a) $t = 0.0$ (b) $t = 0.5$ (c) $t = 1.0$

(d) $t = 1.5$ (e) $t = 2.5$ (f) $t = 5$

(g) $t = 8.5$ (h) $t = 12.5$

Figure 5.21: Simulation of the Heat-Diffusion by using Green's function for 1-D in a bounded domain.

We can see in the pictures that for $\tau = 0$, $c = 1$ and $n = 20$ we get directly the same pictures in the Chapter2 (Dirichlet B.C.) for 1-D case.

5.9.1.3 For 2-D Case

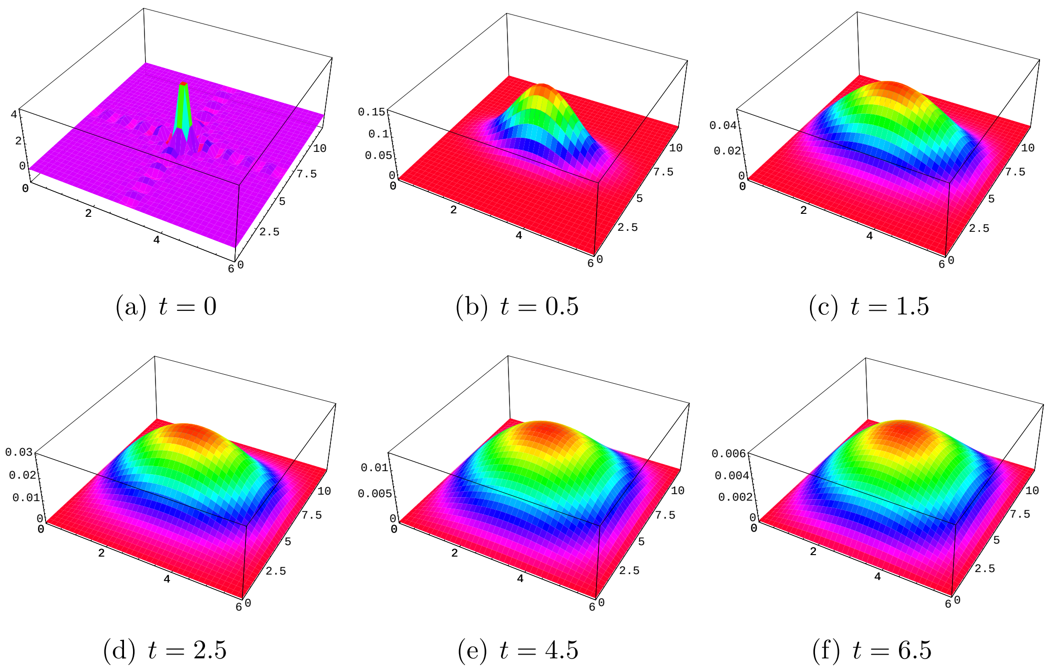
This section deals with modeling and the simulation of Heat-Diffusion equation by Green's function. We have the formula for the Green's function of the form

$$G = \sum_{i,j=1}^{\infty} c^2 \theta(t-\tau) e^{-c^2 \lambda_{ij}(t-\tau)} V_{ij}(\xi) V_{ij}(x), \tag{5.9.10}$$

where

$$\theta(t-\tau) = \begin{cases} 0 \quad , & t < \tau \\ 1 \quad , & t \geq \tau \end{cases} ,$$

$\xi = (\xi_1, \xi_2)$ is the position of the pulse point source, $x = (x_1, x_2)$ is the space variable, τ is the time when the pulse point source starts to act.



(a) $t = 0$ (b) $t = 0.5$ (c) $t = 1.5$

(d) $t = 2.5$ (e) $t = 4.5$ (f) $t = 6.5$

Figure 5.22: Simulation of the Heat-Diffusion by using Green's function for 2-D in a bounded domain.

We can see in the pictures that for $\tau = 0$, $c = 1$ and $n = 20$ we get directly the same pictures in the Chapter2 (Dirichlet B.C.) for 2-D case.

5.9.1.4 For 3-D Case

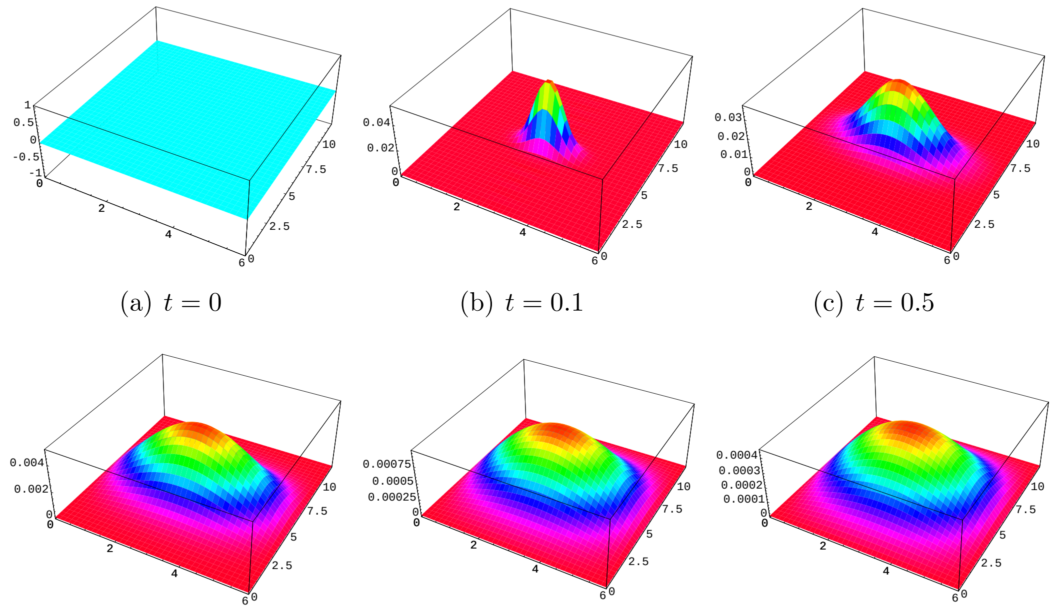
This section deals with modeling and the simulation of Heat-Diffusion equation by Green's function. We have the formula for the Green's function of the form

$$G = \sum_{i,j,k=1}^{\infty} c^2 \theta(t-\tau) e^{-c^2 \lambda_{ijk}(t-\tau)} V_{ijk}(\xi) V_{ijk}(x), \tag{5.9.11}$$

where

$$\theta(t-\tau) = \begin{cases} 0 \quad , & t < \tau \\ 1 \quad , & t \geq \tau \end{cases} ,$$

$\xi = (\xi_1, \xi_2, \xi_3)$ is the position of the pulse point source, $x = (x_1, x_2, x_3)$ is the space variable, τ is the time when the pulse point source starts to act. We can



(a) $t = 0$ (b) $t = 0.1$ (c) $t = 0.5$

(d) $t = 1.5$ (e) $t = 2.5$ (f) $t = 3.0$

Figure 5.23: Simulation of the Heat-Diffusion by using Green's function for 3-D in a bounded domain.

see in the pictures that for $\tau = 0$, $c = 1$ and $n = 20$ we get directly the same pictures in the Chapter2 (Dirichlet B.C.) for 3-D case.

5.10 Analysis of the chapter5 study

1. Exact and approximate formulae for the solutions of IBVPs with Dirichlet boundary condition for the diffusion (heat) equation on a string, in a rectangle and in a parallelepiped were obtained by using Green's function method.

2. These formulae were adjusted to cases when initial data or inhomogeneous term are the Dirac delta function and Heaviside function with a support in a point center the bounded domain D.

3. Obtained formulae for generalized solutions of IBVPs for the heat-diffusion equations were used for modeling and simulations of diffusion processes in bounded domain D arising from the pulse point sources.

4. Results of diffusion processes simulation are presented by 1-D, 2-D and 3-D pictures and animated movies.

5. Obtained formulae and results of simulation were analyzed.

CHAPTER SIX
FOURIER TRANSFORM METHOD FOR CONSTRUCTING GREEN'S FUNCTION OF IVP FOR HEAT-DIFFUSION OPERATOR

The operator

$$\left(\frac{\partial}{\partial t} - a^2\frac{\partial^2}{\partial x^2}\right) \; is\ called\ 1D\ Heat\ Diffusion\ operator\ for\ x \in \mathbf{R}\,,$$

$$\left(\frac{\partial}{\partial t} - a^2\Delta x\right) \; is\ called\ 2D\ Heat\ Diffusion\ operator\ for\ x \in \mathbf{R^2}\,,$$

$$\left(\frac{\partial}{\partial t} - a^2\Delta x\right) \; is\ called\ 3D\ Heat\ Diffusion\ operator\ for\ x \in \mathbf{R^3}\,.$$

6.1 Green's Function of IVP for 1-D Heat-Diffusion Operator

Definition 6.1.1. A generalized function $G(x,t,\tau)$ satisfying

$$\frac{\partial}{\partial t}G(x,t,\tau) - a^2\frac{\partial}{\partial x}G(x,t,\tau) = \delta(x,t-\tau),\ x \in \mathbf{R},\ t \in \mathbf{R}\ , \tag{6.1.1}$$

$$G(x,t,\tau)|_{t<\tau} = 0\ , \tag{6.1.2}$$

is called the Green's function of IVP for 1D Heat Diffusion operator. Here τ is a parameter from $\mathbf{R}$.

6.1.1 Constructing The Green's Function $G(x,t,\tau)$

Applying the Fourier transform F_x with respect to $x \in \mathbf{R}$ to (6.1.1),(6.1.2) we find

$$\frac{\partial}{\partial t}\widetilde{G}(\nu,t,\tau) + a^2\nu^2\widetilde{G}(\nu,t,\tau) = \delta(t-\tau),\ t \in \mathbf{R}\ , \tag{6.1.3}$$

$$\widetilde{G}(\nu,t,\tau)|_{t<\tau} = 0\ , \tag{6.1.4}$$

where $\widetilde{G}(\nu,t,\tau) = F_x[G(x,t,\tau)](\nu)$, $\nu \in \mathbf{R}$ is a parameter of the Fourier transform.

Remark 6.1.1. *The following properties of the Fourier transform were used here*

$$\delta(x,t-\tau) = \delta(x)\delta(t-\tau)\ ,$$

$$F_x[\delta(x,t-\tau)](\nu) = F_x[\delta(x)\delta(t-\tau)] = F_x[\delta(x)]\delta(t-\tau) = \delta(t-\tau) \ ,$$

$$F_x[\frac{\partial^2}{\partial x^2}G(x,t,\tau)](\nu) = (-i\nu)^2 F_x[G(x,t,\tau)](\nu) = -\nu^2\widetilde{G}(\nu,t,\tau) \ .$$

Remark 6.1.2. *The function $\widetilde{G}(\nu,t,\tau)$ satisfying (6.1.3),(6.1.4) is the Green's function of IVP for the Ordinary differential equation $\left(\frac{d}{dt}+a^2\nu^2\right)$. We have studied the construction of this Green function.*

The formula for $\widetilde{G}(\nu,t,\tau)$ is

$$\widetilde{G}(\nu,t,\tau) = \theta(t-\tau)e^{-a^2\nu^2(t-\tau)} \ . \tag{6.1.5}$$

The formula (6.1.5) was obtained from appendix(2.2).

$$G(x,t,\tau) = F_\nu^{-1}[\widetilde{G}(\nu,t,\tau)](x) = \frac{\theta(t-\tau)}{2\pi}\int_{-\infty}^{\infty} e^{-a^2\nu^2(t-\tau)}e^{-i\nu x}d\nu \ .$$

Calculating the integral we find

$$G(x,t,\tau) = \frac{\theta(t-\tau)}{2a\sqrt{\pi(t-\tau)}} \ \exp\left(-\frac{x^2}{4a^2(t-\tau)}\right). \tag{6.1.6}$$

Remark 6.1.3. *Here we used to the formula from calculus*

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}\exp\left(-a^2\nu^2(t-\tau)\right)e^{-i\nu x}dx = \frac{1}{2a\sqrt{\pi(t-\tau)}} \ \exp\left(-\frac{x^2}{4a^2(t-\tau)}\right).$$

6.1.2 Properties of Green's Function

Let $G(x,t,\tau)$ be the Green's function of IVP for $1D$ Heat-Diffusion operator then $G(x,t,\tau)$ satisfies

$$\frac{\partial}{\partial t}G(x-\xi,t,\tau) - a^2\frac{\partial^2}{\partial x^2}G(x-\xi,t,\tau) = \delta(x-\xi,t-\tau) \ , x\in\mathbf{R}, \ x\in\mathbf{R} \ , \tag{6.1.7}$$

for any parameters $\xi\in\mathbf{R}$ and $\tau\in\mathbf{R}$.

$$G(x-\xi,t,\tau)|_{t<\tau} = 0 \, . \tag{6.1.8}$$

Proof. Let $\overline{x} = x-\xi$. According to definition the Green's function $G(\overline{x},t,\tau)$

satisfies

$$\frac{\partial}{\partial t}G(\overline{x},t,\tau) - a^2\frac{\partial^2}{\partial \overline{x}^2}G(\overline{x},t,\tau) = \delta(x-\xi,t-\tau)\,, \tag{6.1.9}$$

$$G(\overline{x},t,\tau)|_{\,t<\tau} = 0\,. \tag{6.1.10}$$

Substituting $\overline{x} = x - \xi$ into (6.1.9), (6.1.10) and using equality

$$\frac{\partial^2}{\partial \overline{x}^2}G(\overline{x},t,\tau)|_{\,\overline{x}=x-\xi} = \frac{\partial^2}{\partial x^2}G(x-\xi,t,\tau)$$

We find (6.1.7), (6.1.8) from (6.1.9), (6.1.10). □

6.1.3 Applications of Green's Function

Let $G(x,t,\tau)$ be Green's function of IVP for $1D$ Heat-Diffusion operator; $f(x,t)$ be continuous function;

$$\overline{f}(x,t) = \begin{cases} f(x,t) & , \quad t \geq 0 \\ 0 & , \quad t < 0 \end{cases}$$

Then the solution of the following IVP

$$\frac{\partial}{\partial t}u(x,t) - a^2\frac{\partial^2}{\partial x^2}u(x,t) = f(x,t)\;, t > 0\,, \tag{6.1.11}$$

$$u(x,0) = 0\,, \tag{6.1.12}$$

is given by the following formula

$$u(x,t) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} G(x-\xi,t,\tau)\overline{f}(\xi,\tau)d\xi d\tau\,. \tag{6.1.13}$$

Proof. Applying the operators $\frac{\partial}{\partial t}$ and $\frac{\partial^2}{\partial x^2}$ to (6.1.13) we find

$$\frac{\partial}{\partial t}u(x,t) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{\partial}{\partial t}(G(x-\xi,t,\tau))\overline{f}(\xi,\tau)d\xi d\tau\,, \tag{6.1.14}$$

$$\frac{\partial^2}{\partial x^2}u(x,t) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{\partial^2}{\partial x^2}(G(x-\xi,t,\tau))\overline{f}(\xi,\tau)d\xi d\tau\,, \tag{6.1.15}$$

Using (6.1.14), (6.1.15) we have

$$\frac{\partial}{\partial t}u(x,t) - a^2\frac{\partial^2}{\partial x^2}u(x,t)$$

$$= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left\{\frac{\partial}{\partial t}G(x-\xi,t,\tau)-a^2\frac{\partial^2}{\partial x^2}G(x-\xi,t,\tau)\right\}\overline{f}(\xi,\tau)d\xi d\tau\,,$$

using (6.1.7) we get

$$\frac{\partial}{\partial t}u(x,t)-a^2\frac{\partial^2}{\partial x^2}u(x,t)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\delta(x-\xi,t-\tau)\overline{f}(\xi,\tau)d\xi d\tau$$

using the property of $f(x,y)$ we get

$$\frac{\partial}{\partial t}u(x,t)-a^2\frac{\partial^2}{\partial x^2}u(x,t)=\overline{f}(x,t)=f(x,t)\;,for\;t>0\,.$$

This means that (6.1.11) is proved.

To prove (6.1.12) we will consider (6.1.13) where $G(x,t,\tau)$ is defined as (6.1.6). Substituting (6.1.6) into the equation (6.1.13) we have

$$u(x,t)=\frac{1}{2a\sqrt{\pi}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{\theta(t-\tau)}{\sqrt{t-\tau}}\exp\left\{-\frac{(x-\xi)^2}{4a^2(t-\tau)}\right\}\overline{f}(\xi,\tau)d\xi d\tau$$

$$=\left|\begin{array}{lcl}\overline{f}(x,t)=0 & , & \tau<0\\ \theta(t-\tau)=0 & , & t<\tau\end{array}\right|$$

then we have

$$u(x,t)=\frac{1}{2a\sqrt{\pi}}\int_{0}^{t}\int_{-\infty}^{\infty}\frac{1}{\sqrt{t-\tau}}\exp\left\{-\frac{(x-\xi)^2}{4a^2(t-\tau)}\right\}f(\xi,\tau)d\xi d\tau$$

Then we have for $t=0$

$$u(x,0)=\frac{1}{2a\sqrt{\pi}}\int_{0}^{0}\int_{-\infty}^{\infty}\frac{1}{\sqrt{t-\tau}}\exp\left\{-\frac{(x-\xi)^2}{4a^2(t-\tau)}\right\}f(\xi,\tau)d\xi d\tau=0\,.$$

The condition (6.1.12) is proved. $\square$

6.2 Green's Function of IVP for 2-D Heat-Diffusion Operator

Definition 6.2.1. Let $x = (x_1, x_2) \in \mathbf{R^2}$, $t \in \mathbf{R}$. A generalized function $G(x, t, \tau)$ satisfying

$$\frac{\partial}{\partial t}G(x,t,\tau) - a^2\Delta_x G(x,t,\tau) = \delta(x)\delta(t-\tau),\ x \in \mathbf{R^2},\ t \in \mathbf{R}\ , \tag{6.2.1}$$

$$G(x,t,\tau)|_{t<\tau} = 0\ , \tag{6.2.2}$$

is called the Green's function of IVP for 2D Heat Diffusion operator. Here τ is a parameter from $\mathbf{R}$ and $\delta(x) = \delta(x_1)\delta(x_2)$ is 2D Dirac delta function concentrated $x_1 = 0$, $x_2 = 0$.

6.2.1 Constructing The Green's Function $G(x, t, \tau)$

Applying the fourier transform F_x with respect to $x \in \mathbf{R^2}$ to (6.2.1),(6.2.2) we find

$$\frac{\partial}{\partial t}\widetilde{G}(\nu,t,\tau) + a^2|\nu|^2\widetilde{G}(\nu,t,\tau) = \delta(t-\tau),\ t \in \mathbf{R}\ , \tag{6.2.3}$$

$$\widetilde{G}(\nu,t,\tau)|_{t<\tau} = 0\ , \tag{6.2.4}$$

where $\widetilde{G}(\nu, t, \tau) = F_x[G(x, t, \tau)](\nu)$, $\nu \in \mathbf{R^2}$ is a parameter of the fourier transform.

Remark 6.2.1. *The following properties of the Fourier transform were used here*

$$\delta(x, t-\tau) = \delta(x_1)\delta(x_2)\delta(t-\tau)\ ,$$

$$F_x[\delta(x,t-\tau)](\nu) = F_x[\delta(x_1)\delta(x_2)\delta(t-\tau)] = F_x[\delta(x_1)]F_x[\delta(x_2)]\delta(t-\tau) = \delta(t-\tau)\ ,$$

$$F_x[\Delta_x G(x,t,\tau)](\nu) = (-i\nu_1)^2 + (-i\nu_2)^2 F_x[G(x,t,\tau)](\nu) = -(\nu_1^2+\nu_2^2)\widetilde{G}(\nu,t,\tau)\ .$$

And $\nu = (\nu_1, \nu_2) \in \mathbf{R^2}$, $\nu^2 = \nu_1^2 + \nu_2^2$ *and* $F_x[\delta(x_1)](\nu) = F_x[\delta(x_2)](\nu) = 1$.

Remark 6.2.2. *The function $\widetilde{G}(\nu, t, \tau)$ satisfying (6.2.3),(6.2.4) is the Green's function of IVP for the Ordinary differential equation $\left(\frac{d}{dt} + a^2|\nu|^2\right)$. We have studied the construction of this Green function.*

The formula for $\widetilde{G}(\nu, t, \tau)$ is

$$\widetilde{G}(\nu,t,\tau) = \theta(t-\tau)e^{-a^2|\nu|^2(t-\tau)}\ . \tag{6.2.5}$$

The formula (6.2.5) was obtained from appendix(2.2).

$$G(x,t,\tau) = F_\nu^{-1}[\widetilde{G}(\nu,t,\tau)](x) = \frac{\theta(t-\tau)}{(2\pi)^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-a^2|\nu|^2(t-\tau)}e^{-i(\nu_1x_1+\nu_2x_2)}d\nu_1 d\nu_2$$

or equivalently

$$G(x,t,\tau) = \frac{\theta(t-\tau)}{(2a\sqrt{\pi(t-\tau)})^2}\ \exp\left(-\frac{|x|^2}{4a^2(t-\tau)}\right). \qquad (6.2.6)$$

Here $|x|^2 = x_1^2 + x_2^2$ *and* $|\nu|^2 = \nu_1^2 + \nu_2^2$.

Remark 6.2.3. *Here we used to the formula from calculus*

$$\frac{1}{(2\pi)^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\exp\left(-a^2|\nu|^2(t-\tau)\right)e^{-i(\nu_1x_1+\nu_2x_2)}d\nu_1 d\nu_2\ ,$$

$$= \frac{1}{(2a\sqrt{\pi(t-\tau)})^2}\ \exp\left(-\frac{|x|^2}{4a^2(t-\tau)}\right).$$

6.2.2 Properties of Green's Function

Let $G(x,t,\tau)$ be the Green's function of IVP for $2D$ Heat-Diffusion operator then $G(x,t,\tau)$ satisfies

$$\frac{\partial}{\partial t}G(x-\xi,t,\tau) - a^2\Delta_x G(x-\xi,t,\tau) = \delta(x-\xi,t-\tau)\,, \qquad (6.2.7)$$

$$G(x-\xi,t,\tau)|_{t<\tau} = 0\,. \qquad (6.2.8)$$

where $x-\xi = (x_1-\xi_1, x_2-\xi_2) \in \mathbf{R^2}$

Proof. Let $\overline{x} = x-\xi$. According to definition the Green's function $G(\overline{x},t,\tau)$ satisfies

$$\frac{\partial}{\partial t}G(\overline{x},t,\tau) - a^2\Delta_x G(\overline{x},t,\tau) = \delta(x-\xi,t-\tau)\,, \qquad (6.2.9)$$

$$G(\overline{x},t,\tau)|_{\,t<\tau} = 0\,. \qquad (6.2.10)$$

Substituting $\overline{x} = x-\xi$ into (6.2.9), (6.2.10) and using equality

$$\frac{\partial^2}{\partial\overline{x}^2}G(\overline{x},t,\tau)|_{\,\overline{x}=x-\xi} = \frac{\partial^2}{\partial x^2}G(x-\xi,t,\tau)$$

We find (6.2.7), (6.2.8) from (6.2.9), (6.2.10). $\square$

6.2.3 Applications of Green's Function

Let $G(x,t,\tau)$ be Green's function of IVP for $2D$ Heat-Diffusion operator; $f(x,t)$ be continuous function, $x=(x_1,x_2)\in \mathbf{R^2}$;

$$\overline{f}(x,t)=\begin{cases} f(x,t) & , \quad t\geq 0 \\ 0 & , \quad t<0 \end{cases}$$

then the solution of the following IVP

$$\frac{\partial}{\partial t}u(x,t)-a^2\Delta_x u(x,t)=f(x,t)\ ,t>0\,, \tag{6.2.11}$$

$$u(x,0)=0\,, \tag{6.2.12}$$

is given by the following formula

$$u(x,t)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}G(x-\xi,t,\tau)\overline{f}(\xi,\tau)d\xi d\tau\,. \tag{6.2.13}$$

Proof. Applying the operators $\frac{\partial}{\partial t}$ and Δ_x to (6.2.13) we find

$$\frac{\partial}{\partial t}u(x,t)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{\partial}{\partial t}(G(x-\xi,t,\tau))\overline{f}(\xi,\tau)d\xi d\tau\,, \tag{6.2.14}$$

$$\frac{\partial^2}{\partial x^2}u(x,t)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\Delta_x(G(x-\xi,t,\tau))\overline{f}(\xi,\tau)d\xi d\tau\,, \tag{6.2.15}$$

Using (6.2.14), (6.2.15) we have

$$\frac{\partial}{\partial t}u(x,t)-a^2\Delta_x u(x,t)$$

$$=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left\{\frac{\partial}{\partial t}G(x-\xi,t,\tau)-a^2\Delta_x G(x-\xi,t,\tau)\right\}\overline{f}(\xi,\tau)d\xi d\tau\,,$$

using (6.2.7) we get

$$\frac{\partial}{\partial t}u(x,t)-a^2\Delta_x u(x,t)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\delta(x-\xi,t-\tau)\overline{f}(\xi,\tau)d\xi d\tau$$

using the property of $f(x,y)$ we get

$$\frac{\partial}{\partial t}u(x,t)-a^2\Delta_x u(x,t)=\overline{f}(x,t)=f(x,t)\ ,for\ t>0\,.$$

Where $d\xi = d\xi_1 d\xi_2$, $\Delta_x = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}$. This means that (6.2.11) is proved. To prove (6.2.12) we will consider (6.2.13) where $G(x,t,\tau)$ is defined as (6.2.6). Substituting (6.2.6) into the equation (6.2.13) we have

$$u(x,t) = \frac{1}{(2a\sqrt{\pi})^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\theta(t-\tau)}{(t-\tau)} \exp\left\{-\frac{|x-\xi|^2}{4a^2(t-\tau)}\right\} \overline{f}(\xi,\tau) d\xi d\tau$$

$$= \left| \begin{array}{lcl} \overline{f}(x,t) = 0 & , & \tau < 0 \\ \theta(t-\tau) = 0 & , & t < \tau \end{array} \right|$$

then we have

$$u(x,t) = \frac{1}{(2a\sqrt{\pi})^2} \int_{0}^{t} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{1}{(t-\tau)} \exp\left\{-\frac{|x-\xi|^2}{4a^2(t-\tau)}\right\} f(\xi,\tau) d\xi d\tau$$

Then we have for $t = 0$

$$u(x,0) = \frac{1}{(2a\sqrt{\pi})^2} \int_{0}^{0} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{1}{(t-\tau)} \exp\left\{-\frac{|x-\xi|^2}{4a^2(t-\tau)}\right\} f(\xi,\tau) d\xi d\tau = 0\,.$$

Where $|x-\xi|^2 = (x_1-\xi_1)^2 + (x_2-\xi_2)^2$ and $d\xi = d\xi_1 d\xi_2$. The condition (6.1.12) is proved. $\square$

6.3 Green's Function of IVP for 3-D Heat-Diffusion Operator

Definition 6.3.1. Let $x = (x_1, x_2, x_3) \in \mathbf{R^3}$, $t \in \mathbf{R}$. A generalized function $G(x, t, \tau)$ satisfying

$$\frac{\partial}{\partial t}G(x,t,\tau) - a^2\Delta_x G(x,t,\tau) = \delta(x)\delta(t-\tau),\ x \in \mathbf{R^3},\ t \in \mathbf{R}\ , \tag{6.3.1}$$

$$G(x,t,\tau)|_{t<\tau} = 0\ , \tag{6.3.2}$$

is called the Green's function of IVP for 3D Heat Diffusion operator. Here τ is a parameter from $\mathbf{R}$ and $\delta(x) = \delta(x_1)\delta(x_2)\delta(x_3)$ is 3D Dirac delta function concentrated $x_1 = 0$, $x_2 = 0$, $x_3 = 0$.

6.3.1 Constructing The Green's Function $G(x, t, \tau)$

Applying the fourier transform F_x with respect to $x \in \mathbf{R^3}$ to (6.3.1),(6.3.2) we find

$$\frac{\partial}{\partial t}\widetilde{G}(\nu,t,\tau) + a^2|\nu|^2\widetilde{G}(\nu,t,\tau) = \delta(t-\tau),\ t \in \mathbf{R}\ , \tag{6.3.3}$$

$$\widetilde{G}(\nu,t,\tau)|_{t<\tau} = 0\ , \tag{6.3.4}$$

where $\widetilde{G}(\nu,t,\tau) = F_x[G(x,t,\tau)](\nu)$, $\nu \in \mathbf{R^3}$ is a parameter of the fourier transform.

Remark 6.3.1. *The following properties of the Fourier transform were used here*

$$\delta(x,t-\tau) = \delta(x_1)\delta(x_2)\delta(x_3)\delta(t-\tau)\ ,$$

$$F_x[\delta(x,t-\tau)](\nu) = F_x[\delta(x_1)\delta(x_2)\delta(x_3)\delta(t-\tau)]$$

$$= F_x[\delta(x_1)]F_x[\delta(x_2)]F_x[\delta(x_3)])\delta(t-\tau) = \delta(t-\tau)\ ,$$

$$F_x[\Delta_x G(x,t,\tau)](\nu) = (-i\nu_1)^2 + (-i\nu_2)^2 + (-i\nu_3)^2 F_x[G(x,t,\tau)](\nu)$$

$$= -(\nu_1^2 + \nu_2^2 + \nu_3^2)\widetilde{G}(\nu,t,\tau)\ .$$

And $\nu = (\nu_1, \nu_2, \nu_3) \in \mathbf{R^3}$, $\nu^2 = \nu_1^2 + \nu_2^2 + \nu_3^2$ *and* $F_x[\delta(x_1)](\nu) = F_x[\delta(x_2)](\nu) = F_x[\delta(x_3)](\nu) = 1$.

Remark 6.3.2. *The function $\widetilde{G}(\nu,t,\tau)$ satisfying (6.3.3),(6.3.4) is the Green's function of IVP for the Ordinary differential equation $\left(\frac{d}{dt} + a^2|\nu|^2\right)$. We have* *studied the construction of this Green function.*

The formula for $\widetilde{G}(\nu, t, \tau)$ *is*

$$\widetilde{G}(\nu, t, \tau) = \theta(t-\tau)e^{-a^2|\nu|^2(t-\tau)} \,. \tag{6.3.5}$$

The formula (6.3.5) was obtained from appendix(2.2).

$$G(x,t,\tau) = F_\nu^{-1}[\widetilde{G}(\nu,t,\tau)](x)$$

$$= \frac{\theta(t-\tau)}{(2\pi)^3}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-a^2|\nu|^2(t-\tau)}e^{-i(\nu_1x_1+\nu_2x_2+\nu_3x_3)}d\nu_1 d\nu_2 d\nu_3 \,,$$

or equivalently

$$G(x,t,\tau) = \frac{\theta(t-\tau)}{(2a\sqrt{\pi(t-\tau)})^{3/2}}\ \exp\left(-\frac{|x|^2}{4a^2(t-\tau)}\right). \tag{6.3.6}$$

Here $|x|^2 = x_1^2 + x_2^2 + x_3^2$ *and* $|\nu|^2 = \nu_1^2 + \nu_2^2 + \nu_3^2$.

Remark 6.3.3. *Here we used to the formula from calculus*

$$\frac{1}{(2\pi)^3}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \exp\left(-a^2|\nu|^2(t-\tau)\right) e^{-i(\nu_1x_1+\nu_2x_2+\nu_3x_2)}d\nu_1 d\nu_2 d\nu_3$$

$$= \frac{1}{(2a\sqrt{\pi(t-\tau)})^{3/2}}\ \exp\left(-\frac{|x|^2}{4a^2(t-\tau)}\right).$$

6.3.2 Properties of Green's Function

Let $G(x,t,\tau)$ be the Green's function of IVP for $3D$ Heat-Diffusion operator then $G(x,t,\tau)$ satisfies

$$\frac{\partial}{\partial t}G(x-\xi,t,\tau) - a^2\Delta_x G(x-\xi,t,\tau) = \delta(x-\xi,t-\tau)\,, \tag{6.3.7}$$

$$G(x-\xi,t,\tau)|_{t<\tau} = 0\,. \tag{6.3.8}$$

where $x-\xi = (x_1-\xi_1, x_2-\xi_2, x_3-\xi_3) \in \mathbf{R^3}$

Proof. Let $\overline{x} = x - \xi$. According to definition the Green's function $G(\overline{x},t,\tau)$

satisfies

$$\frac{\partial}{\partial t}G(\overline{x},t,\tau) - a^2\Delta_x G(\overline{x},t,\tau) = \delta(x-\xi,t-\tau)\,, \tag{6.3.9}$$

$$G(\overline{x},t,\tau)|_{\,t<\tau} = 0\,. \tag{6.3.10}$$

Substituting $\overline{x} = x - \xi$ into (6.3.9), (6.3.10) and using equality

$$\frac{\partial^2}{\partial \overline{x}^2}G(\overline{x},t,\tau)|_{\,\overline{x}=x-\xi} = \frac{\partial^2}{\partial x^2}G(x-\xi,t,\tau)$$

We find (6.3.7), (6.3.8) from (6.3.9), (6.3.10). □

6.3.3 Applications of Green's Function

Let $G(x,t,\tau)$ be Green's function of IVP for $3D$ Heat-Diffusion operator; $f(x,t)$ be continuous function, $x = (x_1,x_2,x_3) \in \mathbf{R^3}$;

$$\overline{f}(x,t) = \begin{cases} f(x,t) & , \quad t \geq 0 \\ 0 & , \quad t < 0 \end{cases}$$

then the solution of the following IVP

$$\frac{\partial}{\partial t}u(x,t) - a^2\Delta_x u(x,t) = f(x,t)\ , t > 0\,, \tag{6.3.11}$$

$$u(x,0) = 0\,, \tag{6.3.12}$$

is given by the following formula

$$u(x,t) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} G(x-\xi,t,\tau)\overline{f}(\xi,\tau)d\xi d\tau\,. \tag{6.3.13}$$

Proof. Applying the operators $\frac{\partial}{\partial t}$ and Δ_x to (6.3.13) we find

$$\frac{\partial}{\partial t}u(x,t) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{\partial}{\partial t}(G(x-\xi,t,\tau))\overline{f}(\xi,\tau)d\xi d\tau\,, \tag{6.3.14}$$

$$\frac{\partial^2}{\partial x^2}u(x,t) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \Delta_x(G(x-\xi,t,\tau))\overline{f}(\xi,\tau)d\xi d\tau\,, \tag{6.3.15}$$

Using (6.3.14), (6.3.15) we have

$$\frac{\partial}{\partial t}u(x,t) - a^2\Delta_x u(x,t)$$

$$= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left\{\frac{\partial}{\partial t}G(x-\xi,t,\tau) - a^2\Delta_x G(x-\xi,t,\tau)\right\}\overline{f}(\xi,\tau)d\xi d\tau\,,$$

using (6.3.7) we get

$$\frac{\partial}{\partial t}u(x,t) - a^2\Delta_x u(x,t) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\delta(x-\xi,t-\tau)\overline{f}(\xi,\tau)d\xi d\tau$$

using the property of $f(x,y)$ we get

$$\frac{\partial}{\partial t}u(x,t) - a^2\Delta_x u(x,t) = \overline{f}(x,t) = f(x,t)\ , for\ t > 0\,.$$

Where $d\xi = d\xi_1 d\xi_2 d\xi_3$, $\Delta_x = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2}$. This means that (6.3.11) is proved. To prove (6.3.12) we will consider (6.3.13) where $G(x,t,\tau)$ is defined as (6.3.6). Substituting (6.3.6) into the equation (6.3.13) we have

$$u(x,t) = \frac{1}{(2a\sqrt{\pi})^{3/2}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{\theta(t-\tau)}{(t-\tau)^{3/2}}\exp\left\{-\frac{|x-\xi|^2}{4a^2(t-\tau)}\right\}\overline{f}(\xi,\tau)d\xi d\tau$$

$$= \left|\begin{array}{ccc} \overline{f}(x,t) = 0 & , & \tau < 0 \\ \theta(t-\tau) = 0 & , & t < \tau \end{array}\right|$$

then we have

$$u(x,t) = \frac{1}{(2a\sqrt{\pi})^{3/2}}\int_{0}^{t}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{1}{(t-\tau)^{3/2}}\exp\left\{-\frac{|x-\xi|^2}{4a^2(t-\tau)}\right\}f(\xi,\tau)d\xi d\tau\ .$$

Then we have for $t = 0$

$$u(x,0) = 0\,.$$

Where $|x-\xi|^2 = (x_1-\xi_1)^2 + (x_2-\xi_2)^2 + (x_3-\xi_3)^2$ and $d\xi = d\xi_1 d\xi_2 d\xi_3$. The condition (6.1.12) is proved. $\square$

6.4 Examples of simulations of IVP for Heat-Diffusion equation

This section contains some examples of modeling and simulations of heat-diffusion equation in 1-D, 2-D and 3-D IVPs. Solutions will be simulated by using mathematical tools. We have an unbounded domain and we took a pulse point source described by the Dirac delta function.

6.4.1 1-D Heat-Diffusion equation

In this case we have a string on $[-3, 3]$

Example 6.4.1. Let us consider the problem (6.1.11)-(6.1.12). Where $f(x,t)$ is given by

$$f(x,t) = \delta(x)\delta(t) ,$$

and $\delta(x)$ is the Dirac delta function. Using formula for $f(x,t)$ and the properties of the Dirac delta function the solution of the problem (6.1.11)-(6.1.12) can be found by the following formula

$$u(x,t) = \frac{1}{2a\sqrt{\pi}} \int_0^t \int_{-\infty}^{\infty} \frac{1}{\sqrt{t-\tau}} \exp\left\{ -\frac{(x-\xi)^2}{4a^2(t-\tau)} \right\} \delta(\xi)\delta(\tau) d\xi d\tau , \qquad (6.4.1)$$

and substitutions gives that

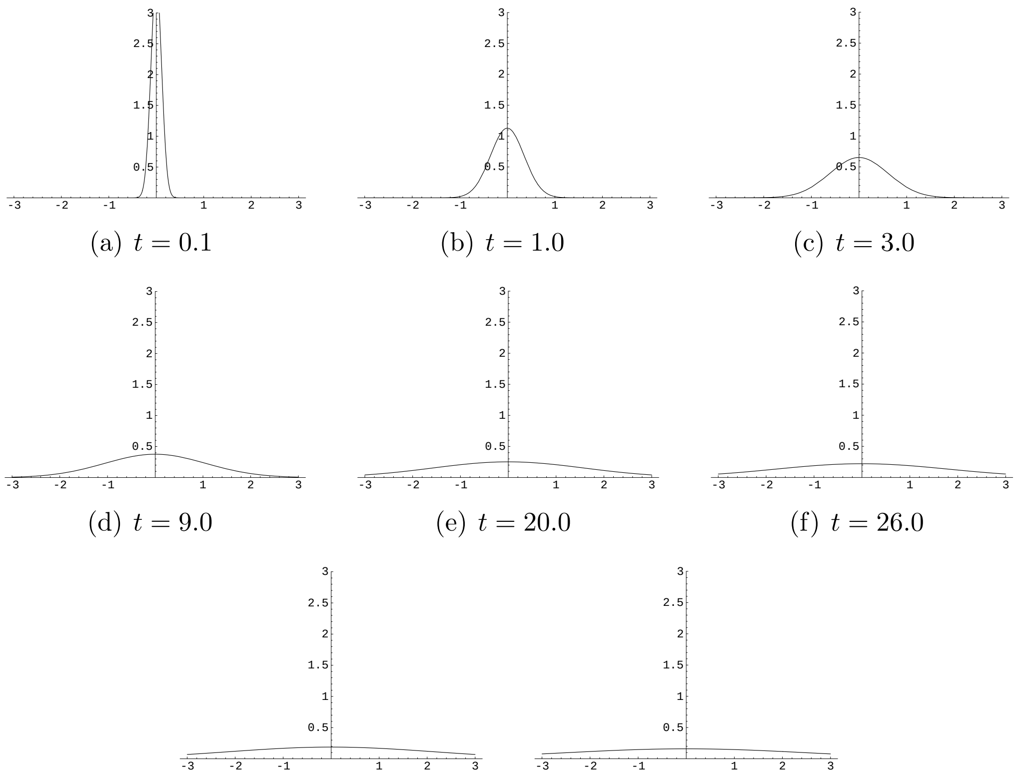
$$u(x,t) = \frac{1}{2a\sqrt{\pi(t-\tau)}} \exp\left\{ -\frac{x^2}{4a^2(t-\tau)} \right\} . \qquad (6.4.2)$$

Equation (6.4.2) is the special solution of the problem (6.1.11)-(6.1.12).

For the given data of Example 6.4.1, we used Mathematica codes for finding simulations.

6.4.1.1 *Simulations of 1-D Heat-Diffusion equation (IVP)*

Using the formula (6.4.2) and Mathematica codes we simulated the diffusion processes from the pulse point source which is located in the center of the domain D. The simulations for different times shown in figures below. And the speed of the propagation was taken as $a = 0.25$



(a) $t = 0.1$ (b) $t = 1.0$ (c) $t = 3.0$

(d) $t = 9.0$ (e) $t = 20.0$ (f) $t = 26.0$

(g) $t = 36.0$ (h) $t = 50.0$

Figure 6.24: Example 6.4.1: IVP for 1-D heat-diffusion equation .

We can see in the pictures that in the first picture we have a big pick, and the other pictures shows us this source propagates everywhere. If the domain is bounded we have some reflections (we did it in Chapters 2,3,4) but in this case there is no reflection.

6.4.2 2-D Heat-Diffusion equation

In this case we have a string on $[-10, 10] \times [-10, 10]$

Example 6.4.2. Let us consider the problem (6.2.11)-(6.2.12). Where $f(x_1, x_2, t)$ is given by

$$f(x_1, x_2, t) = \delta(x_1)\delta(x_2)\delta(t) \ ,$$

and $\delta(\cdot)$ is the Dirac delta function. Using formula for $f(x_1, x_2, t)$ and the properties of the Dirac delta function the solution of the problem (6.2.11)-(6.2.12) can be found by the following formula

$$u(x_1, x_2, t) = \frac{1}{2a\sqrt{\pi}} \int_0^t \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{1}{\sqrt{t-\tau}} \exp\left\{ -\frac{|x-\xi|^2}{4a^2(t-\tau)} \right\} \delta(\xi)\delta(\tau) d\xi d\tau \ , \tag{6.4.3}$$

where $|x - \xi|^2 = (x_1 - \xi_1)^2 + (x_2 - \xi_2)^2$, $\delta(\xi) = \delta(\xi_1)\delta(\xi_2)$ and $d\xi = d\xi_1 d\xi_2$ substitutions gives that

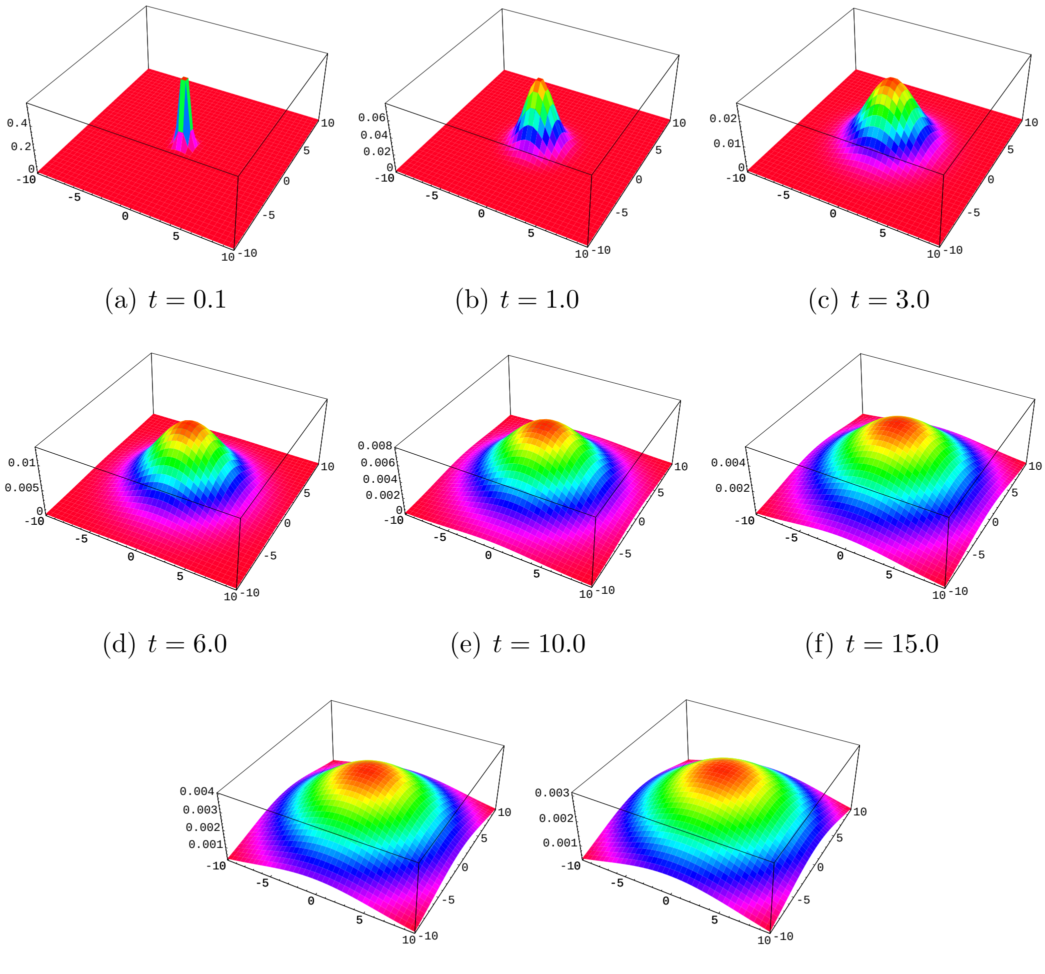
$$u(x_1, x_2, t) = \frac{1}{4a^2\pi(t-\tau)} \exp\left\{ -\frac{x_1^2 + x_2^2}{4a^2(t-\tau)} \right\} \ . \tag{6.4.4}$$

Equation (6.4.4) is the special solution of the problem (6.2.11)-(6.2.12).

For the given data of Example 6.4.2, we used Mathematica codes for finding simulations.

6.4.2.1 Simulations of 2-D Heat-Diffusion equation (IVP)

Using the formula (6.4.4) and Mathematica codes we simulated the diffusion processes from the pulse point source which is located in the center of the domain D. The simulations for different times shown in figures below. And the speed of the propagation was taken as $a = 1$



(a) $t = 0.1$ (b) $t = 1.0$ (c) $t = 3.0$

(d) $t = 6.0$ (e) $t = 10.0$ (f) $t = 15.0$

(g) $t = 20.0$ (h) $t = 26.0$

Figure 6.25: Example 6.4.2: IVP for 2-D heat-diffusion equation .

We can see in the pictures that in the first picture we have a big pick, and the other pictures shows us this source propagates everywhere. If the domain is bounded we have some reflections (we did it in Chapters 2,3,4) but in this case there is no reflection.

6.4.3 3-D Heat-Diffusion equation

In this case we have a string on $[-10,10]\times[-10,10]\times[-10,10]$

Example 6.4.3. Let us consider the problem (6.3.11)-(6.3.12). Where $f(x_1,x_2,x_3,t)$ is given by

$$f(x_1,x_2,x_3,t)=\delta(x_1)\delta(x_2)\delta(x_3)\delta(t)\ ,$$

and $\delta(\cdot)$ is the Dirac delta function. Using formula for $f(x_1,x_2,x_3,t)$ and the properties of the Dirac delta function the solution of the problem (6.3.11)-(6.3.12) can be found by the following formula

$$u(x_1,x_2,x_3,t)=\frac{1}{2a\sqrt{\pi}}\int_0^t\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{1}{\sqrt{t-\tau}}\exp\left\{-\frac{|x-\xi|^2}{4a^2(t-\tau)}\right\}\delta(\xi)\delta(\tau)d\xi d\tau\ , \tag{6.4.5}$$

where $|x-\xi|^2=(x_1-\xi_1)^2+(x_2-\xi_2)^2+(x_3-\xi_3)^2$, $\delta(\xi)=\delta(\xi_1)\delta(\xi_2)\delta(\xi_3)$ and $d\xi=d\xi_1d\xi_2d\xi_3$ substitutions gives that

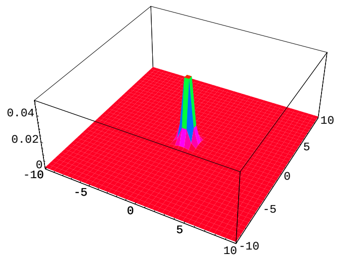
$$u(x_1,x_2,x_3,t)=\frac{1}{(2a\sqrt{\pi(t-\tau)})^{3/2}}\exp\left\{-\frac{x_1^2+x_2^2+x_3^2}{4a^2(t-\tau)}\right\}\ . \tag{6.4.6}$$

Equation (6.4.6) is the special solution of the problem (6.3.11)-(6.3.12).

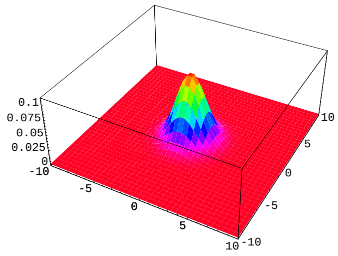
For the given data of Example 6.4.3, we used Mathematica codes for finding simulations.

6.4.3.1 Simulations of 3-D Heat-Diffusion equation (IVP)

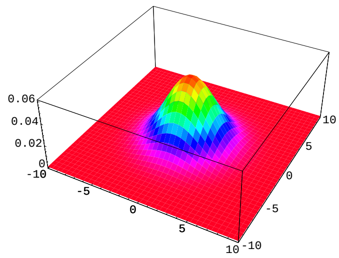
Using the formula (6.4.6) and Mathematica codes we simulated the diffusion processes from the pulse point source which is located in the center of the domain D. The simulations for different times shown in figures below. And the speed of the propagation was taken as $a = 1$



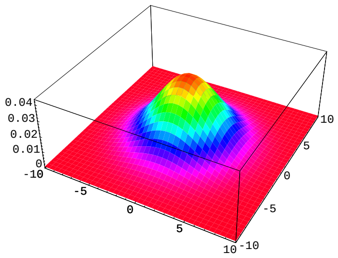
(a) $t = 0.1$



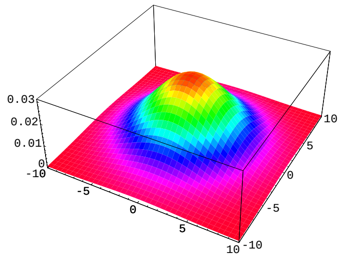
(b) $t = 1.0$



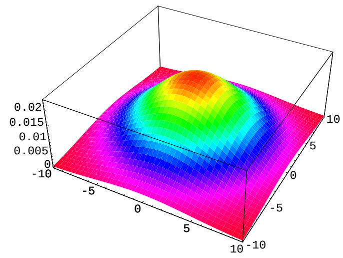
(c) $t = 3.0$



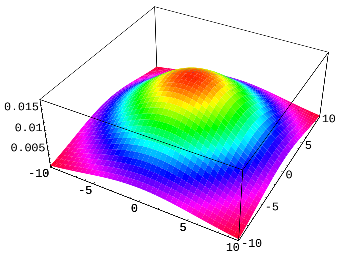
(d) $t = 5.0$



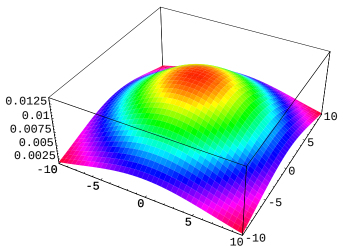
(e) $t = 8.0$



(f) $t = 12.0$



(g) $t = 18.0$



(h) $t = 25.0$

Figure 6.26: Example 6.4.2: IVP for 2-D heat-diffusion equation .

We can see in the pictures that in the first picture we have a big pick, and the other pictures shows us this source propagates everywhere. If the domain is bounded we have some reflections (we did it in Chapters 2,3,4) but in this case there is no reflection.

6.5 Analysis of the chapter6 study

1. By using Green's function method the exact solutions of the IVPs are found.
2. These formulae were adjusted to cases when inhomogeneous term is the Dirac delta function with a support in a point center the bounded domain D.
3. Obtained formulae for generalized solutions of IVPs for the heat-diffusion equation were used for modeling and simulations of diffusion processes in unbounded domain arising from the pulse point sources.
4. Results of diffusion processes simulation are presented by 1-D, 2-D and 3-D pictures and animated movies.
5. Obtained formulae and results of simulation were analyzed.

CHAPTER SEVEN
ELECTRIC FIELD IN DIFFUSION APPROXIMATION

In this section diffusion processes for electric fields will be studied. Using the symbolic and algebraic computations in MATLAB a new method of constructing the exact solution of the initial value problem is obtained. The formulaes will be generated and using these formulaes simulations will be found.

7.1 Definitions of the IVP for systems

By using the articles (Weiss & Newman (2003)), (V.G.Yakhno & T.M.Yakhno & Kasap (2006)) we can define the following IVP for diffusion processes. Let $\sigma = (\sigma_{ij})_{3\times3}$ is a symmetric positive definite matrix with constant elements, σ and j be given and $j = (j_1, j_2, j_3)$ is defined as the density of electric current. Here $\mathbf{E} = (\mathbf{E_1}, \mathbf{E_2}, \mathbf{E_3})$ be the electric fields.

Consider the following IVP :

$$curl_x curl_x \mathbf{E} + \sigma \frac{\partial \mathbf{E}}{\partial t} = -\frac{\partial \mathbf{j}}{\partial t} \; , x \in \mathbf{R^3} \; , t \in \mathbf{R} \; , \tag{7.1.1}$$

$$\mathbf{E}\Big|_{t\leq 0} = 0 \; . \tag{7.1.2}$$

For finding the solution of IVP system we will apply some steps which were written in the next section.

7.2 Finding the exact solution of (7.1.1) and (7.1.2)

Let $\widetilde{\mathbf{E}}(\nu, t)$, $\widetilde{\mathbf{j}}(\nu, t)$ be the Fourier transform images of the electric fields $\mathbf{E}(x, t)$ and current $\mathbf{j}(x, t)$ with respect to $x = (x_1, x_2, x_3) \in \mathbf{R^3}$ i.e

$$\widetilde{\mathbf{E}}(\nu, t) = \mathcal{F}_x[\mathbf{E}](\nu, t) \; , \quad \widetilde{\mathbf{j}}(\nu, t) = \mathcal{F}_x[\mathbf{j}](\nu, t) \; ,$$

where

$$\mathcal{F}_x[\mathbf{E}](\nu, t) = \int_{-\infty}^{-\infty} \int_{-\infty}^{-\infty} \int_{-\infty}^{-\infty} \mathbf{E}(x, t)\, e^{i\nu x} dx_1 dx_2 dx_3 \; ,$$

where $\nu = (\nu_1, \nu_2, \nu_3)$, $x\nu = x_1\nu_1 + x_2\nu_2 + x_3\nu_3$ and $i^2 = -1$.

Applying Fourier transform to equations (7.1.1), (7.1.2) we get the following problem

$$\sigma \frac{\partial \widetilde{\mathbf{E}}}{\partial t} + A(\nu)\widetilde{\mathbf{E}} = -\frac{\partial \widetilde{\mathbf{j}}}{\partial t}\;, t \in \mathbf{R}\;, \nu \in \mathbf{R^3}\;, \tag{7.2.1}$$

$$\widetilde{\mathbf{E}}\big|_{t\leq 0} = 0\;, \nu \in \mathbf{R^3}\;, \tag{7.2.2}$$

where

$$A(\nu) = \begin{pmatrix} \nu_2^2 + \nu_3^2 & -\nu_1\nu_2 & -\nu_1\nu_3 \\ -\nu_1\nu_2 & \nu_1^2 + \nu_3^2 & -\nu_2\nu_3 \\ -\nu_1\nu_3 & -\nu_2\nu_3 & \nu_1^2 + \nu_2^2 \end{pmatrix} . \tag{7.2.3}$$

The method of exact solution contains several steps. In the first step, using the transfer matrix formalism for given $A(\nu)$ and the symmetric positive definite matrix σ we can construct a non-singular matrix $\mathcal{T}(\nu)$ and a diagonal matrix $D(\nu)$ with non-negative elements such that

$$\mathcal{T}^T(\nu)\,\sigma\,\mathcal{T}(\nu) = \mathcal{I}\;, \tag{7.2.4}$$

$$\mathcal{T}^T(\nu)\,A(\nu)\,\mathcal{T}(\nu) = D(\nu)\;, \tag{7.2.5}$$

where $\mathcal{I}$ is the identity matrix, $\mathcal{T}^T(\nu)$ is the transposed matrix to $\mathcal{T}(\nu)$.

In the second step we are looking for the solution of (7.1.1), (7.1.2) in the form

$$\widetilde{\mathbf{E}}(\nu, t) = \mathcal{T}(\nu)\mathbf{Y}(\nu, t)\;, \tag{7.2.6}$$

where the matrix $\mathcal{T}(\nu)$ is constructed in the first step and a vector function $\mathbf{Y}(\nu, t)$ is unknown. Substituting (7.2.6) into (7.2.1) and (7.2.2) we find

$$\sigma\mathcal{T}\frac{\partial \mathbf{Y}}{\partial t} + A(\nu)\mathcal{T}\,\mathbf{Y} = -\frac{\partial \widetilde{\mathbf{j}}}{\partial t}\;, t \in \mathbf{R}\;, \nu \in \mathbf{R^3}\;, \tag{7.2.7}$$

$$\mathbf{Y}(\nu, t)\big|_{t\leq 0} = 0\;, \nu \in \mathbf{R^3}\;, \tag{7.2.8}$$

Multiplying (7.2.7) by $\mathcal{T}^T(\nu)$ and using (7.2.4), (7.2.5) we have

$$\frac{\partial \mathbf{Y}}{\partial t} + D(\nu)\mathcal{T}\mathbf{Y} = -\mathcal{T}^T(\nu)\frac{\partial \widetilde{\mathbf{j}}}{\partial t}\ , t \in \mathbf{R}\ , \nu \in \mathbf{R^3}\ . \tag{7.2.9}$$

In the third step of the method, using the ordinary differential equations technique, see, for example, (Boyce & Diprima (1992)), a solution of the initial value problem (7.2.8), (7.2.9) is given by

$$\mathbf{Y}(\nu, t) = column(Y_1(\nu, t), Y_2(\nu, t), Y_3(\nu, t))\ , \tag{7.2.10}$$

where for $t < 0$ the function $\mathbf{Y}_n(\nu, t)$ vanishes and for $t \geq 0$ is defined by

$$\begin{aligned} \mathbf{Y}_n(\nu, t) &= -[\,\mathcal{T}^T(\nu)\,\widetilde{\mathbf{j}}(\nu, t)\,]_n + d_n(\nu)\int_0^t e^{-d_n(\nu)(t-\tau)}[\,\mathcal{T}^T(\nu)\,\widetilde{\mathbf{j}}(\nu, \tau)\,]_n d\tau \\ &\qquad\qquad if\ d_n(\nu) > 0\ , \qquad (7.2.11) \\ \mathbf{Y}_n(\nu, t) &= -[\,\mathcal{T}^T(\nu)\,\widetilde{\mathbf{j}}(\nu, t)\,]_n \quad if\ d_n(\nu) = 0\ , \qquad (7.2.12) \end{aligned}$$

where $d_n(\nu)$, $n = 1, 2, 3$ are elements of the matrix $D(\nu)$; $[\mathcal{T}^T(\nu)\widetilde{\mathbf{j}}(\nu, \tau)]_n$ is the nth component of the vector.

Proof 7.2.1. *(Solution of (7.2.7), (7.2.6))) The homogeneous part of the problem (7.2.7)*

$$\frac{d\boldsymbol{Y}}{dt} + D(\nu)\,\boldsymbol{Y} = 0\ ,$$

has the solution of the form

$$\boldsymbol{Y}(\nu, t) = C\,e^{-D(\nu)t}\ ,$$

where C is a constant.

Using the variation of parameters technique (writing C with parameter t) we can write the solution

$$\boldsymbol{Y}(\nu, t) = C(t)\,e^{-D(\nu)t}\ ,$$

and the last equation satisfy (7.2.7).

Substitution gives that

$$C'(t)\,e^{-D(\nu)t} - D(\nu)\,C(t)\,e^{-D(\nu)t} + D(\nu)C(t)\,e^{-D(\nu)t} = -\mathcal{T}^T(\nu)\frac{\partial \widetilde{\boldsymbol{j}}}{\partial t}\ ,$$

or equivalently

$$C'(t)\, e^{-D(\nu)t} = -\mathcal{T}^T(\nu)\frac{\partial \widetilde{\boldsymbol{j}}}{\partial t}\ ,$$

then we have

$$C'(t) = -e^{D(\nu)t}\mathcal{T}^T(\nu)\frac{\partial \widetilde{\boldsymbol{j}}}{\partial t}\ .$$

Integrating the last equation from 0 to t with respect to t we get

$$C(t) - C(0) = -\int_0^t e^{D(\nu)\tau}\, [\mathcal{T}^T(\nu)\frac{\partial \widetilde{\boldsymbol{j}}}{\partial \tau}]d\tau\ ,$$

Substitution gives that

$$\boldsymbol{Y}(\nu, t) = C(0)e^{-D(\nu)t} - \int_0^t e^{-D(\nu)(t-\tau)}\, [\, \mathcal{T}^T(\nu)\frac{\partial \boldsymbol{j}}{\partial \tau}\,]d\tau\ .$$

Setting

$$e^{-D(\nu)(t-\tau)} = u \quad \Rightarrow \quad D(\nu)\, e^{-D(\nu)(t-\tau)}d\tau = du\ ,$$

and

$$\mathcal{T}^T(\nu)\frac{\partial \widetilde{\boldsymbol{j}}}{\partial \tau}\, d\tau = dv \quad \Rightarrow \quad \mathcal{T}^T(\nu)\, \widetilde{\boldsymbol{j}} = v\ .$$

Now, using integration by parts we have

$$\boldsymbol{Y}(\nu, t) = C(0)e^{-D(\nu)t} - \left\{ e^{-D(\nu)(t-\tau)}\mathcal{T}^T(\nu)\, \widetilde{\boldsymbol{j}}\, \Big|_0^t - \int_0^t D(\nu)\, e^{-D(\nu)(t-\tau)}[\, \mathcal{T}^T(\nu)\, \widetilde{\boldsymbol{j}}]d\tau \right\}\ .$$

Using (7.2.6) we have

$$\boldsymbol{Y}(\nu, t) = -[\, \mathcal{T}^T(\nu)\, \widetilde{\boldsymbol{j}}(\nu, t)\,] + D(\nu)\int_0^t e^{-D(\nu)(t-\tau)}[\, \mathcal{T}^T(\nu)\, \widetilde{\boldsymbol{j}}(\nu, \tau)\,]d\tau\ ,$$

and if $d_n(\nu) > 0$ we have

$$\boldsymbol{Y}_n(\nu, t) = -[\, \mathcal{T}^T(\nu)\, \widetilde{\boldsymbol{j}}(\nu, t)\,]_n + d_n(\nu)\int_0^t e^{-d_n(\nu)(t-\tau)}[\, \mathcal{T}^T(\nu)\, \widetilde{\boldsymbol{j}}(\nu, \tau)\,]_n d\tau\ ,$$

if $d_n(\nu) = 0$ we have

$$\boldsymbol{Y}_n(\nu, t) = -[\, \mathcal{T}^T(\nu)\, \widetilde{\boldsymbol{j}}(\nu, t)\,]_n\ ,$$

where $d_n(\nu)$, $n = 1, 2, 3$ are elements of the matrix $D(\nu)$; $[\mathcal{T}^T(\nu)\widetilde{\boldsymbol{j}}(\nu, \tau)]_n$ is the nth component of the vector.

Using formulae (7.2.8), (7.2.10)-(7.2.11) and given matrices $\mathcal{T}(\nu)$, $\mathcal{T}^T(\nu)$, $D(\nu)$

found in the first step we find the Fourier image of the electric fields $\widetilde{\mathbf{E}}(\nu, t)$. In the last step the electric fields $\mathbf{E}(x, t)$ is determined by inverse Fourier transform $\mathcal{F}_\nu^{-1}$ of $\widetilde{\mathbf{E}}(\nu, t)$, i.e

$$\mathbf{E}(x,t) = \mathcal{F}_\nu^{-1}[\widetilde{\mathbf{E}}](x,t) \ ,$$

$$\mathcal{F}_\nu^{-1}[\widetilde{\mathbf{E}}](x,t) = \frac{1}{(2\pi)^3} \int_{-\infty}^{-\infty} \int_{-\infty}^{-\infty} \int_{-\infty}^{-\infty} \widetilde{\mathbf{E}}(\nu, t)\, e^{-i\nu x} d\nu_1 d\nu_2 d\nu_3 \ , \tag{7.2.13}$$

7.3 Matrix formalism and symbolic implementation in MATLAB

Let us consider in details this matrix formalism and its computer implementation, which simultaneously transfer the symmetric positive definite matrix σ and the matrix $A(\nu)$ defined by (7.2.3) into the identity matrix and diagonal matrix with non-negative respectively. This matrix formalism is based on the following procedures of the matrix theory (Goldberg (1992)): finding $\sigma^{-1/2}$, constructing an orthogonal matrix $\mathcal{L}$ of eigenvectors of $\sigma^{-1/2}A(\nu)\sigma^{-1/2}$ and a diagonal matrix $D(\nu)$ of eigenvalues of $\sigma^{-1/2}A(\nu)\sigma^{-1/2}$.

7.3.1 Finding $\sigma^{-1/2}$

Let us consider a symmetric positive definite matrix σ. Matrix $\mathcal{Z}$ such that $\mathcal{Z}^2 = \sigma$ is denoted as $\sigma^{1/2}$. The inverse matrix to $\sigma^{1/2}$ is denoted as $\sigma^{-1/2}$, i.e $\sigma^{-1/2} = (\sigma^{1/2})^{-1}$. There are the following properties of $\sigma^{-1/2}$:

$$\sigma^{-1/2}\sigma = \sigma^{1/2} , \quad (\sigma^{-1/2})^{-1} = \sigma^{1/2} ;$$

$\sigma^{-1/2}$ is symmetric positive definite. The procedure of finding $\sigma^{-1/2}$ contains the following operations.

(O1) Find three linear independent eigenvectors of σ. From these eigenvectors form the matrix where each eigenvector is a column. This matrix is denoted by $\mathcal{P}$

(O2) Find three eigenvalues of σ. Form the diagonal matrix with these eigenvalues on diagonal. Denote this matrix as $\mathcal{M}$ i.e $\mathcal{M} = diag(\mu_1, \mu_2, \mu_3)$, where μ_1, μ_2 and μ_3 are eigenvalues of σ

Remark 7.3.1. *Since σ is positive definite then all its eigenvalues μ_1, μ_2 and μ_3 are real and positive.*

(O3) Calculate the square root of $\mathcal{M}$ by the formula

$$\mathcal{M}^{1/2} = diag(\sqrt{\mu_1}, \sqrt{\mu_2}, \sqrt{\mu_3}) ,$$

(O4) Find the matrix $\sigma^{1/2}$ by the formula $\sigma^{1/2} = \mathcal{P}\mathcal{M}^{1/2}\mathcal{P}^{-1}$, where is the matrix found by (O1), $\mathcal{P}^{-1}$is the inverse to $\mathcal{P}$, $\mathcal{M}^{1/2}$ is the matrix defined by (O3).

(O5) Find the matrix $\sigma^{-1/2}$ by means of the formula $\sigma^{-1/2} = (\sigma^{1/2})^{-1}$, where $(\sigma^{1/2})^{-1}$ is the inverse to $\sigma^{1/2}$

MATLAB commands of above mentioned matrix operations are listed below.

```
INPUT: Eps;
[EigVecSgm,EigValSgm] = eig(Sgm);
P=EigVecSgm;
PT=P'.;
M=EigValSgm;
Mh=sqrt(M);
SqrSgm=P*Mh*PT;
InvSrtSgm=inv(SqrSgm)
OUTPUT: SqrSgm, InvSrtSgm.
Here
Sgm, SqrSgm, InvSrtSgm
```

are σ, $\sigma^{1/2}$, $\sigma^{-1/2}$ respectively.

7.3.2 Constructing $D(\nu)$, $\mathcal{T}(\nu)$

Using the procedure described in Section(1.3.1) the matrix $\sigma^{-1/2}$ is found, if σ is known. As a result of it the matrix $\sigma^{-1/2}A(\nu)\sigma^{-1/2}$ may be found as well. The procedure of constructing matrices $D(\nu)$, $\mathcal{T}(\nu)$ satisfying (7.2.4) and (7.2.5) for given σ and $A(\nu)$ consists of the following operations.

(O6) Find three linear independent orthonormal eigenvectors of $\sigma^{-1/2}A(\nu)\sigma^{-1/2}$. From these eigenvectors form the matrix where each eigenvector is a column. Denote this matrix by $\mathcal{L}$.

(O7) Find three eigenvalues of $\sigma^{-1/2}A(\nu)\sigma^{-1/2}$. Form the diagonal matrix with these eigenvalues on diagonal. Denote this matrix as $D(\nu)$ i.e $D(\nu) = diag(d_1(\nu), d_2(\nu), d_3(\nu))$, where $d_1(\nu)$, $d_2(\nu)$, $d_3(\nu)$ are eigenvalues of $\sigma^{-1/2}A(\nu)\sigma^{-1/2}$.

Remark 7.3.2. *Since $\sigma^{-1/2}A(\nu)\sigma^{-1/2}$ is positive semi-definite then all its eigenvalues $d_1(\nu)$, $d_2(\nu)$ and $d_3(\nu)$ are real and non-negative.*

(O8) Calculate the matrix $\mathcal{T}(\nu)$ by the formula

$$\mathcal{T}(\nu) = \sigma^{-1/2}\mathcal{L}(\nu)\,.$$

(O9) Find the matrix $\mathcal{T}^T(\nu)$ as transpose to $\mathcal{T}(\nu)$.

MATLAB commands of constructing $D(\nu)$, $\mathcal{T}(\nu)$ are listed below.

```
INPUT: InvSrtSgm , S;
A = simplify(InvSrtSgm*S*InvSrtSgm);
[EigVecA, EigValA] = eig(A);
D = simplify(EigValA);
Q = simplify(EigVecA);
Q(:,1) = Q(:,1) ./ sqrt(sum (Q(:,1).^2));
Q(:,2) = Q(:,2) ./ sqrt(sum (Q(:,2).^2));
Q(:,3) = Q(:,3) ./ sqrt(sum (Q(:,3).^2));
T = InvSrtSgm * Q;
transT = T.';
OUTPUT: D, T, transT.
Here
InvSrtSgm, D, T, transT
```

are $\sigma^{-1/2}$, $D(\nu)$, $\mathcal{T}(\nu)$, $\mathcal{T}^T(\nu)$ respectively.

7.4 Image of the simulation of electric fields by (7.2.13)

We consider now examples of electric fields simulations obtained by the exact formula (7.2.13) for the solution of initial value problems for the time-dependent Maxwell's system with different tensors of dielectric permittivity. For all these examples the current density $\mathbf{j}$ was taken in the form

$$\mathbf{j}(x,t) = \mathbf{e^1}\,\delta(x_1)\delta(x_2)\delta(x_3)\delta(t)\ , \quad x = (x_1, x_2, x_3) \in \mathbf{R^3} \tag{7.4.1}$$

where $\mathbf{e^1} = (1,0,0)$, $\delta(\cdot)$ is the Dirac delta function. This form of the current density is related to a directional pulse electric source concentrated at the origin of coordinates at the time $t = 0$ in the direction $\mathbf{e}^1$. Results of the electric fields simulation are pictures of the all components of electric fields $\mathbf{E_1}(x_1, x_2, x_3, t)$, $\mathbf{E_2}(x_1, x_2, x_3, t)$, $\mathbf{E_3}(x_1, x_2, x_3, t)$ obtained for $x_1 = 0$ for different time.

And applying fourier transform to $\mathbf{j}$ with respect to x, we get $\widetilde{\mathbf{j}}$ in the form

$$\widetilde{\mathbf{j}} = \mathbf{e^1}\delta(t)\ . \tag{7.4.2}$$

Remark 7.4.1. *For simulations, substituting (7.4.2) into the equations (7.2.11) and (7.2.12) gives*
for $d_n(\nu) > 0$ we have;

$$\boldsymbol{Y}_n(\nu,t) = -[\,\mathcal{T}^T(\nu)\,\boldsymbol{e^1}\delta(t)\,]_n + d_n(\nu)\int_0^t e^{-d_n(\nu)(t-\tau)}[\,\mathcal{T}^T(\nu)\,\boldsymbol{e^1}\delta(\tau)\,]_n d\tau\ ,$$

or equivalently

$$\boldsymbol{Y}_n(\nu,t) = -[\,\mathcal{T}^T(\nu)\,\boldsymbol{e^1}\delta(t)\,]_n + d_n(\nu)\,e^{-d_n(\nu)t}[\,\mathcal{T}^T(\nu)\,\boldsymbol{e^1}\,]_n\ ,$$

and for $d_n(\nu) = 0$ we have;

$$\boldsymbol{Y}_n(\nu,t) = -[\,\mathcal{T}^T(\nu)\,\boldsymbol{e^1}\delta(t)\,]_n\ .$$

Using (Barton (1991)) we can write $\delta(t)$ as

$$\delta(t) = \lim_{\varepsilon\to 0}\frac{\sin(t/\varepsilon)}{\pi t}$$

where ε is a given small number and we can substitute $\delta(t)$ numerically into the last two equations for finding numerical solutions and simulations.

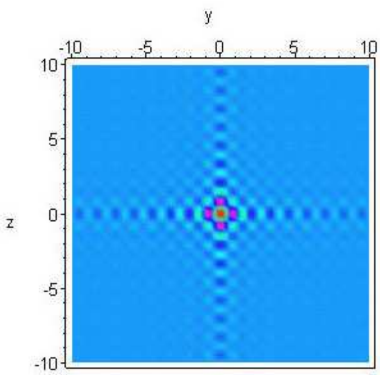
7.5 Examples of simulations for IVP systems

This section contains some examples of simulations for IVP for electric fields. Solutions will be simulated by using mathematical tools. For different matrix σ we have the different system. And also numerical results were used for simulations.

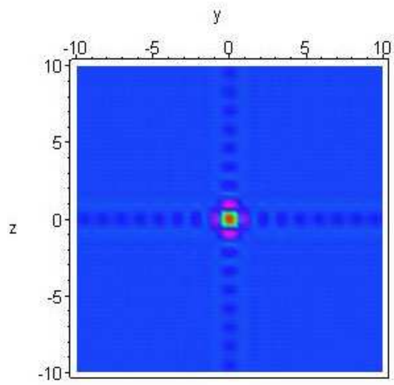
Example 7.5.1. The matrix σ is given by

$$\sigma = diag(10, 10, 40).$$

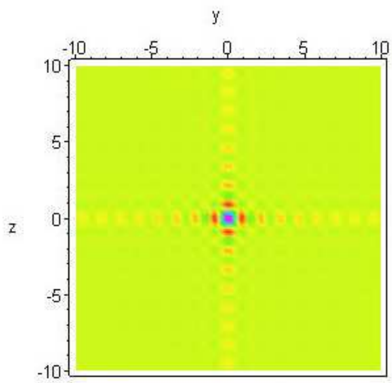
And $x = (x_1, x_2, x_3) \in \mathbf{R^3}$ and using numerical representation of Dirac delta function, 2-D level plots were generated for fixed t and given value for one of the coordinate, the other two coordinate were plotted in $[-10, 10] \times [-10, 10]$ interval. For the function $\mathbf{E_1}(x_1, x_2, x_3, t)$ we have this simulations;



(a) $t = 0$



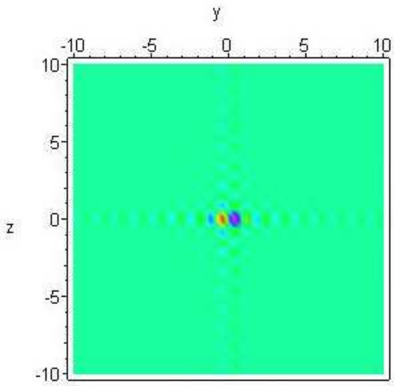
(b) $t = 2.0$



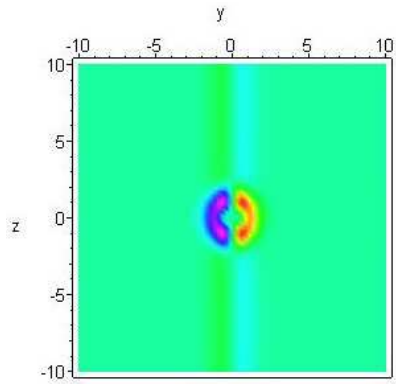
(c) $t = 6.0$

Figure 7.27: Example 6.4.1: 2D level plots of $\mathbf{E_1}$, (a) $\mathbf{E_1}(0, x_2, x_3, 0)$, (b) $\mathbf{E_1}(0, x_2, x_3, 2)$, (c) $\mathbf{E_1}(0, x_2, x_3, 6)$.

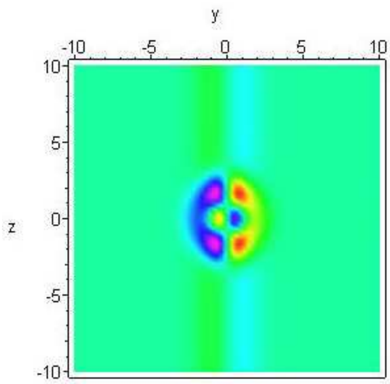
For the function $\mathbf{E_2}(x_1, x_2, x_3, t)$ we have the simulations as shown in below;



(a) $t = 0$



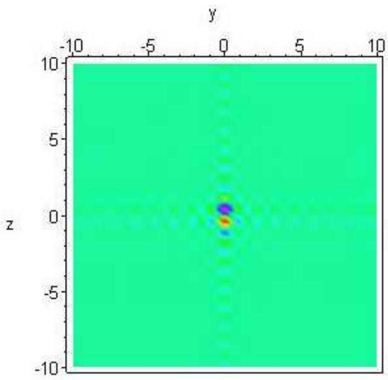
(b) $t = 2.0$



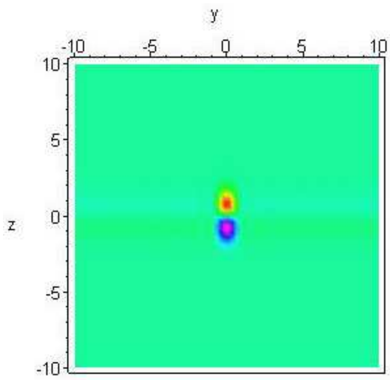
(c) $t = 6.0$

Figure 7.28: Example 6.4.1: 2D level plots of $\mathbf{E_2}$, (a) $\mathbf{E_2}(0, x_2, x_3, 0)$, (b) $\mathbf{E_2}(0, x_2, x_3, 3)$, (c) $\mathbf{E_2}(0, x_2, x_3, 6)$.

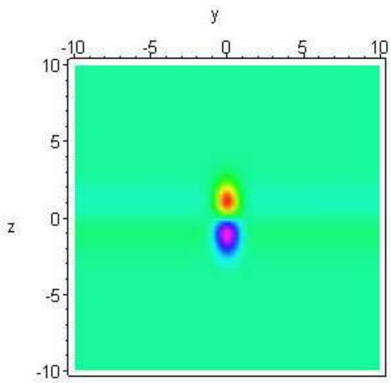
For the function $\mathbf{E_3}(x_1, x_2, x_3, t)$ we have the simulations as shown in below;



(a) $t = 0$



(b) $t = 2.0$



(c) $t = 6.0$

Figure 7.29: Example 6.4.1: 2D level plots of $\mathbf{E_3}$, (a) $\mathbf{E_3}(0, x_2, x_3, 0)$, (b) $\mathbf{E_3}(0, x_2, x_3, 3)$, (c) $\mathbf{E_3}(0, x_2, x_3, 6)$.

7.6 Analysis of the chapter7 study

1. We describe the efficient method for modeling electric fields by system (7.1.1)-(7.1.2).

2. Exact solution was found by matrix symbolic calculations and the inverse Fourier transform which is done numerically.

3. Results of electric fields are presented by 3-D pictures and animated movies.

4. Obtained formulae and results of simulation were analyzed.

CHAPTER EIGHT
CONCLUSION

The main result of this thesis are the following;

- Explicit formulae for solutions of initial boundary value problems with the Dirichlet, Neumann and Mixed boundary conditions were obtained.
- Explicit formulae for solutions of initial boundary value problems with the Dirichlet boundary condition were obtained by using generalized Green's function method.
- Explicit formulae for solutions of initial value problems with unbounded domain were obtained by using Fourier transform method for constructing Green's function.
- Explicit formulae for electric fields were obtained by using Fourier transform and matrix formalism.
- Obtained formulae were adjusted for the case of pulse point sources described by the Dirac delta function.
- using obtained formulae, 'Mathematica5' and 'MATLAB6.5' the simulations of diffusion phenomena were obtained.
- Results of simulations were presented by 1-D, 2-D and 3-D pictures and animated movies.
- Analysis of obtained formulas and results of simulations were described.

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Appendix A

STURM-LIOUVILLE PROBLEMS (SLP)

This part of the Appendix contains the solutions of the Sturm-Liouville problems (SLP) for an ordinary differential equations with different boundary conditions.

A.1 SLP with Dirichlet Boundary Condition

Consider the following SLP

$$y''(x) + \lambda y(x) = 0 \ , \quad x \in (0, \ell) \ , \tag{A.1.1}$$

$$y(0) = y(\ell) = 0 \ , \tag{A.1.2}$$

where ℓ is a given positive number, λ is a parameter.

For finding the solution of the SLP we have three cases for the parameter λ.

$$\lambda < 0 \quad (Case1) \ , \quad \lambda = 0 \quad (Case2) \ , \quad \lambda > 0 \quad (Case3) \ .$$

1. ***Case1*** For $\lambda < 0$ we have a general solution for (A.1.1) as in the form

$$y(x) = C_1 \exp(-\sqrt{-\lambda}x) + C_2 \exp(\sqrt{-\lambda}x) \ . \tag{A.1.3}$$

Substituting (A.1.3) to (A.1.1) we get :

$$y(0) = C_1 + C_2 = 0 \ ,$$

$$y(\ell) = C_1 \exp(-\sqrt{-\lambda}\ell) + C_2 \exp(\sqrt{-\lambda}\ell) = 0 \ .$$

This system has trivial solution, $C_1 = C_2 = 0$, so we conclude for $\lambda < 0$ there is no eigenvalues and eigenfunctions.

2. ***Case2*** For $\lambda = 0$ we have a general solution for (A.1.1) as in the form

$$y(x) = C_1 x + C_2 \ . \tag{A.1.4}$$

Substituting (A.1.4) to (A.1.1) we get :

$$y(0) = C_1\, 0 + C_2 = 0 \quad \Rightarrow \quad C_2 = 0 \ ,$$

and using the last equation we have

$$y(\ell) = C_1 \ell = 0 \quad \Rightarrow \quad C_1 = 0 \ ,$$

since $\ell \neq 0$. This implies that for $\lambda = 0$ we have zero solution, so we conclude for $\lambda = 0$ there is no eigenvalues and eigenfunctions.

3. ***Case3*** For $\lambda > 0$ we have a general solution for (A.1.1) as in the form

$$y(x) = C_1 \cos(\sqrt{\lambda}x) + C_2 \sin(\sqrt{\lambda}x) \ . \tag{A.1.5}$$

Substituting (A.1.5) to (A.1.1) we get :

$$y(0) = C_1 \cos(\sqrt{\lambda}0) + C_2 \sin(\sqrt{\lambda}0) = 0 \quad \Rightarrow \quad C_1 = 0 \ ,$$

and using the last equation we have

$$y(0) = C_2 \sin(\sqrt{\lambda}\ell) = 0 \ ,$$

for finding a solution we may select $C_2 \neq 0$ and this implies that $\sin(\sqrt{\lambda}\ell) = 0$ and $\sqrt{\lambda}\ell = k\pi$ for $k = 1, 2, ...$ that is

$$\lambda_k = \left(\frac{k\pi}{\ell}\right)^2 , \quad k = 1, 2, ...$$

So we have eigenvalues λ_k and corresponding eigenvectors $y_k(x) = C_2 \sin(\sqrt{\lambda_k} x)$ for $k = 1, 2, ...$ We can normalize this orthogonal functions by choosing $C_2 = \sqrt{\frac{2}{\ell}}$.

4. ***Conclusion:*** Generally the eigenvalue-eigenfunction problem (A.1.1), (A.1.2) has the solution

$$\lambda_k = (\frac{k\pi}{\ell})^2 , \quad y_k(x) = \sqrt{\frac{2}{\ell}} \sin(\sqrt{\lambda_k} x) , \quad k = 1, 2, ...$$

where λ_k are eigenvalues and $y_k(x)$ are eigenvectors corresponding to them.

A.2 SLP with Neumann Boundary Condition

Consider the following SLP

$$y''(x) + \lambda y(x) = 0 , \quad x \in (0, \ell) , \tag{A.2.1}$$

$$y'(0) = y'(\ell) = 0 , \tag{A.2.2}$$

where ℓ is a given positive number, λ is a parameter.

For finding the solution of the SLP we have three cases for the parameter λ.

$$\lambda < 0 \quad (Case1) , \quad \lambda = 0 \quad (Case2) , \quad \lambda > 0 \quad (Case3) .$$

1. ***Case1*** For $\lambda < 0$ we have a general solution for (A.2.1) as in the form

$$y(x) = C_1 \exp(-\sqrt{-\lambda} x) + C_2 \exp(\sqrt{-\lambda} x) , \tag{A.2.3}$$

and

$$y'(x) = C_1(-\sqrt{-\lambda}) \exp(-\sqrt{-\lambda} x) + C_2(\sqrt{-\lambda}) \exp(\sqrt{-\lambda} x) . \tag{A.2.4}$$

Substituting (A.2.4) to (A.2.1) we get :

$$y'(0) = (C_1 - C_2) = 0 ,$$

$$y'(\ell) = C_1 \exp(-\sqrt{-\lambda}\ell) - C_2 \exp(\sqrt{-\lambda}\ell) = 0 .$$

This system has trivial solution, $C_1 = C_2 = 0$, so we conclude for $\lambda < 0$ there is no eigenvalues and eigenfunctions.

2. ***Case2*** For $\lambda = 0$ we have a general solution for (A.2.1) as in the form

$$y(x) = C_1 x + C_2 \ . \tag{A.2.5}$$

Substituting (A.2.5) to (A.2.1) we get :

$$y'(0) = C_1 = 0 \ ,$$

and using the last equation we have

$$y'(\ell) = C_1 \ell = 0 \quad \Rightarrow \quad C_1 = 0 \ ,$$

since $\ell \neq 0$. This implies that for $\lambda = 0$ we have a solution if we choose $C_2 \neq 0$. So we have $y(x) = C_2$. So we conclude $\lambda = 0$ is an eigenvalue and $y(x) = C_2$ is corresponding eigenfunctions to $\lambda = 0$.

3. ***Case3*** For $\lambda > 0$ we have a general solution for (A.2.1) as in the form

$$y(x) = C_1 \cos(\sqrt{\lambda} x) + C_2 \sin(\sqrt{\lambda} x) \ , \tag{A.2.6}$$

$$y(x) = -\sqrt{\lambda} C_1 \sin(\sqrt{\lambda} x) + \sqrt{\lambda} C_2 \cos(\sqrt{\lambda} x) \ , \tag{A.2.7}$$

Substituting (A.2.7) to (A.2.1) we get :

$$y'(0) = -\sqrt{\lambda} C_1 \sin(\sqrt{\lambda} 0) + \sqrt{\lambda} C_2 \cos(\sqrt{\lambda} 0) = 0 \quad \Rightarrow \quad C_2 = 0 \ ,$$

and using the last equation we have

$$y'(\ell) = -\sqrt{\lambda} C_1 sin(\sqrt{\lambda} \ell) = 0 \ ,$$

for finding a solution we may select $C_2 \neq 0$ and this implies that $sin(\sqrt{\lambda}\ell) = 0$ and $\sqrt{\lambda}\ell = k\pi$ for $k = 1, 2, ...$ that is

$$\lambda_k = \left(\frac{k\pi}{\ell}\right)^2, \quad k = 1, 2, ...$$

So we have eigenvalues λ_k and corresponding eigenvectors $y_k(x) = C_1 \cos(\sqrt{\lambda_k} x)$ for $k = 1, 2, ...$ We can normalize this orthogonal functions by choosing $C_2 = \sqrt{\frac{2}{\ell}}$.

4. ***Conclusion:*** Generally the eigenvalue-eigenfunction problem (A.2.1), (A.2.2) has the solution

$$\lambda_k = \left(\frac{k\pi}{\ell}\right)^2 \ , \quad y_k(x) = \sqrt{\frac{2}{\ell}}\cos(\sqrt{\lambda_k}x) \ , \quad k = 0, 1, 2, ...$$

   where λ_k are eigenvalues and $y_k(x)$ are eigenvectors corresponding to them.

A.3 SLP with Mixed Boundary Condition

Consider the following SLP

$$y''(x) + \lambda y(x) = 0 \ , \quad x \in (0, \ell) \ , \tag{A.3.1}$$

$$y'(0) - \alpha y(0) = 0 \ , \tag{A.3.2}$$

$$y'(\ell) - \alpha y(\ell) = 0 \ , \tag{A.3.3}$$

where ℓ is a given positive number, λ is a parameter.

For finding the solution of the SLP we have three cases for the parameter λ.

$$\lambda < 0 \quad (Case1) \ , \quad \lambda = 0(\quad Case2) \ , \quad \lambda > 0 \quad (Case3) \ .$$

1. ***Case1*** For $\lambda < 0$ we have a general solution for (A.3.1) as in the form

$$y(x) = C_1 \exp(-\sqrt{-\lambda}x) + C_2 \exp(\sqrt{-\lambda}x) \ ,$$

   Set $-\lambda = \vartheta^2$. Then;

$$y(x) = C_1 e^{-\vartheta x} + C_2 e^{\vartheta x} \ , \tag{A.3.4}$$

$$y(x) = -C_1 \vartheta e^{-\vartheta x} + C_2 \vartheta e^{\vartheta x} \ . \tag{A.3.5}$$

   Substituting (A.3.4), (A.3.5) into (A.3.2), (A.3.3) we get;

$$y'(0) - \alpha y(0) = -C_1\vartheta + C_2\vartheta - \alpha(C_1 + C_2) = 0 \ ,$$

$$y'(\ell) + \alpha y(\ell) = -C_1 \vartheta e^{-\vartheta\ell} + C_2 \vartheta e^{\vartheta\ell} + \alpha(C_1 e^{-\vartheta\ell} + C_2 e^{\vartheta\ell}) = 0 \ .$$

We need to solve this system for C_1, C_1:

$$-C_1\vartheta + C_2\vartheta - \alpha(C_1 + C_2) = 0 \ ,$$

$$-C_1\vartheta e^{-\vartheta\ell} + C_2\vartheta e^{\vartheta\ell} + \alpha(C_1 e^{-\vartheta\ell} + C_2 e^{\vartheta\ell}) = 0 \ .$$

Or equivalently:

$$C_1(-\vartheta - \alpha) + C_2(\vartheta - \alpha) = 0 \ ,$$

$$C_1(-\vartheta + \alpha)e^{-\vartheta\ell} + C_2(\vartheta + \alpha)e^{\vartheta\ell} = 0 \ .$$

To find a non-zero solution we must have;

$$\begin{vmatrix} (-\vartheta - \alpha) & (\vartheta - \alpha) \\ (-\vartheta + \alpha)e^{-\vartheta\ell} & (\vartheta + \alpha)e^{\vartheta\ell} \end{vmatrix} = 0 \ ,$$

$$(-\vartheta - \alpha)(\vartheta + \alpha)e^{\vartheta\ell} - (\vartheta - \alpha)(-\vartheta + \alpha)e^{-\vartheta\ell} = 0$$

$$-(\vartheta + \alpha)^2 e^{\vartheta\ell} + (\vartheta - \alpha)^2 e^{-\vartheta\ell} = 0 \ ,$$

$$(\vartheta + \alpha)^2 e^{\vartheta\ell} = (\vartheta - \alpha)^2 e^{-\vartheta\ell} \ ,$$

$$\frac{(\vartheta + \alpha)^2}{(\vartheta - \alpha)^2} = e^{-2\vartheta\ell} \ ,$$

$$\left|\frac{(\vartheta + \alpha)}{(\vartheta - \alpha)}\right| = e^{-\vartheta\ell} \ .$$

But the last equation is true for $\vartheta = 0$. And this implies that $\lambda = 0$. That is for $\lambda < 0$ we have no eigenvalues and correspondingly no eigenfunctions.

2. ***Case2*** For $\lambda = 0$ we have a general solution for (A.3.1) as in the form

$$y(x) = C_1 x + C_2 \ ,$$

and

$$y'(x) = C_1 \ .$$

Substitution gives that;

$$y'(0) - \alpha y(0) = C_1 - \alpha C_2 = 0 \ ,$$

$$y'(\ell) + \alpha y(\ell) = C_1 + \alpha(C_1\ell + C_2) = 0 \ .$$

So we need to solve:

$$C_1 - \alpha C_2 = 0 \ ,$$

$$C_1 + \alpha(C_1\ell + C_2) = 0 \ .$$

But we have the following non-zero determinant

$$\begin{vmatrix} 1 & -\alpha \\ 1+\alpha & \alpha \end{vmatrix} = \alpha + (\alpha + \alpha^2\ell) = \alpha(2+\alpha\ell) \neq 0 \ .$$

Since $\alpha > 0$ and $\ell > 0$. We conclude that $\lambda = 0$ is not eigenvalue and there is no eigenfunction for $\lambda = 0$.

3. ***Case3*** For $\lambda > 0$ we have a general solution for (A.3.1) as in the form

$$y(x) = C_1 \cos(\sqrt{\lambda}x) + C_2 \sin(\sqrt{\lambda}x) \ ,$$

Set $-\lambda = \vartheta^2$. Then;

$$y(x) = C_1 \cos(\vartheta x) + C_2 \sin(\vartheta x) \ ,$$

$$y'(x) = -C_1\vartheta \sin(\vartheta x) + C_2\vartheta \cos(\vartheta x) \ .$$

Substituting these into (A.3.1), (A.3.2) we will find:

$$y'(0) - \alpha y(0) = C_2\vartheta - \alpha C_1 = 0 \ ,$$

$$y'(\ell)+\alpha y(\ell) = -C_1\vartheta \sin(\vartheta\ell)+C_2\vartheta \cos(\vartheta\ell)+\alpha(C_1 \cos(\vartheta\ell)+C_2 \sin(\vartheta\ell)) = 0 \ .$$

Hence we need to find:

$$\begin{vmatrix} -\alpha & \vartheta \\ -\vartheta \sin(\vartheta\ell) + \alpha \cos(\vartheta\ell) & \vartheta \cos(\vartheta\ell) + \alpha \sin(\vartheta\ell) \end{vmatrix} = 0 \ .$$

So,

$$-\alpha(\vartheta \cos(\vartheta\ell) + \alpha \sin(\vartheta\ell)) - \vartheta(-\vartheta \sin(\vartheta\ell) + \alpha \cos(\vartheta\ell)) = 0 \ ,$$

$$-\alpha\vartheta \cos(\vartheta\ell) - \alpha^2 \sin(\vartheta\ell) + \vartheta^2 \sin(\vartheta\ell) - \vartheta\alpha \cos(\vartheta\ell) = 0 \ ,$$

$$-2\alpha\vartheta \cos(\vartheta\ell) + (\vartheta^2 - \alpha^2) \sin(\vartheta\ell) = 0 \ .$$

Hence after rearranging we have;

$$\frac{\cos(\vartheta\ell)}{\sin(\vartheta\ell)} = \frac{(\vartheta^2 - \alpha^2)}{2\alpha\vartheta} \ ,$$

$$\frac{\cos(\vartheta\ell)}{\sin(\vartheta\ell)} = \frac{1}{2}\left(\frac{\vartheta}{\alpha} - \frac{\alpha}{\vartheta}\right) \ ,$$

$$\cot(\vartheta\ell) = \frac{1}{2}\left(\frac{\vartheta}{\alpha} - \frac{\alpha}{\vartheta}\right) ,$$

The last equation implies that there are infinitely many ϑ_k, $k = 1, 2, ...$ which satisfies the equation. So correspondingly there are infinitely many eigenvalues of the problem for $\lambda > 0$. Since, it was $\lambda = \vartheta^2$. So we have eigenfunctions

$$y_k(x) = C_1 \cos(\vartheta_k x) + C_2 \sin(\vartheta_k x) .$$

Choose

$$C_1 = \frac{\vartheta_k}{\alpha} C_k , \quad C_2 = C_k .$$

We get

$$\begin{aligned} y_k(x) &= \frac{\vartheta_k}{\alpha}\cos(\vartheta_k x) + C_k \sin(\vartheta_k x) \\ &= C_k \left(\frac{\vartheta_k}{\alpha}\cos(\vartheta_k x) + \sin(\vartheta_k x)\right) \\ &= C_k \sin(\vartheta_k x + \varphi_k) , \end{aligned}$$

where

$$\varphi_k = \arctan\left(\frac{\vartheta_k}{\alpha}\right) , \quad k = 1, 2, ...$$

4. ***Conclusion:*** We have eigenfunctions

$$y_k(x) = C_k \sin(\vartheta_k x + \varphi_k) , \quad k = 1, 2, ...$$

and correspondingly the eigenvalues $\lambda_k = \vartheta_k^2$, where ϑ_k, $k = 1, 2, ...$ are a solutions of

$$\cot(\vartheta_k\ell) = \frac{1}{2}\left(\frac{\vartheta_k}{\alpha} - \frac{\alpha}{\vartheta_k}\right) ,$$

and C_k is chosen as follows

$$\int_0^\ell y_k^2(x)dx = \int_0^\ell C_k^2 \sin^2(\vartheta_k x + \varphi_k)dx = C_k^2 \int_0^\ell \sin^2(\vartheta_k x + \varphi_k)dx = 1 .$$

Hence

$$C_k = \frac{1}{(\int_0^\ell \sin^2(\vartheta_k x + \varphi_k)dx)^{1/2}} .$$

So

$$\begin{aligned} \int_0^\ell \sin^2(\vartheta_k x + \varphi_k)dx &= \int_0^\ell \frac{1 - \cos 2(\vartheta_k x + \varphi_k)}{2} dx \\ &= \frac{x}{2}\bigg|_0^\ell - \frac{\sin 2(\vartheta_k x + \varphi_k)}{4\vartheta_k}\bigg|_0^l \end{aligned}$$

$$
\begin{aligned}
&= \frac{\ell}{2} - \frac{\sin 2(\ell x + \varphi_k)}{4\vartheta_k} + \frac{\sin 2\vartheta_k}{4\vartheta_k} \\
&= \frac{2\ell\vartheta_k - \sin 2(\ell x + \varphi_k) + \sin 2\vartheta_k}{4\vartheta_k}
\end{aligned}
$$

Hence

$$
C_k = \sqrt{\frac{4\vartheta_k}{2\ell\vartheta_k - \sin 2(\ell x + \varphi_k) + \sin 2\vartheta_k}}\ , \quad k = 1, 2, ...
$$

Appendix B

B.1 Definitions of Dirac Delta Function

A generalized function $\delta(x - x^0)$ defined by

$$\int_{-\infty}^{\infty} \delta(x - x^0)\varphi(x)dx = \varphi(x^0)$$

for any continuous function $\varphi(x^0)$ is called the Dirac delta function concentrated at $x = x^0$. Here $x \in \mathbf{R^1}$ and $x^0 \in \mathbf{R^1}$ is a parameter.

Let $x = (x_1, x_2, \ldots, x_n)$, $x^0 = (x_1^0, x_2^0, \ldots, x_n^0)$ then the Dirac delta function $\delta(x - x^0) = \delta(x_1 - x_1^0) \ldots \delta(x_n - x_n^0)$ defined by

$$\int_{-\infty}^{\infty} \delta(x - x^0)\varphi(x)dx = \varphi(x^0)$$

for any $\varphi(x) = \varphi(x_1^0, x_2^0, \ldots, x_n^0)$ continuous function of $x_1^0, x_2^0, \ldots, x_n^0$ variables.

B.1.1 Properties Of The Dirac Delta Function

1. Let $x \in \mathbf{R}$, $x^0 \in \mathbf{R}$, $\theta(x)$ be the Heaviside (step) function, which is defined by

   $$\theta(x) = \begin{cases} 1, & x \geq 0 \\ 0, & x < 0 \end{cases}$$

   then

   $$\frac{d}{dx}[\theta(x)] = \delta(x)$$

2. Let $f(x) \in \mathbf{C^1}(x \geq x^0) \cap \mathbf{C^1}(x \leq x^0)$. Then a generalized derivative $\frac{d}{dx}f$ is defined by
$$\frac{d}{dx}[f(x)] = \{f'(x)\} + [f]_{x=x^0}\ \delta(x - x^0)\ ,$$
where $\{f'(x)\}$ is the classical derivative at all points where this derivative exists.

Remark B.1.1. *$\{f'(x)\}$ is not defined at $x = x^0$*

$$[f]_{x=x^0} = f(x^0 + 0) - f(x^0 - 0) \qquad (Jump)$$

Remark B.1.2. *Let $\theta(x - x^0)$ be Heaviside function*

$$\frac{d}{dx}[\theta(x - x^0)] = \{0\} + 1.\delta(x - x^0)$$

or equivalently we have

$$\frac{d}{dx}[\theta(x - x^0)] = \delta(x - x^0)$$

where
$$\theta(x - x^0) = \begin{cases} 1, & x \geq x^0 \\ 0, & x < x^0 \end{cases}$$

definition of derivative for any function such that $f(x)$;

$$\lim_{x \to a} \frac{f(x) - f(a)}{x - a}$$

is not defined,
$$\theta(x - x^0) = \begin{cases} 0, & x > x^0 \\ 0, & x < x^0 \end{cases}$$

for $x = x^0$, $\{\theta(x - x^0)\}$ is not defined

3. Let $x = (x_1, x_2, \ldots, x_n) \in \mathbf{R^n}$, $(x_1^0, x_2^0, \ldots, x_n^0) \in \mathbf{R^n}$ then

$$f(x)\delta(x - x^0) = f(x^0)\delta(x - x^0)$$

Appendix C

C.1 1D Fourier Transform And Its Properties

Let $\mathbf{C}_0^\infty$ be a class of infinitely differentiable functions which are equal to zero outside of interval $[-A, A]$ (for each function, A is different).

Definition C.1.1. The transform F_x defined by

$$F_x[\varphi](\nu) = \int_{-\infty}^{\infty} \varphi(x) e^{i\nu x} dx \ , \tag{C.1.1}$$

is called the Fourier transform with respect to x variable; ν is a parameter of Fourier transform; $\widetilde{\varphi}(\nu) = F_x[\varphi](\nu)$ is the image of Fourier transform; $i^2 = -1$, $\nu \in \mathbf{R}$.

This is $1 - D$ Fourier transform.

PROPERTIES :

1.
$$\frac{d^m}{d\nu^m}\widetilde{\varphi}(\nu) = \frac{d^m}{d\nu^m}F_x[\varphi(x)](\nu) = F_x[(ix)^m \varphi(x)](\nu)$$

Proof: Substituting (C.1.1) into the property(1) we have

$$\frac{d^m}{d\nu^m}\widetilde{\varphi}(\nu) = \frac{d^m}{d\nu^m}F_x[\varphi(x)](\nu) = \frac{d^m}{d\nu^m}[\int_{-\infty}^{\infty} \varphi(x) e^{i\nu x} dx]$$

$$= \int_{-\infty}^{\infty} \frac{d^m}{d\nu^m}[\varphi(x) e^{i\nu x}] dx = \int_{-\infty}^{\infty} \varphi(x) \frac{d^m}{d\nu^m}[e^{i\nu x}] dx$$

$$= \int_{-\infty}^{\infty} \varphi(x)(ix)^m e^{i\nu x} dx = F_x[(ix)^m \varphi(x)](\nu) \ .$$

Property(1) is proved.

2.
$$F_x \left[\frac{d^m}{dx^m} \varphi(x) \right] (\nu) = (-i\nu)^m F_x[\varphi](\nu)$$

Proof: Using (C.1.1) we have

$$F_x \left[\frac{d^m}{dx^m} \varphi(x) \right] (\nu) = \int_{-\infty}^{\infty} \frac{d^m}{dx^m} \varphi(x) e^{i\nu x} dx$$

By using integration by parts we get

$$\frac{d^{m-1}}{dx^{m-1}} e^{i\nu x}|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{d^{m-1}}{dx^{m-1}} \varphi(x) \left[\frac{d}{dx}(e^{i\nu x}) \right] dx$$

or equivalently
$$(-i\nu) \int_{-\infty}^{\infty} \frac{d^{m-1}}{dx^{m-1}} \varphi(x) e^{i\nu x} dx$$

Applying integration by parts $m-1$ times we get

$$F_x \left[\frac{d^m}{dx^m} \varphi(x) \right] (\nu) = \int_{-\infty}^{\infty} \varphi(x) e^{i\nu x} dx = (-i\nu)^m F_x[\varphi](\nu) \ .$$

Property(2) is proved.

3. Let
$$(f * g)(x) = \int_{-\infty}^{\infty} f(\xi) g(x - \xi) d\xi$$

be the convolution of f and g.
Then

$$F_x[(f * g)(\nu)] = F_x[f(x)](\nu) \cdot F_x[g(x)](\nu) = \widetilde{f}(\nu) \widetilde{g}(\nu) \ , \forall f, g \in \mathbf{C}_0^\infty$$

4.
$$F_x[\delta(x - x^0)](\nu) = e^{i\nu x^0} \ ,$$

in particular if $x^0 = 0$ then

$$F_x[\delta(x)](\nu) = 1 \ .$$

5. Let the operator F_ν^{-1} is defined by

$$F_\nu^{-1}[\psi(\nu)](x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \psi(\nu)e^{-i\nu x}d\nu$$

for any $\psi(\nu) \in \mathbf{C}_0^\infty$ for which the integral $\int_{-\infty}^{\infty} |\psi(\nu)|d\nu$ exists.

Then

$$F_\nu^{-1}[F_x[\varphi](\nu)](x) = \varphi(x) \ , \quad \forall\, \varphi(x) \in \mathbf{C}_0^\infty \ .$$

Definition C.1.2. The operator F_ν^{-1} is called the inverse Fourier transform operator.

C.2 2D Fourier Transform And Its Properties

Let $\mathbf{C}_0^\infty$ be a class of infinitely differentiable functions depending on $x_1,\ x_2$ variables which are equal to zero outside $x_1^2+x_2^2<A^2$.

Definition C.2.1. The transform of the form

$$\widetilde{\varphi}(\nu)=F_x[\varphi(x)](\nu)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\varphi(x)e^{i\nu x}dx\ , \tag{C.2.1}$$

where $dx=dx_1dx_2$ and $\nu x=\nu_1x_1+\nu_2x_2$, for any $\varphi(x)\in\mathbf{C}_0^\infty$ is called the Fourier transform with respect to $x=(x_1,x_2)\in\mathbf{R^2}$; $\nu=(\nu_1,\nu_2)\in\mathbf{R^2}$ is a parameter, $\widetilde{\varphi}(\nu)=F_x[\varphi(x)](\nu)$ is the image of Fourier transform; $i^2=-1$, $\nu\in\mathbf{R^2}$.

This is 2D Fourier transform.

PROPERTIES :

1.
$$\begin{aligned}\frac{d^{m_1+m_2}}{d\nu_1^{m_1}d\nu_2^{m_2}}\widetilde{\varphi}(\nu_1,\nu_2)&=\frac{d^{m_1+m_2}}{d\nu_1^{m_1}d\nu_2^{m_2}}F_{x_1,x_2}[\varphi(x_1,x_2)](\nu_1,\nu_2)\\&=F_{x_1,x_2}\left[(ix_1)^{m_1}(ix_2)^{m_2}\varphi(x_1,x_2)\right](\nu_1,\nu_2)\end{aligned}$$

2.
$$F_x\left[\frac{d^{m_1+m_2}}{dx_1^{m_1}dx_2^{m_2}}\varphi(x_1,x_2)\right](\nu_1,\nu_2)=(-i\nu_1)_1^m(-i\nu_2)_2^mF_{x_1,x_2}[\varphi(x_1,x_2)](\nu_1,\nu_2)$$

3. Let
$$(f\star g)(x_1,x_2)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}f(\xi)g(x_1-\xi_1,x_2-\xi_2)d\xi_1d\xi_2$$
be the convolution of f and g.
Then
$$F_{x_1,x_2}[(f\star g)(\nu_1,\nu_2)]=F_{x_1,x_2}[f(x_1,x_2)](\nu_1,\nu_2).F_{x_1,x_2}[g(x_1,x_2)](\nu_1,\nu_2)$$
$$=\widetilde{f}(\nu_1,\nu_2)\widetilde{g}(\nu_1,\nu_2)$$
for all $f,g\in\mathbf{C}_0^\infty$.

4.
$$F_{x_1,x_2}[\delta(x_1-x_1^0)\delta(x_2-x_2^0)](\nu)=e^{i\nu_1x_1^0}e^{i\nu_2x_2^0}\ ,$$

in particular if $x_1^0 = x_2^0 = 0$ then

$$F_{x_1,x_2}[\delta(x_1)\delta(x_2)](\nu_1, \nu_2) = 1 \ .$$

5. Let the operator F_ν^{-1} is defined by

$$F_{\nu_1,\nu_2}^{-1}[\psi(\nu_1, \nu_2)](x) = (\frac{1}{2\pi})^2 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi(\nu_1, \nu_2) e^{-i(\nu_1 x_1 + \nu_2 x_2)} d\nu_1 d\nu_{12} \ ,$$

for any $\psi(\nu_1, \nu_2) \in \mathbf{C}_0^\infty$

Then

$$F_{\nu_1,\nu_2}^{-1} \left[F_{x_1,x_2}[\varphi](\nu_1, \nu_2) \right] (x_1, x_2) = \varphi(x_1, x_2) \ , \quad \forall \ \varphi(x_1, x_2) \in \mathbf{C}_0^\infty \ .$$

Definition C.2.2. The operator F_{ν_1,ν_2}^{-1} is called the inverse Fourier transform operator.

Appendix D

D.1 Green's function of IVP for the Operator $\left(\frac{d}{dt} + a^2\right)$

Definition D.1.1. A generalized function $G(t,\tau)$ is called Green's function of IVP for $(\frac{d}{dt} + a^2)$ if

$$\frac{d}{dt}G(t,\tau) + a^2 G(t,\tau) = \delta(t-\tau)\ , t \in \mathbf{R}, \tag{D.1.1}$$

$$G(t,\tau)|_{t<\tau} = 0\ . \tag{D.1.2}$$

Here τ is a parameter, $\tau \in \mathbf{R}$.

Lemma D.1.1. *let $\theta(t)$ be the Heaviside function; $\mathbb{Z}(t,\tau)$ be a solution of*

$$\frac{d}{dt}\mathbb{Z}(t,\tau) + a^2\mathbb{Z}(t,\tau) = 0\ , \quad t > \tau\ , \tag{D.1.3}$$

$$\mathbb{Z}(\tau,\tau) = 1\ . \tag{D.1.4}$$

Then $G(t,\tau) = \theta(t-\tau)\mathbb{Z}(t,\tau)$ is the Green's function for $(\frac{d}{dt} + a^2)$.

Proof D.1.1. *Let $\theta(t-\tau)$ be the Heaviside function; $\mathbb{Z}(t,\tau)$ be a solution of (D.2.3),(D.2.4)*

$$G(t,\tau) = \theta(t-\tau)\mathbb{Z}(t,\tau)\ . \tag{D.1.5}$$

Applying operators $\frac{d}{dt}$ and $\frac{d}{dt} + a^2$ we find

$$\frac{d}{dt}G(t,\tau) = \frac{d}{dt}\left\{\theta(t-\tau)\mathbb{Z}(t,\tau)\right\}$$

$$= \frac{d}{dt}(\theta(t-\tau))\mathbb{Z}(t,\tau) + \theta(t-\tau)\frac{d}{dt}(\mathbb{Z}(t,\tau))$$

by using the property(1) we get

$$= \delta(t-\tau)\mathbb{Z}(t,\tau) + \theta(t-\tau)\frac{d}{dt}(\mathbb{Z}(t,\tau)) \ ,$$

by using property(3) we have

$$= \mathbb{Z}(\tau,\tau)\delta(t-\tau) + \theta(t-\tau)\frac{d}{dt}(\mathbb{Z}(t,\tau)) \ ,$$

using eqn(D.2.4) we get

$$\frac{d}{dt}G(t,\tau) = \delta(t-\tau) + \theta(t-\tau)\frac{d}{dt}(\mathbb{Z}(t,\tau)) \ .$$

Using the last relation we find

$$\frac{d}{dt}G(t,\tau) + a^2G(t,\tau) = \delta(t-\tau) + \theta(t-\tau)\frac{d}{dt}(\mathbb{Z}(t,\tau)) + a^2\theta(t-\tau)\mathbb{Z}(t,\tau)$$

$$= \delta(t-\tau) + \theta(t-\tau)\left\{\frac{d}{dt}(\mathbb{Z}(t,\tau)) + a^2\mathbb{Z}(t,\tau)\right\} = \delta(t-\tau)$$

And also by using the definition of Heaviside function we can say that

$$G(t,\tau)|_{t<\tau} = \{\theta(t-\tau)\mathbb{Z}(t,\tau)\}\,|_{t<\tau} = 0 \ .$$

Therefore $G(t,\tau)$ is the Green's function of IVP for the operator $(\frac{d}{dt} + a^2)$.

Lemma D.1.2. *The solution of (D.2.3), (D.2.4) is given by*

$$\mathbb{Z}(t,\tau) = e^{-a^2(t-\tau)} \ , \quad t > \tau \ . \tag{D.1.6}$$

Proof D.1.2. *A generalized solution of (D.2.3) is given by*

$$\mathbb{Z}(t,\tau) = c_1 e^{-a^2(t-\tau)} \ , \tag{D.1.7}$$

c_1 is an arbitrary constant, substituting (D.1.7) into (D.2.4) we find

$$\mathbb{Z}(\tau,\tau) = 1 \ \Rightarrow \ c_1 e^{-a^2(\tau-\tau)} = 1 \ \Rightarrow \ c_1 e^{-a^2(0)} = 1 \ \Rightarrow \ c_1 = 1 \ .$$

Hence $\mathbb{Z}(t,\tau) = e^{-a^2(t-\tau)}$ satisfies (D.2.3),(D.2.4).

Corollary D.1.3. *The Green's function of IVP for $(\frac{d}{dt} + a^2)$ is given by*

$$G(t,\tau) = \theta(t-\tau)e^{-a^2(t-\tau)} \ , t \in \mathbf{R}, \ \tau \in \mathbf{R} \ ,$$

where $\theta(t)$ is the Heaviside function.

Lemma D.1.4. *Let $G(t,\tau)$ be the Green's function of IVP for $(\frac{d}{dt}+a^2)$; $f(t)$ be an arbitrary continuous function.*

Then

$$y(t) = \int_{-\infty}^{\infty} G(t,\tau)\overline{f(\tau)}d\tau \ , \tag{D.1.8}$$

is a solution of the following IVP

$$\frac{d}{dt}y(t) + a^2 y(t) = f(t), \ t > 0 \ , \tag{D.1.9}$$

$$y(0) = 0 \ , \tag{D.1.10}$$

here

$$\overline{f}(\tau) = \begin{cases} f(t) & , \quad t \geq 0 \\ 0 & , \quad t < 0 \end{cases}$$

Proof D.1.3. *Applying operators $\frac{d}{dt}$, $\frac{d}{dt}+a^2$ to (D.1.8) we find*

$$\frac{d}{dt}y(t) = \frac{d}{dt}\left[\int_{-\infty}^{\infty} G(t,\tau)\overline{f(\tau)}d\tau\right] = \int_{-\infty}^{\infty}\frac{d}{dt}[G(t,\tau)]\overline{f(\tau)}d\tau$$

and

$$\frac{d}{dt}y(t) + a^2 y(t) = \int_{-\infty}^{\infty}\frac{d}{dt}[G(t,\tau)]\overline{f(\tau)}d\tau + a^2\int_{-\infty}^{\infty} G(t,\tau)\overline{f(\tau)}d\tau$$

$$\int_{-\infty}^{\infty}\left\{\frac{d}{dt}G(t,\tau) + a^2 G(t,\tau)\right\}\overline{f(\tau)}d\tau = \int_{-\infty}^{\infty}\delta(t-\tau)\overline{f(\tau)}d\tau = \overline{f(t)} = f(t), \ t > 0 \ .$$

This means that $y(t)$ satisfies (D.1.9).

Let us consider (D.1.8);

$$y(t) = \int_{-\infty}^{\infty} G(t,\tau)\overline{f(\tau)}d\tau = y(t) = \int_{-\infty}^{\infty}\theta(t-\tau)e^{-a^2(t-\tau)}\overline{f(\tau)}d\tau$$

$$\left| \begin{array}{lcl} \overline{f(\tau)} = 0 & , & \tau < 0 \\ \theta(t-\tau) = 0 & , & t < \tau \end{array} \right|$$

implies that

$$y(t) = \int_{-\infty}^{0} 0.d\tau + \int_{0}^{t} e^{-a^2(t-\tau)}f(\tau)d\tau + \int_{0}^{\infty} 0.d\tau = \int_{0}^{t} e^{-a^2(t-\tau)}f(\tau)d\tau \ ,$$

so we have

$$y(t) = \int_0^t e^{-a^2(t-\tau)} f(\tau) d\tau \ .$$

Using the last equality we find that $y(0) = 0$, *therefore* $y(t)$ *satisfies (D.1.9),(D.1.10).*

D.2 Green's function of IVP for the Operator $\left(\frac{d^2}{dt^2}+a^2\right)$

Definition D.2.1. A generalized function $G(t,\tau)$ is called Green's function of IVP for $(\frac{d^2}{dt^2}+a^2)$ if

$$\frac{d^2}{dt^2}G(t,\tau)+a^2G(t,\tau)=\delta(t-\tau)\ ,t\in\mathbf{R}, \tag{D.2.1}$$

$$G(t,\tau)|_{t<\tau}=0\ . \tag{D.2.2}$$

Here τ is a parameter, $\tau\in\mathbf{R}$.

Lemma D.2.1. *let $\theta(t)$ be the Heaviside function; $\mathbb{Z}(t,\tau)$ be a solution of*

$$\frac{d^2}{dt^2}\mathbb{Z}(t,\tau)+a^2\mathbb{Z}(t,\tau)=0\ ,\quad t>\tau\ , \tag{D.2.3}$$

$$\mathbb{Z}(\tau,\tau)=0\ ,\qquad \frac{d}{dt}\mathbb{Z}(t,\tau)=1. \tag{D.2.4}$$

Then $G(t,\tau)=\theta(t-\tau)\mathbb{Z}(t,\tau)$ is the Green's function for $(\frac{d^2}{dt^2}+a^2)$.

Proof D.2.1. *Let $\theta(t-\tau)$ be the Heaviside function; $\mathbb{Z}(t,\tau)$ be a solution of (D.2.3),(D.2.4)*

$$G(t,\tau)=\theta(t-\tau)\mathbb{Z}(t,\tau)\ . \tag{D.2.5}$$

Applying operators $\frac{d}{dt}$, $\frac{d^2}{dt^2}$, $\frac{d^2}{dt^2}+a^2$ we find

$$\frac{d}{dt}G(t,\tau)=\frac{d}{dt}\left\{\theta(t-\tau)\mathbb{Z}(t,\tau)\right\}$$

$$=\frac{d}{dt}(\theta(t-\tau))\mathbb{Z}(t,\tau)+\theta(t-\tau)\frac{d}{dt}(\mathbb{Z}(t,\tau))$$

by using the property(1) we get

$$=\delta(t-\tau)\mathbb{Z}(t,\tau)+\theta(t-\tau)\frac{d}{dt}(\mathbb{Z}(t,\tau))\ ,$$

by using property(3) we have

$$=\mathbb{Z}(\tau,\tau)\delta(t-\tau)+\theta(t-\tau)\frac{d}{dt}(\mathbb{Z}(t,\tau))\ ,$$

using eqn(D.2.4) we get

$$\frac{d}{dt}G(t,\tau)=\theta(t-\tau)\frac{d}{dt}(\mathbb{Z}(t,\tau))\ ,$$

and applying $\frac{d}{dt}$ to the last equality we get

$$\frac{d^2}{dt^2}G(t,\tau) = \frac{d}{dt}\left\{\theta(t-\tau)\frac{d}{dt}(\mathbb{Z}(t,\tau))\right\}$$

$$= \frac{d}{dt}\theta(t-\tau)\frac{d}{dt}\mathbb{Z}(t,\tau) + \theta(t-\tau)fracd^2dt^2\mathbb{Z}(t,\tau)\ ,$$

by using the property(1) we get

$$= \delta(t-\tau)\frac{d}{dt}\mathbb{Z}(t,\tau) + \theta(t-\tau)fracd^2dt^2\mathbb{Z}(t,\tau)\ ,$$

by using property(3) we have

$$= \delta(t-\tau)\frac{d}{dt}\mathbb{Z}(t,\tau)|_{t=\tau} + \theta(t-\tau)fracd^2dt^2\mathbb{Z}(t,\tau)\ ,$$

using eqn(D.2.4) we get

$$= \delta(t-\tau) + \theta(t-\tau)fracd^2dt^2\mathbb{Z}(t,\tau)\ .$$

Then we have

$$\frac{d^2}{dt^2}G(t,\tau) + a^2G(t,\tau) = \delta(t-\tau) + \theta(t-\tau)\frac{d^2}{dt^2}(\mathbb{Z}(t,\tau)) + a^2\theta(t-\tau)\mathbb{Z}(t,\tau)$$

$$= \delta(t-\tau) + \theta(t-\tau)\left\{\frac{d^2}{dt^2}(\mathbb{Z}(t,\tau)) + a^2\mathbb{Z}(t,\tau)\right\} = \delta(t-\tau)$$

And also by using the definition of Heaviside function we can say that

$$G(t,\tau)|_{t<\tau} = \{\theta(t-\tau)\mathbb{Z}(t,\tau)\}\,|_{t<\tau} = 0\ .$$

Therefore $G(t,\tau)$ is the Green's function of IVP for the operator $(\frac{d}{dt} + a^2)$.

Lemma D.2.2. *The solution of (D.2.3), (D.2.4) is given by*

$$\mathbb{Z}(t,\tau) = \frac{sin[a(t-\tau)]}{a}\ ,\quad t>\tau\ . \tag{D.2.6}$$

Proof D.2.2. *We will apply $\frac{d}{dt}$ and $\frac{d^2}{dt^2}$ to (D.2.6)*

$$\frac{d}{dt}\left\{\frac{sin[a(t-\tau)]}{a}\right\} = \frac{cos[a(t-\tau)]}{a}\ , a = cos[a(t-\tau)]\ ,$$

$$\frac{d^2}{dt^2}\left\{\frac{sin[a(t-\tau)]}{a}\right\} = \frac{d}{dt}\{cos[a(t-\tau)]\} = -a\ , sin[a(t-\tau)]\ .$$

Then we get

$$\frac{d^2}{dt^2}\mathbb{Z}(t,\tau) + a^2\mathbb{Z}(t,\tau) = -asin[a(t-\tau)] + a\frac{a^2 sin[a(t-\tau)]}{a} = 0\ .$$

Therefore $\mathbb{Z}(t,\tau)$ satisfies the differential equation (D.2.3), and using (D.2.4) we have

$$\mathbb{Z}(\tau,\tau) = \frac{sin[a(\tau-\tau)]}{a} = 0$$

and

$$\frac{d}{dt}\mathbb{Z}(t,\tau)|_{t=\tau} = cos[a(\tau-\tau)] = 0\ .$$

that is $\mathbb{Z}(t,\tau)$ is the solution of (D.2.3), (D.2.4).

Corollary D.2.3. *The Green's function of IVP for $(\frac{d^2}{dt^2} + a^2)$ is given by*

$$G(t,\tau) = \theta(t-\tau)\frac{sin[a(t-\tau)]}{a}\ , t \in \mathbf{R},\ \tau \in \mathbf{R}\ ,$$

where $\theta(t)$ is the Heaviside function.