VALUE OF LAMBDA, $\lambda$ FOR CRANK-NICOLSON
SCHEME ON SOLVING DIFFUSION EQUATION

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I declare that the work presented in this thesis is to the best of my knowledge and belief, original and my own work except as acknowledged in the text.

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ABSTRACT

The main purpose of this study is to investigate if a specific value of lambda,
\[ \lambda = \frac{k(\Delta t)}{2\rho C_p(\Delta x)^2} \]
exists where \( \Delta t \), \( \Delta x \), \( k \), \( \rho \) and \( C_p \) represent time step, length increment in x direction, coefficient thermal diffusivity, density and specific heat, respectively. The specific value is able to achieve the most desirable approximate solution for any combination of \( \Delta t \) and \( \Delta x \) base on the Crank-Nicolson scheme. A basic diffusion equation is discretized by Crank-Nicolson scheme and the tridiagonal matrix system is solved by Crout decomposition algorithm. All the data have been processed by diffusion equation being use in analysis to compare with the analytical solution. The specific value of the \( \lambda \) is not exist for any combination of \( \Delta t \) and \( \Delta x \). However, the study resulted that a value of \( \lambda \) is happened to exist for each \( \Delta t = 0.3\Delta x \) which is able to ensure the approximate solution executed in the highly accuracy.
NILAI LAMBDA, \( \lambda \) BAGI KAEDAH CRANK-NICOLSON DALAM PENYELESAIAN PERSAMAAN PENYEBARAN HABA

ABSTRAK

Penyelidikan ini dijalankan untuk mengenal pasti sama ada lambda, \( \lambda = \frac{k(\Delta t)}{2\rho C_p (\Delta x)^2} \) dengan \( \Delta t \) adalah perubahan masa, \( \Delta x \) adalah perubahan jarak secara melintang, \( k \) adalah pekali penyebaran terma, \( \rho \) adalah ketumpatan bahan dan \( C_p \) adalah haba tentu, wujud pada sesuatu nilai yang khusus apabila nilai khusus tersebut mencapai hasil penyelesaian berangka yang paling hampir kepada penyelesaian analitikal untuk mana-mana kombinasi \( \Delta t \) dan \( \Delta x \) dengan kaedah Crank-Nicolson. Persamaan penyebaran haba ini diselesaikan dengan menggunakan kaedah Crank-Nicolson dan matriks tiga penpejuru yang terhasil diselesaikan dengan algorithm penguraian Crout. Keseluruhan data yang telah diproses oleh persamaan penyebaran telah digunakan dalam analisis bagi membuat perbandingan dengan penyelesaian analitikal. Secara keseluruhan, nilai khusus pada \( \lambda \) adalah tidak wujud. Namun begitu, kajian ini mendapati nilai \( \lambda \) secara kebetulannya wujud pada setiap \( \Delta t = 0.3\Delta x \) yang mampu memastikan bahawa penyelesaian yang paling hampir kepada penyelesaian analitikal dapat dilaksanakan pada ketepatan yang tinggi.
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LIST OF SYMBOLS

\( C_p \) specific heat, \( \text{cal/g} \cdot ^\circ\text{C} \)

\( H \) heat, \( \text{cal} \)

\( k \) coefficient thermal conductivity, \( \text{cal/(s} \cdot \text{cm} \cdot ^\circ\text{C}) \)

\( m \) the number of equal size length increment in \( x \) direction

\( M \) dimensionless pressure

\( q \) heat flux, \( \text{cal/(cm}^2\text{s}) \)

\( Q_{\text{gen}} \) heat generated in element

\( t \) time, \( s \)

\( T \) temperature, \( ^\circ\text{C} \)

\( \alpha \) coefficient thermal diffusivity, \( \text{cm}^2/\text{s} \)

\( \rho \) Density, \( \text{g/cm}^3 \)

\( \Delta x \) length increment in \( x \) direction, \( \text{cm} \)

\( \Delta t \) time increment, \( s \)

\( x \) horizontal coordinate, \( \text{cm} \)

\( i \) index position of \( x \)

\( j \) index position of \( t \)

\( \lambda \) lambda, dimensionless variable
1.1 Overview

Numerical analysis plays a very important role in science and engineering problems solving since approximately 2000 B.C. (Hosking et al., 1996). For example, linear interpolation was using to fill the gaps in tables with the astronomical data since antiquity. The applications of numerical analysis was increased dramatically in recent centuries where the invention of computers was successfully solve the problems of the tedious and repetitive works in numerical analysis where computer is able to do the calculation rapidly without making mistakes meanwhile the accuracy of the numerical results is desirable. Numerical analysis is a technique that scientists and engineers use to convert the problems to the mathematics model which can be solved by arithmetic operations transform to the computer language with the results in the form of approximation and the error which generated during the process of transformation must be taking into consideration. However, for a very small error the approximation that was obtained during the calculation are in very high accuracy. On the other hand, analytical solution is a technique that to obtain the mathematical functions from the problems which the results can be evaluated for specific instances. Although, analytical solution provided exact results for the problem but it was limited for only
certain class of problems. Numerical solution is important due to most of the problems arise from science and engineering do not possess a closed form solution which means the analytical solution could not be found. For example, integral of \( e^{-x^2} \). There is no analytical solution for this problem thus; the only way to obtain the solution is using numerical method.

The number of scientific and engineering problems involving partial differential equation is already very large and still growing. Those problems normally not only limited for single independent variable but it may be two or more. Additionally, in natural form, those problems involving its partial derivatives with respect to the independent variables which can be formulated to partial differential equation. According to the definition, partial differential equation (PDE) is an equation involving partial derivatives of an unknown function of two or more independent variables (Steven et al., 2006). Various type families of PDEs allow of ordinarily statement about the behaviour of their solutions. There exists a long-standing close connection between this field and the physical sciences, especially physics, thermodynamics, and quantum mechanics due to the geneses of the problem and the qualitative nature of the solutions are best understood by characterizing the homologous result in physics. PDEs are usually solved in the presence of boundary condition as well as initial condition.

Dirichlet problem is the easiest boundary condition problem where the boundary of the domain is given by a set of values for the problem. For instance, a thin rod is insulated from surrounding but one of its end hold at absolute zero then the value of the problem would be known at the point in space as illustrated in Figure 1.1a.
On the other hand, derivative boundary condition which is currently referred as a Neumann boundary condition where the boundary of domain gives a value to the derivative of the problem. For example, a thin rod is insulated from surrounding except its both ends. One of the ends is held absolute zero and another end is provided with thermal energy at a constant rate but the actual temperature will not be known, see Figure 1.1b.

![Diagram](image)

**Figure 1.1**  (a) Dirichlet boundary condition and (b) Neumann boundary condition for a thin rod.

Irregular boundary problem can be depicted as the problem with nonrectangular boundary which is more realistic geometry which normally occurs in engineering problem as shown in Figure 1.2. Cauchy boundary condition is the one corresponding to Dirichlet and Neumann boundary conditions where the solution of a differential equation is given by the value of the domain and also the directional derivative or normal derivative at the boundary. On the other hand, the initial value is usually used for the problem which distributed in space and time where specify values of the problem is given for all space at a given time. For example, in a middle of still pond if someone taps the water with a known force that would create a ripple and give an initial condition.
With the equation of form

\[ A(x, y) \frac{\partial^2 u(x, y)}{\partial x^2} + B(x, y) \frac{\partial^2 u(x, y)}{\partial x \partial y} + C(x, y) \frac{\partial^2 u(x, y)}{\partial y^2} + D(x, y) = 0 \]  \hspace{1cm} (1.1)

where \( A(x, y) \), \( B(x, y) \), \( C(x, y) \) and \( D(x, y) \) are the functions of the independent variables, \( x \) and \( y \), and dependent variable, \( u(x, y) \). However, \( A \), \( B \), \( C \) and \( D \) will be defined constant functions for the following explanation. Equation (1.1) is called elliptic, parabolic or hyperbolic at a point whenever the discriminant, \( B^2 - 4AC \) is negative, zero or positive, respectively, at the point. Equation (1.1) classified to this three categories is based on the method of characteristics which is useful because each category relates to specific and distinct scientific and engineering problem context that demand special solution techniques.

In thermal science, heat transfer is the problem that always interested by engineers due to understand and control the flow of the heat through the use of insulators, heat exchangers, and other device. Heat flow is a concern about passage of the thermal energy where it always occurs from regions of high to low temperature, the boundary condition set up a potential that leads to heat flow from the hot to the cool boundaries. The system will eventually reach the stable distribution of temperature or say as a steady-state of distribution is achieved by a sufficient time.
elapsed. As mentioned above, for this situation if the problem with absence of time derivative hence the problem can be solved by elliptic equation. In contrast, the parabolic or hyperbolic equation will be considered to use for solving the problem which called unsteady-state problem.

Parabolic equation determines how an unknown variety in both space and time. A parabolic solution may be characterized as a conic section where the result usually shows in symmetry. Some of the problems that influenced by gravitational field will follow a parabolic trajectory. For instance, a basketball is flying through the air. The famous application of parabolic equation is heat conduction equation.

The hyperbolic PDE, where the discriminant shows positive which means there have two distinct real roots. Hyperbolic equation deals with the propagation problem but more in propagation in sound or light. Wave equation is categorized into hyperbolic PDE which the unknown is characterized by a second derivative with respect to time. Hyperbolic equation is the disconnected conic section and able to support solutions with discontinuities. Besides, it is also the solution of oscillation such as vibrating string or in a swinging pendulum most occur in physical system.

Heat conduction equation is concerned about the propagation problem, typically propagation of heat through a solid by time. Evidently, heat conduction equation is categorized into parabolic equation. For instance, the temperatures of ends of a long, thin and adiabatic rod are prefixed as one end with higher temperature than another one. Assume that the rod’s thinness is allowed the heat distribute evenly over its cross section as x-axis. The temperature of the interior latitude is vary from time to
time can be observed. Therefore, the solution consists of a series of spatial distribution corresponding to the state of the rod at various times.

Finite difference method (FDM) is one of the classical and straightforward numerical solutions for PDEs. The FDM is the techniques of discretization where the continuous domain of solution is discretized into a mesh of discrete points. The PDE is converted into a set of finite difference equations which can be derived using Taylor series expansion. However, the appropriated boundary condition is subjected with finite difference scheme. Discrete derivatives are replaced by finite difference approximations which derive by using finite difference operators. There are three kinds of common finite difference operators which are forward difference, backward difference and central difference and denoted as $\Delta$, $\nabla$ and $\delta$, respectively.

Figure 1.3 Computational molecules demonstrating the fundamental differences between (a) explicit, (b) implicit and (c) Crank-Nicolson schemes.

For parabolic PDEs, there have two fundamental solution approaches which are explicit and implicit schemes. Explicit scheme is used to calculate the values of
each node for a future time from the values of node and its adjacent nodes at current
time where a small time step is required in order to keep the error in the result
bounded (Figure 1.3a). For implicit scheme, the spatial derivatives are approximated
at an advanced time level hence resulting the difference equation contains several
unknown and produce a system of equations must be solved simultaneously
(Figure 1.3b). Though, the stability of implicit scheme is much better than explicit
scheme but its accuracy is limited while using large time step.

Hence, an alternative implicit scheme that is second-order accurate in both
space and time is chosen for this study which called Crank-Nicolson scheme. The
difference approximations of Crank-Nicolson scheme are developed at the midpoint of
the time increment as shown in Figure 1.3c. The derivatives are taking half way
between the beginning and the end of the time increment. The average difference
approximations produce a second-order convergence where the first-order error term
was dropped out. Therefore, it is numerically stable for any values of time step but
small values are more accurate. The Crank-Nicolson scheme involves solving a
tridiagonal system of linear equation.

This study will concentrate in solving the basic linear parabolic diffusion
equation as

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2}, \quad (0 < x < 1, t > 0)$$

(1.2)

by using Crank-Nicolson method where initial condition is given as $T = \sin \pi x$ when
$t = 0$ for $0 \leq x \leq 1$, and the boundary conditions are $T = 0$ when $x = 0$, $x = 1$ and
$t > 0$. The analytical solution $T = e^{-\alpha^2 t} \sin(\pi x)$ will be used to compare with the
numerical solution and the accuracy of the Crank-Nicolson method will be discussed (Smith, 1996). The computation for numerical solution will be executed by a program which is developed by C language based on Crank-Nicolson scheme.

1.2 Objective

The main purpose of this study is to investigate if a particular value of

\[ \lambda = \frac{K(\Delta t)}{2\rho C_p(\Delta x)^2} \]

exists hence a high accurate numerical solution can be conducted where \( \Delta t \), \( \Delta x \), \( K \), \( \rho \) and \( C_p \) represent time step, length increment in \( x \) direction, coefficient thermal diffusivity, density and specific heat, respectively.
2.1 Heat Conduction Equation

Heat transfer is naturally occurred when a temperature gradient exists. Normally, the transfer of heat is in energy term from higher temperature region to lower temperature region. Conduction is one of the types of heat transfer where the propagation heat is happened within a substance by agitation of molecules without any motion of the substance as a whole. Heat conduction equation can be defined as a diffusion equation. Many studies were introduced due to the widely application of heat conduction equation in distinct field. This literature review is according to the different fields follows by the years.

Asan and Sancaktar (1998) have proposed a method to determine the effects of the thickness and the thermophysical properties of a wall on time lag and decrement factor where time lag means the time was taken for the heat wave to propagate from outer surface to the inner surface while decrement factor is the decreasing ratio of heat wave’s amplitude during the process of propagation. The investigation of thermal storage buildings based on the different materials is considered importance due to a good material for floors and walls are able to stored energy in it during day period
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