APPLICATION OF SMOOTHED PARTICLE HYDRODYNAMICS METHOD IN TWO-DIMENSIONAL HEAT EQUATION

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To my beloved father and mother

Omar Sarbini

&

Norrimi Abdul Malik

And also

to my dearest sister

Nur Athirah Omar

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Syukur alhamdulillah, finally this research has been completed successfully. I will not manage to complete this research without the help from people around me.

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ABSTRACT

Solution to the two-dimensional (2D) heat equation has been done by many researchers earlier. Numerical methods always being used in solving 2D heat equation. The usual numerical method being chosen is the finite difference techniques such as explicit finite difference method, Crank-Nicolson method and alternating direction implicit (ADI) method. However, in this research, the smoothed particle hydrodynamics (SPH) method is chosen and being studied to be applied in solving the 2D heat equation. The algorithm for SPH method is also being developed. As for making the comparisons to study on the accuracy of SPH method, 2D heat equation also being solved using ADI method. FORTRAN programming is used as a calculation medium for both the ADI and SPH method.

ABSTRAK

Penyelesaian terhadap persamaan haba dua-dimensi telah banyak dijalankan dalam kajian-kajian oleh para penyelidik terdahulu. Kaedah berangka seringkali digunakan bagi menyelesaikan persamaan haba dua-dimensi. Antaranya adalah dengan menggunakan pelbagai teknik beza terhingga seperti kaedah beza terhingga eksplisit, kaedah Crank-Nicolson dan kaedah arah ulang-alik implisit (ADI). Namun begitu, dalam kajian ini kaedah zarah hidrodinamik lancar (SPH) dipilih dan dikaji untuk diaplikasikan dalam menyelesaikan masalah persamaan haba dua-dimensi tersebut. Algoritma bagi kaedah SPH turut dirumuskan. Sebagai perbandingan bagi mengkaji tentang ketepatan kaedah SPH, persamaan haba dua-dimensi dalam kajian ini akan turut diselesaikan dengan menggunakan kaedah ADI dan pengaturcaraan Fortran digunakan sebagai medium pengiraan bagi kedua-dua kaedah ADI dan SPH tersebut.

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LIST OF SYMBOLS

Δ, ∇^2	-	Laplacian operator
f	-	Function
$\mathbf{F}(\mathbf{x})$	-	Vector notation of f_i
k	-	Constant
N	-	Number of particles
$\boldsymbol{x}$	-	Vector
$\lim_{h \to 0} W(\boldsymbol{x} - \boldsymbol{x}', h)$	-	Definition of continuous for function W at point "0"

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CHAPTER 1

INTRODUCTION

1.1 Background of the Problem

Heat is a form of energy in transition where it flows from one system to another. However, there will not be any transfer of mass whenever there is a temperature difference between the systems. Heat transfer process is the exchange in internal energy between the systems. It is almost in every phase of scientific and engineering work processes, there will be dealing with the flow of heat energy [1].

Heat equation is one of the most important partial differential equation which describes the distribution of heat (or variation in temperature) in a given region over time. Looking at the real world situations, there are many problems involving heat conduction which could not be suitable to be solved using those classical mathematical methods such as the separation of variables techniques or the implementation of Green's function. In conjunction with that matter, there are now a lot of procedures especially the numerical solutions have been proposed in order to obtain an approximate solution for those problems [2]. As for this research, we are interested in solving two dimensional heat equations. One of the most practical methods that can be used to solve it is the finite difference technique since it is one of the earliest developed methods that allow determining temperature values at discrete spatial points and temporal points [3]. Alternating direction implicit (ADI) method is one of the most suitable finite difference techniques which can be applied in the two-dimensional heat equation.

ADI method is one of the finite difference techniques which have been introduced in the previous research papers by Peaceman and Rachford, and Douglas [4; 5]. The ADI method has first suggested for approximating the solution of transient and permanent heat flow problems in two space variables. The method then has been extended for mildly nonlinear problems, three space variables and nonsymmetrical problem [6].

In the field of numerical analysis, ADI method is a finite difference technique which is used to solve parabolic and elliptic partial differential equations. It is particularly being used in solving heat conduction problem or diffusion equation in two or more dimensions [5]. Normally, Crank-Nicolson method is always being chosen as the method for solving heat conduction equation. However, this method is quite costly. The advantage of using ADI method is that, in every iteration, the equations that have to be solved in the ADI scheme provides a simple structure and therefore it is easier to be solved.

At first place, validation of the method has been established only in the case of a rectangular domain. After all, procedure of the method is then being tested successfully on several more complex examples [7]. Other than that, in the approximation of the solutions of parabolic and elliptic differential equations in two and three variables cases, ADI method has proved valuable [6].

ADI method also provides a better scheme for solving heat equations in two spatial dimensions using tridiagonal matrices but it requires more effort in developing a program. However, Ayunni [8] had mentioned that the convergence rate of ADI is faster than Successive Over-Relation (SOR) method and it was the reason why this ADI method became so popular.

In the previous study, Shafiqah [9] stated that implementing the von Neumann stability analysis yields an amplification factor which ensures that ADI method is unconditionally stable. In additional, ADI method is second order accurate in both time and space. ADI also has become an ideal choice due to its accuracy and unconditional stability.

However, our main focus in this research is to solve two-dimensional heat equation using a meshless method called the smoothed particle hydrodynamics (SPH) method. The purpose of applying the ADI method first in solving the two dimensional heat equation is to enable us for making observations and comparisons on the solution of both methods later in order to validate the present SPH method as well as its accuracy.

The Smoothed Particle Hydrodynamics (SPH) method, which is a meshfree particle method, is one of the meshless method branches. Before we go any further on SPH method, we will first discuss on the meshless method. Generally, meshless method can be divided into three main groups. The first group consists of those methods which based on strong formulations. These types of methods are computationally efficient and completely meshless but often unstable and less accurate. While for the second group, it consists of methods that based on weak formulations which are very stable and accurate but there is a need of a background mesh. Examples of those methods are such as the Element Free Galerkin (EFG), Meshless Local Petrov-Galerkin (MLPG) and Point Interpolation Method (PIM). Finally, for the third group, it is stand up by the particle method such as the Molecular Dynamic (MD), Monte Carlo (MC) and Smoothed Particle Hydrodynamics (SPH) method, where those methods are actually similar to the methods based on weak formulations and are stable for arbitrary distributed nodes and excellently cope with large deformations, which the accuracy mostly depends on the smoothing function [10].

In this research, we are dealing with smoothed particle hydrodynamics; a particle method where the advantages of the method is discretised with particles that are not connected with a mesh which allows for a simple and accurate solution at large deformations. The discretisation of complex geometries is less complicated and also, the physical values and paths of particles are easy to follow and evaluate such that it is also consequently simple to determine the free surface of movable interfaces or deformable boundaries [11].

In the SPH method, the state of the system is represented by a set of particles, which possesses individual material properties and move according to the governing conservation equations [11]. Smoothed particle hydrodynamics (SPH) as a meshfree, Lagrangian particle method for modeling fluid flows, was first invented to solve astrophysical problems in three-dimensional (3D) open space, in particular polytropes [12; 13], since the collective movement of those particles is similar to the movement of a liquid or gas flow, and it can be modeled by the governing equations of the classical Newtonian hydrodynamics.

SPH was also invented to simulate non-axisymmetric phenomena in astrophysics. It is easy to work with and reasonably accurate. SPH is a particle method and does not need a grid to calculate spatial derivatives. Instead, they are found by analytic differentiation of interpolation formulae. The continuity equation, the equation of motion and the energy equation become sets of ordinary differential equations, which are easy to understand in mechanical and thermodynamic grounds. The key to SPH is an interpolation method that allows any function to be expressed in terms of its values at a set of disordered points. These points lie at the location of the particles.

The idea behind SPH is to replace the equations of fluid dynamics by equations for particles. In effect we replace the continuum equations by a set of particle equations that approximates the continuum and at the same time, provides a rigorous model of the underlying and more fundamental molecular system. There are many other particle methods but as for this research, we only concerned with Smoothed Particle Hydrodynamics (SPH) devised by Gingold and Monaghan [13] and by Lucy [12]. Useful reviews are those of Benz [14] and Monaghan [15].

As being mentioned above, the SPH method has been applied in many fields such as in the astrophysics. The adaptive resolution of smoothed particle hydrodynamics (SPH) combined with its ability to simulate phenomena covering many orders of magnitude, make it ideal for computations in theoretical astrophysics. Simulations of galaxy formation, star formation, stellar collisions, supernovae and meteor impacts are some of the wide variety of astrophysical and cosmological uses of this method.

Generally speaking, SPH is used to model hydrodynamic flows, including possible effects of gravity, incorporating other astrophysical processes which may be important, such as radiative transfer and magnetic fields in an active area of research in the astronomical community, and has had some limited success.

Smoothed particle hydrodynamics (SPH) is being increasingly used to model fluid motion as well. This is due to several benefits over traditional grid-based techniques. First, SPH guarantees conservation of mass without extra computation since the particles themselves represent mass. Secondly, SPH computes pressure from weighted contributions of neighboring particles rather than by solving linear systems of equations. Finally, unlike grid-base technique which must track fluid boundaries, SPH creates a free surface for two-phase interacting fluids directly since the particles represent the denser fluid (usually water) and empty space represents the lighter fluid (usually air). For these reasons it is possible to simulate fluid motion using SPH in real time. However, both grid-base and SPH techniques still require the generation of renderable free surface geometry using a polygonization technique such as metaballs and marching cubes, point splatting, or “carpet” visualization. For gas dynamics it is more appropriate to use the kernel function itself to produce a rendering of gas column density, for example, as done in the SPLASH visualization package.

One drawback over grid-based techniques is the need for large numbers of particles to produce simulations of equivalent resolution. In the typical implementation of both uniform grids and SPH particle techniques, many voxels or particles will be used to fill water volumes which are never rendered. However, accuracy can be significantly higher with sophisticated grid-based techniques, especially those coupled with particle methods, such as particle level sets.

In the other field, William G. Hoover had used SPH to study impact fracture in solids. Hoover and others use the acronym SPAM (smoothed-particle applied mechanics) to refer to the numerical method. The application of smoothed-particle methods to solid mechanics remains a relatively unexplored field.

SPH method also had been applied in the problem of hydraulic erosion. A paper published by P. Kristof et. al. [16] has presented a new technique for modification of 3D terrains by hydraulic erosion. Here, a Lagrangian approach, which is the SPH method and a physically-based erosion model adopted from an Eulerian approach had been used for efficiently couples the fluid simulation. The eroded sediment is associated with the SPH particles and is advected both implicity due to the particle motion and explicity through an additional velocity field which accounts for the sediment transfer between the particles. A new donor-acceptor scheme for the explicit advection in SPH was also being proposed. Sediment exchange between the SPH particles and the terrain itself were being mediated using the boundary particles associated to the terrain. The final results show that this particle-based method is efficient for the erosion of dense, large and sparse fluid. Implementation of this research by P. Kristof et. al. also provides interactive results for scenes with up to 25,000 particles. A solution to coupling hydraulic erosion with SPH-based fluid simulation also has been presented. The design choices by the researchers were motivated by the goal to keep the overhead of erosion simulation small. For that very reason, rather than introducing separate sediment particles, they represent the dissolved sediment as a volume fraction in SPH particles. Since the sediment does not entirely follow the water flow, an additional advection by the gravity field was introduced. A novel donor-acceptor scheme for sediment exchange also being proposed. The results also had shown that SPH affords for interactive erosion simulation in a moderately complex environment with fully 3D water.

In the other research project by Charles Thomas Wolfe and Sudhanshu Kumar Semwal [17], SPH method had been applied in the acoustic modeling of reverberation. Basically, current methods for digital acoustic modeling of reverberation can be categorized into two main areas that are DSP algorithms and sound tracing algorithms. DSP algorithms are usually chosen for their speed and ease of use. Generally DSP methods are fast, but do not accurately represent complex environments. For example, beam tracing, which is one of the sound tracing algorithms, can accurately model static environments but have difficulty with complex and/or moving geometry. It is then involves SPH which is also has become one of the Computational Fluid Dynamics (CFD) method that has recently gained interest as a method for accurately simulating fluid flow using discrete particles. SPH method is then being extended by adding the ability to model the sound wave propagation through fluids. A generalized method that integrates sound generation and reception is also being presented. This method provides a basis for acoustic sound effects such as reverberation.

Other than that, a research paper entitled Smoothed Particle Hydrodynamics on GPUs by Takahiro et. al. has been produced [18]. SPH as a simulation method of free surface flow is being accelerated by the use of Graphics Processing Units

(GPUs). No study has so far accomplished acceleration of particle-based fluid simulation by implementing the entire algorithm on GPUs. This is because a neighboring particle search cannot be easily implemented on GPUs. The researchers developed a method that can search for neighboring particles on GPUs by introducing a 3D grid. The proposed method can exploit the computational power of GPUs because all of the computation is done on the GPU. As a result, SPH simulation is accelerated drastically and tens of thousands of particles are simulated in real-time.

The SPH method, a truly meshfree, free Lagrangian, particle method, promises alternatives ways of solutions in many classes of problems especially for those which are characterized by large deformations and moving discontinuities [19].

SPH as a Lagrangian method also has been introduced specifically in order to simulate self-gravitating fluids moving freely in three dimensions. One of the key ideas of SPH is to calculate pressure gradient forces by kernel estimation, directly from the particle positions rather than by finite differencing on a grid, as in older particle methods such as Particle In Cell (PIC) method. SPH was first introduced by Lucy [12] and Gingold and Monaghan [13], who used it to study dynamical fission instabilities in rapidly rotating stars. Since then, a wide variety of astrophysical fluid dynamics problems have been tackled using SPH [22].

Smoothed particle hydrodynamics (SPH) reduces the time to create a mesh, because gaps and overlapping surfaces do not prevent mesh generation. The generation and modification of finite element and control volume meshes can take a significant proportion of the time available in a modeling project. Reducing the time required to build meshes would improve the turnaround time and reduce the cost of solutions. One important accelerator would be eliminating the need to modify CAD geometries to make them suitable for model generation. Solution adaptivity through mesh refinement and coarsening is a desirable feature in many analyses because it enables important features to be resolved accurately. Traditionally this has required the regeneration of meshes based on preceding simulations. SPH enables the creation and deletion of particles as dictated by the solution, and there is no need to remesh because there is no connectivity between particles.

In additional, as a Lagrangian meshless method, SPH can be applied for the solution of partial differential equations. Spatial discretisation is achieved via a distribution of interpolation points (pseudo-particles) that place no requirement on connectivity. This provides a mechanism for reducing the model set up time and is naturally suited to problems involving complex free surface behavior, fracture and penetration. SPH tracks the movement of material and can therefore model problems involving history dependent material properties, such as resin cure. SPH method is particularly suited to fluid and structural dynamic problems involving free surfaces, fragmentation and complex physics. SPH is also very well suited to the solution of problems involving large material deformations. One such example is birdstrike where the bird model experiences very large distortions when it impacts a structure.

In other cases, SPH method is being applied for modeling heat and mass flows. Materials are approximated by particles that are free to move rather than by fixed grids or meshes. The governing PDE are converted into equations of motion for these particles. The SPH method has been developed over the past two decades for astrophysical applications [15]. More recently the method has been extended to incompressible enclosed flows [23]. There are several advantages that make SPH particularly well suited to this type of problem. The main thing is that SPH can handles momentum dominated flows well. In surroundings of complex free surfaces which involve fragmentations break-up, it can be modeled naturally using SPH. For a complicated physics such as multi-phase, realistic equations of state, compressibility, radiation and solidification, those can be added easily by SPH. In additional, SPH can also easily able to handle complex geometries in two and three dimensions.

Unlike the meshfree nodes in other meshfree methods, which are only used as interpolation points, the SPH particles also carry material properties, functioning as both approximation points and material components. These particles are capable of moving in space, carry all the computational information, and thus form the computational frame for solving the partial differential equations describing the conservation laws. The numerical solution procedure of the SPH formulation consists of the following steps [11].

The first step is focusing on generating the meshless numerical model where the problem domain is dicretised with a finite number of arbitrary located particles without mesh connectivity between them. Secondly, integral representation or also known as the kernel approximation is used for the field function approximation. For the next step, particle approximation is being done by replacing the integration in integral representation with summations for the values of neighboring particles in the support domain. The steps then come to the adaptation stage where the particle approximation is performed at every step and depends on the current local particle distribution. However, it does not depend on the particle locations in the previous time step. Finally, for the last step, it is on the dynamical analysis. Here, the direct time integration of the governing equation is performed with explicit integration scheme allowing for fast time stepping and obtaining time history for all field variables of particles assembling the problem domain [10].

Computations of both the SPH and ADI method will be performed using FORTRAN program since it is impossible to do the calculations manually for large scale problem and also in order to assure the accuracy of the solution. In additional, SPH method do involves tedious and complex calculation. Thus, it is ideal to be applied numerically in FORTRAN program.

1.2 Statement of the Problem

Grid or mesh based numerical methods such as finite difference methods (FDM) and finite element methods (FEM) have been widely applied to various areas such as fluid dynamics and solid mechanics. These methods are currently the dominant methods in solving problems of engineering and science.

However, mesh-based methods such as FEM suffer from some difficulties. One of the problem arise is expensive process of generating or regenerating the mesh due to large deformation of structures. In order to overcome this time consuming problem, meshfree method is developed which successfully avoid the process of regenerating the whole mesh in the large deformation scenario. One of the meshfree methods is smoothed particle hydrodynamics (SPH) method which can solve problem of large deformation without remeshing process.

The aim of this research is to solve two-dimensional heat equation using SPH method. In order to study on the accuracy of the SPH method, a finite difference technique, which is the alternating direction implicit (ADI) method has first being applied to solve the two-dimensional heat equation. Solution obtained from the ADI method is then being used to make a comparison with the solution of SPH method in order to study on the accuracy of the SPH method. FORTRAN programming will be used in order to reduce the computational effort.

1.3 Objectives of the Study

The main objectives of this research are:

1. To study the basic concepts of SPH method.
2. To solve a problem of two-dimensional heat equation using SPH method.
3. To solve the problem of two-dimensional heat equation numerically using a finite difference technique, which is the alternating direction implicit (ADI) method.
4. To validate and compare the accuracy of solution between SPH method with the results of ADI method.

1.4 Scope of the Study

This research mainly focuses on the concept of SPH method. Numerical algorithm of the SPH method will be constructed in order to make use of the method later. The SPH method is then be applied to solve a two-dimensional heat equation. Observations on the accuracy of SPH method will also be done by doing the comparison with the results of a finite difference technique, which is the alternating direction implicit (ADI) method.

1.5 Significance of the Study

The results of this research can be used for further research in related areas. One of the goals of this research is that, this research will gives a clearer view of the SPH method, where it will finally lead to further understanding on the application and implementation of the SPH method in solving related problems especially in the science and engineering fields. The non-uniform grid nodes are applicable in SPH method which enables the application of the method in complex geometry. Last but not least, the ability of avoiding remeshing process indicates that SPH method is better than traditional mesh-based method such as FDM.

1.6 Organization of the Study

This research has been divided into five chapters. In chapter 1, we discuss about the background of the study, problem statement, objectives, scope, significant of the study, organization of the study and the research methodology.

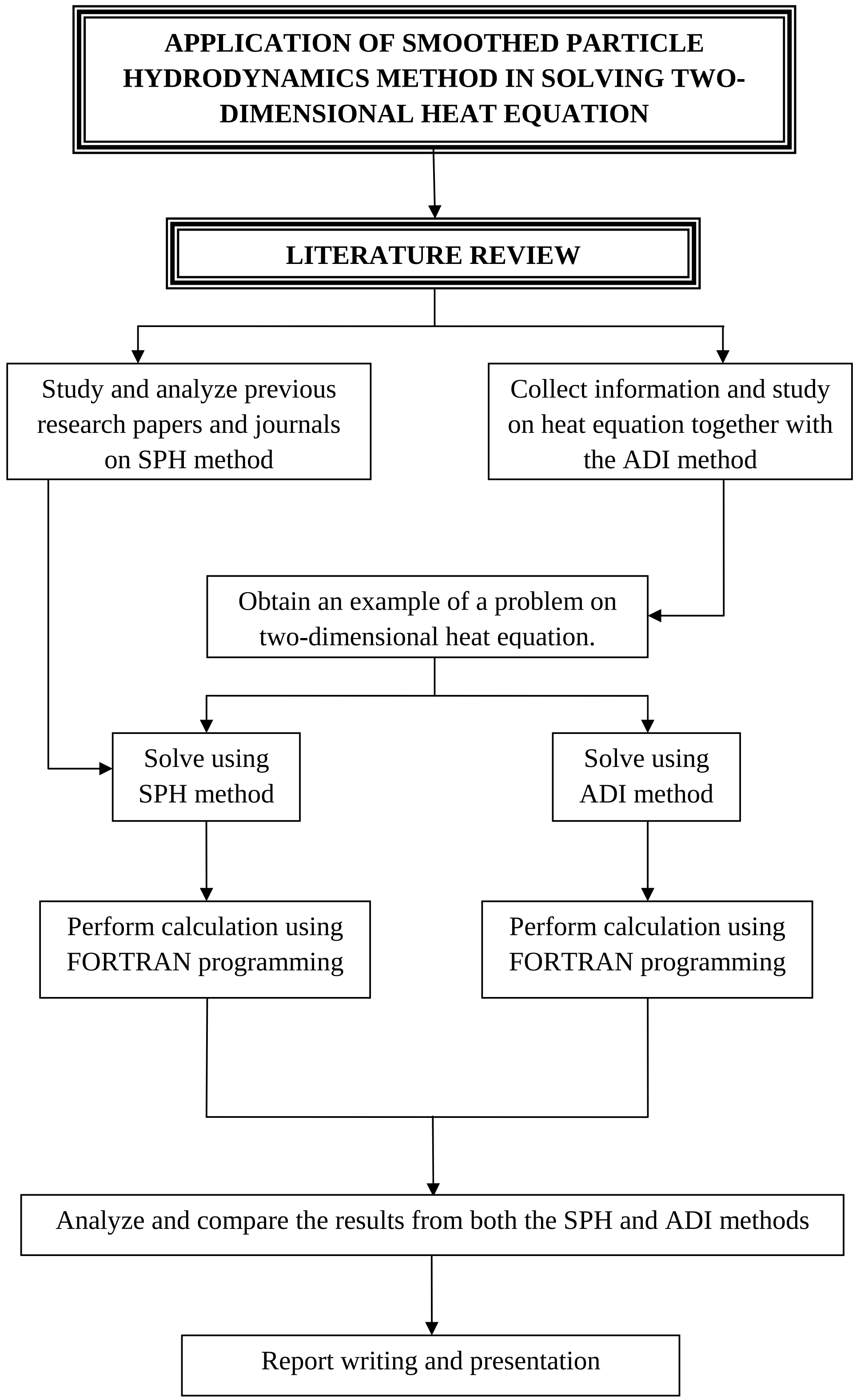
In chapter 2, we discuss on the heat equation. The discussion involved one- and two-dimensional heat equation. The numerical methods that can be used to solve the heat equation also be mentioned.

Chapter 3 is focusing on the alternating direction implicit (ADI) method. The two-dimensional heat equation will be solved using the ADI method including with one numerical example.

Chapter 4 is mainly discussing on the smoothed particle hydrodynamics (SPH) method. SPH method then will also being applied to solve the two-dimensional heat equation. Comparisons of the solution from both the ADI and SPH method will then being compared in order to look at the accuracy.

Chapter 5 is the final chapter of this research where conclusion and recommendation of the whole research is being discussed.

1.7 Research Methodology



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