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Solving One-Dimensional Diffusion Problem by using Finite Element Method

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Abstract
Finite element method is a technique to solve partial differential equations by splitting the physical region into a smaller piece linked at nodes and can be applied to solve diffusion problem. The Galerkin method is a particular approach within the weighted residual methods to choose the basis function. The purpose of this study is to solve one-dimensional diffusion equation by using finite element method by applying on linear and quadratic basis functions. The strong and weak form are first derived. To be more specific, a portion of dye in an infinitesimal long pipe is considered. Fick's law of diffusion is expressed in a partial differential equation. It states that the flux of a substance through a unit area per unit time is proportional to the negative gradient of the concentration. The goal of solving a linear and quadratic system of equations is to find the values of the variables that satisfy all the equations simultaneously. Thomas algorithm is used to find a concentration in diffusion problem where it provides an efficient and accurate solution to the linear equations that arise during the analysis of structures and systems. This study focused on diffusion problem in one dimensional linear shape function and quadratic shape function on a pipe consisting of four nodes with three elements and three nodes with two elements have been solved. As a result, quadratic elements can represent curved boundaries and model problem domains more accurately than linear elements
Keywords: Finite element method; One-dimensional diffusion problem; Fick's Law; Linear and quadratic shape functions; Galerkin method

1. Introduction

The Finite Element Method, sometimes known as FEM, is a numerical method for addressing physics and engineering-related issues. Problems in structure analysis, heat transfer, fluid flow, mass movement, and electromagnetic potential are all common areas of study. FEM subdivides a big problem into smaller, easier, parts, called finite elements. Then, these simple equations that model these limited parts are put together to make a bigger set of equations that model the whole problem.

The FEM is a powerful way to solve differential and integral equations that come up in many engineering and applied science fields. There are various methods for obtaining a numerical solution to a differential equation. If the governing differential equation is a first-order ordinary differential equation, we may find numerical solutions using well-known techniques such as the Euler Method, a variety of Runge-Kutta Methods, or multi-step approaches such as the Adam-Bashforth and Adam-Moulten Methods. And if the governing equation is a higher-order ordinary differential equation, it can be turned into a system of coupled first-order equations and then solved using any of the standard methods for first-order equations [1].

There are several weighted residual approaches. Some of the standard methods are the point collocation method, the subdomain collocation method, the least squares method, and the Galerkin method [2]. In the Galerkin model of the weighted residual method, the trial functions themselves are used as the weight functions. The Galerkin method makes symmetric positive definite coefficient matrices if the differential operator is self-adjoint, and it takes less time to compute than the least squares method.

The Galerkin method is a common numerical approach for solving partial differential equations (PDEs) in numerical analysis and computing. Based on [3] previous work, the Galerkin method is also used in other FEM variants, such as the discontinuous Galerkin method. Then [4] used a FEM hybridisable discontinuous Galerkin method. In the Galerkin method, the problem is turned into a weak form, a set of basis functions and then the factors that make the residue as compact as possible are determined.

By using the Galerkin method, the PDE is turned into a set of algebraic equations, which is usually shown as a matrix equation. This system of equations must be solved in order to get the unknown coefficients of the linear combination of basis functions. To solve the resulting problem, different computational approaches like the finite element method, the finite difference method, or the spectral method can be used.

In FEM, shape functions are one of the most important parts of estimating how a physical system will respond. They are mathematical concepts equations that are used to estimate the unknown values of each finite element. The idea that quadratic shape functions were introduces in [5] and were used to grow the displacement field in the group. By specifying the shape functions, the FEM may estimate the unknowns at any location within an element using the values at the nodes of the element. This makes it possible to put together a set of equations that show how the whole structure or system in question works.

In math and physics, a diffusion problem is usually the study of how a quantity, such as temperature, concentration, or pressure, changes over a period due to diffusion. The goal of the problem is to figure out how and why so much changes based on how it starts and ends. Mathematically, diffusion problems are often explained by PDEs like the heat equation or the diffusion equation, which link the rate of change of a number to how it changes in space and time. These equations show the basic rules of diffusion, such as Fick's law, which says that the rate of diffusion is related to the difference in concentration.

This study is mostly about getting the main idea behind the finite element method, specifically the Galerkin method, which includes figuring out the strong formulation, the weak formulation, shape function of linear and quadratic system and the stiffness matrix for one-dimensional diffusion issues. The solution in this research also employs the elementwise approximation, which follows the Galerkin technique and makes use of the global shape function and weight function. As a result, this study ought to be able to clear the introduction of a method that is effective for resolving issues with irregular boundary conditions with irregular and complicated geometries.

2. Literature Review

2.1 Finite Element Method

Early In 1956, [6] introduced the use of finite elements for the study of aircraft structures, which is considered one of the major contributions to the advancement of the Finite Element Method (FEM). One of the earliest implementations of this computational approach was his essay, which was published in 1956. He introduced the concept of finite elements in a 1960 paper. Next, in 1982, [7] introduced that the FEM is a numerical technique that has become so well known that it now seems to be one of the best ways to figure out how well a wide range of real-world problems work. In fact, applied mathematicians are now doing research on this method.

Later in 1992, [8] reintroduced the FEM is based on the idea that you can solve a hard problem by making it into a simpler one. In 2004, [9] determined that FEM is an accurate computational method used to find approximations of solutions to boundary value problems in engineering. For convenience, the FEM process allows the continuum to be discretized into a limited number of parts or elements and highlights that the continuous domain characteristics may be calculated by collecting the comparable qualities of discrete components per node. In 2004 [10], the FEM has been used rigorously to solve a wide range of problems in applied science and engineering, and it has grown quickly over the years.

2.2 Diffusion Problem

In 1990, [11] describe a new way to solve the diffusion problem with computers. In particular, the researcher builds a generalized state-space system and figure out the impulse response of a shortened state-space system that is equivalent to the generalized one. They use a 3D FEM to get the state-space structure for this project. Next, in 2012 [12] study the two-dimensional equilibrium radiation diffusion problem that solved with the help of the discontinuous Galerkin method. The semi-implicit integration factor method is used on the nonlinear ordinary differential equations that are created by the discontinuous Galerkin spatial discretization.

Based on [13] in previous study, they are using numerical method for solving parabolic interface problems with nonhomogeneous flux jump conditions and nonlinear jump conditions. To deal with nonlinearity, the main idea is to use the standard finite element method on a semi-Cartesian mesh along with Newton's method.

3. Mathematical Formulation

3.1 Basic Concept

According to [14], finite element analysis (FEA), which was initially created for aerospace structural analysis, is now widely used in other industries, such as automotive, structural engineering, composite design, and manufacturing, as a practical and quick method for approximating the resolution to a range of challenging engineering issues. The Finite Element Method (FEM) is used in FEA. FEM is simply a different way to solve engineering problems automatically. Instead of using standard differential equations and partial differential equations. The general step are as follows [15]

1) Discretization. In this step, the domain of the problem is subdivided into a mesh of smaller elements.
2) Formulation of Element Equations. Within each element, the governing equations are made using variational principles involving the principle of minimum potential energy or the principle of virtual work.
3) Assembly. When the equations for the elements are put together, they make up a system of equations for the full problem area. This means putting together the matrices and vectors of each part into a global stiffness matrix and load vector.
4) Solution. By solving the system of equations, you can find the values of the unknown factors, such as temperature or concentration. For solving the problem, different computational methods can be used, such as direct methods for example using Gaussian elimination or iterative methods for example using the conjugate gradient method.
5) Post-processing. Once the answer has been found, post-processing is used to get the results that were wanted.

3.2 Derivation of Strong Formulation of One-Dimensional Diffusion Problem

Diffusion issues in one dimension has been considered in order to illustrate the fundamental stages in developing the strong and weak forms. The strong forms for these problems will be formed along with the boundary conditions.

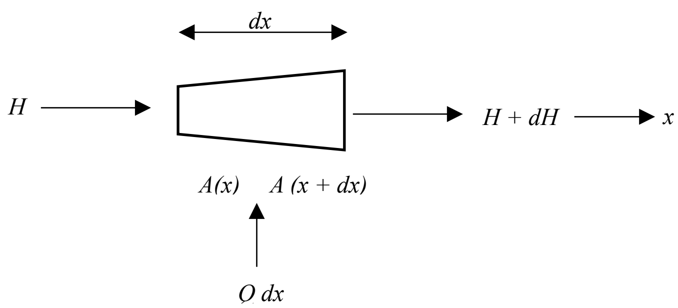

Figure 1 A portion of the dye in an infinitesimal long pipe.

Consider an indefinitely tiny component dx of the pipe, as illustrated in Figure 1. In this diagram, the H and $H+dH$ stand for the flow in and flow out, respectively, per unit time. When facing the x-axis, both H and $H+dH$ are positive. It seems that we also have a supply of per unit of time, as shown by Qdx. We can state the fact that the total inflow equals the total outflow per unit time since we only address stationary problems and the issue is time independent. We can see this in Figure 1.

$$H + Qdx = H + dH$$

Fick's law of diffusion assumes the mass flux H across a cross section of the pipe is given by $H = Aq$. Where q is the flow of atom and liquid movement in the x-direction is seen as a positive flux q. Equation (3.1) adopts the following form using this expression for H as given by.

$$Q = \frac{dH}{dx}(Aq). \tag{3.2}$$

Relationship between flux and concentration is known as Fick's first law, which give as

$$q = -k\frac{dc}{dx} \tag{3.3}$$

A negative sign appears in (3.3) indicates that diffusion occurs in a direction opposite to that of the increasing concentration. Insert (3.3) into (3.2) yields

$$\frac{d}{dx}\left(Ak\frac{dc}{dx}\right) + Q = 0 \qquad a \le x \le b \tag{3.4}$$

To show how weak forms are developed, from the strong form equation (3.4), multiply the result by the arbitrary weight function w, to get the weak form of the one-dimensional problem and integrate over the body.

$$\int_a^b w\left[\frac{d}{dx}\left(Ak\frac{dc}{dx}\right) + Q(x)\right]dx = 0 \tag{3.5}$$

Thus

$$\int_a^b w\frac{d}{dx}\left(Ak\frac{dc}{dx}\right)dx + \int_a^b w\,Q(x)\,dx = 0. \tag{3.6}$$

By using integration by part, integrated the first term of equation (3.6) and the equation become

$$\int_a^b Ak\frac{dc}{dx}\left(\frac{dw}{dx}\right)dx = \left(w.AK\frac{dw}{dx}\right)_a^b + \int_a^b w\,Q\,dx. \tag{3.7}$$

By using Fick' Law $q = -k\frac{dc}{dx}$, substitute into equation (3.7),

$$\int_a^b Ak\frac{dc}{dx}\left(\frac{dw}{dx}\right)dx = -\left(w.Aq\right)_a^b + \int_a^b w\,Q\,dx. \tag{3.8}$$

Therefore equation (3.8) is the weak form of the diffusion problem The solution for the diffusion problem can be obtained by system of equations $\mathbf{Ka} = \mathbf{F}$ where $\mathbf{a}$ is the vector of nodal displacements, $\mathbf{K}$ is the global stiffness matrix and $\mathbf{F}$ is the total of load boundary vector This system of equations can be solved for **a** to find the displacements at each node in the system due to the applied loads.

4 Result and Discussion

4.1 One-dimensional linear element

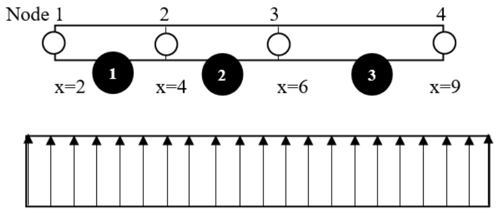

Figure 2 One-dimensional pipe diffusion with four nodes and three elements

Figure 2 shows that one-dimensional pipe diffusion. Consider on a consisting of four nodes and three elements, as shown in the Figure 2. Based on the strong formulation differential equation (3.4) We consider the values of $A = 10$, $k = 4$ and $Q = 50.$ The boundary conditions are $c_1 = c|_{x=2} = 0$ and the flux, $q_4 = q|_{x=9} = 20$. By using Galerkin method for approximation on the linear model $c = \alpha_1 + \alpha_2 x,$ we need to find the concentration at each nodal point, $c_2 = c|_{x=4}, c_3 = c|_{x=6}$ and $c_4 = c|_{x=9}$ and. Next to find the flux at the left end of the pipe, $q_1 = q|_{x=2}$.

Table 1: The global shape functions and their piecewise function derivatives

$N_1(x) = \begin{cases} N_1^1(x) = -\dfrac{x}{2} + 2, & 2 \le x \le 4, \\ 0, & otherwise \end{cases}$	$\dfrac{dN_1(x)}{dx} = \begin{cases} \dfrac{dN_1^1(x)}{dx} = -\dfrac{1}{2}, & 2 \le x \le 4, \\ 0, & otherwise \end{cases}$
$N_2(x) = \begin{cases} N_2^1(x) = \dfrac{x}{2} - 1, & 2 \le x \le 4 \\ N_2^2(x) = -\dfrac{x}{2} + 3, & 4 \le x \le 6 \\ 0, & otherwise \end{cases}$	$\dfrac{dN_2(x)}{dx} = \begin{cases} \dfrac{dN_2^1(x)}{dx} = \dfrac{1}{2}, & 2 \le x \le 4 \\ \dfrac{dN_2^2(x)}{dx} = -\dfrac{1}{2}, & 4 \le x \le 6 \\ 0, & otherwise \end{cases}$
$N_3(x) = \begin{cases} N_3^2(x) = \dfrac{x}{2} - 2, & 4 \le x \le 6, \\ N_3^3(x) = -\dfrac{x}{3} + 3, & 6 \le x \le 9, \\ 0, & otherwise \end{cases}$	$\dfrac{dN_3(x)}{dx} = \begin{cases} \dfrac{dN_3^2(x)}{dx} = \dfrac{1}{2}, & 4 \le x \le 6, \\ \dfrac{dN_3^3(x)}{dx} = -\dfrac{1}{3}, & 6 \le x \le 9, \\ 0, & otherwise \end{cases}$
$N_4(x) = \begin{cases} N_4^3(x) = \dfrac{x}{3} - 2, & 6 \le x \le 9, \\ 0, & otherwise \end{cases}$	$\dfrac{dN_4(x)}{dx} = \begin{cases} \dfrac{dN_4^3(x)}{dx} = \dfrac{1}{3}, & 6 \le x \le 9, \\ 0, & otherwise \end{cases}$

Then, the stiffness matrix $\mathbf{K}$, in the element are integrate with respect to x

$$K_{ij} = \int_a^b \frac{dN_i}{dx} Ak \frac{dN_j}{dx} dx$$

The element will produce the stiffness matrix such as below

$$\mathbf{K} = \begin{pmatrix} K_{11} & K_{12} & K_{13} & K_{14} \\ K_{21} & K_{22} & K_{23} & K_{24} \\ K_{31} & K_{32} & K_{33} & K_{34} \\ K_{41} & K_{42} & K_{43} & K_{44} \end{pmatrix} = \begin{pmatrix} 20 & -20 & 0 & 0 \\ -20 & 40 & -20 & 0 \\ 0 & -20 & \frac{100}{3} & -\frac{40}{3} \\ 0 & 0 & -\frac{40}{3} & \frac{40}{3} \end{pmatrix}$$

Next the boundary vector and load vector are calculated which are

$$f_b = -10\begin{pmatrix} N_1(9)q(9) - N_2(2)q(2) \\ N_2(9)q(9) - N_2(2)q(2) \\ N_3(9)q(9) - N_3(2)q(2) \\ N_4(9)q(9) - N_4(2)q(2) \end{pmatrix} = \begin{pmatrix} 10q_2 \\ 0 \\ 0 \\ 200 \end{pmatrix}$$

$$f_L = \begin{pmatrix} 50\int_2^4 -\frac{x}{2} + 2\,dx \\ 50\int_2^4 \frac{x}{2} - 1\,dx + 50\int_4^6 -\frac{x}{2} + 3\,dx \\ 50\int_4^6 \frac{x}{2} - 2\,dx + 50\int_6^9 -\frac{x}{3} + 3\,dx \\ 50\int_6^9 \frac{x}{3} - 2\,dx \end{pmatrix} = \begin{pmatrix} 50 \\ 100 \\ 125 \\ 75 \end{pmatrix}$$

Therefore, solving the system of linear equation by using Thomas algorithm $\mathbf{Ka} = \mathbf{f_b} + \mathbf{f_L}$, give the following value

$$\begin{pmatrix} 20 & -20 & 0 & 0 \\ -20 & 40 & -20 & 0 \\ 0 & -20 & 100/3 & -40/3 \\ 0 & 0 & -40/3 & 40/3 \end{pmatrix} \begin{pmatrix} 0 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix} = \begin{pmatrix} 10q_2 \\ 0 \\ 0 \\ -200 \end{pmatrix} + \begin{pmatrix} 50 \\ 100 \\ 125 \\ 75 \end{pmatrix}$$

$$10q_3 + 50 = 20(c_1) + (-20)(c_2) + 0(c_3) + 0(c_4)$$
$$10q_3 + 50 = -20(5)$$
$$q_3 = -150$$

4.2 One-dimensional quadratic element

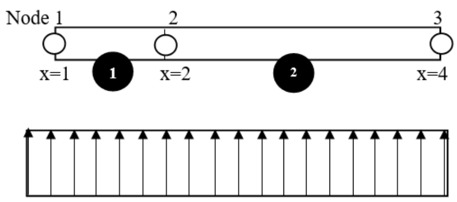

Figure 3 One-dimensional pipe diffusion with two nodes and three elements

Based on the strong formulation differential equation (3.4) We consider the values of $A = 10$, $k = 4$ *and* $Q = 100$. The boundary conditions are $c_1 = c|_{x=1} = 0$ and the flux, $q_4 = q|_{x=4} = 20$. By using Galerkin method for approximation on the quadratic model, $c = a + bx + dx^2$ we need to find the concentration at each nodal point, at *x=2* and *x=4*, and the flux at the left of the pipe end.

First, we used Kronecker delta to describe the shape function for a certain node equals 1 at that node and 0 at all other nodes. The shape functions and their derivatives are defined as table below

Table 2: The global shape functions and their piecewise function derivatives

$N_1(x) = \begin{cases} N_1^1(x) = 6 - 7x + 2x^2 & 1 \le x \le 2, \\ 0, & otherwise \end{cases}$	$\dfrac{dN_1(x)}{dx} = \begin{cases} \dfrac{dN_1^1(x)}{dx} = -7 + 4x, & 1 \le x \le 2, \\ 0, & otherwise \end{cases}$
$N_2(x) = \begin{cases} N_2^1(x) = -8 + 12x - 4x^2, & 1 \le x \le 2 \\ 0, & otherwise \end{cases}$	$\dfrac{dN_2(x)}{dx} = \begin{cases} \dfrac{dN_2^1(x)}{dx} = 12 - 8x, & 1 \le x \le 2 \\ 0, & otherwise \end{cases}$
$N_3(x) = \begin{cases} N_3^1(x) = 3 - 5x + 2x^2, & 1 \le x \le 2, \\ N_3^2(x) = 6 - 3.5x + 0.5x^2, & 2 \le x \le 4, \\ 0, & otherwise \end{cases}$	$\dfrac{dN_3(x)}{dx} = \begin{cases} \dfrac{dN_3^1(x)}{dx} = -5 + 4x, & 1 \le x \le 2, \\ \dfrac{dN_3^2(x)}{dx} = -3.5 + x, & 2 \le x \le 4, \\ 0, & otherwise \end{cases}$
$N_4(x) = \begin{cases} N_4^2(x) = -8 + 6x - x^2, & 2 \le x \le 4, \\ 0, & otherwise \end{cases}$	$\dfrac{dN_4(x)}{dx} = \begin{cases} \dfrac{dN_4^1(x)}{dx} = 6 - 2x, & 2 \le x \le 4, \\ 0, & otherwise \end{cases}$
$N_5(x) = \begin{cases} N_5^2(x) = 3 - 2.5x + 0.5x^2, & 2 \le x \le 4, \\ 0, & otherwise \end{cases}$	$\dfrac{dN_5(x)}{dx} = \begin{cases} \dfrac{dN_5^2(x)}{dx} = -2.5 + x, & 2 \le x \le 4, \\ 0, & otherwise \end{cases}$

Then, the stiffness matrix $\mathbf{K}$, in the element are integrate with respect to x

$$K_{ij} = \int_a^b \frac{dN_i}{dx} Ak \frac{dN_j}{dx} dx$$

The element produces the stiffness matrix such as below

$$\boldsymbol{K} = \begin{pmatrix} K_{11} & K_{12} & K_{13} & K_{14} & K_{15} \\ K_{21} & K_{22} & K_{23} & K_{24} & K_{25} \\ K_{31} & K_{32} & K_{33} & K_{34} & K_{35} \\ K_{41} & K_{42} & K_{43} & K_{44} & K_{45} \\ K_{51} & K_{52} & K_{53} & K_{54} & K_{55} \end{pmatrix} = \begin{pmatrix} \frac{280}{3} & -\frac{320}{3} & \frac{40}{3} & 0 & 0 \\ -\frac{320}{3} & \frac{640}{3} & -\frac{320}{3} & 0 & 0 \\ \frac{40}{3} & -\frac{320}{3} & 140 & -\frac{160}{3} & \frac{20}{3} \\ 0 & 0 & -\frac{160}{3} & \frac{320}{3} & -\frac{160}{3} \\ 0 & 0 & \frac{20}{3} & -\frac{160}{3} & \frac{140}{3} \end{pmatrix}$$

Next the boundary vector and load vector are calculated which are

$$\boldsymbol{f_b} = -10\begin{pmatrix} N_1(4)q(4) - N_1(1)q(1) \\ N_2(4)q(4) - N_2(1)q(1) \\ N_3(4)q(4) - N_3(1)q(1) \\ N_4(4)q(4) - N_4(1)q(1) \\ N_5(4)q(4) - N_5(1)q(1) \end{pmatrix} == -10\begin{pmatrix} 0 - q(1) \\ 0 - 0 \\ 0 - 0 \\ 0 - 0 \\ q(4) - 0 \end{pmatrix} = \begin{pmatrix} 10q_1 \\ 0 \\ 0 \\ 0 \\ -200 \end{pmatrix}$$

$$\mathbf{f_L} = \begin{pmatrix} 100\int_1^2 x^2 - 7x + 6\,dx \\ 100\int_1^2 -4x^2 + 12x - 8x\,dx \\ 100\int_1^2 2x^2 - 5x + 3\,dx + 100\int_2^4 0.5x^2 - 3.5x + 6\,dx \\ 100\int_2^4 -x^2 + 6x - 8\,dx \\ 100\int_2^4 0.5x^2 - 2.5x + 3\,dx \end{pmatrix} = \begin{pmatrix} -\frac{650}{3} \\ \frac{200}{3} \\ 50 \\ \frac{400}{3} \\ \frac{100}{3} \end{pmatrix}$$

Therefore, solving the system of linear equation by using Thomas algorithm $\mathbf{Ka} = \mathbf{f_b} + \mathbf{f_L}$, give the following values

$$\begin{pmatrix} \frac{640}{3} & -\frac{320}{3} & 0 & 0 \\ -\frac{320}{3} & 140 & -\frac{160}{3} & \frac{20}{3} \\ 0 & -\frac{160}{3} & \frac{320}{3} & -\frac{160}{3} \\ 0 & \frac{20}{3} & -\frac{160}{3} & \frac{140}{3} \end{pmatrix}\begin{pmatrix} T_2 \\ T_3 \\ T_4 \\ T_5 \end{pmatrix} = \begin{pmatrix} \frac{200}{3} \\ 50 \\ \frac{400}{3} \\ -\frac{500}{3} \end{pmatrix}$$

$$10q_1 - \frac{650}{3} = \frac{280}{3}\left(c_1\right) + \left(-\frac{320}{3}\right)\left(c_2\right) + \frac{40}{3}\left(c_3\right) + 0\left(c_4\right) + 0\left(c_5\right)$$

$$10q_1 - \frac{650}{3} = \left(-\frac{320}{3}\right)\left(\frac{115}{176}\right) + \frac{40}{3}\left(\frac{15}{22}\right)$$

$$q_1 = \frac{515}{33}$$

$$= 15.6061$$

5 Conclusion

In this study we have identified that the FEM is a technique to solve partial differential equations. Generally, FEM is a mathematical method used to predict how a structure will behave based on a finite element analysis (FEA) of any physical phenomenon. The problems discussed on the behaviour of Fick's Law related with FEM, several methods that related to solve linear equation system and numerical method be used to solve a diffusion problem in one-dimensional system. The basis concept and the derivation of strong formulation of one-dimensional diffusion problem is derived in this study. The formulation of Thomas algorithm and shape function for linear and quadratic equation are showed. To summarise, the several examples of one-dimensional linear diffusion problem and one-dimensional quadratic problem with different elements and node has been completed. This chapter needs to obtain global shape function and their derivatives, find stiffness matrix **K**, obtain the boundary vector, and load vector. From this example, we can conclude that it showed that three element is better than two elements. And the number of elements influenced shape function.

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