Computational Fluid Dynamics
Coursework 1

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1. The Laplace equation models the heat conduction and is defined as:

$$\nabla^2 \mathbf{T} = \mathbf{0} \tag{1}$$

a) Discretise equation (1) in one dimension using a centered approximation.

The Laplace equation given above in one dimension can be written as:

$$\nabla^2 \mathrm{T} = 0 \rightarrow \frac{\partial^2 T}{\partial x^2} = 0$$

The 1-D Laplace equation can be discretized into Finite Difference form using the Taylor series expansion which is given by:

$$T(x + \Delta x) = T(x) + \Delta x \frac{\partial T}{\partial x} + \frac{(\Delta x)^2}{2} \frac{\partial^2 T}{\partial x^2} + \cdots + \frac{(\Delta x)^n}{n!} \frac{\partial^n T}{\partial x^n}$$

The 1-D central approximation uses the point before and after the current point to update the current point. So, one step forward and one step backward of Taylor expansion are needed to get the central approximation:

$$T_{i+1} = T_i + \Delta x \frac{\partial T}{\partial x} + \frac{(\Delta x)^2}{2} \frac{\partial^2 T}{\partial x^2} + \frac{(\Delta x)^3}{6} \frac{\partial^3 T}{\partial x^3} + O(\Delta x^4)$$

$$T_{i-1} = T_i - \Delta x \frac{\partial T}{\partial x} + \frac{(-\Delta x)^2}{2} \frac{\partial^2 T}{\partial x^2} - \frac{(\Delta x)^3}{6} \frac{\partial^3 T}{\partial x^3} + O(\Delta x^4)$$

$$T_{i+1} + T_{i-1} = 2T_i + (\Delta x)^2 \frac{\partial^2 T}{\partial x^2} + O(\Delta x^4) \rightarrow \frac{\partial^2 T}{\partial x^2} = \frac{T_{i+1} - 2T_i + T_{i-1}}{(\Delta x)^2} - O(\Delta x^2) = 0$$

As can be seen from the final expression of the second order derivative, the dependent variable in truncation error has a power of 2, which implies that this central approximation is a second order accurate scheme.

b) The domain is a square in the region $0 \leq x \leq 1$, $0 \leq y \leq 1$ what boundary conditions are needed/possible on the edges? Justify your answer.

One of the possible types of boundary condition that can be applied on the edges is the Dirichlet boundary condition. It specifies the value of $\phi(x, y)$, or in this case, the value of $T(x, y)$ on the edges of the domain, and then the adjacent points' solution can be obtained by using the scheme, so the solution will propagate inwards to the domain while doing iterations and should converge after some amount of iterations depending on the size of the mesh. Laplace equation totally depends on the boundary conditions, any changes on boundary conditions will result in different final solution. The Dirichlet boundary condition to be imposed could be a constant or a known function, as long as the values on the edges are specified the Laplace equation can be solved by numerical schemes.

It is also possible to apply Neumann and Robin condition for the Laplace equation, Neumann condition specifies the normal derivative $\frac{\partial T(x,y)}{\partial \boldsymbol{n}}$ on each points along the boundaries and Robin condition is a combination of Dirichlet and Neumann, it specifies $T(x, y) + \frac{\partial T(x,y)}{\partial \boldsymbol{n}}$ on the boundaries. It is very important to mention that the Dirichlet boundary condition need to be imposed at least on one edge. For example, in the given case, which is in a 2D domain, Neumann and Robin conditions can be only imposed on maximum 3 edges, and the last one should have a Dirichlet condition in order to solve numerically the Laplace equation. If Neumann or Robin conditions are applied at all four edges, there will be infinite possible solutions for the Laplace equation, since there is infinite value for $T(x, y)$ with the same gradient, infinite possible solution is not a valid solution.

c) Use TWO numerical schemes to discretize your equation and solve the PDE assuming the following boundary conditions T = 1@x = 0, T = cos(6 * 3 2 πy) + 1@x = 1, T = 1@y = 1. T = (1 + x)@y = 0. In the domain there is a point at T = 1.5@x = 0.5, y = 0.5 Discuss the advantage of one scheme against the other and plot the iso-contours of the two dimensional thermal field in both cases.

The domain to model the heat conduction is two dimensional, this implies that a new dimension should be added to the temperature $T(x, y)$, and the Laplace equation in two dimension will have the following form:

$$\nabla^2 \mathrm{T} = 0 \rightarrow \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$$

Two different schemes will be used in this coursework. The first scheme which make the discretization is the five-point central Finite Difference approximation. This scheme uses 4 surrounding points to update the solution on each point, the scheme can be deduced from the 2D Taylor series expansion in x and y direction and they are given by the following expressions:

$$T(x + \Delta x, y) = T(x, y) + \Delta x \frac{\partial T(x, y)}{\partial x} + \frac{(\Delta x)^2}{2} \frac{\partial^2 T(x, y)}{\partial x^2} + \cdots + \frac{(\Delta x)^n}{n!} \frac{\partial^n T(x, y)}{\partial x^n}$$

$$T(x, y + \Delta y) = T(x, y) + \Delta y \frac{\partial T(x, y)}{\partial y} + \frac{(\Delta y)^2}{2} \frac{\partial^2 T(x, y)}{\partial y^2} + \cdots + \frac{(\Delta y)^n}{n!} \frac{\partial^n T(x, y)}{\partial y^n}$$

As can be observed from the above Taylor series expansions with two variables, the form of these expansions is really the same as the form of Taylor expansion with one variable. Thus, the central finite difference expression found in section a) can be directly used but with a slight modification in sub-index. Since it is 2D now, a new sub-index j is incorporated to represent the second dimension. The 2D central finite difference using 4 surrounding points can be then written as following:

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = \frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{(\Delta x)^2} + \frac{T_{i,j+1} - 2T_{i,j} + T_{i,j-1}}{(\Delta y)^2} = 0$$

Rearrange the Laplace equation in Finite Difference form above to obtain the update scheme of each point:

$$T_{i,j} = \left(\frac{\Delta x^2 \Delta y^2}{2\Delta x^2 + 2\Delta y^2}\right)\left(\frac{T_{i+1,j} + T_{i-1,j}}{\Delta x^2} + \frac{T_{i,j+1} + T_{i,j-1}}{\Delta y^2}\right)$$

The found scheme above is second order accurate, this scheme uses the four neighbour points to update the solution at each point. Note the points along the four edges of the domain should not be included in the update scheme, the values on the boundaries are fixed and specified by the given condition. So, the sub-index of the scheme should be limited to $2 \le i \le m-1$ and $2 \le j \le m-1$ for a domain with $m \times n$ points. Apart from four boundary conditions on the edges, there is another boundary condition which is not situated at the edges. One of the ways to impose this boundary condition in the code is let the update scheme to include this point, and after this point is updated by the scheme, replae the specified value back to this point immediately, so this point remains the same value after each iteration and the surrounding points can take this specified value into the calculation. The resultant iso-contour plot of the two-dimensional thermal field using five-point central scheme is shown below:

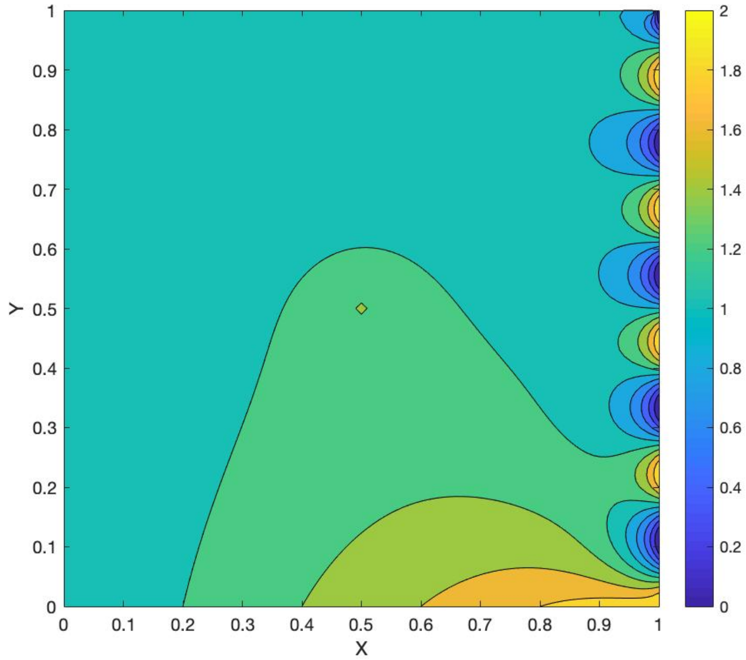

Figure 1: Iso-contour plot of thermal field using five-point central scheme

The second scheme to discretize the Laplace equation is the nine-point central finite difference scheme. This scheme is very similar to the five-point scheme which was described previously, the difference between is that this scheme uses 8 surrounding points to update the solution at each point, which means that in addition to the four surrounding points, four more outer points are taken into account. To deduce this scheme, 2D Taylor expansions of 2-step sizes are needed:

$$T_{i+2,j} = T_{i,j} + 2\Delta x \frac{\partial T}{\partial x} + \frac{(2\Delta x)^2}{2}\frac{\partial^2 T}{\partial x^2} + \frac{(2\Delta x)^3}{6}\frac{\partial^3 T}{\partial x^3} + O(\Delta x^4)$$

$$T_{i-2,j} = T_{i,j} - 2\Delta x \frac{\partial T}{\partial x} + \frac{(-2\Delta x)^2}{2}\frac{\partial^2 T}{\partial x^2} + \frac{(-2\Delta x)^3}{6}\frac{\partial^3 T}{\partial x^3} + O(\Delta x^4)$$

$$T_{i,j+2} = T_{i} + 2\Delta y \frac{\partial T}{\partial y} + \frac{(2\Delta y)^2}{2}\frac{\partial^2 T}{\partial y^2} + \frac{(2\Delta y)^3}{6}\frac{\partial^3 T}{\partial y^3} + O(\Delta y^4)$$

$$T_{i,j-2} = T_{i} - 2\Delta y \frac{\partial T}{\partial y} + \frac{(-2\Delta y)^2}{2}\frac{\partial^2 T}{\partial y^2} + \frac{(-2\Delta y)^3}{6}\frac{\partial^3 T}{\partial y^3} + O(\Delta y^4)$$

And just to remember, the Taylor expansions of one-step size are:

$$T_{i+1,j} = T_{i,j} + \Delta x \frac{\partial T}{\partial x} + \frac{(\Delta x)^2}{2}\frac{\partial^2 T}{\partial x^2} + \frac{(\Delta x)^3}{6}\frac{\partial^3 T}{\partial x^3} + O(\Delta x^4)$$

$$T_{i-1,j} = T_{i,j} - \Delta x \frac{\partial T}{\partial x} + \frac{(-\Delta x)^2}{2}\frac{\partial^2 T}{\partial x^2} - \frac{(\Delta x)^3}{6}\frac{\partial^3 T}{\partial x^3} + O(\Delta x^4)$$

$$T_{i,j+1} = T_{i,j} + \Delta y \frac{\partial T}{\partial y} + \frac{(\Delta x)^2}{2}\frac{\partial^2 T}{\partial y^2} + \frac{(\Delta x)^3}{6}\frac{\partial^3 T}{\partial y^3} + O(\Delta x^4)$$

$$T_{i,j-1} = T_{i,j} - \Delta y \frac{\partial T}{\partial y} + \frac{(-\Delta y)^2}{2}\frac{\partial^2 T}{\partial y^2} - \frac{(\Delta y)^3}{6}\frac{\partial^3 T}{\partial y^3} + O(\Delta y^4)$$

Summing all the Taylor expansions in x-direciton will get:

$$T_{i+2,j} + T_{i-2,j} + T_{i+1,j} + T_{i-1,j} = 4T_{i,j} + 5(\Delta x)^2 \frac{\partial^2 T}{\partial x^2} + O(\Delta x^4)$$

$$\frac{\partial^2 T}{\partial x^2} = \frac{T_{i-2,j} + T_{i-1,j} - 4T_{i,j} + T_{i+1,j} + T_{i+2,j}}{5(\Delta x)^2}$$

Similarly, in y-direciton:

$$\frac{\partial^2 T}{\partial y^2} = \frac{T_{i,j-2} + T_{i,j-1} - 4T_{i,j} + T_{i,j+1} + T_{i,j+2}}{5(\Delta y)^2}$$

Nine-point Finite difference scheme of Laplace equation:

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = \frac{T_{i-2,j} + T_{i-1,j} - 4T_{i,j} + T_{i+1,j} + T_{i+2,j}}{5(\Delta x)^2} + \frac{T_{i,j-2} + T_{i,j-1} - 4T_{i,j} + T_{i,j+1} + T_{i,j+2}}{5(\Delta y)^2} = 0$$

Rearrange the expression and omitting the intermediate process, it was found that the update scheme at each point is given by:

$$T_{i,j} = \left(\frac{\Delta x^2 \Delta y^2}{4\Delta x^2 + 4\Delta y^2}\right)\left(\frac{T_{i-2,j} + T_{i-1,j} + T_{i+1,j} + T_{i+2,j}}{\Delta x^2} + \frac{T_{i,j-2} + T_{i,j-1} + T_{i,j+1} + T_{i,j+2}}{\Delta y^2}\right)$$

Note the nine-point scheme uses 2 points forward and backward in each direction, this will cause a problem at the points just next to the boundaries, these points will need points outside the edges to update their solution. One way to solve this problem is to create extra halo points outside the boundaries, another way is to use five-point central scheme at the points next to boundary. Since five-point scheme only need one point forward and backward, so the solution on points next to edges can be updated without the halo points. The second mentioned way to solve the Laplace equation is used in this coursework. it is really a mixed five-point and nine-point scheme. The following sketch could be helpful to understand what is done in order to make this scheme to work.

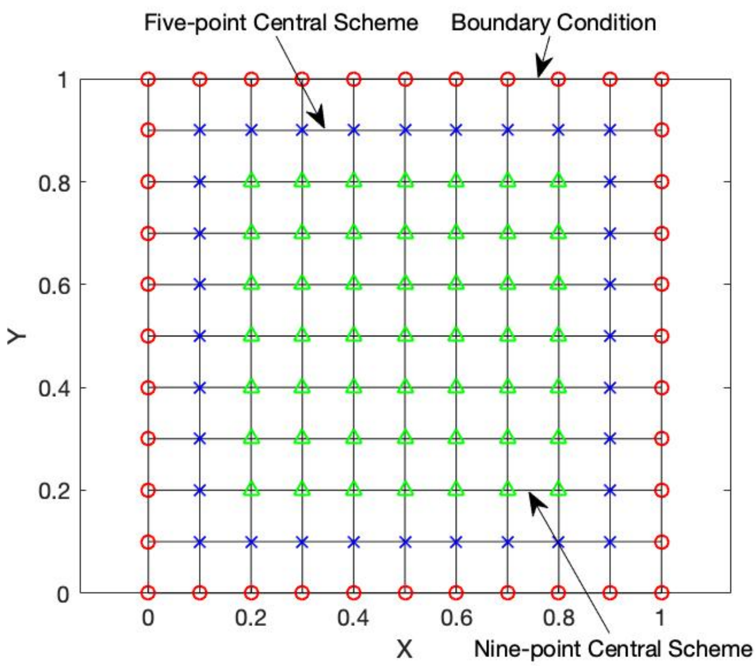

Figure 2: Diagrammatic sketch of the scheme

The resultant iso-contour plot using the nine-point scheme is very similar as the one of five-point scheme and is shown below:

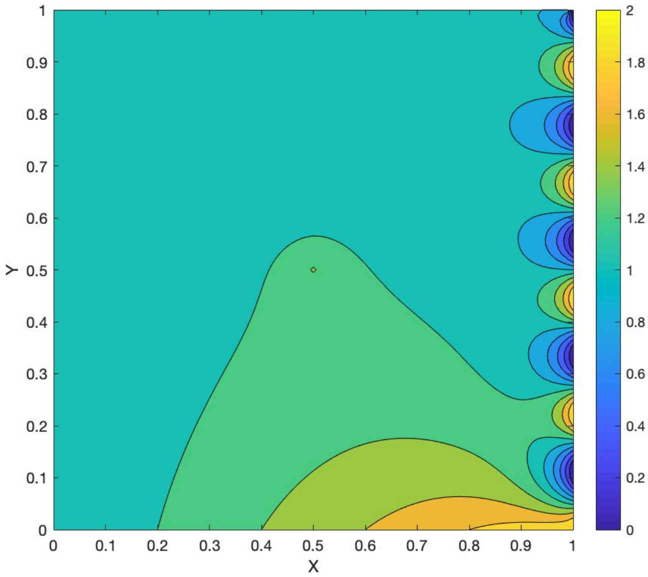

Figure 3: Iso-contour plot of thermal field using nine-point central scheme

Comparing the resultant iso-contour in Figure *1* and Figure *3*, they do not seem to have many difference, this implies that both schemes are able to solve the Laplace equation and give the approximated solution of the Laplace equation. Both schemes have their own advantages and disadvantages. In order to show the advantages and disadvantages of each scheme in a more intuitive way, the following plots were made:

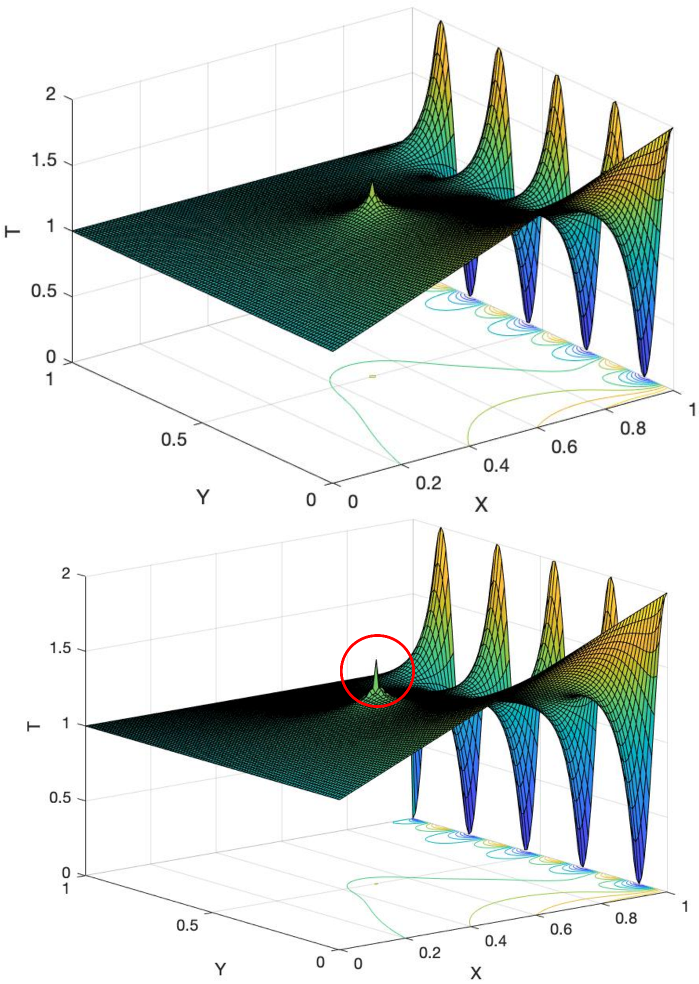

Figure 4: 3D view of the thermal field using five-point scheme (up) and nine-point scheme (down)

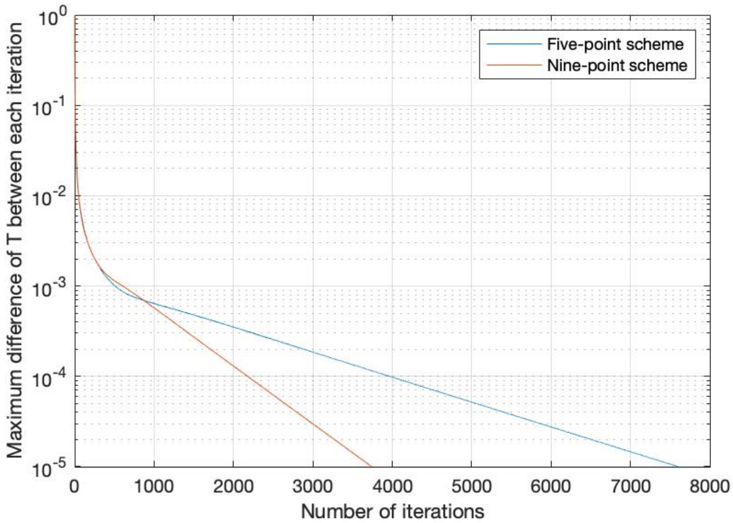

Figure 5: Number of iterations needed to converge

Although no difference can be found between contour plots of five-point and nine-point plots, but when looking at 3D views of the thermal field shown in *Figure 4*, the difference becomes much clearer. It can be observed that the middle region, around the peak, of the nine-point scheme has less smooth results than the one of the five-point scheme. This is because the nine-point scheme need to take the 2 points away from current point to update, this implies that the 4 surrounding points just next to the peak will take the points on the other side of the peak into the scheme, so the value at peak point will be less weighted in the update scheme for these points which will consequently result in lower values of T at these 4 points.

Now looking the *Figure 5*, it shows the convergence rate of both schemes. The y-axis represents the maximum value difference of T among all points in the domain. As can be seen that there is no big difference between two schemes in terms of iteration number to reach a convergence criteria of 10^{-3}, but for the convergence criteria above this level, the five-point scheme needs much more iteration numbers than the nine-point scheme need. For example, in order to reach a convergence criteria of 10^{-5} for a mesh of 101×101 points, five-point scheme (3743 iterations) need to take double iteration number (7604 iterations) than nine-point scheme need. The reason that nine-point scheme converges faster is that it takes 8 surrounding points to update at each point, so more information is propagated to each point for each iteration.

In conclusion, the advantage of the nine-point scheme is that it converges much faster, so in large simulations, this scheme will save a lot of time; one of the disadvantages of this scheme is that it does not work very well for the points around the peak, another disadvantage is that it is quite complicated to implement in the code, since the points just next to the boundaries need to be specify, which means extra "boundary conditions" are needed. On the other hand, the five-point scheme does not have problem when dealing with the points around the peak, and it is relatively easy to implement in the code; the disadvantage is that this scheme need to spend a lot of time to reach the convergence.

d) Using the same boundary conditions of question c, plot ϵ_{max} versus Δx on a set of log-log axes and comment on the form of the plot. Mesh with Δx=Δy, at least 3 different mesh sizes. Explain how you have decided the minimum Δx=Δy of your computational domain.

Six different mesh sizes were used to solve the Laplace equation, the number of mesh points used are 321×321, 161×161, 81×81, 41×41, 21×21, 11×11. The results on the finest mesh was assumed to be the "true solution", and the error was calculated by comparing results on other mesh sizes with the results on finest mesh. Since the domain is two dimensional, every comparison will produce a set of errors, to see the effect of mesh size on the error, the maximum error value of each set was taken. The following log-log scaled plot shows that the maximum error versus different mesh size:

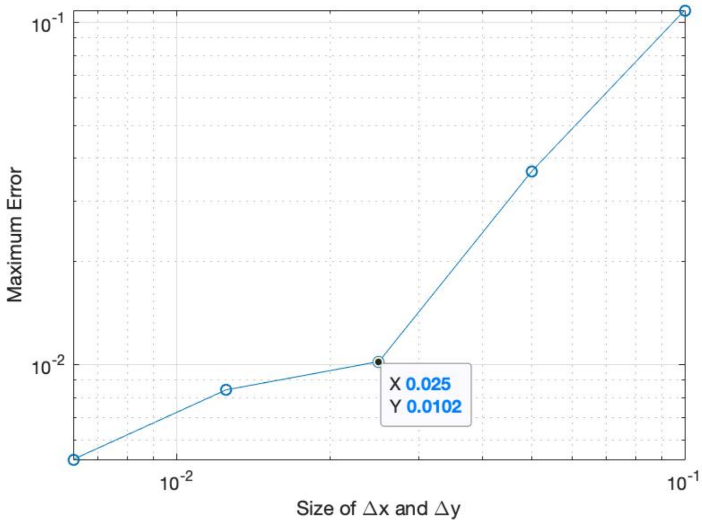

Figure 6: Maximum error with different size of **Δx=Δy**

Looking at the Figure *6*, the main tendency of the curve is behaving as expected, increasing the size of $\Delta x = \Delta y$ will result a larger error. The curve is clearly not linear, as can be seen from the graph, it is divided into a high gradient region and a low gradient region, entering low gradient region implies that the effect of decreasing mesh size is reduced, so the optimum minimum mesh size would be 0.025, it is the point where the high gradient becomes low gradient. Using mesh sizes below this value will not improve remarkably the results, and at the same time it will increase significantly the cost in time and computational resource, which is very inefficient. Thus, 0.025 would be the optimum minimum mesh size. Additionally, since there is a sinusoidal function on the right edge, which is $\cos(9\pi x) + 1$, a minimum of 10 points are needed in order to catch the oscillatory behaviour of the function, otherwise the shape or the frequency of the sinusoidal function will be altered.