Proceedings of the course Computational Heat and Fluid Flow ME6151
Indian Institute of Technology Madras
January-May, 2025, Chennai, India

DIFFUSION ON TWO-DIMENSIONAL UNSTRUCTURED ORTHOGONAL AND NON-ORTHOGONAL MESHES IN A SQUARE DOMAIN

Anushka Venkatesh
ME21B026
Department of Mechanical Engineering
Indian Institute of Technology Madras
Chennai 600036
Email: me21b026@smail.iitm.ac.in

Ronalyn Sequeira
ME21B186
Department of Mechanical Engineering
Indian Institute of Technology Madras
Chennai 600036
Email: me21b186@smail.iitm.ac.in

ABSTRACT

Many physics problems require the use of unstructured meshes due to their complex geometries. This study focuses on building a Python code for a simple square domain using the Finite Volume Method for the Diffusion Problem over unstructured meshes which is not as easily formulated as structured meshes. These codes can then be further expanded over more complicated domains.

INTRODUCTION

The main goal of this study is to develop a solver that can solve the Finite-Volume 2D diffusion equation with both Dirichlet and Nuemann boundary conditions on unstructured meshes of the orthogonal and non-orthogonal kind.

Many engineering problems often require PDEs to be solved over domains with complex shapes. Structured meshes which have square or rectangular cells do not conform to these complex geometries well. Unstructured meshes can virtually conform to any domain shape, as they have no restriction on the cell shape. However, this comes at the cost of increased memory usage and reduced speeds as each cell and its neighbours need to be stored separately.

Further, non-orthogonal unstructured meshes also allow for local refinement of meshes which proves to be very useful for regions of the mesh where the gradients are high. On the other hand, structured meshes for these cases would require that entire rows and columns be refined to capture regions with high gradients.

Given the advantages mentioned above, unstructured meshes find extensive application in CFD problems such as engine combustion, flow over aircraft wings, and blood flow in arteries, where accurate mesh geometry representation is critical.

PROBLEM STATEMENT

We're solving for temperature distribution over a square domain of unit side with unit diffusion constant. The upper and lower boundaries are maintained at 200 K and the left and right boundaries at 100 K without heat generation in the domain. Four methods of obtaining the solution were implemented: a structured square mesh, an unstructured equilateral triangle mesh, and an unstructured non-orthogonal triangular mesh for the Finite-Volume method. Additionally, the square-mesh was also solved using the Finite-Difference method to verify the solution.

GOVERNING EQUATIONS

The 2D steady-state diffusion equation for a scalar field $\phi(x,y)$, with a constant diffusion coefficient D and a source term $S(\phi)$, is given by:

$$\nabla \cdot (D\nabla\phi) + S(\phi) = 0 \quad \text{in the domain } \Omega \tag{1}$$

Assuming D is constant:

$$D\nabla^2\phi + S(\phi) = 0 \tag{2}$$

Integrating over a control volume $C.V$, we obtain:

$$\int_{C.V} \nabla \cdot (D\nabla\phi)\, dV + \int_{C.V} S(\phi)\, dV = 0 \tag{3}$$

Applying the Gauss divergence theorem:

$$\int_{C.S} D\nabla\phi \cdot \hat{n}\, dA + \int_{C.V} S(\phi)\, dV = 0 \tag{4}$$

where $\hat{n}$ is the outward unit normal to the control surface.

DISCRETIZATION

Unstructured Orthogonal Mesh

The discretized diffusion equation gives:

$$\sum_{faces} D\nabla\phi.\delta A_{face} + S(\phi)\delta V = 0 \tag{5}$$

Following the local coordinate system of the triangular cell to obtain $\nabla\phi$:

$$\nabla\phi = \frac{\partial\phi}{\partial\xi}\hat{\xi} + \frac{\partial\phi}{\partial\eta}\hat{\eta} \tag{6}$$

Applying the Central Difference scheme and assuming $\Delta\xi = \Delta\eta = h$ i.e. an equilateral mesh, the final discretized equation for an unstructured orthogonal mesh is :

$$D\left(\frac{\phi_1 + \phi_2 + \phi_3 - 3\phi_p}{\Delta\xi}\right)\Delta\eta + S_\phi \Delta\xi\Delta\eta = 0 \tag{7}$$

Simplifying :

$$\phi_P = \frac{1}{3}(\phi_1 + \phi_2 + \phi_2) + \frac{h^2}{3D}S_\phi \tag{8}$$

Unstructured Non-Orthogonal Mesh

For a non-orthogonal mesh, the local coordinate system can be expressed as:

$$\begin{aligned} \vec{e}_\xi &= x_\xi \hat{i} + y_\xi \hat{j} \\ \vec{e}_\eta &= x_\eta \hat{i} + y_\eta \hat{j} \end{aligned} \tag{9}$$

The gradient is:

$$\nabla\phi = \frac{\partial\phi}{\partial x}\hat{i} + \frac{\partial\phi}{\partial y}\hat{j} \tag{10}$$

In local coordinates:

$$\begin{aligned} \phi_\xi &= \phi_x x_\xi + \phi_y y_\xi \\ \phi_\eta &= \phi_x x_\eta + \phi_y y_\eta \end{aligned} \tag{11}$$

The face area vector is given by:

$$\vec{A}_f = A_x \hat{i} + A_y \hat{j} \tag{12}$$

Substituting the coordinate and gradient expressions into the diffusion term $D\nabla\phi \cdot \vec{A}_f$, we obtain:

$$D(\nabla\phi)_f \cdot \vec{A}_f = D\left[\frac{\partial\phi}{\partial\xi}\frac{A_x y_\eta - A_y x_\eta}{J} + \frac{\partial\phi}{\partial\eta}\frac{A_y x_\xi - A_x y_\xi}{J}\right] \tag{13}$$

where $J = x_\xi y_\eta - x_\eta y_\xi$ is the Jacobian determinant. Upon simplifying :

$$D(\nabla\phi)_f \cdot \vec{A}_f = D_f\left(\frac{A_f.A_f}{A_f.e_\xi}\phi_\xi\right) - D_f\left(\frac{A_f.A_f}{A_f.e_\xi}(e_\xi.e_\eta)\phi_\eta\right) \tag{14}$$

Where ϕ_ξ is called the primary gradient and ϕ_η is the secondary / non-orthogonal gradient.
The non-orthogonal gradient is found using the green-gauss method using values from the previous iteration.

Structured Orthogonal Mesh

For a structured Cartesian mesh with uniform grid spacing $\Delta x = \Delta y = h$, the finite volume discretization with central differences gives:

$$D\left(\frac{\phi_E + \phi_W - 2\phi_P}{h^2} + \frac{\phi_N + \phi_S - 2\phi_P}{h^2}\right) + S_\phi = 0 \tag{15}$$

Simplifying:

$$\phi_P = \frac{1}{4}(\phi_E + \phi_W + \phi_N + \phi_S) + \frac{h^2}{4D} S_\phi \tag{16}$$

PROCEDURE

This study looks at a numerical example of **steady-state pure diffusion** in two dimensions. The computational domain is a square region with a side length of **1.0 m**. Thermal conductivity is assumed to be constant and uniform, *1 kW/m*. In this example, we do not consider any internal source terms.

The problem is solved for three different types of computational meshes:

1. **Structured mesh** consisting of quadrilateral elements.
2. **Orthogonal unstructured mesh** composed of triangular elements.
3. **Non-orthogonal unstructured mesh** made up of triangular elements.

The study has been carried out for the case ”Dirichlet boundary conditions for all four walls, **left and right wall** at **100K** and **top and bottom wall** at **200K**”.

It can also be expanded to different combinations of Dirichlet and Neumann conditions (which is not used as a case in this report).

The governing equation, without the source term, then reduces to:

$$k\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right) = 0 \tag{17}$$

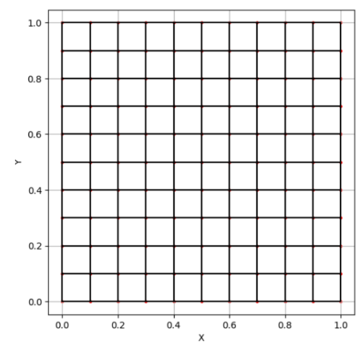
To verify the Temperature Distribution Profile obtained we use the results obtained from Finite Difference Method, which is:

$$\frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{(\Delta x)^2} + \frac{T_{i,j+1} - 2T_{i,j} + T_{i,j-1}}{(\Delta y)^2} = 0 \tag{18}$$

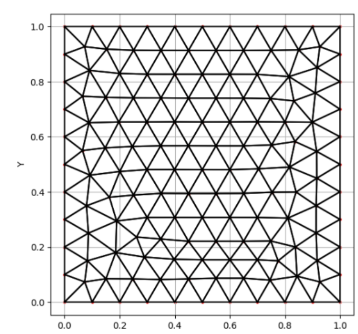
applied over structured mesh, with the above given boundary conditions.

METHODOLOGY

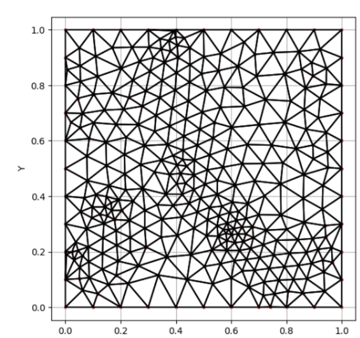
1. Mesh is generated using the *gmsh library* in Python or can also be imported from *GMSH software* as a *.msh* file.
2. The mesh function takes the input parameters on whether the user wants to generate an orthogonal or a non-orthogonal mesh.
3. Using the Finite Difference Method to find the temperature profile as the basis of comparison with code written by the Finite Volume Method (FVM).
4. The FVM method here, uses the cell centroid method, where the temperatures are stored at the centroids of each cell.
5. The functions for all three of the meshes can be altered to run for both Dirichlet and Neumann Boundary Conditions.



(a)



(b)



(c)

FIGURE 1: Mesh configurations used in the simulations (a) Structured,(b) Unstructured Orthogonal and (c) Unstructured Non-orthogonal

The boundary conditions for the numerical problem we are solving is:

1. **Left** and **Right** walls at **100K**.
2. **Top** and **Bottom** walls at **200K**.

OBSERVATIONS AND RESULTS

The meshes generated for the numerical problem analysis are given in figure 1.
The **Temperature Profile** obtained through FDM over a structured mesh is given as follows:

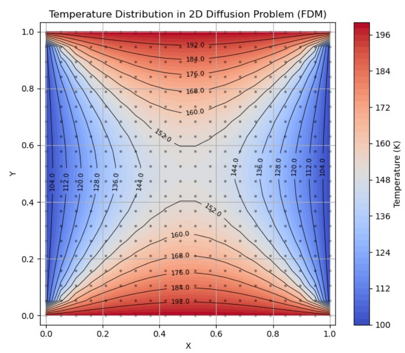


FIGURE 2: Temperature Profile from FDM

In Figure 2, we can see...
The Temperature Profiles for the three meshes and the number of iterations after which it has converged are given as:

1. Structured Mesh:

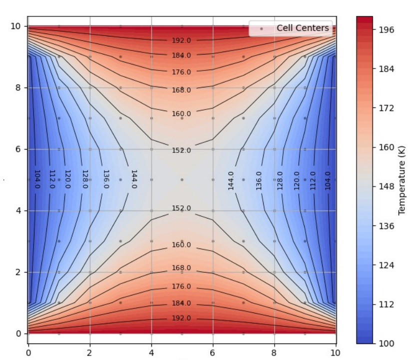


FIGURE 3: **118** iterations

2. Unstructured Orthogonal Mesh:
3. Unstructured Non-Orthogonal Mesh:

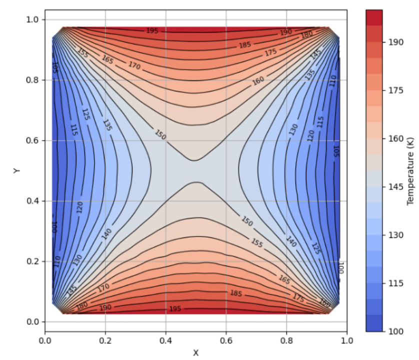


FIGURE 4: **473** iterations

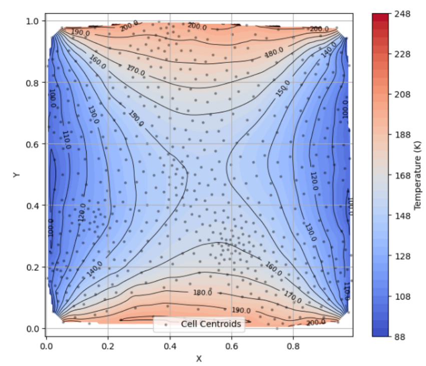


FIGURE 5: **3785** iterations

Results

1. In Figure 3, 4 and 5, the temperature profiles obtained are identical.Due to the differences in the locations of centroids and distances between two centroids of cells, the contours obtained are not smooth and the color-map is not identical.
2. The number of iterations for convergence increase from structured mesh to unstructured orthogonal mesh to unstructured non-orthogonal mesh.

CONCLUSION

A Python Code is developed for Finite Volume Method to solve steady-state pure diffusion equation over unstructured mesh (orthogonal and non-orthogonal) case considering both Dirichlet and Neumann conditions at any wall. This study used a numerical example over a square domain with three different meshes and compared the results with the solution obtained from Finite Difference Method which is generally used to solve Laplace Equation, which validates the code written.

REFERENCES

[1] Suhas V Patankar. *Numerical Heat Transfer and Fluid Flow*, volume 53, 1980.

[2] H.K. Versteeg and W. Malalasekera. *Introduction to Computational Fluid Dynamics*, volume 44, 2005.