Computational Fluid Dynamics
Fundamentals Course

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Disclaimer

The exercises, software, code and equations in this course are for educational and demonstrative purposes only. They should not be used to analyse, design, test, accredit or validate real scientific/engineering/mathematical structures and flow systems. For such applications, appropriate trained, qualified and accredited engineers/scientists should be consulted. Fluid Mechanics 101 and Dr. Aidan Wimshurst are not accountable or liable in any form for the use or misuse of the information contained in this course beyond the specific educational and demonstrative purpose for which it was intended.

Foreward

Welcome to my Computational Fluid Dynamics Fundamentals Course! I put together this course to help you develop a deep understanding of computational fluid dynamics (CFD), so that you can set up, run and post-process engineering simulations of fluids (liquids and gases) more effectively. This course starts from the absolute basics, with the only prior knowledge required being basic calculus, differential equations and vector operations. These basics are typically taught during first year college/university courses and in some cases secondary/high school lessons. Hence, this course is perfect for anyone with a foundational background in science/mathematics/engineering or physics.

Having carried out several years of CFD studies myself, I found that many areas of the CFD process were hidden or poorly explained. This often made it difficult for me and my colleagues to set up and analyse simple flow simulations. The aim of this course is to guide you through some simple flow simulations interactively, with working CFD code that you can set up and run yourself. The entire process if transparent and documented/explained and no specific CFD code is required. By the end of this course, you will have set up and run CFD simulations from scratch and observed first hand the effect of different discretisation schemes on the solution. Having carried out these simulations yourself, you can return to full-scale CFD codes with confidence and a deep understanding of how the CFD code is operating. This will ultimately lead to better simulations, results and problem solving skills.
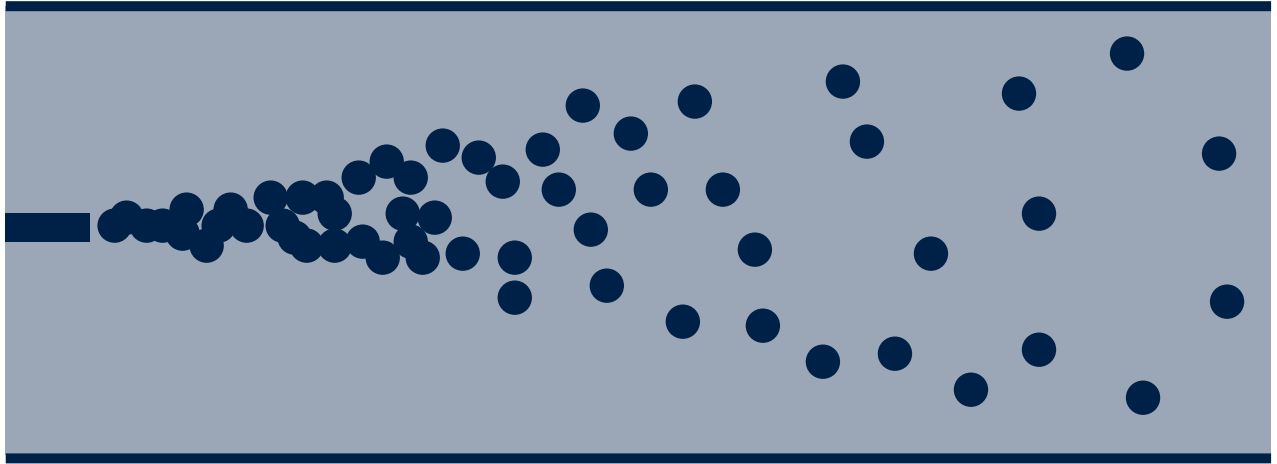
I am really excited to bring you this course and know that you will find it as useful as I have. The interactive exercises may even answer some long standing technical questions that you never found the answer to ...

All the best
Aidan

How To Use This Course

This course contains a comprehensive set of equations, explantations and diagrams, which are all contained in this PDF book. It is recommended that you follow along with the content in this book from start to finish, as Chapter 3 and 4 follow chronologically from Chapter 1 and 2. As you proceed through Chapter 2, 3 and 4, worked examples are provided. When instructed, it is advied that you open the example code (either in Microsoft Excel or in a suitable text editor/graphical user interface (GUI) for Python). Here you will be able to examine the code, modify the input variables and run the CFD simuations yourself. This is where the majority of the learning is likely to take place and is highly encouraged for all readers.

All of the exercises can be completed using either the Excel or Python scripts. Use whichever approach is more appealing and straightforward for you to follow. Alternatively, you can use the equations that are provided in the text to write your own code/scripts to solve the equations! The aim of this course is not to develop knowledge of a specific language or CFD code, but to learn and observe the overall process. Hence, it is highly encouraged for you to take your preferred approach.

Chapter 1

Introduction to Transport Equations

1   Introduction to Transport Equations

A solid body will remain stationary or in motion at constant velocity unless acted on by external forces. When acted on by external forces, the momentum of a solid body will change according to Newton's second law. For a solid body with constant mass, Newton's second law can be written concisely in differential form as:

$$\boldsymbol{F} = m\boldsymbol{a} \qquad \rightarrow \qquad \boldsymbol{F} = m\frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} \tag{1}$$

where $\boldsymbol{F}$ is the sum of the forces acting on the body, $\boldsymbol{v}$ is the velocity of the body, m is the mass of the body and bold symbols represent vector quantities. If the mass of the solid body changes with time, then equation 1 becomes:

$$\boldsymbol{F} = \frac{\mathrm{d}(m\boldsymbol{v})}{\mathrm{d}t} \tag{2}$$

Hence, Newton's second law physically states that the rate of change of momentum (mass multiplied by velocity), is equal to the sum of the external forces acting on the body. The solid body velocity ($\boldsymbol{v}$) is a vector quantity. In a Cartesian coordinate system, the solid body velocity can be resolved into components in the x, y and z directions ($\boldsymbol{v} = (v_x, v_y, v_z)$). Hence, when written in vector form, Newton's second law is a compact way of expressing three individual equations for the change of momentum of the body in the x, y and z directions.

$$F_x = \frac{\mathrm{d}(mv_x)}{\mathrm{d}t} \qquad F_y = \frac{\mathrm{d}(mv_y)}{\mathrm{d}t} \qquad F_z = \frac{\mathrm{d}(mv_z)}{\mathrm{d}t} \tag{3}$$

If the mass of the object and the forces acting on it are known, then Newton's second law can be solved to calculate the velocity ($\boldsymbol{v}$) of the object at a given time. The equations are solved by integration. In the same way that the velocity of a solid body can be calculated by solving Newton's second law, the velocity of a fluid (liquid or gas) can be calculated by solving the *Navier-Stokes* equations. The Navier-Stokes equations are analogous to Newton's second law and state that the rate of change of momentum of a fluid is equal to the sum of the external forces acting on the fluid. However, the Navier-Stokes equations are applied to a parcel/finite volume of fluid rather than a solid body.

Figure 1 shows an example of a fluid parcel/volume that forms a part of the fluid continuum. The parcel has a volume V and can be any size. In concise vector form, the Navier-Stokes equations can be written as:

$$\frac{\mathrm{D}\left(m\boldsymbol{U}\right)}{\mathrm{D}t} = \boldsymbol{F} \tag{4}$$

where m is the mass of the fluid parcel, $\boldsymbol{U}$ is the velocity of the fluid parcel and $\boldsymbol{F}$ is the sum of the external forces acting on a fluid parcel. Note the similarities between this form of the Navier-Stokes equations and Newton's second law for a solid body (equation 2). It is standard practice to divide the Navier-Stokes equations by the volume of the fluid parcel, as this is constant. This simplification leads to:

$$\frac{\mathrm{D}\left(\rho\boldsymbol{U}\right)}{\mathrm{D}t} = \boldsymbol{f} \tag{5}$$

where ρ is the fluid density and $\boldsymbol{f}$ is the sum of the external forces per unit volume, acting on the fluid parcel. In the same manner that Newton's second law can be solved by integration to
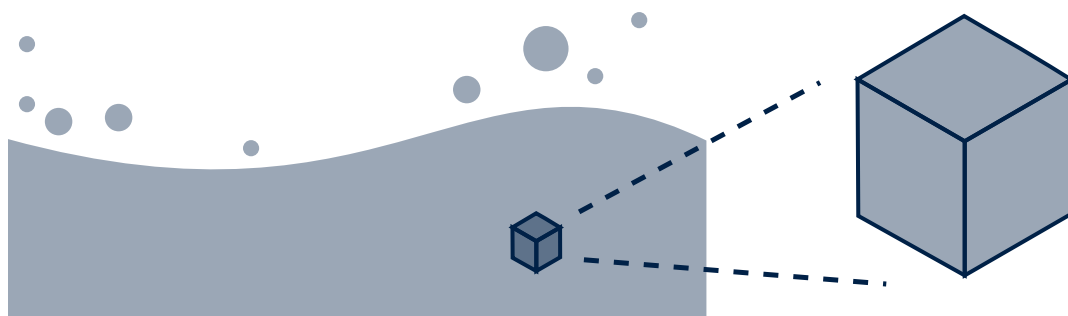
Figure 1: A finite parcel/volume of fluid that forms a part of the fluid continuum.
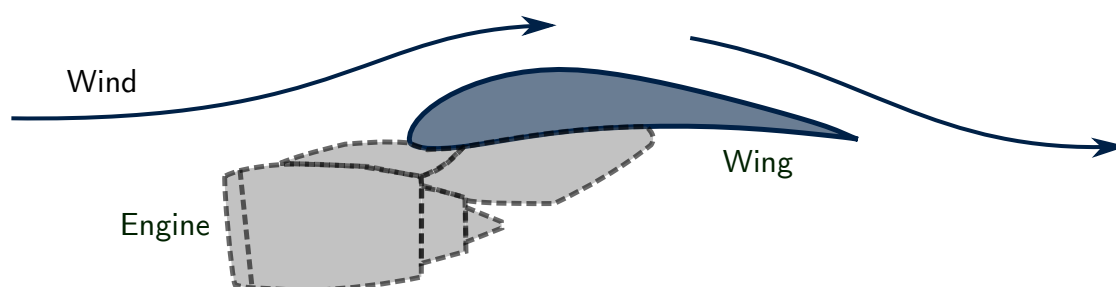

Figure 2: Calculating the flow of air over a wing allows the lift and drag forces acting on the wing to be calculated.

calculate the velocity of a solid body, the Navier-Stokes equations can be solved to calculate the velocity (motion) of the fluid. Once the velocity of the fluid has been determined, the forces acting on the solid surfaces that are in contact with the fluid can be computed. For example, solving the Navier-Stokes equations for the flow of air around a wing allows pressure and skin friction forces acting on the wing to be calculated (see Figure 2). These forces generate lift and drag and allow the plane to fly. Hence, solving the Navier-Stokes equations numerically (for real geometries) is of considerable interest to scientists and engineers. Solving the Navier-Stokes equations numerically will be the focus of this fundamentals course.

Fluid Acceleration

In the Navier-Stokes equation (equation 5), the change in momentum of the fluid parcel has been written as:

$$\frac{\mathrm{D}(\rho \boldsymbol{U})}{\mathrm{D}t} \tag{6}$$

where $\mathrm{D}/\mathrm{D}t$ is the *total derivative*. The total derivative has been used instead of the temporal derivative $(\mathrm{d}/\mathrm{d}t)$ in the Navier-Stokes equation. The reason for this change is the fluid volume may change its momentum in *time* and also change its momentum as it moves through *space*. For example, consider the flow of water through a garden hose (Figure 3), which is held at a constant flow rate. The overall flow rate of water will be constant with time if the tap is kept open at the same setting. However, the water accelerates (in space) as it moves into the nozzle. As time advances while the water moves through space, the water experiences an acceleration in time as it moves through the nozzle. The total derivative can be expanded to show the change in time and the change in space. Adopting a Cartesian coordinate system for the spatial dimensions (x, y and z):
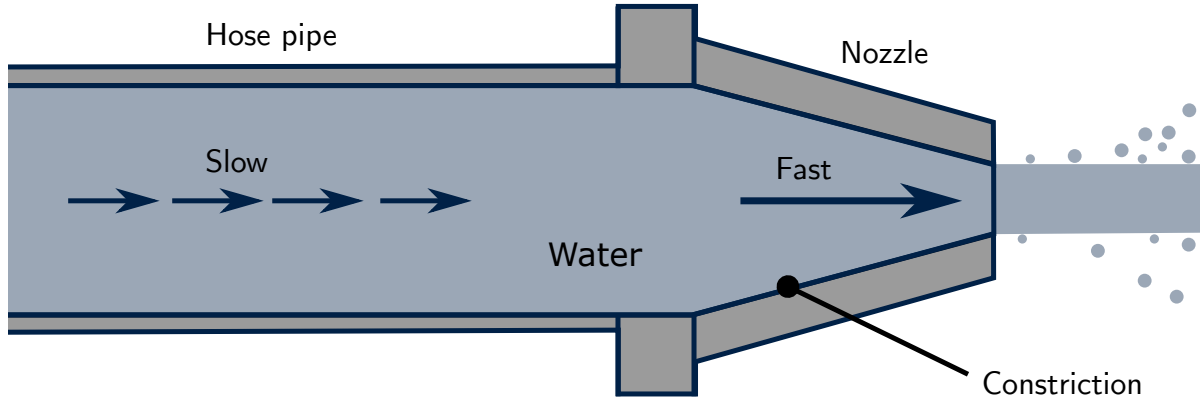
Figure 3: The flow of water through a garden hose. The water accelerates as it moves through the nozzle due to the contraction. Even if the global flow does not change in time, a fluid parcel accelerates in time as it moves through the nozzle due to the contraction.

$$\frac{\mathrm{D}}{\mathrm{D}t} = \underbrace{\frac{\partial}{\partial t}}_{\text{Time}} + \underbrace{U_x \frac{\partial}{\partial x} + U_y \frac{\partial}{\partial y} + U_z \frac{\partial}{\partial z}}_{\text{Space}} \tag{7}$$

The first term represents the change in momentum in time and the second, third and fourth terms represent the change in momentum in the x, y and z spatial directions respectively, as the fluid parcel is convected through the flow field. In vector form, the total derivative can be written compactly as:

$$\frac{\mathrm{D}}{\mathrm{D}t} = \frac{\partial}{\partial t} + \boldsymbol{U} \cdot \nabla \tag{8}$$

By using the expanded form of the total derivative, the Navier-Stokes equations can be written:

$$\frac{\partial (\rho \boldsymbol{U})}{\partial t} + \boldsymbol{U} \cdot \nabla (\rho \boldsymbol{U}) = \boldsymbol{f} \tag{9}$$

Equation 9 can be simplified slightly by applying conservation of mass and the product rule. For conciseness, the details are not included here.

$$\frac{\partial (\rho \boldsymbol{U})}{\partial t} + \nabla \cdot (\rho \boldsymbol{U}\boldsymbol{U}) = \boldsymbol{f} \tag{10}$$

While the Navier-Stokes equations have been expanded and rewritten, their physical interpretation remains the same. The change in momentum of a fluid parcel in time is equal to the sum of the forces acting on the fluid parcel.

External Forces

Depending on the flow condition, a variety of external forces may act to change the momentum of a fluid. Three of the most common forces that act to change the momentum of fluids are pressure, viscosity and gravity. These terms are included in the Navier-Stokes equations as forces (per unit volume) on the right hand side of the equation:

$$\frac{\partial (\rho \boldsymbol{U})}{\partial t} + \nabla \cdot (\rho \boldsymbol{U}\boldsymbol{U}) = \underbrace{-\nabla p}_{\text{Pressure}} + \underbrace{\nabla \cdot \boldsymbol{\tau}}_{\text{Shear Stress}} + \underbrace{\rho \boldsymbol{g}}_{\text{Gravity}} \tag{11}$$
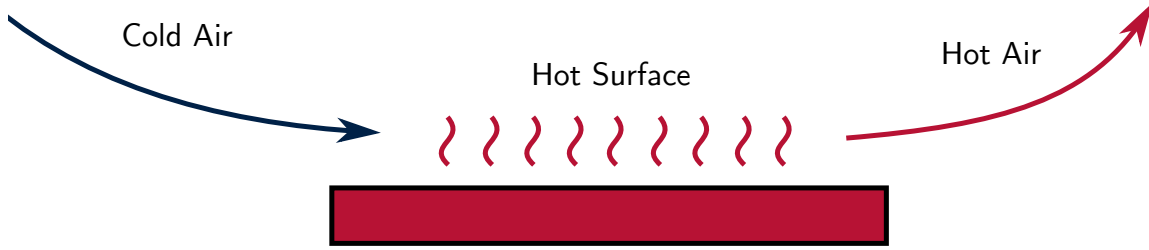
Figure 4: The flow of cold air over a hot plate, cooling the plate.

where p is the static pressure (normal stress), $\boldsymbol{\tau}$ is the shear stress (which includes the action of viscosity) and $\boldsymbol{g}$ is the acceleration due to gravity. All of the terms on the right hand-side represent forces acting on the fluid parcel, while the terms on the left hand-side represent the acceleration of the fluid parcel in response to the forces. Physically, the equations state that pressure, gravity and viscosity all act to change the momentum of the fluid ($\rho \boldsymbol{U}$). By solving the equations numerically, the velocity of the fluid can be computed in response to these forces. Once the equations are solved, the forces acting on the solid surfaces that contact the fluid can be computed.

In this course, the *Finite Volume Method* will be examined, which is the most popular method for solving the Navier-Stokes equations numerically. By following this course, you will develop an understanding of the fundamentals of how the finite volume method can be used to solve the Navier-Stokes and other transport equations.

Transport Equations

In addition to solving the Navier-Stokes equations to determine the fluid velocity ($\boldsymbol{U}$), additional equations may need to be solved, depending on the application. For example, the fluid flow may be used to cool a hot surface, as shown in Figure 4. In this instance, the fluid transports heat away from the surface, cooling the surface. In order to determine rate of cooling of the hot surface by the fluid, the temperature (and velocity) of the fluid need to be computed. For air or water cooling at low velocity (incompressible flow), the following equation can be solved to compute the temperature T of the fluid:

$$\frac{\partial \left(\rho c_p T \right)}{\partial t} + \underbrace{\nabla \cdot \left(\rho c_P \boldsymbol{U} T \right)}_{\text{Convection}} = \underbrace{\nabla \cdot \left(k \nabla T \right)}_{\text{Diffusion}} + S \tag{12}$$

where c_p is the specific heat capacity of the fluid, k is the thermal conductivity of the fluid and S is a heat source (per unit fluid volume). This type of equation is called a *transport equation*, as the temperature (representing the thermal energy of the fluid) is transported by the motion of the fluid ($\boldsymbol{U}$).

Thermal energy is transported through the fluid by two main mechanisms: convection and diffusion. Thermal energy is also transported by radiation, but this will not be considered here. The mathematical form of the convective and diffusive transport mechanisms are highlighted in equation 12. Diffusion represents the physical process where thermal energy moves from areas of high temperature to areas of low temperature due to the temperature gradient (see Figure 5). The diffusion of heat takes the following mathematical form:

$$\nabla \cdot \left(k \nabla T \right) \quad \equiv \quad \frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left(k \frac{\partial T}{\partial z} \right) \tag{13}$$
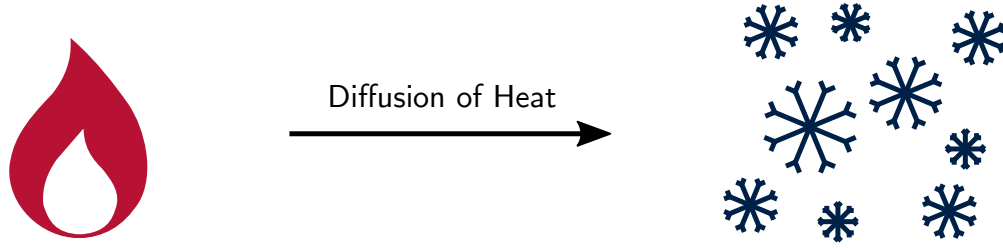
Figure 5: Heat diffuses from regions of high temperature to regions of low temperature. This diffusion is represented mathematically by $\nabla \cdot (k\nabla T)$.

The thermal conductivity k gives the strength of diffusion. A highly conductive material (such as copper) will transfer significant quantities of heat with a small temperature gradient. On the other hand, thermal insulators (like oven gloves) have low thermal conductivity k and will transmit relatively little heat, even with a large temperature gradient.

Diffusion occurs in moving and stationary fluids, hence it does not depend on the velocity of the fluid $\boldsymbol{U}$. Diffusion is often referred to as conduction, when applied to solids. In a stationary fluid where the velocity $\boldsymbol{U} = 0$, the convection term is zero and the temperature equation reduces to:

$$\frac{\partial (\rho c_p T)}{\partial t} = \underbrace{\nabla \cdot (k\nabla T)}_{\text{Diffusion}} + S \tag{14}$$

Convection of heat is the transport of thermal energy by the motion (velocity) of the fluid. It has the following mathematical form:

$$\nabla \cdot (\rho c_p \boldsymbol{U} T) \quad \equiv \quad \frac{\partial}{\partial x} (\rho c_p T U_x) + \frac{\partial}{\partial y} (\rho c_p T U_y) + \frac{\partial}{\partial z} (\rho c_p T U_z) \tag{15}$$

The thermal energy is physically transported by the motion of the moving fluid ($\boldsymbol{U}$). This is similar to the transport of leaves and branches that are dropped into a moving river. The leaves and branches are physically transported by the motion of the fluid and are carried along with the river. Convection increases the rate of heat transfer and is the reason why blowing over the surface of a hot drink reduces its temperature, so that we can drink it!

Other Transport Equations

A variety of quantities that are transported by fluids follow a similar transport equation to the temperature/thermal energy equation. On example is the injection of dye or fine solid particles into a flow stream, as shown in Figure 6. The particles will be convected by the fluid and will also diffuse from areas of high concentration to low concentration. Hence, the concentration C of dye/solid particles follows a similar transport equation to temperature:

$$\frac{\partial(\rho C)}{\partial t} + \underbrace{\nabla \cdot (\rho \boldsymbol{U} C)}_{\text{Convection}} = \underbrace{\nabla \cdot (D\nabla C)}_{\text{Diffusion}} + S_c \tag{16}$$

where D is the diffusivity of the dye/solid particles. The transport equations that govern the convection and diffusion of quantities in a fluid flow (velocity, temperature, concentration etc.) all share the same common form:

$$\frac{\partial (\rho \phi)}{\partial t} + \nabla \cdot (\rho \boldsymbol{U} \phi) = \nabla \cdot (\Gamma \nabla \phi) + S_\phi \tag{17}$$
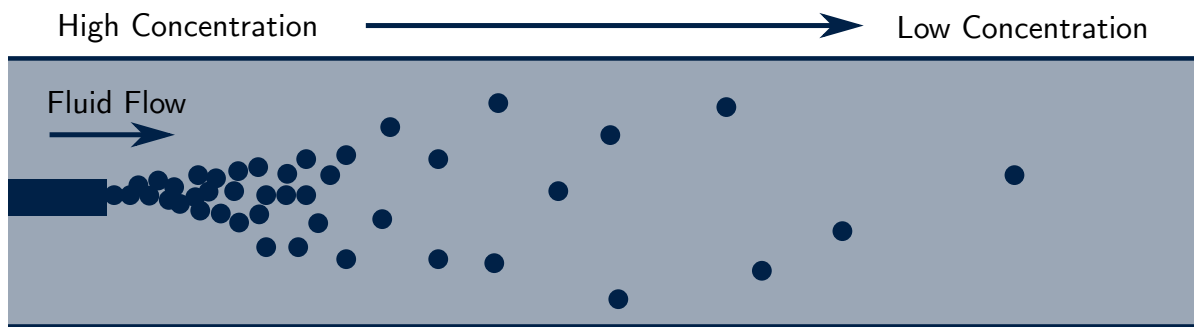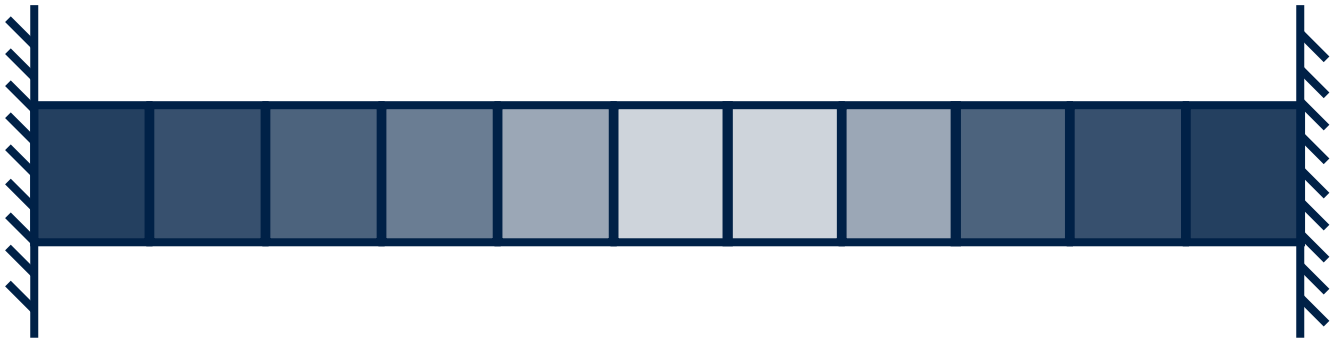
Figure 6: The concentration of dye/solid particles diffuses from regions of high concentration to regions of low concentration. This diffusion is represented mathematically by $\nabla \cdot (D\nabla C)$

where ϕ is a transported quantity (velocity, temperature, concentration etc.), ρ is the fluid density, Γ is the diffusivity of the quantity and S_ϕ is the additional source per unit volume of the quantity ϕ. In this course, the finite volume method will be used to solve a general transport equation that includes convection, diffusion and a source term. As the governing equations of fluid flow all share the same general form, the same method can then be applied to any transport equation (velocity, temperature, concentration etc.) that is required.

In the three remaining chapters in this course, the finite volume method will be applied to a transport equation for temperature. Temperature has been chosen specifically in this course, as it is conceptually the most straightforward quantity to understand while applying the method. The same techniques applied in this course can then be applied to any transported quantity of interest, by following the same analysis steps. The diffusion and source terms will be considered first, to develop a general understanding of the method. The convection term will then be added in the third chapter of this course, allowing the effects of diffusion and convection to be studies simultaneously. In the fourth chapter of this course, a special technique called *upwind differencing* will be introduced. This technique is essential to solve the majority of convection-diffusion equations and is adopted by all modern CFD codes.

Chapter 2

The 1D Diffusion Equation

2 The 1D Diffusion Equation

In the previous chapter, the convection-diffusion equation for the transport of temperature (thermal energy) was introduced.

$$\frac{\partial(\rho c_p T)}{\partial t} + \nabla \cdot (\rho c_p \boldsymbol{U} T) = \nabla \cdot (\kappa \nabla T) + S \tag{18}$$

In this chapter, the transport equation for temperature will be solved for the limited case of one-dimensional (1D) steady-state diffusion. This limited case will be used to introduce the finite volume method and demonstrate how it works. The same approach can also be applied to other transport equations (momentum, species concentration, turbulence etc.). Temperature has been specifically chosen for this chapter, as it is conceptually the most straightforward to follow and understand. In the next chapter, the one-dimensional steady-state diffusion example will be extended to also include convection. Starting with the three-dimensional (3D) transport equation for thermal energy (temperature), the temporal derivative and the convection term will be neglected in this chapter.

$$\cancel{\frac{\partial(\rho c_p T)}{\partial t}}^{0} + \cancel{\nabla \cdot (\rho c_p \boldsymbol{U} T)}^{0} = \nabla \cdot (\kappa \nabla T) + S \tag{19}$$

$$0 = \nabla \cdot (\kappa \nabla T) + S \tag{20}$$

Expand the gradient (∇) and dot product ($\nabla \cdot$) operators in Cartesian coordinates:

$$0 = \frac{\partial}{\partial x}\left(\kappa\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(\kappa\frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(\kappa\frac{\partial T}{\partial z}\right) + S \tag{21}$$

For one-dimensional diffusion, the y and z derivatives are zero.

$$0 = \frac{\partial}{\partial x}\left(\kappa\frac{\partial T}{\partial x}\right) + \cancel{\frac{\partial}{\partial y}\left(\kappa\frac{\partial T}{\partial y}\right)}^{0} + \cancel{\frac{\partial}{\partial z}\left(\kappa\frac{\partial T}{\partial z}\right)}^{0} + S \tag{22}$$

$$\boxed{0 = \frac{d}{dx}\left(k\frac{dT}{dx}\right) + S} \tag{23}$$

Equation 23 is the 1D steady-state heat diffusion equation. This equation will be solved using the *finite-volume method*, which is the most common approach used by modern CFD codes. The finite volume method can also be applied to more detailed equations and is not limited to one dimensional analysis. However, one dimensional flow has been specifically selected here to illustrate the principals of the method clearly.

Equation 23 is a differential equation (not an algebraic equation). Hence, the solution of this equation requires integration and the application of boundary conditions. Rather than integrate the equation over the entire domain of interest, the first stage in the finite volume method is to integrate the equation over a small piece of the domain. This piece is called a finite volume or parcel of fluid. Figure 7 shows an example of a finite volume of fluid, which forms a part of the continuum of fluid. Remember that the differential equation is valid for every finite volume of fluid in the domain, regardless of the size of the volume and its location. Mathematically, the integration process is described as:

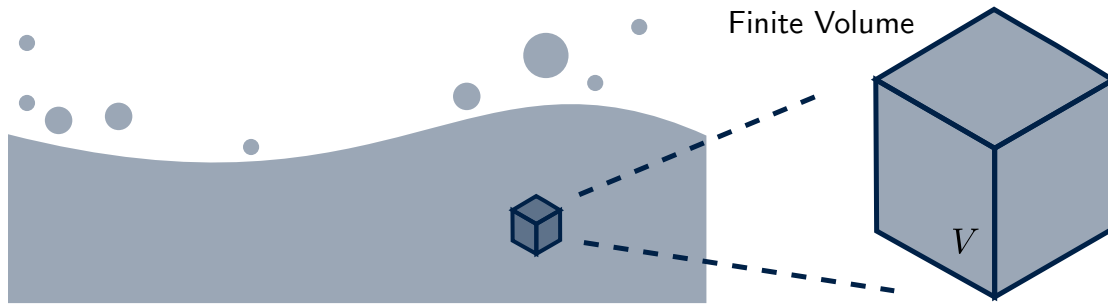$$\int_V \left[\frac{d}{dx}\left(k\frac{dT}{dx}\right) + S\right] dV = 0 \tag{24}$$

Figure 7: A finite volume of fluid, which has been isolated from the fluid continuum.
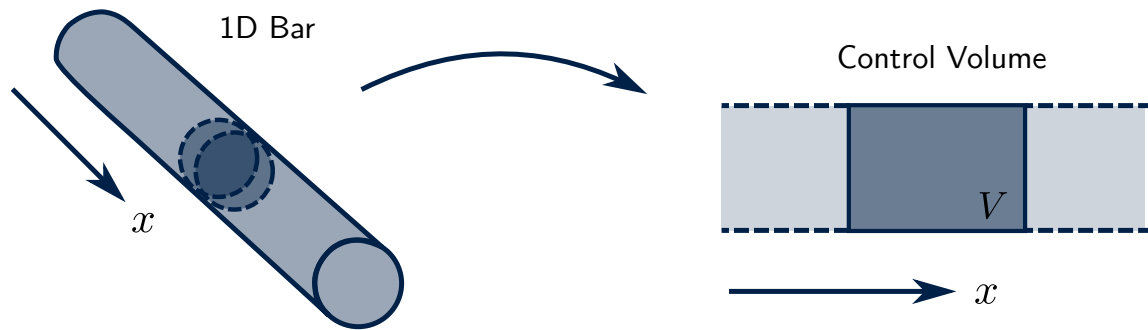

Figure 8: A 1D finite volume of fluid with volume V, which has been isolated from the bar.

The integration of each term can be considered separately, as addition and integration are commutative operations (it does not matter which order they are carried out in).

$$\int_V \left[\frac{d}{dx} \left(k \frac{dT}{dx} \right) \right] \mathrm{d}V + \int_V [S] \, \mathrm{d}V = 0 \tag{25}$$

In one-dimension, the control volume forms a part of a one-dimensional geometry, as shown in Figure 8. This control volume can be thought of as a piece of a bar that is conducting heat from one-end to the other, with constant properties over its cross-section. The second term in equation 25 represents the heat source generated in the finite volume. Assume that the heat source is constant across the control volume, with a value of $\overline{S}$ (the volume average heat source). The second term in the finite volume integral can now be simplified.

$$\int_V \left[\frac{d}{dx} \left(k \frac{dT}{dx} \right) \right] \mathrm{d}V + \overline{S} \int_V \mathrm{d}V = 0 \tag{26}$$

$$\int_V \left[\frac{d}{dx} \left(k \frac{dT}{dx} \right) \right] \mathrm{d}V + \overline{S} V = 0 \tag{27}$$

The source term $\overline{S}$ has units of W/m^3. Hence, the product $\overline{S}V$ has units of W.

   The first term in equation 25 is the volume integral of the heat diffusion inside the control volume. To simplify and evaluate this term, the *divergence theorem* is required. Physically, the divergence theorem states that the rate of accumulation of a vector field inside a control volume is equal to the flux of the vector field across the surfaces of the control volume. When applied to the heat diffusion equation, this theorem can be thought of as an expression of conservation of energy. Heat accumulating inside the control volume by diffusion must cross the surfaces of the control volume if there are no additional sources of heat in the volume,
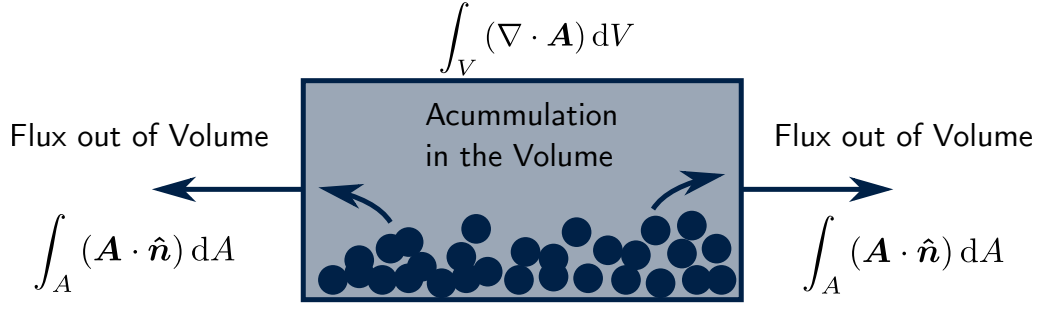
Figure 9: A diagram to show the physical significance of the divergence theorem applied to vector field $\boldsymbol{A}$. The accumulation of $\boldsymbol{A}$ in the volume equals the flux of $\boldsymbol{A}$ over the surfaces of the volume.
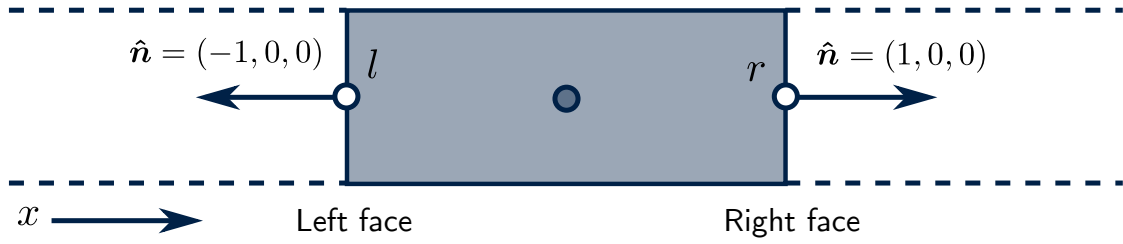

Figure 10: A diagram to show the face normal vectors on the left and right faces of the 1D cell. The cell normal vectors always point out of the cell.

as shown in Figure 9. Mathematically, the divergence theorem for a general vector field $\boldsymbol{A}$ is written as:

$$\int_V (\nabla \cdot \boldsymbol{A})\, \mathrm{d}V = \int_A (\boldsymbol{A} \cdot \hat{\boldsymbol{n}})\, \mathrm{d}A \tag{28}$$

$$\int_V \left(\frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z} \right) \mathrm{d}V = \int_A (A_x n_x + A_y n_y + A_z n_z)\, \mathrm{d}A \tag{29}$$

where $\hat{\boldsymbol{n}}$ is the unit normal vector pointing out of the control volume and A is the surface area of the control volume. In 1D, the divergence theorem can be written:

$$\int_V \left(\frac{\mathrm{d}A_x}{\mathrm{d}x} \right) \mathrm{d}V = \int_A (A_x \hat{n}_x)\, \mathrm{d}A \tag{30}$$

For the 1D heat diffusion equation $\boldsymbol{A} = k\nabla T$. Hence $A_x = k\, \mathrm{d}T/\mathrm{d}x$. Applying the 1D divergence theorem to the 1D heat diffusion equation leads to:

$$\int_A \left(\kappa \frac{\mathrm{d}T}{\mathrm{d}x} n_x \right) \mathrm{d}A + \overline{S}V = 0 \tag{31}$$

Physically, equation 31 states that the flux of heat out of the cell by diffusion must balance the heat generated within the cell. To simplify this equation further, consider the 1D cell in Figure 10. The cell has a left face l and a right face r. Lower-case letters l and r are used in this course to refer to the left and right faces of the cell, while upper-case L and R are used to refer to the centroids of the neighbour cell that are on the left and right of the cell under consideration. The flow quantities (temperature, thermal conductivity etc.) are constant on the cell face. Hence, the first integral can be simplified:

$$\left(\kappa \frac{\mathrm{d}T}{\mathrm{d}x} n_x \right) \int_A \mathrm{d}A + \overline{S}V = 0 \tag{32}$$

(a) Interior Cell   (b) Boundary Cell

Figure 11: A comparison of interior cells (a) and boundary cells (b) in the mesh.

$$\left(k\frac{dT}{dx}n_xA\right)_r + \left(k\frac{dT}{dx}n_xA\right)_l + \overline{S}V = 0 \tag{33}$$

As shown in Figure 10, n_x is positive on the right face and negative on the left face. Hence:

$$\left(kA\frac{dT}{dx}\right)_r - \left(kA\frac{dT}{dx}\right)_l + \overline{S}V = 0 \tag{34}$$

This simplified form of the 1D heat-diffusion equation is valid for all cells in the mesh. However, it cannot be solved yet numerically, as the equation is written in terms of variables on the cell faces (l and r). In the cell-centred finite volume method, the equation is solved in terms of variables at the cell centroids (L, R and P). To carry out the necessary simplification, *interior cells* and *boundary cells* need to be considered separately. As shown in Figure 11, interior cells are in the interior of the geometry and are connected to other cells. However, boundary cells are connected to a boundary of the domain (such as an inlet or wall) on one or more of their faces. In the sections that follow, the interior and boundary cells will be considered separately when simplifying equation 34.

Interior Cells

Start with the general finite volume discretisation of the 1D heat-diffusion equation.

$$\left(kA\frac{dT}{dx}\right)_r - \left(kA\frac{dT}{dx}\right)_l + \overline{S}V = 0 \tag{35}$$

To simplify and solve this equation for the interior cells, the temperature gradient on the cell faces (l and r) need to be expressed in terms of temperatures at the cell centroids (L, R and P). This simplification can be accomplished with linear interpolation, which is often called *central-differencing*. To help understand this simplification, remember that the spatial gradient of temperature can be thought of as:

$$\frac{dT}{dx} \sim \frac{\Delta T}{\Delta x} = \frac{\text{Change in Temperature}}{\text{Distance}} \tag{36}$$

As shown in Figure 12, the temperature gradient on the left face can be expressed using central differencing as:

$$\left(\frac{dT}{dx}\right)_l = \frac{T_P - T_L}{d_{LP}} \tag{37}$$

where d_{LP} is the distance between the cell centroids L and P. In a similar manner, the temperature gradient on the right face can also be expressed using central differencing:

$$\left(\frac{dT}{dx}\right)_r = \frac{T_R - T_P}{d_{PR}} \tag{38}$$

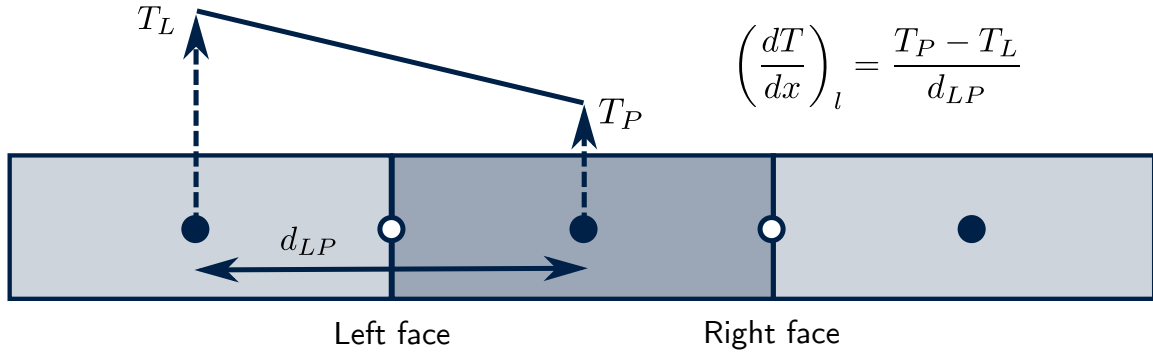$$\left(\frac{dT}{dx}\right)_l = \frac{T_P - T_L}{d_{LP}}$$

Figure 12: Central differencing (linear interpolation) of the temperature gradient on the left face of the cell using the values at the cell centroids of the interior cell (T_P) and the left cell (T_L).

Substitute this simplification into the 1D heat-diffusion equation (equation 35).

$$\left(k_r A_r \frac{T_R - T_P}{d_{PR}}\right) - \left(k_l A_l \frac{T_P - T_L}{d_{LP}}\right) + \overline{S}V = 0 \tag{39}$$

The 1D diffusion equation can now be solved for the temperatures at the cell centroids (T_L, T_R and T_P). To simplify this process, rearrange the equation and collect the terms in terms of temperature of the interior cell (T_P), temperature of the left cell (T_L) and the temperature of the right cell (T_R).

$$T_P \left(\frac{k_l A_l}{d_{LP}} + \frac{k_r A_r}{d_{PR}}\right) = T_L \left(\frac{k_l A_l}{d_{LP}}\right) + T_R \left(\frac{k_r A_r}{d_{PR}}\right) + \overline{S}V \tag{40}$$

For convenience, introduce the notation $D = k/d$. This quantity can be thought of as the diffusive flux of heat per unit area through the cell face and has units of W/m^{2}K.

$$T_P (D_l A_l + D_r A_r) = T_L (D_l A_l) + T_R (D_r A_r) + \overline{S}V \tag{41}$$

For consistency with other equations that will be introduced later, write the above equation in the following form:

$$a_p T_P = a_L T_L + a_R T_R + S_u \tag{42}$$

$$T_P \underbrace{(D_l A_l + D_r A_r + 0)}_{a_p} = T_L \underbrace{(D_l A_l)}_{a_L} + T_R \underbrace{(D_r A_r)}_{a_R} + \underbrace{\overline{S}V}_{S_u} \tag{43}$$

Hence, the following coefficients can be identified. These coefficients will be compared with other formulations of the convection-diffusion equation in the next two chapters.

$$a_p = a_L + a_R - S_p \qquad a_L = D_l A_l \qquad a_R = D_r A_r \tag{44}$$

$$S_P = 0 \qquad S_u = \overline{S}V \tag{45}$$

At this stage, we now have an algebraic equation for the temperature at the centroid of the cell T_P. This is the unknown in the equation that we want to solve for. However, the temperature of the cells on the left and right of this cell (T_L and T_R) are also unknown. To overcome this difficulty, one equation will be written for every cell in the mesh, with the unknown of each euqation being the temperature of that cell centroid T_P. Each of these equations is coupled to the equations of the cells on the left and right of the cell through the variables T_L and T_R, as shown in equation 43. Before proceeding to assemble and solve these equations, separate treatment is required for the boundary cells.
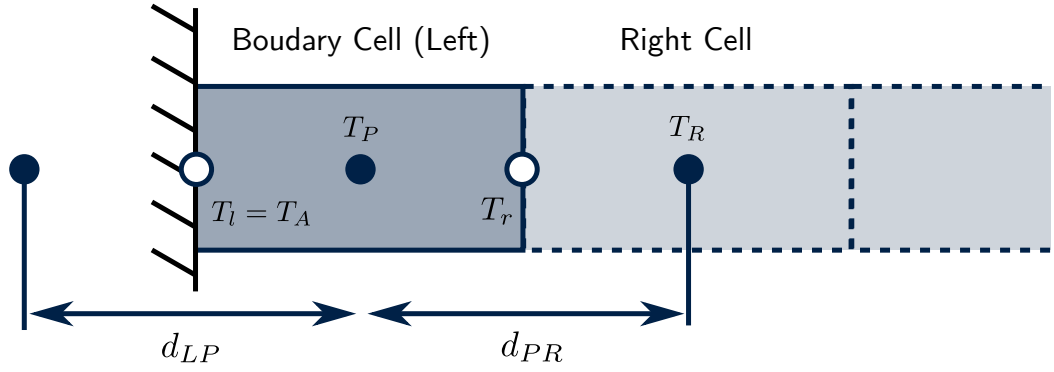
Figure 13: The left boundary cell with temperature T_P at its centroid. The shared face between the boundary cell and the right cell is at a temperature T_r and the wall has a temperature $T_l = T_A$.

Boundary Cell (Left)

Figure 13 shows the boundary cell at the left end of the bar. The cell is connected to the boundary (wall) at the left face, where a fixed temperature T_A is applied. The finite volume discretisation of the 1D heat-diffusion equation (equation 34) is:

$$\left(kA\frac{dT}{dx}\right)_r - \left(kA\frac{dT}{dx}\right)_l + \overline{S}V = 0 \tag{46}$$

The right face of the boundary cell is connected to an interior cell. Hence, the same central differencing scheme for the temperature gradient from the previous section can be used. However, the left face is connected to a boundary. As shown in Figure 13, the temperature gradient term for the left face is:

$$\left(\frac{dT}{dx}\right)_l = \frac{T_P - T_A}{d_{LP}/2} \tag{47}$$

The factor of $1/2$ is required as the distance from the cell centroid to the face is $1/2$ of d_{LP} (the distance from the cell centroid to the cell centroid of the adjacent cell). The finite volume discretisation of the 1D heat-diffusion equation for the left boundary cell is now:

$$\left(k_r A_r \frac{T_R - T_P}{d_{PR}}\right) - \left(k_l A_l \frac{T_P - T_A}{d_{LP}/2}\right) + \overline{S}V = 0 \tag{48}$$

Again, introduce the notation $D = k/d$ for the diffusive heat flux per unit area.

$$T_P \left(2D_l A_l + D_r A_r\right) = T_R \left(D_r A_r\right) + T_A \left(2D_l A_l\right) + \overline{S}V \tag{49}$$

For consistency with the interior cell, write in the following form:

$$a_p T_P = a_L T_L + a_R T_R + S_u \tag{50}$$

$$T_P \underbrace{\left(0 + D_r A_r + 2D_l A_l\right)}_{a_P} = T_L \underbrace{(0)}_{a_L} + T_R \underbrace{\left(D_r A_r\right)}_{a_R} + \underbrace{T_A \left(2D_l A_l\right) + \overline{S}V}_{S_u} \tag{51}$$

For comparison with the interior cell, the boundary cell (left) has the following coefficients:

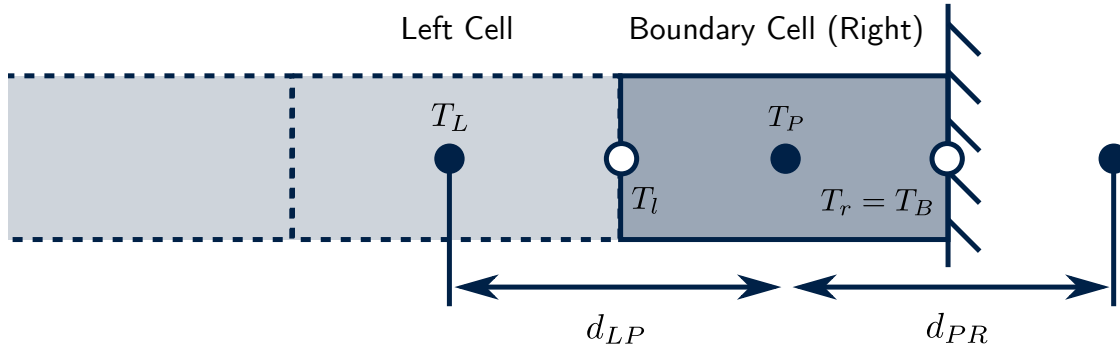$$a_L = 0 \qquad a_R = D_r A_r \qquad a_p = a_L + a_R - S_p \tag{52}$$

Figure 14: The right boundary cell with temperature T_P at its centroid. The shared face between the boundary cell and the left cell is at a temperature T_l and the boundary has a temperature $T_r = T_B$.

$$S_P = -2D_l A_l \qquad S_u = T_A(2D_l A_l) + \overline{S}V \tag{53}$$

Comparing these coefficients with the coefficients for the interior cell, it can be seen that the left coefficient a_L is zero. This makes sense physically, because the boundary cell is not connected to another cell on the left. The influence of the boundary condition is introduced into the equation through the source terms S_p and S_u.

Boundary Cell (Right)

The boundary cell on the right of the domain is shown in Figure 14. The cell is connected to the boundary at the right face, where a fixed temperature T_B is applied. The finite volume discretisation of the 1D heat-diffusion equation from equation 34 is:

$$\left(kA\frac{dT}{dx}\right)_r - \left(kA\frac{dT}{dx}\right)_l + \overline{S}V = 0 \tag{54}$$

The left face of the boundary cell is connected to an interior cell. Hence, the same face interpolation schemes from the previous section can be used. However, the right face is connected to a boundary. As shown in Figure 14, the temperature gradient term for the right face is:

$$\left(\frac{dT}{dx}\right)_r = \frac{T_B - T_P}{d_{PR}/2} \tag{55}$$

The factor of $1/2$ is required as the distance from the cell centroid to the face is $1/2$ of d_{PR} (the distance from the cell centroid to the cell centroid of the adjacent cell). The finite volume discretisation of the 1D heat-diffusion equation is now:

$$\left(k_r A_r \frac{T_B - T_P}{d_{PR}/2}\right) - \left(k_l A_l \frac{T_P - T_L}{d_{LP}}\right) + \overline{S}V = 0 \tag{56}$$

Again, introduce the notation $D = k/d$ for the diffusive heat flux per unit area.

$$T_P \left(D_l A_l + 2D_r A_r\right) = T_L \left(D_l A_l\right) + T_B \left(2D_r A_r\right) + \overline{S}V \tag{57}$$

For consistency with the interior cell, write in the standard form:

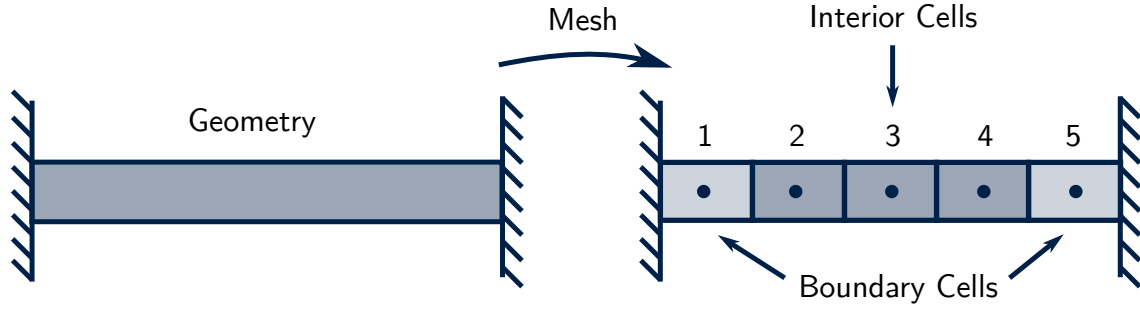$$a_p T_p = a_L T_L + a_R T_R + S_u \tag{58}$$

Figure 15: An example of the meshing process, where a 1D bar is divided into 5 cells/finite volumes. Cell 1 and cell 5 are boundary cells, whereas cells 2, 3 and 4 are interior cells.

$$T_P \underbrace{(D_l A_l + 0 + 2D_r A_r)}_{a_p} = T_L \underbrace{(D_l A_l)}_{a_L} + T_R \underbrace{0}_{a_R} + \underbrace{T_B (2D_r A_r) + \overline{S}V}_{S_u} \tag{59}$$

For comparison with the interior cell, the boundary cell (right) has the following coefficients:

$$a_L = D_l A_l \qquad a_R = 0 \qquad a_p = a_L + a_R - S_p \tag{60}$$

$$S_P = -2D_r A_r \qquad S_u = T_B(2D_r A_r) + \overline{S}V \tag{61}$$

Summary of Coefficients

A summary of the finite volume coefficients is provided in the table below for interior and boundary cells. Notice that the boundary cells have zero contribution from the cells that would extend outside of the domain. The boundary conditions are introduced through the source terms S_u and S_p.

	a_L	a_R	a_P	S_p	S_u
Boundary (L)	0	$D_R A_R$	$a_l + a_r - S_p$	$-2D_L A_L$	$T_A(2D_L A_L) + \overline{S}V$
Interior	$D_L A_L$	$D_R A_R$	$a_l + a_r - S_p$	0	$\overline{S}V$
Boundary (R)	$D_L A_L$	0	$a_l + a_r - S_p$	$-2D_R A_R$	$T_B(2D_R A_R) + \overline{S}V$

Meshing the Geometry

Before solving the finite volume equations, the physical geometry of interest needs to be divided into discrete cells/ volumes. This process is called *meshing* and is the most significant part of the CFD solution process because the quality of the mesh affects the accuracy and stability of the solution. The meshing process will not be examined here, as the primary aim of this course is the implementation of the finite volume method. An ideal quadrilateral mesh will be used for the 1D geometry, as shown in Figure 15. In the next section, the set of finite volume equations will be assembled for the all cells in the mesh.

Write an Equation for Every Cell in the Mesh

Conceptually, the next stage in the finite volume method is to construct an equation for every cell in the mesh individually. The equation written for each cell is coupled to the equations

written for the neighbours of that cell. As an example, consider a 1D mesh with 5 cells, as shown in Figure 15. Cell 1 is the left boundary cell and cell 5 is the right boundary cell. Cells 2, 3 and 4 are interior cells. The individual finite volume equations are:

Cell 1	Boundary Cell (Left)	$a_{p1}T_1 = a_{r1}T_2 + S_{u1}$
Cell 2	Interior Cell	$a_{p2}T_2 = a_{l2}T_1 + a_{r2}T_3 + S_{u2}$
Cell 3	Interior Cell	$a_{p3}T_3 = a_{l3}T_2 + a_{r3}T_4 + S_{u3}$
Cell 4	Interior Cell	$a_{p4}T_4 = a_{l4}T_3 + a_{r4}T_5 + S_{u4}$
Cell 5	Boundary Cell (Right)	$a_{p5}T_5 = a_{l5}T_4 + S_{u5}$

where the coefficients a_p, a_L, a_R and S_u are given in the summary in the previous section. Notice that the interior cells are coupled to the temperature of the cells on the left and right hand side of them. In contrast, the boundary cells are only coupled to the temperature of a single cell centroid (the interior cell that they are in contact with). The boundary conditions enter the equations through the source terms S_u.

Assemble the Matrices

To assemble the matrices, rearrange the equations by bringing all the temperature terms to the left hand side. Leave the source terms on the right hand side.

Cell 1	Boundary Cell (Left)	$a_{p1}T_1 - a_{r1}T_2 = S_{u1}$
Cell 2	Interior Cell	$-a_{l2}T_1 + a_{p2}T_2 - a_{r2}T_3 = S_{u2}$
Cell 3	Interior Cell	$-a_{l3}T_2 + a_{p3}T_3 - a_{r3}T_4 = S_{u3}$
Cell 4	Interior Cell	$-a_{l4}T_3 + a_{p4}T_4 - a_{r4}T_5 = S_{u4}$
Cell 5	Boundary Cell (Right)	$-a_{l5}T_4 + a_{p5}T_5 = S_{u5}$

Add additional zero values for the missing temperatures in each equation.

Cell 1	Boundary Cell (Left)	$a_{p1}T_1 - a_{r1}T_2 + 0T_3 + 0T_4 + 0T_5 = S_{u1}$
Cell 2	Interior Cell	$-a_{l2}T_1 + a_{p2}T_2 - a_{r2}T_3 + 0T_4 + 0T_5 = S_{u2}$
Cell 3	Interior Cell	$0T_1 - a_{l3}T_2 + a_{p3}T_3 - a_{r3}T_4 + 0T_5 = S_{u3}$
Cell 4	Interior Cell	$0T_1 - a_{l3}T_2 + a_{p3}T_3 - a_{r3}T_4 + 0T_5 = S_{u3}$
Cell 5	Boundary Cell (Right)	$0T_1 + 0T_2 + 0T_3 - a_{l5}T_4 + a_{p5}T_5 = S_{u5}$

Write the equations in matrix form:

$$
\begin{bmatrix}
a_{p1} & -a_{r1} & 0 & 0 & 0 \\
-a_{l2} & a_{p2} & -a_{r2} & 0 & 0 \\
0 & -a_{l3} & a_{p3} & -a_{r3} & 0 \\
0 & 0 & -a_{l4} & a_{p4} & -a_{r4} \\
0 & 0 & 0 & -a_{l5} & a_{p5}
\end{bmatrix}
\begin{bmatrix}
T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5
\end{bmatrix}
=
\begin{bmatrix}
S_{u1} \\ S_{u2} \\ S_{u3} \\ S_{u4} \\ S_{u5}
\end{bmatrix}
\qquad \boldsymbol{AT = B} \qquad (62)
$$

which is the standard form used in linear algebra. Commercial CFD solvers populate the matrices by calculating the coefficients (a_l, a_p and a_r) automatically for the user and then solve the matrix equations. In the next section, the entire process will be demonstrated with an example problem. A mesh will be defined, the coefficients will be calculated and then the matrices will be constructed and solved.
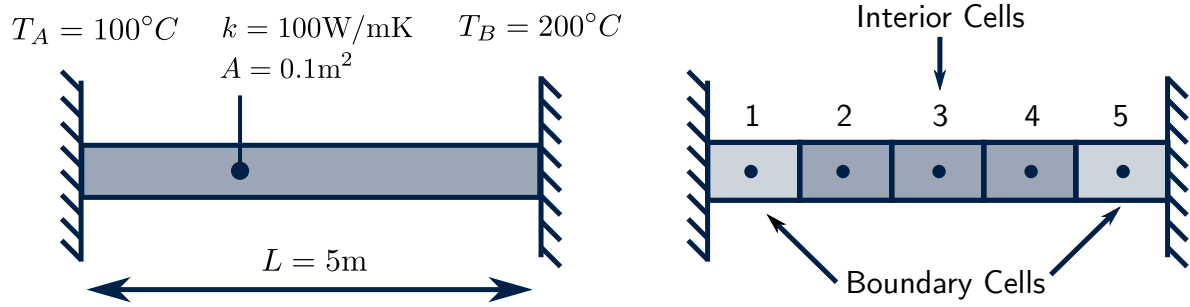
Figure 16: An example problem to demonstrate 1D heat-diffusion in a bar.

Example Problem: Heat Diffusion in a Bar

Consider 1D steady-state diffusion of heat in a bar, as shown in Figure 16. The bar has a length of 5m, a cross-sectional area of 0.1 m^2 and a thermal conductivity of 100 W/mK. The temperature at the left end of the bar (T_A) is $100°C$ and the temperature at the right end (T_B) is $200°C$. There is a constant heat source of 1000 W/m^3 in the bar. The temperature field in the bar is governed by the 1D steady-state diffusion equation.

$$\frac{d}{dx}\left(k\frac{dT}{dx}\right) + S = 0 \tag{63}$$

Step 1: Divide the Geometry into a Mesh

For the example in Figure 16, divide the geometry into a mesh of 5 cells of equal length. The length of each cell (L_{cell}) is given by:

$$L_{\text{cell}} = \frac{L}{N} = \frac{5}{5} = 1\text{m} \tag{64}$$

Because the cells are uniformly distributed and have equal size, the distance between cell centroids d is equivalent to the length of the cells. Hence:

$$d_{LP} = d_{PR} = d = 1\text{m} \tag{65}$$

Step 2: Assign Material Properties

The thermal conductivity k and the cross-sectional area A are the same for every cell in the mesh. Hence, the parameter DA is given by:

$$DA = \frac{kA}{d} = \frac{100 * 0.1}{1} = 10 \text{ [W/K]} \tag{66}$$

$$D_l A_l = D_r A_r = DA = 10 \text{ [W/K]} \tag{67}$$

The heat source per unit volume in each cell is given by:

$$\overline{SV} = \overline{S}AL_{\text{cell}} = 1000 * 0.1 * 1 = 100 \text{ [W]} \tag{68}$$

Step 3: Calculate Matrix Coefficients

Now calculate the coefficients required to assemble the matrices. The most straightforward way is to fill in the table of coefficients:

	a_L	a_R	S_p	S_u	a_p
Boundary (Left)	0	10	-20	2100	30
Interior	10	10	0	100	20
Boundary (Right)	10	0	-20	4100	30

Step 4: Assemble the Matrices

Assign the coefficients to their correct location in the matrix.

$$\begin{bmatrix} 30 & -10 & 0 & 0 & 0 \\ -10 & 20 & -10 & 0 & 0 \\ 0 & -10 & 20 & -10 & 0 \\ 0 & 0 & -10 & 20 & -10 \\ 0 & 0 & 0 & -10 & 30 \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \end{bmatrix} = \begin{bmatrix} 2100 \\ 100 \\ 100 \\ 100 \\ 4100 \end{bmatrix} \tag{69}$$

Step 5: Solve the Equations

Now that the matrices have been assembled, the matrix equation can solved with an appropriate *iterative method*. An iterative method (such as Gauss-Seidel or Pre-conditioned Conjugate Gradient) is usually chosen by modern CFD codes, as the equations are usually too large for a *direct method* (like Gaussian Elimination) to be feasible. For example, a mesh with 1 million cells will require the solution of a matrix equation with 1 million unknowns. This is not feasible to solve in a reasonable time with a direct method. In this course, different algorithms to solve the matrix equation $AT = B$ will not be considered, as details can be found in any comprehensive text on linear algebra. The default solvers for linear algebra will be used instead.

Run the Example Problem Yourself!

Now, open either the Excel spreadsheet or the Python source code and solve the problem yourself.

Excel   *solve1DDiffusionEquation.xlsx*

Python   *solve1DDiffusionEquation.py*

Examine the calculation of the coefficients, the assembly of the matrices and run the code. You can even try changing some of the geometric and material properties of the problem

(such as the thermal conductivity or the length of the bar) and examine the changes in the solution.

Results

The blue circles in Figure 17 show the temperature variation in the 1D bar computed with the CFD code. The dashed line shows the analytical solution of the 1D heat diffusion equation with a constant heat source (S) which is given by:

$$T = T_A + \frac{x}{L}\left(T_B - T_A\right) + \frac{S}{2k}x\left(L - x\right) \tag{70}$$

As shown in Figure 17 (a), there is a small error between the CFD solution and the analytical solution. This is because the finite volume method assumes a *linear variation* between cells, whereas the analytical solution (for this flow scenario) is quadratic in nature. To reduce the error in the CFD solution, the mesh needs to be refined by increasing the number of cells. Figure 17 (b) shows the CFD solution of the same problem, with the number of cells increased from 5 to 20. The error in the CFD solution is reduced. However, the computational cost of the simulation has increased significantly. Hence, for practical CFD applications, a careful balance must be made between increased accuracy and increased cost of the simulations.
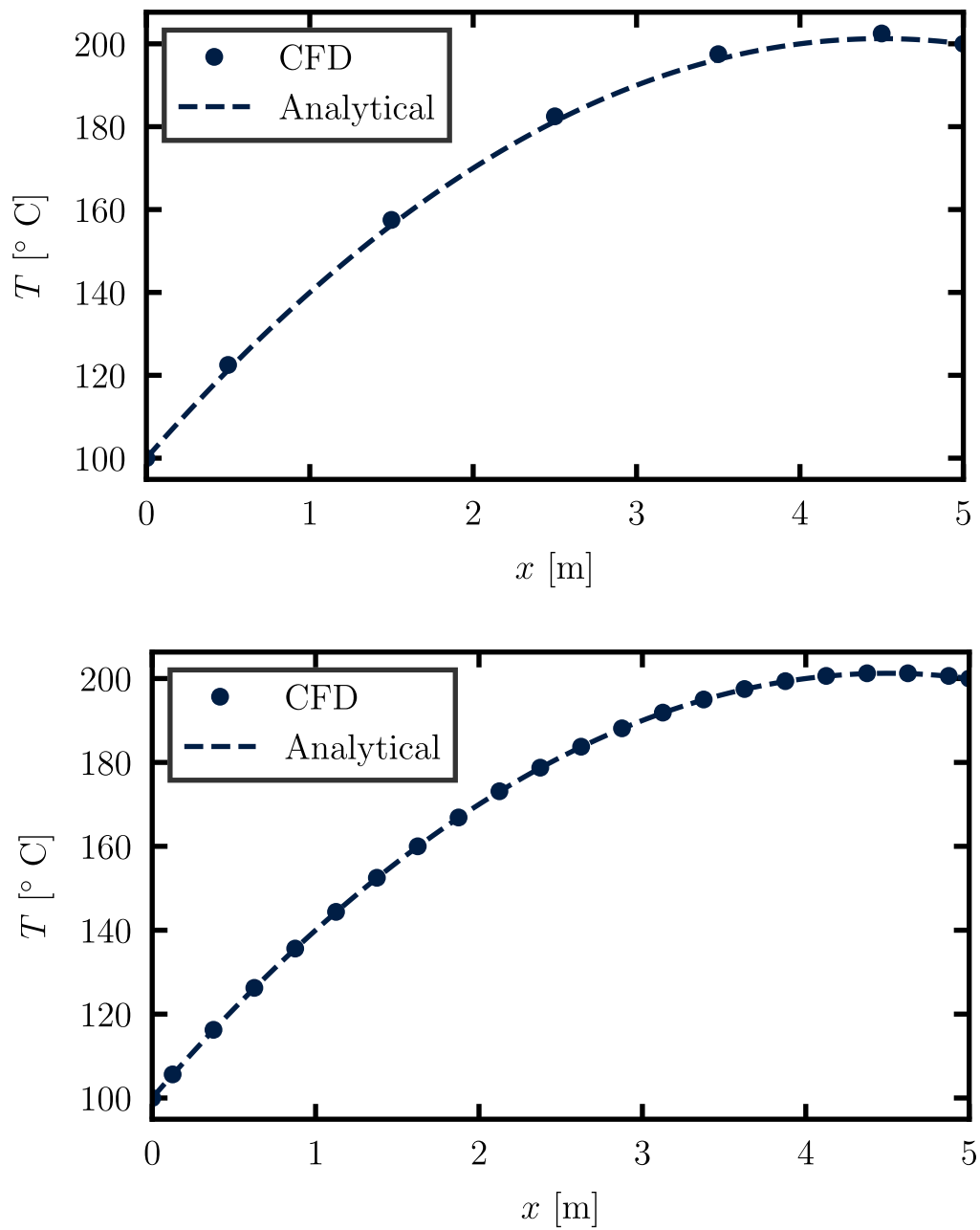
Figure 17: Temperature variation along the 1D bar for a mesh of (a) 5 cells and (b) 20 cells.

Chapter 3

The 1D Convection-Diffusion Equation

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Chapter 4

Upwind Differencing

[Upgrade to the full product for Chapter 3 and 4]