The Finite Volume Method for Transport Equations
Chapter 1

MXB324 Computational Fluid Dynamics
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Outline

1. Introduction to FVM
2. FVM in one dimension
3. Diffusion equation
4. Advection-diffusion equation
5. Treatment of Nonlinearity
6. Introduction to FVM in two dimensions

Transport eq^{n}s

Introduction

$$\frac{\partial \varphi}{\partial t} + \nabla \cdot (\varphi \underline{v}) = S$$

- The **Finite Volume Method** (FVM) is a method designed particularly for solving transport equations.
- In the field of computational fluid dynamics, especially in modern CFD software packages, it is much more widely used than the finite difference method. FLUENT.
- One important reason for its popularity is that it *conserves*, even at the discrete level. Thus, even though the numerical solution is only approximate, it nevertheless obeys the laws of conservation of mass, momentum and energy.
- Other desirable features of the method are its applicability on unstructured meshes and its natural handling of boundary conditions.

Meshes

- The basic geometric structure that underlies the finite volume method is called the **mesh**.
- A mesh consists of a set of **nodes**, and a set of connections between the nodes to form **elements**.
- Elements can be of any shape, but commonly used shapes are triangles and quadrilaterals in two dimensions, and tetrahedra and hexahedra in three dimensions.
- An **unstructured** mesh is one for which there is no regular grid underlying the mesh.
- These are difficult to construct (fortunately there is a wealth of software, both free and commercial, that can build these meshes), but very versatile—able to take the shape of complex domains and be refined in regions of interest.

Examples of Meshes

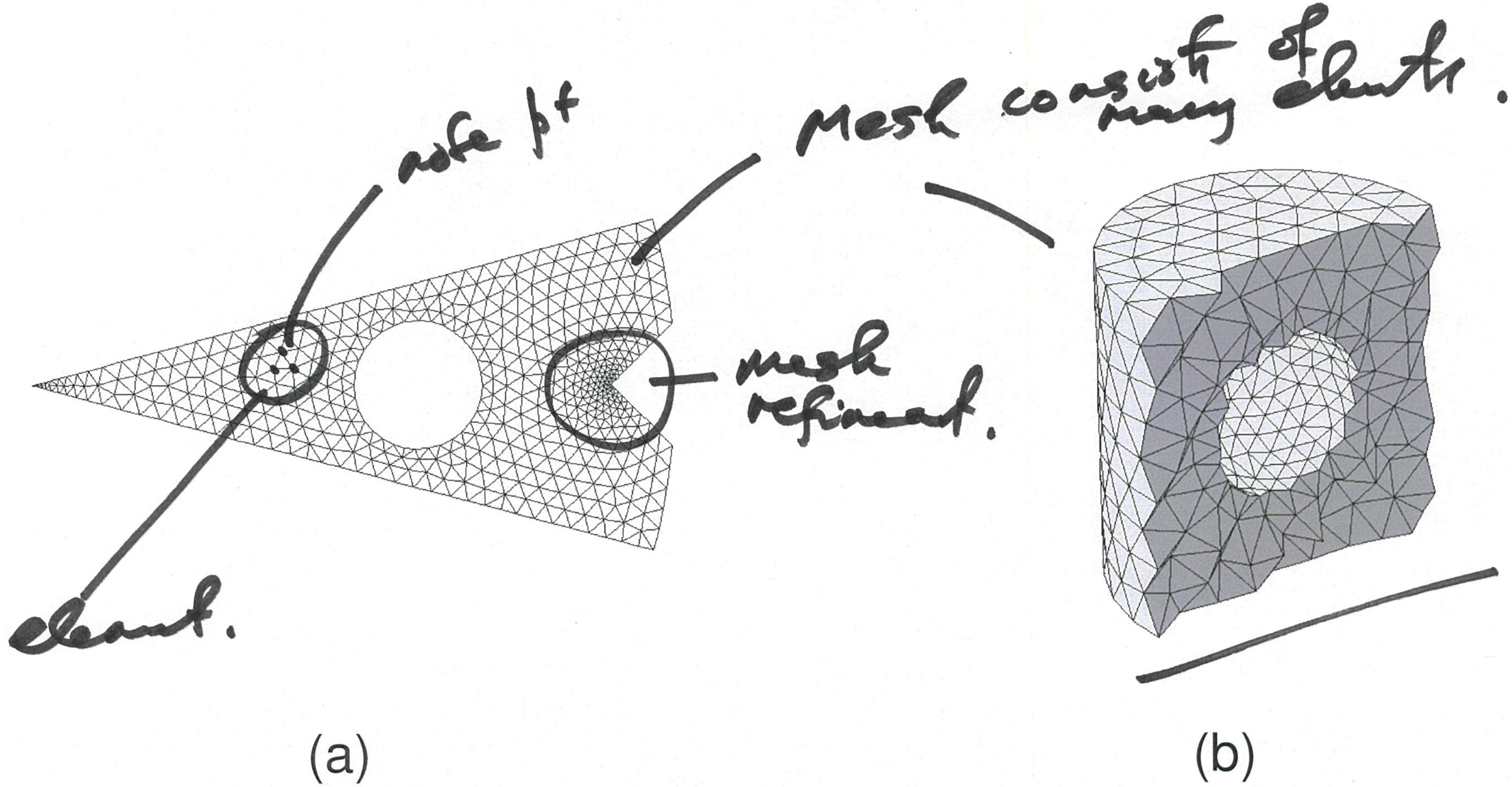


Figure: Unstructured meshes: (a) triangular; (b) tetrahedral.

Control Volume Construction

- The finite volume method uses the mesh to construct **control volumes** over which conservation is enforced.
  - Although technically these structures are only "volumes" when working in three dimensions, it is standard terminology even when working in one or two dimensions.
- There are a number of ways in which these control volumes can be constructed.
- In a **cell-centred** approach, the elements themselves form the control volumes, and a new set of nodes is constructed at the element centroids.
- In a **vertex-centred** approach, control volumes are constructed around the existing nodes, forming a **dual mesh** over the top of the existing mesh.

Illustration of Control Volume Construction in 3D

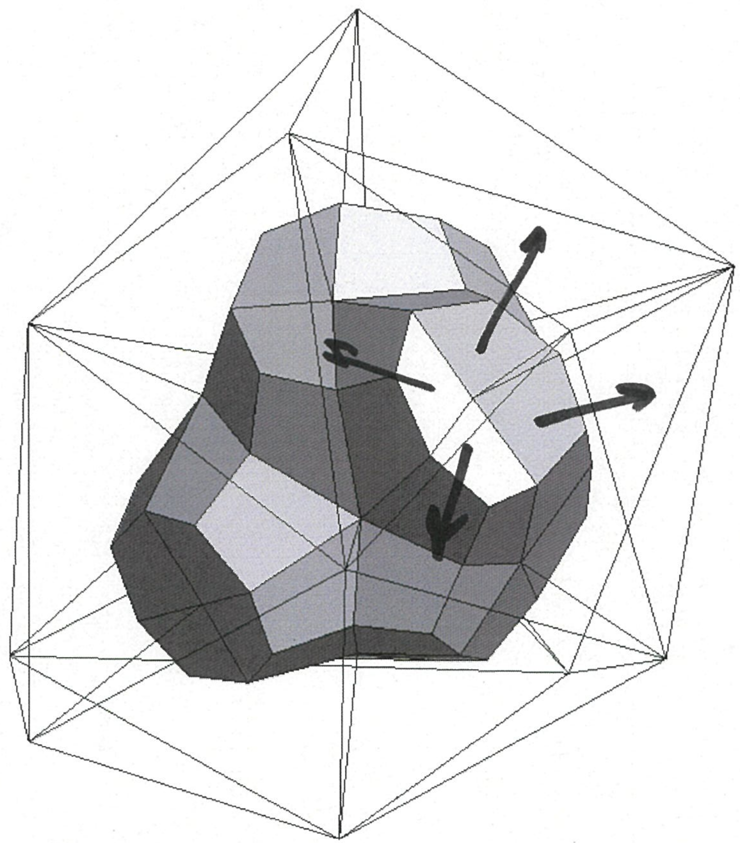


Figure: Vertex-centred control volume in three dimensions

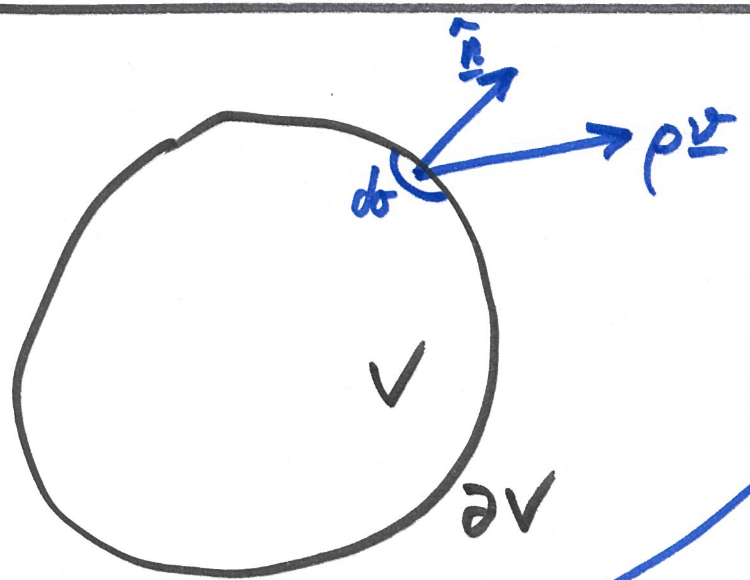
Control Volume Construction (continued)

Vertex - centred

Whichever approach is used to construct control volumes, the finite volume method works in the same way:

1. the PDE is integrated over each control volume,
2. numerical approximations are introduced,
3. the resulting system of equations is solved to yield a solution at each node.

Conservation of Mass :



R.E.V. representive elementary Volume ?

Rate of change of Mass in V = the mass flowing into/out of V + Volumetric Sources/Sinks of mass.

translate maths

$$\frac{d}{dt}\int_V \rho(\underline{x},t)\,dV \quad \frac{1}{s}\cdot\frac{kg}{m^3}\cancel{m^3} \quad \underline{kg\,s^{-1}}$$

$$= -\oint\!\!\oint_{\partial V} \rho\underline{v}\cdot\underline{n}\,d\sigma \quad \frac{kg}{m^3}\cdot\frac{m}{s}\,m^2 \quad kg\,s^{-1}$$

RHS $kg\,s^{-1}$ ✓

$$+\int_V S(\underline{x},t)\,\underline{dV} \quad \frac{kg}{s\,\cancel{m^3}}\,\cancel{m^3}$$

Divergence Thm

LHS $kg\,s^{-1}$

$$\int_V\left\{\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\underline{v}) - S\right\}dV = 0$$

Since V is arbitrary ; it must be that

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\underline{v}) - S = 0$$

Conservation of Mass :

$$\boxed{\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \underline{v}) = S}$$

$$\overline{\psi} = \frac{1}{\Delta V_i} \iiint_{V_i} \psi \, dV . \quad \leftarrow \text{Average of function over } V_i$$

$$\overline{S} = \frac{1}{\Delta V_i} \iiint_{V_i} S(x_i, t) \, dV \quad \leftarrow \text{Average of source over } V_i$$

General Transport Equation

We consider the general transport equation

$$\overbrace{\frac{\partial(\rho\varphi)}{\partial t}}^{\text{accumulation}} + \underbrace{\nabla\cdot(\rho\varphi\mathbf{v})}_{\text{advective term}} = \underbrace{\nabla\cdot(\Gamma\nabla\varphi)}_{\text{Diffusive Dispersion}} + \underbrace{S_\varphi}_{\text{Source/Sink}} \qquad (1)$$

or, as it is sometimes written for compactness,

$$\underbrace{\frac{\partial\psi}{\partial t}}_{\text{Unsteady term}} + \underbrace{\nabla\cdot\mathbf{J}}_{\text{Flux term}} = \underbrace{S_\varphi}_{\text{Source term}} \qquad (2)$$

where $\psi = \rho\varphi$, and $\mathbf{J} = \rho\varphi\mathbf{v} - \Gamma\nabla\varphi$ is the **flux vector**, representing both advective and diffusive fluxes.

Note: capital **J** is used, to avoid confusion with the coordinate vector **j**.

Control Volume Formulation

If we integrate (2) over the ith control volume V_i, we obtain

$$\iiint_{V_i} \frac{\partial \psi}{\partial t}\, \mathrm{d}V + \iiint_{V_i} \boldsymbol{\nabla} \cdot \mathbf{J}\, \mathrm{d}V = \iiint_{V_i} S_\varphi\, \mathrm{d}V\,.$$

Rearranging, and applying the divergence theorem gives

$$\frac{\mathrm{d}}{\mathrm{d}t} \underbrace{\iiint_{V_i} \psi\, \mathrm{d}V}_{\Delta V_i \overline{\psi}_i} = -\iint_{\partial V_i} \mathbf{J} \cdot \hat{\mathbf{n}}\, \mathrm{d}\sigma + \underbrace{\iiint_{V_i} S_\varphi\, \mathrm{d}V}_{\Delta V_i \overline{S}_{\varphi_i}}\,.$$

Control Volume Formulation

Defining the control volume averaged values of ψ and S_φ over V_i as $\overline{\psi}_i$ and $\overline{S_{\varphi}}_i$ respectively, we obtain

$$\frac{\mathrm{d}\overline{\psi}_i}{\mathrm{d}t}\cancel{\Delta V_i} = -\frac{1}{\Delta V_i}\iint_{\partial V_i} \mathbf{J}\cdot\hat{\mathbf{n}}\,\mathrm{d}\sigma + \overline{S_{\varphi}}_i\,\cancel{\Delta V_i}$$

or

$$\boxed{\frac{\mathrm{d}\overline{\psi}_i}{\mathrm{d}t} = \frac{-1}{\Delta V_i}\iint_{\partial V_i} \mathbf{J}\cdot\hat{\mathbf{n}}\,\mathrm{d}\sigma + \overline{S_{\varphi}}_i\,.} \qquad (3)$$

At this point, the first step is complete: (3) is an *exact* reformulation of (2), in control volume form.

Control Volume Formulation

To proceed we must introduce numerical approximations.

First, we replace the control volume averaged values $\overline{\psi_i}$ and $\overline{S_{\varphi_i}}$ with their values at the control volume node, ψ_i and S_{φ_i} respectively, to obtain the following *approximate* form of (3):

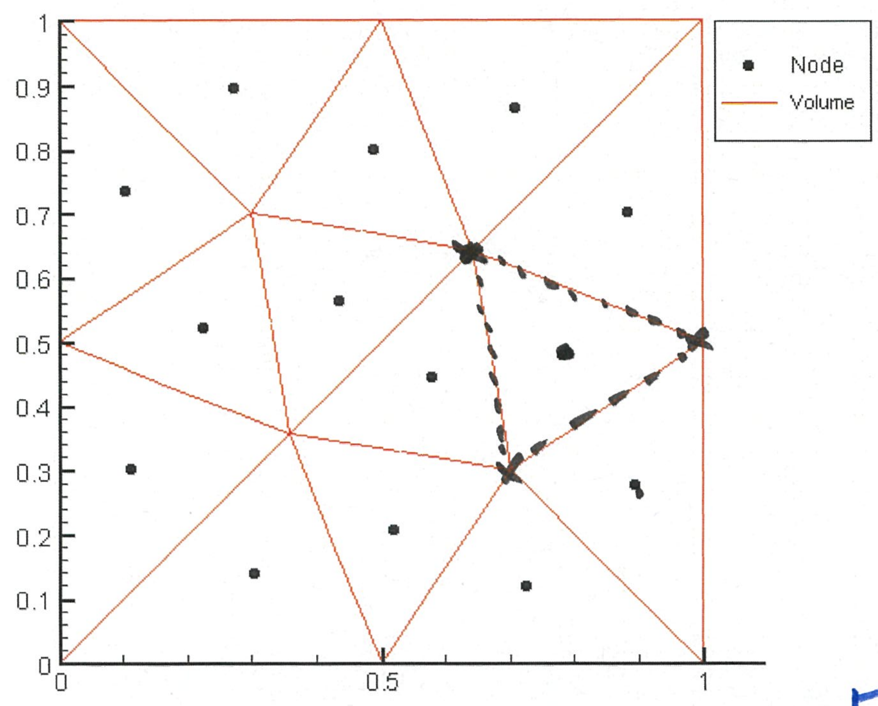
$$\frac{\mathrm{d}\psi_i}{\mathrm{d}t} = \frac{-1}{\Delta V_i} \iint_{\partial V_i} \mathbf{J} \cdot \hat{\mathbf{n}} \, \mathrm{d}\sigma + S_{\varphi_i} \, .$$

We also require an approximation for the integral of $\mathbf{J} \cdot \hat{\mathbf{n}}$ over the control volume surface ∂V_i.

Much of the rest of this chapter will be spent addressing how to do this appropriately.

Illustration of Control Volume Construction in 2D

cell-centred.



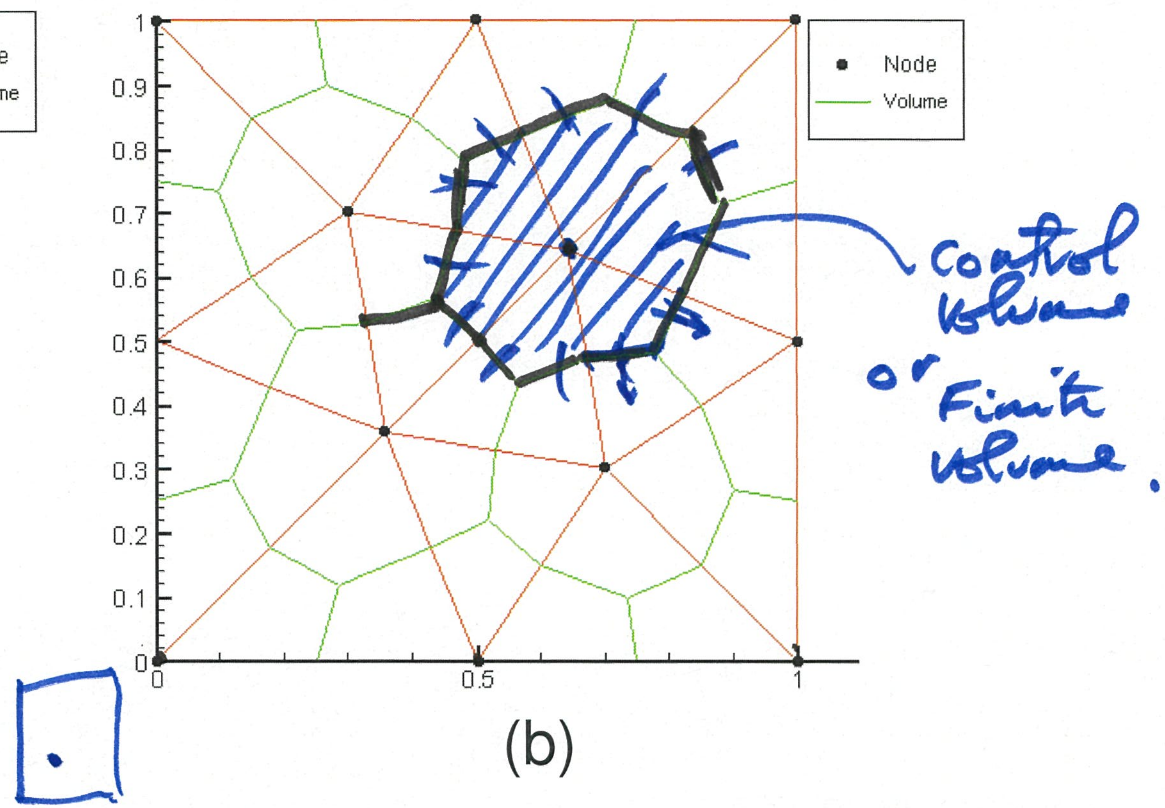
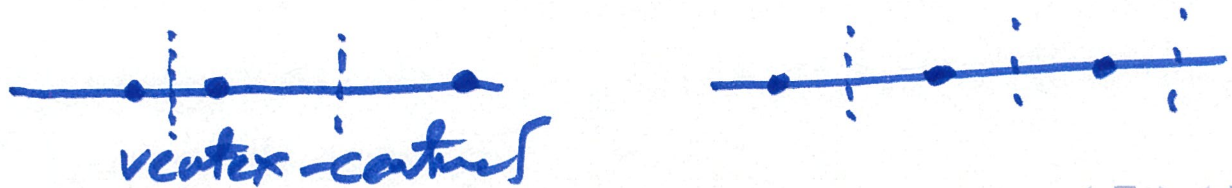


Figure: Constructing control volumes in two dimensions: (a) cell-centred; (b) vertex-centred.



Notation in one dimension

The one-dimensional version of the general transport equation (1) for a problem with a constant value of ρ and where $\mathbf{v} = u\,\mathbf{i}$ with u, S_φ and Γ potentially functions of the dependent variable φ, is expressed as

$$\frac{\partial \varphi}{\partial t} + \frac{\partial}{\partial x}\Big(\underbrace{u\,\varphi - D\frac{\partial \varphi}{\partial x}}_{J}\Big) = S \qquad (4)$$

where we have divided throughout by ρ and set $D = \Gamma/\rho$ and $S = S_\varphi/\rho$.

In (4) the i^{th} component of the flux vector J is given by $J = u\,\varphi - D\frac{\partial \varphi}{\partial x}$.

$$\boxed{\frac{\partial \varphi}{\partial t} + \frac{\partial J}{\partial x} = S}\ , \ \mathcal{I}$$

When working in one dimension, we adopt the notation illustrated in the figure for a particular control volume of interest. Extending the control volume faces in the vertical direction is done purely for illustrative purposes: these are one-dimensional structures.

control volume.

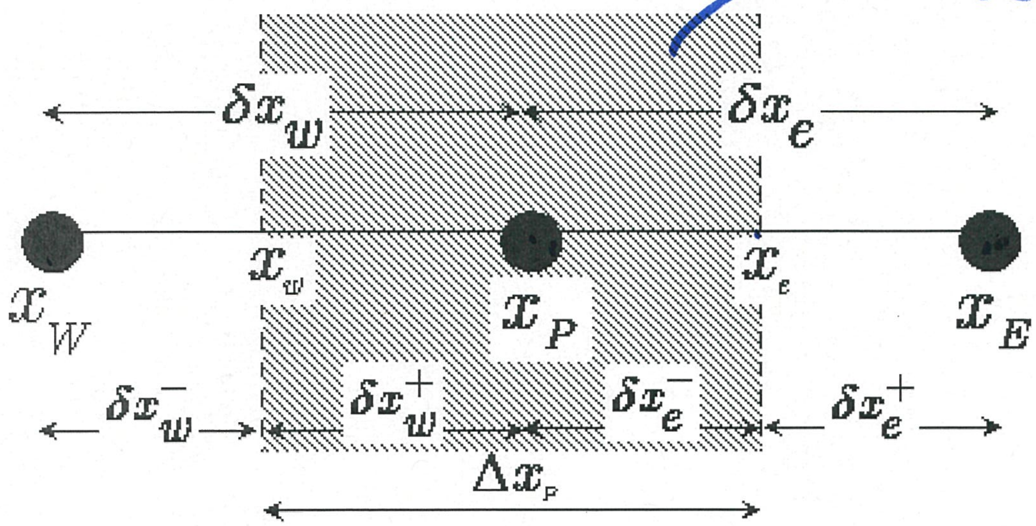


Figure: Control volume in one dimension

Illustration of Cell–Centred & Vertex–Centred Schemes in 1D

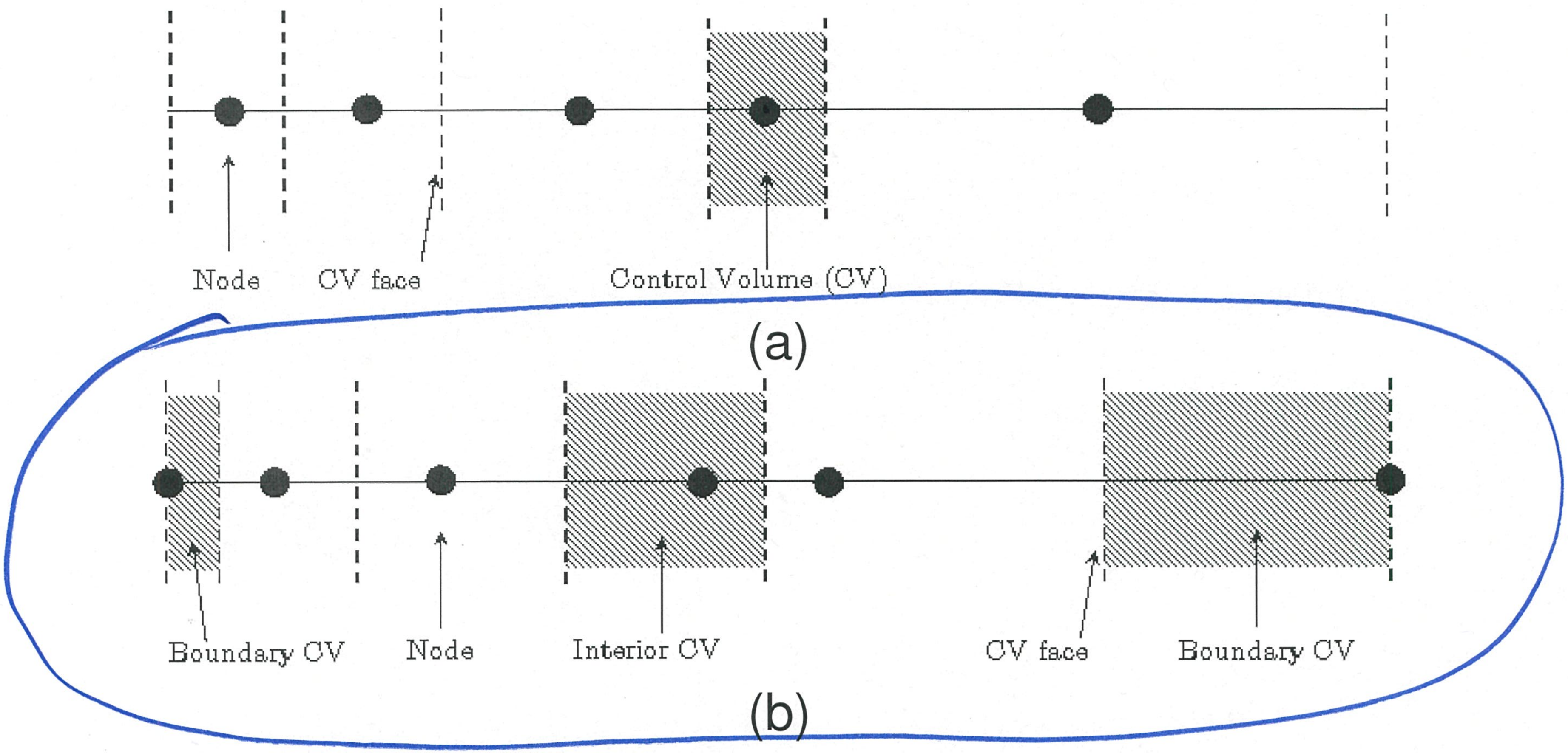


Figure: Constructing control volumes in one dimension: (a) cell-centred; (b) vertex-centred.

Diffusion Equation

We begin by considering the linear *diffusion equation with source term* on the interval $[0, L]$:

Diffusivity

$$\frac{\partial \varphi}{\partial t} + \frac{\partial}{\partial x}\Big(\underbrace{-D\frac{\partial \varphi}{\partial x}}_{J}\Big) = S, \qquad 0 < x < L, \quad t > 0 \tag{5}$$

subject to

$$-\cancel{B_0}^{D}\frac{\partial \varphi}{\partial x} = \frac{D}{B_0}\left(C_0 - A_0\varphi\right)$$

$$-D\frac{\partial \varphi}{\partial x} = K(C^{*} - \varphi)$$

$$\begin{aligned} &\text{at } x = 0, \quad A_0\varphi - B_0\frac{\partial \varphi}{\partial x} = C_0, \quad t > 0 \\ &\text{at } x = L, \quad A_L\varphi + B_L\frac{\partial \varphi}{\partial x} = C_L, \quad t > 0 \end{aligned} \tag{6}$$

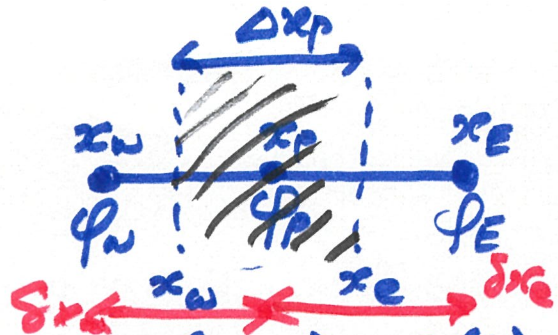
and initially

$$\varphi(x, 0) = \varphi_0(x), \qquad 0 \le x \le L.$$

$$\cancel{\rho C_p} \frac{\partial \varphi}{\partial t} = \boxed{\frac{k}{\rho C_p}} \frac{\partial^2 \varphi}{\partial x^2}$$

thermal diffusivity.

Spatial Discretisation



$\varphi(x_P, t) := \varphi_P(t)$
$\varphi(x_E, t) := \varphi_E(t)$
$\varphi(x_W, t) := \varphi_W(t)$

First we integrate from x_w to x_e to obtain

$$\int_{x_w}^{x_e} \frac{\partial \varphi}{\partial t}\, \mathrm{d}x + \int_{x_w}^{x_e} \frac{\partial J}{\partial x}\, \mathrm{d}x = \int_{x_w}^{x_e} S\, \mathrm{d}x\,.$$

Then, proceeding as in the previous section, we obtain

$$\frac{\mathrm{d}\varphi_P}{\mathrm{d}t} = \frac{1}{\Delta x_P}(J_w - J_e) + S_P\,. \tag{7}$$

However, in order to apply this equation, we need expressions for J_w and J_e: the fluxes evaluated at the west and east face respectively.

We approximate $\left(\frac{\partial \varphi}{\partial x}\right)_w$ by $\frac{\varphi_P - \varphi_W}{\delta x_w}$ and $\left(\frac{\partial \varphi}{\partial x}\right)_e$ by $\frac{\varphi_E - \varphi_P}{\delta x_e}$, and hence

$$J_w = \left(-D\frac{\partial \varphi}{\partial x}\right)_w \approx -D\left(\frac{\varphi_P - \varphi_W}{\delta x_w}\right), \quad J_e = \left(-D\frac{\partial \varphi}{\partial x}\right)_e \approx -D\left(\frac{\varphi_E - \varphi_P}{\delta x_e}\right). \tag{8}$$

$$\frac{d}{dt}\int_{x_w}^{x_e}\varphi(x,t)\,dx + \left\{ J(x_e,t) - J(x_w,t) \right\} = \int_{x_w}^{x_e} S(x,t)\,dx$$

$$\overline{\varphi_P} = \frac{1}{\Delta x_P}\int_{x_w}^{x_e}\varphi(x,t)\,dx \; ; \quad \overline{S_P} = \frac{1}{\Delta x_P}\int_{x_w}^{x_e} S(x,t)\,dx$$

$$\therefore \quad \frac{d\overline{\varphi_P}}{dt} + \frac{1}{\Delta x_P}\left\{ \underline{J_e(t)} - \underline{J_w(t)} \right\} = \overline{S_P} .$$

How should we approximate these terms?

IDEA: $\overline{\varphi_P} \simeq \varphi_P \,, \quad \overline{S_P} \simeq S_P$

$$J_e = \left[-D\frac{\partial\varphi}{\partial x} \right]_{x=x_e} , \quad J_w = \left[-D\frac{\partial\varphi}{\partial x} \right]_{x=x_w}$$

$$J_e \simeq -D_e\frac{(\varphi_E - \varphi_P)}{\delta x_e} , \quad J_w \simeq -D_w\frac{(\varphi_P - \varphi_W)}{\delta x_w}$$

substitution gives :

$$\frac{d\varphi_P}{dt} = -\frac{1}{\Delta x_P}\left\{-\frac{D_e}{\delta x_e}\left(\varphi_E(t)-\varphi_P(t)\right)+\frac{D_w}{\delta x_w}\left(\varphi_P(t)-\varphi_W(t)\right)\right\} + S_P$$

Rearranging : (constant diffusivity $D = D_e = D_w$).

$$\boxed{\frac{d\varphi_P}{dt} = \frac{D}{\Delta x_P}\left[\frac{1}{\delta x_e}\varphi_E(t) - \left(\frac{1}{\delta x_e}+\frac{1}{\delta x_w}\right)\varphi_P(t) + \frac{1}{\delta x_w}\varphi_W(t)\right] + S_P(t).}$$

- Finite Volume eq^n (FVE).
- Finite Volume discretisation eq^n.

Substituting (8) into (7) we obtain, after rearrangement,

$$\frac{\mathrm{d}\varphi_P}{\mathrm{d}t} = \frac{D}{\Delta x_P}\left[\left(\frac{1}{\delta x_w}\right)\varphi_W - \left(\frac{1}{\delta x_w} + \frac{1}{\delta x_e}\right)\varphi_P + \left(\frac{1}{\delta x_e}\right)\varphi_E\right] + S_P \quad (9)$$

which is the **finite volume discretisation** of (5).

Note

Note that this is a discretisation in space only: the derivative in time remains.