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

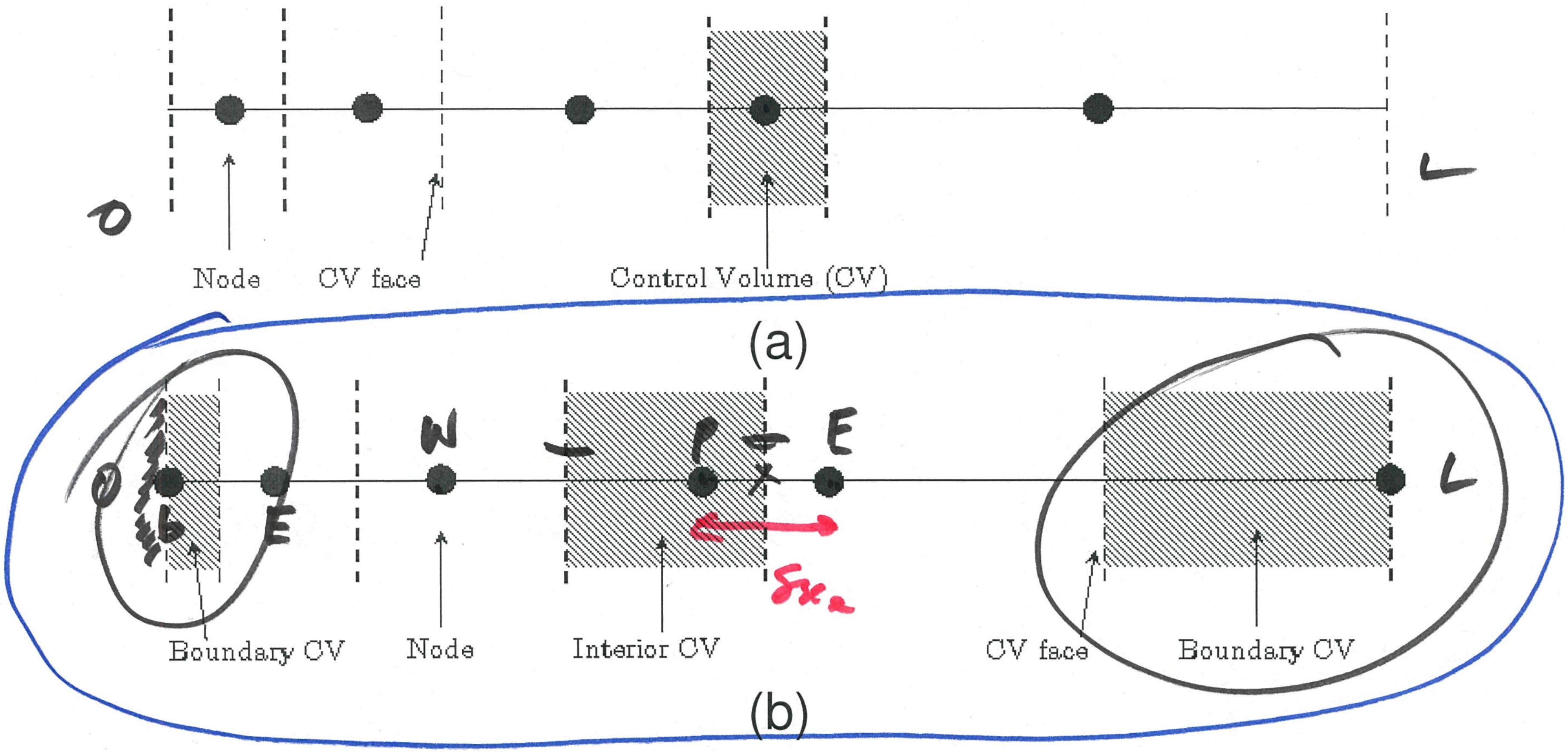
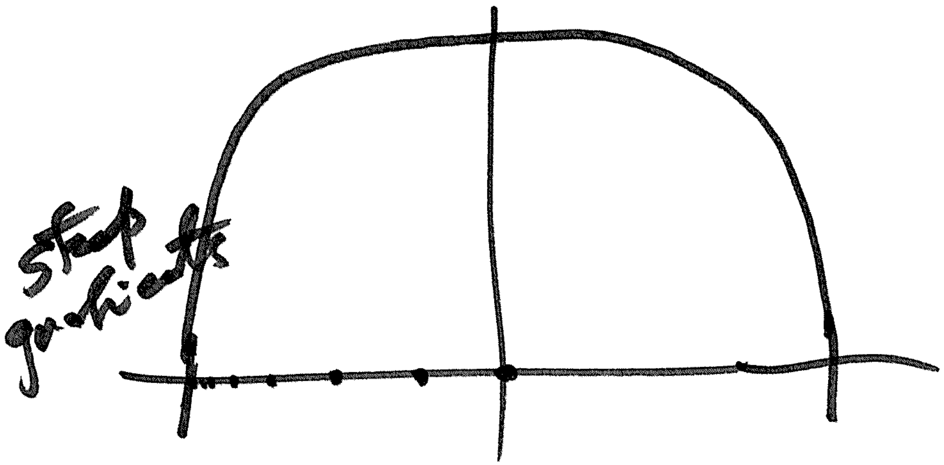
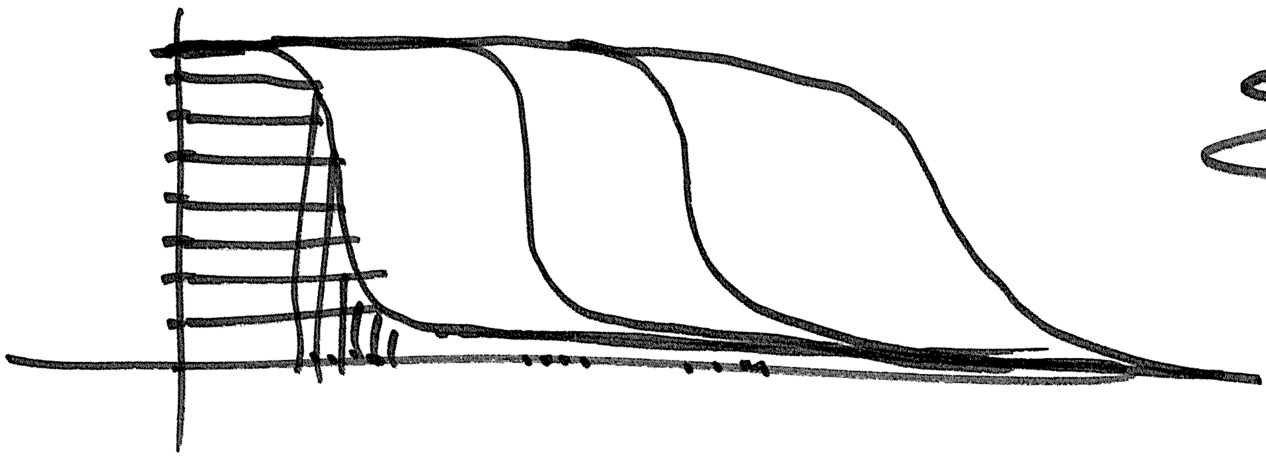


Figure: Constructing control volumes in one dimension: (a) cell-centred; (b) vertex-centred.



GRIDS ARE DESIGNED TO CAPTURE PHYSICS



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.

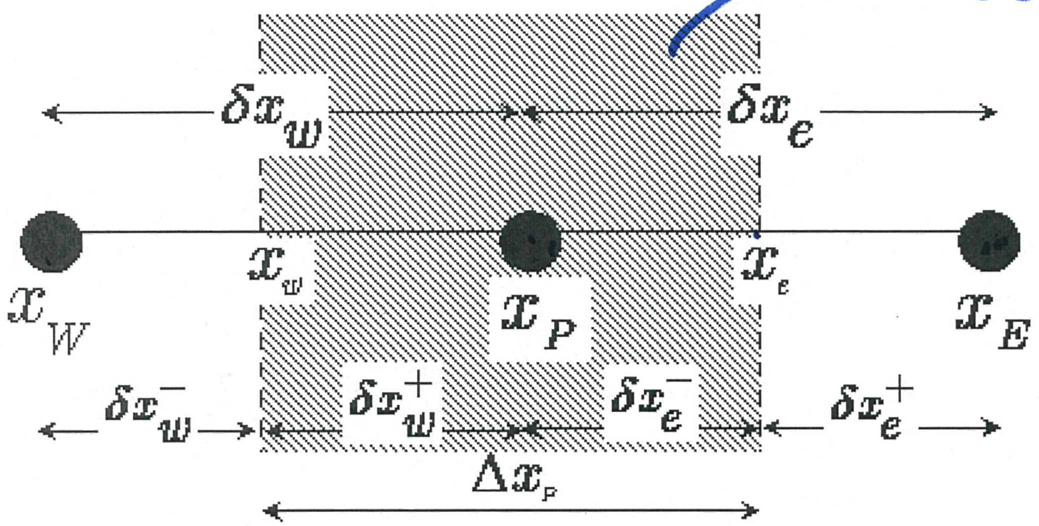


Figure: Control volume in one dimension

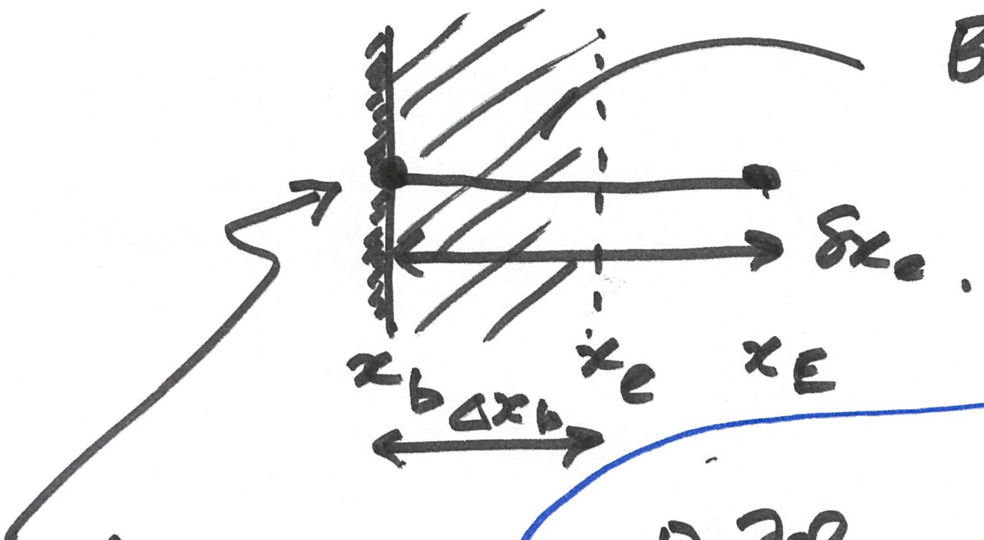
substitution gives :

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

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.



BCV. boundary control volume.

at $x=0$: $-D\dfrac{\partial \varphi}{\partial x} = \dfrac{D}{B_0}\left(C_0 - A_0\varphi\right)$.

$$\int_{x_b}^{x_E} \frac{\partial \varphi}{\partial t}\,dx + \int_{x_b}^{x_e} \frac{\partial J}{\partial x}\,dx = \int_{x_b}^{x_E} S\,dx.$$

$$\Delta x_b \frac{d\varphi_b}{dt} + \left\{ J_e - \underset{\uparrow}{J_b} \right\} = \Delta x_b S_b$$

$$\left[-D\frac{\partial \varphi}{\partial x}\right]_{x=x_b}.$$

$$\Delta x_b \frac{d\varphi_b}{dt} + \left\{ -\frac{D_e}{\delta x_e}(\varphi_E - \varphi_b) - \frac{D_b}{B_0}(C_0 - A_0 \varphi_b) \right\} = \Delta x_b S_b.$$

Rearranging: (Assumption $D = D_e = D_b$)

$x = 0$:
$$\frac{d\varphi_b}{dt} = \frac{D}{\Delta x_b}\left[\frac{1}{\delta x_e}\varphi_E - \left(\frac{1}{\delta x_e} + \frac{A_0}{B_0}\right)\varphi_b + \frac{C_0}{B_0} \right] + S_b.$$

Boundary F.V.E.

Diffusion Equation

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

Diffusivity $\quad S(\varphi)$

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

$D(\varphi)$

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

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

subject to

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

and initially

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

Hence, we obtain the equations for the boundary nodes:

$$\text{at } x = 0, \quad \frac{\mathrm{d}\varphi_P}{\mathrm{d}t} = \frac{D}{\Delta x_P}\left[-\left(\frac{1}{\delta x_e} + \frac{A_0}{B_0}\right)\varphi_P + \left(\frac{1}{\delta x_e}\right)\varphi_E + \frac{C_0}{B_0}\right] + S_P$$

$$\text{at } x = L, \quad \frac{\mathrm{d}\varphi_P}{\mathrm{d}t} = \frac{D}{\Delta x_P}\left[\left(\frac{1}{\delta x_w}\right)\varphi_W - \left(\frac{1}{\delta x_w} + \frac{A_L}{B_L}\right)\varphi_P + \frac{C_L}{B_L}\right] + S_P\,.$$

Note

If Dirichlet boundary conditions are imposed ($B_0 = 0, A_0 = 1$ and/or $B_L = 0, A_L = 1$) we simply set the boundary value accordingly as $\varphi = C_0$ at $x = 0$ and/or $\varphi = C_L$ at $x = L$.

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

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

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

Note

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

At $x = 0$ we use

$$J_w = \left(-D\frac{\partial \varphi}{\partial x}\right)_w = -\frac{DA_0}{B_0}\varphi_P + \frac{DC_0}{B_0}.$$

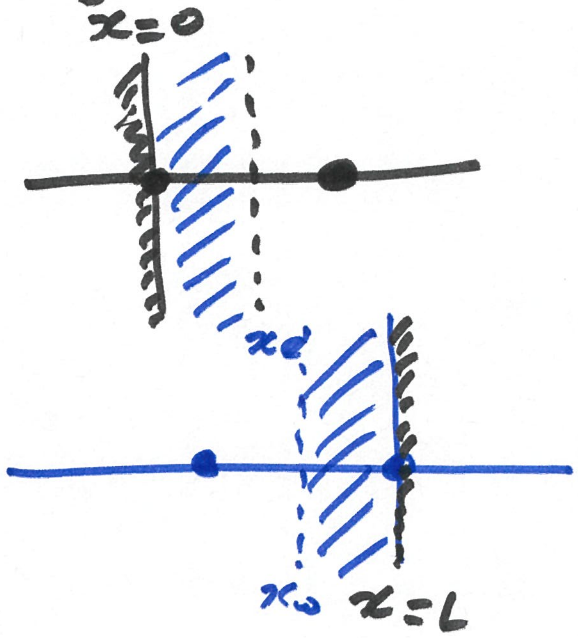
A similar situation applies at $x = L$, where we require the boundary condition to compute J_e. We use

$$J_e = \left(-D\frac{\partial \varphi}{\partial x}\right)_e = \frac{DA_L}{B_L}\varphi_P - \frac{DC_L}{B_L}.$$

Note

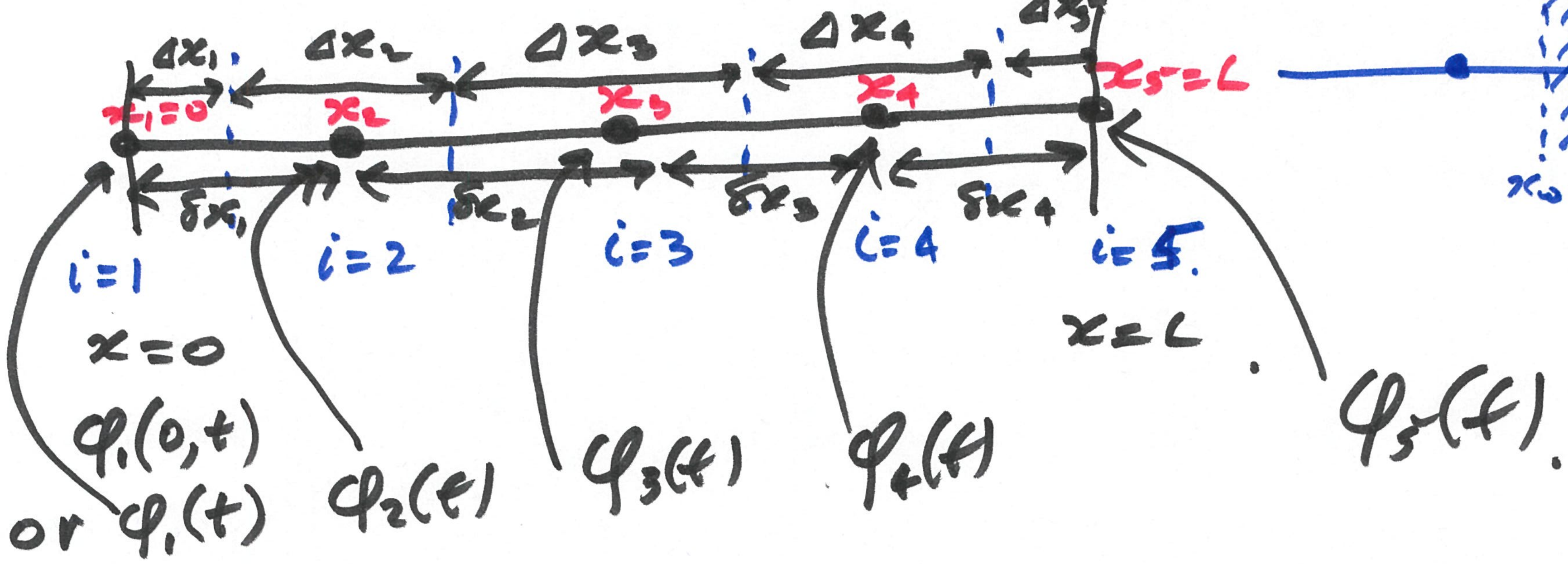
No approximations are required here. The boundary conditions provide exact values for the fluxes.

$$\frac{d\varphi_b}{dt} = \frac{1}{\Delta x_b}\left[J_e - J_b \right] + S_b$$



Vertex-centred FVM.

TEST MESH (EXAMPLE)



We now use our FVEs to obtain a system of ODEs:

$$\frac{d\varphi_1}{dt} = \frac{D}{\Delta x_1}\left[-\left(\frac{1}{\delta x_1}+\frac{A_0}{B_0}\right)\varphi_1 + \left(\frac{1}{\delta x_1}\right)\varphi_2 + \frac{C_0}{B_0}\right] + S_1$$

$$\frac{d\varphi_i}{dt} = \frac{D}{\Delta x_i}\left[\frac{1}{\delta x_{i-1}}\varphi_{i-1} - \left(\frac{1}{\delta x_{i-1}}+\frac{1}{\delta x_i}\right)\varphi_i + \frac{1}{\delta x_i}\varphi_{i+1}\right] + S_i,$$

$$i = 2,3,4.$$

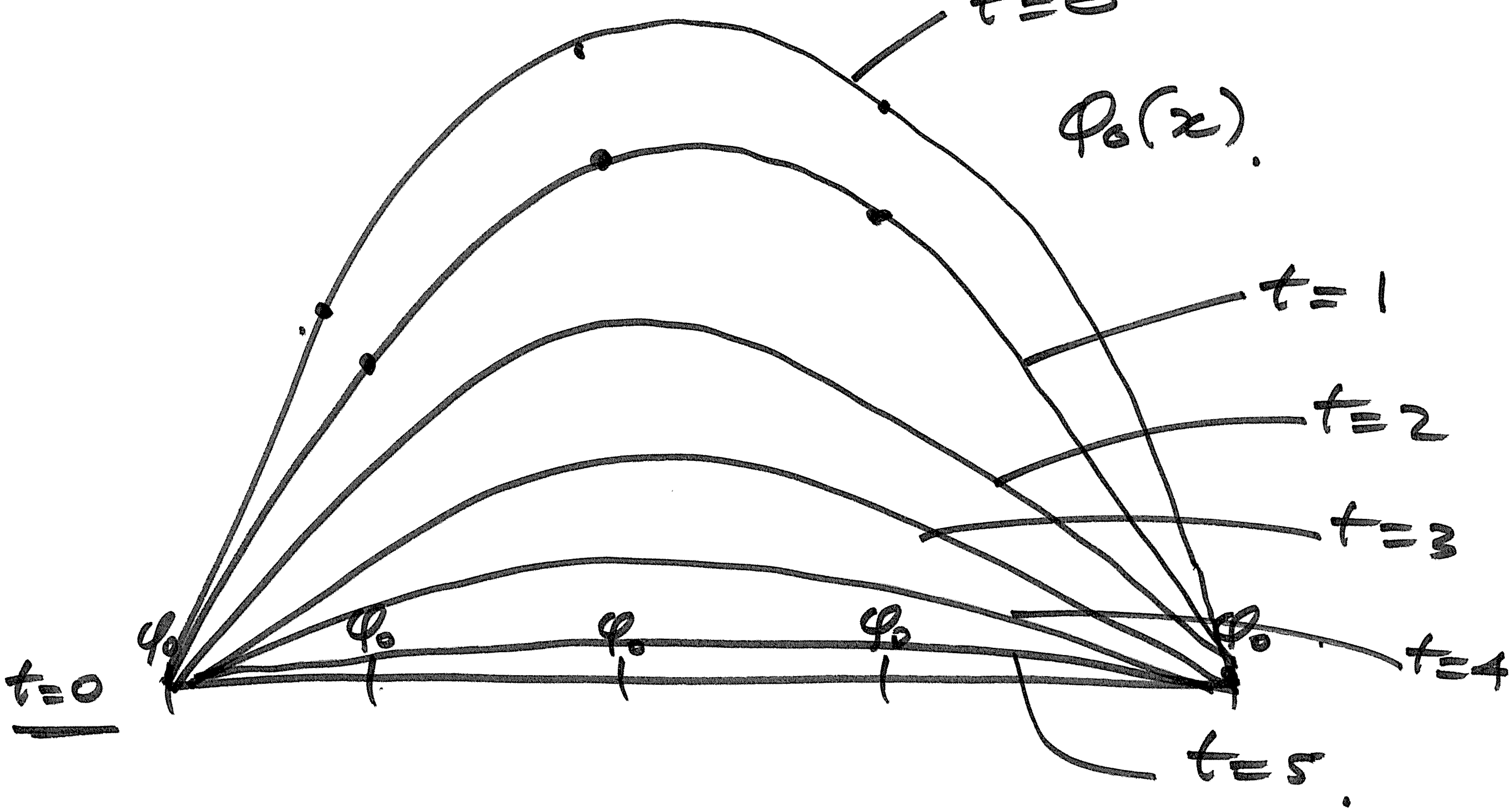
$$\frac{d\varphi_5}{dt} = \frac{D}{\Delta x_5}\left[\frac{1}{\delta x_4}\varphi_4 - \left(\frac{1}{\delta x_4}+\frac{A_L}{B_L}\right)\varphi_5 + \frac{C_L}{B_L}\right] + S_5.$$

$$\underline{u}(t) = (\varphi_1(t), \varphi_2(t), \varphi_3(t), \varphi_4(t), \varphi_5(t))^T.$$

$$\frac{d\underline{u}}{dt} = \underline{g}(\underline{u}) = A\underline{u} + \underline{b}$$

tri diagonal ~~matrix~~

Subject to $\underline{u}(0) = \underline{u}_0 = (\varphi_0(0), \varphi_0(x_2), \varphi_0(x_3), \varphi_0(x_4), \varphi_0(\cancel{x_5}\,L))^T.$



$t=0$
$\varphi_0(x)$.
$t=1$
$t=2$
$t=3$
$t=4$
$t=5$.
φ_0
φ_0
φ_0
φ_0
φ_0
$\underline{t=0}$

Control Volume Average

We now consider the accuracy of the approximations made in formulating the finite volume discretisation (9).

The transient and source terms involve the control volume averaged values of φ and S, utilising the approximations

$$\boxed{\overline{\varphi}_P \equiv \frac{1}{\Delta x_P}\int_{x_w}^{x_e} \varphi \, dx \approx \varphi_P} \tag{10}$$

and

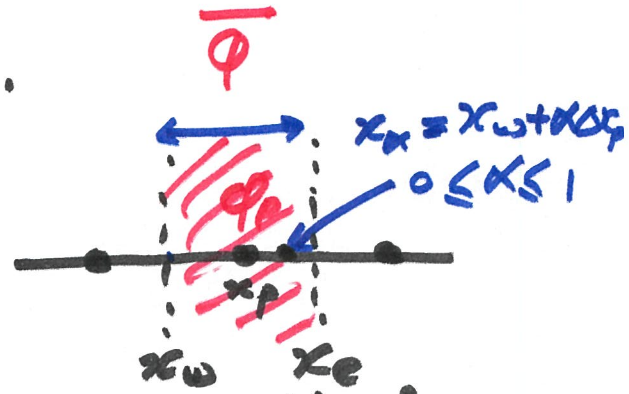
$$\overline{S}_P \equiv \frac{1}{\Delta x_P}\int_{x_w}^{x_e} S \, dx \approx S_P \tag{11}$$

respectively.

Exercises

1. Use Taylor series for φ about x_P to show that (10) is accurate to second order in the cell-centred case, but only to first order in the vertex-centred case.
2. Use Taylor series for φ about x_w and x_e to show that the derivative approximations are accurate to second order in the vertex-centred case, but only to first order in the cell-centred case.

ERROR ANALYSIS : (SPACE).



Expand a Taylor series for $\varphi(x,t)$ about $x = x_\alpha$.

$$\varphi(x,t) = \varphi(x_\alpha,t) + (x - x_\alpha)\frac{\partial \varphi}{\partial x}(x_\alpha,t) + \frac{(x-x_\alpha)^2}{2}\frac{\partial^2 \varphi}{\partial x^2}(\xi(x),t)$$

$$x_w < \xi(x) < x_e$$

Next, integrate

$$\int_{x_w}^{x_e} \varphi(x,t)\,dx = \Delta x_p\, \varphi(x_\alpha,t) + \frac{\partial \varphi}{\partial x}(x_\alpha,t)\int_{x_w}^{x_e}(x - x_\alpha)\,dx$$
$$+ \frac{1}{2}\int_{x_w}^{x_e} \underline{(x-x_\alpha)^2}\, \frac{\partial^2 \varphi}{\partial x^2}(\xi(x),t)\,dx$$

$I = \int_{x_w}^{x_e} f(x) g(x)\,dx$. If $f(x) > 0$ on $[x_w, x_e]$ then by the weighted. M. V. T for integrals, there is a point $c \in [x_w, x_e]$ s.t.

$$I = g(c)\int_{x_w}^{x_e} f(x)\,dx.$$

Hence, $\frac{1}{\Delta x_p}\int_{x_w}^{x_e} \varphi(x,t)\,dx = \cancel{\Delta x_p}\,\varphi(x_\alpha, t) + \frac{1}{\Delta x_p}\frac{\partial \varphi}{\partial x}(x_\alpha, t)\left[\frac{(x-x_\alpha)^2}{2}\right]_{x_w}^{x_e}$

$$+ \frac{1}{6\Delta x_p}\frac{\partial^2 \varphi}{\partial x^2}(\xi^*, t)\left[(x-x_\alpha)^3\right]_{x_w}^{x_e}$$

$$\therefore\ \overline{\varphi}_p = \varphi(x_\alpha, t) + \frac{1}{\cancel{\Delta x_p}}\frac{\partial \varphi}{\partial x}(x_\alpha, t)\,\frac{\Delta x_p^{\cancel{2}}}{2}(1-2\alpha)$$

$$+ \frac{1}{6\cancel{\Delta x_p}}\frac{\partial^2 \varphi}{\partial x^2}(\xi^*, t)\,\Delta x_p^{\cancel{3}\,2}(1-3\alpha+3\alpha^2).$$

For the choice $\alpha = 1/2$

$$\overline{\varphi}_p = \varphi(x_p, t) + O(\Delta x_p^2)$$

cell-centred

i.e, second order scheme (approx).

vertex-centred scheme (α might not be 1/2 in general) first order scheme.

Flux Approximation

The flux term requires evaluating $\frac{\partial \varphi}{\partial x}$ at the control volume face.

In the previous section, we developed the approximations

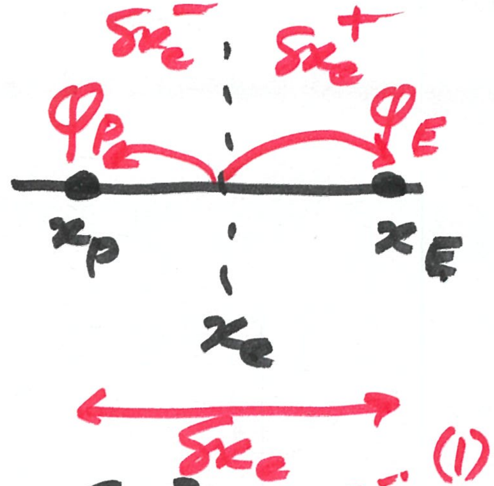
$$\left(\frac{\partial \varphi}{\partial x}\right)_w \approx \frac{\varphi_P - \varphi_W}{\delta x_w}$$

what is the error?

and

$$\left(\frac{\partial \varphi}{\partial x}\right)_e \approx \frac{\varphi_E - \varphi_P}{\delta x_e}.$$

Next $\displaystyle \left[\frac{\partial\varphi}{\partial x}\right]_{x_e} \simeq \frac{(\varphi_E - \varphi_P)}{\delta x_e}$



$$\varphi_E = \varphi(x_E,t) = \varphi(x_e + \delta x_e^+)$$
$$= \varphi_e + \delta x_e^+ \frac{\partial\varphi}{\partial x}(x_e,t) + \frac{\delta x_e^{+2}}{2}\frac{\partial^2\varphi}{\partial x^2}(x_e,t) + \frac{\delta x_e^{+3}}{6}\frac{\partial^3\varphi}{\partial x^3}(\xi^+,t) \quad \dots (1)$$

$$x_e < \xi^+ < x_E$$

$$\varphi_P = \varphi(x_P,t) = \varphi(x_e - \delta x_e^-)$$
$$= \varphi_e - \delta x_e^- \frac{\partial\varphi}{\partial x}(x_e,t) + \frac{\delta x_e^{-2}}{2}\frac{\partial^2\varphi}{\partial x^2}(x_e,t) - \frac{\delta x_e^{-3}}{6}\frac{\partial^3\varphi}{\partial x^3}(\xi^-,t) \quad \dots (2)$$

$$x_P < \xi^- < x_e$$

(1) − (2) gives

$$\frac{\varphi_E - \varphi_P}{\delta x_e} = \cancel{\delta x_e}\frac{\partial\varphi}{\partial x}(x_e,t) + \frac{\cancel{\delta x_e}}{2}\frac{\partial^2\varphi}{\partial x^2}(x_e,t)\cdot(\delta x_e^+ - \delta x_e^-)$$
$$+ \frac{1}{\delta x_e 6}\left[\delta x_e^{+3}\frac{\partial^3\varphi}{\partial x^3}(\xi^+,t) + \delta x_e^{-3}\frac{\partial^3\varphi}{\partial x^3}(\xi^-,t)\right]$$

$$\frac{(\varphi_E - \varphi_P)}{\delta x_e} = \left[\frac{\partial \varphi}{\partial x}\right]_{x_e} + \frac{\delta x_e \overbrace{\left(\frac{\delta x_e^+}{\delta x_e} - \frac{\delta x_e^-}{\delta x_e}\right)}^{O(\delta x_e)}}{2}\left[\frac{\partial^2 \varphi}{\partial x^2}\right]_{x_e}$$

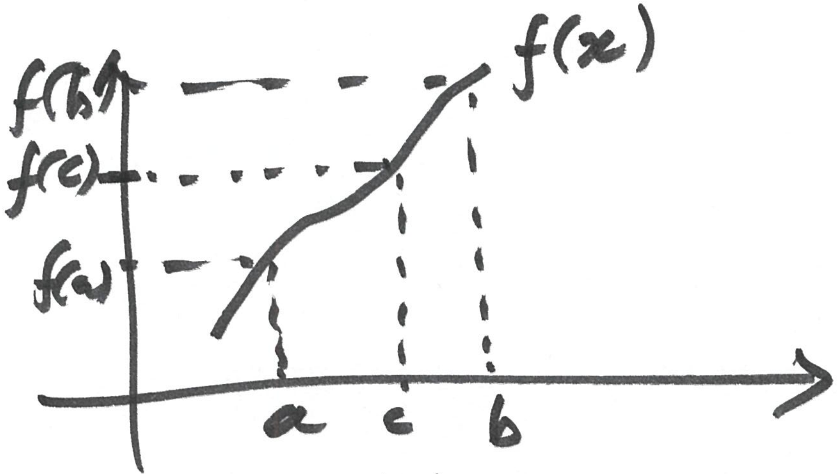
$$+ \frac{1}{6\delta x_e}\left[\delta x_e^{+3}\frac{\partial^3 \varphi}{\partial x^3}(\xi^+, t) + \delta x_e^{-3}\frac{\partial^3 \varphi}{\partial x^3}(\xi^-, t)\right]$$

Consider vertex-centred case : $\delta x_e^+ = \delta x_e^- = \frac{\delta x_e}{2}$

$$\frac{(\varphi_E - \varphi_P)}{\delta x_e} = \left[\frac{\partial \varphi}{\partial x}\right]_{x_e} + \frac{\delta x_e^2}{24}\left[\frac{1}{2}\left(\frac{\partial^3 \varphi}{\partial x^3}(\xi^+, t) + \frac{\partial^3 \varphi}{\partial x^3}(\xi^-, t)\right)\right]$$

$$+ \frac{\delta x_e^2}{24}\frac{\partial^3 \varphi}{\partial x^3}(\xi^*, t) \qquad \xi^- < \xi^* < \xi^+.$$

$$O(\delta x^2)$$



I.V.Th^m.

Temporal Discretisation

The temporal discretisation is carried out by choosing a time stepsize δt and letting $t_n = n\delta t$ for $n = 0, 1, \ldots$. Returning to (7), one way to proceed is to integrate from time t_n to t_{n+1} to obtain

$$\int_{t_n}^{t_{n+1}} \frac{\mathrm{d}\varphi_P}{\mathrm{d}t}\,\mathrm{d}t = \int_{t_n}^{t_{n+1}} \frac{1}{\Delta x_P}(J_w - J_e)\,\mathrm{d}t + \int_{t_n}^{t_{n+1}} S_P\,\mathrm{d}t\,.$$

We consider a general **theta method** for approximating the integrals in time:

$$\varphi_P^{n+1} - \underset{\displaystyle \varphi_P^n}{\overset{\displaystyle \varphi_P(t_n)}{\shortparallel}} = \frac{\delta t}{\Delta x_P}\left[\theta_1\left(J_w^{n+1} - J_e^{n+1}\right) + (1-\theta_1)\,(J_w^n - J_e^n)\right]$$

$$+\,\delta t\left[\theta_2 S_P^{n+1} + (1-\theta_2) S_P^n\right]. \qquad (12)$$

$\varphi_P(t)$

$\varphi_P(t_{n+1}) := \varphi_P^{n+1}$

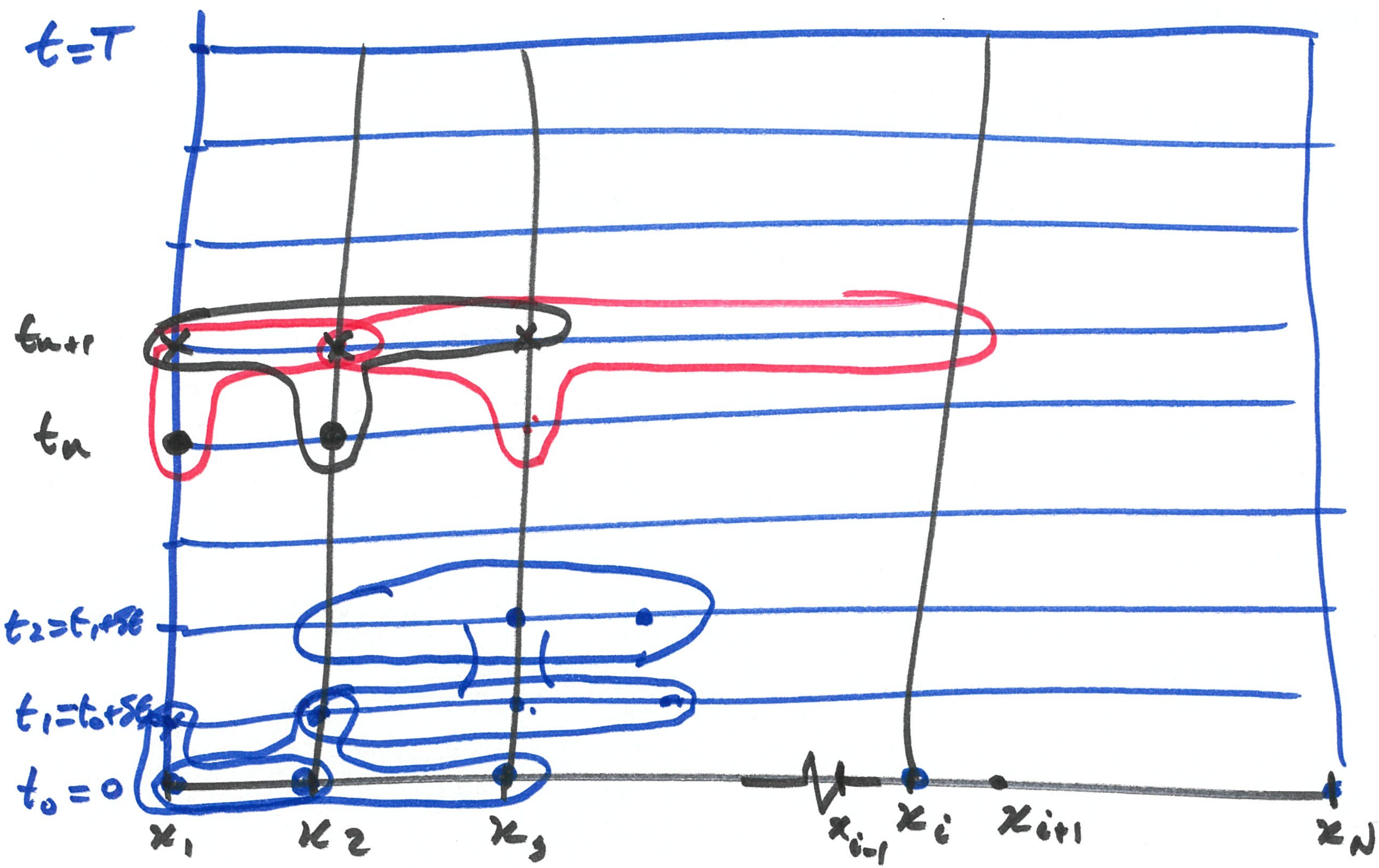
Temporal Discretisation

To understand the temporal error associated with (12), consider the approximation:

$$\int_{t_n}^{t_{n+1}} f(t)\,\mathrm{d}t \approx \delta t\big((1-\theta)f(t_n) + \theta f(t_{n+1})\big). \tag{13}$$

Exercise

1. Expand $f(t)$ as a Taylor polynomial about $t_{n+\theta} = t_n + \theta\delta t$, $0 \leq \theta \leq 1$ and integrate this polynomial from t_n to t_{n+1} to show that (13) is accurate to second order for the choice $\theta = 1/2$ and first order accurate for $\theta = 0$ or $\theta = 1$.



$t=T$
t_{n+1}
t_n
$t_2=t_1+\delta t$
$t_1=t_0+\delta t$
$t_0=0$
x_1
x_2
x_3
x_{i-1}
x_i
x_{i+1}
x_N

left-hand rule.

The above exercise allows us to conclude that if $\theta = 0$, which is known as the **forward Euler method**, then

Explicit

$$\int_{t_n}^{t_{n+1}} f(t)\,\mathrm{d}t = \delta t\, f(t_n) + \mathcal{O}(\delta t^2)$$

and the *local* error associated with the temporal discretisation is $\mathcal{O}(\delta t^2)$, and hence the *global* error is $\mathcal{O}(\delta t)$: it is *first order in time*.

right-hand rule.

The same is true for the choice $\theta = 1$, which is known as the **backward Euler method**, where

Implicit.

$$\int_{t_n}^{t_{n+1}} f(t)\,\mathrm{d}t = \delta t\, f(t_{n+1}) + \mathcal{O}(\delta t^2).$$

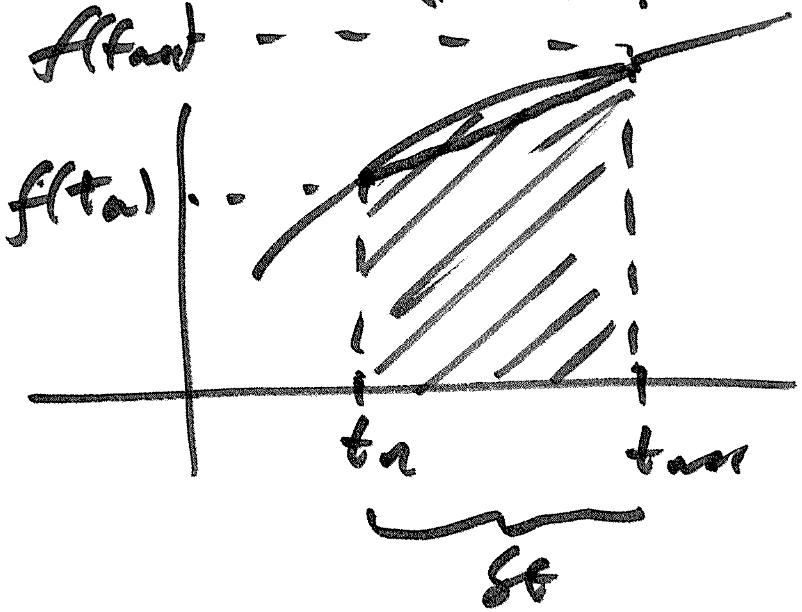
$$\int_{t_n}^{t_{n+1}} f(t)\,dt \simeq \delta t\left[(1-\theta)f(t_n)+\theta f(t_{n+1})\right]$$

$0 \leq \theta \leq 1$

$\theta = 0: \quad \simeq \delta t\, f(t_n) \leftarrow$ left-hand rule

$\theta = 1: \quad \simeq \delta t\, f(t_{n+1}) \leftarrow$ right-hand rule

$\theta = 1/2: \quad \simeq \frac{\delta t}{2}\left[f(t_n)+f(t_{n+1})\right]$



1940's

For the choice $\theta = 1/2$, known as the **Crank-Nicolson method**, we have that

$\theta = 1/2$

$$\int_{t_n}^{t_{n+1}} f(t)\,\mathrm{d}t = \frac{\delta t}{2}\left(f(t_n) + f(t_{n+1})\right) + \mathcal{O}(\delta t^3)$$

and the *local* error associated with the temporal discretisation is $\mathcal{O}(\delta t^3)$, and hence the *global* error is $\mathcal{O}(\delta t^2)$: it is *second order in time*.

The fact that we have used two values θ_1 and θ_2 in (12) emphasises that different methods can be used for different terms.

For example, one might use $\theta_1 = 1$ (backward Euler) for the flux term, and $\theta_2 = 0$ (forward Euler) for the source term.

This approach is sometimes called an **IMEX method** (short for implicit-explicit).

Note

It is conventional, as we have done, to use subscripts for spatial indices and superscripts for temporal indices. Do not interpret the superscript *n* as a power – it is not.

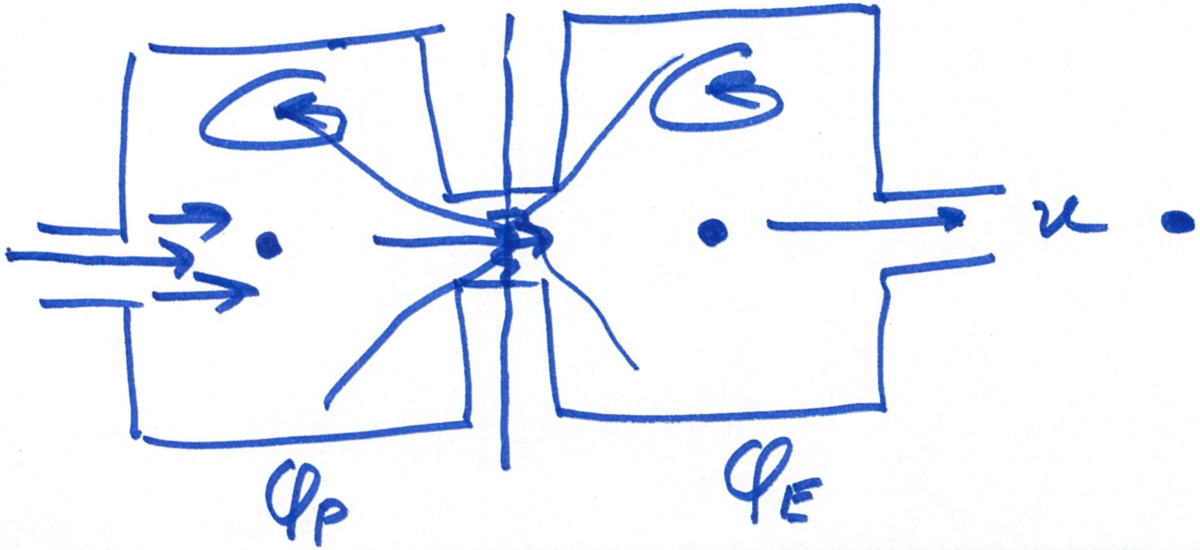
φ_p^{k+1}

Advection-diffusion Equation

We now consider the linear *advection-diffusion equation with source term*:

$$\frac{\partial \varphi}{\partial t} + \frac{\partial}{\partial x}\underbrace{\left(\boxed{u\varphi} - D\frac{\partial \varphi}{\partial x}\right)}_{J} = S \qquad 0 < x < L, \quad t > 0 \qquad (14)$$

subject to the same initial and boundary conditions as before. $u \approx$



$\varphi_e = \frac{1}{2}(\varphi_E + \varphi_P)$

$u \gg$

$\varphi_e = \varphi_P$