Computational Mathematics 2

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Contents

1 The Transport Equation

1.1 Transport Phenomena

Transport phenomena broadly comprises three disciplines; fluid dynamics, heat transfer, and mass transfer. **Fluid dynamics** is the study of the motion of fluids, including liquids and gases. **Heat transfer** is the study of how heat (thermal energy) is transported, generated, dissipated, and/or converted in a physical system. **Mass transfer** is the study of the movement of mass from one location to another.
The mathematical equations used to describe the above phenomena involve three fundamental mechanisms of transport:

1. Diffusion
2. Advection
3. Reaction

1.1.1 Diffusion

Diffusion is the gradual movement of a substance from regions of high concentration to regions of low concentration. The direction of diffusion is determined by the sign of the negative gradient of the concentration.

1.1.2 Advection

Advection is the transport of a substance by bulk motion of a fluid. Advection is driven by a vector field in which the substance is transported.

1.1.3 Reaction

Reaction is the process in which substances are created or destroyed. Reaction is represented as a source or sink function.

1.2 Transport Equation

The general form of the transport equation is given by

$$\underbrace{\frac{\partial u}{\partial t}}_{\text{unsteady term}} + \underbrace{\boldsymbol{\nabla} \cdot (\mathbf{v}u)}_{\text{advection term}} = \underbrace{\boldsymbol{\nabla} \cdot (\mathbf{D}\boldsymbol{\nabla} u)}_{\text{diffusion term}} + \underbrace{R}_{\text{reaction term}}$$

where $u(\mathbf{x},\ t)$ is the quantity being transported at position $\mathbf{x}$ and time t, $\mathbf{v}(\mathbf{x},\ t) \in \mathbb{R}^n$ is a velocity vector field which drives u, $\mathbf{D} \in \mathbb{R}^{n\times n}$ is the diffusion matrix, and R is a reaction term. n represents the dimension of the spatial domain of the problem, which can be 1, 2, or 3.
An alternative form of the transport equation combines the divergence terms

$$\underbrace{\frac{\partial u}{\partial t}}_{\text{unsteady term}} + \underbrace{\boldsymbol{\nabla} \cdot \mathbf{q}}_{\text{flux term}} = \underbrace{R}_{\text{reaction term}}$$

where $\mathbf{q} = \mathbf{v}u - \mathbf{D}\boldsymbol{\nabla} u$ is the *flux vector*.

1.2.1 Domain

This PDE is defined on a specified domain Ω which is an open connected subset of $\mathbb{R}^n$, with the boundary $\partial\Omega$.

1.2.2 Derivation

The transport equation can be derived from the conservation of mass principle: the rate of change of the quantity u within a region D must be balanced by the net flow of u in/out of the boundary ∂D of D, and the rate of creation or destruction of u within D. Consider an arbitrarily small sub-domain D of Ω with boundary ∂D, then:

$$\begin{aligned}
\left\{\begin{array}{c}\text{Rate of change}\\ \text{of } u \text{ in } D\end{array}\right\} &= -\left\{\begin{array}{c} u \text{ leaving } D\\ \text{across } \partial D\end{array}\right\} + \left\{\begin{array}{c}\text{Generation/Destruction}\\ \text{of } u \text{ within } D\end{array}\right\}\\
\frac{\mathrm{d}}{\mathrm{d}t}\int_D u\,\mathrm{d}V &= -\int_{\partial D}\mathbf{q}\cdot\mathbf{n}\,\mathrm{d}s + \int_D R\,\mathrm{d}V\\
\int_D \frac{\partial u}{\partial t}\,\mathrm{d}V &= -\int_D \boldsymbol{\nabla}\cdot\mathbf{q}\,\mathrm{d}V + \int_D R\,\mathrm{d}V\\
\int_D\left(\frac{\partial u}{\partial t} + \boldsymbol{\nabla}\cdot\mathbf{q} - R\right)\mathrm{d}V &= 0\\
\frac{\partial u}{\partial t} + \boldsymbol{\nabla}\cdot\mathbf{q} &= R.
\end{aligned}$$

1.3 Special Cases

1.3.1 One Spatial Dimension

In one spatial dimension, the transport equation reduces to

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}(vu) = \frac{\partial}{\partial x}\left(D\frac{\partial u}{\partial x}\right) + R.$$

where $u(x,\, t)$ is a function of one spatial dimension and time, v is the velocity, and $D > 0$ is the diffusivity.

1.3.2 Two Spatial Dimensions

In two spatial dimensions, the transport equation reduces to

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}(v_x u) + \frac{\partial}{\partial y}(v_y u) = \frac{\partial}{\partial x}\left(D_{xx}\frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_{yy}\frac{\partial u}{\partial y}\right) + R.$$

where $u(x,\, y,\, t)$ is a function of two spatial dimensions and time, v_x and v_y are the velocities in the x and y directions, and D_{xx} and D_{yy} are the diffusivities in the x and y directions.

1.3.3 Eliminating Terms

The transport equation is also called the *advection-diffusion-reaction equation*.

- If the *velocity term* $\mathbf{v}$ is the zero vector, the equation reduces to the *diffusion-reaction equation*.
- If the *diffusion term* $\mathbf{D}$ is the zero matrix, the equation reduces to the *advection-reaction equation*.
- If the *reaction term* R is zero, the equation reduces to the *advection-diffusion equation*.

1.4 Classification

While the terms in the transport equation may be constant or variable, certain combinations of these terms lead to different solution methods.

- The velocity vector $\mathbf{v}$ may be a constant vector or a function of space $\mathbf{x}$, time t, and/or the solution u.
- The diffusion matrix $\mathbf{D}$ may be a constant matrix or a function of space $\mathbf{x}$, time t, and/or the solution u.
- The reaction term R may be a constant or a function of space $\mathbf{x}$, time t, and/or the solution u.

When $\mathbf{v}$ and $\mathbf{D}$ are <u>not</u> functions of u, and R is a <u>linear</u> function of u, the transport equation is called *linear*. The equation is *nonlinear* otherwise. The domain Ω is called *heterogeneous* if any of the coefficients $\mathbf{v}$, $\mathbf{D}$, or R are functions of space $\mathbf{x}$, and *homogeneous* otherwise.

1.5 Dimensional Analysis

Performing a dimensional analysis on the transport equation allows us to associate physical units with the coefficients of the equation. This analysis is useful for verifying the correctness of the equation and for scaling the equation to a dimensionless form. The terms in the equation

$$\frac{\partial u}{\partial t} + \boldsymbol{\nabla} \cdot (\mathbf{v} u) = \boldsymbol{\nabla} \cdot (\mathbf{D} \boldsymbol{\nabla} u) + R$$

may only be added or subtracted if they have the same units. Therefore, given that

$$\left[\frac{\partial u}{\partial t}\right] \equiv \frac{[u]}{[t]} = \frac{[u]}{\mathsf{T}}$$

we can deduce the units of other terms in the equation.

$$\begin{aligned}
[\boldsymbol{\nabla} \cdot (\mathbf{v} u)] \equiv \frac{[\mathbf{v}]\,[u]}{[x]} &= \frac{[u]}{\mathsf{T}} \implies [\mathbf{v}] = \frac{\mathsf{L}}{\mathsf{T}} \\
[\boldsymbol{\nabla} \cdot (\mathbf{D} \boldsymbol{\nabla} u)] \equiv \frac{[\mathbf{D}]\,[\boldsymbol{\nabla} u]}{[x]} = \frac{[\mathbf{D}]\,[u]}{[x]^2} &= \frac{[u]}{\mathsf{T}} \implies [\mathbf{D}] = \frac{\mathsf{L}^2}{\mathsf{T}} \\
[R] &\equiv \frac{[u]}{[t]} \implies [R] = \frac{[u]}{\mathsf{T}}
\end{aligned}$$

1.6 Initial and Boundary Conditions

In addition to the transport equation, which describes the behaviour of u within the domain Ω, the problem must also specify how u behaves at the boundary $\partial\Omega$ with *boundary conditions*. Some common boundary conditions include:

- Specified value: $u(\mathbf{x},\, t) = u_b$ on $\partial\Omega$
- Specified flux: $\mathbf{q} \cdot \mathbf{n} = q_b$ on $\partial\Omega$
- Specified gradient: $\boldsymbol{\nabla} u \cdot \mathbf{n} = d_b$ on $\partial\Omega$

Here u_b, q_b, and d_b may be constants or scalar functions of $\mathbf{x}$ and/or t, and $\mathbf{n}$ is the unit normal vector to $\partial\Omega$, directed outward from Ω.
We may also wish to use a Robin condition to describe a general boundary condition of the form:

$$au + b\left(\boldsymbol{\nabla} u \cdot \mathbf{n}\right) = c$$

where a, b, and c are constants or scalar functions of $\mathbf{x}$ and/or t. When $c = 0$, the condition is called *homogeneous*, and *nonhomogeneous* otherwise.
In addition to these conditions, an *initial condition* is required to specify the profile of u at time $t = 0$.

1.7 Steady-State Problems

If it exists, the *steady-state solution* of the transport equation is the solution of the equation when the time-derivative of u is zero:

$$\frac{\partial u}{\partial t} = 0.$$

The steady-state solution is useful for understanding the long-term behaviour of the system, where it is assumed that the system is no longer time-dependent. The steady-state solution is expressed as $u_\infty = \lim_{t\to\infty} u(\mathbf{x},\, t)$.

2 Finite Volume Method

The *Finite Volume Method* (FVM) is a method for solving the transport equation at discrete points (nodes) in space: $u_i(t) \approx u(\mathbf{x}_i,\, t)$ for $i = 1,\, 2,\, \dots,\, N$. FVM is a *spatial discretisation* method that converts a spatially-continuous initial-boundary value problem to a satially-discrete initial-value problem.
The FVM is used in transport phenomena because the approximate solution obeys the laws of conservation of mass and energy. This is generally not true for finite differences or finite element methods. FVM also has the advantage of being able to handle complex geometries and irregular grids.

2.1 Discretising the Domain

The basic geometric structure used in the FVM is called the **mesh**. A mesh is a partitioning of the domain Ω into smaller sub-domains called **elements**. The intersection of edges in this mesh are called **vertices**. An example of a 1D mesh is shown below.

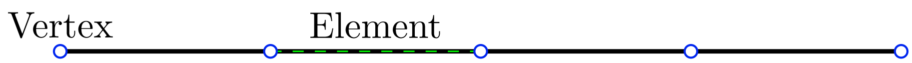
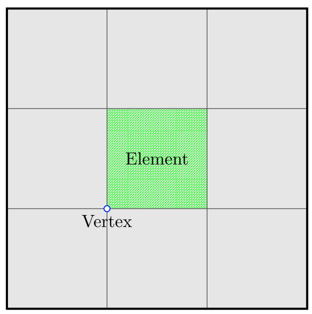
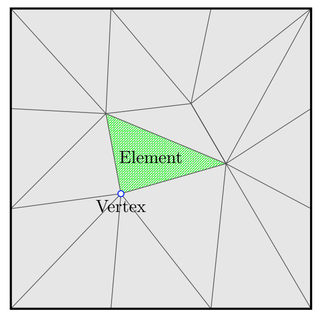


Figure 1: 1D mesh.

In two and three dimensions, the mesh may be either *structured* or *unstructured* as shown below. Unstructured meshes typically consist of triangles (or tetrahedra in 3D).



(a) 2D structured mesh.



(b) 2D unstructured mesh.

The FVM defines:

- **Nodes $\mathbf{x}_i$**, at which the solution is approximated by u_i
- **Control volumes Ω_i**, over which the conservation principle is applied

where $i = 1, 2, \dots, N$ is the index of the nodes. There are several ways to define the control volumes. Two common approaches are:

- **Cell-Centred Control Volumes**: Nodes are positioned at the centroids of elements, and control volumes are defined over elements.
- **Vertex-Centred Control Volumes**: Nodes are positioned at vertices, and control volumes are constructed using the centroids of adjacent element boundaries.

This is illustrated in 1D and 2D in the following figures.

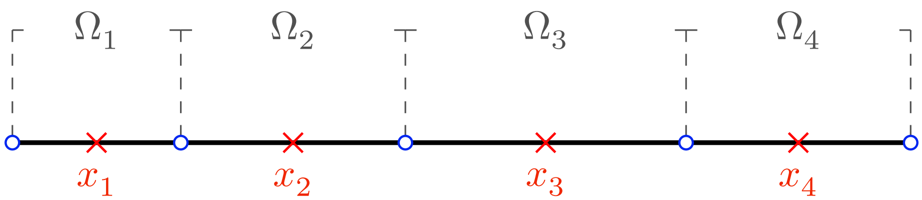


Figure 3: 1D mesh with cell-centred control volumes.

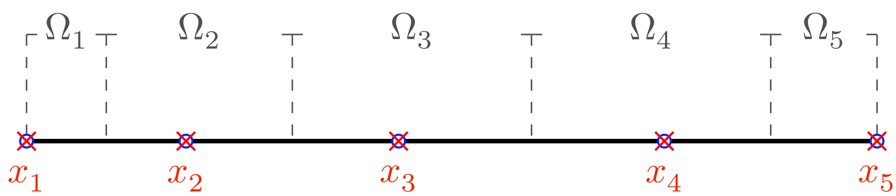
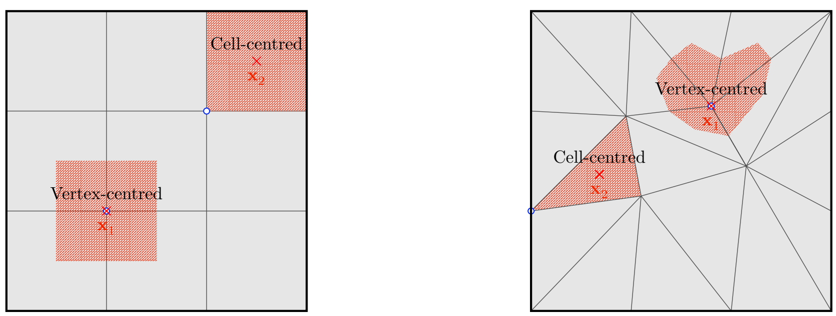


Figure 4: 1D mesh with vertex-centred control volumes.



(a) 2D structured mesh with vertex-/cell-centred control volumes.

(b) 2D unstructured mesh with vertex-/cell-centred control volumes.

For problems in three dimensions using structured meshes, control volumes are cubes (or rectangular prisms). For unstructured meshes with control volumes using the cell-centred approach, elements themselves are used as control volumes. For the vertex-centred approach, control volume boundaries are defined using the centroids of adjacent element boundaries.

2.2 General Strategy

Consider a mesh with N nodes and N control volumes:

1. Label the nodes x_1, x_2, ..., x_N and the unknowns u_1, u_2, ..., u_N.
2. Identify the control volume types (interior node, boundary node).

3. Integrate the transport equation over each control volume and apply the Divergence theorem to the flux term.
4. Incorporate the boundary conditions to approximate/discretise all remaining terms.

To discretise the transport equation, let us integrate the transport equation over each control volume Ω_i:

$$\frac{\partial u}{\partial t} + \boldsymbol{\nabla} \cdot \mathbf{q} = R$$
$$\int_{\Omega_i} \frac{\partial u}{\partial t} \, \mathrm{d}V + \int_{\Omega_i} (\boldsymbol{\nabla} \cdot \mathbf{q}) \, \mathrm{d}V = \int_{\Omega_i} R \, \mathrm{d}V$$

Applying the divergence theorem to the flux term, we have

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\Omega_i} u \, \mathrm{d}V + \int_{\partial \Omega_i} (\mathbf{q} \cdot \mathbf{n}) \, \mathrm{d}s = \int_{\Omega_i} R \, \mathrm{d}V$$

where $\partial \Omega_i$ is the control volume boundary of Ω_i, and $\mathbf{n}$ is the outward unit vector normal to $\partial \Omega_i$, directed out of Ω_i. Consider the spatial average of u and R over Ω_i:

$$\bar{u}_i = \frac{1}{V_i} \int_{\Omega_i} u \, \mathrm{d}V, \qquad \bar{R}_i = \frac{1}{V_i} \int_{\Omega_i} R \, \mathrm{d}V$$

where V_i is the volume of Ω_i. Using this quantity, we can rewrite the transport equation as

$$\frac{\mathrm{d}\bar{u}_i}{\mathrm{d}t} + \frac{1}{V_i} \int_{\partial \Omega_i} (\mathbf{q} \cdot \mathbf{n}) \, \mathrm{d}s = \bar{R}_i.$$

We can now approximate this ODE using the discrete approximations, u_i and R_i, at each node $\mathbf{x}_i$.

$$\frac{\mathrm{d}u_i}{\mathrm{d}t} = -\frac{1}{V_i} \int_{\partial \Omega_i} (\mathbf{q} \cdot \mathbf{n}) \, \mathrm{d}s + R_i$$

2.3 FVM in 1D

Before we consider the 1D case for the FVM, let us define the following geometric quantities (for the vertex-centred control volume strategy):

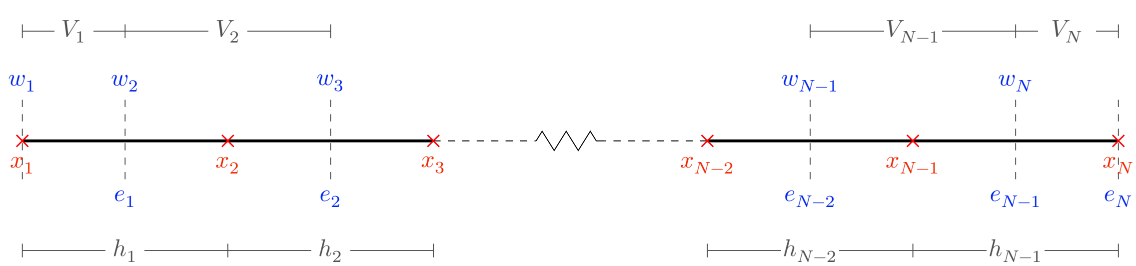


Figure 6: 1D FVM.

where

- $\Omega = (x_1, x_N)$
- $\Omega_i = (w_i, e_i)$ is the control volume for node i
- h_i is the spacing between nodes i and $i+1$

$$h_i = x_{i+1} - x_i \quad \text{for } i = 1,\ \dots,\ N-1$$

- V_i is the volume of control volume Ω_i

$$V_i = \begin{cases} \dfrac{h_1}{2}, & i = 1 \\ \dfrac{h_{i-1} + h_i}{2}, & 2 \leqslant i \leqslant N-1 \\ \dfrac{h_{N-1}}{2}, & i = N \end{cases}$$

- w_i and e_i are the west and east boundaries of control volume Ω_i

$$w_i = \begin{cases} x_1, & i = 1 \\ \dfrac{x_{i-1} + x_i}{2}, & 2 \leqslant i \leqslant N \end{cases}$$
$$e_i = \begin{cases} \dfrac{x_i + x_{i+1}}{2}, & 1 \leqslant i \leqslant N-1 \\ x_N, & i = N \end{cases}$$

Then, if we integrate over all control volumes Ω_i in 1D, the spatial averages simplify to:

$$\bar{u}_i = \frac{1}{V_i} \int_{w_i}^{e_i} u \, \mathrm{d}x, \qquad \bar{R}_i = \frac{1}{V_i} \int_{w_i}^{e_i} R \, \mathrm{d}x$$

likewise, the flux term becomes,

$$\begin{aligned} \int_{\Omega_i} (\boldsymbol{\nabla} \cdot \mathbf{q}) \, \mathrm{d}V &= \int_{w_i}^{e_i} \frac{\partial q}{\partial x} \, \mathrm{d}x \\ &= q_{e_i} - q_{w_i} \end{aligned}$$

Then using the strategy outlined in the previous section, we find:

$$\frac{\mathrm{d}u_i}{\mathrm{d}t} = \frac{1}{V_i} \left(q_{w_i} - q_{e_i} \right) + R_i$$

where $u_i \approx \bar{u}_i$ and $R_i \approx \bar{R}_i$. This equation can now be used to solve an initial-boundary value problem using the FVM. This is done by applying the finite-difference method at internal nodes, using:

$$\begin{aligned} \frac{\partial u}{\partial x} (w_i,\ t) &= \frac{u_i - u_{i-1}}{h_{i-1}} \\ \frac{\partial u}{\partial x} (e_i,\ t) &= \frac{u_{i+1} - u_i}{h_i} \end{aligned}$$

and at boundary nodes, using the boundary conditions:

$$\frac{\partial u}{\partial x}(w_1,\, t) = \frac{\partial u}{\partial x}(0,\, t) \qquad \frac{\partial u}{\partial x}(e_1,\, t) = \frac{u_2 - u_1}{h_1} \qquad \text{(left boundary)}$$
$$\frac{\partial u}{\partial x}(w_N,\, t) = \frac{u_N - u_{N-1}}{h_{N-1}} \qquad \frac{\partial u}{\partial x}(e_N,\, t) = \frac{\partial u}{\partial x}(L,\, t) \qquad \text{(right boundary)}$$

we find a linear ODE of the form:

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \mathbf{A}\mathbf{u} + \mathbf{b}(t), \qquad \mathbf{u}(0) = \mathbf{u}^{(0)}$$

where $\mathbf{u} = (u_1,\, \dots,\, u_N)^\top$ is the numerical solution vector at time t containing the solution at each node x_i and $\mathbf{u}^{(0)} = (f(x_1),\, \dots,\, f(x_N))^\top$ is the initial solution vector.
$\mathbf{A} \in \mathbb{R}^{N\times N}$ is a tridiagonal matrix containing the coefficients of the finite-difference method, and $\mathbf{b}(t)$ contains any time-dependent terms in the transport equation. This ODE can be solved using standard ODE solving techniques. When the transport equation is nonlinear, the RHS cannot be written as a matrix-vector product, so that

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \mathbf{F}(t,\, \mathbf{u}(t)).$$

2.4 Time Discretisation

The resulting ODE can be solved using a time-stepping method such as the Forward Euler, the Backward Euler, or the Crank-Nicolson methods. To solve this initial value problem, we will consider a sufficiently large final time, T, so that the problem is solved between $t = 0$ and $t = T$. Then, we will discretise the time domain into M time steps of size $\delta t = T/M = t_{n+1} - t_n$, such that $t_n = n\,\delta t$ for $n = 0,\, 1,\, \dots,\, M$.
Let us rewrite the ODE in the equivalent form:

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \mathbf{A}\mathbf{u} + \mathbf{b}_1 + \mathbf{b}_2(t), \qquad \mathbf{u}(0) = \mathbf{u}^{(0)}$$

such that $\mathbf{b}_2(t) = (R(x_1,\, t),\, \dots,\, R(x_N,\, t))^\top$ is the time-dependent flux term, and $\mathbf{b}_1 = \mathbf{b}(t) - \mathbf{b}_2(t)$ contains the time-independent reaction term. We will now compute $\mathbf{u}^{(n)} = \left(u_1^{(n)},\, \dots,\, u_N^{(n)}\right)^\top$, where $u_i^{(n)} \approx u_i(t_n) = u(x_i,\, t_n)$, is the solution at $x = x_i$ and time $t = t_n$, using the θ-method.
Let us first integrate the ODE over the time interval (t_n, t_{n+1}):

$$\begin{aligned}
\int_{t_n}^{t_{n+1}} \frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t}\,\mathrm{d}t &= \int_{t_n}^{t_{n+1}} (\mathbf{A}\mathbf{u} + \mathbf{b}_1 + \mathbf{b}_2(t))\,\mathrm{d}t \\
\mathbf{u}(t_{n+1}) - \mathbf{u}(t_n) &= \mathbf{A}\int_{t_n}^{t_{n+1}} \mathbf{u}\,\mathrm{d}t + \int_{t_n}^{t_{n+1}} \mathbf{b}_1\,\mathrm{d}t + \int_{t_n}^{t_{n+1}} \mathbf{b}_2(t)\,\mathrm{d}t \\
\mathbf{u}^{(n+1)} - \mathbf{u}^{(n)} &= \mathbf{A}\int_{t_n}^{t_{n+1}} \mathbf{u}\,\mathrm{d}t + \mathbf{b}_1(t_{n+1} - t_n) + \int_{t_n}^{t_{n+1}} \mathbf{b}_2(t)\,\mathrm{d}t
\end{aligned}$$

To integrate the time-dependent terms, we will use the weighted θ approximation, where

$$\int_{t_n}^{t_{n+1}} f(t)\,\mathrm{d}t \approx \delta t\left[(1-\theta) f(t_n) + \theta f(t_{n+1})\right].$$

Therefore, we have

$$\begin{aligned}
\mathbf{u}^{(n+1)} - \mathbf{u}^{(n)} &= \delta t\mathbf{A}\left[(1-\theta_1)\,\mathbf{u}^{(n)} + \theta_1\mathbf{u}^{(n+1)}\right] + \mathbf{b}_1\,\delta t + \delta t\left[(1-\theta_2)\,\mathbf{b}_2^{(n)} + \theta_2\mathbf{b}_2^{(n+1)}\right] \\
\mathbf{u}^{(n+1)} - \mathbf{A}\theta_1\,\delta t\mathbf{u}^{(n+1)} &= \mathbf{u}^{(n)} + \delta t\,(1-\theta_1)\,\mathbf{A}\mathbf{u}^{(n)} + \delta t\mathbf{b}_1 + \delta t\left[(1-\theta_2)\,\mathbf{b}_2^{(n)} + \theta_2\mathbf{b}_2^{(n+1)}\right] \\
(\mathbf{I} - \delta t\theta_1\mathbf{A})\,\mathbf{u}^{(n+1)} &= \left[\mathbf{I} + \delta t\,(1-\theta_1)\,\mathbf{A}\right]\mathbf{u}^{(n)} + \delta t\left[\mathbf{b}_1 + (1-\theta_2)\,\mathbf{b}_2^{(n)} + \theta_2\mathbf{b}_2^{(n+1)}\right] \\
\tilde{\mathbf{A}}\mathbf{u}^{(n+1)} &= \tilde{\mathbf{b}}
\end{aligned}$$

for two choices of θ_1 and θ_2. Setting $\theta_1 = \theta_2 = 0$, we obtain the Forward Euler method:

$$\mathbf{u}^{(n+1)} = (\mathbf{I} + \delta t\mathbf{A})\,\mathbf{u}^{(n)} + \delta t\left(\mathbf{b}_1 + \mathbf{b}_2^{(n)}\right)$$

which is an explicit method. Setting $\theta_1 = \theta_2 = 1$, yields the Backward Euler method:

$$(\mathbf{I} - \delta t\mathbf{A})\,\mathbf{u}^{(n+1)} = \mathbf{u}^{(n)} + \delta t\left(\mathbf{b}_1 + \mathbf{b}_2^{(n+1)}\right)$$

while setting $\theta_1 = \theta_2 = \frac{1}{2}$ gives the Crank-Nicolson method:

$$\left(\mathbf{I} - \frac{\delta t}{2}\mathbf{A}\right)\mathbf{u}^{(n+1)} = \left(\mathbf{I} + \frac{\delta t}{2}\mathbf{A}\right)\mathbf{u}^{(n)} + \frac{\delta t}{2}\left(2\mathbf{b}_1 + \mathbf{b}_2^{(n)} + \mathbf{b}_2^{(n+1)}\right)$$

which are both implicit methods. Using different values for θ_1 and θ_2 is also possible, and is called the IMEX method (Implicit-Explicit).

2.5 Time Discretisation for the 1D FVM

We can apply the same time discretisation to the 1D FVM. Let us consider the 1D FVM with the following ODE:

$$\frac{\mathrm{d}u_i}{\mathrm{d}t} = \frac{1}{V_i}\left(q_{w_i} - q_{e_i}\right) + R_i$$

where $u_i \approx \bar{u}_i$ and $R_i \approx \bar{R}_i$. We will now compute $u_i^{(n)} = u_i(t_n) = u(x_i,\, t_n)$ using the θ-method. We will first integrate the ODE over the time interval (t_n, t_{n+1}):

$$\begin{aligned}
\int_{t_n}^{t_{n+1}} \frac{\mathrm{d}u_i}{\mathrm{d}t}\,\mathrm{d}t &= \int_{t_n}^{t_{n+1}} \left(\frac{1}{V_i}\left(q_{w_i} - q_{e_i}\right) + R_i\right)\mathrm{d}t \\
u_i(t_{n+1}) - u_i(t_n) &= \frac{1}{V_i}\int_{t_n}^{t_{n+1}} q_{w_i} - q_{e_i}\,\mathrm{d}t + \int_{t_n}^{t_{n+1}} R_i\,\mathrm{d}t \\
u_i^{(n+1)} - u_i^{(n)} &= \frac{\delta t}{V_i}\left[(1-\theta_1)\left(q_{w_i}^{(n)} - q_{e_i}^{(n)}\right) + \theta_1\left(q_{w_i}^{(n+1)} - q_{e_i}^{(n+1)}\right)\right] \\
&\quad + \delta t\left[(1-\theta_2)\,R_i^{(n)} + \theta_2 R_i^{(n+1)}\right]
\end{aligned}$$

2.6 Dirichlet Boundary Conditions

Given the above linear system, we can also modify the system to account for Dirichlet boundary conditions rather than Neumann boundary conditions by replacing the first row of the matrix $\tilde{\mathbf{A}}$ with $(1, 0, \ldots, 0)^\top \in \mathbb{R}^{1\times N}$ and the first element of the RHS vector $\tilde{\mathbf{b}}$ with the Dirichlet boundary condition.