Computational Mathematics 2

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Contents

1 Finite Volume Methods

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 $u_\infty = \lim_{t\to\infty} u(\mathbf{x},\, t)$.