Chapter 2
Review of Vector Calculus

Abstract This chapter sets the ground for the derivation of the conservation
equations by providing a brief review of the continuum mechanics tools needed for
that purpose while establishing some of the mathematical notations and procedures
that will be used throughout the book. The review is by no mean comprehensive
and assumes a basic knowledge of the fundamentals of continuum mechanics.
A short introduction of the elements of linear algebra including vectors, matrices,
tensors, and their practices is given. The chapter ends with an examination of the
fundamental theorems of vector calculus, which constitute the elementary building
blocks needed for manipulating and solving these conservation equations either
analytically or numerically using computational fluid dynamics.

2.1 Introduction

The transfer phenomena of interest here can be mathematically represented by
equations involving physical variables that fall under three categories: scalars,
vectors, and tensors [1–3]. Throughout this book scalars are designated by lightface
italic, vectors by lower boldface Roman, and tensors by boldface Greek letters. In
addition, matrices are identified by upper boldface Roman letters.

A scalar represents a quantity that has magnitude such as volume \( V \), pressure \( p \),
temperature \( T \), time \( t \), mass \( m \), and density \( \rho \). A vector represents a quantity of a
given magnitude and direction such as velocity \( \mathbf{v} \), momentum \( \mathbf{L} = m\mathbf{v} \), and force \( \mathbf{F} \).
A matrix is a rectangular array of quantities ordered along rows and columns.
A tensor is a mathematical object analogous to but more general than a vector,
represented by an array of components, such as the shear stress tensor. Moreover,
the conservation equations are composed of terms that represent the product of two
or more variables. The multiplication involved may be of various types to be
detailed later and the variables could be a combination of the three types described
above. Whenever the multiplication results in a scalar, the product will be enclosed
by parentheses “(product)”, if it results in a vector it will be enclosed by square brackets “[product]”, and if it results in a tensor it will be enclosed by curly brackets “{product}”.

2.2 Vectors and Vector Operations

The most frequently used vector in fluid dynamics is the velocity vector that will be designated by \( \mathbf{v} \). The components of the velocity vector in a three-dimensional Cartesian coordinate system will be denoted by \( u, v, \) and \( w \) in the \( x \), \( y \), and \( z \) direction, respectively (Fig. 2.1). In Cartesian coordinates, \( \mathbf{v} \) is written as

\[
\mathbf{v} = u \mathbf{i} + v \mathbf{j} + w \mathbf{k}
\]

(2.1)

where \( \mathbf{i}, \mathbf{j}, \) and \( \mathbf{k} \) are unit vectors in the \( x \), \( y \), and \( z \) direction, respectively. A vector is usually presented in a column format with its transpose, denoted with a superscript \( T \), in a row format as

\[
\mathbf{v} = \begin{bmatrix} u \\ v \\ w \end{bmatrix} \quad \mathbf{v}^T = [u \quad v \quad w]
\]

(2.2)

The magnitude of a vector is given by

\[
\|\mathbf{v}\| = \sqrt{u^2 + v^2 + w^2}
\]

(2.3)

The sum of two vectors \( \mathbf{v}_1 \) and \( \mathbf{v}_2 \) is the sum of their components, i.e.,

\[
\mathbf{v}_1 = u_1 \mathbf{i} + v_1 \mathbf{j} + w_1 \mathbf{k} \quad \mathbf{v}_2 = u_2 \mathbf{i} + v_2 \mathbf{j} + w_2 \mathbf{k}
\]

\[
\Rightarrow \mathbf{v}_1 + \mathbf{v}_2 = (u_1 + u_2)\mathbf{i} + (v_1 + v_2)\mathbf{j} + (w_1 + w_2)\mathbf{k}
\]

(2.4)

Fig. 2.1 The components of a vector \( \mathbf{v} \) in a three-dimensional Cartesian coordinate system.
or

\[ \mathbf{v}_1 = \begin{bmatrix} u_1 \\ v_1 \\ w_1 \end{bmatrix} \quad \mathbf{v}_2 = \begin{bmatrix} u_2 \\ v_2 \\ w_2 \end{bmatrix} \Rightarrow \mathbf{v}_1 + \mathbf{v}_2 = \begin{bmatrix} u_1 + u_2 \\ v_1 + v_2 \\ w_1 + w_2 \end{bmatrix} \]  \hspace{1cm} (2.5)

The multiplication of a vector \( \mathbf{v} \) by a scalar \( s \) results in the vector \( s\mathbf{v} \) such that

\[ s\mathbf{v} = s(u\mathbf{i} + v\mathbf{j} + w\mathbf{k}) = su\mathbf{i} + sv\mathbf{j} + sw\mathbf{k} = \begin{bmatrix} su \\ sv \\ sw \end{bmatrix} \]  \hspace{1cm} (2.6)

The product of two vectors is not as straightforward. When multiplying a vector \( \mathbf{v}_1 \) by another vector \( \mathbf{v}_2 \) two types of multiplications arise [4–6]. The first is denoted by the scalar or dot product, \( \mathbf{v}_1 \cdot \mathbf{v}_2 \), and the second by vector or cross product \( \mathbf{v}_1 \times \mathbf{v}_2 \).

### 2.2.1 The Dot Product of Two Vectors

By definition, the dot product of two vectors \( \mathbf{v}_1 \) and \( \mathbf{v}_2 \) is a scalar quantity given by

\[ \mathbf{v}_1 \cdot \mathbf{v}_2 = \|\mathbf{v}_1\|\|\mathbf{v}_2\|\cos(\mathbf{v}_1, \mathbf{v}_2) \]  \hspace{1cm} (2.7)

where \( \cos(\mathbf{v}_1, \mathbf{v}_2) \) denotes the cosine of the angle between \( \mathbf{v}_1 \) and \( \mathbf{v}_2 \). From the definition of the vector dot product, it follows that

\[ \mathbf{i} \cdot \mathbf{i} = \mathbf{j} \cdot \mathbf{j} = \mathbf{k} \cdot \mathbf{k} = 1 \]
\[ \mathbf{i} \cdot \mathbf{j} = \mathbf{j} \cdot \mathbf{i} = \mathbf{k} \cdot \mathbf{i} = \mathbf{k} \cdot \mathbf{j} = 0 \]  \hspace{1cm} (2.8)

In terms of orthonormal Cartesian components, the dot product of the two vectors \( \mathbf{v}_1 \) and \( \mathbf{v}_2 \) can be calculated as

\[ \mathbf{v}_1 \cdot \mathbf{v}_2 = (u_1\mathbf{i} + v_1\mathbf{j} + w_1\mathbf{k}) \cdot (u_2\mathbf{i} + v_2\mathbf{j} + w_2\mathbf{k}) = u_1u_2 + v_1v_2 + w_1w_2 \]  \hspace{1cm} (2.9)

### 2.2.2 Vector Magnitude

From Eq. (2.9) it follows that the magnitude of a vector \( \mathbf{v} \) can be obtained as

\[ \|\mathbf{v}\| = \sqrt{\mathbf{v} \cdot \mathbf{v}} = \sqrt{u^2 + v^2 + w^2} \]  \hspace{1cm} (2.10)
2.2.3 The Unit Direction Vector

A unit vector \( \mathbf{e}_v \) in the direction of \( \mathbf{v} \) can be derived from the definition of the dot product as

\[
\mathbf{v} \cdot \mathbf{v} = \| \mathbf{v} \| \| \mathbf{v} \| \cos(\mathbf{v}, \mathbf{v}) = \| \mathbf{v} \|^2 \Rightarrow \mathbf{v} \cdot \frac{\mathbf{v}}{\| \mathbf{v} \|} = \| \mathbf{v} \| \]

\[
\mathbf{v} \cdot \mathbf{e}_v = \| \mathbf{v} \| \| \mathbf{e}_v \| \cos(\mathbf{v}, \mathbf{e}_v) = \| \mathbf{v} \| \Rightarrow \mathbf{v} \cdot \mathbf{e}_v = \| \mathbf{v} \| = \| \mathbf{e}_v \| = \frac{\mathbf{v}}{\| \mathbf{v} \|}
\]

Therefore the component of a vector in the direction of another vector (i.e., magnitude of the projected length) can be viewed as the dot product of the vector to be projected with the unit direction of the other vector as shown in Fig. 2.2a, b.

2.2.4 The Cross Product of Two Vectors

Whereas the dot product of two vectors \( \mathbf{v}_1 \) and \( \mathbf{v}_2 \) is a scalar quantity, their cross or vector product is a vector \( \mathbf{v}_3 \) normal to the plane formed by the vectors \( \mathbf{v}_1 \) and \( \mathbf{v}_2 \), of magnitude calculated as

\[
\| \mathbf{v}_3 \| = \| \mathbf{v}_1 \times \mathbf{v}_2 \| = \| \mathbf{v}_1 \| \| \mathbf{v}_2 \| \sin(\mathbf{v}_1, \mathbf{v}_2),
\]

and of direction given by the right hand rule. As shown in Fig. 2.3, the magnitude of the cross product of two vectors represents the area of the parallelogram spanned by the two vectors. Since, in addition, the resulting vector is normal to the plane.
formed by the vectors, the cross product of two vectors represents their surface vector.

It is then clear that the cross product of two collinear vectors is zero as they define no area, and that the cross product of two orthogonal unit vectors is a unit vector perpendicular to the two unit vectors. Adopting the right hand rule to define the direction of the resulting vector, the following cross product operations hold:

\[ \mathbf{i} \times \mathbf{i} = \mathbf{j} \times \mathbf{j} = \mathbf{k} \times \mathbf{k} = 0 \]
\[ \mathbf{i} \times \mathbf{j} = \mathbf{k} = -\mathbf{j} \times \mathbf{i} \]
\[ \mathbf{j} \times \mathbf{k} = \mathbf{i} = -\mathbf{k} \times \mathbf{j} \]
\[ \mathbf{k} \times \mathbf{i} = \mathbf{j} = -\mathbf{i} \times \mathbf{k} \]  \hfill (2.13)

Using the above relations, the cross product of two vectors in terms of their Cartesian components is given by

\[
\mathbf{v}_1 \times \mathbf{v}_2 = (u_1 \mathbf{i} + v_1 \mathbf{j} + w_1 \mathbf{k}) \times (u_2 \mathbf{i} + v_2 \mathbf{j} + w_2 \mathbf{k}) \\
= u_1 u_2 \mathbf{i} \times \mathbf{i} + u_1 v_2 \mathbf{i} \times \mathbf{j} + u_1 w_2 \mathbf{i} \times \mathbf{k} \\
+ v_1 u_2 \mathbf{j} \times \mathbf{i} + v_1 v_2 \mathbf{j} \times \mathbf{j} + v_1 w_2 \mathbf{j} \times \mathbf{k} \\
+ w_1 u_2 \mathbf{k} \times \mathbf{i} + w_1 v_2 \mathbf{k} \times \mathbf{j} + w_1 w_2 \mathbf{k} \times \mathbf{k} \\
= u_1 u_2 0 + u_1 v_2 \mathbf{k} + u_1 w_2 (-\mathbf{j}) \\
+ v_1 u_2 (-\mathbf{k}) + v_1 v_2 0 + v_1 w_2 \mathbf{i} \\
+ w_1 u_2 \mathbf{j} + w_1 v_2 (-\mathbf{i}) + w_1 w_2 0 \\
= (v_1 w_2 - v_2 w_1) \mathbf{i} - (u_1 w_2 - u_2 w_1) \mathbf{j} + (u_1 v_2 - u_2 v_1) \mathbf{k} \]  \hfill (2.14)

which can be written using determinant notation as

\[
\mathbf{v}_1 \times \mathbf{v}_2 = \begin{vmatrix}
\mathbf{i} & \mathbf{j} & \mathbf{k} \\
u_1 & v_1 & w_1 \\
u_2 & v_2 & w_2
\end{vmatrix} = \begin{bmatrix}
v_1 w_2 - v_2 w_1 \\
u_2 w_1 - u_1 w_2 \\
u_1 v_2 - u_2 v_1
\end{bmatrix} \]  \hfill (2.15)
Example 1
Compute the area of the triangle formed by points (Fig. 2.4):
P_1(0, 0, 0), P_2(1, 0, 0) and P_3(0.5, 1, 0).

Solution
The surface defined by the triangle \((P_1, P_2, P_3)\) can be computed using the cross product of two sides as

\[
S_{123} = 0.5 \overrightarrow{P_1 P_2} \times \overrightarrow{P_1 P_3}
\]

\[
\overrightarrow{P_1 P_2} = (x_2 - x_1)\hat{i} + (y_2 - y_1)\hat{j} + (z_2 - z_1)\hat{k} = \hat{i}
\]

\[
\overrightarrow{P_1 P_3} = (x_3 - x_1)\hat{i} + (y_3 - y_1)\hat{j} + (z_3 - z_1)\hat{k} = 0.5\hat{i} + \hat{j}
\]

\[
S_{123} = 0.5\hat{i} \times (0.5\hat{i} + \hat{j}) = 0.5\hat{k} \Rightarrow \|S_{123}\| = 0.5
\]

2.2.5 The Scalar Triple Product

In addition, combined products of three vectors \(v_1, v_2,\) and \(v_3\) may arise such as \((v_1 \cdot [v_2 \times v_3]),\) which can be calculated using the following determinant (to be explained later):

\[
(v_1 \cdot [v_2 \times v_3]) = \begin{vmatrix}
  u_1 & v_1 & w_1 \\
  u_2 & v_2 & w_2 \\
  u_3 & v_3 & w_3 \\
\end{vmatrix}
\]

(2.16)

As shown in Fig. 2.5, the absolute value of the scalar triple product represents the volume of the parallelepiped formed by the vectors \(v_1, v_2,\) and \(v_3.\)
Example 2

Compute the volume of the pyramid defined by the points: $P_1(0, 0, 0), P_2(1, 0, 0), P_3(0.5, 1, 0), \text{ and } P_4(0.5, 0.5, 1)$ shown in Fig. 2.6.

Solution

The volume of the pyramid can be computed using the scalar triple product as

\[
V = 0.25 \mathbf{P}_1 \mathbf{P}_4 \cdot \left( \mathbf{P}_1 \mathbf{P}_2 \times \mathbf{P}_1 \mathbf{P}_3 \right)
\]

\[
= 0.25(0.5\mathbf{i} + 0.5\mathbf{j} + \mathbf{k}) \cdot \mathbf{k}
\]

\[
= 0.25
\]

2.2.6 Gradient of a Scalar and Directional Derivatives

An important vector operator, which arises frequently in fluid dynamics, is the “del” (or “nabla”) operator defined as

\[
\nabla = \frac{\partial}{\partial x}\mathbf{i} + \frac{\partial}{\partial y}\mathbf{j} + \frac{\partial}{\partial z}\mathbf{k}
\]  

(2.17)

When the “del” operator is applied on a scalar variable $s$ it results in the gradient of $s$ [7, 8] given by

\[
\nabla s = \frac{\partial s}{\partial x}\mathbf{i} + \frac{\partial s}{\partial y}\mathbf{j} + \frac{\partial s}{\partial z}\mathbf{k}
\]  

(2.18)

Thus the gradient of a scalar field is a vector field indicating that the value of $s$ changes with position in both magnitude and direction.

The projection of $\nabla s$ in a certain direction of unit vector $\mathbf{e}_l$ is given by

\[
\frac{ds}{dl} = \nabla s \cdot \mathbf{e}_l = ||\nabla s|| \cos(\nabla s, \mathbf{e}_l)
\]  

(2.19)

and is called the directional derivative of $s$ along the direction of the unit vector $\mathbf{e}_l$, as schematically depicted in Fig. 2.7. The maximum value of the directional derivative is $||\nabla s||$ and is obtained when $\cos(\nabla s, \mathbf{e}_l) = 1$, that is in the direction of $\nabla s$. Therefore, it can be stated that the gradient of a scalar field $s$ indicates the direction and magnitude of the largest change in $s$ at every point in space. Moreover, $\nabla s$ is normal to the constant $s$ surface that passes through that point.
Example 3
Let \( f(x, y, z) = x^2y + y^2z + z^2x \)

(a) find \( \nabla f \) at point \((3, 2, 0)\).
(b) find the derivative at point \((3, 2, 0)\) along the direction \((1, 2, 2)\).

Solution

(a) \[ \frac{\partial f}{\partial x} = 2xy + z^2 \quad \frac{\partial f}{\partial y} = x^2 + 2yz \quad \frac{\partial f}{\partial z} = y^2 + 2xz \]

\[ \nabla f = (2xy + z^2)i + (x^2 + 2yz)j + (y^2 + 2xz)k \]

Thus

\[ \nabla f\big|_{(3,2,0)} = 12i + 9j + 4k \]

(b) The unit vector along direction \((1, 2, 2)\) is

\[ \mathbf{e}_l = \frac{1i + 2j + 2k}{\sqrt{1^2 + 2^2 + 2^2}} = \frac{1i + 2j + 2k}{3} \]
The derivative along the direction \((1, 2, 2)\) is
\[
\frac{df}{dl}(3, 2, 0) = \nabla f(3, 2, 0) \cdot \mathbf{e}_l
\]
\[
= (12\mathbf{i} + 9\mathbf{j} + 4\mathbf{k}) \cdot \frac{\mathbf{i} + 2\mathbf{j} + 2\mathbf{k}}{3}
\]
\[
= (12 + 18 + 8)/3 = 38/3
\]

### 2.2.7 Operations on the Nabla Operator

The dot product of the del operator with a vector \(\mathbf{v}\) of components \(u, v,\) and \(w\) in the \(x, y,\) and \(z\) direction, respectively, results in the divergence of the vector \([7, 8]\), which is a scalar quantity written as

\[
\nabla \cdot \mathbf{v} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}
\]  

(2.20)

Physically the divergence of a vector field over a region is a measure of how much the vector field points into or out of the region.

The divergence of the gradient of a scalar variable \(s\) is denoted by the Laplacian of \(s\) and is a scalar given by

\[
\nabla \cdot (\nabla s) = \nabla^2 s = \frac{\partial^2 s}{\partial x^2} + \frac{\partial^2 s}{\partial y^2} + \frac{\partial^2 s}{\partial z^2}
\]  

(2.21)

The Laplacian of a vector follows from the above definition of the Laplacian operator and is a vector computed as

\[
\nabla^2 \mathbf{v} = (\nabla^2 u)\mathbf{i} + (\nabla^2 v)\mathbf{j} + (\nabla^2 w)\mathbf{k}
\]  

(2.22)

**Example 4**

*Find the divergence of \(\mathbf{v} = (u, v, w) = (3x, 2xy, 4z)\)*

**Solution**

Then divergence of \(\mathbf{v}\) is obtained as

\[
\nabla \cdot \mathbf{v} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}
\]

\[
= 3 + 2x + 4
\]

\[
= 7 + 2x
\]
Another quantity of interest is the curl of a vector field \([7, 8]\) formed between the “del” operator and the vector \(\mathbf{v}\), resulting in the following vector:

\[
\nabla \times \mathbf{v} = \left( \frac{\partial}{\partial x} \mathbf{i} + \frac{\partial}{\partial y} \mathbf{j} + \frac{\partial}{\partial z} \mathbf{k} \right) \times (u\mathbf{i} + v\mathbf{j} + w\mathbf{k})
\]

\[
= \begin{vmatrix}
\mathbf{i} & \mathbf{j} & \mathbf{k} \\
\frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\
u & v & w
\end{vmatrix}
= \left( \frac{\partial w}{\partial y} - \frac{\partial v}{\partial z} \right) \mathbf{i} + \left( \frac{\partial u}{\partial z} - \frac{\partial w}{\partial x} \right) \mathbf{j} + \left( \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \right) \mathbf{k}
\]

(2.23)

Examples of the divergence and curl of a vector field are schematically displayed in Fig. 2.8. The radial vector field shown in Fig. 2.8a has only divergence with zero curl. In fluid mechanics this vector field represents the velocity field of a sink/source flow. On the other hand Fig. 2.8b depicts a rotational vector field which has only curl with zero divergence (i.e., a divergence free vector field). Such a field corresponds to the velocity field of a vortex flow.

The divergence of a vector \(\mathbf{v}\) with its gradient also arises in the equations of interest in this book and is computed as

\[
[(\nabla \cdot \mathbf{v})] = (u\mathbf{i} + v\mathbf{j} + w\mathbf{k}) \cdot \left( \frac{\partial}{\partial x} \mathbf{i} + \frac{\partial}{\partial y} \mathbf{j} + \frac{\partial}{\partial z} \mathbf{k} \right) (u\mathbf{i} + v\mathbf{j} + w\mathbf{k})
\]

\[
= \left( u \frac{\partial}{\partial x} + v \frac{\partial}{\partial y} + w \frac{\partial}{\partial z} \right) (u\mathbf{i} + v\mathbf{j} + w\mathbf{k})
\]

\[
= \left( u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} \right) \mathbf{i} + \left( u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} \right) \mathbf{j} + \left( u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} \right) \mathbf{k}
\]

(2.24)

Fig. 2.8  a A radial vector field, b a solenoidal vector field
Example 5
Determine for the flow fields shown in Fig. 2.9a, b, c which is divergence free (i.e., neither expanding nor compressing) and which is irrotational (i.e., does not undergo a rotation)

(a) \( \nabla \cdot \mathbf{F} = 0 \) \( \nabla \times \mathbf{F} = 0 \mathbf{i} + 0 \mathbf{j} + 2 \mathbf{k} \)
(b) \( \nabla \cdot \mathbf{F} = 0 \) \( \nabla \times \mathbf{F} = 0 \mathbf{i} + 0 \mathbf{j} + 0 \mathbf{k} \)
(c) \( \nabla \cdot \mathbf{F} = 2 + 2 = 4 \) \( \nabla \times \mathbf{F} = 0 \mathbf{i} + 0 \mathbf{j} + 0 \mathbf{k} \)

2.2.8 Additional Vector Operations

If \( s \) is a scalar function, and \( \mathbf{v}_1, \mathbf{v}_2 \) and \( \mathbf{v}_3 \) are vector fields, then the following relations, which are listed without proof, apply:

\[ \nabla \cdot (\nabla \times \mathbf{v}) = 0 \]  \hspace{1cm} (2.25)
\[ \nabla \times (\nabla s) = 0 \]  \hspace{1cm} (2.26)
\[ \nabla \cdot (s \mathbf{v}) = s \nabla \cdot \mathbf{v} + \mathbf{v} \cdot \nabla s \]  \hspace{1cm} (2.27)
\[ \nabla \times (s \mathbf{v}) = s \nabla \times \mathbf{v} + \nabla s \times \mathbf{v} \]  \hspace{1cm} (2.28)
\[ \nabla (\mathbf{v}_1 \cdot \mathbf{v}_2) = \mathbf{v}_1 \times (\nabla \times \mathbf{v}_2) + \mathbf{v}_2 \times (\nabla \times \mathbf{v}_1) + (\mathbf{v}_1 \cdot \nabla) \mathbf{v}_2 + (\mathbf{v}_2 \cdot \nabla) \mathbf{v}_1 \]  \hspace{1cm} (2.29)
\[ \nabla \cdot (\mathbf{v}_1 \times \mathbf{v}_2) = \mathbf{v}_2 \cdot (\nabla \times \mathbf{v}_1) - \mathbf{v}_1 \cdot (\nabla \times \mathbf{v}_2) \]  \hspace{1cm} (2.30)
\[ \nabla \times (\mathbf{v}_1 \times \mathbf{v}_2) = \mathbf{v}_1 (\nabla \cdot \mathbf{v}_2) - \mathbf{v}_2 (\nabla \cdot \mathbf{v}_1) + (\mathbf{v}_2 \cdot \nabla) \mathbf{v}_1 - (\mathbf{v}_1 \cdot \nabla) \mathbf{v}_2 \]  \hspace{1cm} (2.31)
\[ \nabla \times (\nabla \times \mathbf{v}) = \nabla (\nabla \cdot \mathbf{v}) - \nabla^2 \mathbf{v} \]  \hspace{1cm} (2.32)
\[ (\nabla \times \mathbf{v}) \times \mathbf{v} = \mathbf{v} \cdot (\nabla \mathbf{v}) - \nabla (\mathbf{v} \cdot \mathbf{v}) \]  \hspace{1cm} (2.33)
2.3 Matrices and Matrix Operations

A matrix $A$ of order $M \times N$ is a rectangular array of quantities (numbers or expressions) arranged in $M$ rows and $N$ columns [9–11]. An element of $A$ located on the $i$th row and $j$th column is denoted by $a_{ij}$. For example, element $a_{32}$ of the $4 \times 3$ matrix shown in Fig. 2.10 is 12.

Based on this definition it follows that a column vector $v$ of dimensionality $N$ is a matrix of order $N \times 1$ and a scalar $s$ is a matrix of order $1 \times 1$.

The transpose of a matrix $A$ of order $M \times N$ is another matrix denoted by $A^T$ of order $N \times M$ for which the rows of $A$ are the columns of $A^T$ and the columns of $A$ are the rows of $A^T$. Mathematically, this can be written as

$$A = [a_{ij}] \Rightarrow A^T = [a_{ji}]$$ (2.34)

Two matrices of the same order are equal if their corresponding elements are equal. Two matrices of the same order can be added or subtracted element by element. For example, if $A$ and $B$ are given by

$$A = \begin{bmatrix} 1 & 2 & 4 \\ 3 & -1 & 7 \end{bmatrix} \quad B = \begin{bmatrix} -2 & 1 & 4 \\ -3 & 1 & 6 \end{bmatrix}$$

then $A + B$ and $A - B$ are found to be

$$A + B = \begin{bmatrix} -1 & 3 & 8 \\ 0 & 0 & 13 \end{bmatrix} \quad A - B = \begin{bmatrix} 3 & 1 & 0 \\ 6 & -2 & 1 \end{bmatrix}$$

If a matrix is multiplied by a scalar $s$ than all its elements are multiplied by $s$. Mathematically this is written as

$$A = [a_{ij}] \Rightarrow sA = [sa_{ij}]$$ (2.35)

To multiply two matrices $A$ and $B$, the number of columns of $A$ must be equal to the number of rows of $B$. Therefore, if $A$ is of size $M \times X$ for the product $P = AB$

$$\begin{array}{ccc} 1 & 2 & 3 \\ \downarrow & & \\ 1 & \begin{bmatrix} -1 & 2 & -4 \\ 5 & 4 & 7 \\ 0 & 12 & -2 \\ 3 & 6 & 3 \end{bmatrix} & \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \\ a_{41} & a_{42} & a_{43} \end{bmatrix} = \begin{bmatrix} a_{ij} \end{bmatrix} \end{array}$$

Fig. 2.10 Example of a $4 \times 3$ matrix
to be possible, \( B \) must be of size \( X \times N \). The size of \( P \) will be \( M \times N \) with its element \( p_{ij} \) obtained as

\[
p_{ij} = \sum_{k=1}^{X} a_{ik} b_{kj}
\]  

(2.36)

If \( A \) is a \( 3 \times 2 \) matrix and \( B \) a \( 2 \times 4 \) matrix given by

\[
A = \begin{bmatrix}
1 & 2 \\
-1 & 3 \\
2 & -5
\end{bmatrix}
\quad B = \begin{bmatrix}
2 & -1 & 0 & 4 \\
-3 & 0 & 3 & 2
\end{bmatrix}
\]

then \( P = AB \) will be a \( 3 \times 4 \) matrix computed as

\[
P = \begin{bmatrix}
1 & 2 \\
-1 & 3 \\
2 & -5
\end{bmatrix}
\begin{bmatrix}
2 & -1 & 0 & 4 \\
-3 & 0 & 3 & 2
\end{bmatrix} = \begin{bmatrix}
p_{11} & p_{12} & p_{13} & p_{14} \\
p_{21} & p_{22} & p_{23} & p_{24} \\
p_{31} & p_{32} & p_{33} & p_{34}
\end{bmatrix}
\]

\[
p_{11} = 1 \times 2 + 2 \times (-3) = -4
\]

\[
p_{12} = 1 \times (-1) + 2 \times 0 = -1
\]

\[
p_{13} = \ldots
\]

\[
p_{14} = \ldots
\]

\[
P = \begin{bmatrix}
-3 & -1 & 6 & 8 \\
-11 & 1 & 9 & 2 \\
19 & -2 & -15 & -2
\end{bmatrix}
\]

2.3.1 Square Matrices

If the number of columns \( N \) of matrix \( A \) is equal to its number of rows, then \( A \) is a square matrix of order \( N \). The elements \( a_{ii} \) of a square matrix \( A \) form its main diagonal which stretches from top left to bottom right. The diagonal composed of elements \( a_{ij} \) for which \( i + j = N + 1 \) is called the cross diagonal and it extends from the bottom left to top right.

Square matrices possess properties that are not applicable to other types of matrices such as symmetry and antisymmetry. In addition, many operations such as taking determinants and calculating eigenvalues are only defined for square matrices.

The result of multiplying a square matrix of order \( N \) by itself is a square matrix of order \( N \). Therefore a square matrix can be multiplied by itself as many times as needed and the notation \( A^k \) designates \( A \) multiplied by itself \( k \) times, i.e.,

\[
A^k = A \times A \times A \ldots \times A
\]

(2.37)
A square matrix $A$ is symmetric if $a_{ij} = a_{ji}$ (i.e., $A^T = A$), and antisymmetric if $a_{ij} = -a_{ji}$. An example of a symmetric square matrix of order 3 is

$$
\begin{bmatrix}
  5 & 3 & -2 \\
  3 & 2 & 7 \\
 -2 & 7 & -1 \\
\end{bmatrix}
$$

and of an antisymmetric square matrix of order 4 is

$$
\begin{bmatrix}
  0 & 3 & -2 & 4 \\
 -3 & 0 & 1 & -3 \\
 2 & -1 & 0 & -2 \\
-4 & 3 & 2 & 0 \\
\end{bmatrix}
$$

A diagonal square matrix $D$ is one for which all elements off the main diagonal are zero while elements on the main diagonal are arbitrary. An example of a square diagonal matrix of order 3 is

$$
\begin{bmatrix}
  5 & 0 & 0 \\
  0 & 0 & 0 \\
  0 & 0 & -2 \\
\end{bmatrix}
$$

A diagonal matrix of order $N$ for which all elements on the main diagonal are 1 (i.e., $a_{ii} = 1$) is called an identity matrix of order $N$ and is designated by $I$. An identity matrix of order 4 is given by

$$
I = \begin{bmatrix}
  1 & 0 & 0 & 0 \\
  0 & 1 & 0 & 0 \\
  0 & 0 & 1 & 0 \\
  0 & 0 & 0 & 1 \\
\end{bmatrix}
$$

The inverse of a square matrix $A$ of order $N$ is the square matrix $A^{-1}$ of order $N$ satisfying

$$
A^{-1}A = AA^{-1} = I
$$

(2.38)

An upper triangular matrix $U$ is a square matrix in which all elements below the main diagonal are zero. Mathematically this can be expressed as

$$
U = \begin{cases}
  u_{ij} & i \leq j \\
  0 & i > j
\end{cases}
$$

(2.39)
A lower triangular matrix \( \mathbf{L} \) is a square matrix in which all elements above the main diagonal are zero. Using mathematical notation, this is written as

\[
\mathbf{L} = \begin{cases} 
\ell_{ij} & i \geq j \\
0 & i < j 
\end{cases}
\] (2.40)

Examples of upper and lower triangular square matrices of order 3 are

\[
\mathbf{U} = \begin{bmatrix} 1 & 2 & 6 \\ 0 & 4 & 5 \\ 0 & 0 & -7 \end{bmatrix} \quad \mathbf{L} = \begin{bmatrix} 3 & 0 & 0 \\ -1 & 2 & 0 \\ -9 & -2 & 4 \end{bmatrix}
\]

2.3.2 Using Matrices to Describe Systems of Equations

Matrices can be used to compactly describe systems of equations [12]. A system of \( N \) equations in \( N \) unknowns can be written as

\[
a_{11}\phi_1 + a_{12}\phi_2 + a_{13}\phi_3 + \ldots + a_{1N}\phi_N = b_1 \\
a_{21}\phi_1 + a_{22}\phi_2 + a_{23}\phi_3 + \ldots + a_{2N}\phi_N = b_2 \\
a_{31}\phi_1 + a_{32}\phi_2 + a_{33}\phi_3 + \ldots + a_{3N}\phi_N = b_3 \\
\vdots \quad \vdots \quad \vdots \quad \vdots \\
a_{N1}\phi_1 + a_{N2}\phi_2 + a_{N3}\phi_3 + \ldots + a_{NN}\phi_N = b_N
\] (2.41)

In matrix notation, this system of equations is equivalent to

\[
\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & \cdots & a_{1N} \\ a_{21} & a_{22} & a_{23} & \cdots & \cdots & a_{2N} \\ a_{31} & a_{32} & a_{33} & \cdots & \cdots & a_{3N} \\ \vdots & \vdots & \vdots & \ddots & \cdots & \vdots \\ a_{N1} & a_{N2} & a_{N3} & \cdots & \cdots & a_{NN} \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \vdots \\ \vdots \\ \phi_N \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ \vdots \\ b_N \end{bmatrix}
\] (2.42)

or in compact form as

\[
\mathbf{A}\phi = \mathbf{b}
\] (2.43)

2.3.3 The Determinant of a Square Matrix

A determinant is a value associated with a square matrix \( \mathbf{A} \) that can be computed from the elements of the matrix through a mathematical procedure and is denoted by \( \det(\mathbf{A}) \) or \( |\mathbf{A}| \) (which should not be confused with the absolute value notation) [13].
The calculation of the determinant of a matrix of order 2 is straightforward and is the product of the elements in the main diagonal minus the product of the elements in the cross diagonal. If \( A \) is a square matrix of order 2 then,

\[
A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \Rightarrow \text{det}(A) = a_{11}a_{22} - a_{21}a_{12}
\] (2.44)

For higher order matrices the procedure is more involved and is based on the notion of minors and cofactors.

A minor \((mi)_{ij}\) for an element \(a_{ij}\) is the determinant that results when the \(i\)th row and \(j\)th column are deleted. The cofactor \((co)_{ij}\) of an element \(a_{ij}\) is the value of the minor multiplied by either a positive or a negative sign depending on whether \((i + j)\) is even or odd, respectively. The mathematical relation between cofactors and minors can be written as

\[
(co)_{ij} = (-1)^{i+j}(mi)_{ij}
\] (2.45)

The determinant of a square matrix \( A \) of order \( N \) is computed by finding the cofactors of one of its rows or its columns, multiplying each cofactor by the corresponding element, and adding the results. Mathematically this is given by

\[
\text{det}(A) = \begin{cases} 
\sum_{i=1}^{N} a_{ij}(co)_{ij} & \text{for any } j \\
\text{or} \\
\sum_{j=1}^{N} a_{ij}(co)_{ij} & \text{for any } i
\end{cases}
\] (2.46)

It should be clarified that the calculation of the cofactors may require further decomposition of the minor determinants. This decomposition may give rise to further decompositions until a determinant with a size of 2 is reached. Moreover, based on the above discussion it is easily demonstrated that the determinant of an upper, a lower, or a diagonal matrix \( A \) of order \( N \) is the product of the elements along its main diagonal, i.e., \( \text{det}(A) = \prod_{i=1}^{N} a_{ii} \).

**Example 6**

Calculate the determinant of matrix \( A \) of order 4 given by

\[
A = \begin{bmatrix} 1 & 1 & 1 & 0 \\ 1 & 2 & 0 & 5 \\ 2 & 3 & -2 & 0 \\ 4 & 1 & -5 & 3 \end{bmatrix}
\]
Solution

As mentioned above, the determinant can be calculated based on the cofactors of any selected row or column. A smart choice would be a row or a column with the largest number of zeros. Therefore computations will be reduced by selecting either the first row or the last column. The determinant will be calculated using both to further show that the end results will be the same.

The signs of cofactors are

\[
\begin{pmatrix}
+ & - & + & - \\
- & + & - & + \\
+ & - & + & - \\
- & + & - & + \\
\end{pmatrix}
\]

The determinant using cofactors of row 1 is computed as

\[
\text{det}(A) = 1 \times (co)_{11} + 1 \times (co)_{13} = \begin{vmatrix}
2 & 0 & 5 \\
3 & -2 & 0 \\
1 & -5 & 3
\end{vmatrix} + \begin{vmatrix}
1 & 2 & 5 \\
2 & 3 & 0 \\
4 & 1 & 3
\end{vmatrix}
\]

The first new determinant is calculated using the cofactors of row 1 while the second determinant is calculated using cofactors of column 3 as

\[
\text{det}(A) = 2 \begin{vmatrix}
-2 & 0 \\
-5 & 3
\end{vmatrix} + 5 \begin{vmatrix}
3 & -2 \\
1 & -5
\end{vmatrix} + 5 \begin{vmatrix}
2 & 3 \\
4 & 1
\end{vmatrix} + 3 \begin{vmatrix}
1 & 2 \\
2 & 3
\end{vmatrix}
\]

\[
= 2(-6 - 0) + 5(-15 + 2) + 5(2 - 12) + 3(3 - 4)
\]

\[
= -12 - 65 - 50 - 3
\]

\[
\text{det}(A) = -130
\]

The determinant using cofactors of column 4 is calculated as

\[
\text{det}(A) = 5 \times (co)_{24} + 3 \times (co)_{44} = 5 \begin{vmatrix}
1 & 0 & 1 \\
2 & 3 & -2 \\
4 & 1 & -5
\end{vmatrix} + 3 \begin{vmatrix}
1 & 0 & 1 \\
2 & 3 & 0 \\
4 & 1 & 3
\end{vmatrix}
\]

The first and second new determinants are calculated using the cofactors of row 1 as

\[
\text{det}(A) = 5 \begin{vmatrix}
3 & -2 \\
1 & -5
\end{vmatrix} + 5 \begin{vmatrix}
2 & 3 \\
4 & 1
\end{vmatrix} + 3 \begin{vmatrix}
2 & 0 \\
3 & -2
\end{vmatrix} + 3 \begin{vmatrix}
1 & 2 \\
2 & 3
\end{vmatrix}
\]

\[
= 5(-15 + 2) + 5(2 - 12) + 3(-4 - 0) + 3(3 - 4)
\]

\[
= -65 - 50 - 12 - 3
\]

\[
\text{det}(A) = -130
\]

As expected, the same value is obtained.
2.3.4 Eigenvectors and Eigenvalues

Consider a square matrix \( A \) and a vector \( v \). The vector \( v \) is an eigenvector of \( A \) if the product \( Av \) results in a vector that has the same direction as \( v \) [14–19]. Therefore an eigenvector of a matrix is a nonzero vector that does not rotate when is applied to it. As shown in Fig. 2.11, the only effects may be to change its length and/or reverse its direction. Thus, there exist a scalar \( \lambda \) such that \( Av = \lambda v \). The value of \( \lambda \) is an eigenvalue of \( A \). It is clear that for any constant \( z \) the vector \( zv \) is also an eigenvector of \( A \) because \( A(zv) = zAv = z\lambda v = \lambda(zv) \). Thus, a scaled eigenvector is also an eigenvector.

If \( A \) is symmetric of order \( N \), then it can be shown that \( A \) has a set of linearly independent eigenvectors denoted \( v_1, v_2, v_3, \ldots, v_N \). As proved above this set is not unique. However the corresponding set of their eigenvalues, denoted \( \lambda_1, \lambda_2, \lambda_3, \ldots, \lambda_N \), which may or may not be equal to each other, is unique. The eigenvalues of the identity matrix are all ones, and every nonzero vector is an eigenvector of \( I \).

In general the eigenvalues of a square matrix \( A \) of order \( N \) are obtained from solving the following equation:

\[
Av = \lambda v \Rightarrow Av = \lambda I v \Rightarrow (A - \lambda I)v = 0
\]  \hspace{1cm} (2.47)

Since, by definition, eigenvectors are nonzero, then

\[
A - \lambda I = 0 \Rightarrow \det(A - \lambda I) = 0
\]  \hspace{1cm} (2.48)

The expanded form of Eq. (2.48) is given by

\[
\begin{vmatrix}
  a_{11} - \lambda & a_{12} & a_{13} & \cdots & a_{1N} \\
a_{21} & a_{22} - \lambda & a_{23} & \cdots & a_{2N} \\
a_{31} & a_{32} & a_{33} - \lambda & \cdots & a_{3N} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
a_{N1} & a_{N2} & a_{N3} & \cdots & a_{NN} - \lambda
\end{vmatrix} = 0
\]  \hspace{1cm} (2.49)

Fig. 2.11 Effects of multiplying a matrix \( A \) by one of its Eigenvectors \( v \)
As an example, the eigenvalues of the following square matrix of order 2 are found as:

\[
A = \begin{bmatrix} 3 & 1 \\ 8 & 1 \end{bmatrix} \Rightarrow \begin{vmatrix} \lambda - 3 & 1 \\ 8 & \lambda - 1 \end{vmatrix} = 0 \Rightarrow (\lambda - 3)(\lambda - 1) - 8 = 0
\]
\[
\therefore \lambda^2 - 4\lambda - 5 = 0 \Rightarrow (\lambda + 1)(\lambda - 5) = 0 \Rightarrow \lambda_1 = -1 \text{ or } \lambda_2 = 5
\]

### 2.3.5 A Symmetric Positive-Definite Matrix

A symmetric matrix \( A = [a_{ij}] \) of order \( N \) is positive-definite if for all column vectors \( p \) in \( \mathbb{R}^N \) the following inequality holds:

\[
p^T A p > 0
\]  

(2.50)

For example, if \( A \) is an order 3 symmetric matrix given by

\[
A = \begin{bmatrix} 5 & 3 & 1 \\ 3 & 7 & 4 \\ 1 & 4 & 8 \end{bmatrix}
\]

then Eq. (2.50) for any column vector \( p \) of order 3 gives

\[
p^T A p = \begin{bmatrix} a \\ b \\ c \end{bmatrix}^T \begin{bmatrix} 5 & 3 & 1 \\ 3 & 7 & 4 \\ 1 & 4 & 8 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = 3(a + b)^2 + (a + c)^2 + 4(b + c)^2 + a^2 + 4b^2 + 3c^2 > 0
\]

which is positive-definite.

If \( A \) is a symmetric positive-definite matrix given by

\[
A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & \cdots & a_{1N} \\ a_{21} & a_{22} & a_{23} & \cdots & \cdots & a_{2N} \\ a_{31} & a_{32} & a_{33} & \cdots & \cdots & a_{3N} \\ \vdots & \vdots & \vdots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \ddots & \vdots \\ a_{N1} & a_{N2} & a_{N3} & \cdots & \cdots & a_{NN} \end{bmatrix}
\]  

(2.51)
then, among others, the following properties apply:

1. Any sub-matrix $\mathbf{P}$ of $\mathbf{A}$ of order $M(1 \leq M \leq N)$ of the form

$$
\mathbf{P} = \begin{bmatrix}
  a_{11} & a_{12} & \cdots & a_{1M} \\
  a_{21} & a_{22} & \cdots & a_{2M} \\
  \vdots & \vdots & \ddots & \vdots \\
  a_{M1} & a_{M2} & \cdots & a_{MM}
\end{bmatrix}
$$

is also positive-definite.

2. The $N$ eigenvalues of $\mathbf{A}$, $\lambda_1, \lambda_2, \lambda_3, \ldots, \lambda_N$ are positive.

3. If all the eigenvalues of a matrix $\mathbf{A}$ are positive, then $\mathbf{A}$ is positive-definite.

4. $\mathbf{A}$ has a unique decomposition of the form $\mathbf{A} = \mathbf{LL}^T$, where $\mathbf{L}$ is a lower triangular matrix. This decomposition is known as the Cholesky decomposition.

### 2.3.6 Additional Matrix Operations

If $s_1$ and $s_2$ are scalar functions, $\mathbf{I}$ an identity matrix, and $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$ are matrices, then the various matrix operations, addition, subtraction, scalar multiplication, and matrix multiplication, have the following properties listed without proof:

$$
\mathbf{A} + (\mathbf{B} + \mathbf{C}) = (\mathbf{A} + \mathbf{B}) + \mathbf{C}
$$

$$
\mathbf{A} + \mathbf{B} = \mathbf{B} + \mathbf{A}
$$

$$
s_1(\mathbf{A} + \mathbf{B}) = s_1\mathbf{A} + s_1\mathbf{B}
$$

$$
(s_1 + s_2)\mathbf{A} = s_1\mathbf{A} + s_2\mathbf{A}
$$

$$
\mathbf{A}(\mathbf{BC}) = (\mathbf{AB})\mathbf{C}
$$

$$
\mathbf{AI} = \mathbf{IA} = \mathbf{A}
$$

$$
\mathbf{A}(\mathbf{B} + \mathbf{C}) = \mathbf{AB} + \mathbf{AC}
$$

$$
(\mathbf{A} + \mathbf{B})\mathbf{C} = \mathbf{AC} + \mathbf{BC}
$$

$$
(\mathbf{A} + \mathbf{B})^T = \mathbf{A}^T + \mathbf{B}^T
$$

$$
(s_1\mathbf{A})^T = s_1\mathbf{A}^T
$$

$$
(\mathbf{AB})^T = \mathbf{B}^T\mathbf{A}^T
$$

$$
(\mathbf{AB})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1}
$$
2.4 Tensors and Tensor Operations

Tensors can be thought of as extensions to the ideas already used when defining quantities like scalars and vectors [2, 20, 21]. A scalar is a tensor of rank zero, and a vector is a tensor of rank one. Tensors of higher rank (2, 3, etc.) can be developed and their main use is to manipulate and transform sets of equations. Since within the scope of this book only tensors of rank two are needed, they will be referred to simply as tensors.

Similar to the flow velocity vector \( \mathbf{v} \), the deviatoric stress tensor \( \mathbf{\tau} \) (Fig. 2.12) will be referred to frequently in this book and is used here to illustrate tensor operations.

Let \( x, y, \) and \( z \) represent the directions in an orthonormal Cartesian coordinate system, then the stress tensor \( \tau \) and its transpose designated with superscript \( T \) are represented in terms of their components as

\[
\tau = \begin{bmatrix}
\tau_{xx} & \tau_{xy} & \tau_{xz} \\
\tau_{yx} & \tau_{yy} & \tau_{yz} \\
\tau_{zx} & \tau_{zy} & \tau_{zz}
\end{bmatrix} \\
\tau^T = \begin{bmatrix}
\tau_{xx} & \tau_{yx} & \tau_{zx} \\
\tau_{xy} & \tau_{yy} & \tau_{zy} \\
\tau_{xz} & \tau_{yz} & \tau_{zz}
\end{bmatrix}
\] (2.65)

Similar to writing a vector in terms of its components, defining the unit vectors \( \mathbf{i}, \mathbf{j}, \) and \( \mathbf{k} \) in the \( x, y, \) and \( z \) direction, respectively, the tensor \( \tau \) given by Eq. (2.65) can be written in terms of its components as

\[
\tau = i_i \tau_{xx} + i_j \tau_{xy} + i_k \tau_{xz} + j_i \tau_{yx} + j_j \tau_{yy} + j_k \tau_{yz} + k_i \tau_{zx} + k_j \tau_{zy} + k_k \tau_{zz}
\] (2.66)

Equation (2.66) allows defining a third type of vector product for multiplying two vectors, known as the dyadic product, and resulting in a tensor with its components formed by ordered pairs of the two vectors. In specific, the dyadic product

Fig. 2.12  Schematic of a stress tensor field
of a vector \( \mathbf{v} \) by itself, arising in the formulation of the momentum equation of fluid flow, gives

\[
\{ \mathbf{vv} \} = (ui + vj + wk)(ui + vj + wk) \\
= iiu + ijv + ikw + \\
jivu + jjvv + jkvw + \\
kiwu + kjvw + kkww
\]

\[
\Rightarrow \{ \mathbf{vv} \} = \begin{bmatrix} uu & uv & uw \\ vu & vv & vw \\ wu & wv & ww \end{bmatrix} \tag{2.67}
\]

The gradient of a vector \( \mathbf{v} \) is a tensor given by

\[
\{ \nabla \mathbf{v} \} = \left( \frac{\partial}{\partial x} \mathbf{i} + \frac{\partial}{\partial y} \mathbf{j} + \frac{\partial}{\partial z} \mathbf{k} \right) (ui + vj + wk) \\
= ii \frac{\partial u}{\partial x} + ij \frac{\partial v}{\partial x} + ik \frac{\partial w}{\partial x} + \\
ju \frac{\partial u}{\partial y} + jjv + jk \frac{\partial w}{\partial y} + \\
ku \frac{\partial u}{\partial z} + kjv + kk \frac{\partial w}{\partial z}
\]

\[
\Rightarrow \{ \nabla \mathbf{v} \} = \begin{bmatrix} \frac{\partial u}{\partial x} & \frac{\partial v}{\partial x} & \frac{\partial w}{\partial x} \\ \frac{\partial u}{\partial y} & \frac{\partial v}{\partial y} & \frac{\partial w}{\partial y} \\ \frac{\partial u}{\partial z} & \frac{\partial v}{\partial z} & \frac{\partial w}{\partial z} \end{bmatrix} \tag{2.68}
\]

The sum of two tensors \( \sigma \) and \( \tau \) is a tensor \( \Sigma \) whose components are the sum of the corresponding components of the two tensors, i.e.,

\[
\Sigma = \sigma + \tau = \begin{bmatrix} \sigma_{xx} + \tau_{xx} & \sigma_{xy} + \tau_{xy} & \sigma_{xz} + \tau_{xz} \\ \sigma_{yx} + \tau_{yx} & \sigma_{yy} + \tau_{yy} & \sigma_{yz} + \tau_{yz} \\ \sigma_{zx} + \tau_{zx} & \sigma_{zy} + \tau_{zy} & \sigma_{zz} + \tau_{zz} \end{bmatrix} \tag{2.69}
\]

Multiplying a tensor \( \tau \) by a scalar \( s \) results in a tensor whose components are multiplied by that scalar, i.e.,

\[
\{ s\tau \} = \begin{bmatrix} s\tau_{xx} & s\tau_{xy} & s\tau_{xz} \\ s\tau_{yx} & s\tau_{yy} & s\tau_{yz} \\ s\tau_{zx} & s\tau_{zy} & s\tau_{zz} \end{bmatrix} \tag{2.70}
\]

The dot product of a tensor \( \tau \) by a vector \( \mathbf{v} \) results in the following vector:

\[
[\tau \cdot \mathbf{v}] = \left( ii\tau_{xx} + ij\tau_{xy} + ik\tau_{xz} + ji\tau_{yx} + \\
jj\tau_{yy} + jk\tau_{yz} + kii\tau_{zx} + kj\tau_{zy} + kk\tau_{zz} \right) \cdot (ui + vj + wk) \tag{2.71}
\]
which upon expanding becomes

\[
[\mathbf{\tau} \cdot \mathbf{v}] = ii \cdot i\tau_{xx}u + ii \cdot j\tau_{xx}v + ii \cdot k\tau_{xx}w + ij \cdot i\tau_{xy}u + ij \cdot j\tau_{xy}v + ij \cdot k\tau_{xz}w + ji \cdot i\tau_{yx}u + ji \cdot j\tau_{yx}v + ji \cdot k\tau_{yx}w + jk \cdot i\tau_{yz}u + jk \cdot j\tau_{yz}v + jk \cdot k\tau_{yz}w + kk \cdot i\tau_{zz}v + kk \cdot j\tau_{zz}v + kk \cdot k\tau_{zz}w
\]

(2.72)

Using Eq. (2.8), Eq. (2.72) reduces to

\[
[\mathbf{\tau} \cdot \mathbf{v}] = (\tau_{xx}u + \tau_{xy}v + \tau_{xz}w)i + (\tau_{yx}u + \tau_{yy}v + \tau_{yz}w)j + (\tau_{zx}u + \tau_{zy}v + \tau_{zz}w)k
\]

(2.73)

The above equation can be derived using matrix multiplication as

\[
[\mathbf{\tau} \cdot \mathbf{v}] = \begin{bmatrix} \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \tau_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \tau_{zz} \end{bmatrix} \begin{bmatrix} u \\ v \\ w \end{bmatrix} = \begin{bmatrix} \tau_{xx}u + \tau_{xy}v + \tau_{xz}w \\ \tau_{yx}u + \tau_{yy}v + \tau_{yz}w \\ \tau_{zx}u + \tau_{zy}v + \tau_{zz}w \end{bmatrix}
\]

(2.74)

In a similar way the divergence of a tensor \( \mathbf{\tau} \) is found to be a vector given by

\[
[\nabla \cdot \mathbf{\tau}] = \left( \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z} \right)i + \left( \frac{\partial \tau_{yx}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{yz}}{\partial z} \right)j + \left( \frac{\partial \tau_{zx}}{\partial x} + \frac{\partial \tau_{zy}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} \right)k
\]

(2.75)

The double dot product of two tensors \( \mathbf{\tau} \) and \( \{\nabla \mathbf{v}\} \) is a scalar computed as

\[
(\mathbf{\tau} : \nabla \mathbf{v}) = \begin{bmatrix} ii\tau_{xx} + ij\tau_{xy} + ik\tau_{xz} + & ij\tau_{xy} + jj\tau_{yy} + jk\tau_{yz} + \\
jk\tau_{zx} + kj\tau_{zy} + kk\tau_{zz} \end{bmatrix} \begin{bmatrix} ii \frac{\partial u}{\partial x} + ij \frac{\partial v}{\partial x} + ik \frac{\partial w}{\partial x} + \\
ji \frac{\partial u}{\partial y} + jj \frac{\partial v}{\partial y} + jk \frac{\partial w}{\partial y} + \\
ki \frac{\partial u}{\partial z} + kj \frac{\partial v}{\partial z} + kk \frac{\partial w}{\partial z} \end{bmatrix}
\]

(2.76)

The final value is obtained by expanding the above product and performing the double dot product on the various terms. For example,

\[
i \cdot j \tau_{xy} : \frac{\partial u}{\partial y} = i \cdot j \tau_{xy} \frac{\partial u}{\partial y} = i \cdot j \tau_{xy} \frac{\partial y}{\partial y} = i \cdot j \tau_{xy} \frac{\partial y}{\partial y}
\]

(2.77)
Performing the same steps on every term in the expanded product, the final form of \((\tau : \nabla \nu)\) is obtained as

\[
(\tau : \nabla \nu) = \tau_{xx} \frac{\partial u}{\partial x} + \tau_{xy} \frac{\partial u}{\partial y} + \tau_{xz} \frac{\partial u}{\partial z} + \tau_{yx} \frac{\partial v}{\partial x} + \tau_{yy} \frac{\partial v}{\partial y} + \tau_{yz} \frac{\partial v}{\partial z} + \tau_{zx} \frac{\partial w}{\partial x} + \tau_{zy} \frac{\partial w}{\partial y} + \tau_{zz} \frac{\partial w}{\partial z}
\]

(2.78)

### 2.5 Fundamental Theorems of Vector Calculus

All mathematical formulations presented in this book will be performed using vectors. Therefore a good knowledge of the fundamental theorems of vector calculus is helpful. A brief review of some of these theorems is presented next.

#### 2.5.1 Gradient Theorem for Line Integrals

The gradient theorem for line integrals relates a line integral to the values of a function at its endpoints [22]. It states that if \(C\) is a smooth curve, as shown in Fig. 2.13, described by the vector \(\mathbf{r}(t) = [x(t), y(t), z(t)]\) for \(a \leq t \leq b\), and \(s\) is a scalar function whose gradient, \(\nabla s\), is continuous on \(C\), then

\[
\int_C \nabla s \cdot d\mathbf{r} = s(r(b)) - s(r(a))
\]

(2.79)

where \(a\) and \(b\) are the endpoints of \(C\). It follows that the value of the integral over a closed contour is zero.

**Fig. 2.13** A schematic depiction of a curve \(C\) of a scalar function \(s\) showing its end points and the position vector \(\mathbf{r}(t)\).
2.5.2 Green’s Theorem

Green’s theorem expresses the contour integral of a simple closed curve \( C \) in terms of the double integral of the two dimensional region \( R \) bounded by \( C \) [23–26].

Let \( C \) denotes the closed contour (Fig. 2.14) of a two dimensional region \( R \). If \( u(x,y) \) and \( v(x,y) \) are functions of continuous partial derivatives defined on \( R \), then

\[
\oint_C (u \, dx + v \, dy) = \iint_R \left( \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \right) \, dx \, dy \tag{2.80}
\]

In Eq. (2.80) the contour integral along \( C \) is taken positive in the counterclockwise direction.

![Schematic of a region R and its closed contour C](image)

Green’s theorem can be written in a more compact form using vectors. For that purpose defining \( d\mathbf{r} \), \( \mathbf{v} \) and the area vector \( d\mathbf{S} \) as

\[
d\mathbf{r} = dx \mathbf{i} + dy \mathbf{j} \quad \mathbf{v} = u \mathbf{i} + v \mathbf{j} \quad d\mathbf{S} = dxdy \mathbf{k}
\]

then the vector form of Green’s theorem is given by

\[
\oint_C \mathbf{v} \cdot d\mathbf{r} = \iint_R [\nabla \times \mathbf{v}] \cdot d\mathbf{S} \tag{2.82}
\]

Green’s theorem is helpful for computing line integrals arising in two-dimensional flows.

**Example 7**

Compute \( \oint_C 2y^3 \, dx + 3xy^2 \, dy \) where \( C \) is the CCW-oriented boundary of the region \( R \) shown in Fig. 2.15.

The vector field in the above integral is \((u, v) = (2y^3, 3xy^2)\). The line integral can be computed directly. But, it is more easily computed using Green’s theorem using a double integral. Applying Green’s theorem the integrand is obtained as
\[ \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} = 3y^2 - 6y^2 = -3y^2 \]

Since the line integral is over a semi circle, the region \( R \) is mathematically given by

\[
-1 \leq x \leq 1 \\
0 \leq y \leq \sqrt{1-x^2}
\]

The value of the integral is obtained as

\[
\oint \limits_C 2y^3 \, dx + 3xy^2 \, dy = \iint \limits_D \left( \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \right) \, dA = -3 \int_{-1}^{1} \int_{0}^{\sqrt{1-x^2}} y^2 \, dy \, dx
\]

\[
= -3 \int_{-1}^{1} \left( \frac{y^3}{3} \right)_{y=0}^{y=\sqrt{1-x^2}} \, dx = -\int_{-1}^{1} (1-x^2)^{3/2} \, dx
\]

Let \( x = \cos \theta \Rightarrow dx = -\sin \theta \, d\theta \)

Thus

\[
\oint \limits_C 2y^3 \, dx + 3xy^2 \, dy = -\int_{0}^{\pi} \sin^2 \theta d\theta + \int_{0}^{\pi} \sin^2 \theta \cos^2 \theta d\theta
\]

\[
= -\left[ \frac{\theta - \sin 2\theta}{2} \right]_0^\pi + \left[ \frac{\theta - \sin 4\theta}{8} \right]_0^\pi
\]

\[
= -\frac{3\pi}{8}
\]

### 2.5.3 Stokes’ Theorem

Stokes’ theorem is a higher dimensional version of Green’s theorem [27–29]. Whereas Green’s theorem relates a line integral to a double integral, Stokes theorem relates a line integral to a surface integral. Let \( \mathbf{v} \) be a vector field, \( S \) an oriented surface, and \( C \) the boundary curve of \( S \), oriented using the right-hand rule, as depicted in Fig. 2.16. Stokes’ theorem states the following:
where \( \mathbf{r} \) is such that \( d\mathbf{r}/ds \) is the unit tangent vector and \( s \) the arc length of \( C \). The curve of the line integral, \( C \), must have positive orientation, meaning that \( d\mathbf{r} \) points counterclockwise when the surface normal, \( dS \), points toward the viewer, following the right-hand rule.

### 2.5.4 Divergence Theorem

Let \( V \) represents a volume in three-dimensional space (Fig. 2.17) of boundary \( S \). Let \( \mathbf{n} \) be the outward pointing unit vector normal to \( S \). If \( \mathbf{v} \) is a vector field defined on \( V \), then the divergence theorem [30, 31] (also known as Gauss’ theorem) states that

\[
\int_{V} \left( \nabla \times \mathbf{v} \right) \cdot dV = \oint_{S} \mathbf{v} \cdot d\mathbf{r} \tag{2.83}
\]

The divergence theorem implies that the net flux of a vector field through a closed surface is equal to the total volume of all sources and sinks (i.e., the volume integral of its divergence) over the region inside the surface. It is an important theorem for fluid dynamics.
The divergence theorem can be used in different contexts to derive many other useful identities (corollaries) [32]. In specific it can be applied to the product of a scalar function, \( s \), and a non-zero constant vector, to derive the following important relation:

\[
\int_V \nabla s \, dV = \oint_S s \, dS
\]  

(2.85)

The divergence theorem is equally applicable to tensors, in which case it is written as

\[
\int_V [\nabla \cdot \mathbf{\tau}] \, dV = \oint_S [\mathbf{\tau} \cdot \mathbf{n}] \, dS
\]  

(2.86)

**Example 8**

Use the divergence theorem to evaluate

\[
\iiint_V \mathbf{F} \cdot dS
\]

where \( \mathbf{F} = (3x + z^2)\mathbf{i} + (y^2 - \sin(x^2z))\mathbf{j} + (xz + ye^{x^2})\mathbf{k} \)

and \( V \) is a box defined by

\[0 \leq x \leq 1 \quad 0 \leq y \leq 3 \quad 0 \leq z \leq 2\]

with an outward pointing surface.
Solution
This is a difficult field to integrate however using the divergence theorem it can be transformed to

\[ \iiint_{\partial V} \mathbf{F} \cdot d\mathbf{S} = \iiint_{V} (\nabla \cdot \mathbf{F}) dV \]

where the divergence of \( \mathbf{F} \) is obtained as

\[ \nabla \cdot \mathbf{F} = 3 + 2y + x \]

integrating over the box, the integral is evaluated as

\[ \iiint_{\partial V} \mathbf{F} \cdot d\mathbf{S} = \int_{0}^{1} \int_{0}^{2} \int_{0}^{3} (3 + 2y + x) dzdydx = \int_{0}^{1} \int_{0}^{2} (6 + 4y + 2x) dydx \]

\[ = \int_{0}^{1} (18 + 18 + 6x) dx = 36 + 3 = 39 \]

2.5.5 Leibniz Integral Rule

The Leibniz integral rule gives a formula for differentiating a definite integral whose limits are functions of the differential variable [33–36]. Let \( \phi(x, t) \) represents a function that depends on a space variable \( x \) and time \( t \). Then Leibniz integral rule can be stated as follows

\[ \frac{d}{dt} \int_{a(t)}^{b(t)} \phi(x, t) dx = \int_{a(t)}^{b(t)} \frac{\partial \phi}{\partial t} dx + \phi(b(t), t) \frac{\partial b}{\partial t} - \phi(a(t), t) \frac{\partial a}{\partial t} \quad (2.87) \]

The meaning of the various terms in Eq. (2.87) can be inferred from Fig. 2.18. The first term on the right side gives the change in the integral because \( \phi \) is changing with time \( t \), while the second and third terms accounts for the gain and loss in area as the upper and lower bounds are moved, respectively.
The three-dimensional form of this formula applied to a volume \( V(t) \) enclosed by a surface \( S(t) \) with its surface elements moving with a velocity \( \mathbf{v}_s \) can be written as

\[
\frac{d}{dt} \int_{V(t)} \phi dV = \int_{V(t)} \frac{\partial \phi}{\partial t} dV + \int_{S(t)} \phi \mathbf{v}_s \cdot \mathbf{n} dS \tag{2.88}
\]

where \( \phi(t, \mathbf{x}) \) is a scalar function of space and time. For a non-moving volume \( V \), the equation reduces to

\[
\frac{d}{dt} \int_{V} \phi dV = \int_{V} \frac{\partial \phi}{\partial t} dV \tag{2.89}
\]

The above equations are also applicable to vectors and tensors.

### 2.6 Closure

The chapter offered a brief review of vector and tensor operations. In addition the fundamental theorems of vector calculus were presented. The next chapter will rely on information presented in this chapter to derive the conservation equations governing the transfer phenomena of interest in this book.
2.7 Exercises

Exercise 1
Let \( \mathbf{v}_1, \mathbf{v}_2 \) and \( \mathbf{v}_3 \) be three vectors given by

\[
\mathbf{v}_1 = \begin{bmatrix} 1 \\ 2 \\ -5 \end{bmatrix}, \quad \mathbf{v}_2 = \begin{bmatrix} -1 \\ 10 \\ -2 \end{bmatrix}, \quad \mathbf{v}_3 = \begin{bmatrix} 8 \\ -5 \end{bmatrix}
\]

Find:

a. \( \mathbf{v}_1 + \mathbf{v}_2, \quad \mathbf{v}_1 + 2\mathbf{v}_2, \quad 3\mathbf{v}_2 - 4\mathbf{v}_3 \)

b. \( |\mathbf{v}_1|, |\mathbf{v}_2|, |\mathbf{v}_3| \)

c. \( \mathbf{v}_1 \cdot \mathbf{v}_2, \quad \mathbf{v}_3 \times \mathbf{v}_2, \quad \mathbf{v}_2 \cdot (\mathbf{v}_1 \times \mathbf{v}_3) \)

d. A unit vector in the direction of \( (\mathbf{v}_1 + \mathbf{v}_2 + \mathbf{v}_3) \)

Exercise 2
Let \( \mathbf{i}, \mathbf{j} \), and \( \mathbf{k} \) be unit vectors in the \( x, y \), and \( z \) direction, respectively, and let \( \mathbf{v} \) be any vector, which in a Cartesian coordinate system is given by

\[
\mathbf{v} = u\mathbf{i} + v\mathbf{j} + w\mathbf{k}
\]

Prove that

\[
\mathbf{v} = C[\mathbf{i} \times (\mathbf{v} \times \mathbf{i}) + \mathbf{j} \times (\mathbf{v} \times \mathbf{j}) + \mathbf{k} \times (\mathbf{v} \times \mathbf{k})]
\]

where \( C \) is a constant to be determined.

Exercise 3
Find \( \nabla s \) if \( s \) is the scalar function given by

a. \( s = y^2e^{2x-3z} \)

b. \( s = \ln(x + y^2 + z^3) \)

c. \( s = \tan^{-1}\left(\frac{z}{\sqrt{xy}}\right) \)

Exercise 4
If \( s \) is a scalar function and \( \mathbf{v} \) is a vector function, prove the following identities:

a. \( \nabla \times (\nabla s) = \mathbf{0} \)

b. \( \nabla \cdot (\mathbf{s}\mathbf{v}) = \mathbf{s} \cdot \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{s} \)

c. \( \nabla \times (\mathbf{s}\mathbf{v}) = \mathbf{s} \nabla \times \mathbf{v} + \nabla \mathbf{s} \times \mathbf{v} \)

d. \( \nabla \cdot (\mathbf{v}_1 \times \mathbf{v}_2) = \mathbf{v}_2 \cdot (\nabla \times \mathbf{v}_1) - \mathbf{v}_1 \cdot (\nabla \times \mathbf{v}_2) \)
Exercise 5
Use Green’s theorem to calculate the area enclosed by an ellipse of semi-major and semi-minor axes \(a\) and \(b\), respectively.

Exercise 6
Find the Laplacian of the scalar \(s (\nabla^2 s)\) for the cases when \(s\) is given by:

a. \(s = x^3 + z^2 e^{2y - 3x}\)
b. \(s = z + \ln(x + y)\)
c. \(s = \sin^{-1}(x + y + z)\)

Exercise 7
Verify the divergence theorem for the parallelepiped with centre at the origin and faces in the planes \(x = \pm 2, y = \pm 1, z = \pm 4\) and \(\mathbf{v}\) given by

a. \(\mathbf{v} = 5\mathbf{i} + 7\mathbf{j} - 3\mathbf{k}\)
b. \(\mathbf{v} = \mathbf{i}(y - z) + \mathbf{j}(x - z) + \mathbf{k}(x - y)\)
c. \(\mathbf{v} = \mathbf{i}y^2 z + \mathbf{j}xz^2 + \mathbf{k}x^2 y\)

Exercise 8
For a surface \(S\) representing the upper half of a cube centered at the origin, with one of its vertices at \((1, 1, 1)\), and with edges parallel to the axes, verify Stokes’s theorem for the case when the curve \(C\) is the intersection of \(S\) with the \(xy\) plane and the vector \(\mathbf{v}\) is given by

\[\mathbf{v} = \mathbf{i}(y + z) + \mathbf{j}(x + z) + \mathbf{k}(x + y)\]

Exercise 9
Find a function \(F\) for which the divergence is the given function \(K\) in the following cases:

a. \(K(x, y, z) = \pi.\)
b. \(K(x, y, z) = x^2.\)
c. \(K(x, y, z) = \sqrt{x^2 + z^2}\)

Exercise 10
Use the divergence theorem to evaluate the integral \(\iint \frac{\partial}{\partial F} (6\mathbf{i} + 4\mathbf{j}) \cdot d\mathbf{F}\) where the surface is a sphere defined as \(\partial F \rightarrow x^2 + y^2 + z^2 = 10.\)
Exercise 11
Let $F$ be a radial vector field defined as $F = xi + yj + zk$ and let $C$ to be a solid cylinder of radius $r$ and height $h$ with its axis coinciding with the $x$-axis and its bottom and top faces located along the $x = 0$ and $x = b$ plane, respectively. Verify Gauss theorem in both flux and divergence forms.

Exercise 12
Given a square matrix $A$ defined as

$$A = \begin{pmatrix}
a_{11} & a_{12} & \cdots \\
a_{21} & \ddots & \vdots \\
\vdots & \cdots & \cdots 
\end{pmatrix}$$

decompose it as

$$A = \frac{1}{2}(A + A^T) + \frac{1}{2}(A - A^T)$$

and show that

a. $\frac{1}{2}(A + A^T)$ is symmetric

b. $\frac{1}{2}(A - A^T)$ is anti-symmetric

Exercise 13
Given two tensors $A$ and $B$ defined as

$$A = \begin{pmatrix}
a_{11} & a_{12} & \cdots \\
a_{21} & \ddots & \vdots \\
\vdots & \cdots & \cdots 
\end{pmatrix} \quad B = \begin{pmatrix}
b_{11} & b_{12} & \cdots \\
b_{21} & \ddots & \vdots \\
\vdots & \cdots & \cdots 
\end{pmatrix}$$

a. Calculate the double inner product $A : B$.

b. Prove that $(A + B)^T = A^T + B^T$ and $(AB)^T = B^T A^T$

c. Evaluate $\nabla \cdot A + \nabla \cdot B$.

References

The Finite Volume Method in Computational Fluid Dynamics
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