

Appendix A

Vector differential operators

In this Appendix we introduce orthogonal curvilinear coordinates and derive the general expressions of the vector differential operators in this kind of coordinates. Moreover, we give the expressions of the differential operators for the particular cases of cylindrical and spherical coordinates. The presentation follows closely the treatment given in *Calculus of Several Variables* (Adams [2, p. 336]) from which the figures have been borrowed, by gentle permission of the author.

A.1 Orthogonal curvilinear coordinates

We assume that (u, v, w) are a set of *orthogonal* curvilinear coordinates in xyz -space defined via the transformation

$$x = x(u, v, w), \quad y = y(u, v, w), \quad z = z(u, v, w).$$

We also assume that the coordinate surfaces are smooth at any nonsingular point and that the local basis vectors $\hat{\mathbf{u}}$, $\hat{\mathbf{v}}$ and $\hat{\mathbf{w}}$ at any such point form a right-handed triad.

The position vector \mathbf{r} of a point P in xyz -space can be expressed in terms of the curvilinear coordinates:

$$\mathbf{r} = x(u, v, w) \mathbf{i} + y(u, v, w) \mathbf{j} + z(u, v, w) \mathbf{k}.$$

If we hold $v = v_0$ and $w = w_0$ fixed and let u vary, then $\mathbf{r} = \mathbf{r}(u, v_0, w_0)$ defines a u -curve in xyz -space. At any point P on this curve, the vector

$$\frac{\partial \mathbf{r}}{\partial u} = \frac{\partial x}{\partial u} \mathbf{i} + \frac{\partial y}{\partial u} \mathbf{j} + \frac{\partial z}{\partial u} \mathbf{k}$$

is tangent to the u -curve at P . In general, the three vectors

$$\frac{\partial \mathbf{r}}{\partial u}, \quad \frac{\partial \mathbf{r}}{\partial v}, \quad \frac{\partial \mathbf{r}}{\partial w}$$

are tangent, respectively, to the the u -curve, the v -curve and the w -curve through P . They are also normal, respectively, to the u -surface, the v -surface and the w -surface through P , so they are mutually perpendicular. (See Figure A.1) The lengths of these tangent vectors are called the *scale factors* of the coordinate system and are therefore defined by

$$h_u = \left| \frac{\partial \mathbf{r}}{\partial u} \right|, \quad h_v = \left| \frac{\partial \mathbf{r}}{\partial v} \right|, \quad h_w = \left| \frac{\partial \mathbf{r}}{\partial w} \right|.$$

The scale factors are nonzero at a nonsingular point P of the coordinate system, so a local basis for the coordinate system at P can be obtained by dividing the tangent vectors to the coordinate curves by their lengths. Denoting the local basis vectors by $\hat{\mathbf{u}}$, $\hat{\mathbf{v}}$ and $\hat{\mathbf{w}}$, we have

$$\frac{\partial \mathbf{r}}{\partial u} = h_u \hat{\mathbf{u}}, \quad \frac{\partial \mathbf{r}}{\partial v} = h_v \hat{\mathbf{v}}, \quad \frac{\partial \mathbf{r}}{\partial w} = h_w \hat{\mathbf{w}}.$$

The basis vectors $\hat{\mathbf{u}}$, $\hat{\mathbf{v}}$ and $\hat{\mathbf{w}}$ will form a right-handed triad provided we have chosen a suitable order for the coordinates u , v and w .

The volume element in an orthogonal curvilinear coordinate system is the volume of an infinitesimal *coordinate box* bounded by pairs of u -, v - and w -surfaces corresponding to values u and $u + du$, v and $v + dv$ and w and $w + dw$, respectively. See Figure A.1. Since these coordinate surfaces are assumed smooth, and since they intersect at right angles, the coordinate box is rectangular and is spanned by the vectors

$$\frac{\partial \mathbf{r}}{\partial u} du = h_u du \hat{\mathbf{u}}, \quad \frac{\partial \mathbf{r}}{\partial v} dv = h_v dv \hat{\mathbf{v}}, \quad \frac{\partial \mathbf{r}}{\partial w} dw = h_w dw \hat{\mathbf{w}}.$$

Therefore, the volume element is given by

$$dV = h_u h_v h_w du dv dw.$$

Furthermore, the surface area elements on the u -, v - and w -surfaces are the areas of the appropriate faces of the coordinate box:

$$dS_u = h_v h_w dv dw, \quad dS_v = h_u h_w du dw, \quad dS_w = h_u h_v du dv.$$

The arc length elements along the u -, v - and w -coordinate curves are the edges of the coordinate box:

$$ds_u = h_u du, \quad ds_v = h_v dv, \quad ds_w = h_w dw.$$

A.2 Differential operators

The gradient ∇f of a scalar field f can be expressed in terms of the local basis at any point P with curvilinear coordinates (u, v, w) in the form

$$\nabla f = F_u \hat{\mathbf{u}} + F_v \hat{\mathbf{v}} + F_w \hat{\mathbf{w}}.$$

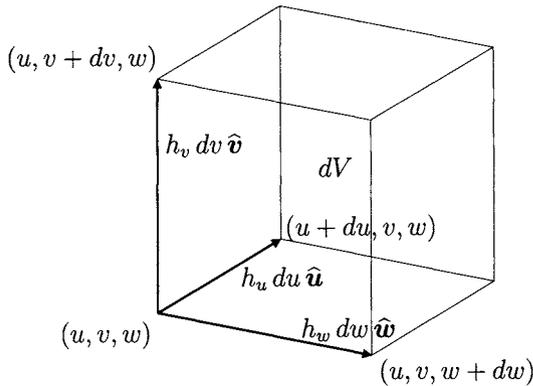


Figure A.1: Infinitesimal coordinate box of an orthogonal coordinate system.

In order to determine the coefficients F_u , F_v and F_w in this formula, we will compare two expressions for the directional derivative of f along an arbitrary curve in xyz -space.

If the curve \mathcal{C} has parametrization $\mathbf{r} = \mathbf{r}(s)$ in terms of arc length s , then the directional derivative of f along \mathcal{C} is given by

$$\frac{df}{ds} = \frac{\partial f}{\partial u} \frac{du}{ds} + \frac{\partial f}{\partial v} \frac{dv}{ds} + \frac{\partial f}{\partial w} \frac{dw}{ds}.$$

On the other hand, this directional derivative is also given by $\frac{df}{ds} = \nabla f \cdot \hat{\gamma}$, where $\hat{\gamma}$ is the unit tangent vector to \mathcal{C} . We have

$$\begin{aligned} \hat{\gamma} &= \frac{d\mathbf{r}}{ds} = \frac{\partial \mathbf{r}}{\partial u} \frac{du}{ds} + \frac{\partial \mathbf{r}}{\partial v} \frac{dv}{ds} + \frac{\partial \mathbf{r}}{\partial w} \frac{dw}{ds} \\ &= h_u \frac{du}{ds} \hat{\mathbf{u}} + h_v \frac{dv}{ds} \hat{\mathbf{v}} + h_w \frac{dw}{ds} \hat{\mathbf{w}}. \end{aligned}$$

Thus

$$\frac{df}{ds} = \nabla f \cdot \hat{\gamma} = F_u h_u \frac{du}{ds} + F_v h_v \frac{dv}{ds} + F_w h_w \frac{dw}{ds}.$$

Comparing these two expressions for df/ds along \mathcal{C} , we see that

$$F_u h_u = \frac{\partial f}{\partial u}, \quad F_v h_v = \frac{\partial f}{\partial v}, \quad F_w h_w = \frac{\partial f}{\partial w}.$$

Therefore, we have shown that

$$\nabla f(u, v, w) = \frac{1}{h_u} \frac{\partial f}{\partial u} \hat{\mathbf{u}} + \frac{1}{h_v} \frac{\partial f}{\partial v} \hat{\mathbf{v}} + \frac{1}{h_w} \frac{\partial f}{\partial w} \hat{\mathbf{w}}.$$

Now consider a vector field \mathbf{F} expressed in terms of the curvilinear coordinates:

$$\mathbf{F}(u, v, w) = F_u(u, v, w) \hat{\mathbf{u}} + F_v(u, v, w) \hat{\mathbf{v}} + F_w(u, v, w) \hat{\mathbf{w}}.$$

The flux of \mathbf{F} out of the infinitesimal coordinate box of Figure A.1 is the sum of the fluxes of \mathbf{F} out of the three pairs of opposite surfaces of the box. The flux out of the u -surfaces corresponding to u and $u + du$ is

$$\begin{aligned} & \mathbf{F}(u + du, v, w) \cdot \hat{\mathbf{u}} dS_u - \mathbf{F}(u, v, w) \cdot \hat{\mathbf{u}} dS_u \\ &= (F_u(u + du, v, w) h_v(u + du, v, w) h_w(u + du, v, w) \\ &\quad - F_u(u, v, w) h_v(u, v, w) h_w(u, v, w)) dv dw \\ &= \frac{\partial}{\partial u} (h_v h_w F_u) du dv dw. \end{aligned}$$

Similar expressions hold for the fluxes out of the other pairs of coordinate surfaces.

The divergence at P of \mathbf{F} is the flux per unit volume out of the infinitesimal coordinate box at P . Thus it is given by

$$\begin{aligned} \nabla \cdot \mathbf{F}(u, v, w) &= \frac{1}{h_u h_v h_w} \left[\frac{\partial}{\partial u} (h_v h_w F_u(u, v, w)) + \frac{\partial}{\partial v} (h_u h_w F_v(u, v, w)) \right. \\ &\quad \left. + \frac{\partial}{\partial w} (h_u h_v F_w(u, v, w)) \right]. \end{aligned}$$

To calculate the curl of a vector field expressed in terms of orthogonal curvilinear coordinates we can make use of some previously obtained vector identities. First, observe that the gradient of the scalar field $f(u, v, w) = u$ is $\hat{\mathbf{u}}/h_u$, so that $\hat{\mathbf{u}} = h_u \nabla u$. Similarly, $\hat{\mathbf{v}} = h_v \nabla v$ and $\hat{\mathbf{w}} = h_w \nabla w$. Therefore, the vector field

$$\mathbf{F} = F_u \hat{\mathbf{u}} + F_v \hat{\mathbf{v}} + F_w \hat{\mathbf{w}}$$

can be written in the form

$$\mathbf{F} = F_u h_u \nabla u + F_v h_v \nabla v + F_w h_w \nabla w.$$

Using the identity $\nabla \times (f \nabla g) = \nabla f \times \nabla g$, we can calculate the curl of each term in the expression above. We have

$$\begin{aligned} \nabla \times (F_u h_u \nabla u) &= \nabla (F_u h_u) \times \nabla u \\ &= \left[\frac{1}{h_u} \frac{\partial}{\partial u} (F_u h_u) \hat{\mathbf{u}} + \frac{1}{h_v} \frac{\partial}{\partial v} (F_u h_u) \hat{\mathbf{v}} + \frac{1}{h_w} \frac{\partial}{\partial w} (F_u h_u) \hat{\mathbf{w}} \right] \times \frac{\hat{\mathbf{u}}}{h_u} \\ &= \frac{1}{h_u h_w} \frac{\partial}{\partial w} (F_u h_u) \hat{\mathbf{v}} - \frac{1}{h_u h_v} \frac{\partial}{\partial v} (F_u h_u) \hat{\mathbf{w}} \\ &= \frac{1}{h_u h_v h_w} \left[\frac{\partial}{\partial w} (F_u h_u) (h_v \hat{\mathbf{v}}) - \frac{\partial}{\partial v} (F_u h_u) (h_w \hat{\mathbf{w}}) \right]. \end{aligned}$$

We have used the facts that $\hat{\mathbf{u}} \times \hat{\mathbf{u}} = \mathbf{0}$, $\hat{\mathbf{v}} \times \hat{\mathbf{u}} = -\hat{\mathbf{w}}$ and $\hat{\mathbf{w}} \times \hat{\mathbf{u}} = \hat{\mathbf{v}}$ to obtain the result above. This is why we assumed that the curvilinear coordinate system was right-handed. Corresponding expressions can be calculated for the other two terms in the formula for $\nabla \times \mathbf{F}$.

Combining the three terms, we conclude that the curl of

$$\mathbf{F} = F_u \hat{\mathbf{u}} + F_v \hat{\mathbf{v}} + F_w \hat{\mathbf{w}}$$

is given by

$$\nabla \times \mathbf{F}(u, v, w) = \frac{1}{h_u h_v h_w} \begin{vmatrix} h_u \hat{\mathbf{u}} & h_v \hat{\mathbf{v}} & h_w \hat{\mathbf{w}} \\ \frac{\partial}{\partial u} & \frac{\partial}{\partial v} & \frac{\partial}{\partial w} \\ F_u h_u & F_v h_v & F_w h_w \end{vmatrix}.$$

A.3 Cylindrical coordinates

A.3.1 Definition

For cylindrical coordinates we have $\mathbf{r} = r \cos \phi \mathbf{i} + r \sin \phi \mathbf{j} + z \mathbf{k}$, so

$$\frac{\partial \mathbf{r}}{\partial r} = \cos \phi \mathbf{i} + \sin \phi \mathbf{j}, \quad \frac{\partial \mathbf{r}}{\partial \phi} = -r \sin \phi \mathbf{i} + r \cos \phi \mathbf{j}, \quad \frac{\partial \mathbf{r}}{\partial z} = \mathbf{k}.$$

It should be noted that here r does not denote the magnitude of the position vector \mathbf{r} , but the distance of \mathbf{r} from the z -axis. Similarly, the vector $\hat{\mathbf{r}}(\phi)$ does not represent the unit vector in direction of \mathbf{r} , but the directions orthogonal to the z -axis.

The scale factors for the cylindrical coordinate system are given by

$$h_r = \left| \frac{\partial \mathbf{r}}{\partial r} \right| = 1, \quad h_\phi = \left| \frac{\partial \mathbf{r}}{\partial \phi} \right| = r, \quad h_z = \left| \frac{\partial \mathbf{r}}{\partial z} \right| = 1,$$

and the local basis consists of the vectors

$$\hat{\mathbf{r}} = \cos \phi \mathbf{i} + \sin \phi \mathbf{j}, \quad \hat{\boldsymbol{\phi}} = -\sin \phi \mathbf{i} + \cos \phi \mathbf{j}, \quad \hat{\mathbf{z}} = \mathbf{k}.$$

See Figure A.2. The local basis is right-handed. The unit vectors do not change with r or z , but

$$\frac{\partial \hat{\mathbf{r}}}{\partial \phi} = \hat{\boldsymbol{\phi}}, \quad \frac{\partial \hat{\boldsymbol{\phi}}}{\partial \phi} = -\hat{\mathbf{r}}, \quad \frac{\partial \hat{\mathbf{z}}}{\partial \phi} = 0.$$

The volume element is given by

$$dV = h_r h_\phi h_z dr d\phi dz = r dr d\phi dz.$$

Its boundary consists of surface elements on the cylinder $r = \text{constant}$, the half-plane $\phi = \text{constant}$ and the plane $z = \text{constant}$. These elements are given, respectively, by

$$dS_r = r d\phi dz, \quad dS_\phi = dr dz, \quad dS_z = r dr d\phi.$$

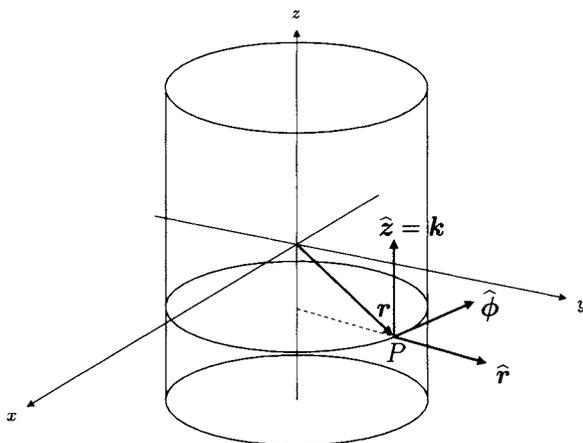


Figure A.2: Cylindrical coordinate system.

A.3.2 Gradient, divergence and curl

In terms of cylindrical coordinates, the gradient of the scalar field $f(r, \phi, z)$ is given by

$$\nabla f(r, \phi, z) = \frac{\partial f}{\partial r} \hat{\mathbf{r}} + \frac{1}{r} \frac{\partial f}{\partial \phi} \hat{\boldsymbol{\phi}} + \frac{\partial f}{\partial z} \hat{\mathbf{z}}.$$

Since for cylindrical coordinates $h_r = h_z = 1$ and $h_\theta = r$, the divergence of $\mathbf{F} = F_r \hat{\mathbf{r}} + F_\phi \hat{\boldsymbol{\phi}} + F_z \hat{\mathbf{z}}$ is

$$\begin{aligned} \nabla \cdot \mathbf{F} &= \frac{1}{r} \left[\frac{\partial}{\partial r}(rF_r) + \frac{\partial}{\partial \phi} F_\phi + \frac{\partial}{\partial z}(rF_z) \right] \\ &= \frac{\partial F_r}{\partial r} + \frac{1}{r} F_r + \frac{1}{r} \frac{\partial F_\phi}{\partial \phi} + \frac{\partial F_z}{\partial z}. \end{aligned}$$

The curl of \mathbf{F} is given by

$$\begin{aligned} \nabla \times \mathbf{F} &= \frac{1}{r} \begin{vmatrix} \hat{\mathbf{r}} & r\hat{\boldsymbol{\phi}} & \hat{\mathbf{z}} \\ \frac{\partial}{\partial r} & \frac{\partial}{\partial \phi} & \frac{\partial}{\partial z} \\ F_r & rF_\phi & F_z \end{vmatrix} \\ &= \left(\frac{1}{r} \frac{\partial F_z}{\partial \phi} - \frac{\partial F_\phi}{\partial z} \right) \hat{\mathbf{r}} + \left(\frac{\partial F_r}{\partial z} - \frac{\partial F_z}{\partial r} \right) \hat{\boldsymbol{\phi}} + \left(\frac{\partial F_\phi}{\partial r} + \frac{F_\phi}{r} - \frac{1}{r} \frac{\partial F_r}{\partial \phi} \right) \hat{\mathbf{z}}. \end{aligned}$$

A.3.3 Laplace and advection operators

Remembering that the Laplacian of a function f is defined by the relationship

$$\nabla^2 f = \nabla \cdot \nabla f,$$

the results just obtained for the gradient and the divergence lead to the following expression for the Laplacian in cylindrical coordinates

$$\begin{aligned} \nabla^2 f &= \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial f}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 f}{\partial \phi^2} + \frac{\partial^2 f}{\partial z^2} \\ &= \frac{\partial^2 f}{\partial r^2} + \frac{1}{r} \frac{\partial f}{\partial r} + \frac{1}{r^2} \frac{\partial^2 f}{\partial \phi^2} + \frac{\partial^2 f}{\partial z^2} + \frac{\partial^2 f}{\partial z^2}. \end{aligned}$$

As far as the Laplacian of a vector field \mathbf{F} is concerned, its explicit expression can be derived from the vector identity

$$\nabla^2 \mathbf{F} = -\nabla \times (\nabla \times \mathbf{F}) + \nabla (\nabla \cdot \mathbf{F}),$$

and using some previously obtained results. We obtain

$$\begin{aligned} \nabla^2 \mathbf{F} &= \left(\nabla^2 F_r - \frac{F_r}{r^2} - \frac{2}{r^2} \frac{\partial F_\phi}{\partial \phi} \right) \hat{\mathbf{r}} \\ &\quad + \left(\nabla^2 F_\phi - \frac{F_\phi}{r^2} + \frac{2}{r^2} \frac{\partial F_r}{\partial \phi} \right) \hat{\boldsymbol{\phi}} \\ &\quad + (\nabla^2 F_z) \hat{\mathbf{z}}. \end{aligned}$$

Finally, we give the expression in cylindrical coordinates of the advection operators for both a scalar and a vector field:

$$\mathbf{a} \cdot \nabla u = a_r \frac{\partial u}{\partial r} + \frac{a_\phi}{r} \frac{\partial u}{\partial \phi} + a_z \frac{\partial u}{\partial z},$$

$$\begin{aligned} (\mathbf{a} \cdot \nabla) \mathbf{u} &= \left[(\mathbf{a} \cdot \nabla) u_r - \frac{a_\phi u_\phi}{r} \right] \hat{\mathbf{r}} \\ &\quad + \left[(\mathbf{a} \cdot \nabla) u_\phi + \frac{a_\phi u_r}{r} \right] \hat{\boldsymbol{\phi}} \\ &\quad + [(\mathbf{a} \cdot \nabla) u_z] \hat{\mathbf{z}}. \end{aligned}$$

A.4 Spherical coordinates

A.4.1 Definition

For spherical coordinates we have

$$\mathbf{r} = r \sin \theta \cos \phi \mathbf{i} + r \sin \theta \sin \phi \mathbf{j} + r \cos \theta \hat{\mathbf{z}}.$$

Thus the tangent vectors to the coordinate curves are

$$\frac{\partial \mathbf{r}}{\partial r} = \sin \theta \cos \phi \mathbf{i} + \sin \theta \sin \phi \mathbf{j} + \cos \theta \hat{\mathbf{z}}$$

$$\frac{\partial \mathbf{r}}{\partial \theta} = r \cos \theta \cos \phi \mathbf{i} + r \cos \theta \sin \phi \mathbf{j} - r \sin \theta \hat{\mathbf{z}}$$

$$\frac{\partial \mathbf{r}}{\partial \phi} = -r \sin \theta \sin \phi \mathbf{i} + r \sin \theta \cos \phi \mathbf{j},$$

and the scale factors are given by

$$h_r = \left| \frac{\partial \mathbf{r}}{\partial r} \right| = 1, \quad h_\theta = \left| \frac{\partial \mathbf{r}}{\partial \theta} \right| = r, \quad h_\phi = \left| \frac{\partial \mathbf{r}}{\partial \phi} \right| = r \sin \theta.$$

The local basis consists of the vectors

$$\hat{\mathbf{r}} = \sin \theta \cos \phi \mathbf{i} + \sin \theta \sin \phi \mathbf{j} + \cos \theta \hat{\mathbf{z}}$$

$$\hat{\boldsymbol{\theta}} = \cos \theta \cos \phi \mathbf{i} + \cos \theta \sin \phi \mathbf{j} - \sin \theta \hat{\mathbf{z}}$$

$$\hat{\boldsymbol{\phi}} = -\sin \phi \mathbf{i} + \cos \phi \mathbf{j}.$$

See Figure A.3. The local basis is right-handed. The unit vectors do not change with r , but

$$\begin{aligned} \frac{\partial \hat{\mathbf{r}}}{\partial \theta} &= \hat{\boldsymbol{\theta}}, & \frac{\partial \hat{\boldsymbol{\theta}}}{\partial \theta} &= -\hat{\mathbf{r}}, & \frac{\partial \hat{\boldsymbol{\phi}}}{\partial \theta} &= 0, \\ \frac{\partial \hat{\mathbf{r}}}{\partial \phi} &= \sin \theta \hat{\boldsymbol{\phi}}, & \frac{\partial \hat{\boldsymbol{\theta}}}{\partial \phi} &= \cos \theta \hat{\boldsymbol{\phi}}, & \frac{\partial \hat{\boldsymbol{\phi}}}{\partial \phi} &= -\sin \theta \hat{\mathbf{r}} - \cos \theta \hat{\boldsymbol{\theta}}. \end{aligned}$$

The volume element in spherical coordinates is

$$dV = h_r h_\theta h_\phi dr d\theta d\phi = r^2 \sin \theta dr d\theta d\phi.$$

The area element on the sphere $r = \text{constant}$ is

$$dS_r = h_\theta h_\phi d\theta d\phi = r^2 \sin \theta d\theta d\phi.$$

The area element on the cone $\theta = \text{constant}$ is

$$dS_\theta = h_r h_\phi dr d\phi = r \sin \theta dr d\phi.$$

The area element on the half-plane $\phi = \text{constant}$ is

$$dS_\phi = h_r h_\theta dr d\theta = r dr d\theta.$$

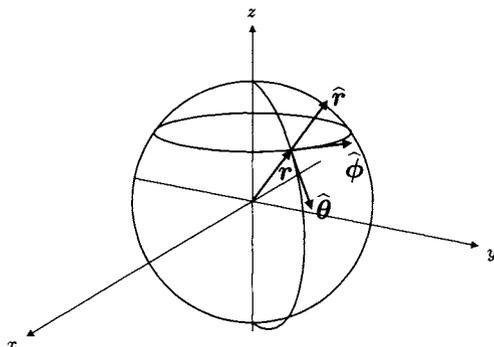


Figure A.3: Spherical coordinate system.

A.4.2 Gradient, divergence and curl

In terms of spherical coordinates, the gradient of the scalar field $f(r, \theta, \phi)$ is expressed by

$$\nabla f(r, \theta, \phi) = \frac{\partial f}{\partial r} \hat{r} + \frac{1}{r} \frac{\partial f}{\partial \theta} \hat{\theta} + \frac{1}{r \sin \theta} \frac{\partial f}{\partial \phi} \hat{\phi}.$$

For spherical coordinates, $h_r = 1$, $h_\theta = r$ and $h_\phi = r \sin \theta$. The divergence of the vector field $\mathbf{F} = F_r \hat{r} + F_\theta \hat{\theta} + F_\phi \hat{\phi}$ is

$$\begin{aligned} \nabla \cdot \mathbf{F} &= \frac{1}{r^2 \sin \theta} \left[\frac{\partial}{\partial r} (r^2 \sin \theta F_r) + \frac{\partial}{\partial \theta} (r \sin \theta F_\theta) + \frac{\partial}{\partial \phi} (r F_\phi) \right] \\ &= \frac{\partial}{\partial r} (r^2 F_r) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta F_\theta) + \frac{1}{r \sin \theta} \frac{\partial F_\phi}{\partial \phi} \\ &= \frac{\partial F_r}{\partial r} + \frac{2}{r} F_r + \frac{1}{r} \frac{\partial F_\theta}{\partial \theta} + \frac{\cot \theta}{r} F_\theta + \frac{1}{r \sin \theta} \frac{\partial F_\phi}{\partial \phi}. \end{aligned}$$

The curl of \mathbf{F} is given by

$$\begin{aligned}\nabla \times \mathbf{F} &= \frac{1}{r^2 \sin \theta} \begin{vmatrix} \hat{\mathbf{r}} & r\hat{\boldsymbol{\theta}} & r \sin \theta \hat{\boldsymbol{\phi}} \\ \frac{\partial}{\partial r} & \frac{\partial}{\partial \theta} & \frac{\partial}{\partial \phi} \\ F_r & rF_\theta & r \sin \theta F_\phi \end{vmatrix} \\ &= \frac{1}{r \sin \theta} \left(\cos \theta F_\phi + \sin \theta \frac{\partial F_\phi}{\partial \theta} - \frac{\partial F_\theta}{\partial \phi} \right) \hat{\mathbf{r}} \\ &\quad + \frac{1}{r \sin \theta} \left(\frac{\partial F_r}{\partial \phi} - \sin \theta F_\phi - r \sin \theta \frac{\partial F_\phi}{\partial r} \right) \hat{\boldsymbol{\theta}} \\ &\quad + \frac{1}{r} \left(F_\theta + r \frac{\partial F_\theta}{\partial r} - \frac{\partial F_r}{\partial \theta} \right) \hat{\boldsymbol{\phi}}.\end{aligned}$$

A.4.3 Laplace and advection operators

Using the results above, the expressions of the Laplacian operators in spherical coordinates are easily found. The Laplacian of the scalar field $f(r, \theta, \phi)$ assumes the form

$$\begin{aligned}\nabla^2 f &= \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial f}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial f}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 f}{\partial \phi^2} \\ &= \frac{\partial^2 f}{\partial r^2} + \frac{2}{r} \frac{\partial f}{\partial r} + \frac{\cot \theta}{r^2} \frac{\partial f}{\partial \theta} + \frac{1}{r^2} \frac{\partial^2 f}{\partial \theta^2} + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 f}{\partial \phi^2},\end{aligned}$$

whereas the Laplacian of the vector field $\mathbf{F} = F_r \hat{\mathbf{r}} + F_\theta \hat{\boldsymbol{\theta}} + F_\phi \hat{\boldsymbol{\phi}}$ is

$$\begin{aligned}\nabla^2 \mathbf{F} &= \left(\nabla^2 F_r - \frac{2F_r}{r^2} - \frac{2}{r^2 \sin \theta} \frac{\partial(\sin \theta F_\theta)}{\partial \theta} - \frac{2}{r^2 \sin \theta} \frac{\partial F_\phi}{\partial \phi} \right) \hat{\mathbf{r}} \\ &\quad + \left(\nabla^2 F_\theta - \frac{F_\theta}{r^2 \sin^2 \theta} - \frac{2 \cos \theta}{r^2 \sin^2 \theta} \frac{\partial F_\phi}{\partial \phi} + \frac{2}{r^2} \frac{\partial F_r}{\partial \theta} \right) \hat{\boldsymbol{\theta}} \\ &\quad + \left(\nabla^2 F_\phi - \frac{F_\phi}{r^2 \sin^2 \theta} + \frac{2 \cos \theta}{r^2 \sin^2 \theta} \frac{\partial F_\theta}{\partial \phi} + \frac{2}{r^2 \sin \theta} \frac{\partial F_r}{\partial \phi} \right) \hat{\boldsymbol{\phi}}.\end{aligned}$$

Finally, the advection operators in spherical coordinates assume the form

$$\mathbf{a} \cdot \nabla u = a_r \frac{\partial u}{\partial r} + \frac{a_\theta}{r} \frac{\partial u}{\partial \theta} + \frac{a_\phi}{r \sin \theta} \frac{\partial u}{\partial \phi},$$

$$\begin{aligned}(\mathbf{a} \cdot \nabla) \mathbf{u} &= \left[(\mathbf{a} \cdot \nabla) u_r - \frac{a_\theta u_\theta + a_\phi u_\phi}{r} \right] \hat{\mathbf{r}} \\ &+ \left[(\mathbf{a} \cdot \nabla) u_\theta + \frac{a_\theta u_r - \cot \theta a_\phi u_\phi}{r} \right] \hat{\boldsymbol{\theta}} \\ &+ \left[(\mathbf{a} \cdot \nabla) u_\phi + \frac{a_\phi u_r + \cot \theta a_\theta u_\theta}{r} \right] \hat{\boldsymbol{\phi}}.\end{aligned}$$

Appendix B

Separation of vector elliptic equations

B.1 Introduction

Many of the methods discussed in this study for the approximate solution of the incompressible Navier–Stokes require to solve Poisson and Helmholtz equations of vector type, supplemented by Dirichlet boundary conditions. As well known, this kind of boundary value problems for a vector field separates into uncoupled Dirichlet problems for the scalar components of the unknown only in Cartesian coordinates. On the contrary, when the vector elliptic equation is expressed in polar, cylindrical or spherical coordinates, the Laplace operator acting on a vector field produces a system of coupled elliptic equations for the orthogonal components of the unknown. The aim of the present Appendix is to describe the similarity transformations which reduce the vector Poisson equation expressed in these orthogonal coordinate systems into a set of uncoupled elliptic equations for scalar unknowns.

Four different geometrical situations will be analyzed. Firstly, the vector two-dimensional Poisson equation in polar coordinates is examined (section B.2). Secondly, the case of elliptic equations for a vector field defined on, and tangential to, a spherical surface is considered, using the latitude and the longitude as orthogonal coordinates (section B.3). For both cases, the same similarity transformation is found to be effective.

Three-dimensional equations are then addressed, starting with the examination of cylindrical coordinates (section B.4). Here, the solution domain of the Poisson equation is assumed to consist of an entire annular region of the three-dimensional space, so that the dependence on the angular variable can be represented by Fourier analysis. A convenient complex representation of the vector field is introduced to obtain a real (*i.e.*, noncomplex) characterization

of the operator occurring in the Fourier-transformed problem. In this way, the three-dimensional vector problem is reduced to a set of two-dimensional problems, but always of vector type. Two of the three cylindrical components of each Fourier mode, with the exception of the first mode, are found to be coupled together by the elliptic operator, like the cylindrical components of the original three-dimensional vector problem. This coupling is eliminated by a similarity transformation which reduces the operator to a diagonal form.

A similar analysis is finally conducted for the 3D vector Poisson equation in annular regions radially bounded by two concentric spherical surfaces, using spherical coordinates (section B.5). In this case, after the Fourier analysis of the longitudinal dependence, the three spherical components of each Fourier mode of the vector unknown are found to be solution of a system of three two-dimensional elliptic equations which are coupled together. The coupling is eliminated by an appropriate similarity transformation and the solution of the original problem is thus reduced to a sequence of purely scalar elliptic equations in two dimensions, plus the operations for performing the transformation, the Fourier analysis of the data as well as the synthesis of the solution.

As it will be shown, the similarity transformations which allow the uncoupling (in 3D after Fourier analysis) of the orthogonal components of the vector unknown are so simple that some of them, if not all, may have been already considered and employed in other studies. However, since the complete set of these transformations is not easily available in the computational literature, it is collected here, also with the purpose of showing how the use of solution algorithms for scalar two-dimensional elliptic equations can be extended to the solution of Dirichlet problems for vector fields in two and three dimensions.

B.2 Polar coordinates

Let us consider the vector Poisson equation $\nabla^2 \mathbf{u} = \mathbf{f}$ in two dimensions expressed in polar coordinates (r, ϕ) . The Laplace operator in this coordinate system is

$$\nabla^2 = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2}{\partial \phi^2},$$

the vector field \mathbf{u} being expressed in its polar components (u_r, u_ϕ) according to

$$\mathbf{u}(r, \phi) = u_r(r, \phi) \hat{\mathbf{r}}(\phi) + u_\phi(r, \phi) \hat{\boldsymbol{\phi}}(\phi),$$

where $\hat{\mathbf{r}}(\phi)$ and $\hat{\boldsymbol{\phi}}(\phi)$ are the unit vectors of the polar coordinate system. Due to the dependence of the unit vectors on the angle ϕ , the action of the Laplace operator on a vector field is such that the vector Poisson equation becomes, in

polar components, (see, e.g., Acheson [1])

$$\begin{aligned} \left(\nabla^2 - \frac{1}{r^2}\right) u_r - \frac{2}{r^2} \frac{\partial u_\phi}{\partial \phi} &= f_r, \\ \left(\nabla^2 - \frac{1}{r^2}\right) u_\phi + \frac{2}{r^2} \frac{\partial u_r}{\partial \phi} &= f_\phi. \end{aligned}$$

Thus, a system of two coupled scalar elliptic equations for the polar components of the unknown is obtained. Introducing the matrix differential operator

$$\nabla^2 = \begin{pmatrix} \nabla^2 - \frac{1}{r^2} & -\frac{2}{r^2} \frac{\partial}{\partial \phi} \\ \frac{2}{r^2} \frac{\partial}{\partial \phi} & \nabla^2 - \frac{1}{r^2} \end{pmatrix},$$

the vector Poisson equation $\nabla^2 \mathbf{u} = \mathbf{f}$ can be written in the matrix form:

$$\nabla^2 \begin{pmatrix} u_r \\ u_\phi \end{pmatrix} = \begin{pmatrix} f_r \\ f_\phi \end{pmatrix}.$$

Let us now consider the change of variables defined by the following linear transformation

$$\mathbf{t}(\phi) = \begin{pmatrix} \sin \phi & \cos \phi \\ \cos \phi & -\sin \phi \end{pmatrix}, \quad \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \mathbf{t}(\phi) \begin{pmatrix} u_r \\ u_\phi \end{pmatrix}.$$

The matrix $\mathbf{t}(\phi)$ is such that $\mathbf{t}(\phi) = \mathbf{t}(\phi)^{\text{tr}} = \mathbf{t}(\phi)^{-1}$, and thus is both symmetric and orthogonal. As usual, the superscript “tr” denotes transposition. By simple calculations one can show that the similarity transformation provided by matrix $\mathbf{t}(\phi)$ is such that

$$\mathbf{t}(\phi) \nabla^2 \mathbf{t}(\phi) = \begin{pmatrix} \nabla^2 & 0 \\ 0 & \nabla^2 \end{pmatrix},$$

i.e., it diagonalizes the matrix operator of the vector Poisson equation in polar coordinates. As a consequence, the solution of such an equation can be calculated by first applying the transformation $\mathbf{t}(\phi)$ to the source field \mathbf{f} , then solving the two independent equations

$$\begin{aligned} \nabla^2 u_1 &= f_1, \\ \nabla^2 u_2 &= f_2, \end{aligned}$$

and finally backtransforming the two computed solutions u_1 and u_2 according to

$$\begin{pmatrix} u_r \\ u_\phi \end{pmatrix} = \mathbf{t}(\phi) \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}.$$

Of course, the transformation $\mathbf{t}(\phi)$ must be applied also to the prescribed data of the boundary conditions associated with the original vector elliptic problem.

The same transformation can be obviously applied also to the Dirichlet vector problem for the Helmholtz operator $(\nabla^2 - \gamma)$, with $\gamma > 0$. More generally, the

similarity transformation is effective in separating the polar components in any Dirichlet problem for the operator $(\nabla^2 - \Gamma(r))$, where $\Gamma(r)$ is a given function, possibly satisfying some suitable conditions.

In the particular case of an annular domain, $[r_1 \leq r \leq r_2, 0 \leq \phi < 2\pi]$, the two-dimensional scalar Poisson equation $\nabla^2 u = f$ could be solved by introducing a Fourier representation of the dependence on ϕ in f and u by means of complex Fourier series, namely,

$$f(r, \phi) = \sum_{m=-\infty}^{\infty} f_m(r) e^{im\phi}, \quad u(r, \phi) = \sum_{m=-\infty}^{\infty} u_m(r) e^{im\phi}.$$

This decomposition reduces the two-dimensional Poisson equation to a set of ordinary differential equations for the second-order operator

$$\mathcal{D}_m^2 = \frac{1}{r} \frac{d}{dr} \left(r \frac{d}{dr} \right) - \frac{m^2}{r^2} = \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} - \frac{m^2}{r^2}.$$

The equation governing the Fourier coefficient $u_m(r)$, namely,

$$\mathcal{D}_m^2 u_m = f_m,$$

is an Euler (equidimensional) equation whose solution can be written as

$$u_m(r) = A_m r^m + B_m r^{-m} + F_m(r),$$

where A_m and B_m are constants determined by the boundary conditions, and $F_m(r)$ is any particular solution to the equation (14).

It is interesting to note that, always with reference to the annular domain, the solution method above is not the only method allowing the reduction of the vector elliptic equation to a set of uncoupled ordinary differential equations for scalar unknowns. Another method consists in introducing the Fourier decomposition *before* uncoupling the vector components of the unknown by means of the similarity transformation. In fact, let the vector field $\mathbf{u}(r, \phi)$, $0 \leq \phi < 2\pi$, be represented by means of the following complex Fourier series:

$$\mathbf{u}(r, \phi) = \mathbf{u}_0(r; \phi) + \sum_{\substack{m=-\infty \\ m \neq 0}}^{\infty} \mathbf{u}_m(r; \phi) e^{im\phi},$$

where

$$\mathbf{u}_0(r; \phi) = u_{r,0}(r) \hat{\mathbf{r}}(\phi) + u_{\phi,0}(r) \hat{\boldsymbol{\phi}}(\phi)$$

and

$$\mathbf{u}_m(r; \phi) = u_{r,m}(r) \hat{\mathbf{r}}(\phi) + u_{\phi,m}(r) \hat{\boldsymbol{\phi}}(\phi) i.$$

In the expansion above, the coefficient of the angular component of the Fourier mode, with the exclusion of the first mode, has been multiplied by the imaginary

unit in order to obtain a purely real representation of the second-order matrix operator acting on the Fourier coefficients of the vector mode. The condition that the vector function \mathbf{u} be real-valued implies that the complex coefficients

$$\begin{aligned} u_{r,m}(r) &= v_{r,m}(r) + i w_{r,m}(r), \\ u_{\phi,m}(r) &= v_{\phi,m}(r) + i w_{\phi,m}(r), \end{aligned}$$

for $m > 0$, satisfy the following conditions:

$$\begin{aligned} v_{r,-m} &= v_{r,m}, & w_{r,-m} &= -w_{r,m}; \\ v_{\phi,-m} &= -v_{\phi,m}, & w_{\phi,-m} &= w_{\phi,m}. \end{aligned}$$

According to this Fourier representation, the Laplace operator ∇^2 acting on the Fourier coefficients of the m th vector mode becomes

$$\mathcal{D}_m^2 = \begin{pmatrix} \mathcal{D}_m^2 - \frac{1}{r^2} & \frac{2m}{r^2} \\ \frac{2m}{r^2} & \mathcal{D}_m^2 - \frac{1}{r^2} \end{pmatrix}.$$

Therefore, the conditions of reality mean that the complex system

$$\mathcal{D}_m^2 \begin{pmatrix} u_{r,m} \\ u_{\phi,m} \end{pmatrix} = \begin{pmatrix} f_{r,m} \\ f_{\phi,m} \end{pmatrix}$$

has to be solved only for $m > 0$. Of course, such a complex system is equivalent to the two real systems

$$\mathcal{D}_m^2 \begin{pmatrix} v_{r,m} \\ v_{\phi,m} \end{pmatrix} = \begin{pmatrix} g_{r,m} \\ g_{\phi,m} \end{pmatrix}, \quad \mathcal{D}_m^2 \begin{pmatrix} w_{r,m} \\ w_{\phi,m} \end{pmatrix} = \begin{pmatrix} h_{r,m} \\ h_{\phi,m} \end{pmatrix},$$

where the right hand sides are the real and imaginary parts of the complex Fourier coefficients of \mathbf{f} , *i.e.*, $\mathbf{f}_m = \mathbf{g}_m + i \mathbf{h}_m$.

Introducing the similarity transformation

$$\mathbf{s} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix},$$

the matrix ordinary differential operator \mathcal{D}_m is diagonalized as follows

$$\mathbf{s} \mathcal{D}_m^2 \mathbf{s} = \begin{pmatrix} \mathcal{D}_{m-1}^2 & 0 \\ 0 & \mathcal{D}_{m+1}^2 \end{pmatrix}.$$

This uncoupling is exploited in section 4 to deal with the three-dimensional vector Poisson equation expressed in cylindrical coordinates.

Once the pairs $v_{r,m}, v_{\phi,m}$, and $w_{r,m}, w_{\phi,m}$, have been determined, the solution \mathbf{u} can be expressed in real form according to

$$\begin{aligned} \mathbf{u}(r, \phi) &= \left\{ u_{r,0}(r) + 2 \sum_{m=1}^{\infty} [v_{r,m}(r) \cos(m\phi) - w_{r,m}(r) \sin(m\phi)] \right\} \hat{\mathbf{r}}(\phi) \\ &+ \left\{ u_{\phi,0}(r) - 2 \sum_{m=1}^{\infty} [v_{\phi,m}(r) \sin(m\phi) + w_{\phi,m}(r) \cos(m\phi)] \right\} \hat{\boldsymbol{\phi}}(\phi). \end{aligned}$$

B.3 Spherical coordinates on the unit sphere

The similarity transformation $\mathbf{t}(\phi)$ is effective also in diagonalizing the Poisson equation which governs a vector field defined on, and tangential to, the surface of a sphere. Consider the unit sphere and an orthogonal coordinate system on it, consisting of the angular variables latitude θ ($0 \leq \theta \leq \pi$) and longitude ϕ ($0 \leq \phi < 2\pi$). The Laplace operator over the unit sphere is

$$\nabla^2 = \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2},$$

and a vector field \mathbf{u} “belonging” to the spherical surface can be expressed in terms of its spherical components u_θ and u_ϕ according to

$$\mathbf{u}(\theta, \phi) = u_\theta(\theta, \phi) \hat{\boldsymbol{\theta}}(\theta, \phi) + u_\phi(\theta, \phi) \hat{\boldsymbol{\phi}}(\theta, \phi),$$

where $\hat{\boldsymbol{\theta}}(\theta, \phi)$ and $\hat{\boldsymbol{\phi}}(\theta, \phi)$ denote the two unit vectors of the spherical coordinate system over the spherical surface.

It is to be noted that the Laplacian and the other related second-order differential operators introduced in each section of this Appendix represent the operators in different coordinates, but are indicated by identical symbols in the various sections to avoid a cumbersome notation. In other words, the definite meaning of these operators changes in each section although they are denoted identically, since the range of validity of each definition is limited only to a specific section.

Considering now the vector Poisson equation $\nabla^2 \mathbf{u} = \mathbf{f}$, in terms of its spherical components it becomes

$$\begin{aligned} \left(\nabla^2 - \frac{1}{\sin^2 \theta} \right) u_\theta - \frac{2 \cos \theta}{\sin^2 \theta} \frac{\partial u_\phi}{\partial \phi} &= f_\theta, \\ \left(\nabla^2 - \frac{1}{\sin^2 \theta} \right) u_\phi + \frac{2 \cos \theta}{\sin^2 \theta} \frac{\partial u_\theta}{\partial \phi} &= f_\phi. \end{aligned}$$

Introducing the matrix differential operator

$$\nabla^2 = \begin{pmatrix} \nabla^2 - \frac{1}{\sin^2 \theta} & -\frac{2 \cos \theta}{\sin^2 \theta} \frac{\partial}{\partial \phi} \\ \frac{2 \cos \theta}{\sin^2 \theta} \frac{\partial}{\partial \phi} & \nabla^2 - \frac{1}{\sin^2 \theta} \end{pmatrix},$$

the Poisson equation can be written in the matrix form

$$\nabla^2 \begin{pmatrix} u_\theta \\ u_\phi \end{pmatrix} = \begin{pmatrix} f_\theta \\ f_\phi \end{pmatrix}.$$

Now, the partial derivative $\frac{\partial}{\partial\phi}$ occurs in this matrix operator ∇^2 as well as in the Laplacian ∇^2 exactly as it occurs in the corresponding operators in polar coordinates. Therefore, the similarity transformation $\mathbf{t}(\phi)$ introduced in the previous section,

$$\mathbf{t}(\phi) = \begin{pmatrix} \sin\phi & \cos\phi \\ \cos\phi & -\sin\phi \end{pmatrix}, \quad \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \mathbf{t}(\phi) \begin{pmatrix} u_\theta \\ u_\phi \end{pmatrix},$$

diagonalize also the matrix operator ∇^2 for spherical coordinates, namely,

$$\mathbf{t}(\phi) \nabla^2 \mathbf{t}(\phi) = \begin{pmatrix} \nabla^2 & 0 \\ 0 & \nabla^2 \end{pmatrix}.$$

Similarly to polar coordinates, the solution of the equation $\nabla^2 \mathbf{u} = \mathbf{f}$ on the unit sphere can be calculated by applying the transformation $\mathbf{t}(\phi)$ to the source field \mathbf{f} , solving the two independent equations

$$\nabla^2 u_1 = f_1,$$

$$\nabla^2 u_2 = f_2,$$

and backtransforming the calculated solutions through

$$\begin{pmatrix} u_\theta \\ u_\phi \end{pmatrix} = \mathbf{t}(\phi) \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}.$$

The same transformation can be applied to more general elliptic equations, such as, for instance, the Helmholtz equation $(\nabla^2 - \gamma)\mathbf{u} = \mathbf{f}$, with $\gamma > 0$, or the equation $(\nabla^2 - \Gamma(\theta))\mathbf{u} = \mathbf{f}$, where $\Gamma(\theta)$ is a given function possibly satisfying convenient conditions.

As for polar coordinates, if the domain is such that $0 \leq \phi < 2\pi$, it would be possible to reduce each scalar Poisson equation $\nabla^2 u = f$ to a set of second-order ordinary differential equations by introducing a Fourier decomposition of the involved functions.

B.4 Cylindrical coordinates

Coming to three-dimensional problems, we examine first the case of cylindrical coordinates (r, z, ϕ) . Let us consider the Poisson equation $\nabla^2 \mathbf{u} = \mathbf{f}$, with the Laplace operator defined by

$$\nabla^2 = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} \right) + \frac{\partial^2}{\partial z^2} + \frac{1}{r^2} \frac{\partial^2}{\partial \phi^2}.$$

If the vector field \mathbf{u} is expressed in terms of its cylindrical components u_r , u_z and u_ϕ , the Laplacian pertaining to the vector problem is found to be given by the matrix (see section A.3.3 of Appendix A)

$$\nabla^2 = \begin{pmatrix} \nabla^2 - \frac{1}{r^2} & 0 & -\frac{2}{r^2} \frac{\partial}{\partial \phi} \\ 0 & \nabla^2 & 0 \\ \frac{2}{r^2} \frac{\partial}{\partial \phi} & 0 & \nabla^2 - \frac{1}{r^2} \end{pmatrix}.$$

We assume now that the domain of definition of the elliptic equation goes all around the z -axis, that is, $0 \leq \phi < 2\pi$. Under these circumstances, the vector field $\mathbf{u}(r, z, \phi)$ can be represented by means of a complex Fourier series, which we will write in the following form

$$\mathbf{u}(r, z, \phi) = \mathbf{u}_0(r, z; \phi) + \sum_{\substack{m=-\infty \\ m \neq 0}}^{\infty} \mathbf{u}_m(r, z; \phi) e^{im\phi},$$

where

$$\mathbf{u}_0(r, z; \phi) = u_0^r(r, z) \hat{\mathbf{r}}(\phi) + u_0^z(r, z) \hat{\mathbf{z}} + u_0^\phi(r, z) \hat{\boldsymbol{\phi}}(\phi)$$

and

$$\mathbf{u}_m(r, z; \phi) = u_m^r(r, z) \hat{\mathbf{r}}(\phi) + u_m^z(r, z) \hat{\mathbf{z}} + u_m^\phi(r, z) \hat{\boldsymbol{\phi}}(\phi) i.$$

In the two expressions above, $\hat{\mathbf{r}}(\phi)$, $\hat{\mathbf{z}}$ and $\hat{\boldsymbol{\phi}}(\phi)$ denote the unit vectors of the cylindrical coordinate system. (Note that here $\hat{\mathbf{r}}(\phi)$ represents the direction orthogonal to the z -axis and is not the radial unit vector pointing out from the origin.)

Being interested in the solution of only *real* vector fields, we have multiplied the coefficient of the angular component of the Fourier mode, with the exclusion of the first mode, by the imaginary unit in order to obtain a purely real representation of the second-order matrix operator acting on the Fourier coefficients of the vector mode (see later). Then, the condition of reality for \mathbf{u} expressed by the Fourier series above implies that the real and imaginary parts of its Fourier coefficients $\mathbf{u}_m = \mathbf{v}_m + i\mathbf{w}_m$ with $m \neq 0$ must satisfy the conditions:

$$\begin{aligned} v_{-m}^r &= v_m^r, & w_{-m}^r &= -w_m^r; \\ v_{-m}^z &= v_m^z, & w_{-m}^z &= -w_m^z; \\ v_{-m}^\phi &= -v_m^\phi, & w_{-m}^\phi &= w_m^\phi. \end{aligned}$$

It follows that the Fourier expansion of a real vector field in cylindrical coordi-

nates can be written also in the following form

$$\begin{aligned} \mathbf{u}(r, z, \phi) = & \left\{ u_0^r(r, z) + 2 \sum_{m=1}^{\infty} [v_m^r(r, z) \cos(m\phi) - w_m^r(r, z) \sin(m\phi)] \right\} \hat{\mathbf{r}}(\phi) \\ & + \left\{ u_0^z(r, z) + 2 \sum_{m=1}^{\infty} [v_m^z(r, z) \cos(m\phi) - w_m^z(r, z) \sin(m\phi)] \right\} \hat{\mathbf{z}} \\ & + \left\{ u_0^\phi(r, z) - 2 \sum_{m=1}^{\infty} [v_m^\phi(r, z) \sin(m\phi) + w_m^\phi(r, z) \cos(m\phi)] \right\} \hat{\boldsymbol{\phi}}(\phi). \end{aligned}$$

According to the adopted Fourier representation, the Laplace operator for the Fourier coefficient of the m th mode assumes the form

$$\partial_m^2 = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} \right) + \frac{\partial^2}{\partial z^2} - \frac{m^2}{r^2}.$$

Furthermore, the matrix Laplace operator for the Fourier coefficients of a vector field becomes

$$\boldsymbol{\partial}_m^2 = \begin{pmatrix} \partial_m^2 - \frac{1}{r^2} & 0 & \frac{2m}{r^2} \\ 0 & \partial_m^2 & 0 \\ \frac{2m}{r^2} & 0 & \partial_m^2 - \frac{1}{r^2} \end{pmatrix}.$$

Thus, for $m \neq 0$ there is a coupling between the two components of the vector mode normal to the z -axis, whereas the axial component is always uncoupled. Consider the change of variables given by the following linear transformation:

$$\mathbf{S} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 \\ 0 & \sqrt{2} & 0 \\ 1 & 0 & -1 \end{pmatrix}, \quad \begin{pmatrix} u_m^1 \\ u_m^2 \\ u_m^3 \end{pmatrix} = \mathbf{S} \begin{pmatrix} u_m^r \\ u_m^z \\ u_m^\phi \end{pmatrix},$$

which lineary combines only the first and the third components ($u_m^2 = u_m^z$). The matrix \mathbf{S} is such that $\mathbf{S} = \mathbf{S}^{\text{tr}} = \mathbf{S}^{-1}$ and that

$$\mathbf{S} \boldsymbol{\partial}_m^2 \mathbf{S} = \begin{pmatrix} \partial_{m-1}^2 & 0 & 0 \\ 0 & \partial_m^2 & 0 \\ 0 & 0 & \partial_{m+1}^2 \end{pmatrix}.$$

The solution of the vector mode with $m \neq 0$ can be determined by first applying the transformation \mathbf{S} to the the Fourier coefficient \mathbf{f}_m of the source term \mathbf{f} , then solving the three uncoupled equations

$$\begin{aligned} \partial_{m-1}^2 u_m^1 &= f_m^1, \\ \partial_m^2 u_m^2 &= f_m^2, \\ \partial_{m+1}^2 u_m^3 &= f_m^3. \end{aligned}$$

and finally backtransforming the solutions according to

$$\begin{pmatrix} u_m^r \\ u_m^z \\ u_m^\phi \end{pmatrix} = \mathbf{S} \begin{pmatrix} u_m^1 \\ u_m^2 \\ u_m^3 \end{pmatrix}.$$

For the first Fourier mode $m = 0$, the similarity transformation is not needed since the three equations for the cylindrical components are already uncoupled; in fact, the operator of the first mode is already in the diagonal form

$$\partial_0^2 = \begin{pmatrix} \partial_1^2 & 0 & 0 \\ 0 & \partial_0^2 & 0 \\ 0 & 0 & \partial_1^2 \end{pmatrix}.$$

Of course, a Fourier analysis of the source term \mathbf{f} and of the data for the boundary conditions is required before the solution process, and a final Fourier synthesis of the solutions \mathbf{u}_m , $m = 1, 2, \dots, M$, is to be performed as the last step of the solution process.

B.5 Spherical coordinates

We are now ready for the most interesting case, *i.e.*, the three-dimensional vector Poisson equation in spherical coordinates (r, θ, ϕ) , assuming that the domain goes all around the polar axis, namely, $0 \leq \phi < 2\pi$. The Laplace operator in spherical coordinates is (cf. section A.4.3 of Appendix A)

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2}.$$

When the Laplacian acts on a vector field \mathbf{u} expressed in terms of its spherical coordinates u_r , u_θ and u_ϕ , the following matrix differential operator has to be considered

$$\nabla^2 = \begin{pmatrix} \nabla^2 - \frac{2}{r^2} & -\frac{2}{r^2 \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta \dots) & -\frac{2}{r^2 \sin \theta} \frac{\partial}{\partial \phi} \\ \frac{2}{r^2} \frac{\partial}{\partial \theta} & \nabla^2 - \frac{1}{r^2 \sin^2 \theta} & -\frac{2 \cos \theta}{r^2 \sin^2 \theta} \frac{\partial}{\partial \phi} \\ \frac{2}{r^2 \sin \theta} \frac{\partial}{\partial \phi} & \frac{2 \cos \theta}{r^2 \sin^2 \theta} \frac{\partial}{\partial \phi} & \nabla^2 - \frac{1}{r^2 \sin^2 \theta} \end{pmatrix}.$$

Let us now represent the dependence on the cyclic coordinate ϕ by means of the Fourier series

$$\mathbf{u}(r, \theta, \phi) = \mathbf{u}_0(r, \theta; \theta, \phi) + \sum_{\substack{m=-\infty \\ m \neq 0}}^{\infty} \mathbf{u}_m(r, \theta; \theta, \phi) e^{im\phi},$$

where

$$\mathbf{u}_0(r, \theta; \theta, \phi) = u_0^r(r, \theta) \hat{\mathbf{r}}(\theta, \phi) + u_0^\theta(r, \theta) \hat{\boldsymbol{\theta}}(\theta, \phi) + u_0^\phi(r, \theta) \hat{\boldsymbol{\phi}}(\theta, \phi)$$

and

$$\mathbf{u}_m(r, \theta; \theta, \phi) = u_m^r(r, \theta) \hat{\mathbf{r}}(\theta, \phi) + u_m^\theta(r, \theta) \hat{\boldsymbol{\theta}}(\theta, \phi) + u_m^\phi(r, \theta) \hat{\boldsymbol{\phi}}(\theta, \phi) i.$$

In the two expressions above, $\hat{\mathbf{r}}(\theta, \phi)$, $\hat{\boldsymbol{\theta}}(\theta, \phi)$ and $\hat{\boldsymbol{\phi}}(\theta, \phi)$ denote the unit vectors of the spherical coordinate system. The coefficients of the ϕ component of the Fourier modes with $m \neq 0$ have been multiplied by the imaginary unit to obtain a purely real representation of the second-order matrix operator acting on the Fourier coefficients of the vector mode.

The condition of reality of the vector field \mathbf{u} expressed in spherical coordinates implies that its complex Fourier coefficients $\mathbf{u}_m = \mathbf{v}_m + i \mathbf{w}_m$ with $m \neq 0$ have real and imaginary parts satisfying the following conditions

$$\begin{aligned} v_{-m}^r &= v_m^r, & w_{-m}^r &= -w_m^r; \\ v_{-m}^\theta &= v_m^\theta, & w_{-m}^\theta &= -w_m^\theta; \\ v_{-m}^\phi &= -v_m^\phi, & w_{-m}^\phi &= w_m^\phi. \end{aligned}$$

As a consequence, the Fourier series above of a real vector field \mathbf{u} can be written also in the form

$$\begin{aligned} \mathbf{u}(r, \theta, \phi) &= \left\{ u_0^r(r, \theta) + 2 \sum_{m=1}^{\infty} \left[v_m^r(r, \theta) \cos(m\phi) - w_m^r(r, \theta) \sin(m\phi) \right] \right\} \hat{\mathbf{r}}(\theta, \phi) \\ &+ \left\{ u_0^\theta(r, \theta) + 2 \sum_{m=1}^{\infty} \left[v_m^\theta(r, \theta) \cos(m\phi) - w_m^\theta(r, \theta) \sin(m\phi) \right] \right\} \hat{\boldsymbol{\theta}}(\theta, \phi) \\ &+ \left\{ u_0^\phi(r, \theta) - 2 \sum_{m=1}^{\infty} \left[v_m^\phi(r, \theta) \sin(m\phi) + w_m^\phi(r, \theta) \cos(m\phi) \right] \right\} \hat{\boldsymbol{\phi}}(\theta, \phi) \end{aligned}$$

which may be more convenient for the computations.

By virtue of the adopted Fourier expansion, the operator representing the Laplace operator ∇^2 in the space of the Fourier coefficients of a scalar function is

$$\partial_m^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) - \frac{m^2}{r^2 \sin^2 \theta},$$

whereas the operator representing the Laplace matrix operator ∇^2 in the space of the Fourier coefficients of a vector field is

$$\boldsymbol{\partial}_m^2 = \begin{pmatrix} \partial_m^2 - \frac{2}{r^2} & -\frac{2}{r^2 \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta \dots) & \frac{2m}{r^2 \sin \theta} \\ \frac{2}{r^2} \frac{\partial}{\partial \theta} & \partial_m^2 - \frac{1}{r^2 \sin^2 \theta} & \frac{2m \cos \theta}{r^2 \sin^2 \theta} \\ \frac{2m}{r^2 \sin \theta} & \frac{2m \cos \theta}{r^2 \sin^2 \theta} & \partial_m^2 - \frac{1}{r^2 \sin^2 \theta} \end{pmatrix}.$$

Thus, for $m \neq 0$, the three spherical components of the vector Fourier mode are coupled together, whilst for the first mode, $m = 0$, only the first two components are coupled.

The similarity transformation which uncouples the three equations is constructed in two steps: first, the coupling between the r and θ components due to the off-diagonal terms containing the first-order derivative $\frac{\partial}{\partial\theta}$ is eliminated; then, the remaining coupling between the first new variable and the third unchanged variable (the ϕ component) is eliminated by means of the same similarity transformation considered in the analysis of the cylindrical coordinates.

Let us consider the (partial) change of variables defined by the linear transformation

$$\mathbf{T}(\theta) = \begin{pmatrix} \sin\theta & \cos\theta & 0 \\ \cos\theta & -\sin\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} \bar{u}_m^1 \\ \bar{u}_m^2 \\ u_m^\phi \end{pmatrix} = \mathbf{T}(\theta) \begin{pmatrix} u_m^r \\ u_m^\theta \\ u_m^\phi \end{pmatrix}.$$

As for matrix $\mathbf{t}(\phi)$ occurring in the previous analysis of polar coordinates, matrix $\mathbf{T}(\theta)$ is such that $\mathbf{T}(\theta) = \mathbf{T}^{\text{tr}}(\theta) = \mathbf{T}^{-1}(\theta)$. Furthermore, by standard calculations, it is possible to show that the similarity transformation provided by matrix $\mathbf{T}(\theta)$ gives the following partial diagonalization of the matrix operator ∂_m^2 :

$$\mathbf{T}(\theta) \partial_m^2 \mathbf{T}(\theta) = \begin{pmatrix} \partial_m^2 - \frac{1}{r^2 \sin^2\theta} & 0 & \frac{2m}{r^2 \sin\theta} \\ 0 & \partial_m^2 & 0 \\ \frac{2m}{r^2 \sin\theta} & 0 & \partial_m^2 - \frac{1}{r^2 \sin^2\theta} \end{pmatrix}.$$

It is important to note that, even though the matrix $\mathbf{T}(\theta)$ is coincident (apart from its dimension) with $\mathbf{t}(\phi)$, this demonstration is different from, and less elementary than, that given for the polar coordinates because of the presence of the function $\sin\theta$ inside and outside the derivative $\frac{\partial}{\partial\theta}$ in the operator ∂_m^2 as well as in its matrix counterpart ∂_m^2 .

Very easy is instead the elimination of the coupling still remaining between the first (new) and the third (old) components of the vector mode, the structure of the coupling being identical to that encountered for the cylindrical coordinates. Thus, introducing a second linear transformation defined by the matrix

$$\mathbf{S} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 \\ 0 & \sqrt{2} & 0 \\ 1 & 0 & -1 \end{pmatrix}, \quad \begin{pmatrix} u_m^1 \\ u_m^2 \\ u_m^3 \end{pmatrix} = \mathbf{S} \begin{pmatrix} \bar{u}_m^1 \\ \bar{u}_m^2 \\ u_m^\phi \end{pmatrix},$$

with, as before, $\mathbf{S} = \mathbf{S}^{\text{tr}} = \mathbf{S}^{-1}$, one obtains immediately

$$\mathbf{S} \mathbf{T}(\theta) \partial_m^2 \mathbf{T}(\theta) \mathbf{S} = \begin{pmatrix} \partial_{m-1}^2 & 0 & 0 \\ 0 & \partial_m^2 & 0 \\ 0 & 0 & \partial_{m+1}^2 \end{pmatrix}.$$

Therefore, defining the complete transformation $\mathbf{R}(\theta) = \mathbf{S}\mathbf{T}(\theta)$, it is immediate to obtain

$$\mathbf{R}(\theta) = \frac{1}{\sqrt{2}} \begin{pmatrix} \sin \theta & \cos \theta & 1 \\ \sqrt{2} \cos \theta & -\sqrt{2} \sin \theta & 0 \\ \sin \theta & \cos \theta & -1 \end{pmatrix}, \quad \begin{pmatrix} u_m^1 \\ u_m^2 \\ u_m^3 \end{pmatrix} = \mathbf{R}(\theta) \begin{pmatrix} u_m^r \\ u_m^\theta \\ u_m^\phi \end{pmatrix},$$

and the previous complete diagonalization of the matrix operator ∂_m^2 can be written as

$$\mathbf{R}(\theta) \partial_m^2 \mathbf{R}(\theta)^{\text{tr}} = \begin{pmatrix} \partial_{m-1}^2 & 0 & 0 \\ 0 & \partial_m^2 & 0 \\ 0 & 0 & \partial_{m+1}^2 \end{pmatrix},$$

since $\mathbf{T}(\theta)\mathbf{S} = \mathbf{T}(\theta)^{\text{tr}}\mathbf{S}^{\text{tr}} = (\mathbf{S}\mathbf{T}(\theta))^{\text{tr}} = \mathbf{R}(\theta)^{\text{tr}}$, by the properties of matrices $\mathbf{T}(\theta)$ and \mathbf{S} . It is interesting to note that the same properties imply $\mathbf{T}(\theta)\mathbf{S} = \mathbf{T}(\theta)^{-1}\mathbf{S}^{-1} = (\mathbf{S}\mathbf{T}(\theta))^{-1} = \mathbf{R}(\theta)^{-1}$, so that $\mathbf{R}(\theta)^{\text{tr}} = \mathbf{R}(\theta)^{-1}$ and $\mathbf{R}(\theta)$ is orthogonal, but $\mathbf{R}(\theta) \neq \mathbf{R}(\theta)^{\text{tr}}$ since $\mathbf{T}(\theta)$ and \mathbf{S} do not commute.

The solution of the equations for the m th Fourier mode with $m \neq 0$ proceeds as follows: first, the transformation $\mathbf{R}(\theta)$ is applied to the Fourier coefficient \mathbf{f}_m of the source term \mathbf{f} of the Poisson equation; then, the three uncoupled elliptic 2D equations

$$\begin{aligned} \partial_{m-1}^2 u_m^1 &= f_m^1, \\ \partial_m^2 u_m^2 &= f_m^2, \\ \partial_{m+1}^2 u_m^3 &= f_m^3, \end{aligned}$$

are solved; finally, the spherical components of the m th Fourier mode are obtained through the backtransformation

$$\begin{pmatrix} u_m^r \\ u_m^\theta \\ u_m^\phi \end{pmatrix} = \mathbf{R}(\theta)^{\text{tr}} \begin{pmatrix} u_m^1 \\ u_m^2 \\ u_m^3 \end{pmatrix}.$$

The problem for the first Fourier mode $m = 0$ is simpler, since the corresponding matrix operator in the Fourier space is

$$\partial_0^2 = \begin{pmatrix} \partial_0^2 - \frac{2}{r^2} & -\frac{2}{r^2} \frac{\partial}{\sin \theta} \frac{\partial}{\partial \theta} (\sin \theta \dots) & 0 \\ \frac{2}{r^2} \frac{\partial}{\partial \theta} & \partial_1^2 & 0 \\ 0 & 0 & \partial_1^2 \end{pmatrix}.$$

Thus, the similarity transformation performing the diagonalization is easily found to be

$$\mathbf{T}(\theta) \partial_0^2 \mathbf{T}(\theta) = \begin{pmatrix} \partial_1^2 & 0 & 0 \\ 0 & \partial_0^2 & 0 \\ 0 & 0 & \partial_1^2 \end{pmatrix}.$$

The solution procedure for the first mode $m = 0$ amounts therefore to transforming the source term \mathbf{f}_0 by means of matrix $\mathbf{T}(\theta)$, solving the three uncoupled equations

$$\begin{aligned}\partial_1^2 u_0^1 &= f_0^1, \\ \partial_0^2 u_0^2 &= f_0^2, \\ \partial_1^2 u_0^3 &= f_0^3,\end{aligned}$$

and backtransforming the computed solutions through

$$\begin{pmatrix} u_0^r \\ u_0^\theta \\ u_0^\phi \end{pmatrix} = \mathbf{T}(\theta) \begin{pmatrix} u_0^1 \\ u_0^2 \\ u_0^3 \end{pmatrix}.$$

Needless to say, all of the transformations above must be performed also on the data of the boundary conditions. Moreover, steps of Fourier analysis and synthesis must precede and follow the solution procedure.

The same procedure can be applied to solve Dirichlet vector problems for the Helmholtz operator $(\nabla^2 - \gamma)$, with $\gamma > 0$, as well as for more general elliptic operators of the form $(\nabla^2 - \Gamma(r, \phi))$, where the function $\Gamma(r, \phi)$ can be subject to suitable conditions.

To conclude, we recall that the similarity transformation described in this Appendix can be combined with existing algorithms for the numerical solution of scalar elliptic equations in two dimensions to obtain solution methods for vector Dirichlet problems in any plane region and in annular three-dimensional regions.

Appendix C

Spatial difference operators

C.1 Introduction

This Appendix contains the various difference operators which are involved in the spatial discretization of the transient advection equation for a scalar unknown by means of finite elements. We consider the equations both in two and three dimensions and assume a uniform mesh of square and cubic elements, respectively, with a multilinear interpolation of the unknown variable. We will give also the explicit expressions of the operators produced by the application of the Taylor–Galerkin method to the advection equation. The Fourier representation of the various spatial operators is provided to allow the study of numerical stability and response properties of integration schemes for multidimensional problems.

C.2 2D equation: four-node bilinear element

Let a variable $u(x, y)$ be approximated over a uniform mesh of square elements of size h by means of bilinear functions which match with continuity at interelement boundaries. When the Galerkin method is applied to solve an advection equation of the type $u_t + (\mathbf{a} \cdot \nabla)u = s$, approximately, one obtains a semidiscrete equation which involves spatial difference operators of first order and also of second order due to the presence of the consistent mass matrix. Such operators are obtained from the following elementary first-order operators:

$$(\Delta_x U)_{j,k} = \frac{1}{2}(U_{j+1,k} - U_{j-1,k}),$$

$$(\Delta_y U)_{j,k} = \frac{1}{2}(U_{j,k+1} - U_{j,k-1}),$$

$$(\Delta_{xy} U)_{j,k} = \frac{1}{2}(U_{j+1,k+1} - U_{j-1,k-1}),$$

$$(\Delta_{yx} U)_{j,k} = \frac{1}{2}(U_{j+1,k-1} - U_{j-1,k+1}),$$

$$\widehat{\Delta}_x = \frac{2}{3} \left(\Delta_x + \frac{1}{4} \Delta_{xy} + \frac{1}{4} \Delta_{yx} \right),$$

$$\widehat{\Delta}_y = \frac{2}{3} \left(\Delta_y + \frac{1}{4} \Delta_{xy} - \frac{1}{4} \Delta_{yx} \right);$$

and from the following elementary second-order operators:

$$\left(\delta_x^2 U \right)_{j,k} = U_{j+1,k} - 2U_{j,k} + U_{j-1,k},$$

$$\left(\delta_y^2 U \right)_{j,k} = U_{j,k+1} - 2U_{j,k} + U_{j,k-1},$$

$$\left(\delta_{xy}^2 U \right)_{j,k} = U_{j+1,k+1} - 2U_{j,k} + U_{j-1,k-1},$$

$$\left(\delta_{yx}^2 U \right)_{j,k} = U_{j+1,k-1} - 2U_{j,k} + U_{j-1,k+1},$$

$$\widehat{\delta}_x^2 = \frac{2}{3} \delta_x^2 + \frac{1}{6} \left(\delta_{xy}^2 + \delta_{yx}^2 \right) - \frac{1}{3} \delta_y^2,$$

$$\widehat{\delta}_y^2 = \frac{2}{3} \delta_y^2 + \frac{1}{6} \left(\delta_{xy}^2 + \delta_{yx}^2 \right) - \frac{1}{3} \delta_x^2.$$

The Galerkin method applied to the equation $u_t + (\mathbf{a} \cdot \nabla)u = 0$ gives the semidiscrete equation

$$M \frac{dU}{dt} = -\frac{1}{h} \mathbf{a} \cdot \widehat{\Delta} U,$$

where

$$M = 1 + \frac{1}{9} \left(\delta_x^2 + \delta_y^2 + \frac{1}{4} \delta_{xy}^2 + \frac{1}{4} \delta_{yx}^2 \right)$$

$$= \left(1 + \frac{1}{6} \delta_x^2 \right) \left(1 + \frac{1}{6} \delta_y^2 \right),$$

$$\widehat{\Delta} = \left(\widehat{\Delta}_x, \widehat{\Delta}_y \right).$$

It is worth noting the factorization of the consistent mass matrix operator, which allowed to develop a very efficient method for the solution of the linear system of the consistent mass on Cartesian (possibly nonuniform) meshes (Staniforth and Mitchell 1978 and 1987).

The application of the Taylor–Galerkin method would lead instead to the fully discrete equation

$$M_{\text{TG}}(\boldsymbol{\nu})(U^{n+1} - U^n) = -\boldsymbol{\nu} \cdot \widehat{\Delta} U^n + K(\boldsymbol{\nu})U^n,$$

where $\boldsymbol{\nu} = (\Delta t/h)\mathbf{a}$ and

$$\widehat{\Delta} = \left(\widehat{\Delta}_x, \widehat{\Delta}_y \right),$$

$$K(\boldsymbol{\nu}) = \nu_x^2 \widehat{\delta}_x^2 + 2\nu_x \nu_y \Delta_x \Delta_y + \nu_y^2 \widehat{\delta}_y^2,$$

$$M_{\text{TG}}(\boldsymbol{\nu}) = M - \frac{1}{6} K(\boldsymbol{\nu}).$$

In other words, one has the following correspondences

$$\begin{aligned}\Delta t \mathbf{a} \cdot \nabla &\longrightarrow \boldsymbol{\nu} \cdot \widehat{\Delta}, \\ (\Delta t)^2 (\mathbf{a} \cdot \nabla)^2 &\longrightarrow K(\boldsymbol{\nu}).\end{aligned}$$

Introducing a Fourier analysis with mode $\exp(i\mathbf{k} \cdot \mathbf{x})$ and the dimensionless wave number $\boldsymbol{\xi} = h\mathbf{k}$, it is not difficult to find the Fourier image of the relevant difference operators:

$$\begin{aligned}M(\boldsymbol{\xi}) &= \frac{4}{9} \left(1 + \frac{1}{2} \cos \xi\right) \left(1 + \frac{1}{2} \cos \eta\right) \\ &= \left(1 - \frac{2}{3} \sin^2 \frac{1}{2} \xi\right) \left(1 - \frac{2}{3} \sin^2 \frac{1}{2} \eta\right), \\ A(\boldsymbol{\xi}, \boldsymbol{\nu}) &= \frac{2}{3} i \nu_x \sin \xi \left(1 + \frac{1}{2} \cos \eta\right) + \frac{2}{3} i \nu_y \sin \eta \left(1 + \frac{1}{2} \cos \xi\right), \\ K(\boldsymbol{\xi}, \boldsymbol{\nu}) &= -\frac{4}{3} \nu_x^2 (1 - \cos \xi) \left(1 + \frac{1}{2} \cos \eta\right) - 2 \nu_x \nu_y \sin \xi \sin \eta \\ &\quad - \frac{4}{3} \nu_y^2 (1 - \cos \eta) \left(1 + \frac{1}{2} \cos \xi\right), \\ M_{\text{TG}}(\boldsymbol{\xi}, \boldsymbol{\nu}) &= M(\boldsymbol{\xi}) - \frac{1}{6} K(\boldsymbol{\xi}, \boldsymbol{\nu}).\end{aligned}$$

Of course $A(\boldsymbol{\xi}, \boldsymbol{\nu})$ denotes the Fourier transform of $\boldsymbol{\nu} \cdot \widehat{\Delta}$.

C.3 3D equation: eight-node trilinear element

The approximate solution of the three-dimensional equation $u_t + (\mathbf{a} \cdot \nabla)u = 0$ on a uniform cubic mesh of trilinear elements requires to consider the following elementary spatial difference operators. The first-order operators are

$$\begin{aligned}(\Delta_x U)_{j,k,l} &= \frac{1}{2}(U_{j+1,k,l} - U_{j-1,k,l}), \\ (\Delta_y U)_{j,k,l} &= \frac{1}{2}(U_{j,k+1,l} - U_{j,k-1,l}), \\ (\Delta_z U)_{j,k,l} &= \frac{1}{2}(U_{j,k,l+1} - U_{j,k,l-1}), \\ (\Delta_{xy} U)_{j,k,l} &= \frac{1}{2}(U_{j+1,k+1,l} - U_{j-1,k-1,l}), \\ (\Delta_{yx} U)_{j,k,l} &= \frac{1}{2}(U_{j+1,k-1,l} - U_{j-1,k+1,l}), \\ (\Delta_{zx} U)_{j,k,l} &= \frac{1}{2}(U_{j+1,k,l+1} - U_{j-1,k,l-1}), \\ (\Delta_{xz} U)_{j,k,l} &= \frac{1}{2}(U_{j+1,k,l-1} - U_{j-1,k,l+1}), \\ (\Delta_{yz} U)_{j,k,l} &= \frac{1}{2}(U_{j,k+1,l+1} - U_{j,k-1,l-1}), \\ (\Delta_{zy} U)_{j,k,l} &= \frac{1}{2}(U_{j,k+1,l-1} - U_{j,k-1,l+1}),\end{aligned}$$

$$\begin{aligned}
(\Delta_{xyz}U)_{j,k,l} &= \frac{1}{2}(U_{j+1,k+1,l+1} - U_{j-1,k-1,l-1}), \\
(\Delta_{xy\bar{z}}U)_{j,k,l} &= \frac{1}{2}(U_{j+1,k+1,l-1} - U_{j-1,k-1,l+1}), \\
(\Delta_{x\bar{y}z}U)_{j,k,l} &= \frac{1}{2}(U_{j+1,k-1,l+1} - U_{j-1,k+1,l-1}), \\
(\Delta_{\bar{x}yz}U)_{j,k,l} &= \frac{1}{2}(U_{j-1,k+1,l+1} - U_{j+1,k-1,l-1}),
\end{aligned}$$

$$\widehat{\Delta}_x = \frac{4}{9} \left[\Delta_x + \frac{1}{4}(\Delta_{xy} + \Delta_{yx} + \Delta_{zx} + \Delta_{xz}) + \frac{1}{16}(\Delta_{xyz} + \Delta_{xy\bar{z}} + \Delta_{x\bar{y}z} - \Delta_{\bar{x}yz}) \right],$$

$$\widehat{\Delta}_y = \frac{4}{9} \left[\Delta_y + \frac{1}{4}(\Delta_{xy} - \Delta_{yx} + \Delta_{yz} + \Delta_{zy}) + \frac{1}{16}(\Delta_{xyz} + \Delta_{xy\bar{z}} - \Delta_{x\bar{y}z} + \Delta_{\bar{x}yz}) \right],$$

$$\widehat{\Delta}_z = \frac{4}{9} \left[\Delta_z + \frac{1}{4}(\Delta_{zx} - \Delta_{xz} + \Delta_{yz} - \Delta_{zy}) + \frac{1}{16}(\Delta_{xyz} - \Delta_{xy\bar{z}} + \Delta_{x\bar{y}z} + \Delta_{\bar{x}yz}) \right].$$

The second-order operators are

$$(\delta_x^2 U)_{j,k,l} = U_{j+1,k,l} - 2U_{j,k,l} + U_{j-1,k,l},$$

$$(\delta_y^2 U)_{j,k,l} = U_{j,k+1,l} - 2U_{j,k,l} + U_{j,k-1,l},$$

$$(\delta_z^2 U)_{j,k,l} = U_{j,k,l+1} - 2U_{j,k,l} + U_{j,k,l-1},$$

$$(\delta_{xy}^2 U)_{j,k,l} = U_{j+1,k+1,l} - 2U_{j,k,l} + U_{j-1,k-1,l},$$

$$(\delta_{yx}^2 U)_{j,k,l} = U_{j+1,k-1,l} - 2U_{j,k,l} + U_{j-1,k+1,l},$$

$$(\delta_{zx}^2 U)_{j,k,l} = U_{j+1,k,l+1} - 2U_{j,k,l} + U_{j-1,k,l-1},$$

$$(\delta_{xz}^2 U)_{j,k,l} = U_{j+1,k,l-1} - 2U_{j,k,l} + U_{j-1,k,l+1},$$

$$(\delta_{yz}^2 U)_{j,k,l} = U_{j,k+1,l+1} - 2U_{j,k,l} + U_{j,k-1,l-1},$$

$$(\delta_{zy}^2 U)_{j,k,l} = U_{j,k+1,l-1} - 2U_{j,k,l} + U_{j,k-1,l+1},$$

$$(\delta_{xyz}^2 U)_{j,k,l} = U_{j+1,k+1,l+1} - 2U_{j,k,l} + U_{j-1,k-1,l-1},$$

$$(\delta_{xy\bar{z}}^2 U)_{j,k,l} = U_{j+1,k+1,l-1} - 2U_{j,k,l} + U_{j-1,k-1,l+1},$$

$$(\delta_{x\bar{y}z}^2 U)_{j,k,l} = U_{j+1,k-1,l+1} - 2U_{j,k,l} + U_{j-1,k+1,l-1},$$

$$(\delta_{\bar{x}yz}^2 U)_{j,k,l} = U_{j-1,k+1,l+1} - 2U_{j,k,l} + U_{j+1,k-1,l-1},$$

$$\widetilde{\delta^2} = \delta_{xy}^2 + \delta_{yx}^2 + \delta_{zx}^2 + \delta_{xz}^2 + \delta_{yz}^2 + \delta_{zy}^2,$$

$$\overline{\delta^2} = \delta_{xyz}^2 + \delta_{xy\bar{z}}^2 + \delta_{x\bar{y}z}^2 + \delta_{\bar{x}yz}^2,$$

$$\begin{aligned}\widehat{\delta}_x^2 &= \frac{4}{9} \left[\delta_x^2 - \frac{1}{2} (\delta_y^2 + \delta_z^2) + \frac{1}{4} \widetilde{\delta}^2 - \frac{3}{8} (\delta_{yz}^2 + \delta_{zy}^2) + \frac{1}{16} \overline{\delta}^2 \right], \\ \widehat{\delta}_y^2 &= \frac{4}{9} \left[\delta_y^2 - \frac{1}{2} (\delta_x^2 + \delta_z^2) + \frac{1}{4} \widetilde{\delta}^2 - \frac{3}{8} (\delta_{zx}^2 + \delta_{xz}^2) + \frac{1}{16} \overline{\delta}^2 \right], \\ \widehat{\delta}_z^2 &= \frac{4}{9} \left[\delta_z^2 - \frac{1}{2} (\delta_x^2 + \delta_y^2) + \frac{1}{4} \widetilde{\delta}^2 - \frac{3}{8} (\delta_{xy}^2 + \delta_{yx}^2) + \frac{1}{16} \overline{\delta}^2 \right].\end{aligned}$$

The application of the Galerkin method to the advection equation in three dimensions gives the semidiscrete equation

$$M \frac{dU}{dt} = -\frac{1}{h} \mathbf{a} \cdot \widehat{\Delta} U,$$

where

$$\begin{aligned}M &= 1 + \frac{2}{27} \left[\delta_x^2 + \delta_y^2 + \delta_z^2 + \frac{1}{4} \widetilde{\delta}^2 + \frac{1}{16} \overline{\delta}^2 \right], \\ \widehat{\Delta} &= (\widehat{\Delta}_x, \widehat{\Delta}_y, \widehat{\Delta}_z).\end{aligned}$$

As in two dimensions, the consistent mass matrix allows a factorization in one-dimensional operators

$$M = \left(1 + \frac{1}{6} \delta_x^2\right) \left(1 + \frac{1}{6} \delta_y^2\right) \left(1 + \frac{1}{6} \delta_z^2\right)$$

which can be exploited for the efficient solution of advection problems over a Cartesian mesh of brick elements.

The application of the Taylor–Galerkin method introduces the additional operators

$$\begin{aligned}K(\boldsymbol{\nu}) &= \nu_x^2 \widehat{\delta}_x^2 + \nu_y^2 \widehat{\delta}_y^2 + \nu_z^2 \widehat{\delta}_z^2 + 2\nu_x \nu_y \Delta_x \Delta_y + 2\nu_x \nu_z \Delta_x \Delta_z + 2\nu_y \nu_z \Delta_y \Delta_z, \\ M_{\text{TG}}(\boldsymbol{\nu}) &= M - \frac{1}{6} K(\boldsymbol{\nu}),\end{aligned}$$

where $\boldsymbol{\nu} = (\Delta t/h) \mathbf{a}$. Finally, the Fourier analysis of the numerical schemes can be done by means of the following explicit expressions

$$\begin{aligned}M(\boldsymbol{\xi}) &= \frac{8}{27} \left(1 + \frac{1}{2} \cos \xi\right) \left(1 + \frac{1}{2} \cos \eta\right) \left(1 + \frac{1}{2} \cos \zeta\right) \\ &= \left(1 - \frac{2}{3} \sin^2 \frac{1}{2} \xi\right) \left(1 - \frac{2}{3} \sin^2 \frac{1}{2} \eta\right) \left(1 - \frac{2}{3} \sin^2 \frac{1}{2} \zeta\right),\end{aligned}$$

$$\begin{aligned}A(\boldsymbol{\xi}, \boldsymbol{\nu}) &= \frac{4}{9} i \nu_x \sin \xi \left(1 + \frac{1}{2} \cos \eta\right) \left(1 + \frac{1}{2} \cos \zeta\right) \\ &\quad + \frac{4}{9} i \nu_y \sin \eta \left(1 + \frac{1}{2} \cos \xi\right) \left(1 + \frac{1}{2} \cos \zeta\right) \\ &\quad + \frac{4}{9} i \nu_z \sin \zeta \left(1 + \frac{1}{2} \cos \xi\right) \left(1 + \frac{1}{2} \cos \eta\right),\end{aligned}$$

$$\begin{aligned}K(\boldsymbol{\xi}, \boldsymbol{\nu}) &= -\frac{8}{9} \nu_x^2 (1 - \cos \xi) \left(1 + \frac{1}{2} \cos \eta\right) \left(1 + \frac{1}{2} \cos \zeta\right) \\ &\quad - \frac{8}{9} \nu_y^2 (1 - \cos \eta) \left(1 + \frac{1}{2} \cos \xi\right) \left(1 + \frac{1}{2} \cos \zeta\right) \\ &\quad - \frac{8}{9} \nu_z^2 (1 - \cos \zeta) \left(1 + \frac{1}{2} \cos \xi\right) \left(1 + \frac{1}{2} \cos \eta\right) \\ &\quad - 2\nu_x \nu_y \sin \xi \sin \eta - 2\nu_x \nu_z \sin \xi \sin \zeta - 2\nu_y \nu_z \sin \eta \sin \zeta.\end{aligned}$$

Appendix D

Time derivative of integrals over moving domains

In this Appendix we provide some vector differential identities expressing the time derivative of integrals over domains which move and change in shape in an arbitrary manner. We consider the integrals over curves and surfaces moving and deforming themselves in the three-dimensional space, as well as integrals over three-dimensional regions whose boundary has a velocity specified at each point.

These identities generalize to the three-dimensional space the well known theorem of calculus expressing the derivative of a definite integral with respect to a variable which the limits of integration and possibly the integrand depend on. If the variable involved in the derivation is denoted by t and referred to as “time,” and the integration interval $\mathcal{I}_t = [a(t), b(t)]$ depends on time, the theorem states

$$\frac{d}{dt} \int_{a(t)}^{b(t)} f(x, t) dx = \int_{a(t)}^{b(t)} \frac{\partial f(x, t)}{\partial t} dx + f(b(t), t) \frac{db(t)}{dt} - f(a(t), t) \frac{da(t)}{dt}.$$

The time derivative of $a(t)$ and $b(t)$ represents the “velocity” of the end points of \mathcal{I}_t , according to the definition:

$$v_a(t) = \frac{da(t)}{dt} \quad \text{and} \quad v_b(t) = \frac{db(t)}{dt},$$

so that the previous identity can also be written in the form

$$\frac{d}{dt} \int_{a(t)}^{b(t)} f(x, t) dx = \int_{a(t)}^{b(t)} \frac{\partial f(x, t)}{\partial t} dx + f(b(t), t) v_b(t) - f(a(t), t) v_a(t).$$

This expression is now generalized to integrals expressing the circulation along a curve and the flux across a surface both evolving in the three-dimensional space in a known manner. The expression of the time derivative of the three-dimensional

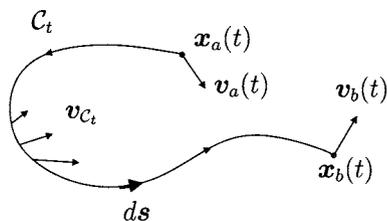


Figure D.1: Curve moving and deforming in space.

integrals of scalar and vector fields over a moving and deforming volume will be also given.

The scalar functions and vector fields to be integrated in the following are defined not only on the integration domain but in the entire spatial region where the integration domain is evolving. We assume that the various functions are smooth enough so that the standard operations of calculus may be performed on them.

D.1 Circulation along a moving curve

Let us consider a continuous curve \mathcal{C}_t which moves and deforms itself with time and let $\mathbf{x}_{\mathcal{C}_t}(s)$ be its parametric representation at time t with s the arclength parameter. The end points of \mathcal{C}_t will be (see Figure D.1)

$$\mathbf{x}_a(t) = \mathbf{x}_{\mathcal{C}_t}(s_a(t)) \quad \text{and} \quad \mathbf{x}_b(t) = \mathbf{x}_{\mathcal{C}_t}(s_b(t)).$$

The velocity of points of \mathcal{C}_t at time t will be indicated by

$$\mathbf{v}_{\mathcal{C}_t} = \mathbf{v}_{\mathcal{C}_t}(\mathbf{x}_{\mathcal{C}_t}),$$

where $\mathbf{x}_{\mathcal{C}_t} \in \mathcal{C}_t$.

Let $\mathbf{F}(\mathbf{x}, t)$ denote a time-dependent vector field which is defined in the three-dimensional region of evolution of \mathcal{C}_t . The generalization of the previous differential identity to the circulation integral of $\mathbf{F}(\mathbf{x}, t)$ along the moving curve \mathcal{C}_t is:

$$\begin{aligned} \frac{d}{dt} \int_{\mathcal{C}_t} \mathbf{F} \cdot d\mathbf{s} &= \int_{\mathcal{C}_t} \frac{\partial \mathbf{F}}{\partial t} \cdot d\mathbf{s} + \int_{\mathcal{C}_t} (\nabla \times \mathbf{F}) \times \mathbf{v}_{\mathcal{C}_t} \cdot d\mathbf{s} \\ &\quad + \mathbf{F}(\mathbf{x}_b(t), t) \cdot \mathbf{v}_b(t) - \mathbf{F}(\mathbf{x}_a(t), t) \cdot \mathbf{v}_a(t), \end{aligned}$$

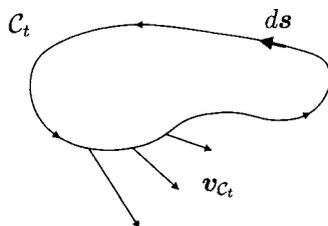


Figure D.2: Closed curve moving in space.

where, of course,

$$\mathbf{v}_a(t) = \mathbf{v}_{C_t}(\mathbf{x}_a(t)) \quad \text{and} \quad \mathbf{v}_b(t) = \mathbf{v}_{C_t}(\mathbf{x}_b(t)).$$

In particular, if the curve C_t is assumed to be closed (see Figure D.2), this result simplifies to

$$\frac{d}{dt} \oint_{C_t} \mathbf{F} \cdot d\mathbf{s} = \oint_{C_t} \frac{\partial \mathbf{F}}{\partial t} \cdot d\mathbf{s} + \oint_{C_t} (\nabla \times \mathbf{F}) \times \mathbf{v}_{C_t} \cdot d\mathbf{s}.$$

Notice that this identity gives a straightforward proof of Kelvin circulation theorem.

D.2 Flux across a moving surface

Let us consider the flux of a vector field across a surface S_t which has a boundary C_t and which moves with a velocity given by

$$\mathbf{v}_{S_t} = \mathbf{v}_{S_t}(\mathbf{x}_{S_t}),$$

where $\mathbf{x}_{S_t} \in S_t$ (see Figure D.3).

The time derivative of the flux of $\mathbf{F}(\mathbf{x}, t)$ across S_t is given by the following identity

$$\begin{aligned} \frac{d}{dt} \iint_{S_t} \mathbf{F} \cdot \mathbf{n} \, dS &= \iint_{S_t} \frac{\partial \mathbf{F}}{\partial t} \cdot \mathbf{n} \, dS + \iint_{S_t} (\nabla \cdot \mathbf{F}) \mathbf{v}_{S_t} \cdot \mathbf{n} \, dS \\ &\quad + \oint_{C_t} \mathbf{F} \times \mathbf{v}_{C_t} \cdot d\mathbf{s}, \end{aligned}$$

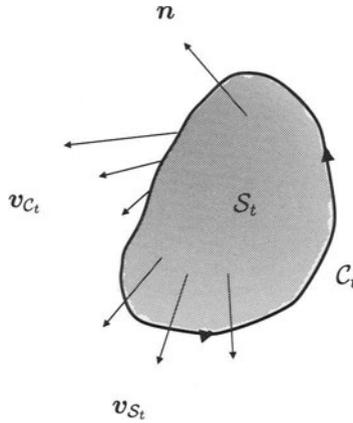


Figure D.3: Bounded surface moving and deforming in space.

where, of course, $\mathbf{v}_{C_t} = \mathbf{v}_{S_t}(\mathbf{x}_{C_t})$. This identity allows a direct demonstration of Helmholtz first vorticity theorem, see, *e.g.*, Acheson [1, p. 162].

In particular, if the surface S_t is *closed* (see Figure D.4), the curvilinear integral along the boundary C_t disappears and the time derivative of the flux becomes

$$\frac{d}{dt} \iint_{S_t} \mathbf{F} \cdot \mathbf{n} dS = \iint_{S_t} \frac{\partial \mathbf{F}}{\partial t} \cdot \mathbf{n} dS + \iint_{S_t} (\nabla \cdot \mathbf{F}) \mathbf{v}_{S_t} \cdot \mathbf{n} dS.$$

D.3 Integrals over a moving volume

Consider finally a varying three-dimensional domain \mathcal{V}_t bounded by the closed surface S_t whose points at time t move with the velocity

$$\mathbf{v}_{S_t} = \mathbf{v}_{S_t}(\mathbf{x}_{S_t}).$$

The derivative of the integral of a scalar function $f(\mathbf{x}, t)$ over the varying domain \mathcal{V}_t with respect to time is given by the well known expression:

$$\frac{d}{dt} \iiint_{\mathcal{V}_t} f(\mathbf{x}, t) dV = \iiint_{\mathcal{V}_t} \frac{\partial f(\mathbf{x}, t)}{\partial t} dV + \iint_{S_t} f \mathbf{v}_{S_t} \cdot \mathbf{n} dS.$$

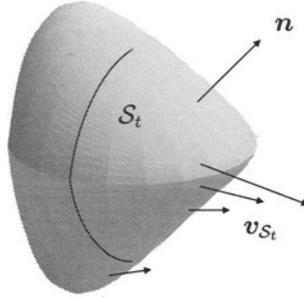


Figure D.4: Closed surface moving and deforming in space.

The last term represents the flux of the quantity f across the moving boundary of the integration domain.

A similar expression holds for the integral of a vector quantity $\mathbf{F}(\mathbf{x}, t)$ which is defined over a three-dimensional region containing \mathcal{V}_t , namely,

$$\frac{d}{dt} \iiint_{\mathcal{V}_t} \mathbf{F}(\mathbf{x}, t) dV = \iiint_{\mathcal{V}_t} \frac{\partial \mathbf{F}(\mathbf{x}, t)}{\partial t} dV + \iint_{S_t} \mathbf{F}(\mathbf{v}_{S_t} \cdot \mathbf{n}) dS.$$

It is to be remarked that these results are obtained without considering any velocity field at points in the interior of the integration domain \mathcal{V}_t . In other words, the identities provide the relationship implied by the *kinematics* of the boundary S_t and by the possible time dependence of the integrand, with no reference to any dynamical aspect associated with the field variable appearing in the integral.

The two vector identities above can be useful to establish the relationship existing between the local and material (substantial) forms of the conservation laws for a fluid. In fact they eliminate the need of Lagrangian coordinates and of the change of variables associated with the flow map which gives the configuration at time t in terms of the initial one. In particular, the analysis of the conservation of momentum will be possible using the following extension of the divergence theorem:

$$\iint_S \mathbf{F}(\mathbf{G} \cdot \mathbf{n}) dS = \iiint_V [\mathbf{F}(\nabla \cdot \mathbf{G}) + (\mathbf{G} \cdot \nabla)\mathbf{F}] dV,$$

which holds for any two differentiable vector fields \mathbf{F} and \mathbf{G} .

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