Differentiation in non-Cartesian coordinates.

We have Cartesian coordinates ($x = x_1, y = x_2, z = x_3$) and another coordinate system $Q = (q_1, q_2, q_3)$ so that

$$x_k = \chi_k(q_1, q_2, q_3),\ k = 1, 2, 3.$$

Consider a point with Q coordinates $q_1 = c_1, q_2 = c_2, q_3 = c_3$ and the corresponding Cartesian coordinates $x_1 = \chi_1(c_1, c_2, c_3), x_2 = \chi_2(c_1, c_2, c_3), x_3 = \chi_3(c_1, c_2, c_3)$. The **$Q$-coordinate curves** through this point *in the Q coordinates* are $\vec{r}_1(t) = (c_1 + t, c_2, c_3), \vec{r}_2(t) = (c_1, c_2 + t, c_3), \vec{r}_3(t) = (c_1, c_2, c_3 + t)$. The same curves *in Cartesian coordinates* are

$$\begin{aligned}\vec{r}_1(t) &= \langle \chi_1(c_1 + t, c_2, c_3), \chi_2(c_1 + t, c_2, c_3), \chi_3(c_1 + t, c_2, c_3)\rangle,\\ \vec{r}_2(t) &= \langle \chi_1(c_1, c_2 + t, c_3), \chi_2(c_1, c_2 + t, c_3), \chi_3(c_1, c_2 + t, c_3)\rangle,\\ \vec{r}_3(t) &= \langle \chi_1(c_1, c_2, c_3 + t), \chi_2(c_1, c_2, c_3 + t), \chi_3(c_1, c_2, c_3 + t)\rangle.\end{aligned}$$

We have the corresponding unit vectors $\hat{q}_1, \hat{q}_2, \hat{q}_3$ in the direction of $\vec{r}_1{}'(0), \vec{r}_2{}'(0), \vec{r}_3{}'(0)$, respectively, and the numbers $h_k = \|\vec{r}_k{}'(0)\|$, $k = 1, 2, 3$. *Note that, to compute the length of $\vec{r}_k{}'(0)$, we have to write $\vec{r}_k$ in Cartesian coordinates.*

We assume that the Q-system is orthogonal, that is, $\hat{q}_k \cdot \hat{q}_n = 0$ for $k \neq k$. Both cylindrical and spherical coordinates are orthogonal.

Coords Q (q_1, q_2, q_3)	h_1	h_2	h_3
Cylindrical (r, θ, z)	1	r	1
Spherical (r, θ, φ)	1	$r \sin\varphi$	r

If we have a scalar function f defined at different points in space, then the *values* of the function and of its gradient do not depend on the coordinate system, but the *representations* of the function and its gradient depend on the coordinate system. For example, if $f = x + yz = x_1 + x_2x_3$ in Cartesian coordinates and $q_1 = r, q_2 = \theta, q_3 = \varphi$ are the spherical coordinates, then $x_1 = r\cos\theta\sin\phi, x_2 = r\sin\theta\sin\varphi,\ x_3 = r\cos\phi$, and $f = r\cos\theta\sin\varphi + r^2\sin\theta\sin\varphi\cos\varphi$. We can then compute partial derivatives f_{x_k}, which immediately give us the gradient in the Cartesian coordinates, but it is not at all clear how the partial derivative f_r, f_θ, and f_φ relate to the gradient of f in the spherical coordinates.

Consider a function with a given representation $f = f(q_1, q_2, q_3)$ in the Q coordinates and consider the point in space with Q coordinates $q_1 = c_1, q_2 = c_2, q_3 = c_3$. Since the Q coordinates are orthogonal, we have the expression for the gradient as

$$\nabla f(c_1, c_2, c_3) = (\nabla f(c_1, c_2, c_3) \cdot \hat{q}_1)\hat{q}_1 + (\nabla f(c_1, c_2, c_3) \cdot \hat{q}_2)\hat{q}_2 + (\nabla f(c_1, c_2, c_3) \cdot \hat{q}_3)\hat{q}_3.$$

We need to write $\nabla f(c_1, c_2, c_3) \cdot \hat{q}_k$ in terms of the partial derivatives of f with respect to its variables q_1, q_2, q_3 at the point (c_1, c_2, c_3). To this end, consider the functions $g_k(t) = f(\vec{r}_k(t))$, $k = 1, 2, 3$. For example, $g_1(t) = f(c_1 + t, c_2, c_3)$. Then

$$g_k'(0) = \nabla f(c_1, c_2, c_3) \cdot \vec{r}_k{}'(0) = h_k \nabla f(c_1, c_2, c_3) \cdot \hat{q}_k.$$

On the other hand, the special form of the vectors $\vec{r}_k(t)$, together with the definition of the partial derivative, implies that

$$g_k'(0) = \frac{\partial f(c_1, c_2, c_3)}{\partial q_k}.$$

For example,

$$g_1'(0) = \lim_{t\to 0} \frac{f(c_1 + t, c_2, c_3) - f(c_1, c_2, c_3)}{t} = \frac{\partial f(c_1 + t, c_2, c_3)}{\partial q_1}.$$

As a result, $h_k \nabla f(c_1, c_2, c_3) \cdot \hat{q}_k = \frac{\partial f(c_1, c_2, c_3)}{\partial q_k}$, and so

$$\nabla f = \frac{1}{h_1}\frac{\partial f}{\partial q_1}\hat{q}_1 + \frac{1}{h_2}\frac{\partial f}{\partial q_2}\hat{q}_2 + \frac{1}{h_3}\frac{\partial f}{\partial q_3}\hat{q}_3,$$

where $f = f(q_1, q_2, q_3)$ is the representation of the function in the Q coordinates.

For example, if the function f is originally defined in Cartesian coordinates by

$$f = x + yz$$

then

$$f = r\cos\theta\sin\varphi + r^2\sin\theta\sin\varphi\cos\varphi = r\cos\theta\sin\varphi + \frac{r^2}{2}\sin\theta\sin 2\varphi,$$

and

$$\begin{aligned}\nabla f &= \frac{\partial f}{\partial r}\hat{r} + \frac{1}{r\sin\varphi}\frac{\partial f}{\partial\theta}\hat{\theta} + \frac{1}{r}\frac{\partial f}{\partial\varphi}\hat{\varphi}\\ &= (\cos\theta\sin\varphi + r\sin\theta\sin 2\varphi)\hat{r} + (-\sin\theta + r\cos\theta\cos\varphi)\hat{\theta} + (\cos\theta\cos\varphi + r\sin\theta\cos 2\varphi)\hat{\varphi}.\end{aligned}$$

Next, we derive the expression for the DIVERGENCE in Q coordinates. Recall that, to compute the divergence in the cartesian coordinates, we consider a family of shrinking cubes with faces parallel to the coordinate planes. The same approach works in any coordinates by considering rectangular boxes whose sides are parallel to the *local* basis vectors $\hat{q}_1, \hat{q}_2, \hat{q}_3$. Let P be a point with Q coordinates (c_1, c_2, c_3), and, for sufficiently small $a > 0$, consider a rectangular box with vertices at the points with the Q coordinates $(c_1 \pm (a/2), c_2 \pm (a/2), c_3 \pm (a/2))$. The volume of this box is approximately $a^3|\vec{r}_1{}'(0)\cdot(\vec{r}_2{}'(0)\times\vec{r}_3{}'(0))| = a^3h_1h_2h_3$ Because the vectors $\hat{q}_k$ are orthogonal, the vector $\hat{q}_k$ is normal to two of the faces so that the area of each of those faces is approximately $a^2h_mh_n$, where $k \neq m \neq n$. Consider a continuously differentiable vector field $\vec{F}$ written in the Q coordinates as $\vec{F}(q_1,q_2,q_3) = F_1(q_1,q_2,q_3)\,\hat{q}_1 + F_2(q_1,q_2,q_3)\,\hat{q}_2 + F_3(q_1,q_2,q_3)\,\hat{q}_3$. Then the flux of this vector field through the pair of faces with the normal vector $\hat{q}_1$ is approximately

$$\begin{aligned}&a^2\Big(h_2\big(c_1+(a/2),c_2,c_3\big)h_3\big(c_1+(a/2),c_2,c_3\big)F_1\big(c_1+(a/2),c_2,c_3\big)\\ &-h_2\big(c_1-(a/2),c_2,c_3\big)h_3\big(c_1-(a/2),c_2,c_3\big)F_1\big(c_1-(a/2),c_2,c_3\big)\Big)\\ &\approx a^3\frac{\partial(h_2h_3F_1)}{\partial q_1},\end{aligned}$$

with the approximation getting better as $a \to 0$. Similar expressions hold for the fluxes across the other two pairs of faces. Summing up all the fluxes, dividing by the volume of the box, and passing to the limit $a \to 0$, we get the formula for the divergence of $\vec{F}$ in Q coordinates:

$$\mathrm{div}\vec{F} = \frac{1}{h_1h_2h_3}\left(\frac{\partial(h_2h_3F_1)}{\partial q_1} + \frac{\partial(h_1h_3F_2)}{\partial q_2} + \frac{\partial(h_1h_2F_3)}{\partial q_3}\right).$$

In particular, in cylindrical coordinates,

$$\mathrm{div}\vec{F} = \frac{1}{r}\left(\frac{\partial(rF_1)}{\partial r} + \frac{\partial F_2}{\partial\theta} + \frac{\partial(rF_3)}{\partial z}\right);$$

in spherical coordinates,

$$\mathrm{div}\vec{F} = \frac{1}{r^2\sin\varphi}\left(\frac{\partial(r^2\sin\varphi\,F_1)}{\partial r} + \frac{\partial(rF_2)}{\partial\theta} + \frac{\partial(r\sin\varphi\,F_3)}{\partial\varphi}\right).$$

Recall that the Laplacian $\nabla^2 f$ of a scalar field f is defined in every coordinate system as $\nabla^2 f = \mathrm{div}(\mathrm{grad} f)$. Let $f = f(q_1,q_2,q_3)$ be a scalar field defined in an orthogonal coordinate system Q. The

$$\nabla^2 f = \frac{1}{h_1h_2h_3}\left(\frac{\partial}{\partial q_1}\left(\frac{h_2h_3}{h_1}\frac{\partial f}{\partial q_1}\right) + \frac{\partial}{\partial q_2}\left(\frac{h_1h_3}{h_2}\frac{\partial f}{\partial q_2}\right) + \frac{\partial}{\partial q_3}\left(\frac{h_1h_2}{h_3}\frac{\partial f}{\partial q_3}\right)\right).$$

In particular, in cylindrical coordinates,

$$\nabla^2 f = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial f}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 f}{\partial\theta^2} + \frac{\partial^2 f}{\partial z^2};$$

in spherical coordinates,

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

Next, we derive the formula for the CURL. Consider a continuously differentiable vector field $\vec{F}$ written in the Q coordinates as $\vec{F}(q_1,q_2,q_3) = F_1(q_1,q_2,q_3)\,\hat{q}_1 + F_2(q_1,q_2,q_3)\,\hat{q}_2 + F_3(q_1,q_2,q_3)\,\hat{q}_3$. Let us compute $\operatorname{curl}\vec{F}(P)\cdot\hat{q}_1$, where the point P has Q-coordinates (c_1, c_2, c_3). For a sufficiently small $a > 0$, consider a rectangle spanned by the vectors $a\vec{r}_k'(0)$, $k = 2, 3$, so that P is at the center of the rectangle. The vertices of the rectangle have the Q coordinates $(c_1, c_2 \pm (a/2), c_3 \pm (a/2))$ and the area of this rectangle is approximately $a^2 h_2 h_3$. The line integral of $\vec{F}$ along the two sides parallel to $\hat{q}_2$ is approximately

$$\begin{aligned}
&a\Big(h_2\big(c_1, c_2, c_3 - (a/2)\big)F_2\big(c_1, c_2, c_3 - (a/2)\big)\\
&- h_2\big(c_1, c_2, c_3 + (a/2)\big)F_2\big(c_1, c_2, c_3 + (a/2)\big)\Big)\\
&\approx -a^2\frac{\partial(h_2F_2)}{\partial q_3},
\end{aligned}$$

with the quality of approximation improving as $a \to 0$. The line integral over the remaining two sides is approximately $a^2\partial(h_3F_3)/\partial q_2$. Dividing by the area of the rectangle and passing to the limit $a \to 0$, we find that

$$\operatorname{curl}\vec{F}(P)\cdot\hat{q}_1 = \frac{1}{h_1h_2h_3}\left(\frac{\partial(h_3F_3)}{\partial q_2} - \frac{\partial(h_2F_2)}{\partial q_3}\right)h_1$$

The other two components, $\operatorname{curl}\vec{F}(P)\cdot\hat{q}_2$ and $\operatorname{curl}\vec{F}\cdot\hat{q}_3$ are computed similarly. As a result,

$$\operatorname{curl}\vec{F} = \frac{1}{h_1h_2h_3}\begin{vmatrix} h_1\hat{q}_1 & h_2\hat{q}_2 & h_3\hat{q}_3 \\ \frac{\partial}{\partial q_1} & \frac{\partial}{\partial q_2} & \frac{\partial}{\partial q_3} \\ h_1F_1 & h_2F_2 & h_3F_3 \end{vmatrix}.$$