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Let x, y and z be our usual Cartesian coordinates and consider the general change of coordinates

$$\begin{aligned} x &= x(q_1, q_2, q_3) \\ y &= y(q_1, q_2, q_3) \\ z &= z(q_1, q_2, q_3) \end{aligned}$$
(1)

or, more succinctly, let  $x = x_1$ ,  $y = x_2$ ,  $z = x_3$  so

$$x_i = x_i(q_1, q_1, q_3), \quad i = 1, 2, 3.$$
 (2)

The position vector  $\mathbf{r}$  can be expressed in terms of the  $q_j$ 's through the Cartesian expression:

$$\boldsymbol{r} = \hat{\boldsymbol{x}} x(q_1, q_2, q_3) + \hat{\boldsymbol{y}} y(q_1, q_2, q_3) + \hat{\boldsymbol{z}} z(q_1, q_2, q_3) = \sum_{i=1}^3 \hat{\boldsymbol{x}}_i x_i(q_1, q_2, q_3).$$
(3)

Fixing  $q_2, q_3$  and varying  $q_1$ , the vector function  $\mathbf{r} = \mathbf{r}(q_1, q_2, q_3)$  describes a curve. The derivative  $\partial \mathbf{r}/\partial q_1$  is tangent to that curve. Likewise,  $\mathbf{r} = \mathbf{r}(q_1, q_2, q_3)$  with  $q_1, q_3$  fixed and varying  $q_2$  gives another family of curves, one curve for each value of  $q_1, q_3$ , with tangents  $\partial \mathbf{r}/\partial q_2$ . Finally,  $\mathbf{r} = \mathbf{r}(q_1, q_2, q_3)$  with  $q_1, q_2$  fixed and varying  $q_3$  is the third family of curves with tangents  $\partial \mathbf{r}/\partial q_3$ . On the other hand, fixing  $q_1$  and varying  $q_2, q_3$ , the vector function  $\mathbf{r} = \mathbf{r}(q_1, q_2, q_3)$  now describes a family of surfaces, one for each  $q_1$ , while  $q_2$  fixed with varying  $q_1, q_3$  is another surface and  $q_3$  fixed, varying  $q_1, q_2$  is the third family of surfaces.

Line Element (Displacement vector) The general line element dr in curvilinear coordinates is given by (chain rule):

$$d\mathbf{r} = \frac{\partial \mathbf{r}}{\partial q_1} dq_1 + \frac{\partial \mathbf{r}}{\partial q_2} dq_2 + \frac{\partial \mathbf{r}}{\partial q_3} dq_3 = \sum_{i=1}^3 \frac{\partial \mathbf{r}}{\partial q_i} dq_i.$$
(4)

**Surface Elements** The surface element on the surface  $q_3 = constant$ , for example, is given by

$$d\mathbf{A}_3 = \left(\frac{\partial \mathbf{r}}{\partial q_1} \times \frac{\partial \mathbf{r}}{\partial q_2}\right) dq_1 dq_2,\tag{5}$$

and likewise for other area elements. An orientation is built into the order of the coordinates.

Volume Element The volume element is given by the mixed (i.e. triple scalar) product

$$dV = \left(\frac{\partial \boldsymbol{r}}{\partial q_1} \times \frac{\partial \boldsymbol{r}}{\partial q_2}\right) \cdot \frac{\partial \boldsymbol{r}}{\partial q_3} \, dq_1 dq_2 dq_3. \tag{6}$$

This volume element is positive if  $q_1, q_2, q_3$  correspond to a right-handed frame, negative otherwise. This important formula, which corresponds to change of variables in multiple integrals, can be written in the form of a determinant – the *Jacobian determinant* or simply *Jacobian*, often denoted J– which generalizes directly to any dimensions

$$dV = \begin{vmatrix} \frac{\partial x}{\partial q_1} & \frac{\partial x}{\partial q_2} & \frac{\partial x}{\partial q_3} \\ \frac{\partial y}{\partial q_1} & \frac{\partial y}{\partial q_2} & \frac{\partial y}{\partial q_3} \\ \frac{\partial z}{\partial q_1} & \frac{\partial z}{\partial q_2} & \frac{\partial z}{\partial q_3} \end{vmatrix} dq_1 dq_2 dq_3 = det\left(\frac{\partial x_i}{\partial q_j}\right) dq_1 dq_2 dq_3.$$
(7)

## **Orthogonal Coordinates**

The vectors  $\partial \mathbf{r}/\partial q_i$  are key to the coordinates. They provide a natural vector basis. The coordinates are said to be orthogonal if these tangent vectors are orthogonal to each other. It is useful to define the unit vector in the  $q_i$  coordinate direction by

$$\frac{\partial \boldsymbol{r}}{\partial q_i} = h_i \hat{\boldsymbol{q}}_i \tag{8}$$

where  $h_i$  is therefore

$$h_i = ||\frac{\partial \boldsymbol{r}}{\partial q_i}|| = \sqrt{\sum_{k=1}^3 \left(\frac{\partial x_k}{\partial q_i}\right)^2}.$$
(9)

These  $h_i$ 's are called the *scale* or *metric* factors. The distance traveled in x-space when changing  $q_i$  by  $dq_i$ , keeping the other q's fixed, is  $ds_i = h_i dq_i$ .

In curvilinear coordinates, the unit vectors  $\hat{q}_i$  depend on the coordinates. We need to know their derivatives with respect to the  $q_j$ ,  $\partial \hat{q}_i / \partial q_j$ , for various operations but in particular to determine the appropriate curvilinear expressions for gradient, divergence and curl. These derivative are perpendicular to  $\hat{q}_i$  as, by definition,  $\hat{q}_i \cdot \hat{q}_i = 1$ . Differentiating that expression with respect to  $q_j$  yields

$$\hat{\boldsymbol{q}}_i \cdot \frac{\partial \hat{\boldsymbol{q}}_i}{\partial q_j} = 0. \tag{10}$$

The rate of change of a unit vector is always perpendicular to the unit vector.

Orthogonal coordinates are such that  $\hat{q}_i \cdot \hat{q}_j = \delta_{ij}$ ,  $\forall i, j$ . We'll now derive compact expressions for  $\partial \hat{q}_i / \partial q_j$  in terms of the  $\hat{q}_i$ 's and the  $h_i$ 's, in the case of orthogonal coordinates.

The key relationship arises from the equality of mixed partials

$$\frac{\partial^2 \boldsymbol{r}}{\partial q_i \partial q_j} = \frac{\partial^2 \boldsymbol{r}}{\partial q_j \partial q_i} \tag{11}$$

if these 2nd derivatives exist and are continuous, which we assume. Expanding these derivatives in terms of  $\hat{q}_i$  and  $\hat{q}_j$  defined as in (8) gives

$$\hat{\boldsymbol{q}}_i \frac{\partial h_i}{\partial q_j} + h_i \frac{\partial \hat{\boldsymbol{q}}_i}{\partial q_j} = \hat{\boldsymbol{q}}_j \frac{\partial h_j}{\partial q_i} + h_j \frac{\partial \hat{\boldsymbol{q}}_j}{\partial q_i}.$$
(12)

Let

$$\frac{\partial \hat{\boldsymbol{q}}_i}{\partial q_j} = \sum_{k=1}^3 C_{ijk} \, \hat{\boldsymbol{q}}_k, \qquad C_{ijk} = \hat{\boldsymbol{q}}_k \cdot \frac{\partial \hat{\boldsymbol{q}}_i}{\partial q_j} \,. \tag{13}$$

Then (10) implies that

$$C_{iji} = 0, \qquad \forall i, j \tag{14}$$

and projecting (12) onto  $\hat{q}_{j}$ , with i, j distinct, gives

$$C_{ijj} = \frac{1}{h_i} \frac{\partial h_j}{\partial q_i}, \qquad \forall i \neq j.$$
(15)

as  $\hat{q}_i$  is orthogonal to  $\partial \hat{q}_i / \partial q_i$ . Projecting (12) onto  $\hat{q}_k$  now, with  $i \neq k, j \neq k$ , gives

$$h_i C_{ijk} = h_j C_{jik}, \quad \forall i \neq k, j \neq k.$$
 (16)

Finally, orthogonality of the unit vectors  $\hat{\boldsymbol{q}}_k \cdot \hat{\boldsymbol{q}}_i = \delta_{ik}$ , implies  $\partial(\hat{\boldsymbol{q}}_k \cdot \hat{\boldsymbol{q}}_i)/\partial q_j = 0$ . Expanding this out and using the definition of  $C_{ijk}$  yields

$$C_{ijk} = -C_{kji}, \qquad \forall i \neq k. \tag{17}$$

The four relationships (14), (15), (16) and (17) determine all the  $C_{ijk}$ 's. There are 27  $C_{ijk}$  coefficients. Eqn. (14) specifies 9 of them and (15) specifies another 6. The remaining 12 coefficients are determined by the 3 equations given by (16) and the 9 equations (17). Indeed (15) and (17) give

$$C_{jji} = -C_{ijj} = -\frac{1}{h_i} \frac{\partial h_j}{\partial q_i}, \qquad \forall i \neq j,$$
(18)

so all coefficients with at least one repeated index, i.e.  $C_{iji}$ ,  $C_{ijj}$  and  $C_{iik}$  are known. When i, j, k are all distincts then (16) and (17) give

$$h_i C_{ijk} = h_j C_{jik} = -h_j C_{kij},$$
  

$$h_j C_{jki} = h_h C_{kji} = -h_k C_{ijk},$$
  

$$h_k C_{kij} = h_i C_{ikj} = -h_i C_{jki}.$$
(19)

The first and last column of these equations give the 3-by-3 system

$$\begin{array}{rcl}
h_i C_{ijk} &+ & h_j C_{kij} &= 0, \\
h_k C_{ijk} &+ & h_j C_{jki} &+ & = 0, \\
& & h_i C_{jki} &+ & h_k C_{kij} &= 0,
\end{array}$$
(20)

whose unique solution is  $C_{ijk} = C_{jki} = C_{kij} = 0$ . Hence all coefficients with no repeated indices vanish. The final results are

$$\frac{\partial \hat{q}_i}{\partial q_i} = \hat{q}_j \frac{1}{h_i} \frac{\partial h_j}{\partial q_i}, \qquad \forall i \neq j$$
(21)

$$\frac{\partial \hat{\boldsymbol{q}}_i}{\partial q_i} = -\hat{\boldsymbol{q}}_j \frac{1}{h_j} \frac{\partial h_i}{\partial q_j} - \hat{\boldsymbol{q}}_k \frac{1}{h_k} \frac{\partial h_i}{\partial q_k}, \quad \forall i, j, k \quad \text{distinct.}$$
(22)

For orthogonal coordinates, the surface and volume elements can be expressed in terms of the  $h_i$ 's as well. For instance, the surface element for the  $q_3 = const$ . surface is

$$d\boldsymbol{A}_3 = \boldsymbol{\hat{q}}_3 \, h_1 h_2 \, dq_1 dq_2, \tag{23}$$

and the volume element

$$dV = h_1 h_2 h_3 \, dq_1 dq_2 dq_3, \tag{24}$$

assuming that  $q_1, q_2, q_3$  is right-handed.

ADD: grad, div, curl... so the h's determine everything when the q coords are orthogonal. Moreover they often have simple expressions in terms of the q's. Let's look at some important examples.

## Cylindrical coordinates

$$x = \rho \cos \varphi, \quad y = \rho \sin \varphi, \quad z = z.$$
 (25)

Spherical coordinates

$$x = r\sin\theta\cos\varphi, \quad y = r\sin\theta\sin\varphi, \quad z = r\cos\theta.$$
(26)

Elliptical coordinates

$$x = \alpha \cosh u \cos v, \quad y = \alpha \sinh u \sin v, \quad z = z \tag{27}$$

## Non-orthogonal Curvilinear Coordinates

When the coordinates are not orthogonal, the length of the natural basis vectors  $h_i = ||\partial r/\partial q_i||$  do not fully determine the geometry. We need to know all the lengths and all the angles between the basis vectors, i.e. all the dot-products

$$g_{ij} \equiv \frac{\partial \boldsymbol{r}}{\partial q_i} \cdot \frac{\partial \boldsymbol{r}}{\partial q_j} = \sum_{l=1}^3 \frac{\partial x_l}{\partial q_i} \frac{\partial x_l}{\partial q_j}.$$
(28)

The  $g_{ij}$ 's are the *metric* coefficients. Note that  $g_{ii} = h_i^2$ .

But there is another important set of basis vectors when the coordinates are non-orthogonal: the  $\nabla q_i$  vectors, i = 1, 2, 3. The  $\nabla q_i$  vector is perpendicular to the  $q_i = constant$  surface. Therefore  $\nabla q_1$ , for instance, is orthogonal both to  $\partial r/\partial q_2$  and  $\partial r/\partial q_3$  which are both tangent to the  $q_1 = constant$  surface, but  $\nabla q_i$  is not parallel to  $\partial r/\partial q_i$  unless the coordinates are orthogonal. However, their dot product is always 1. Indeed, by the chain rule, we have

$$\frac{\partial \boldsymbol{r}}{\partial q_i} \cdot \boldsymbol{\nabla} q_j = \sum_{l=1}^3 \frac{\partial x_l}{\partial q_i} \frac{\partial q_j}{\partial x_l} = \frac{\partial q_j}{\partial q_i} = \delta_{ij} .$$
<sup>(29)</sup>

When the coordinates are orthogonal, then  $\partial \mathbf{r}/\partial q_i$  and  $\nabla q_i$  are parallel and, moreover, their magnitudes are inverse of one another from (29), i.e.  $\partial \mathbf{r}/\partial q_i = h_i \hat{\mathbf{q}}_i$  and  $\nabla q_i = h_i^{-1} \hat{\mathbf{q}}_i$ . Again, in the orthogonal case the  $h_i$ 's and the  $\hat{\mathbf{q}}_i$ 's determine everything. But in the non-orthogonal case, the algebra is simpler if we stick with the non-normalized basis vectors  $\partial \mathbf{r}/\partial q_i$  and  $\nabla q_i$ , i = 1, 2, 3. (Actually, it is useful to normalize those basis vectors and define two sets of non-dimensional unit vectors, as the components of vectors in those normalized bases keep their physical units. One speaks of "physical curvilinear coordinates" when the normalized bases are used).

Note that  $\nabla q_i$  refers to the gradient of the inverse functions  $q_i = q_i(x_1, \ldots, x_n)$ . The **implicit func**tion theorem states that these inverse functions exists provided the Jacobian  $J \equiv det(\partial x_i/\partial q_j)$ is not singular. Geometrically, this means that if the vectors  $\partial r/\partial q_i$ ,  $i = 1, \ldots, n$  are not coplanar, then the  $q_i$ 's are good coordinates (at least locally) and each point in *q*-space corresponds to one and only one point in *x*-space. The equation (29) specifies that the Jacobian matrices,  $\partial x_i/\partial q_j$ and  $\partial q_i/\partial x_j$  are inverses of one another. This is true for their determinant  $J_x = det(\partial x_i/\partial q_j)$  and  $J_q = det(\partial q_i/\partial x_j)$  also:  $J_x J_q = 1$ . The Jacobian determinant (or simply Jacobian) is the amplification factor of a volume element, *i.e.* the volume element in *q*-space:  $dV_q \equiv dq_1dq_2dq_3$  becomes the volume  $dV_x \equiv J_x dV_q$  in *x*-space. Vice-versa: the volume element  $dV_x \equiv dxdydz$  in *x*-space becomes the volume  $dV_q = J_q dV_x$  in *q*-space. We're back in *q*-space so the volume should be the same as originally and that means  $J_x J_q = 1$ . This relation is useful in practice as it may be easier to compute one Jacobian than the other (example: try the Carnot cycle problem posted in the exercises). Note that the chain rule also gives

$$\frac{\partial x_i}{\partial x_j} = \delta_{ij} = \sum_{l=1}^3 \frac{\partial x_i}{\partial q_l} \frac{\partial q_l}{\partial x_j} \,. \tag{30}$$

The  $\partial r/\partial q_i$  basis (displacement basis) is particularly appropriate for displacement type vectors such as the velocity. Indeed the velocity components which are  $\dot{x}_i$  in Cartesian coordinates are simply  $\dot{q}_i$  in the  $q_i$  coordinates when using the displacement basis as by the chain rule

$$\frac{d\boldsymbol{r}}{dt} = \sum_{i} \hat{\boldsymbol{x}}_{i} \dot{\boldsymbol{x}}_{i} = \sum_{j} \dot{q}_{j} \frac{\partial \boldsymbol{r}}{\partial q_{j}}.$$
(31)

On the other hand, the  $\nabla q_i$  basis is particularly appropriate for the gradient operator as by the chain rule again

$$\boldsymbol{\nabla} f = \sum_{i} \hat{\boldsymbol{x}}_{i} \frac{\partial f}{\partial x_{i}} = \sum_{j} \frac{\partial f}{\partial q_{j}} \boldsymbol{\nabla} q_{j}, \qquad (32)$$

so the components of the gradient are simply  $\partial f / \partial q_i$  in the  $\nabla q_i$  basis, how convenient! In general, any vector  $\boldsymbol{v}$  can be expanded in terms of either basis:

$$\boldsymbol{v} \equiv \sum_{i} \hat{\boldsymbol{x}}_{i} v_{i} \equiv \sum_{j} v_{j}^{\prime} \, \frac{\partial \boldsymbol{r}}{\partial q_{j}} \equiv \sum_{j} \bar{v}_{j} \, \boldsymbol{\nabla} q_{j}. \tag{33}$$

Using the relationships (29), one obtains the components of one basis by projecting onto the other, *i.e.* 

$$v_i' = \boldsymbol{v} \cdot \boldsymbol{\nabla} q_i = \sum_k v_k \frac{\partial q_i}{\partial x_k} = \sum_j \bar{v}_j \, \boldsymbol{\nabla} q_i \cdot \boldsymbol{\nabla} q_j \,, \tag{34}$$

and

$$\bar{v}_i = \boldsymbol{v} \cdot \frac{\partial \boldsymbol{r}}{\partial q_i} = \sum_l v_l \frac{\partial x_l}{\partial q_i} = \sum_j v'_j \frac{\partial \boldsymbol{r}}{\partial q_j} \cdot \frac{\partial \boldsymbol{r}}{\partial q_i} \,. \tag{35}$$

These two types of vector components,  $v'_i$  and  $\bar{v}_i$ , are usually referred to as the "contravariant" and "covariant" vectors, respectively. They are usually written  $v^j$  and  $v_j$ , but I won't use that compact but weird notation here. These two sets of components can be directly related to each other through the metric coefficients

$$g_{ij} \equiv \frac{\partial \boldsymbol{r}}{\partial q_i} \cdot \frac{\partial \boldsymbol{r}}{\partial q_j} = \sum_l \frac{\partial x_l}{\partial q_i} \frac{\partial x_l}{\partial q_j},\tag{36}$$

and

$$g^{ij} \equiv \nabla q_i \cdot \nabla q_j = \sum_l \frac{\partial q_i}{\partial x_l} \frac{\partial q_j}{\partial x_l}.$$
(37)

Indeed from (34) and (35) we have

$$v_i' = \sum_j g^{ij} \,\bar{v}_j,\tag{38}$$

and

$$\bar{v}_i = \sum_j g_{ij} \, v'_j. \tag{39}$$

The metric coefficients  $g_{ij}$  and  $g^{ij}$  specify all the lengths and angles of the bases  $\partial \boldsymbol{r}/\partial q_i$  and  $\nabla q_i$ , i = 1, 2, 3, respectively. In orthogonal coordinates, we only needed the 3 h's, but in general we need the 6 g's. (The matrices  $g^{ij}$  and  $g_{ij}$  are inverse of one another again).

We're starting to understand why Einstein introduced the *summation convention* where sums over repeated indices are implicit, *e.g.* Einstein simply writes

$$v_j' \, \frac{\partial x_l}{\partial q_i} \frac{\partial x_l}{\partial q_j}$$

for the double sum

$$\sum_{j} \sum_{l} v_{j}^{\prime} \frac{\partial x_{l}}{\partial q_{i}} \frac{\partial x_{l}}{\partial q_{j}}.$$

The repeated indices j and l implicitly imply a sum over all values of those indices in Einstein's convention. It is a very useful compact notation and you don't quite need to be Einstein to use it. However it does require some care and understanding!