III. TRANSFORMATION RELATIONS

The transformation relations from cartesian coordinates to a general curvilinear system are developed here using certain concepts from differential geometry and tensor analysis, which are introduced only as needed. Warsi [15] has given an extensive collection of concepts from tensor analysis and differential geometry applicable to the generation of curvilinear coordinate systems. Another discussion is given in Eiseman [16], where these concepts are developed as part of a general survey on the generation and use of curvilinear coordinate systems. Eiseman includes a discussion on differential forms, which is a fundamental part of modern differential geometry, but primarily restricts his development to Euclidean space. In contrast, Warsi has given a classical development that includes curved space, but not differential forms.

Partial derivatives with respect to cartesian coordinates are related to partial derivatives with respect to curvilinear coordinates by the chain rule which may be written in either of two ways. If A is a scalar-valued function, then

$$A_{x_i} = \sum_{j=1}^{3} A_{\xi^j} (\xi^j)_{x_i} \qquad (i = 1,2,3) \tag{1}$$

or, equivalently,

$$A_{\xi^i} = \sum_{j=1}^{3} A_{x_j} (x_j)_{\xi^i} \qquad (i = 1,2,3) \tag{2}$$

Either formulation may be used to relate the cartesian and curvilinear derivatives of the function A. However, there is a difference in the transformation derivatives which must be inserted in these relations. In the first ease one must be able to evaluate (or approximate) the vectors

$$\nabla\xi^i \qquad (i = 1,2,3)$$

whereas, the second case requires

$$\mathbf{r}_{\xi^i} \qquad (i = 1,2,3)$$

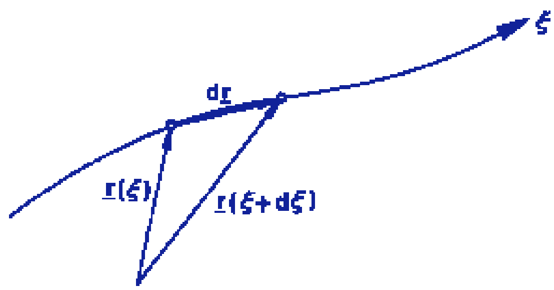
Thus all the transformation relations may be based on either of these two sets of vectors. Various properties of, and relationships between, these vectors are developed and applied in this chapter to provide the necessary transformation relations.

1. Base Vectors

The curvilinear coordinate lines of a three-dimensional system are space curves formed by the intersection of surfaces on which one coordinate is constant. One coordinate varies along a coordinate line, of course, while the other two are constant thereon. The tangents to the coordinate line and the normals to the coordinate surface are the base vectors of the coordinate system.

A. Covariant

Consider first a coordinate line along which only the coordinate ξ varies:



Clearly a tangent vector to the coordinate line is given by

$$\lim_{d\xi \to 0} \frac{\underline{r}(\xi + d\xi) - \underline{r}(\xi)}{d\xi} = \underline{r}_{\xi}$$

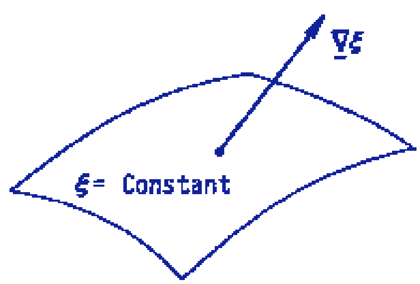
(Coordinates appearing as subscripts will always indicate partial differentiation.) These tangent vectors to the three coordinate lines are the three covariant base vectors of the curvilinear coordinate system, designated

$$\underline{a}_i = \underline{r}_{\xi^i} \quad (i = 1,2,3) \tag{3}$$

where the three curvilinear coordinates are represented by ξ^i (i=1,2,3), and the subscript i indicates the base vector corresponding to the ξ^i coordinate, i.e., the tangent to the coordinate line along which only ξ^i varies.

B. Contravariant

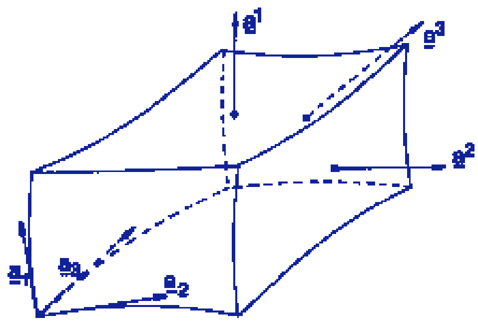
A normal vector to a coordinate surface on which the coordinate ξ is constant is given by $\underline{\nabla}\xi$:



These normal vectors to the three coordinate surfaces are the three contravariant base vectors of the curvilinear coordinate system, designated

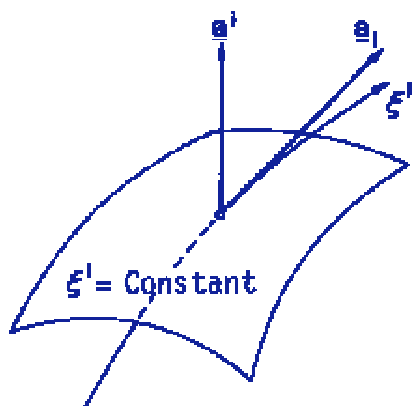
$$\underline{a}^i = \nabla\xi^i \qquad (i = 1,2,3) \tag{4}$$

Here the coordinate index i appears as a superscript on the base vector to differentiate these contravariant base vectors from the covariant base vectors. The two types of base vectors are illustrated in the following figure, showing an element of volume with six sides, each of which lies on some coordinate surface.



C. Orthogonality

Only in an orthogonal coordinate system are the two types of base vectors parallel, since for a non-orthogonal system, the normal to a coordinate surface does not necessarily coincide with the tangent to a coordinate line crossing that surface:



Also for an orthogonal system the three base vectors of each type are obviously mutually perpendicular.

2. Differential Elements

The differential increments of arc length, surface, and volume, which are needed for the formulation of the respective integrals, can be generated directly from the co-variant base vectors. The general arc length increment leads also to the definition of a fundamental metric tensor.

A. Covariant metric tensor

The general differential increment (not necessarily along a coordinate line) of a position vector is given by

$$d\underset{\sim}{r} = \sum_{i=1}^{3} \underset{\sim}{r}_{\xi^i} \, d\xi^i = \sum_{i=1}^{3} \underset{\sim}{a}_i \, d\xi^i$$

An increment of arc length along a general space curve then is given by

$$(ds)^2 = |d\underset{\sim}{r}|^2 = \sum_{i=1}^{3} \sum_{j=1}^{3} \underset{\sim}{a}_i \cdot \underset{\sim}{a}_j \, d\xi^i d\xi^j$$

The general arc length increment thus depends on the nine dot products, $\underset{\sim}{a}_i \cdot \underset{\sim}{a}_j$ (i=1,2,3) and (j= 1,2,3), which form a symmetric tensor. These quantities are the covariant metric tensor components:

$$g_{ij} = \underset{\sim}{a}_i \cdot \underset{\sim}{a}_j = g_{ji} \quad (i = 1,2,3), \ (j = 1,2,3) \tag{5}$$

Thus the general arc length increment can be written as

$$(ds)^2 = \sum_{i=1}^{3} \sum_{j=1}^{3} g_{ij} \, d\xi^i d\xi^j \tag{6}$$

B. Arc length element

An increment of arc length on a coordinate line along which ξ^i varies is given by

$$ds^i = |\underset{\sim}{r}_{\xi^i}| d\xi^i = |\underset{\sim}{a}_i| d\xi^i = \sqrt{g_{ii}} \, d\xi^i \tag{7}$$

C. Surface area element

Also an increment of area on a coordinate surface of constant ξ^i is given by

$$dS^i = |\underset{\sim}{r}_{\xi^j} \times \underset{\sim}{r}_{\xi^k}| d\xi^j d\xi^k = |\underset{\sim}{a}_j \times \underset{\sim}{a}_k| d\xi^j d\xi^k \qquad (i = 1,2,3) \quad (i,j,k) \text{ cyclic} \tag{8}$$

Using the vector identity

$$(\underset{\sim}{A} \times \underset{\sim}{B}) \cdot (\underset{\sim}{C} \times \underset{\sim}{D}) = (\underset{\sim}{A} \cdot \underset{\sim}{C})(\underset{\sim}{B} \cdot \underset{\sim}{D}) - (\underset{\sim}{A} \cdot \underset{\sim}{D})(\underset{\sim}{B} \cdot \underset{\sim}{C}) \tag{9}$$

we have

$$|\mathbf{a}_j \times \mathbf{a}_k|^2 = (\mathbf{a}_j \cdot \mathbf{a}_j)(\mathbf{a}_k \cdot \mathbf{a}_k) - (\mathbf{a}_j \cdot \mathbf{a}_k)^2$$

$$= g_{jj}g_{kk} - g_{jk}^2 \qquad (10)$$

so that the increment of surface area can be written as

$$dS^i = \sqrt{g_{jj}g_{kk} - g_{jk}^2}\, d\xi^j d\xi^k \qquad (i = 1,2,3)$$

$$(i,j,k) \text{ cyclic} \qquad (11)$$

D. Volume element

An increment of volume is given by

$$dV = \mathbf{r}_{\xi^i} \cdot (\mathbf{r}_{\xi^j} \times \mathbf{r}_{\xi^k}) d\xi^i d\xi^j d\xi^k \quad (i,j,k) \text{cyclic}$$

$$= \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) d\xi^1 d\xi^2 d\xi^3 \qquad (12)$$

But, by the identity (9),

$$[\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)]^2 = (\mathbf{a}_1 \cdot \mathbf{a}_1)[(\mathbf{a}_2 \times \mathbf{a}_3) \cdot (\mathbf{a}_2 \times \mathbf{a}_3)]$$

$$- |\mathbf{a}_1 \times (\mathbf{a}_2 \times \mathbf{a}_3)|^2$$

Also from (9),

$$(\mathbf{a}_2 \times \mathbf{a}_3) \cdot (\mathbf{a}_2 \times \mathbf{a}_3) = (\mathbf{a}_2 \cdot \mathbf{a}_2)(\mathbf{a}_3 \cdot \mathbf{a}_3) - (\mathbf{a}_2 \cdot \mathbf{a}_3)^2$$

and by the vector identity

$$\mathbf{A} \times (\mathbf{B} \times \mathbf{C}) = (\mathbf{A} \cdot \mathbf{C})\mathbf{B} - (\mathbf{A} \cdot \mathbf{B})\mathbf{C} \qquad (13)$$

we have

$$\mathbf{a}_1 \times (\mathbf{a}_2 \times \mathbf{a}_3) = (\mathbf{a}_1 \cdot \mathbf{a}_3)\mathbf{a}_2 - (\mathbf{a}_1 \cdot \mathbf{a}_2)\mathbf{a}_3$$

so that with the dot products replaced according to the definition (5),

$$[\underset{\sim}{a}_1 \cdot (\underset{\sim}{a}_2 \times \underset{\sim}{a}_3)]^2 = g_{11}(g_{22}g_{33} - g_{23}^2) - g_{13}^2 g_{22}$$

$$- g_{12}^2 g_{33} + 2g_{13}g_{12}g_{23}$$

$$= g_{11}(g_{22}g_{33} - g_{23}^2)$$

$$- g_{12}(g_{12}g_{33} - g_{13}g_{23})$$

$$+ g_{13}(g_{12}g_{23} - g_{13}g_{22})$$

This last expression is simply the determinant of the (symmetric) covariant metric tensor expanded by cofactors. Therefore

$$[\underset{\sim}{a}_1 \cdot (\underset{\sim}{a}_2 \times \underset{\sim}{a}_3)]^2 = \det|g_{ij}| = g \tag{14}$$

so that the volume increment can be written

$$dV = \sqrt{g}\, d\xi^1 d\xi^2 d\xi^3 \tag{15}$$

where $\sqrt{g}$ (called the Jacobian of the transformation) can be evaluated by either of the following expressions:

$$\sqrt{g} = \sqrt{\det|g_{ij}|} = \underset{\sim}{a}_1 \cdot (\underset{\sim}{a}_2 \times \underset{\sim}{a}_3) \tag{16}$$

3. Derivative Operators

Expressions for the derivative operators, such as gradient, divergence, curl, Laplacian, etc., are obtained by applying the Divergence Theorem to a differential volume increment bounded by coordinate surfaces. The gradient operator then leads to the expression of contravariant base vectors in terms of the covariant base vectors, and to the contravariant metric tensor as the inverse of the covariant metric tensor.

By the Divergence Theorem,

$$\iiint_V \underset{\sim}{\nabla} \cdot \underset{\sim}{A}\, dV = \oiint_S \underset{\sim}{A} \cdot \underset{\sim}{n}\, dS \tag{17}$$

for any tensor $\underset{\sim}{A}$, where $\underset{\sim}{n}$ is the outward-directed unit normal to the closed surface S enclosing the volume V. For a differential surface element lying on a coordinate surface we have, by Eq. (8),

$$\underset{\sim}{n}\, dS^i = \pm\, \underset{\sim}{a}_j \times \underset{\sim}{a}_k\, d\xi^j d\xi^k \qquad (18)$$

with the choice of sign being dependent on the location of the volume relative to the surface. Then considering a differential element of volume, δV, bounded by six faces lying on coordinate surfaces, as shown in the figure on p. 98, we have, using Eq. (15) and (18),

$$\iiint_{\delta V} (\underset{\sim}{\nabla} \cdot \underset{\sim}{A}) \sqrt{g}\, d\xi^1 d\xi^2 d\xi^3$$

$$= \sum_{i=1}^{3} \Big[\iint_{\delta S^i_+} \underset{\sim}{A} \cdot (\underset{\sim}{a}_j \times \underset{\sim}{a}_k) d\xi^j d\xi^k \qquad (19)$$

$$- \iint_{\delta S^i_-} \underset{\sim}{A} \cdot (\underset{\sim}{a}_j \times \underset{\sim}{a}_k) d\xi^j d\xi^k \Big]$$

where the notation δS^i_+ and S^i_- indicates the element on ξ^i two sides of the which ξ is constant and which are located at larger and smaller values, respectively, of ξ. Here, as usual, the indices (i,j,k) are cyclic.

A. Divergence

Proceeding to the limit as the element of volume shrinks to zero we then have an expression for the divergence:

$$\underset{\sim}{\nabla} \cdot \underset{\sim}{A} = \frac{1}{\sqrt{g}} \sum_{i=1}^{3} [(\underset{\sim}{a}_j \times \underset{\sim}{a}_k) \cdot \underset{\sim}{A}]_{\xi^i} \qquad (20)$$

where, as noted, the subscript ξ^i on the bracket indicates partial differentiation.

A basic metric identity is involved here, since

$$\sum_{i=1}^{3} (\underset{\sim}{a}_j \times \underset{\sim}{a}_k)_{\xi^i} = \sum_{i=1}^{3} (\underset{\sim}{r}_{\xi^j} \times \underset{\sim}{r}_{\xi^k})_{\xi^i}$$

$$= \sum_{i=1}^{3} \underset{\sim}{r}_{\xi^j \xi^i} \times \underset{\sim}{r}_{\xi^k} + \sum_{i=1}^{3} \underset{\sim}{r}_{\xi^j} \times \underset{\sim}{r}_{\xi^k \xi^i}$$

The indices (i,j,k) are cyclic, and therefore the last summation may be written equivalently as

$$\sum_{i=1}^{3} \mathbf{r}_{\xi^j} \times \mathbf{r}_{\xi^k \xi^i} = \sum_{i=1}^{3} \mathbf{r}_{\xi^k} \times \mathbf{r}_{\xi^i \xi^j}$$

Since this is then the negative of the first summation we have the identity,

$$\sum_{i=1}^{3} (\mathbf{a}_j \times \mathbf{a}_k)_{\xi^i} = 0 \qquad (21)$$

This is a fundamental metric identity which will be used several times in the developments that follow. This identity also follows directly from Eq. (20) for uniform $\underset{\sim}{A}$. It then follows that the divergence can also be written as

$$\nabla \cdot \mathbf{A} = \frac{1}{\sqrt{g}} \sum_{i=1}^{3} (\mathbf{a}_j \times \mathbf{a}_k) \cdot \mathbf{A}_{\xi^i} \qquad (22)$$

Although the equations (20) and (22) are equivalent expressions for the divergence, because of the identity (21), the numerical representations of these two forms may not be equivalent. The form given by Eq. (20) is called the conservative form, and that of Eq. (22), where the product derivative has been expanded and Eq. (21) has been used, is called the non-conservative form. Recalling that the quantity $(\underset{\sim}{a}_j \times \underset{\sim}{a}_k)$ represents an increment of surface area (cf.Eq. (8)), so that $(\underset{\sim}{a}_j \times \underset{\sim}{a}_k) \cdot \underset{\sim}{A}$ is a flux through this area, it is clear that the difference between the two forms is that the area used in numerical representation of the flux in the conservative form, Eq. (20), is the area of the individual sides of the volume element, but inthe nonconservative form, a common area evaluated at the center of the volume element is used. The conservative form thus gives the telescopic collapse of the flux terms when the difference equations are summed over the field, so that this summation then involves only the boundary fluxes. This would seem to favor the conservative form as the better numerical representation of the net flux through the volume element.

It is important to note that since the conservative form of the divergence, and of the gradient, curl, and Laplacian to follow, is obtained directly from the closed surface integral in the Divergence Theorem, the use of the conservative difference forms for these derivative operators is equivalent to using difference forms for that closed surface integral. Therefore the finite volume difference formulation can be implemented by using these conservative forms directly in the differential equations of motion without the necessity of returning to the integral form of the equations of motion.

B. Curl

Since Eq. (17) is also valid with the dot products replaced by cross products, the conservative and non-conservative expressions for the curl follow immediately from Eq. (20) and (22):

$$\underline{\nabla} \times \underline{A} = \frac{1}{\sqrt{g}} \sum_{i=1}^{3} \left[(\underline{a}_j \times \underline{a}_k) \times \underline{A} \right]_{\xi^i} \tag{23}$$

and

$$\underline{\nabla} \times \underline{A} = \frac{1}{\sqrt{g}} \sum_{i=1}^{3} (\underline{a}_j \times \underline{a}_k) \times \underline{A}_{\xi^i} \tag{24}$$

These expressions can also be written, using Eq. (13), as

$$\underline{\nabla} \times \underline{A} = \frac{1}{\sqrt{g}} \sum_{i=1}^{3} \left[(\underline{a}_j \cdot \underline{A})\underline{a}_k - (\underline{a}_k \cdot \underline{A})\underline{a}_j \right]_{\xi^i} \tag{25}$$

and

$$\underline{\nabla} \times \underline{A} = \frac{1}{\sqrt{g}} \sum_{i=1}^{3} \left[(\underline{a}_j \cdot \underline{A}_{\xi^i})\underline{a}_k - (\underline{a}_k \cdot \underline{A}_{\xi^i})\, \underline{a}_j \right] \tag{26}$$

C. Gradient

Eq. (17) is also valid with $\underline{A}$ replaced by a scalar, and the dot product replaced by simple operation on the left and multiplication on the right. Therefore the conservative and non-conservative expressions for the gradient also follow directly from Eq. (20) and (22) as

$$\underline{\nabla} A = \frac{1}{\sqrt{g}} \sum_{i=1}^{3} \left[(\underline{a}_j \times \underline{a}_k) A \right]_{\xi^i} \tag{27}$$

and

$$\underline{\nabla} A = \frac{1}{\sqrt{g}} \sum_{i=1}^{3} (\underline{a}_j \times \underline{a}_k) A_{\xi^i} \tag{28}$$

D. Laplacian

The expressions for the Laplacian then follow from Eq. (20) or (22), with $\underline{A}$ replaced by $\underline{\nabla}$A from Eq. (27) or (28). Thus the conservative form is

$$\nabla^2 A = \underline{\nabla} \cdot (\underline{\nabla} A)$$

$$= \frac{1}{\sqrt{g}} \sum_{i=1}^{3} \sum_{l=1}^{3} \{\frac{1}{\sqrt{g}}[(\underline{a}_j \times \underline{a}_k) \cdot [(\underline{a}_m \times \underline{a}_n)A]_{\xi^l}\}_{\xi^i} \quad (29)$$

$$(i,j,k) \text{ cyclic} \qquad (l,m,n) \text{ cyclic}$$

and the non-conservative is

$$\nabla^2 A = \frac{1}{\sqrt{g}} \sum_{i=1}^{3} \sum_{l=1}^{3} (\underline{a}_j \times \underline{a}_k) \cdot [\frac{1}{\sqrt{g}}(\underline{a}_m \times \underline{a}_n)A_{\xi^l}]_{\xi^i} \quad (30)$$

$$(i,j,k) \text{ cyclic} \qquad (l,m,n) \text{ cyclic}$$

With the product derivative expanded, the non-conservative form, Eq. (30), can also be written as

$$\nabla^2 A = \frac{1}{g} \sum_{i=1}^{3} \sum_{l=1}^{3} (\underline{a}_j \times \underline{a}_k) \cdot (\underline{a}_m \times \underline{a}_n)A_{\xi^l \xi^i}$$
$$+ \frac{1}{\sqrt{g}} \sum_{i=1}^{3} \sum_{l=1}^{3} (\underline{a}_j \times \underline{a}_k) \cdot [\frac{1}{\sqrt{g}}(\underline{a}_m \times \underline{a}_n)]_{\xi^i} A_{\xi^l} \quad (31)$$

4. Relations Between Covariant and Contravariant Metrics

A. Base vectors

The expression (28) for the gradient allows the contravariant base vectors to be expressed in terms ofthe co-variant base vectors as follows. With A=ξ^m in (28), we have

$$\underline{\nabla}\xi^m = \frac{1}{\sqrt{g}} \sum_{i=1}^{3} (\underline{a}_j \times \underline{a}_k)\delta_i^m$$

since the three curvilinear coordinates are independent of each other. Then

$$\underline{\nabla}\xi^i = \frac{1}{\sqrt{g}} \underline{a}_j \times \underline{a}_k \qquad (i = 1,2,3) \qquad (i,j,k) \text{ cyclic} \quad (32)$$

This gives a relation between the derivatives of the curvilinear coordinates $(\xi^i)_{x_l}$ and the derivatives $(x_r)_{\xi^s}$ of the cartesian coordinates. By Eq. (4) the contravariant base vectors maybe written in terms of the covariant base vectors as

$$a^i = \nabla\xi^i = \frac{1}{\sqrt{g}} a_j \times a_k \tag{33}$$

$$(i = 1,2,3) \qquad (i,j,k) \text{ cyclic}$$

By Eq. (33),

$$a_i \cdot a^j = \frac{1}{\sqrt{g}} a_i \cdot (a_k \times a_l)$$

where here (j,k,l) are cyclic. If $j \neq i$, either k or l must be i, and in that case the right-hand sidevanishessince the three vectors in the triple product may be in any cyclic order and the cross product of any vector with itself vanishes. When j=i, the right-hand side is simply unity. Therefore, in general

$$a_i \cdot a^j = \delta_i^j \tag{34}$$

Because of this relation, any vector $\underset{\sim}{A}$ can be expressed in terms of either set of base vectors as

$$A = \sum_{i=1}^{3} (a^i \cdot A)\, a_i \tag{35}$$

and

$$A = \sum_{i=1}^{3} (a_i \cdot A)\, a^i \tag{36}$$

Here the quantities $A^i = a^i \cdot A$ and $A^i = a_i \cdot A$, are the contravariant and co-variant components, respectively, of the vector $\underset{\sim}{A}$.

B. Metric Tensors

The components of the contravariant metric tensor are the dot products of the contravariant base vectors:

$$g^{ij} = a^i \cdot a^j = g^{ji} \qquad (i = 1,2,3) \quad (j = 1,2,3) \tag{37}$$

The relation between the covariant and contravariant metric tensor components is obtained by use of Eq. (33) in (37). Thus, with (i,j,k) cyclic and (l,m,n) cyclic,

$$g^{il} = \underline{a}^i \cdot \underline{a}^l = \frac{1}{g}(\underline{a}_j \times \underline{a}_k) \cdot (\underline{a}_m \times \underline{a}_n)$$

$$= \frac{1}{g}[(\underline{a}_j \cdot \underline{a}_m)(\underline{a}_k \cdot \underline{a}_n) - (\underline{a}_j \cdot \underline{a}_n)(\underline{a}_k \cdot \underline{a}_m)]$$

by the identity (9). Then from the definition (5),

$$g^{il} = \frac{1}{g}(g_{jm}g_{kn} - g_{jn}g_{km}) \qquad (38)$$

$$(i = 1,2,3) \qquad (l = 1,2,3)$$

$$(i,j,k) \text{ cyclic} \qquad (l,m,n) \text{ cyclic}$$

Since the quantity in parentheses in the above equation is the signed cofactor of the il component of the covariant metric tensor, the right-hand side above is the li component of the inverse of this tensor. Then, since the metric tensor is symmetric we have immediately that the contravariant metric tensor is simply the inverse of the covariant metric tensor. It then follows that

$$\det|g^{ij}| = \frac{1}{\det|g_{ij}|} = \frac{1}{g}$$

so that, in terms of the contravariant base vectors, the Jacobian is

$$\sqrt{g} = (\det|g^{ij}|)^{-1/2} = \frac{1}{\underline{a}^1 \cdot (\underline{a}^2 \times \underline{a}^3)} \qquad (39)$$

The identity (21) can be given, using Eq. (33), as

$$\sum_{i=1}^{3}(\sqrt{g}\,\underline{a}^i)_{\xi^i} = 0 \qquad (40)$$

5. Restatement of Derivative Operators

In view of Eq. (33), the cross products of the co-variant base vectors in the expressions given above for the gradient, divergence, curl, and Laplacian can be replaced directly by the contravariant base vectors (multiplied by the Jacobian). The components of these contravariant base vectors $\underline{a}^i$ in the expressions are the derivatives of the curvilinear coordinates with respect to the cartesian coordinates, and this notation, rather than the cross-products, often appears in the literature. Thus, by Eq. (4), the x_j-component of ai can be written as

$$(\underline{a}^i)_j = (\xi^i)_{x_j} \qquad (41)$$

The expressions for the gradient, divergence, curl, Laplacian, etc., given above in terms of the cross products of the covariant base vectors, $\underset{\sim}{a}_i$, involve the derivatives of the cartesian coordinates with respect to the curvilinear coordinates, e.g. $(x_i)_{\xi^j}$. The expressions given below in terms of the contravariant base vectors, $\underset{\sim}{a}^i$, involve the derivatives $(\xi^i)_{x_j}$ when $\sqrt{g}$ is evaluated from (39). From a coding standpoint, however, the contravariant base vectors $\underset{\sim}{a}^i$ in these expressions would be evaluated from the covariant base vectors using Eq. (33).

A. Conservative

The conservative forms are as follows:

$$\underset{\sim}{\nabla} A = \frac{1}{\sqrt{g}} \sum_{i=1}^{3} (\sqrt{g}\, \underset{\sim}{a}^i A)_{\xi^i} \tag{42}$$

$$\underset{\sim}{\nabla} \cdot \underset{\sim}{A} = \frac{1}{\sqrt{g}} \sum_{i=1}^{3} (\sqrt{g}\, \underset{\sim}{a}^i \cdot \underset{\sim}{A})_{\xi^i} \tag{43}$$

$$\underset{\sim}{\nabla} \times \underset{\sim}{A} = \frac{1}{\sqrt{g}} \sum_{i=1}^{3} (\sqrt{g}\, \underset{\sim}{a}^i \times \underset{\sim}{A})_{\xi^i} \tag{44}$$

$$\nabla^2 A = \frac{1}{\sqrt{g}} \sum_{i=1}^{3} \sum_{j=1}^{3} [\underset{\sim}{a}^i \cdot (\sqrt{g}\, \underset{\sim}{a}^j A)_{\xi^j}]_{\xi^i} \tag{45}$$

By expanding the inner derivative, the Laplacian can be expressed as

$$\nabla^2 A = \frac{1}{\sqrt{g}} \sum_{i=1}^{3} \sum_{j=1}^{3} (\sqrt{g}\, g^{ij} A_{\xi^j})_{\xi^i} \tag{46}$$

For $\underset{\sim}{\nabla} \cdot (\alpha \underset{\sim}{\nabla} A)$ we have

$$\underset{\sim}{\nabla} \cdot (\alpha \underset{\sim}{\nabla} A) = \frac{1}{\sqrt{g}} \sum_{i=1}^{3} \sum_{j=1}^{3} [\alpha \underset{\sim}{a}^i \cdot (\sqrt{g}\, \underset{\sim}{a}^j A)_{\xi^j}]_{\xi^i} \tag{47}$$

or, with the inner derivative expanded,

$$\underset{\sim}{\nabla} \cdot (\alpha \underset{\sim}{\nabla} A) = \frac{1}{\sqrt{g}} \sum_{i=1}^{3} \sum_{j=1}^{3} (\alpha \sqrt{g}\, g^{ij} A_{\xi^j})_{\xi^i} \tag{48}$$

In the expressions for the divergence, $\underset{\sim}{A}$ may be a tensor, in which case we have

$$(\underset{\sim}{\nabla} \cdot \underset{\sim}{A})_k = \sum_{l=1}^{3} (A_{kl})_{x_l}$$

$$= \frac{1}{\sqrt{g}} \sum_{i=1}^{3} \sum_{l=1}^{3} [\sqrt{g}\, (\underset{\sim}{a}^i)_l A_{kl}]_{\xi^i} \qquad (k = 1,2,3) \tag{49}$$

From Eq. (42) we have the conservative expressions for the first derivative:

$$A_{x_j} = (\underset{\sim}{\nabla} A)_j = \frac{1}{\sqrt{g}} \sum_{i=1}^{3} [\sqrt{g}\, (\underset{\sim}{a}^i)_j A]_{\xi^i} \tag{50}$$

where $(\cdot)_j$ is the component in the x_j-direction. Also, for the second derivative,

$$A_{x_j x_k} = [\underset{\sim}{\nabla}(A_{x_j})]_k = \frac{1}{\sqrt{g}} \sum_{i=1}^{3} \sum_{l=1}^{3} \{(\underset{\sim}{a}^i)_k [\sqrt{g}\, (\underset{\sim}{a}^l)_j A]_{\xi^l}\}_{\xi^i} \tag{51}$$

or, with the inner derivative expanded,

$$A_{x_j x_k} = \frac{1}{\sqrt{g}} \sum_{i=1}^{3} \sum_{l=1}^{3} [\sqrt{g}\, (\underset{\sim}{a}^i)_k (\underset{\sim}{a}^l)_j A_{\xi^l}]_{\xi^i} \tag{52}$$

It then follows that all of the above conservative expressions can be written in the form

$$\frac{1}{\sqrt{g}} \sum_{i=1}^{3} (A^i)_{\xi^i} \tag{53}$$

where the quantity A^i takes the following form for the various operatfons, with i = 1,2,3,

$$\underset{\sim}{\nabla} A : \quad A^i = \sqrt{g}\, \underset{\sim}{a}^i A \tag{54}$$

$$\underset{\sim}{\nabla} \cdot \underset{\sim}{A} \text{ (vector } \underset{\sim}{A}) : \quad A^i = \sqrt{g}\, \underset{\sim}{a}^i \cdot \underset{\sim}{A} \tag{55}$$

$$\underset{\sim}{\nabla} \cdot \underset{\sim}{A} \text{ (tensor } \underset{\sim}{A}) : \quad \underset{\sim}{A}^i = \sqrt{g}\, \underset{\sim}{A}\, \underset{\sim}{a}^i \tag{56}$$

matrix product of square matrix $\underset{\sim}{A}$ and column vector $\underset{\sim}{a}^i$. Here $\underset{\sim}{A}^i$ is a vector)

$$\underset{\sim}{\nabla} \times \underset{\sim}{A} : \quad \underset{\sim}{A}^i = \sqrt{g}\, \underset{\sim}{a}^i \times \underset{\sim}{A} \tag{57}$$

$$\nabla^2 A : \quad A^i = \underline{a}^i \cdot \sum_{j=1}^{3} (\sqrt{g}\, \underline{a}^j A)_{\xi^j} \quad \text{(for Eq. (45))} \tag{58}$$

$$A^i = \sqrt{g} \sum_{j=1}^{3} g^{ij} A_{\xi^j} \quad \text{(for Eq. (46))} \tag{59}$$

$$\underline{\nabla} \cdot (\alpha \underline{\nabla} A) : \quad A^i = \alpha \sum_{j=1}^{3} [\underline{a}^i \cdot (\sqrt{g}\, \underline{a}^j A)_{\xi^j}] \quad \text{(for Eq. (47))} \tag{60}$$

$$A^i = \alpha\sqrt{g} \sum_{j=1}^{3} g^{ij} A_{\xi^j} \quad \text{(for Eq. (48))} \tag{61}$$

$$A_{x_j} : \quad A^i = \sqrt{g}\, (\underline{a}^i)_j A \tag{62}$$

$$A_{x_j x_k} : \quad A^i = (\underline{a}^i)_k \sum_{l=1}^{3} [\sqrt{g}\, (\underline{a}^l)_j A]_{\xi^l} \quad \text{(for Eq. (51))} \tag{63}$$

$$A^i = \sqrt{g}\, (\underline{a}^i)_k \sum_{l=1}^{3} (\underline{a}^l)_j A_{\xi^l} \quad \text{(for Eq. (52))} \tag{64}$$

It is computationally more efficient to evaluate the product $\sqrt{g}\, \underline{a}^i$ as an entity from Eq. (33) when the conservative forms are used, in order to avoid the extra multiplication by $\sqrt{g}$. Another alternative is to include $\sqrt{g}$ with $\underline{A}$.

B. Non-conservative

The non-conservative relations are as follows:

$$\underline{\nabla} A = \sum_{i=1}^{3} \underline{a}^i A_{\xi^i} \tag{65}$$

From Eq. (65) the p operator can be represented by

$$\underline{\nabla} = \sum_{i=1}^{3} \underline{a}^i \frac{\partial}{\partial \xi^i} \tag{66}$$

and

$$\nabla \cdot A = \sum_{i=1}^{3} a^i \cdot A_{\xi^i} \tag{67}$$

$$\nabla \times A = \sum_{i=1}^{3} a^i \times A_{\xi^i} \tag{68}$$

$$\nabla^2 A = \sum_{i=1}^{3} \sum_{j=1}^{3} a^i \cdot a^j \; A_{\xi^i \xi^j} + \sum_{i=1}^{3} \sum_{j=1}^{3} a^i \cdot (a^j)_{\xi^i} \; A_{\xi^j} \tag{69}$$

Since

$$\nabla^2 \xi^l = \nabla \cdot (\nabla \xi^l) = \nabla \cdot a^l = \sum_{i=1}^{3} a^i \cdot (a^l)_{\xi^i} \tag{70}$$

by Eq. (37) and (69), the Laplacian can also be written as

$$\nabla^2 A = \sum_{i=1}^{3} \sum_{j=1}^{3} g^{ij} \; A_{\xi^i \xi^j} + \sum_{j=1}^{3} (\nabla^2 \xi^j) A_{\xi^j} \tag{71}$$

Using Eq. (67) and (65) we also have

$$\nabla \cdot (\alpha \nabla A) = \sum_{i=1}^{3} a^i \cdot (\alpha \nabla A)_{\xi^i}$$

$$= \sum_{i=1}^{3} \sum_{j=1}^{3} a^i \cdot (\alpha a^j A_{\xi^j})_{\xi^i}$$

$$= \sum_{i=1}^{3} \sum_{j=1}^{3} a^i \cdot [a^j (\alpha A_{\xi^j})_{\xi^i} + \alpha (a^j)_{\xi^i} A_{\xi^j}]$$

Thus, by Eq. (70), the non-conservative expression is

$$\nabla \cdot (\alpha \nabla A) = \sum_{i=1}^{3} \sum_{j=1}^{3} g^{ij} (\alpha A_{\xi^j})_{\xi^i} + \alpha \sum_{j=1}^{3} (\nabla^2 \xi^j) A_{\xi^j} \tag{72}$$

A more practical equation than Eq. (70) for the evaluation of $\nabla^2\xi^j$ in these expressions can be obtained as follows.

Since $\nabla^2 \underset{\sim}{r}=0$ it follows from Eq. (71) that

$$\sum_{i=1}^{3}\sum_{j=1}^{3} g^{ij}\, r_{\xi^i\xi^j} + \sum_{j=1}^{3} (\nabla^2\xi^j) r_{\xi^j} = 0 \tag{73}$$

But $\underset{\sim}{r}_{\xi^j}=\underset{\sim}{a}_j$. Then dotting $\underset{\sim}{a}^l$ into this equation and using Eq. 34, we have

$$\sum_{i=1}^{3}\sum_{j=1}^{3} g^{ij}\, a^l \cdot r_{\xi^i\xi^j} + \sum_{j=1}^{3} (\nabla^2\xi^j)\delta_j^l = 0$$

so that $\nabla^2\xi^l$ is given by

$$\nabla^2\xi^l = -\sum_{i=1}^{3}\sum_{j=1}^{3} g^{ij}\, a^l \cdot r_{\xi^i\xi^j} \qquad (l = 1,2,3) \tag{74}$$

The non-conservative form of the divergence of a tensor is, by expansion in Eq. (49),

$$(\nabla \cdot A)_k = \sum_{l=1}^{3} (A_{kl})_{x_l} = \sum_{i=1}^{3}\sum_{l=1}^{3} (a^i)_l\, (A_{kl})_{\xi^i} \qquad (k = 1,2,3) \tag{75}$$

From Eq.(65) the non-conservative expressions for the first and second derivatives are

$$A_{x_j} = (\nabla A)_j = \sum_{i=1}^{3} (a^i)_j A_{\xi^i} \tag{76}$$

and

$$\begin{aligned} A_{x_j x_k} = [\nabla(A_{x_j})]_k &= \sum_{i=1}^{3}\sum_{l=1}^{3} (a^i)_k\, [(a^l)_j A_{\xi^l}]_{\xi^i} \\ &= \sum_{i=1}^{3}\sum_{l=1}^{3} (a^i)_k\, [(a^l)_j A_{\xi^l\xi^i} + (a^l_{\xi^i})_j A_{\xi^l}] \end{aligned} \tag{77}$$

This non-conservative form in terms of the contravariant base vectors is referred to by some as the "chain-rule conservation" form (Eq. (76) is equivalent to Eq. (1)). In any case only the conservative form gives the telescopic collapse over the field that characterizes conservative numerical representations, and it is necessary to substitute for the contravariant base vectors from Eq. (33) in implementation, since it is the covariant base vectors that are directly calculated from the grid point locations.

6. Normal and Tangential Derivatives

Expressions for derivatives normal and tangential to coordinate surfaces are needed in boundary conditions and are obtained from the base vectors as follows.

A. Tangent to coordinate lines

Since the covariant base vectors are tangent to the coordinate lines, the tangential derivative on a coordinate line along which ξ^i varies is given by

$$(A)_\tau^i = \frac{\mathbf{a}_i}{|\mathbf{a}_i|} \cdot \nabla A = \frac{1}{|\mathbf{a}_i|} \sum_{j=1}^{3} (\mathbf{a}_i \cdot \mathbf{a}^j) A_{\xi^j}$$

using Eq. (65). In view of Eq. (34), this reduces to

$$(A)_\tau^i = \frac{A_{\xi^i}}{\sqrt{g_{ii}}} \qquad (i = 1,2,3) \tag{78}$$

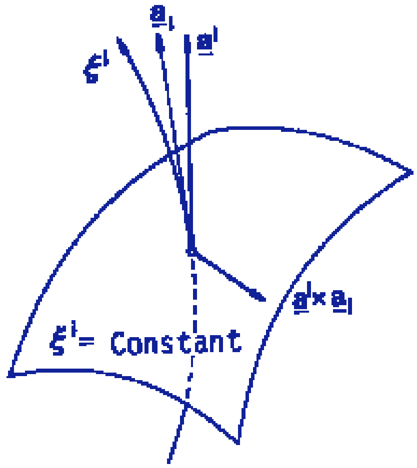
B. Normal to coordinate surfaces

Also, since the contravariant base vectors are normal to the coordinate surfaces, the normal derivative to a coordinate surface on which ξ^i is constant is given by

$$\begin{aligned}(A)_n^i &= \frac{\mathbf{a}^i}{|\mathbf{a}^i|} \cdot \nabla A = \frac{1}{|\mathbf{a}^i|} \sum_{j=1}^{3} (\mathbf{a}^i \cdot \mathbf{a}^j) A_{\xi^j} \\ &= \frac{1}{\sqrt{g^{ii}}} \sum_{j=1}^{3} g^{ij} A_{\xi^j} \qquad (i = 1,2,3)\end{aligned} \tag{79}$$

C. Normal to coordinate lines and tangent to coordinate surfaces

The vector $\mathbf{a}^i \times \mathbf{a}_i$ is normal to the coordinate line on which ξ^i varies and is also tangent to the coordinate surface on which ξ^i is constant:



Using Eq. (33) and the identity (13), this vector is given by

$$\begin{aligned}
\mathbf{a}^i \times \mathbf{a}_i &= \frac{1}{\sqrt{g}} (\mathbf{a}_j \times \mathbf{a}_k) \times \mathbf{a}_i \\
&= -\frac{1}{\sqrt{g}} [(\mathbf{a}_i \cdot \mathbf{a}_k)\mathbf{a}_j - (\mathbf{a}_i \cdot \mathbf{a}_j)\mathbf{a}_k] \qquad (80) \\
&= -\frac{1}{\sqrt{g}} (g_{ik}\mathbf{a}_j - g_{ij}\mathbf{a}_k)
\end{aligned}$$

and the magnitude is given by

$$\begin{aligned}
|\mathbf{a}^i \times \mathbf{a}_i|^2 &= \frac{1}{g} (g_{ik}^2 g_{jj} + g_{ij}^2 g_{kk} - 2 g_{ik} g_{ij} g_{jk}) \\
&= \frac{1}{g} [g_{ik}(g_{ik} g_{jj} - g_{ij} g_{jk}) + g_{ij}(g_{ij} g_{kk} - g_{ik} g_{jk})]
\end{aligned}$$

The bracket is the negative of the second and third terms of the determinant, $g = \det|g_{ij}|$, expanded by cofactors. Therefore, we have

$$\begin{aligned}
|\mathbf{a}^i \times \mathbf{a}_i|^2 &= \frac{1}{g} [g_{ii}(g_{jj} g_{kk} - g_{jk}^2) - g] \\
&= \frac{g_{ii}}{g} (g_{jj} g_{kk} - g_{jk}^2) - 1
\end{aligned} \qquad (81)$$

The derivative normal to the coordinate line on which ξ^i varies and in the coordinate surface on which ξ^i is constant then, using Eq. (65) and (80), is given by

$$(A)_T^i = \frac{\underset{\sim}{a}^i \times \underset{\sim}{a}_i}{|\underset{\sim}{a}^i \times \underset{\sim}{a}_i|} \cdot \underset{\sim}{\nabla} A$$

$$= - \frac{1}{\sqrt{g}|\underset{\sim}{a}^i \times \underset{\sim}{a}_i|} \sum_{l=1}^{3} (g_{ik}\underset{\sim}{a}_j \cdot \underset{\sim}{a}^l A_{\xi^l} - g_{ij}\underset{\sim}{a}_k \cdot \underset{\sim}{a}^l A_{\xi^l})$$

$$= - \frac{1}{\sqrt{g}|\underset{\sim}{a}^i \times \underset{\sim}{a}_i|} (g_{ik}A_{\xi^j} - g_{ij}A_{\xi^k})$$

By Eq. (34). Thus, using Eq. (81),

$$(A)_T^i = \frac{g_{ij}A_{\xi^k} - g_{ik}A_{\xi^j}}{\sqrt{g_{ii}(g_{jj}g_{kk} - g_{jk}^2) - g}} \qquad (i,j,k) \text{ cyclic} \tag{82}$$

7. Integrals

Expressions for surface, volume, and line integrals are easily developed from the base vectors as follow.

A. Surface integral

Returning to the Divergence Theorem, Eq. (17), and its counterparts with the dot product replaced by a cross product or simple operation (the latter with A replaced by a scalar), we have approximate expressions for the surface integrals over the surface of the volume element given, using Eq. (15), by

$$\oiint_{\delta S} \underset{\sim}{A} \circ \underset{\sim}{n}\, dS \doteq \sqrt{g}\, \underset{\sim}{\nabla} \circ \underset{\sim}{A}\, d\xi^1 d\xi^2 d\xi^3 \tag{83}$$

with the open circle indicating the product operation, and using the appropriate expression for $\underset{\sim}{\nabla} \cdot \underset{\sim}{A}$ from those given in the developments above. This emphasizes again that difference representations based on integral formulations, e.g. finite volume, can be obtained by using conservative expressions for the derivative operators directly in the partial differential equations.

B. Volume integral

The approximate expression for the volume integral over the volume element, again using Eq. (15), is simply

$$\iiint_{\delta V} \underset{\sim}{A}\, dV \doteq \sqrt{g}\, \underset{\sim}{A}\, d\xi^1 d\xi^2 d\xi^3 \tag{84}$$

C. Line integrals

Using Eq. (3), the line integral on a coordinate line element on which ξ^i varies is simply

$$\int_{\delta s} \underset{\sim}{A} \circ d\underset{\sim}{r} = \underset{\sim}{A} \circ \underset{\sim}{a}_i\, d\xi^i \tag{85}$$

where again the open circle indicates any type of operation, and $\underset{\sim}{A}$ is any tensor. Also since

$$\oint_c \underset{\sim}{A} \circ d\underset{\sim}{r} = \iint_S (\underset{\sim}{n} \times \underset{\sim}{\nabla}) \circ \underset{\sim}{A}\, dS$$

we have for a closed circuit lying on a coordinate surface on which ξ^i is constant,

$$\oint_{c^i} \underset{\sim}{A} \circ d\underset{\sim}{r} = \sqrt{g} \sum_{l=1}^{3} [(\underset{\sim}{a}^i \times \underset{\sim}{a}^l)\frac{\partial}{\partial \xi^l}] \circ \underset{\sim}{A}\, d\xi^m d\xi^n$$

$$= \sqrt{g} \sum_{l=1}^{3} (\underset{\sim}{a}^i \times \underset{\sim}{a}^l) \circ \underset{\sim}{A}_{\xi^l}\, d\xi^m d\xi^n$$

using Eq. (83), where (l,m,n) are cyclic. But

$$\underset{\sim}{a}^i \times \underset{\sim}{a}^l = \underset{\sim}{a}^i \times (\underset{\sim}{a}_m \times \underset{\sim}{a}_n)/\sqrt{g}$$

Then using the identity (13), we have

$$\underset{\sim}{a}^i \times \underset{\sim}{a}^l = (\underset{\sim}{a}^i \cdot \underset{\sim}{a}_n)\underset{\sim}{a}_m - (\underset{\sim}{a}^i \cdot \underset{\sim}{a}_m)\underset{\sim}{a}_n$$

$$= \delta^i_n\, \underset{\sim}{a}_m - \delta^i_m\, \underset{\sim}{a}_n \tag{86}$$

by using Eq. (34). With (1,j,k) cyclic we have for the circuit integral,

$$\oint_{c^i} \underset{\sim}{A} \circ d\underset{\sim}{r} = \underset{\sim}{a}_k \circ \underset{\sim}{A}_{\xi^j}\, d\xi^j - \underset{\sim}{a}_j \circ \underset{\sim}{A}_{\xi^k}\, d\xi^k \tag{87}$$

8. Two-Dimensional Forms

In two dimensions, let the x_3 direction be the direction of invariance, and let the ξ^3 curvilinear coordinate be identical with x_3. Also, for convenience of notation, let the other coordinates be identified as

$$x_1 = x, \quad x_2 = y, \quad \xi^1 = \xi, \quad \text{and } \xi^2 = \eta$$

A. Metric elements

Then

$$\mathbf{a}_3 = \mathbf{a}^3 = \mathbf{k},$$

and the other base vectors are

$$\mathbf{a}_1 = \mathbf{r}_\xi = \mathbf{i}x_\xi + \mathbf{j}y_\xi$$

$$\mathbf{a}_2 = \mathbf{r}_\eta = \mathbf{i}x_\eta + \mathbf{j}y_\eta \tag{88}$$

The covariant metric components then are

$$g_{33} = \mathbf{k} \cdot \mathbf{k} = 1$$

$$g_{13} = g_{31} = \mathbf{a}_1 \cdot \mathbf{k} = 0$$

$$g_{23} = g_{32} = \mathbf{a}_2 \cdot \mathbf{k} = 0$$

$$g_{11} = x_\xi^2 + y_\xi^2 \tag{89}$$

$$g_{22} = x_\eta^2 + y_\eta^2$$

$$g_{12} = g_{21} = x_\xi x_\eta + y_\xi y_\eta$$

From Eq. (16), the Jacobian is given by

$$\sqrt{g} = \sqrt{\det|g_{ij}|} = \sqrt{g_{11}g_{22} - g_{12}^2}$$

$$= \underline{k} \cdot (\underline{a}_1 \times \underline{a}_2) = |\underline{a}_1 \times \underline{a}_2| \quad (90)$$

$$= x_\xi y_\eta - x_\eta y_\xi$$

The other contravariant base vectors are, from Eq. (33),

$$\underline{a}^1 = \frac{1}{\sqrt{g}}(\underline{a}_2 \times \underline{k}) = \frac{1}{\sqrt{g}}(\underline{i}y_\eta - \underline{j}x_\eta)$$

$$\underline{a}^2 = \frac{1}{\sqrt{g}}(\underline{k} \times \underline{a}_1) = \frac{1}{\sqrt{g}}(-\underline{i}y_\xi + \underline{j}x_\xi) \quad (91)$$

and the contravariant metric components are, from Eq. (37) or (38),

$$g^{33} = \underline{k} \cdot \underline{k} = 1$$

$$g^{13} = g^{31} = \underline{a}^1 \cdot \underline{k} = 0$$

$$g^{23} = g^{32} = \underline{a}^2 \cdot \underline{k} = 0 \quad (92)$$

$$g^{11} = \frac{g_{22}}{g}, \qquad g^{22} = \frac{g_{11}}{g}$$

$$g^{12} = g^{21} = -\frac{g_{12}}{g}$$

From Eq. (4) we have $\underline{\nabla}\xi = \underline{a}^1$ and $\underline{\nabla}\eta = \underline{a}^2$, so that by Eq. (91),

$$\xi_x = \frac{y_\eta}{\sqrt{g}}, \quad \xi_y = -\frac{x_\eta}{\sqrt{g}}, \qquad \eta_x = -\frac{y_\xi}{\sqrt{g}}, \quad \eta_y = \frac{x_\xi}{\sqrt{g}} \quad (93)$$

B. Transformation relations

Divergence (conservative), Eq. (43):

$$\underline{\nabla} \cdot \underline{A} = \frac{1}{\sqrt{g}}[(y_\eta A_1 - x_\eta A_2)_\xi + (-y_\xi A_1 + x_\xi A_2)_\eta] \quad (94)$$

(non-conservative), Eq. (67):

$$\underset{\sim}{\nabla} \cdot \underset{\sim}{A} = \frac{1}{\sqrt{g}}[y_\eta(A_1)_\xi - x_\eta(A_2)_\xi - y_\xi(A_1)_\eta + x_\xi(A_2)_\eta] \tag{95}$$

Gradient (conservative), Eq., (42):

$$f_x = \frac{1}{\sqrt{g}}[(y_\eta f)_\xi - (y_\xi f)_\eta] \tag{96}$$

$$f_y = \frac{1}{\sqrt{g}}[-(x_\eta f)_\xi + (x_\xi f)_\eta] \tag{97}$$

(non-conservative), Eq. (65):

$$f_x = \frac{1}{\sqrt{g}}(y_\eta f_\xi - y_\xi f_\eta) \tag{98}$$

$$f_y = \frac{1}{\sqrt{g}}(-x_\eta f_\xi + x_\xi f_\eta) \tag{99}$$

By Eq. (93), or directly from Eq. (76), these non-conservative forms may be given as

$$f_x = f_\xi \xi_x + f_\eta \eta_x$$

$$f_y = f_\xi \xi_y + f_\eta \eta_y$$

which are the so-called "chain-rule conservative" forms. This form, however, is not conservative and the relations given by Eq. (93) must be substituted in the implementation in any case, since it is x_ξ, etc., rather than ξ_x, that is directly calculated from the grid point locations.

Curl (conservative), Eq. (44):

$$\underset{\sim}{\nabla} \times \underset{\sim}{A} = \frac{\underset{\sim}{k}}{\sqrt{g}}[(y_\eta A_2 + x_\eta A_1)_\xi - (y_\xi A_2 + x_\xi A_1)_\eta] \tag{100}$$

(non-conservative), Eq. (68):

$$\underset{\sim}{\nabla} \times \underset{\sim}{A} = \frac{\underset{\sim}{k}}{\sqrt{g}}[y_\eta(A_2)_\xi + x_\eta(A_1)_\xi - y_\xi(A_2)_\eta - x_\xi(A_1)_\eta] \tag{101}$$

Laplacian (conservative), Eq. (45):

$$\sqrt{g}\,\nabla^2 f = \{[\frac{1}{\sqrt{g}} y_\eta[(y_\eta f)_\xi - (y_\xi f)_\eta]$$

$$- \frac{1}{\sqrt{g}} x_\eta[-(x_\eta f)_\xi + (x_\xi f)_\eta]\}_\xi$$

$$+ \{- \frac{1}{\sqrt{g}} y_\xi[(y_\eta f)_\xi - (y_\xi f)_\eta]$$

$$+ \frac{1}{\sqrt{g}} x_\xi[-(x_\eta f)_\xi + (x_\xi f)_\eta]\}_\eta \tag{102}$$

(non-conservative), Eq. (65):

$$\nabla^2 f = \frac{1}{g}[(x_\eta^2 + y_\eta^2)f_{\xi\xi} - 2(x_\xi x_\eta + y_\xi y_\eta)f_{\xi\eta}$$

$$+ (x_\xi^2 + y_\xi^2)f_{\eta\eta}] + (\nabla^2\xi)f_\xi + (\nabla^2\eta)f_\eta \tag{103}$$

Second derivatives (non-conservative):

$$f_{xx} = (y_\eta^2 f_{\xi\xi} - 2y_\xi y_\eta f_{\xi\eta} + y_\xi^2 f_{\eta\eta})/g$$

$$+ [(y_\eta^2 y_{\xi\xi} - 2y_\xi y_\eta y_{\xi\eta} + y_\xi^2 y_{\eta\eta})(x_\eta f_\xi - x_\xi f_\eta)$$

$$+ (y_\eta^2 x_{\xi\xi} - 2y_\xi y_\eta x_{\xi\eta} + y_\xi^2 x_{\eta\eta})(y_\xi f_\eta - y_\eta f_\xi)]/g^{3/2} \tag{104}$$

$$f_{yy} = (x_\eta^2 f_{\xi\xi} - 2x_\xi x_\eta f_{\xi\eta} + x_\xi^2 f_{\eta\eta})/g$$

$$+ [(x_\eta^2 y_{\xi\xi} - 2x_\xi x_\eta y_{\xi\eta} + x_\xi^2 y_{\eta\eta})(x_\eta f_\xi - x_\xi f_\eta)$$

$$+ (x_\eta^2 x_{\xi\xi} - 2x_\xi x_\eta x_{\xi\eta} + x_\xi^2 x_{\eta\eta})(y_\xi f_\eta - y_\eta f_\xi)]/g^{3/2} \tag{105}$$

$$f_{xy} = [(x_\xi y_\eta + x_\eta y_\xi)f_{\xi\eta} - x_\xi y_\xi f_{\eta\eta} - x_\eta y_\eta f_{\xi\xi}]/g$$

$$+ \{(x_\xi y_{\eta\eta} - x_\eta y_{\xi\eta})/g + [x_\eta y_\eta(\sqrt{g})_\xi - x_\xi y_\eta(\sqrt{g})_\eta]/g^{3/2}\}f_\xi$$

(106)

$$+ \{(x_\eta y_{\xi\xi} - x_\xi y_{\xi\eta})/g + [x_\xi y_\xi(\sqrt{g})_\eta - x_\eta y_\xi(\sqrt{g})_\xi]/g^{3/2}\}f_\eta$$

Normal derivative (conservative):

$$f_{n}(\xi) = \frac{1}{\sqrt{g}\sqrt{x_\eta^2 + y_\eta^2}}\{y_\eta[(y_\eta f)_\xi - (y_\xi f)_\eta]$$

(107)

$$- x_\eta[-(x_\eta f)_\xi + (x_\xi f)_\eta]\}$$

$$f_{n}(\eta) = \frac{1}{\sqrt{g}\sqrt{x_\xi^2 + y_\xi^2}}\{-y_\xi[(y_\eta f)_\xi - (y_\xi f)_\eta]$$

(108)

$$+ x_\xi[-(x_\eta f)_\xi + (x_\xi f)_\eta]\}$$

(non-conservative):

$$f_{n}(\xi) = \frac{1}{\sqrt{g}\sqrt{x_\eta^2 + y_\eta^2}}[(x_\eta^2 + y_\eta^2)f_\xi - (x_\xi x_\eta + y_\xi y_\eta)f_\eta] \quad (109)$$

$$f_{n}(\eta) = \frac{1}{\sqrt{g}\sqrt{x_\xi^2 + y_\xi^2}}[-(x_\xi x_\eta + y_\xi y_\eta)f_\xi + (x_\xi^2 + y_\xi^2)f_\eta] \quad (110)$$

Tangential derivative (conservative):

$$f_{\tau}(\xi) = \frac{1}{\sqrt{g}\sqrt{x_\eta^2 + y_\eta^2}}\{x_\eta[(y_\eta f)_\xi - (y_\xi f)_\eta]$$

(111)

$$- y_\eta[(x_\eta f)_\xi - (x_\xi f)_\eta]\}$$

$$f_{\tau}(\eta) = \frac{1}{\sqrt{g}\sqrt{x_\xi^2 + y_\xi^2}}\{x_\xi[(y_\eta f)_\xi - (y_\xi f)_\eta]$$

(112)

$$- y_\xi[(x_\eta f)_\xi - (x_\xi f)_\eta]\}$$

(non-conservative):

$$f_{\tau}(\xi) = \frac{1}{\sqrt{x_{\eta}^2 + y_{\eta}^2}} f_{\eta} \tag{113}$$

$$f_{\tau}(\eta) = \frac{1}{\sqrt{x_{\xi}^2 + y_{\xi}^2}} f_{\xi} \tag{114}$$

Surface integral:

$$\iint_S f dS = \sqrt{g}\, f d\xi d\eta \tag{115}$$

9. Time derivatives

A. First Derivative

With moving grids the time derivatives must be transformed also. For the first derivative we have

$$\left(\frac{\partial A}{\partial t}\right)_{\xi} = \left(\frac{\partial A}{\partial t}\right)_{\underset{\sim}{x}} + \underset{\sim}{\nabla} A \cdot \left(\frac{\partial \underset{\sim}{x}}{\partial t}\right)_{\xi} \tag{116}$$

where here, and in Eq. (117) below, the subscripts indicate the variable being held constant in the partial differentiation. Here the time derivative on the left side is at a fixed position in the transformed space, i.e., at a given grid point. The time derivative on the right is at a fixed position in the physical space, i.e., the time derivative that appears in the physical equations of motion. The quantity $\partial \underset{\sim}{x} / \partial t_{\xi}$ is the grid point speed, to be written $\dot{\underset{\sim}{x}}$ hereafter. Thus we have, for substitution into the physical equations of motion, the relation

$$\left(\frac{\partial A}{\partial t}\right)_{\underset{\sim}{x}} = \left(\frac{\partial A}{\partial t}\right)_{\xi} - \dot{\underset{\sim}{x}} \cdot \underset{\sim}{\nabla} A \tag{117}$$

with $\underset{\sim}{\nabla}$ to come from thetransformation relations given previously. With the time derivatives transformed, only time derivatives at fixed points in the transformed space will appear in the equations and, therefore, all computation can be done on the fixed uniform grid in the transformed field without interpolation, even though the grid points are in motion in the physical space. The last term in Eq. (117) resembles a convective term and accounts for the motion of the grid.

B. Convective terms

Consider the generic convective terms

$$C = A_t + \nabla \cdot (\underline{u}A) \qquad (118)$$

where $\underline{u}$ is a velocity, which occur in many conservation equations. Using Eq. (117) we have

$$C = A_t - \dot{\underline{x}} \cdot \nabla A + \nabla \cdot (\underline{u}A)$$

where now the time derivative is understood to be at a fixed point in the transformed space. Then using Eq. (42) and (43) for the gradient and divergence, this becomes

$$C = A_t - \frac{1}{\sqrt{g}} \dot{\underline{x}} \cdot \sum_{i=1}^{3} (\sqrt{g}\, \underline{a}^i A)_{\xi^i} + \frac{1}{\sqrt{g}} \sum_{i=1}^{3} (\sqrt{g}\, \underline{a}^i \cdot \underline{u}A)_{\xi^i} \qquad (119)$$

By Eq. (16),

$$(\sqrt{g})_t = [\underline{a}_1 \cdot (\underline{a}_2 \times \underline{a}_3)]_t$$

$$= (\underline{a}_1)_t \cdot (\underline{a}_2 \times \underline{a}_3) + (\underline{a}_2)_t \cdot (\underline{a}_3 \times \underline{a}_1)$$

$$+ (\underline{a}_3)_t \cdot (\underline{a}_1 \times \underline{a}_2)$$

$$= \sqrt{g} \sum_{i=1}^{3} (\underline{a}_i)_t \cdot \underline{a}^i$$

by Eq. (33). But

$$(\underline{a}_i)_t = (\underline{x}_{\xi^i})_t = (\dot{\underline{x}})_{\xi^i}$$

so that

$$(\sqrt{g})_t = \sqrt{g} \sum_{i=1}^{3} \underline{a}^i \cdot (\dot{\underline{x}})_{\xi^i} \qquad (120)$$

We then can write

$$C = A_t + \frac{A(\sqrt{g})_t}{\sqrt{g}} + \frac{1}{\sqrt{g}} \sum_{i=1}^{3} [\sqrt{g}\, \underset{\sim}{a}^i \cdot (\underset{\sim}{u} - \dot{\underset{\sim}{x}})A]_{\xi^i}$$

(121)

$$= \frac{1}{\sqrt{g}} \{(\sqrt{g}\, A)_t + \sum_{i=1}^{3} [(\sqrt{g}\, A)\underset{\sim}{a}^i \cdot (\underset{\sim}{u} - \dot{\underset{\sim}{x}})\,]_{\xi^i}\}$$

which is a conservative form of the generic convective terms with regard to the quantity, $\sqrt{g}$ A. By Eq. (33), the quantity

$$U^i = \underset{\sim}{a}^i \cdot (\underset{\sim}{u} - \dot{\underset{\sim}{x}}) \qquad (i = 1,2,3) \tag{122}$$

is the contravariant velocity component in the ξ^i-direction, relative to the moving grid. Thus Eq. (121) can be written in the conservative form,

$$\sqrt{g}\, C = (\sqrt{g}\, A)_t + \sum_{i=1}^{3} (\sqrt{g}\, AU^i)_{\xi^i} \tag{123}$$

Expanding the derivatives in Eq. (119) and using Eq. (40), we have

$$C = A_t - \dot{\underset{\sim}{x}} \cdot \sum_{i=1}^{3} \underset{\sim}{a}^i A_{\xi^i} + \sum_{i=1}^{3} \underset{\sim}{a}^i \cdot (\underset{\sim}{u} A_{\xi^i} + A\underset{\sim}{u}_{\xi^i}) \tag{124}$$

so that the non-conservative form

$$C = A_t + \sum_{i=1}^{3} U^i A_{\xi^i} + A \sum_{i=1}^{3} \underset{\sim}{a}^i \cdot \underset{\sim}{u}_{\xi^i} \tag{125}$$

The last summation is the divergence of the velocity, $\underset{\sim}{\nabla} \cdot \underset{\sim}{u}$. (Computationally, $\sqrt{g}$ might be included in the definition of U^i for use in the conservative form in the interest of computational efficiency, since by Eq. (33) the product $\sqrt{g}\ \underset{\sim}{a}^i$ can be evaluated directly as the cross product of the co-variant base vectors.)

From Eq. (117) we have, with A taken as ξ^i,

$$\xi^i_t = - \dot{\underset{\sim}{x}} \cdot \underset{\sim}{\nabla}\xi^i = - \dot{\underset{\sim}{x}} \cdot \underset{\sim}{a}^i \tag{126}$$

by Eq. (4). Here the time derivative of ξ^i is, of course, at a fixed position in physical space. The quantity U^i introduced above in Eq. (122), thus could be written as

$$U^i = \mathbf{a}^i \cdot \mathbf{u} + \dot{\xi}^i = \nabla\xi^i \cdot \mathbf{u} + \dot{\xi}^i \quad (i = 1,2,3) \tag{127}$$

Here the $\mathbf{a}^i \cdot \mathbf{u}$ are, of course, the contravariant velocity components.

C. Second derivative

The second time derivative transforms as follows:

$$\left(\frac{\partial^2\phi}{\partial t^2}\right)_{x,y} = \phi_{tt} - 2(\nabla\phi)_t \cdot \dot{\mathbf{r}} + \sum_{i=1}^{3}\sum_{j=1}^{3} \phi_{x_i x_j}\, \dot{x}_i \dot{x}_j - \nabla\phi \cdot \ddot{\mathbf{r}} \tag{128}$$

where the x,y subscripts on the left indicate the variables being held constant, and

$$\nabla\phi = \sum_{i=1}^{3} \mathbf{a}^i\, \phi_{\xi^i} \tag{129}$$

$$(\nabla\phi)_t = \sum_{i=1}^{3} \left(\mathbf{a}^i\, \phi_{t\xi^i} + \dot{\mathbf{a}}^i\, \phi_{\xi^i}\right) \tag{130}$$

$$\phi_{x_i x_j} = \sum_{k=1}^{3}\sum_{l=1}^{3} (\mathbf{a}^k)_i \left[(\mathbf{a}^l)_j\, \phi_{\xi^l \xi^k} + (\mathbf{a}^l_{\xi^k})_j\, \phi_{\xi^l}\right] \tag{131}$$

$$(\mathbf{a}^l)_{\xi^k} = \frac{1}{\sqrt{g}}\left(\mathbf{a}_m \times \mathbf{r}_{\xi^n \xi^k} - \mathbf{a}_n \times \mathbf{r}_{\xi^m \xi^k}\right) - \mathbf{a}^l \sum_{i}^{3}\sum_{j}^{3} g^{ij}\, \mathbf{r}_{\xi^i \xi^j} \tag{132}$$

with (l,m,n) cyclic.

Exercises

1. Obtain the covariant and contravariant base vectors for cylindrical coordinates from Eq. (3) and (4). Show that Eq. (34) holds for this system.

2. Obtain the elements of arc length, surface area, and volume for cylindrical coordinates.

3. Obtain the relations for gradient, divergence, curl, and Laplacian for cylindrical coordinates.

4. Demonstrate that the identity (21) holds for cylindrical coordinates.

5. Demonstrate that Eq. (33), (38) and (39) hold for cylindrical coordinates.

6. Repeat exercises 1 - 5 for spherical coordinates.

7. Show that the covariant base vectors may be written in terms of the contravariant base vectors by

$$a_i = \sqrt{g}\,(a^j \times a^k) \quad (i,j,k) \text{ cyclic}$$

Hint: Cross a^k into Eq. (33) and use (13), rearranging k subscripts at the end. Recalling that $\sqrt{g}$ as can be expressed $(\det|g^{ij}|)^{-1}$, this gives, a relation for $(x_l)_{\xi^i}$ in terms of the derivatives $(\xi^r)_{x_s}$.

8. Show that the elements of the covariant metric tensor can be expressed in terms of the contravariant elements by

$$g_{il} = g(g^{jm}g^{kn} - g^{jn}g^{km}) \quad (i,j,k) \text{ cyclic} \quad (l,m,n) \text{ cyclic}$$

Hint: Follow the development of Eq. (38), but with $a_i \cdot a_l$.

9. Show that Eq. (65) is equivalent to the chain rule expression (1). Also show that the dot product of a_j with Eq. (65) leads, after interchange of indices, to the chain rule expression (4).

10. Show that

$$(\sqrt{g})_{\xi^i} = \sqrt{g} \sum_j \sum_k g^{jk}\, r_{\xi^k \xi^i}$$

Hint: Since $g = \det|g^{ij}|$ depends on ξ only through the g_{ij}, differential g with respect to g_{jk} with respect to ξ^i. Recall Eq. (38).

11. Show that $\nabla^2 r$ =0. Hint: Use cartesian coordinates.

12. Obtain the two-dimensional relations in Section 6 from the general expression.

13. Verify Eq. (74) for cylindrical and spherical coordinates.

14. Obtain the normal and tangential derivatives (Section4) for cylindrical and spherical coordinates.