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Non-orthogonal 3D coordinate systems for dummies

Non-orthogonal coordinates are used all the time in tokamaks and other toroidal plasmas, typically because the poloidal angle θ might not be orthogonal to the flux surface label ψ.

Let us assign three numbers to each point in space. To make the connection to toroidal plasmas clear, I'll denote these numbers (coordinates) by ψ, θ, and ζ. However, nothing in this analysis will be specific to tokamaks or stellarators: it applies to any coordinate system in 3D Euclidean space.

Covariant vs. Contravariant

Associated with the coordinates, there are *two* natural triplets of basis vectors. The first is the set of *gradient* vectors

$$\nabla\psi, \quad \nabla\theta, \quad \nabla\zeta \tag{1}$$

where

$$\nabla\psi = \mathbf{e}_x \frac{\partial\psi}{\partial x} + \mathbf{e}_y \frac{\partial\psi}{\partial y} + \mathbf{e}_z \frac{\partial\psi}{\partial z} \tag{2}$$

and the analogous definition holds for $\nabla\theta$ and $\nabla\zeta$. Above, y and z are held fixed in the $\partial/\partial x$ differentiation, the analogous statements hold for $\partial/\partial y$ and $\partial/\partial z$, and the $\mathbf{e}_i$ are Cartesian unit vectors. The second triplet of basis vectors associated with our coordinates is the set of *tangent* vectors:

$$\frac{\partial\mathbf{r}}{\partial\psi}, \quad \frac{\partial\mathbf{r}}{\partial\theta}, \quad \frac{\partial\mathbf{r}}{\partial\zeta} \tag{3}$$

where $\mathbf{r}$ is the position vector, θ and ζ are held fixed in the $\partial/\partial\psi$ differentiation, and the analogous statements hold for $\partial/\partial\theta$ and $\partial/\partial\zeta$. We can write

$$\frac{\partial\mathbf{r}}{\partial\psi} = \mathbf{e}_x \frac{\partial x}{\partial\psi} + \mathbf{e}_y \frac{\partial y}{\partial\psi} + \mathbf{e}_z \frac{\partial z}{\partial\psi}, \tag{4}$$

and the analogous definitions hold for $\partial\mathbf{r}/\partial\theta$ and $\partial\mathbf{r}/\partial\zeta$. Notice that (2) and (4) are different!

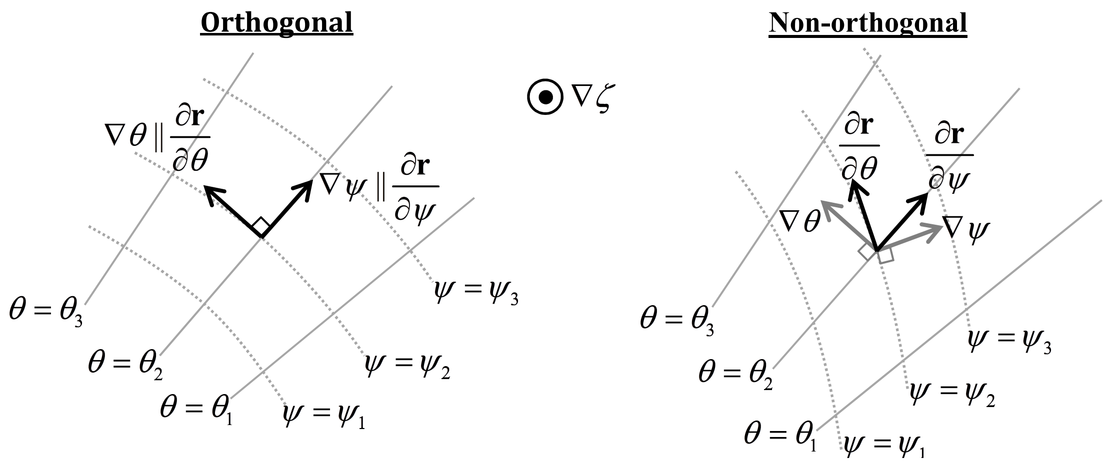
Any vector can be decomposed using either triplet of basis vectors. In the first basis, we can write any vector $\mathbf{B}$ as

$$\mathbf{B} = B_\psi \nabla\psi + B_\theta \nabla\theta + B_\zeta \nabla\zeta \tag{5}$$

where the numbers B_ψ, B_θ, and B_ζ are the *covariant coefficients* of $\mathbf{B}$. Or, decomposing the exact same vector in the second basis, we can write

$$\mathbf{B} = B^\psi \frac{\partial\mathbf{r}}{\partial\psi} + B^\theta \frac{\partial\mathbf{r}}{\partial\theta} + B^\zeta \frac{\partial\mathbf{r}}{\partial\zeta} \tag{6}$$

where the numbers B^ψ, B^θ, and B^ζ are the *contravariant coefficients*. The form (5) is the *covariant representation* of $\mathbf{B}$ and the form (6) is the *contravariant representation*.



We can relate the two sets of basis vectors as follows. First, the vector $\partial\mathbf{r}/\partial\psi$ by definition points in a direction along which θ and ζ do not increase. Thus,

$$\frac{\partial \mathbf{r}}{\partial\psi}\cdot\nabla\theta=0 \qquad \text{and} \qquad \frac{\partial \mathbf{r}}{\partial\psi}\cdot\nabla\zeta=0\,. \tag{7}$$

It follows that

$$\partial\mathbf{r}/\partial\psi = J\nabla\theta\times\nabla\zeta \tag{8}$$

for some coefficient J. To determine this coefficient, consider a step $d\mathbf{r}$ at fixed θ and ζ: $d\psi = d\mathbf{r}\cdot\nabla\psi$, so $\left(\partial\mathbf{r}/\partial\psi\right)\cdot\nabla\psi=1$. (This same result can also be seen by forming the dot product of (2) with (4) and recognizing the result as the chain rule applied to $\partial\psi\left(\mathbf{x}\right)/\partial\psi=1$ where $\mathbf{x}=\mathbf{x}\left(\psi,\theta,\zeta\right)$). The dot product of (8) with $\nabla\psi$ therefore tells us $J=1/\left(\nabla\psi\cdot\nabla\theta\times\nabla\zeta\right)$. Thus,

$$\frac{\partial \mathbf{r}}{\partial\psi}=J\left(\nabla\theta\times\nabla\zeta\right),\quad \frac{\partial \mathbf{r}}{\partial\theta}=J\left(\nabla\zeta\times\nabla\psi\right),\quad \frac{\partial \mathbf{r}}{\partial\zeta}=J\left(\nabla\psi\times\nabla\theta\right) \tag{9}$$

where the last two equalities come from just cyclically permuting the coordinates in the same analysis. The expressions (9) make it clear that if the coordinates are orthogonal (i.e. if $\nabla\psi$, $\nabla\theta$, and $\nabla\zeta$ are mutually orthogonal), then $\nabla\psi$ and $\partial\mathbf{r}/\partial\psi$ will be parallel (similarly for θ and ζ), but in a nonorthogonal system $\nabla\psi$ and $\partial\mathbf{r}/\partial\psi$ represent different directions.

Forming cross products of (9), and applying the vector identity $\left(\mathbf{P}\times\mathbf{Q}\right)\times\left(\mathbf{R}\times\mathbf{S}\right)=\left(\mathbf{P}\cdot\mathbf{Q}\times\mathbf{S}\right)\mathbf{R}-\left(\mathbf{P}\cdot\mathbf{Q}\times\mathbf{S}\right)\mathbf{R}$, we obtain another set of relations between the basis vectors:

$$\nabla\psi=\frac{1}{J}\frac{\partial \mathbf{r}}{\partial\theta}\times\frac{\partial \mathbf{r}}{\partial\zeta},\quad \nabla\theta=\frac{1}{J}\frac{\partial \mathbf{r}}{\partial\zeta}\times\frac{\partial \mathbf{r}}{\partial\psi},\quad \nabla\zeta=\frac{1}{J}\frac{\partial \mathbf{r}}{\partial\psi}\times\frac{\partial \mathbf{r}}{\partial\theta} \tag{10}$$

(again cyclic permutations). Also, the product of the first equations in (9) and (10) gives a new expression for J:

$$J=\frac{1}{\nabla\psi\cdot\nabla\theta\times\nabla\zeta}=\frac{\partial \mathbf{r}}{\partial\psi}\cdot\frac{\partial \mathbf{r}}{\partial\theta}\times\frac{\partial \mathbf{r}}{\partial\zeta}\,. \tag{11}$$

As a final note, observe that we can compute the vector coefficients in (5)-(6) using $B_\psi = \mathbf{B}\cdot(\partial \mathbf{r}/\partial\psi)$, $B^\psi = \mathbf{B}\cdot\nabla\psi$, and the analogous formulae for θ and ζ. These results are obtained by forming the dot product of (5) with (9), or the dot product of (6) with (10), respectively.

Other useful formulae

For any scalar quantity s,

$$\nabla s = \left(\frac{\partial s}{\partial\psi}\right)\nabla\psi + \left(\frac{\partial s}{\partial\theta}\right)\nabla\theta + \left(\frac{\partial s}{\partial\zeta}\right)\nabla\zeta . \qquad (12)$$

This formula is just the chain rule applied to $s\left(\psi(x,y,z),\ \theta(x,y,z),\ \zeta(x,y,z)\right)$.

For any vector $\mathbf{X}$, the divergence is

$$\nabla\cdot\mathbf{X} = \frac{1}{J}\left[\frac{\partial}{\partial\psi}(J\mathbf{X}\cdot\nabla\psi) + \frac{\partial}{\partial\theta}(J\mathbf{X}\cdot\nabla\theta) + \frac{\partial}{\partial\zeta}(J\mathbf{X}\cdot\nabla\zeta)\right] \qquad (13)$$

where $J = (\nabla\psi\cdot\nabla\theta\times\nabla\zeta)^{-1}$. Formulae also exist for the curl, Laplacian, etc.

To perform a surface integral of any vector $\mathbf{X}$ over a constant-ψ surface, use

$$\int d^2\mathbf{n}\cdot\mathbf{X} = \int d\theta \int d\zeta \frac{\mathbf{X}\cdot\nabla\psi}{\nabla\psi\cdot\nabla\theta\times\nabla\zeta} \qquad (14)$$

where $\mathbf{n}$ denotes the normal vector to the surface. To perform surface integrals over constant-θ or constant-ζ surfaces, just use the appropriate cyclic permutation of (14).

As J is the Jacobian determinant for the transformation between Cartesian coordinates and the (ψ,θ,ζ) coordinates, then the volume integral of any scalar quantity s is computed using

$$\int d^3\upsilon\ s = \int d\psi \int d\theta \int d\zeta \frac{s}{\nabla\psi\cdot\nabla\theta\times\nabla\zeta} . \qquad (15)$$

For an axisymmetric magnetic field, $\mathbf{B} = \nabla\zeta\times\nabla\psi + I\nabla\zeta$ where ζ is the toroidal angle. Then notice the inverse Jacobian $1/J$ is $\nabla\psi\cdot\nabla\theta\times\nabla\zeta = \mathbf{B}\cdot\nabla\theta$. Thus, in other books or papers you may encounter the formulae from these notes with $\nabla\psi\cdot\nabla\theta\times\nabla\zeta$ replaced by $\mathbf{B}\cdot\nabla\theta$.

Abstract summary of key formulae

For any coordinates $\left(q^1, q^2, q^3\right)$ which may or may not be orthogonal, any vector $\mathbf{V}$ can be decomposed in the "covariant representation"

$$\mathbf{V} = V_1 \nabla q^1 + V_2 \nabla q^2 + V_3 \nabla q^3 \tag{16}$$

where each coefficient V_i can be computed from $V_i = \mathbf{V} \cdot \left(\partial \mathbf{r} / \partial q^i\right)$ and $\mathbf{r}$ is the position vector. The same vector $\mathbf{V}$ can also be decomposed in the "contravariant representation"

$$\mathbf{V} = V^1 \frac{\partial \mathbf{r}}{\partial q^1} + V^2 \frac{\partial \mathbf{r}}{\partial q^2} + V^3 \frac{\partial \mathbf{r}}{\partial q^3} \tag{17}$$

where the coefficients V^i can be computed from $V^i = \mathbf{V} \cdot \nabla q^i$. Here and throughout this section, $\partial / \partial q^1$ assumes q^2 and q^3 are held fixed, etc. The two sets of basis vectors can be related using the Jacobian, often written as $\sqrt{g}$ instead of J, given by

$$\sqrt{g} = \frac{1}{\nabla q^1 \cdot \nabla q^2 \times \nabla q^3} = \left(\frac{\partial \mathbf{r}}{\partial q^1}\right) \cdot \left(\frac{\partial \mathbf{r}}{\partial q^2}\right) \times \left(\frac{\partial \mathbf{r}}{\partial q^3}\right). \tag{18}$$

Then the basis vectors are related by

$$\frac{\partial \mathbf{r}}{\partial q^1} = \sqrt{g}\left(\nabla q^2 \times \nabla q^3\right), \quad \frac{\partial \mathbf{r}}{\partial q^2} = \sqrt{g}\left(\nabla q^3 \times \nabla q^1\right), \quad \frac{\partial \mathbf{r}}{\partial q^3} = \sqrt{g}\left(\nabla q^1 \times \nabla q^2\right) \tag{19}$$

and

$$\nabla q^1 = \frac{1}{\sqrt{g}}\left(\frac{\partial \mathbf{r}}{\partial q^2} \times \frac{\partial \mathbf{r}}{\partial q^3}\right), \quad \nabla q^2 = \frac{1}{\sqrt{g}}\left(\frac{\partial \mathbf{r}}{\partial q^3} \times \frac{\partial \mathbf{r}}{\partial q^1}\right), \quad \nabla q^3 = \frac{1}{\sqrt{g}}\left(\frac{\partial \mathbf{r}}{\partial q^1} \times \frac{\partial \mathbf{r}}{\partial q^2}\right), \tag{20}$$

i.e. cyclic permutations in each case.

The divergence of a vector is

$$\nabla \cdot \mathbf{V} = \frac{1}{\sqrt{g}} \sum_{i=1,2,3} \frac{\partial}{\partial q^i}\left(\sqrt{g}\mathbf{V} \cdot \nabla q^i\right). \tag{21}$$

Volume integrals are given by

$$\int d^3\mathbf{r}\, s = \int dq^1 \int dq^2 \int dq^3 \sqrt{g} s \tag{22}$$

For more info:

- W. D. D'haeseleer, W. N. G. Hitchon, J. D. Callen, and J. L. Shohet, "Flux coordinates and magnetic field structure", chapter 2.
- Bateman, "MHD Instabilities", p126-127.
- Arfken and Weber, "Mathematical Methods for Physicists," sections 2.10-2.11.