

1 Rotation: definition and meaning

The definition of rotation of vector field $\mathbf{u}(\mathbf{r})$ is given by

$$\text{rot} \mathbf{u} \equiv \nabla \times \mathbf{u} \quad (1)$$

$$= \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ u_x & u_y & u_z \end{vmatrix} \quad (2)$$

$$= \mathbf{i} \left(\frac{\partial u_z}{\partial y} - \frac{\partial u_y}{\partial z} \right) + \mathbf{j} \left(\frac{\partial u_x}{\partial z} - \frac{\partial u_z}{\partial x} \right) + \mathbf{k} \left(\frac{\partial u_y}{\partial x} - \frac{\partial u_x}{\partial y} \right) \quad (3)$$

rot の意味はわかりにくい、長沼伸一郎「物理数学の直感的方法」(通商産業研究社)の5章に記述されている水の流れに中においた微小な水車の回転速度という記述は大変わかりやすい。In the vector analysis the meaning of "rot" is hard to understand, but S. Naganuma gave us a method to understand the meaning of rotation in his book (Intuitive method for physical mathematics(Japanese))

The rotational velocity of the infinitesimal water wheel in water flow field $\mathbf{u}$. The water flow of the right side of the wheel in the upper direction u_y is faster than the left side ($\partial u_y / \partial x > 0$), the wheel rotates in the anticlockwise direction. In the same way the water flow of the upper side of the wheel in the right direction u_x is slower than the lower side ($\partial u_x / \partial y < 0$) the wheel rotates in the anticlockwise direction. Then $\partial u_y / \partial x - \partial u_x / \partial y [\equiv (\text{rot} \mathbf{u})_z]$ contribute the anti. If the wheel rotates the anticlockwise direction the $(\text{rot} \mathbf{u})_z$ has positive value. $(\text{rot} \mathbf{u})_x$ and $(\text{rot} \mathbf{u})_y$ can define in the same way.

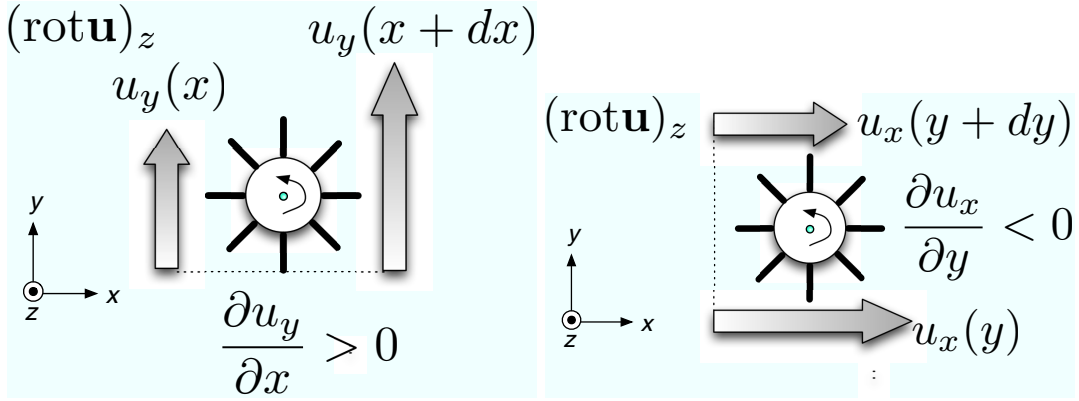


Figure 1: Naganuma's explanation of $\text{rot} \mathbf{u}$

2 Stokes theorem

As shown in Fig. 2 for a general vector field $\mathbf{V}(\mathbf{r})$, Stokes theorem gives

$$\begin{aligned} \oint \mathbf{V} \cdot d\mathbf{r} &= \text{(I)} + \text{(II)} + \text{(III)} + \text{(IV)} \\ &= V_x(x_0, y_0)dx + V_y(x_0 + dx, y_0)dy + V_x(x_0, y_0 + dy)(-dx) + V_y(x_0, y_0)(-dy) \\ &= V_x(x_0, y_0)dx + [V_y(x_0, y_0) + \frac{\partial V_y}{\partial x}dx]dy \\ &\quad - [V_x(x_0, y_0) + \frac{\partial V_x}{\partial y}dy]dx - V_y(x_0, y_0)dy \\ &= \left(\frac{\partial V_y}{\partial x} - \frac{\partial V_x}{\partial y} \right) dxdy = (\text{rot} \mathbf{V})_z dxdy \end{aligned}$$

If we sum-up the line integral as shown in Fig.2, the integral of the neighboring contour cancels out and the contour C only survives, then we have

$$\oint_C \mathbf{V} \cdot d\mathbf{r} = \int_S \text{rot} \mathbf{V} \cdot d\mathbf{S} \quad (4)$$

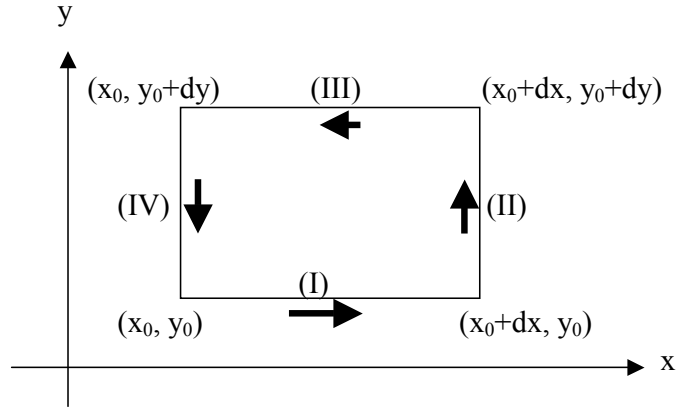


Figure 2: Stokes theorem

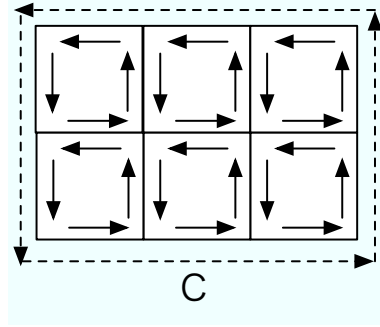


Figure 3: Integral of line and surface integral: Stokes theorem

3 Boundary Conditions at a Interface Between Different Media

Now we think a interface which is at the boundary medium 1 and 2 as shown in Fig.3. From Gauss law, we can get the following for the Gauss box which include the interface inside the box,

$$\int_V d\mathbf{r} \underbrace{\nabla \cdot \mathbf{D}}_{\rho} = \int_S \mathbf{D} \cdot d\mathbf{S} \quad (5)$$

In the limit that the Gauss box is very thin ($\delta h \rightarrow 0$)

$$\int_V d\mathbf{r} \rho = Q_{\text{box}} = \mathbf{n} \cdot [\mathbf{D}_1 - \mathbf{D}_2] S \quad (6)$$

where vector $\mathbf{n}$ means the surface normal unit vector pointing from media 2 to 1.

$$\mathbf{n} \cdot [\mathbf{D}_1 - \mathbf{D}_2] = Q_{\text{box}}/S = \sigma_{12} \quad (7)$$

where σ_{12} means the interface charge density. From $\nabla \cdot \mathbf{B} = 0$

$$\mathbf{n} \cdot [\mathbf{B}_1 - \mathbf{B}_2] = 0 \quad (8)$$

From $\text{rot} \mathbf{E} = -\partial \mathbf{B} / \partial t$ and Stokes theorem we can get

$$\oint_C \mathbf{E} \cdot d\mathbf{r} = \int_S \text{rot} \mathbf{E} \cdot d\mathbf{S} \quad (9)$$

$$= - \int_S \frac{\partial \mathbf{B}}{\partial t} \cdot \mathbf{b} dS \quad (10)$$

$$\delta r [\mathbf{E}_1 \cdot \mathbf{t}_1 + \mathbf{E}_2 \cdot \mathbf{t}_2] = - \frac{\partial \mathbf{B}}{\partial t} \cdot \mathbf{b} \delta r \delta h \longrightarrow 0 \quad (11)$$

$$\mathbf{t} = \mathbf{t}_1 = -\mathbf{t}_2 \quad (12)$$

$$\mathbf{t} \cdot [\mathbf{E}_1 - \mathbf{E}_2] = 0 \quad (13)$$

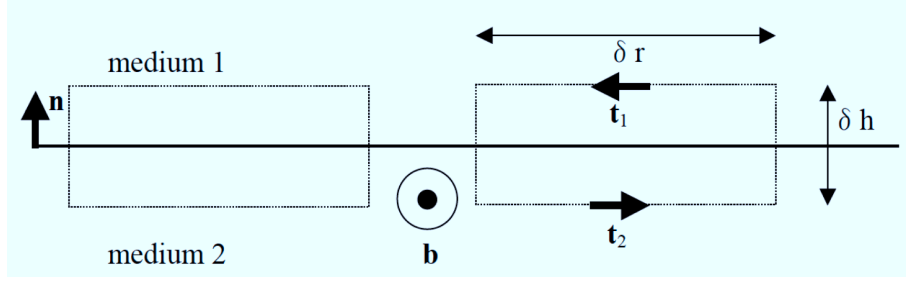


Figure 4: Gauss and Stokes box

Here $\mathbf{b}$ is the unit vector defined by $\mathbf{b} = \mathbf{n} \times \mathbf{t}$. From $\text{rot}\mathbf{H} = \mathbf{J} + \partial\mathbf{D}/\partial t$

$$\oint_C \mathbf{H} \cdot d\mathbf{r} = \int_S \text{rot}\mathbf{H} \cdot d\mathbf{S} \quad (14)$$

$$= \int_S \left(\mathbf{J} + \frac{\partial\mathbf{D}}{\partial t} \right) \cdot \mathbf{b} dS \quad (15)$$

$$\delta r [\mathbf{H}_1 \cdot \mathbf{t}_1 + \mathbf{H}_2 \cdot \mathbf{t}_2] = \left(\mathbf{J} + \frac{\partial\mathbf{D}}{\partial t} \right) \cdot \mathbf{b} \delta r \delta h \longrightarrow \mathbf{J} \cdot \mathbf{b} \delta r \delta h \quad (16)$$

$$\mathbf{t} \cdot [\mathbf{H}_1 - \mathbf{H}_2] = \mathbf{J}_s \quad [\equiv \text{surface current density}(\text{Am}^{-1})] \quad (17)$$

4 Rotation in orthogonal curvilinear coordinates

In the curvilinear coordinate

$$\mathbf{q} = \{q_1, q_2, q_3\} \quad (18)$$

$$\mathbf{q} = \{x, y, z\} : \text{Cartesian coordinates} \quad (19)$$

$$\mathbf{q} = \{r, \theta, z\} : \text{cylindrical coordinates} \quad (20)$$

$$\mathbf{q} = \{r, \theta, \phi\} : \text{spherical coordinates} \quad (21)$$

If we set

$$x = x(q_1, q_2, q_3), \quad dx = \frac{\partial x}{\partial q_1} dq_1 + \frac{\partial x}{\partial q_2} dq_2 + \frac{\partial x}{\partial q_3} dq_3 \quad (22)$$

$$y = y(q_1, q_2, q_3), \quad dy = \frac{\partial y}{\partial q_1} dq_1 + \frac{\partial y}{\partial q_2} dq_2 + \frac{\partial y}{\partial q_3} dq_3 \quad (23)$$

$$z = z(q_1, q_2, q_3), \quad dz = \frac{\partial z}{\partial q_1} dq_1 + \frac{\partial z}{\partial q_2} dq_2 + \frac{\partial z}{\partial q_3} dq_3 \quad (24)$$

$$(25)$$

The distance ds between the two infinitesimal points is given by "metric"

$$ds^2 = dx^2 + dy^2 + dz^2 = \sum_{i,j} g_{ij} dq_i dq_j \quad (26)$$

$$g_{ij} = \frac{\partial x}{\partial q_i} \frac{\partial x}{\partial q_j} + \frac{\partial y}{\partial q_i} \frac{\partial y}{\partial q_j} + \frac{\partial z}{\partial q_i} \frac{\partial z}{\partial q_j} \quad (27)$$

$$(28)$$

For orthogonal curvilinear coordinates such as cylindrical and spherical coordinates

$$g_{ij} = 0, \quad \text{for } i \neq j \quad (29)$$

$$g_{ii} = \left(\frac{\partial x}{\partial q_i} \right)^2 + \left(\frac{\partial y}{\partial q_i} \right)^2 + \left(\frac{\partial z}{\partial q_i} \right)^2 \quad (30)$$

$$ds^2 = g_{11} dq_1 dq_1 + g_{22} dq_2 dq_2 + g_{33} dq_3 dq_3 = ds_1^2 + ds_2^2 + ds_3^2 \quad (31)$$

$$ds_1 \equiv \sqrt{g_{11}} dq_1 \equiv h_1 dq_1 \quad (32)$$

$$ds_2 \equiv \sqrt{g_{22}} dq_2 \equiv h_2 dq_2 \quad (33)$$

$$ds_3 \equiv \sqrt{g_{33}} dq_3 \equiv h_3 dq_3 \quad (34)$$

example 1 : cylindrical coordinates : $x = r \cos \theta, y = r \sin \theta, z = z$

$$g_{11} = \frac{\partial x}{\partial r} \frac{\partial x}{\partial r} + \frac{\partial y}{\partial r} \frac{\partial y}{\partial r} + \frac{\partial z}{\partial r} \frac{\partial z}{\partial r} = \cos^2 \theta + \sin^2 \theta + 0 = 1, \quad h_1 = 1 \quad (35)$$

$$g_{12} = \frac{\partial x}{\partial r} \frac{\partial x}{\partial \theta} + \frac{\partial y}{\partial r} \frac{\partial y}{\partial \theta} + \frac{\partial z}{\partial r} \frac{\partial z}{\partial \theta} = \cos \theta (-r \sin \theta) + \sin \theta (r \cos \theta) + 0 = 0$$

$$g_{13} = \frac{\partial x}{\partial r} \frac{\partial x}{\partial z} + \frac{\partial y}{\partial r} \frac{\partial y}{\partial z} + \frac{\partial z}{\partial r} \frac{\partial z}{\partial z} = 0 + 0 + 0 = 0$$

$$g_{21} = \frac{\partial x}{\partial \theta} \frac{\partial x}{\partial r} + \frac{\partial y}{\partial \theta} \frac{\partial y}{\partial r} + \frac{\partial z}{\partial \theta} \frac{\partial z}{\partial r} = (-r \sin \theta) \cos \theta + r \cos \theta \sin \theta + 0 = 0$$

$$g_{22} = \frac{\partial x}{\partial \theta} \frac{\partial x}{\partial \theta} + \frac{\partial y}{\partial \theta} \frac{\partial y}{\partial \theta} + \frac{\partial z}{\partial \theta} \frac{\partial z}{\partial \theta} = (-r \sin \theta)^2 + (r \cos \theta)^2 + 0 = r^2, \quad h_2 = r \quad (36)$$

$$g_{23} = \frac{\partial x}{\partial \theta} \frac{\partial x}{\partial z} + \frac{\partial y}{\partial \theta} \frac{\partial y}{\partial z} + \frac{\partial z}{\partial \theta} \frac{\partial z}{\partial z} = 0 + 0 + 0 = 0$$

$$g_{31} = \frac{\partial x}{\partial z} \frac{\partial x}{\partial r} + \frac{\partial y}{\partial z} \frac{\partial y}{\partial r} + \frac{\partial z}{\partial z} \frac{\partial z}{\partial r} = 0 + 0 + 0 = 0$$

$$g_{32} = \frac{\partial x}{\partial z} \frac{\partial x}{\partial \theta} + \frac{\partial y}{\partial z} \frac{\partial y}{\partial \theta} + \frac{\partial z}{\partial z} \frac{\partial z}{\partial \theta} = 0 + 0 + 0 = 0$$

$$g_{33} = \frac{\partial x}{\partial z} \frac{\partial x}{\partial z} + \frac{\partial y}{\partial z} \frac{\partial y}{\partial z} + \frac{\partial z}{\partial z} \frac{\partial z}{\partial z} = 0 + 0 + 1^2 = 1, \quad h_3 = 1 \quad (37)$$

example 2 : spherical coordinates : $x = r \sin \theta \cos \phi, y = r \sin \theta \sin \phi, z = r \cos \theta$

$$g_{11} = \frac{\partial x}{\partial r} \frac{\partial x}{\partial r} + \frac{\partial y}{\partial r} \frac{\partial y}{\partial r} + \frac{\partial z}{\partial r} \frac{\partial z}{\partial r} = \sin^2 \theta \cos^2 \phi + \sin^2 \theta \sin^2 \phi + \cos^2 \theta = 1, \quad h_1 = 1 \quad (38)$$

$$g_{12} = \frac{\partial x}{\partial r} \frac{\partial x}{\partial \theta} + \frac{\partial y}{\partial r} \frac{\partial y}{\partial \theta} + \frac{\partial z}{\partial r} \frac{\partial z}{\partial \theta} = \sin \theta \cos \phi (r \cos \theta \cos \phi) + \sin \theta \sin \phi (r \cos \theta \sin \phi) + \cos \theta (-r \sin \theta) = 0$$

$$g_{13} = \frac{\partial x}{\partial r} \frac{\partial x}{\partial \phi} + \frac{\partial y}{\partial r} \frac{\partial y}{\partial \phi} + \frac{\partial z}{\partial r} \frac{\partial z}{\partial \phi} = \sin \theta \cos \phi (-r \sin \theta \sin \phi) + \sin \theta \sin \phi (r \sin \theta \cos \phi) + 0 = 0$$

$$g_{21} = \frac{\partial x}{\partial \theta} \frac{\partial x}{\partial r} + \frac{\partial y}{\partial \theta} \frac{\partial y}{\partial r} + \frac{\partial z}{\partial \theta} \frac{\partial z}{\partial r} = g_{12} = 0$$

$$g_{22} = \frac{\partial x}{\partial \theta} \frac{\partial x}{\partial \theta} + \frac{\partial y}{\partial \theta} \frac{\partial y}{\partial \theta} + \frac{\partial z}{\partial \theta} \frac{\partial z}{\partial \theta} = (r \cos \theta \cos \phi)^2 + (r \cos \theta \sin \phi)^2 + (-r \sin \theta)^2 = r^2, \quad h_2 = r \quad (39)$$

$$g_{23} = \frac{\partial x}{\partial \theta} \frac{\partial x}{\partial \phi} + \frac{\partial y}{\partial \theta} \frac{\partial y}{\partial \phi} + \frac{\partial z}{\partial \theta} \frac{\partial z}{\partial \phi} = r \cos \theta \cos \phi (-r \sin \theta \sin \phi) + r \cos \theta \sin \phi (r \sin \theta \cos \phi) + 0 = 0$$

$$g_{31} = \frac{\partial x}{\partial \phi} \frac{\partial x}{\partial r} + \frac{\partial y}{\partial \phi} \frac{\partial y}{\partial r} + \frac{\partial z}{\partial \phi} \frac{\partial z}{\partial r} = g_{13} = 0$$

$$g_{32} = \frac{\partial x}{\partial \phi} \frac{\partial x}{\partial \theta} + \frac{\partial y}{\partial \phi} \frac{\partial y}{\partial \theta} + \frac{\partial z}{\partial \phi} \frac{\partial z}{\partial \theta} = g_{23} = 0$$

$$g_{33} = \frac{\partial x}{\partial \phi} \frac{\partial x}{\partial \phi} + \frac{\partial y}{\partial \phi} \frac{\partial y}{\partial \phi} + \frac{\partial z}{\partial \phi} \frac{\partial z}{\partial \phi} = (-r \sin \theta \sin \phi)^2 + (r \sin \theta \cos \phi)^2 + 0 = r^2 \sin^2 \theta, \quad h_3 = r \sin \theta \quad (40)$$

The differential distance vector $d\mathbf{r}$ and the unit vector $\mathbf{e}_i$ may be given

$$d\mathbf{r} = h_1 dq_1 \mathbf{e}_1 + h_2 dq_2 \mathbf{e}_2 + h_3 dq_3 \mathbf{e}_3 = \sum_{i=1}^3 h_i q_i \mathbf{e}_i \quad (41)$$

$$\mathbf{e}_i = \frac{1}{h_i} \frac{\partial \mathbf{r}}{\partial q_i} \quad (42)$$

Here we only consider orthogonal curvilinear coordinates such as cylindrical coordinate and spherical coordinates.

The gradient can be defined by the sum of the product of the slope (rate of change) and the unit vector in the i -direction. The slope can be written as

$$\frac{\partial f}{\partial s_i} = \frac{1}{h_i} \frac{\partial f}{\partial q_i} \quad (43)$$

$$(44)$$

Then the gradient in the orthogonal curvilinear coordinates

$$\text{grad}_{\mathbf{q}} f = \nabla_{\mathbf{q}} f = \mathbf{e}_1 \frac{\partial f}{\partial s_1} + \mathbf{e}_2 \frac{\partial f}{\partial s_2} + \mathbf{e}_3 \frac{\partial f}{\partial s_3} \quad (45)$$

$$= \mathbf{e}_1 \frac{1}{h_1} \frac{\partial f}{\partial q_1} + \mathbf{e}_2 \frac{1}{h_2} \frac{\partial f}{\partial q_2} + \mathbf{e}_3 \frac{1}{h_3} \frac{\partial f}{\partial q_3} \quad (46)$$

$$\mathbf{e}_1 = \frac{1}{h_1} \frac{\partial \mathbf{r}}{\partial q_1}, \quad \mathbf{e}_2 = \frac{1}{h_2} \frac{\partial \mathbf{r}}{\partial q_2}, \quad \mathbf{e}_3 = \frac{1}{h_3} \frac{\partial \mathbf{r}}{\partial q_3} \quad (47)$$

In the cartesian coordinates,

$$\mathbf{q} = \{x, y, z\}, \quad \mathbf{r} = (x, y, z) \quad (48)$$

$$h_1 = 1, \quad \frac{\partial \mathbf{r}}{\partial x} = (1, 0, 0), \quad \mathbf{e}_1 = (1, 0, 0) = \mathbf{i} \quad (49)$$

$$h_2 = 1, \quad \frac{\partial \mathbf{r}}{\partial y} = (0, 1, 0), \quad \mathbf{e}_1 = (0, 1, 0) = \mathbf{j} \quad (50)$$

$$h_3 = 1, \quad \frac{\partial \mathbf{r}}{\partial z} = (0, 0, 1), \quad \mathbf{e}_1 = (0, 0, 1) = \mathbf{k} \quad (51)$$

$$\text{grad} f = \nabla f = \left(\mathbf{i} \frac{\partial}{\partial x} + \mathbf{j} \frac{\partial}{\partial y} + \mathbf{k} \frac{\partial}{\partial z} \right) f \quad (52)$$

In the cylindrical coordinates,

$$\mathbf{q} = \{r, \theta, z\}, \quad \mathbf{r} = (x, y, z) = (r \cos \theta, r \sin \theta, z) \quad (53)$$

$$\frac{\partial \mathbf{r}}{\partial r} = (\cos \theta, \sin \theta, 0), \quad h_1 = \left| \frac{\partial \mathbf{r}}{\partial r} \right| = \sqrt{\cos^2 \theta + \sin^2 \theta} = 1, \quad \mathbf{e}_1 = (\cos \theta, \sin \theta, 0) \quad (54)$$

$$\frac{\partial \mathbf{r}}{\partial \theta} = (-r \sin \theta, r \cos \theta, 0), \quad h_2 = \left| \frac{\partial \mathbf{r}}{\partial \theta} \right| = r \sqrt{\cos^2 \theta + \sin^2 \theta} = r, \quad \mathbf{e}_2 = (-\sin \theta, \cos \theta, 0) \quad (55)$$

$$\frac{\partial \mathbf{r}}{\partial z} = (0, 0, 1), \quad h_3 = \left| \frac{\partial \mathbf{r}}{\partial z} \right| = 1, \quad \mathbf{e}_3 = (0, 0, 1) \quad (56)$$

$$\text{grad}_{r,\theta,z} f = \nabla_{r,\theta,z} = \left(\mathbf{e}_1 \frac{\partial}{\partial r} + \mathbf{e}_2 \frac{1}{r} \frac{\partial}{\partial \theta} + \mathbf{e}_3 \frac{\partial}{\partial z} \right) f \quad (57)$$

In the spherical coordinates,

$$\mathbf{q} = \{r, \theta, \phi\}, \quad \mathbf{r} = (x, y, z) = (r \sin \theta \cos \phi, r \sin \theta \sin \phi, r \cos \theta) \quad (58)$$

$$\frac{\partial \mathbf{r}}{\partial r} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta), \quad h_1 = \left| \frac{\partial \mathbf{r}}{\partial r} \right| = \sqrt{\sin^2 \theta (\cos^2 \phi + \sin^2 \phi) + \cos^2 \theta} = 1, \quad \mathbf{e}_1 = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta) \quad (59)$$

$$\frac{\partial \mathbf{r}}{\partial \theta} = (r \cos \theta \cos \phi, r \cos \theta \sin \phi, -r \sin \theta), \quad h_2 = \left| \frac{\partial \mathbf{r}}{\partial \theta} \right| = r \sqrt{\cos^2 \theta (\cos^2 \phi + \sin^2 \phi) + \sin^2 \theta} = r \quad \mathbf{e}_2 = (\cos \theta \cos \phi, \cos \theta \sin \phi, -\sin \theta) \quad (60)$$

$$\frac{\partial \mathbf{r}}{\partial \phi} = (-r \sin \theta \sin \phi, r \sin \theta \cos \phi, 0), \quad h_3 = \left| \frac{\partial \mathbf{r}}{\partial \phi} \right| = r \sqrt{\sin^2 \theta \sin^2 \phi + \sin^2 \theta \cos^2 \phi} = r \sin \theta, \quad \mathbf{e}_3 = (-\sin \phi, \cos \phi, 0) \quad (61)$$

$$\text{grad}_{r,\theta,\phi} f = \nabla_{r,\theta,\phi} = \left(\mathbf{e}_1 \frac{\partial}{\partial r} + \mathbf{e}_2 \frac{1}{r} \frac{\partial}{\partial \theta} + \mathbf{e}_3 \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \right) f \quad (62)$$

We will consider the flux vector $\mathbf{J}$ in Fig.3. The mass balance of the flow-in and flow-out in the J_1 direction can be obtained if we consider the flow-out area also depends on q_1 ¹

$$\left[J_1 ds_2 ds_3 + \frac{\partial(J_1 ds_2 ds_3)}{\partial q_1} dq_1 \right] - J_1 ds_2 ds_3 = \frac{\partial(J_1 h_2 h_3)}{\partial q_1} dq_1 dq_2 dq_3 \quad (63)$$

In the same way we have the total amount for the volume element $ds_1 ds_2 ds_3$

$$\left[\frac{\partial(J_1 h_2 h_3)}{\partial q_1} + \frac{\partial(J_2 h_3 h_1)}{\partial q_2} + \frac{\partial(J_3 h_1 h_2)}{\partial q_3} \right] dq_1 dq_2 dq_3 \quad (64)$$

In the same way as the divergence in x, y, z -coordinate, the divergence is given by the divide of the unit volume

$$\text{div} \mathbf{J}(q_1, q_2, q_3) = \nabla \cdot \mathbf{J}(q_1, q_2, q_3) = \frac{1}{ds_1 ds_2 ds_3} \left[\frac{\partial(J_1 h_2 h_3)}{\partial q_1} + \frac{\partial(J_2 h_3 h_1)}{\partial q_2} + \frac{\partial(J_3 h_1 h_2)}{\partial q_3} \right] dq_1 dq_2 dq_3 \quad (65)$$

$$= \frac{1}{h_1 h_2 h_3} \left[\frac{\partial(J_1 h_2 h_3)}{\partial q_1} + \frac{\partial(J_2 h_3 h_1)}{\partial q_2} + \frac{\partial(J_3 h_1 h_2)}{\partial q_3} \right] \quad (66)$$

$$J_1 = \mathbf{J} \cdot \mathbf{e}_1, \quad J_2 = \mathbf{J} \cdot \mathbf{e}_2, \quad J_3 = \mathbf{J} \cdot \mathbf{e}_3 \quad (67)$$

¹The expansion may be done by s_i but the differentiation should be done by q_i . So the approximation is used here.

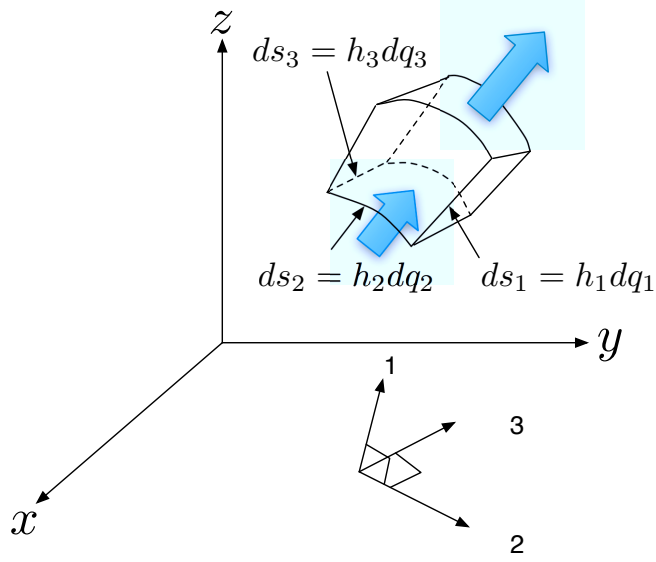


Figure 5:

We also get Laplacian ∇^2 when we use

$$\mathbf{J}(q_1, q_2, q_3) = \text{grad}_{\mathbf{q}} f = \mathbf{e}_1 \frac{1}{h_1} \frac{\partial f}{\partial q_1} + \mathbf{e}_2 \frac{1}{h_2} \frac{\partial f}{\partial q_2} + \mathbf{e}_3 \frac{1}{h_3} \frac{\partial f}{\partial q_3} \quad (68)$$

$$\text{div} \mathbf{J}(q_1, q_2, q_3) = \nabla \cdot \mathbf{J}(q_1, q_2, q_3) = \text{div}(\text{grad}_{\mathbf{q}} f) = \nabla_{\mathbf{q}}^2 f \quad (69)$$

$$\nabla_{\mathbf{q}}^2 f = \frac{1}{h_1 h_2 h_3} \left[\frac{\partial}{\partial q_1} \left(\frac{h_2 h_3}{h_1} \frac{\partial f}{\partial q_1} \right) + \frac{\partial}{\partial q_2} \left(\frac{h_3 h_1}{h_2} \frac{\partial f}{\partial q_2} \right) + \frac{\partial}{\partial q_3} \left(\frac{h_1 h_2}{h_3} \frac{\partial f}{\partial q_3} \right) \right] \quad (70)$$

4.1 Laplacian in P. Chem.

The Laplacian is very important in physical chemistry.

(I) For the diffusion equation

$$\begin{aligned} \frac{\partial c}{\partial t} + \text{div} \mathbf{J} &= 0, \quad \mathbf{J} = -\text{grad} c \\ \frac{\partial c}{\partial t} &= \text{div}(\text{grad} c) = \nabla^2 c \end{aligned}$$

(II) For the wave equation

$$\frac{\partial^2 \xi}{\partial t^2} = v^2 \text{div}(\text{grad} \xi) = v^2 \nabla^2 \xi$$

In the cylindrical coordinates

$$\begin{aligned} h_1 &= 1, \quad h_2 = r, \quad h_3 = 1 \\ \nabla_{\mathbf{q}}^2 f &= \frac{1}{r} \left[\frac{\partial}{\partial r} \left(r \frac{\partial f}{\partial r} \right) + \frac{\partial}{\partial \theta} \left(\frac{1}{r} \frac{\partial f}{\partial \theta} \right) + \frac{\partial}{\partial z} \left(r \frac{\partial f}{\partial z} \right) \right] \\ &= \frac{1}{r} \frac{\partial f}{\partial r} + \frac{\partial^2 f}{\partial r^2} + \frac{1}{r^2} \frac{\partial^2 f}{\partial \theta^2} + \frac{\partial^2 f}{\partial z^2} \end{aligned}$$

In the spherical coordinates

$$\begin{aligned} h_1 &= 1, \quad h_2 = r, \quad h_3 = r \sin \theta \\ \nabla_{\mathbf{q}}^2 f &= \frac{1}{r^2 \sin \theta} \left[\frac{\partial}{\partial r} \left(r^2 \sin \theta \frac{\partial f}{\partial r} \right) + \frac{\partial}{\partial \theta} \left(\frac{r \sin \theta}{r} \frac{\partial f}{\partial \theta} \right) + \frac{\partial}{\partial \phi} \left(\frac{r}{r \sin \theta} \frac{\partial f}{\partial \phi} \right) \right] \\ &= \frac{1}{r^2 \sin \theta} \left[2r \sin \theta \frac{\partial f}{\partial r} + r^2 \sin \theta \frac{\partial^2 f}{\partial r^2} + \cos \theta \frac{\partial f}{\partial \theta} + \sin \theta \frac{\partial^2 f}{\partial \theta^2} + \frac{1}{\sin \theta} \frac{\partial^2 f}{\partial \phi^2} \right] \\ &= \frac{2}{r} \frac{\partial f}{\partial r} + \frac{\partial^2 f}{\partial r^2} + \frac{1}{r^2} \frac{\partial^2 f}{\partial \theta^2} + \frac{\cos \theta}{r^2 \sin \theta} \frac{\partial f}{\partial \theta} + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 f}{\partial \phi^2} \end{aligned}$$

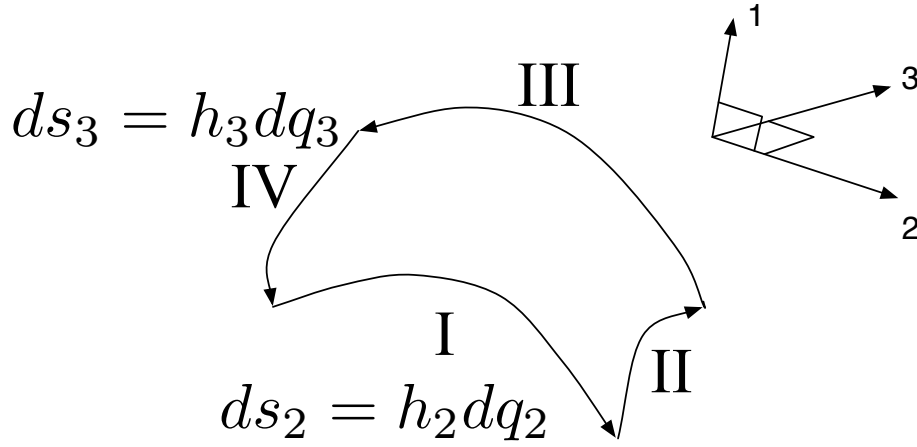


Figure 6: differential surface element in the curvilinear surface $q_1 = \text{constant}$.

4.2 rotation

We will apply the Stokes theorem

$$\int_S \text{rot} \mathbf{J} \cdot d\mathbf{S} = \oint_C \mathbf{J} \cdot \mathbf{r} \quad (71)$$

For the component q_1 direction (as shown in FFig.4.2) the Stokes theorem tells us

$$\int_S (\text{rot} \mathbf{J})_1 (d\mathbf{S})_1 = (\text{rot} \mathbf{J})_1 ds_2 ds_3 = (\text{rot} \mathbf{J})_1 h_2 h_3 dq_2 dq_3 \quad (72)$$

$$\begin{aligned} \oint_C \mathbf{J} \cdot \mathbf{r} &= \underbrace{J_2 h_2 dq_2}_{\text{path I}} + \underbrace{\left(J_3 h_3 dq_3 + \frac{\partial(J_3 h_3)}{\partial q_2} dq_2 dq_3 \right)}_{\text{path II}} - \underbrace{\left(J_2 h_2 dq_2 + \frac{\partial(J_2 h_2)}{\partial q_3} dq_3 dq_2 \right)}_{\text{path III}} - \underbrace{J_3 h_3 dq_3}_{\text{path IV}} \\ &= \frac{\partial(J_3 h_3)}{\partial q_2} dq_2 dq_3 - \frac{\partial(J_2 h_2)}{\partial q_3} dq_3 dq_2 \end{aligned} \quad (73)$$

$$(\text{rot} \mathbf{J})_1 = \frac{1}{h_2 h_3} \left[\frac{\partial(J_3 h_3)}{\partial q_2} - \frac{\partial(J_2 h_2)}{\partial q_3} \right] \quad (74)$$

$$\text{rot} \mathbf{J} \equiv \nabla_{\mathbf{q}} \times \mathbf{J} \quad (75)$$

$$= \frac{1}{h_1 h_2 h_3} \begin{vmatrix} h_1 \mathbf{e}_1 & h_2 \mathbf{e}_2 & h_3 \mathbf{e}_3 \\ \frac{\partial}{\partial q_1} & \frac{\partial}{\partial q_2} & \frac{\partial}{\partial q_3} \\ J_1 h_1 & J_2 h_2 & J_3 h_3 \end{vmatrix} \quad (76)$$

$$\begin{aligned} &= \mathbf{e}_1 \frac{1}{h_2 h_3} \left[\frac{\partial(J_3 h_3)}{\partial q_2} - \frac{\partial(J_2 h_2)}{\partial q_3} \right] \\ &\quad + \mathbf{e}_2 \frac{1}{h_3 h_1} \left[\frac{\partial(J_1 h_1)}{\partial q_3} - \frac{\partial(J_3 h_3)}{\partial q_1} \right] \\ &\quad + \mathbf{e}_3 \frac{1}{h_1 h_2} \left[\frac{\partial(J_2 h_2)}{\partial q_1} - \frac{\partial(J_1 h_1)}{\partial q_2} \right] \end{aligned} \quad (77)$$