

# Divergence(発散) and Laplacian(ラプラシアン) in Orthogonal Curvilinear Coordinate(直交曲線座表)

Masahiro Yamamoto

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## 1 Definition of divergence

Now we consider the vector field  $\mathbf{J}$  that depends on the position. For example, the flux  $\mathbf{J}(\mathbf{r})$  is the vector field of the mass transport per unit time and per unit area at the position  $\mathbf{r}$ . As shown in Fig.1(a), we consider the infinitesimal volume element  $dV = dxdydz$ . The  $x, y, z$ -component of the vector  $\mathbf{J}$  (Fig.1(b)) can be define as

$$\mathbf{J} = J_x \mathbf{i} + J_y \mathbf{j} + J_z \mathbf{k} \quad (1)$$

Here the unit vector in  $x, y, z$  direction is  $\mathbf{i}, \mathbf{j}, \mathbf{k}$ , respectively. The mass transport into this volume element can be obtained as the difference between ingoing-flux  $\times$  area and outgoing-flux  $\times$  area, and that is equal to the change of the total amount of the mass in the volume element.

$$\frac{\partial \rho}{\partial t} dxdydz = -[J_x(x+dx) - J_x(x)]dydz - [J_y(y+dy) - J_y(y)]dxdz - [J_z(z+dz) - J_z(z)]dxdy \quad (2)$$

If we use the following approximation

$$J_x(x+dx) \simeq J_x(x) + \frac{\partial J_x}{\partial x} dx, \quad J_y(y+dy) \simeq J_y(y) + \frac{\partial J_y}{\partial y} dy, \quad J_z(z+dz) \simeq J_z(z) + \frac{\partial J_z}{\partial z} dz \quad (3)$$

we obtained

$$\frac{\partial \rho}{\partial t} dxdydz = -\left[\frac{\partial J_x}{\partial x} dx\right]dydz - \left[\frac{\partial J_y}{\partial y} dy\right]dxdz - \left[\frac{\partial J_z}{\partial z} dz\right]dxdy \quad (4)$$

$$0 = \frac{\partial \rho}{\partial t} + \frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} + \frac{\partial J_z}{\partial z} = \frac{\partial \rho}{\partial t} + \left(\mathbf{i} \frac{\partial}{\partial x} + \mathbf{j} \frac{\partial}{\partial y} + \mathbf{k} \frac{\partial}{\partial z}\right) \cdot (J_x \mathbf{i} + J_y \mathbf{j} + J_z \mathbf{k}) \quad (5)$$

$$= \frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = \frac{\partial \rho}{\partial t} + \text{div} \mathbf{J} \quad (6)$$

The divergence of  $\mathbf{J}$ , we denote  $\nabla \cdot \mathbf{J} \equiv \text{div} \mathbf{J}$ , is the amount of mass in and out from the infinitesimal volume element. As shown in Fig.1(c), the in and out amount correspond to the inner product between the flux  $\mathbf{J}$  and the normal unit vector  $\mathbf{n}$  for the six planes of the volume elements. The normal unit vector is in the ourward direction from the plane.

$$\begin{aligned} & [J_x(x+dx) - J_x(x)]dydz + [J_y(y+dy) - J_y(y)]dxdz + [J_z(z+dz) - J_z(z)]dxdy \\ = & \sum_{\text{six surfaces}} \mathbf{J} \cdot \mathbf{n} dS = \text{div} \mathbf{J} dV \end{aligned} \quad (7)$$

For the case of genaral shape as shown in Fig.1(d), the whole space is divided to the infinitesimal volume elements  $dV$  and take the total sum.  $\mathbf{J} \cdot \mathbf{n} dS$  is cancelled out each other for the neighboring

planes of the volume elements and only the those on the exterior surface will be survived. This is the Gauss law!

$$\sum_{\text{all } dV} \text{div} \mathbf{J} dV = \sum_{\text{exterior surface}} \mathbf{J} \cdot \mathbf{n} dS \quad (8)$$

$$\int dV \text{div} \mathbf{J} = \int dS \mathbf{J} \cdot \mathbf{n} \quad (9)$$

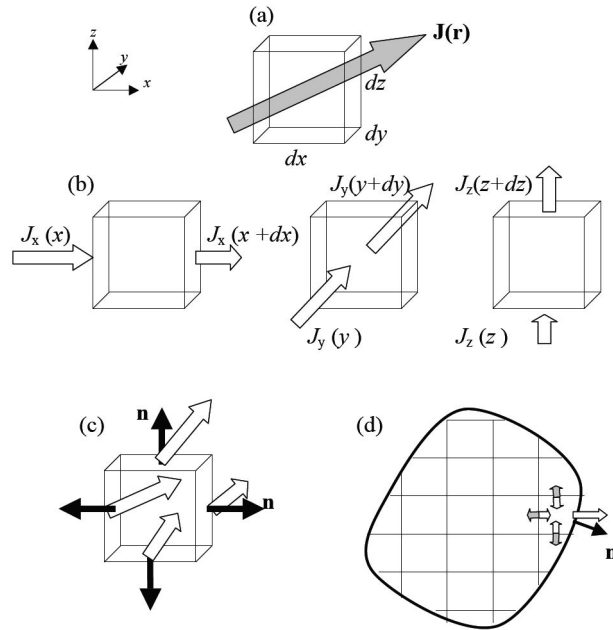


Figure 1:

## 2 Coulomb law, Electric field and Gauss law:クーロンの法則, 電場, ガウスの法則

Now we consider the dielectric medium with dielectric constant  $\epsilon$ . We put a charge  $q_0$  on the origin and the coulomb force  $\mathbf{F}$  between the another charge  $q$  at the position  $\mathbf{r}$  is given by

$$\mathbf{F} = \frac{1}{4\pi\epsilon\epsilon_0} \frac{q_0 q}{r^2} \frac{\mathbf{r}}{r} \quad (10)$$

Here we use  $r = |\mathbf{r}|$  and  $\epsilon_0$  is the permittivity of vacuum. The electric field  $\mathbf{E}$  created by the charge  $q_0$  is given by

$$\mathbf{F} = q\mathbf{E} \quad (11)$$

then we have

$$\mathbf{E} = \frac{1}{4\pi\epsilon\epsilon_0} \frac{q_0}{r^2} \frac{\mathbf{r}}{r} \quad (12)$$

If we apply the Gauss law to the electric field vector  $\mathbf{E}$ , then

$$\int dS \mathbf{E} \cdot \mathbf{n} = \int dV \text{div} \mathbf{E} \quad (13)$$

The electric field  $\mathbf{E}$  has the spherical symmetry, then we consider the sphere shown in Fig.2 and integrate the inner product on the surface. The outward normal unit vector on  $dS$  is given by  $\mathbf{n} = \mathbf{r}/r$ , then

$$\int dS \mathbf{E} \cdot \mathbf{n} = \int dS \frac{1}{4\pi\epsilon\epsilon_0} \frac{q_0}{r^2} \underbrace{\left( \frac{\mathbf{r}}{r} \cdot \frac{\mathbf{r}}{r} \right)}_{=1} = \frac{1}{4\pi\epsilon\epsilon_0} \frac{q_0}{r^2} \int dS = \frac{1}{4\pi\epsilon\epsilon_0} \frac{q_0}{r^2} 4\pi r^2 = \frac{q_0}{\epsilon\epsilon_0} \quad (14)$$

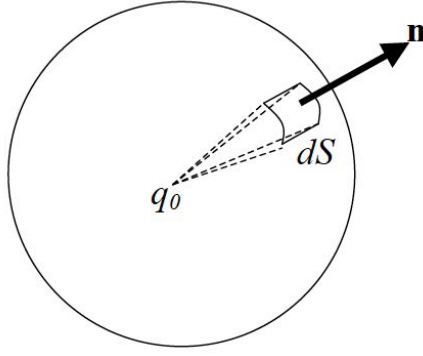


Figure 2:

$q_0$  is the integral of the charge density inside the sphere

$$\frac{q_0}{\epsilon\epsilon_0} = \frac{1}{\epsilon\epsilon_0} \int dV \rho(\mathbf{r}) \quad (15)$$

Therefore,

$$\text{div}\mathbf{E} = \frac{\rho(\mathbf{r})}{\epsilon\epsilon_0} \quad (16)$$

This equation means that the number of the lines of electric force from the charge  $\rho$  in  $dV$  is equal to  $\rho/(\epsilon_0\epsilon)$ . But in general the dielectric constant may become discontinuous at the surface/inteface and the number of the lines of electric force also become discontinuous. To overcome the inconvenience of this discontinuity, we define the electric flux density given by  $\mathbf{D} = \epsilon_0\epsilon\mathbf{E}$ . The electric flux from the volume element  $dV$  does not depend on the dielectric constant but only on the charge  $\rho$ . Then the electric flux is continupous at the surface/interface. The Gauss law becomes

$$\text{div}\mathbf{D} = \rho(\mathbf{r}) \quad (17)$$

ant this is the basic equation of the electirc double layer at the electrode interface.

### 3 Divergence and Laplacian in orthogonal curvilinear coordinates: 直交曲線座標系における発散とラプラシアン

In the curvilinear coordinate

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

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

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

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

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 :  $x = r \cos \theta, y = r \sin \theta, z = z$

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

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

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

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

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

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

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

$$g_{32} = \frac{\partial x}{\partial z} \frac{\partial x}{\partial \theta} + \frac{\partial y}{\partial z} \frac{\partial y}{\partial \theta} + \frac{\partial z}{\partial z} \frac{\partial z}{\partial \theta} = 0 + 0 + 0 = r^2$$

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

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

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

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

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

### 3.1 Gradient: 勾配

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,

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

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

$$h_2 = 1, \quad \frac{\partial \mathbf{r}}{\partial y} = (0, 1, 0), \quad \mathbf{e}_2 = (0, 1, 0) = \mathbf{j} \quad (50)$$

$$h_3 = 1, \quad \frac{\partial \mathbf{r}}{\partial z} = (0, 0, 1), \quad \mathbf{e}_3 = (0, 0, 1) = \mathbf{k} \quad (51)$$

$$\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{i,j}, \quad \delta_{i,j} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases} \quad (52)$$

$$\mathbf{e}_i \times \mathbf{e}_j = \epsilon_{i,j,k} \mathbf{e}_k, \quad \epsilon_{i,j,k} = \begin{cases} 1, & (i, j, k) = (1, 2, 3), (2, 3, 1), (3, 1, 2) \\ -1, & (i, j, k) = (1, 3, 2), (2, 1, 3), (3, 2, 1) \\ 0, & \text{otherwise} \end{cases} \quad (53)$$

$$\text{grad} f = \nabla f = \left( \mathbf{i} \frac{\partial}{\partial x} + \mathbf{j} \frac{\partial}{\partial y} + \mathbf{k} \frac{\partial}{\partial z} \right) f \quad (54)$$

In the cylindrical coordinates,

$$\mathbf{q} = \{r, \theta, z\}, \quad \mathbf{r} = (x, y, z) = (r \cos \theta, r \sin \theta, z) \quad (55)$$

$$\frac{\partial \mathbf{r}}{\partial r} = (\cos \theta, \sin \theta, 0), \quad h_1 = \left| \frac{\partial \mathbf{r}}{\partial r} \right| = \sqrt{\cos^2 \theta + \sin^2 \theta} = 1, \quad \mathbf{e}_1 = (\cos \theta, \sin \theta, 0) \quad (56)$$

$$\frac{\partial \mathbf{r}}{\partial \theta} = (-r \sin \theta, r \cos \theta, 0), \quad h_2 = \left| \frac{\partial \mathbf{r}}{\partial \theta} \right| = r \sqrt{\cos^2 \theta + \sin^2 \theta} = r, \quad \mathbf{e}_2 = (-\sin \theta, \cos \theta, 0) \quad (57)$$

$$\frac{\partial \mathbf{r}}{\partial z} = (0, 0, 1), \quad h_3 = \left| \frac{\partial \mathbf{r}}{\partial z} \right| = 1, \quad \mathbf{e}_3 = (0, 0, 1) \quad (58)$$

$$\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{i,j}, \quad \mathbf{e}_i \times \mathbf{e}_j = \epsilon_{i,j,k} \mathbf{e}_k \quad (59)$$

$$\text{grad}_{r,\theta,z} f = \nabla_{r,\theta,z} f = \left( \mathbf{e}_1 \frac{\partial}{\partial r} + \mathbf{e}_2 \frac{1}{r} \frac{\partial}{\partial \theta} + \mathbf{e}_3 \frac{\partial}{\partial z} \right) f \quad (60)$$

In the spherical coordinates,

$$\mathbf{q} = \{r, \theta, \phi\}, \quad \mathbf{r} = (x, y, z) = (r \sin \theta \cos \phi, r \sin \theta \sin \phi, r \cos \theta) \quad (61)$$

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

$$\mathbf{e}_1 = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta) \quad (62)$$

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

$$\mathbf{e}_2 = (\cos \theta \cos \phi, \cos \theta \sin \phi, -\sin \theta) \quad (63)$$

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

$$\mathbf{e}_3 = (-\sin \phi, \cos \phi, 0) \quad (64)$$

$$\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{i,j}, \quad \mathbf{e}_i \times \mathbf{e}_j = \epsilon_{i,j,k} \mathbf{e}_k \quad (65)$$

$$\text{grad}_{r,\theta,\phi} f = \nabla_{r,\theta,\phi} f = \left( \mathbf{e}_1 \frac{\partial}{\partial r} + \mathbf{e}_2 \frac{1}{r} \frac{\partial}{\partial \theta} + \mathbf{e}_3 \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \right) f \quad (66)$$

### 3.2 Divergence: 発散

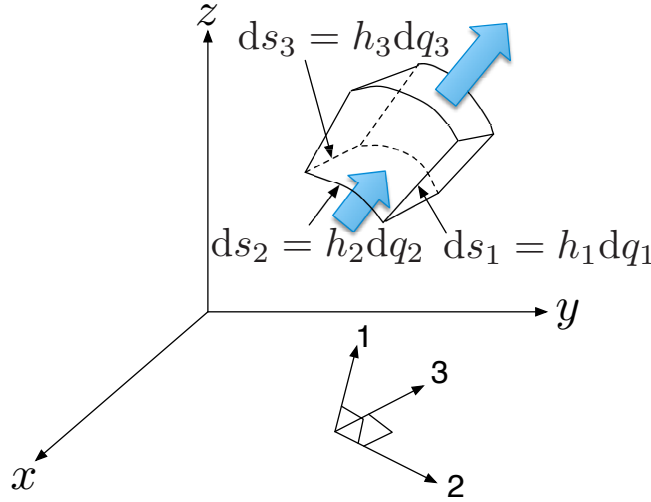


Figure 3:

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  $q_1$ <sup>1</sup>

$$\left[ J_1 ds_2 ds_3 + \frac{\partial(J_1 ds_2 ds_3)}{\partial q_1} dq_1 \right] - J_1 ds_2 ds_3 = \frac{\partial(J_1 h_2 h_3)}{\partial q_1} dq_1 dq_2 dq_3 \quad (67)$$

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

$$\left[ \frac{\partial(J_1 h_2 h_3)}{\partial q_1} + \frac{\partial(J_2 h_3 h_1)}{\partial q_2} + \frac{\partial(J_3 h_1 h_2)}{\partial q_3} \right] dq_1 dq_2 dq_3 \quad (68)$$

In the same way from Eq.(4) to Eq.(5) the divergence is given by the divide of the unit volume

$$\begin{aligned} \text{div} \mathbf{J}(q_1, q_2, q_3) &= \nabla \cdot \mathbf{J}(q_1, q_2, q_3) = \frac{1}{ds_1 ds_2 ds_3} \left[ \frac{\partial(J_1 h_2 h_3)}{\partial q_1} + \frac{\partial(J_2 h_3 h_1)}{\partial q_2} + \frac{\partial(J_3 h_1 h_2)}{\partial q_3} \right] dq_1 dq_2 dq_3 \\ &= \frac{1}{h_1 h_2 h_3} \left[ \frac{\partial(J_1 h_2 h_3)}{\partial q_1} + \frac{\partial(J_2 h_3 h_1)}{\partial q_2} + \frac{\partial(J_3 h_1 h_2)}{\partial q_3} \right] \end{aligned} \quad (69)$$

$$J_1 = \mathbf{J} \cdot \mathbf{e}_1, \quad J_2 = \mathbf{J} \cdot \mathbf{e}_2, \quad J_3 = \mathbf{J} \cdot \mathbf{e}_3 \quad (70)$$

<sup>1</sup>The expansion may be done by  $s_i$  but the differentiation should be done by  $q_i$ . So the approximation is used here.

In the cartesian coordinate

$$\mathbf{q} = (x, y, z) \quad (71)$$

$$h_1 = 1, \quad h_2 = 1, \quad h_3 = 1 \quad (72)$$

$$\operatorname{div}\mathbf{J}(x, y, z) = \frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} + \frac{\partial J_z}{\partial z} \quad (73)$$

In the cylindrical coordinates

$$\mathbf{q} = (r, \theta, z) \quad (74)$$

$$h_1 = 1, \quad h_2 = r, \quad h_3 = 1 \quad (75)$$

$$\operatorname{div}_{r,\theta,z}\mathbf{J} = \nabla_{r,\theta,z} \cdot \mathbf{J} = \frac{1}{r} \left[ \frac{\partial(rJ_r)}{\partial r} + \frac{\partial J_\theta}{\partial \theta} + \frac{\partial(rJ_z)}{\partial z} \right] \quad (76)$$

$$= \frac{1}{r} \left[ \frac{\partial(rJ_r)}{\partial r} + \frac{\partial J_\theta}{\partial \theta} + r \frac{\partial J_z}{\partial z} \right] \quad (77)$$

In the spherical coordinates

$$\mathbf{q} = (r, \theta, \phi) \quad (78)$$

$$h_1 = 1, \quad h_2 = r, \quad h_3 = r \sin \theta \quad (79)$$

$$\operatorname{div}_{r,\theta,\phi}\mathbf{J} = \nabla_{r,\theta,\phi} \cdot \mathbf{J} = \frac{1}{r^2 \sin \theta} \left[ \frac{\partial(r^2 \sin \theta J_r)}{\partial r} + \frac{\partial(r \sin \theta J_\theta)}{\partial \theta} + \frac{\partial(r J_\phi)}{\partial \phi} \right] \quad (80)$$

$$= \frac{1}{r^2 \sin \theta} \left[ \sin \theta \frac{\partial(r^2 J_r)}{\partial r} + r \frac{\partial(\sin \theta J_\theta)}{\partial \theta} + r \frac{\partial J_\phi}{\partial \phi} \right] \quad (81)$$

$$(82)$$

### 3.3 Laplacian: ラプラシアン

We also get Laplacian  $\nabla^2$  when we use

$$\mathbf{J}(q_1, q_2, q_3) = \operatorname{grad}_{\mathbf{q}} f = \mathbf{e}_1 \frac{1}{h_1} \frac{\partial f}{\partial q_1} + \mathbf{e}_2 \frac{1}{h_2} \frac{\partial f}{\partial q_2} + \mathbf{e}_3 \frac{1}{h_3} \frac{\partial f}{\partial q_3} \quad (83)$$

$$\operatorname{div}\mathbf{J}(q_1, q_2, q_3) = \nabla \cdot \mathbf{J}(q_1, q_2, q_3) = \operatorname{div}(\operatorname{grad}_{\mathbf{q}} f) = \nabla_{\mathbf{q}}^2 f \quad (84)$$

$$\nabla_{\mathbf{q}}^2 f = \frac{1}{h_1 h_2 h_3} \left[ \frac{\partial}{\partial q_1} \left( \frac{h_2 h_3}{h_1} \frac{\partial f}{\partial q_1} \right) + \frac{\partial}{\partial q_2} \left( \frac{h_3 h_1}{h_2} \frac{\partial f}{\partial q_2} \right) + \frac{\partial}{\partial q_3} \left( \frac{h_1 h_2}{h_3} \frac{\partial f}{\partial q_3} \right) \right] \quad (85)$$

The Laplacian is very important in physical chemistry.

(a) For the diffusion equation

$$\frac{\partial c}{\partial t} + \operatorname{div}\mathbf{J} = 0, \quad \mathbf{J} = -\operatorname{grad}c \quad (86)$$

$$\frac{\partial c}{\partial t} = \operatorname{div}(\operatorname{grad}c) = \nabla^2 c \quad (87)$$

(b) For the wave equation

$$\frac{\partial^2 \xi}{\partial t^2} = v^2 \operatorname{div}(\operatorname{grad}\xi) = v^2 \nabla^2 \xi \quad (88)$$

In the cartesian coordinate

$$\mathbf{q} = (x, y, z) \quad (89)$$

$$h_1 = 1, \quad h_2 = 1, \quad h_3 = 1 \quad (90)$$

$$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2} \quad (91)$$

In the cylindrical coordinates

$$\mathbf{q} = (r, \theta, z) \quad (92)$$

$$h_1 = 1, \quad h_2 = r, \quad h_3 = 1 \quad (93)$$

$$\nabla_{\mathbf{q}}^2 f = \frac{1}{r} \left[ \frac{\partial}{\partial r} \left( r \frac{\partial f}{\partial r} \right) + \frac{\partial}{\partial \theta} \left( \frac{1}{r} \frac{\partial f}{\partial \theta} \right) + \frac{\partial}{\partial z} \left( r \frac{\partial f}{\partial z} \right) \right] \quad (94)$$

$$= \frac{1}{r} \frac{\partial f}{\partial r} + \frac{\partial^2 f}{\partial r^2} + \frac{1}{r^2} \frac{\partial^2 f}{\partial \theta^2} + \frac{\partial^2 f}{\partial z^2} \quad (95)$$

In the spherical coordinates

$$\mathbf{q} = (r, \theta, \phi) \quad (96)$$

$$h_1 = 1, \quad h_2 = r, \quad h_3 = r \sin \theta \quad (97)$$

$$\nabla_{\mathbf{q}}^2 f = \frac{1}{r^2 \sin \theta} \left[ \frac{\partial}{\partial r} \left( r^2 \sin \theta \frac{\partial f}{\partial r} \right) + \frac{\partial}{\partial \theta} \left( \frac{r \sin \theta}{r} \frac{\partial f}{\partial \theta} \right) + \frac{\partial}{\partial \phi} \left( \frac{r}{r \sin \theta} \frac{\partial f}{\partial \phi} \right) \right] \quad (98)$$

$$= \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial f}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial f}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 f}{\partial \phi^2} \quad (99)$$

$$= \frac{2}{r} \frac{\partial f}{\partial r} + \frac{\partial^2 f}{\partial r^2} + \frac{1}{r^2} \frac{\partial^2 f}{\partial \theta^2} + \frac{\cos \theta}{r^2 \sin \theta} \frac{\partial f}{\partial \theta} + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 f}{\partial \phi^2} \quad (100)$$