Divergence(発散), Gauss Law(ガウスの定理), Orthogonal Curvlinear Coordinate(直交曲線座表)

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1 Definition of divergence

Now we consider the vector field $\mathbf{J}$ that depnends 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 $\mathrm{d}V = \mathrm{d}x\mathrm{d}y\mathrm{d}z$. The x, y, z-component of the vector $\mathbf{J}$ （Fig.1(b)） can be define as

$$\mathbf{J} = J_x\mathbf{i} + J_y\mathbf{j} + J_z\mathbf{k} \tag{1}$$

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 × area and outgoing-flux × area , and that is equal to the change of the total amount of the mass in the volume element.

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

If we use the following approximation

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

we obtained

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

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

$$= \frac{\partial\rho}{\partial t} + \nabla\cdot\mathbf{J} = \frac{\partial\rho}{\partial t} + \mathrm{div}\mathbf{J} \tag{5}$$

$$\tag{6}$$

The divergence of $\mathbf{J}$, we denote $\nabla\cdot\mathbf{J} \equiv \mathrm{div}\mathbf{J}$, 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.

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

For the case of genaral shape as shown in Fig.1(d), the whole space is divided to the infinitesimal volume elements $\mathrm{d}V$ 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!

$$
\begin{aligned}
\sum_{\text{all } dV} \text{div}\mathbf{J}dV &= \sum_{\text{exterior surface}} \mathbf{J}\cdot\mathbf{n}dS && (8)\\
\int dV\text{div}\mathbf{J} &= \int dS\mathbf{J}\cdot\mathbf{n} && (9)
\end{aligned}
$$

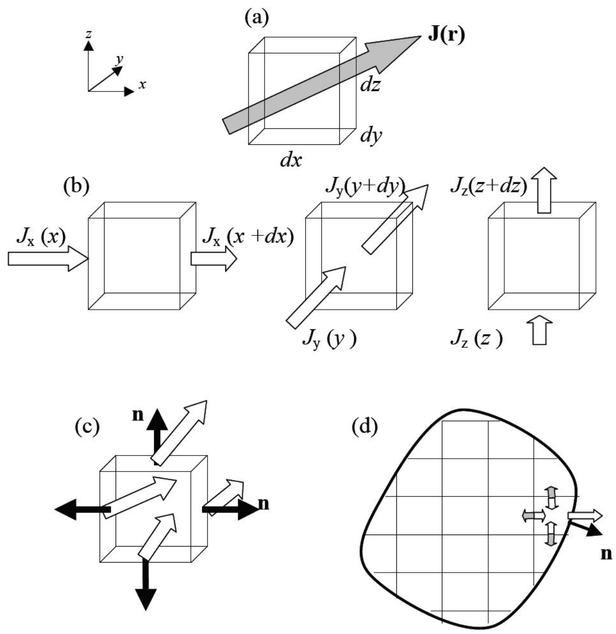

Figure 1:

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 dieletric medium with dielectric constant ϵ. 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

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

Here we use $r = |\mathbf{r}|$ and ϵ_0 is the permittivity of vacuum. The electric field $\mathbf{E}$ created by the charge q_0 is given by

$$\mathbf{F} = q\mathbf{E} \tag{11}$$

then we have

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

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

$$\int dS\mathbf{E}\cdot\mathbf{n} = \int dV\text{div}\mathbf{E} \tag{13}$$

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

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

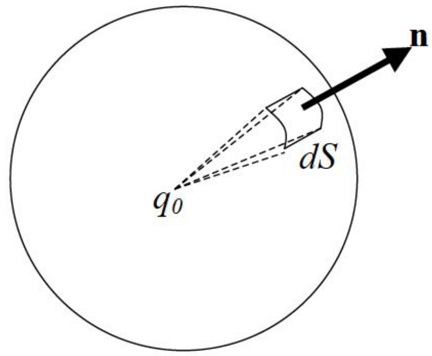

Figure 2:

q_0 is the integral of the charge density inside the sphere

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

Therefore,

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

This equation means that the number of the lines of electric force from the charge ρ 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 ρ. Then the electric flux is continupous at the surface/interface. The Gauss law becomes

$$\mathrm{div}\mathbf{D} = \rho(\mathbf{r}) \tag{17}$$

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

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

In the curvlinear coordinate

$$\mathbf{q} = \{q_1, q_2, q_3\} \tag{18}$$
$$\mathbf{q} = \{x, y, z\} \quad : \text{ Cartesian coordinates} \tag{19}$$
$$\mathbf{q} = \{r, \theta, z\} \quad : \text{ cylindircal coordinates} \tag{20}$$
$$\mathbf{q} = \{r, \theta, \phi\} \quad : \text{ spherical coordinates} \tag{21}$$

If we set

$$x = x(q_1, q_2, q_3), \quad dx = \frac{\partial x}{\partial q_1}dq_1 + \frac{\partial x}{\partial q_2}dq_2 + \frac{\partial x}{\partial q_3}dq_3 \tag{22}$$
$$y = y(q_1, q_2, q_3), \quad dy = \frac{\partial y}{\partial q_1}dq_1 + \frac{\partial y}{\partial q_2}dq_2 + \frac{\partial y}{\partial q_3}dq_3 \tag{23}$$
$$z = z(q_1, q_2, q_3), \quad dz = \frac{\partial z}{\partial q_1}dq_1 + \frac{\partial z}{\partial q_2}dq_2 + \frac{\partial z}{\partial q_3}dq_3 \tag{24}$$
$$\tag{25}$$

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

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

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

$$\tag{28}$$

For orthogonal curvlinear coordinates such as cylindrical and spherical coordinates

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

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

$$ds^2 = g_{11}dq_1dq_1 + g_{22}dq_2dq_2 + g_{33}dq_3dq_3 = ds_1^2 + ds_2^2 + ds_3^2 \tag{31}$$

$$ds_1 \equiv \sqrt{g_{11}}dq_1 \equiv h_1 dq_1 \tag{32}$$

$$ds_2 \equiv \sqrt{g_{22}}dq_2 \equiv h_2 dq_2 \tag{33}$$

$$ds_3 \equiv \sqrt{g_{33}}dq_3 \equiv h_3 dq_3 \tag{34}$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\mathbf{e}_i = \frac{1}{h_i}\frac{\partial \mathbf{r}}{\partial q_i} \tag{42}$$

Here we only consider orthogonal curvlinear 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

$$\frac{\partial f}{\partial s_i} = \frac{1}{h_i}\frac{\partial f}{\partial q_i} \tag{43}$$

$$\tag{44}$$

Then the gradient in the orthogonal curvlinear coordinates

$$\mathrm{grad}_{\mathbf{q}} f = \nabla_{\mathbf{q}} f = \mathbf{e}_1 \frac{\partial f}{\partial s_1} + \mathbf{e}_2 \frac{\partial f}{\partial s_2} + \mathbf{e}_3 \frac{\partial f}{\partial s_1} \tag{45}$$

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

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

In the cartesian coordinates,

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

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

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

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

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

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

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

In the cylindrical coordinates,

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

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

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

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

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

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

In the spherical coordinates,

$$
\begin{aligned}
\mathbf{q} &= \{r, \theta, \phi\}, \quad \mathbf{r} = (x, y, z) = (r\sin\theta\cos\phi, r\sin\theta\sin\phi, r\cos\theta) &(61)\\
\frac{\partial \mathbf{r}}{\partial r} &= (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta), \quad h_1 = \left|\frac{\partial \mathbf{r}}{\partial r}\right| = \sqrt{\sin^2\theta(\cos^2\phi + \sin^2\phi) + \cos^2\theta} = 1, \\
& \mathbf{e}_1 = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta) &(62)\\
\frac{\partial \mathbf{r}}{\partial \theta} &= (r\cos\theta\cos\phi, r\cos\theta\sin\phi, -r\sin\theta), \quad h_2 = \left|\frac{\partial \mathbf{r}}{\partial \theta}\right| = r\sqrt{\cos^2\theta(\cos^2\phi + \sin^2\phi) + \sin^2\theta} = r \\
& \mathbf{e}_2 = (\cos\theta\cos\phi, \cos\theta\sin\phi, -\sin\theta) &(63)\\
\frac{\partial \mathbf{r}}{\partial \phi} &= (-r\sin\theta\sin\phi, r\sin\theta\cos\phi, 0), \quad h_3 = \left|\frac{\partial \mathbf{r}}{\partial \phi}\right| = r\sqrt{\sin^2\theta\sin^2\phi + \sin^2\theta\cos^2\phi} = r\sin\theta, \\
& \mathbf{e}_3 = (-\sin\phi, \cos\phi, 0) &(64)\\
\mathbf{e}_i \cdot \mathbf{e}_j &= \delta_{i,j}, \quad \mathbf{e}_i \times \mathbf{e}_j = \epsilon_{i,j,k}\mathbf{e}_k &(65)\\
\mathrm{grad}_{r,\theta,\phi} f &= \nabla_{r,\theta,\phi} f = \left(\mathbf{e}_1 \frac{\partial}{\partial r} + \mathbf{e}_2 \frac{1}{r}\frac{\partial}{\partial \theta} + \mathbf{e}_3 \frac{1}{r\sin\theta}\frac{\partial}{\partial \phi}\right) f &(66)
\end{aligned}
$$

3.2 Divergence: 発散

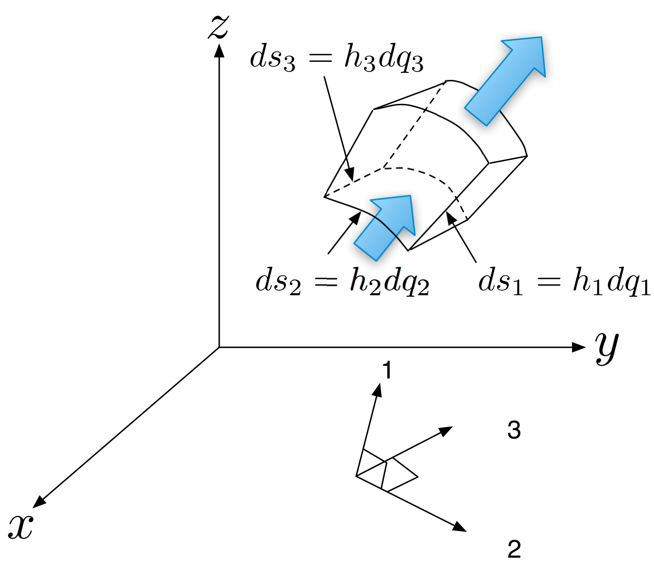

Figure 3:

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 [1]

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

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

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

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

$$
\begin{aligned}
\mathrm{div}\mathbf{J}(q_1, q_2, q_3) &= \nabla \cdot \mathbf{J}(q_1, q_2, q_3) = \frac{1}{ds_1 ds_2 ds_3}\left[\frac{\partial(J_1 h_2 h_3)}{\partial q_1} + \frac{\partial(J_2 h_3 h_1)}{\partial q_2} + \frac{\partial(J_3 h_1 h_2)}{\partial q_3}\right] dq_1 dq_2 dq_3 &(69)\\
&= \frac{1}{h_1 h_2 h_3}\left[\frac{\partial(J_1 h_2 h_3)}{\partial q_1} + \frac{\partial(J_2 h_3 h_1)}{\partial q_2} + \frac{\partial(J_3 h_1 h_2)}{\partial q_3}\right] &(70)\\
J_1 &= \mathbf{J} \cdot \mathbf{e}_1, \quad J_2 = \mathbf{J} \cdot \mathbf{e}_2, \quad J_3 = \mathbf{J} \cdot \mathbf{e}_3 &(71)
\end{aligned}
$$

[1] 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

$$\mathbf{q} = (x, y, z) \tag{72}$$
$$h_1 = 1, \quad h_2 = 1, \quad h_3 = 1 \tag{73}$$
$$\mathrm{div}\mathbf{J}(x, y, z) = \frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} + \frac{\partial J_z}{\partial z} \tag{74}$$

In the cylindrical coordinates

$$\mathbf{q} = (r, \theta, z) \tag{75}$$
$$h_1 = 1, \quad h_2 = r, \quad h_3 = 1 \tag{76}$$
$$\mathrm{div}_{r,\theta,z}\mathbf{J} = \nabla_{r,\theta,z} \cdot \mathbf{J} = \frac{1}{r}\left[\frac{\partial(rJ_r)}{\partial r} + \frac{\partial J_\theta}{\partial \theta} + \frac{\partial(rJ_z)}{\partial z}\right] \tag{77}$$
$$= \frac{1}{r}\left[\frac{\partial(rJ_r)}{\partial r} + \frac{\partial J_\theta}{\partial \theta} + r\frac{\partial J_z}{\partial z}\right] \tag{78}$$

In the spherical coordinates

$$\mathbf{q} = (r, \theta, \phi) \tag{79}$$
$$h_1 = 1, \quad h_2 = r, \quad h_3 = r\sin\theta \tag{80}$$
$$\mathrm{div}_{r,\theta,\phi}\mathbf{J} = \nabla_{r,\theta,\phi} \cdot \mathbf{J} = \frac{1}{r^2\sin\theta}\left[\frac{\partial(r^2\sin\theta J_r)}{\partial r} + \frac{\partial(r\sin\theta J_\theta)}{\partial \theta} + \frac{\partial(rJ_\phi)}{\partial \phi}\right] \tag{81}$$
$$= \frac{1}{r^2\sin\theta}\left[\sin\theta\frac{\partial(r^2 J_r)}{\partial r} + r\frac{\partial(\sin\theta J_\theta)}{\partial \theta} + r\frac{\partial J_\phi}{\partial \phi}\right] \tag{82}$$
$$\tag{83}$$

3.3 Laplacian: ラプラシアン

We also get Laplacian ∇^2 when we use

$$\mathbf{J}(q_1, q_2, q_3) = \mathrm{grad}_{\mathbf{q}} f = \mathbf{e}_1\frac{1}{h_1}\frac{\partial f}{\partial q_1} + \mathbf{e}_2\frac{1}{h_2}\frac{\partial f}{\partial q_2} + \mathbf{e}_3\frac{1}{h_3}\frac{\partial f}{\partial q_3} \tag{84}$$
$$\mathrm{div}\mathbf{J}(q_1, q_2, q_3) = \nabla \cdot \mathbf{J}(q_1, q_2, q_3) = \mathrm{div}(\mathrm{grad}_{\mathbf{q}} f) = \nabla^2_{\mathbf{q}} f \tag{85}$$
$$\nabla^2_{\mathbf{q}} f = \frac{1}{h_1h_2h_3}\left[\frac{\partial}{\partial q_1}\left(\frac{h_2h_3}{h_1}\frac{\partial f}{\partial q_1}\right) + \frac{\partial}{\partial q_2}\left(\frac{h_3h_1}{h_2}\frac{\partial f}{\partial q_2}\right) + \frac{\partial}{\partial q_3}\left(\frac{h_1h_2}{h_3}\frac{\partial f}{\partial q_3}\right)\right] \tag{86}$$

The Laplacian is very important in physical chemistry.
(a) For the diffusion equation

$$\frac{\partial c}{\partial t} + \mathrm{div}\mathbf{J} = 0, \quad \mathbf{J} = -\mathrm{grad}c \tag{87}$$
$$\frac{\partial c}{\partial t} = \mathrm{div}(\mathrm{grad}c) = \nabla^2 c \tag{88}$$

(b) For the wave equation

$$\frac{\partial^2 \xi}{\partial t^2} = v^2\mathrm{div}(\mathrm{grad}\xi) = v^2\nabla^2\xi \tag{89}$$

In the cartesian coordinate

$$\mathbf{q} = (x, y, z) \tag{90}$$
$$h_1 = 1, \quad h_2 = 1, \quad h_3 = 1 \tag{91}$$
$$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2} \tag{92}$$

In the cylindrical coordinates

$$
\begin{aligned}
\mathbf{q} &= (r, \theta, z) && (93)\\
h_1 &= 1, \quad h_2 = r, \quad h_3 = 1 && (94)\\
\nabla^2_{\mathbf{q}} f &= \frac{1}{r}\left[\frac{\partial}{\partial r}\left(r\frac{\partial f}{\partial r}\right) + \frac{\partial}{\partial \theta}\left(\frac{1}{r}\frac{\partial f}{\partial \theta}\right) + \frac{\partial}{\partial z}\left(r\frac{\partial f}{\partial z}\right)\right] && (95)\\
&= \frac{1}{r}\frac{\partial f}{\partial r} + \frac{\partial^2 f}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2 f}{\partial \theta^2} + \frac{\partial^2 f}{\partial z^2} && (96)
\end{aligned}
$$

In the spherical coordinates

$$
\begin{aligned}
\mathbf{q} &= (r, \theta, \phi) && (97)\\
h_1 &= 1, \quad h_2 = r, \quad h_3 = r\sin\theta && (98)\\
\nabla^2_{\mathbf{q}} f &= \frac{1}{r^2\sin\theta}\left[\frac{\partial}{\partial r}\left(r^2\sin\theta\frac{\partial f}{\partial r}\right) + \frac{\partial}{\partial \theta}\left(\frac{r\sin\theta}{r}\frac{\partial f}{\partial \theta}\right) + \frac{\partial}{\partial \phi}\left(\frac{r}{r\sin\theta}\frac{\partial f}{\partial \phi}\right)\right] && (99)\\
&= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial f}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 f}{\partial \phi^2} && (100)\\
&= \frac{2}{r}\frac{\partial f}{\partial r} + \frac{\partial^2 f}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2 f}{\partial \theta^2} + \frac{\cos\theta}{r^2\sin\theta}\frac{\partial f}{\partial \theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 f}{\partial \phi^2} && (101)
\end{aligned}
$$