発散 (divergence), Gauss の定理, 直交曲線座標系

Masahiro Yamamoto

June 25, 2010

1 definition of divergence

今，場所に依存したベクトル場を考えよう。例えば，場所 $\mathbf{r}$ における物質の流速（単位時間，単位面積当たりの物質の移動速度ベクトル）を $\mathbf{J}(\mathbf{r})$ と置く。今，Fig.3(a) のように $\mathbf{r}$ における立方体の微少体積 $dV = dxdydz$ を考える。ベクトル $\mathbf{J}$ を各成分 x, y, z に分けて考える（Fig.3(b)）。

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

微少体積に出入りする物質量は（流速×面積）の差になり，その合計が微少体積内ので物質量（密度×体積）の時間変化になるので

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

ここで，以下の近似を使うと

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

次の関係式が得られる。

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

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

$$= \frac{\partial\rho}{\partial t} + \mathrm{div}\mathbf{J} \tag{6}$$

$$\tag{7}$$

となる。すなわち，$\mathbf{J}$ の発散 $\mathrm{div}\mathbf{J}$ は微少体積 $dV = dxdydz$ に出入りする量を表す。また Eq.(2) の左辺である微少体積に出入りする量は，Fig.3(c) において微少立方体の各面での法線単位ベクトル $\mathbf{n}$(面の外向きに方向をとる。）と $\mathbf{J}$ との内積の和になる。すなわち，

$$\begin{aligned}&[J_x(x+dx) - J_x(x)]dydz + [J_y(y+dy) - J_y(y)]dxdz + [J_z(z+dz) - J_z(z)]dxdy \\ =& \sum_{\text{six surfaces}} \mathbf{J}\cdot\mathbf{n}dS = \mathrm{div}\mathbf{J}dV\end{aligned} \tag{8}$$

Fig.3(d) にあるような一般の形状をしているものを，微少体積に分割し全ての和をとると，立方体で接している面では，$\mathbf{J}\cdot\mathbf{n}dS$ は打ち消し合い，最外表面だけが残る。すなわち，以下の Gauss の定理が成立する。

$$\sum_{\text{all } dV} \mathrm{div}\mathbf{J}dV = \sum_{\text{exterior surface}} \mathbf{J}\cdot\mathbf{n}dS \tag{9}$$

$$\int dV\mathrm{div}\mathbf{J} = \int dS\mathbf{J}\cdot\mathbf{n} \tag{10}$$

2 Coulomb の法則, 電場，ガウスの法則

ϵ の比誘電率をもつ媒体を考える。原点にある電荷 q_0 と $\mathbf{r}$ にある電荷 q の間に働く Coulomb 力 $\mathbf{F}$ は，

$$\mathbf{F} = \frac{1}{4\pi\epsilon\epsilon_0}\frac{q_0 q}{r^2}\frac{\mathbf{r}}{r} \tag{11}$$

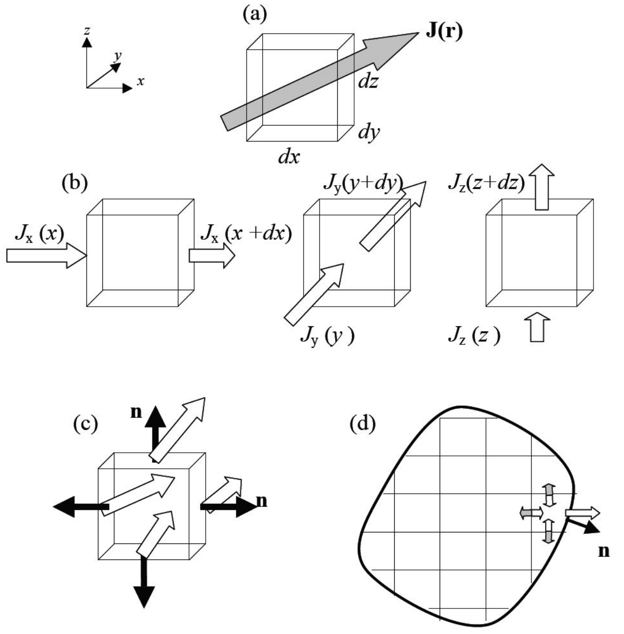

Figure 1:

で与えられる。ここで，$r = |\mathbf{r}|$ で，ϵ_0 は真空の誘電率である。 q_0 が作る電場 $\mathbf{E}$ は,

$$\mathbf{F} = q\mathbf{E} \tag{12}$$

で与えられるので,

$$\mathbf{E} = \frac{1}{4\pi\epsilon\epsilon_0}\frac{q_0}{r^2}\frac{\mathbf{r}}{r} \tag{13}$$

である。この電場ベクトルにガウスの定理を適用すると

$$\int dS\mathbf{E}\cdot\mathbf{n} = \int dV\,\mathrm{div}\mathbf{E} \tag{14}$$

電場ベクトルは球対称なので Fig.2 のような球面を考え，この球面上の面積分を考える。面積要素 dS の法線ベクトルは,

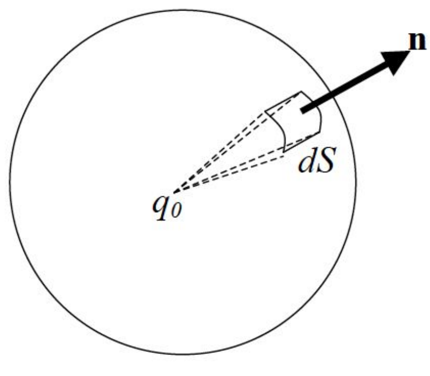

Figure 2:

$\mathbf{n} = \mathbf{r}/r$ となるので

$$\int dS\mathbf{E}\cdot\mathbf{n} \quad = \quad \int dS\frac{1}{4\pi\epsilon\epsilon_0}\frac{q_0}{r^2}\underbrace{\left(\frac{\mathbf{r}}{r}\cdot\frac{\mathbf{r}}{r}\right)}_{=1} = \frac{1}{4\pi\epsilon\epsilon_0}\frac{q_0}{r^2}\int dS = \frac{1}{4\pi\epsilon\epsilon_0}\frac{q_0}{r^2}4\pi r^2 = \frac{q_0}{\epsilon\epsilon_0} \tag{15}$$

q_0 は球体内にある電荷密度の積分量と見なせるので

$$\frac{q_0}{\epsilon\epsilon_0} \quad = \quad \frac{1}{\epsilon\epsilon_0}\int dV\rho(\mathbf{r}) \tag{16}$$

となる。従って，

$$\mathrm{div}\mathbf{E} = \frac{\rho(\mathbf{r})}{\epsilon\epsilon_0} \tag{17}$$

この式は，dV にある電荷 ρ から出る電気力線の数は $\rho/(\epsilon_0\epsilon)$ であることを意味している。ただし，界面・表面では誘電率が不連続になることが多く，電気力線の数も不連続になる。この不便さを解消するために電束を新たに定義し，その密度 $\mathbf{D} = \epsilon_0\epsilon\mathbf{E}$ で定義する。微少体積 dV からでる電束は，誘電率には依存せず電荷 ρ に比例することになり，界面での電束密度は連続につながる。上記の式は

$$\mathrm{div}\mathbf{D} = \rho(\mathbf{r}) \tag{18}$$

となり，電気二重層を考慮する場合はこの式が基本となる。

3 Divergence and Laplacian in orthogonal curvlinear coordinates

In the curvlinear coordinate

$$\mathbf{q} = \{q_1, q_2, q_3\} \tag{19}$$
$$\mathbf{q} = \{x, y, z\} \quad : \text{ Cartesian coordinates} \tag{20}$$
$$\mathbf{q} = \{r, \theta, z\} \quad : \text{ cylindircal coordinates} \tag{21}$$
$$\mathbf{q} = \{r, \theta, \phi\} \quad : \text{ spherical coordinates} \tag{22}$$

If we set

$$x = x(q_1, q_2, q_3), \quad dx = \frac{\partial x}{\partial q_1}dq_1 + \frac{\partial x}{\partial q_2}dq_2 + \frac{\partial x}{\partial q_3}dq_3 \tag{23}$$
$$y = y(q_1, q_2, q_3), \quad dy = \frac{\partial y}{\partial q_1}dq_1 + \frac{\partial y}{\partial q_2}dq_2 + \frac{\partial y}{\partial q_3}dq_3 \tag{24}$$
$$z = z(q_1, q_2, q_3), \quad dz = \frac{\partial z}{\partial q_1}dq_1 + \frac{\partial z}{\partial q_2}dq_2 + \frac{\partial z}{\partial q_3}dq_3 \tag{25}$$
$$\tag{26}$$

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

$$ds^2 = dx^2 + dy^2 + dz^2 = \sum_{i,j} g_{ij}dq_idq_j \tag{27}$$
$$g_{ij} = \frac{\partial x}{\partial q_i}\frac{\partial x}{\partial q_j} + \frac{\partial y}{\partial q_i}\frac{\partial y}{\partial q_j} + \frac{\partial z}{\partial q_i}\frac{\partial z}{\partial q_j} \tag{28}$$
$$\tag{29}$$

For orthogonal curvlinear coordinates such as cylindrical and spherical coordinates

$$g_{ij} = 0, \quad \text{for} \quad i \neq j \tag{30}$$
$$g_{ii} = \left(\frac{\partial x}{\partial q_i}\right)^2 + \left(\frac{\partial y}{\partial q_i}\right)^2 + \left(\frac{\partial z}{\partial q_i}\right)^2 \tag{31}$$
$$ds^2 = g_{11}dq_1dq_1 + g_{22}dq_2dq_2 + g_{33}dq_3dq_3 = ds_1^2 + ds_2^2 + ds_3^2 \tag{32}$$
$$ds_1 \equiv \sqrt{g_{11}}dq_1 \equiv h_1dq_1 \tag{33}$$
$$ds_2 \equiv \sqrt{g_{22}}dq_2 \equiv h_2dq_2 \tag{34}$$
$$ds_3 \equiv \sqrt{g_{33}}dq_3 \equiv h_3dq_3 \tag{35}$$

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

$$g_{11} = \frac{\partial x}{\partial r}\frac{\partial x}{\partial r} + \frac{\partial y}{\partial r}\frac{\partial y}{\partial r} + \frac{\partial z}{\partial r}\frac{\partial z}{\partial r} = \cos^2\theta + \sin^2\theta + 0 = 1, \qquad h_1 = 1 \tag{36}$$
$$g_{12} = \frac{\partial x}{\partial r}\frac{\partial x}{\partial \theta} + \frac{\partial y}{\partial r}\frac{\partial y}{\partial \theta} + \frac{\partial z}{\partial r}\frac{\partial z}{\partial \theta} = \cos\theta(-r\sin\theta) + \sin\theta(r\cos\theta) + 0 = 0$$
$$g_{13} = \frac{\partial x}{\partial r}\frac{\partial x}{\partial z} + \frac{\partial y}{\partial r}\frac{\partial y}{\partial z} + \frac{\partial z}{\partial r}\frac{\partial z}{\partial z} = 0 + 0 + 0 = 0$$
$$g_{21} = \frac{\partial x}{\partial \theta}\frac{\partial x}{\partial r} + \frac{\partial y}{\partial \theta}\frac{\partial y}{\partial r} + \frac{\partial z}{\partial \theta}\frac{\partial z}{\partial r} = (-r\sin\theta)\cos\theta + r\cos\theta\sin\theta + 0 = 0$$

$$
\begin{aligned}
g_{22} &= \frac{\partial x}{\partial \theta}\frac{\partial x}{\partial \theta} + \frac{\partial y}{\partial \theta}\frac{\partial y}{\partial \theta} + \frac{\partial z}{\partial \theta}\frac{\partial z}{\partial \theta} = (-r\sin\theta)^2 + (r\cos\theta)^2 + 0 = r^2, \qquad h_2 = r && (37)\\
g_{23} &= \frac{\partial x}{\partial \theta}\frac{\partial x}{\partial z} + \frac{\partial y}{\partial \theta}\frac{\partial y}{\partial z} + \frac{\partial z}{\partial \theta}\frac{\partial z}{\partial z} = 0 + 0 + 0 = 0\\
g_{31} &= \frac{\partial x}{\partial z}\frac{\partial x}{\partial r} + \frac{\partial y}{\partial z}\frac{\partial y}{\partial r} + \frac{\partial z}{\partial z}\frac{\partial z}{\partial r} = 0 + 0 + 0 = 0\\
g_{32} &= \frac{\partial x}{\partial z}\frac{\partial x}{\partial \theta} + \frac{\partial y}{\partial z}\frac{\partial y}{\partial \theta} + \frac{\partial z}{\partial z}\frac{\partial z}{\partial \theta} = 0 + 0 + 0 = r^2\\
g_{33} &= \frac{\partial x}{\partial z}\frac{\partial x}{\partial z} + \frac{\partial y}{\partial z}\frac{\partial y}{\partial z} + \frac{\partial z}{\partial z}\frac{\partial z}{\partial z} = 0 + 0 + 1^2 = 1, \qquad h_3 = 1 && (38)
\end{aligned}
$$

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

$$
\begin{aligned}
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 && (39)\\
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 && (40)\\
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, \qquad h_3 = r\sin\theta && (41)
\end{aligned}
$$

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

$$
\begin{aligned}
d\mathbf{r} &= h_1 dq_1 \mathbf{e}_1 + h_2 dq_2 \mathbf{e}_2 + h_3 dq_3 \mathbf{e}_3 = \sum_{i=1}^{3} h_i q_i \mathbf{e}_i && (42)\\
\mathbf{e}_i &= \frac{1}{h_i}\frac{\partial \mathbf{r}}{\partial q_i} && (43)
\end{aligned}
$$

Here we only consider orthogonal curvlinear 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

$$
\frac{\partial f}{\partial s_i} = \frac{1}{h_i}\frac{\partial f}{\partial q_i} \qquad (44)
$$

(45)

Then the gradient in the orthogonal curvlinear coordinates

$$
\begin{aligned}
\mathrm{grad}_{\mathbf{q}} f &= \nabla_{\mathbf{q}} f = \mathbf{e}_1\frac{\partial f}{\partial s_1} + \mathbf{e}_2\frac{\partial f}{\partial s_2} + \mathbf{e}_3\frac{\partial f}{\partial s_1} && (46)\\
&= \mathbf{e}_1\frac{1}{h_1}\frac{\partial f}{\partial q_1} + \mathbf{e}_2\frac{1}{h_2}\frac{\partial f}{\partial q_2} + \mathbf{e}_3\frac{1}{h_3}\frac{\partial f}{\partial q_3} && (47)\\
\mathbf{e}_1 &= \frac{1}{h_1}\frac{\partial \mathbf{r}}{\partial q_1}, \quad \mathbf{e}_2 = \frac{1}{h_2}\frac{\partial \mathbf{r}}{\partial q_2}, \quad \mathbf{e}_3 = \frac{1}{h_3}\frac{\partial \mathbf{r}}{\partial q_3} && (48)
\end{aligned}
$$

In the cartesian coordinates,

$$
\begin{aligned}
\mathbf{q} &= \{x, y, z\}, \quad \mathbf{r} = (x, y, z) && (49)\\
h_1 &= 1, \quad \frac{\partial \mathbf{r}}{\partial x} = (1,0,0), \quad \mathbf{e}_1 = (1,0,0) = \mathbf{i} && (50)\\
h_2 &= 1, \quad \frac{\partial \mathbf{r}}{\partial y} = (0,1,0), \quad \mathbf{e}_1 = (0,1,0) = \mathbf{j} && (51)
\end{aligned}
$$

$$h_3 = 1, \quad \frac{\partial \mathbf{r}}{\partial z} = (0,0,1), \quad \mathbf{e}_1 = (0,0,1) = \mathbf{k} \tag{52}$$

$$\mathrm{grad} f = \nabla f = \left(\mathbf{i}\frac{\partial}{\partial x} + \mathbf{j}\frac{\partial}{\partial y} + \mathbf{k}\frac{\partial}{\partial z}\right) f \tag{53}$$

In the cylindrical coordinates,

$$\mathbf{q} = \{r, \theta, z\}, \quad \mathbf{r} = (x, y, z) = (r\cos\theta, r\sin\theta, z) \tag{54}$$

$$\frac{\partial \mathbf{r}}{\partial r} = (\cos\theta, \sin\theta, 0), \quad h_1 = \left|\frac{\partial \mathbf{r}}{\partial r}\right| = \sqrt{\cos^2\theta + \sin^2\theta} = 1, \quad \mathbf{e}_1 = (\cos\theta, \sin\theta, 0) \tag{55}$$

$$\frac{\partial \mathbf{r}}{\partial \theta} = (-r\sin\theta, r\cos\theta, 0), \quad h_2 = \left|\frac{\partial \mathbf{r}}{\partial \theta}\right| = r\sqrt{\cos^2\theta + \sin^2\theta} = r, \quad \mathbf{e}_2 = (-\sin\theta, \cos\theta, 0) \tag{56}$$

$$\frac{\partial \mathbf{r}}{\partial z} = (0,0,1), \quad h_3 = \left|\frac{\partial \mathbf{r}}{\partial z}\right| = 1, \quad \mathbf{e}_3 = (0,0,1) \tag{57}$$

$$\mathrm{grad}_{r,\theta,z} f = \nabla_{r,\theta,z} = \left(\mathbf{e}_1\frac{\partial}{\partial r} + \mathbf{e}_2\frac{1}{r}\frac{\partial}{\partial \theta} + \mathbf{e}_3\frac{\partial}{\partial z}\right) f \tag{58}$$

In the spherical coordinates,

$$\mathbf{q} = \{r, \theta, \phi\}, \quad \mathbf{r} = (x, y, z) = (r\sin\theta\cos\phi, r\sin\theta\sin\phi, r\cos\theta) \tag{59}$$

$$\frac{\partial \mathbf{r}}{\partial r} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta), \quad h_1 = \left|\frac{\partial \mathbf{r}}{\partial r}\right| = \sqrt{\sin^2\theta(\cos^2\phi + \sin^2\phi) + \cos^2\theta} = 1,$$
$$\mathbf{e}_1 = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta) \tag{60}$$

$$\frac{\partial \mathbf{r}}{\partial \theta} = (r\cos\theta\cos\phi, r\cos\theta\sin\phi, -r\sin\theta), \quad h_2 = \left|\frac{\partial \mathbf{r}}{\partial \theta}\right| = r\sqrt{\cos^2\theta(\cos^2\phi + \sin^2\phi) + \sin^2\theta} = r$$
$$\mathbf{e}_2 = (\cos\theta\cos\phi, \cos\theta\sin\phi, -\sin\theta) \tag{61}$$

$$\frac{\partial \mathbf{r}}{\partial \phi} = (-r\sin\theta\sin\phi, r\sin\theta\cos\phi, 0), \quad h_3 = \left|\frac{\partial \mathbf{r}}{\partial \phi}\right| = r\sqrt{\sin^2\theta\sin^2\phi + \sin^2\theta\cos^2\phi} = r\sin\theta,$$
$$\mathbf{e}_3 = (-\sin\phi, \cos\phi, 0) \tag{62}$$

$$\mathrm{grad}_{r,\theta,\phi} f = \nabla_{r,\theta,\phi} = \left(\mathbf{e}_1\frac{\partial}{\partial r} + \mathbf{e}_2\frac{1}{r}\frac{\partial}{\partial \theta} + \mathbf{e}_3\frac{1}{r\sin\theta}\frac{\partial}{\partial \phi}\right) f \tag{63}$$

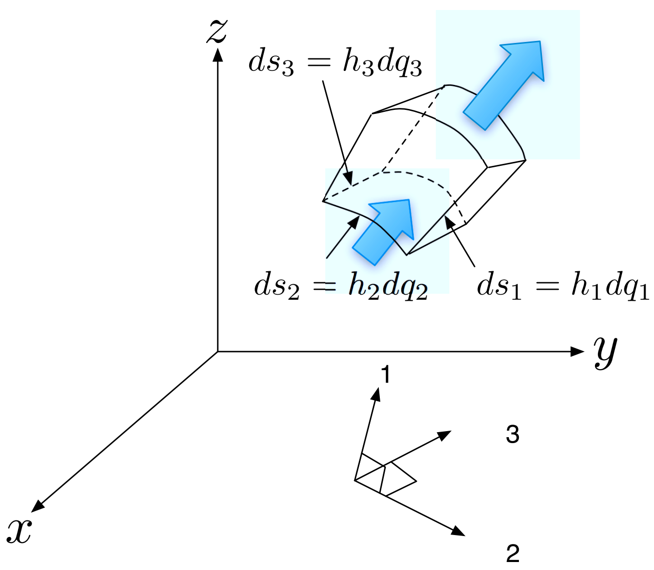

Figure 3:

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]

$$\left[J_1 ds_2 ds_3 + \frac{\partial (J_1 ds_2 ds_3)}{\partial q_1} dq_1\right] - J_1 ds_2 ds_3 = \frac{\partial (J_1 h_2 h_3)}{\partial q_1} dq_1 dq_2 dq_3 \tag{64}$$

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

$$\left[\frac{\partial(J_1 h_2 h_3)}{\partial q_1} + \frac{\partial(J_2 h_3 h_1)}{\partial q_2} + \frac{\partial(J_3 h_1 h_2)}{\partial q_3}\right] dq_1 dq_2 dq_3 \tag{65}$$

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

$$\begin{aligned}
\mathrm{div}\mathbf{J}(q_1,q_2,q_3) &= \nabla\cdot\mathbf{J}(q_1,q_2,q_3) = \frac{1}{ds_1 ds_2 ds_3}\left[\frac{\partial(J_1 h_2 h_3)}{\partial q_1} + \frac{\partial(J_2 h_3 h_1)}{\partial q_2} + \frac{\partial(J_3 h_1 h_2)}{\partial q_3}\right] dq_1 dq_2 dq_3 && (66)\\
&= \frac{1}{h_1 h_2 h_3}\left[\frac{\partial(J_1 h_2 h_3)}{\partial q_1} + \frac{\partial(J_2 h_3 h_1)}{\partial q_2} + \frac{\partial(J_3 h_1 h_2)}{\partial q_3}\right] && (67)\\
J_1 &= \mathbf{J}\cdot\mathbf{e}_1, \quad J_2 = \mathbf{J}\cdot\mathbf{e}_2, \quad J_3 = \mathbf{J}\cdot\mathbf{e}_3 && (68)
\end{aligned}$$

We also get Laplacian ∇^2 when we use

$$\begin{aligned}
\mathbf{J}(q_1,q_2,q_3) &= \mathrm{grad}_{\mathbf{q}} f = \mathbf{e}_1 \frac{1}{h_1}\frac{\partial f}{\partial q_1} + \mathbf{e}_2 \frac{1}{h_2}\frac{\partial f}{\partial q_2} + \mathbf{e}_3 \frac{1}{h_3}\frac{\partial f}{\partial q_3} && (69)\\
\mathrm{div}\mathbf{J}(q_1,q_2,q_3) &= \nabla\cdot\mathbf{J}(q_1,q_2,q_3) = \mathrm{div}(\mathrm{grad}_{\mathbf{q}} f) = \nabla^2_{\mathbf{q}} f && (70)\\
\nabla^2_{\mathbf{q}} f &= \frac{1}{h_1 h_2 h_3}\left[\frac{\partial}{\partial q_1}\left(\frac{h_2 h_3}{h_1}\frac{\partial f}{\partial q_1}\right) + \frac{\partial}{\partial q_2}\left(\frac{h_3 h_1}{h_2}\frac{\partial f}{\partial q_2}\right) + \frac{\partial}{\partial q_3}\left(\frac{h_1 h_2}{h_3}\frac{\partial f}{\partial q_3}\right)\right] && (71)
\end{aligned}$$

3.1 Laplacian in P. Chem.

The Laplacian is very important in physical chemistry.

(I) For the diffusion equation

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

(II) For the wave equation

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

In the cylindrical coordinates

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

In the spherical coordinates

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