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

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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 \( dV = dx dy dz \). The \( x, y, z \)-component of the vector \( \mathbf{J} \) (Fig.1(b)) can be defined as

\[
\mathbf{J} = J_x \mathbf{i} + J_y \mathbf{j} + J_z \mathbf{k}
\]  

(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.

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

(2)

If we use the following approximation

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

(3)

we obtained

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

(4)

\[
0 = \frac{\partial \rho}{\partial t} + \frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} + \frac{\partial J_z}{\partial z} = \frac{\partial \rho}{\partial t} + \left(\mathbf{i} \frac{\partial}{\partial x} + \mathbf{j} \frac{\partial}{\partial y} + \mathbf{k} \frac{\partial}{\partial z}\right) \cdot (J_x \mathbf{i} + J_y \mathbf{j} + J_z \mathbf{k}) = \frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = \frac{\partial \rho}{\partial t} + \text{div}\mathbf{J}
\]  

(5)

(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 outward direction from the plane.

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

(7)

For the case of general 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!

$$\sum_{all \, dV} \text{div} \mathbf{J} dV = \sum_{\text{exterior surface}} \mathbf{J} \cdot \mathbf{n} dS$$  \hspace{1cm} (8)

$$\int dV \text{div} \mathbf{J} = \int dS \mathbf{J} \cdot \mathbf{n}$$  \hspace{1cm} (9)

![Diagram of Gauss law](image)

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

$$\mathbf{F} = \frac{1}{4\pi \epsilon_0} \frac{q_0 q}{r^2} \mathbf{r}$$  \hspace{1cm} (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

$$\mathbf{F} = q \mathbf{E}$$  \hspace{1cm} (11)

then we have

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

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

$$\int dS \mathbf{E} \cdot \mathbf{n} = \int dV \text{div} \mathbf{E}$$  \hspace{1cm} (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

$$\int dS \mathbf{E} \cdot \mathbf{n} = \int dS \frac{1}{4\pi \epsilon_0} \frac{q_0}{r^2} \left( \frac{\mathbf{r}}{r} \cdot \frac{\mathbf{r}}{r} \right) = \frac{1}{4\pi \epsilon_0} \frac{q_0}{r^2} \int dS = \frac{1}{4\pi \epsilon_0} \frac{q_0}{r^2} 4\pi r^2 = \frac{q_0}{\epsilon_0}$$  \hspace{1cm} (14)
\( q_0 \) is the integral of the charge density inside the sphere

\[
\frac{q_0}{\epsilon \epsilon_0} = \frac{1}{\epsilon \epsilon_0} \int dV \rho(r)
\]

(15)

Therefore,

\[
\text{div} E = \frac{\rho(r)}{\epsilon \epsilon_0}
\]

(16)

This equation means that the number of the lines of electric force from the charge \( \rho \) in \( dV \) is equal to \( \rho/(\epsilon \epsilon_0) \). But in general the dielectric constant may become discontinuous at the surface/interface 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 continuous at the surface/interface. The Gauss law becomes

\[
\text{div} \mathbf{D} = \rho(r)
\]

(17)

and this is the basic equation of the electric 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

\[
\mathbf{q} = \{ q_1, q_2, q_3 \}
\]

(18)

\[
\mathbf{q} = \{ x, y, z \} : \text{Cartesian coordinates}
\]

(19)

\[
\mathbf{q} = \{ r, \theta, z \} : \text{cylindrical coordinates}
\]

(20)

\[
\mathbf{q} = \{ r, \theta, \phi \} : \text{spherical coordinates}
\]

(21)

If we set

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

(22)

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

(23)

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

(24)
The distance $ds$ between the two infinitesimal points is given by "metric"

$$ds^2 = dx^2 + dy^2 + dz^2 = \sum_{i,j} g_{ij} dq_i dq_j$$  \hspace{1cm} (26)

$$g_{ij} = \frac{\partial x}{\partial q_i} \frac{\partial x}{\partial q_j} + \frac{\partial y}{\partial q_i} \frac{\partial y}{\partial q_j} + \frac{\partial z}{\partial q_i} \frac{\partial z}{\partial q_j}$$  \hspace{1cm} (27)

For orthogonal curvilinear coordinates such as cylindrical and spherical coordinates

$$g_{ij} = 0, \text{ for } i \neq j$$  \hspace{1cm} (29)

$$g_{ii} = \left(\frac{\partial x}{\partial q_i}\right)^2 + \left(\frac{\partial y}{\partial q_i}\right)^2 + \left(\frac{\partial z}{\partial q_i}\right)^2$$  \hspace{1cm} (30)

$$ds^2 = g_{11} dq_1 dq_1 + g_{22} dq_2 dq_2 + g_{33} dq_3 dq_3 = ds_1^2 + ds_2^2 + ds_3^2$$  \hspace{1cm} (31)

$$ds_1 \equiv \sqrt{g_{11}} dq_1 \equiv h_1 dq_1$$  \hspace{1cm} (32)

$$ds_2 \equiv \sqrt{g_{22}} dq_2 \equiv h_2 dq_2$$  \hspace{1cm} (33)

$$ds_3 \equiv \sqrt{g_{33}} dq_3 \equiv h_3 dq_3$$  \hspace{1cm} (34)

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

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

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

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

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

$$g_{22} = \frac{\partial x}{\partial \theta} \frac{\partial x}{\partial \theta} + \frac{\partial y}{\partial \theta} \frac{\partial y}{\partial \theta} + \frac{\partial z}{\partial \theta} \frac{\partial z}{\partial \theta} = (-r \sin \theta)^2 + (r \cos \theta)^2 + 0 = r^2, \hspace{1cm} h_2 = r$$  \hspace{1cm} (36)

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

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

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

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

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

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

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

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

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

$$g_{22} = \frac{\partial x}{\partial \theta} \frac{\partial x}{\partial \theta} + \frac{\partial y}{\partial \theta} \frac{\partial y}{\partial \theta} + \frac{\partial z}{\partial \theta} \frac{\partial z}{\partial \theta} = (r \cos \theta \cos \phi)^2 + (r \cos \theta \sin \phi)^2 + (-r \sin \theta)^2 = r^2, \hspace{1cm} h_2 = r$$  \hspace{1cm} (39)

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

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

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

$$g_{33} = \frac{\partial x}{\partial \phi} \frac{\partial x}{\partial \phi} + \frac{\partial y}{\partial \phi} \frac{\partial y}{\partial \phi} + \frac{\partial z}{\partial \phi} \frac{\partial z}{\partial \phi} = 0$$
The differential distance vector \(dr\) and the unit vector \(e_i\) may be given

\[
dr = h_1 dq_1 e_1 + h_2 dq_2 e_2 + h_3 dq_3 e_3 = \sum_{i=1}^{3} h_i q_i e_i
\]

(41)

\[
e_i = \frac{1}{h_i} \frac{\partial r}{\partial q_i}
\]

(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

\[
\frac{\partial f}{\partial s_i} = \frac{1}{h_i} \frac{\partial f}{\partial q_i}
\]

(43)

Then the gradient in the orthogonal curvilinear coordinates

\[
\text{grad}_q f = \nabla_q f = e_1 \frac{\partial f}{\partial s_1} + e_2 \frac{\partial f}{\partial s_2} + e_3 \frac{\partial f}{\partial s_3}
\]

(45)

\[
e_1 = \frac{1}{h_1} \frac{\partial r}{\partial q_1}, \quad e_2 = \frac{1}{h_2} \frac{\partial r}{\partial q_2}, \quad e_3 = \frac{1}{h_3} \frac{\partial r}{\partial q_3}
\]

(47)

In the cartesian coordinates,

\[
q = \{x, y, z\}, \quad r = (x, y, z)
\]

(48)

\[
h_1 = 1, \quad \frac{\partial r}{\partial x} = (1, 0, 0), \quad e_1 = (1, 0, 0) = i
\]

(49)

\[
h_2 = 1, \quad \frac{\partial r}{\partial y} = (0, 1, 0), \quad e_1 = (0, 1, 0) = j
\]

(50)

\[
h_3 = 1, \quad \frac{\partial r}{\partial z} = (0, 0, 1), \quad e_1 = (0, 0, 1) = k
\]

(51)

\[
e_i \cdot e_j = \delta_{i,j}, \quad \delta_{i,j} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}
\]

(52)

\[
e_i \times e_j = \epsilon_{i,j,k} e_k, \quad \epsilon_{i,j,k} = \begin{cases} 1, & (i, j, k) = (1, 2, 3), (2, 3, 1), (3, 1, 2) \\ -1, & (i, j, k) = (1, 3, 2), (2, 1, 3), (3, 2, 1) \\ 0, & \text{otherwise} \end{cases}
\]

(53)

\[
\text{grad}_f = \nabla f = \left( \frac{\partial}{\partial x} + j \frac{\partial}{\partial y} + k \frac{\partial}{\partial z} \right) f
\]

(54)

In the cylindrical coordinates,

\[
q = \{r, \theta, z\}, \quad r = (x, y, z) = (r \cos \theta, r \sin \theta, z)
\]

(55)

\[
\frac{\partial r}{\partial r} = (\cos \theta, \sin \theta, 0), \quad h_1 = \left| \frac{\partial r}{\partial r} \right| = \sqrt{\cos^2 \theta + \sin^2 \theta} = 1, \quad e_1 = (\cos \theta, \sin \theta, 0)
\]

(56)

\[
\frac{\partial r}{\partial \theta} = (-r \sin \theta, r \cos \theta, 0), \quad h_2 = \left| \frac{\partial r}{\partial \theta} \right| = r \sqrt{\cos^2 \theta + \sin^2 \theta} = r, \quad e_2 = (-\sin \theta, \cos \theta, 0)
\]

(57)

\[
\frac{\partial r}{\partial z} = (0, 0, 1), \quad h_3 = \left| \frac{\partial r}{\partial z} \right| = 1, \quad e_3 = (0, 0, 1)
\]

(58)

\[
e_i \cdot e_j = \delta_{i,j}, \quad e_i \times e_j = \epsilon_{i,j,k} e_k
\]

(59)

\[
\text{grad}_{r,\theta,z} f = \nabla_{r,\theta,z} f = \left( e_1 \frac{\partial}{\partial r} + e_2 \frac{1}{r} \frac{\partial}{\partial \theta} + e_3 \frac{\partial}{\partial z} \right) f
\]

(60)
In the spherical coordinates,

\[
\begin{align*}
\mathbf{q} &= \{r, \theta, \phi\}, \quad \mathbf{r} = (x, y, z) = (r \sin \theta \cos \phi, r \sin \theta \sin \phi, r \cos \theta) \\
\frac{\partial \mathbf{r}}{\partial r} &= (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta), \quad h_1 = \left| \frac{\partial \mathbf{r}}{\partial r} \right| = \sqrt{\sin^2 \theta (\cos^2 \phi + \sin^2 \phi) + \cos^2 \theta} = 1, \\
\mathbf{e}_1 &= (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta) \\
\frac{\partial \mathbf{r}}{\partial \theta} &= (r \cos \theta \cos \phi, r \cos \theta \sin \phi, -r \sin \theta), \quad h_2 = \left| \frac{\partial \mathbf{r}}{\partial \theta} \right| = r \sqrt{\cos^2 \theta (\cos^2 \phi + \sin^2 \phi) + \sin^2 \theta} = r \\
\mathbf{e}_2 &= (\cos \theta \cos \phi, \cos \theta \sin \phi, -\sin \theta) \\
\frac{\partial \mathbf{r}}{\partial \phi} &= (-r \sin \theta \sin \phi, r \sin \theta \cos \phi, 0), \quad h_3 = \left| \frac{\partial \mathbf{r}}{\partial \phi} \right| = r \sqrt{\sin^2 \theta \sin^2 \phi + \sin^2 \theta \cos^2 \phi} = r \sin \theta, \\
\mathbf{e}_3 &= (-\sin \phi, \cos \phi, 0) \\
\mathbf{e}_i \cdot \mathbf{e}_j &= \delta_{i,j}, \quad \mathbf{e}_i \times \mathbf{e}_j = \epsilon_{i,j,k} \mathbf{e}_k \\
\text{grad}_{r,\theta,\phi} \mathbf{f} &= \nabla_{r,\theta,\phi} \mathbf{f} = \left( \mathbf{e}_1 \frac{\partial}{\partial r} + \mathbf{e}_2 \frac{1}{r} \frac{\partial}{\partial \theta} + \mathbf{e}_3 \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \right) \mathbf{f}.
\end{align*}
\]

3.2 Divergence: 発散

\[ ds_3 = h_3 dq_3 \]
\[ ds_2 = h_2 dq_2 \]
\[ ds_1 = h_1 dq_1 \]

![Figure 3:](image)

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 \( q_1 \)

\[
\begin{align*}
J_1 ds_2 ds_3 + \frac{\partial (J_1 ds_2 ds_3)}{\partial q_1} dq_1 &= J_1 ds_2 ds_3 = \frac{\partial (J_1 h_2 h_3)}{\partial q_1} dq_1 dq_2 dq_3
\end{align*}
\]

In the same way we have the total amount for the volume element \( ds_1 ds_2 ds_3 \)

\[
\begin{align*}
\left[ \frac{\partial (J_1 h_2 h_3)}{\partial q_1} + \frac{\partial (J_2 h_3 h_1)}{\partial q_2} + \frac{\partial (J_3 h_1 h_2)}{\partial q_3} \right] dq_1 dq_2 dq_3
\end{align*}
\]

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

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

\[
J_1 = \mathbf{J} \cdot \mathbf{e}_1, \quad J_2 = \mathbf{J} \cdot \mathbf{e}_2, \quad J_3 = \mathbf{J} \cdot \mathbf{e}_3
\]

\[\text{1 The expansion may be done by } s_i \text{ but the differentiation should be done by } q_i. \text{ So the approximation is used here.}\]
In the cartesian coordinate

\[ \mathbf{q} = (x, y, z) \]  
\[ h_1 = 1, \quad h_2 = 1, \quad h_3 = 1 \]  
\[ \text{div} \mathbf{J}(x, y, z) = \frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} + \frac{\partial J_z}{\partial z} \]  

In the cylindrical coordinates

\[ \mathbf{q} = (r, \theta, z) \]  
\[ h_1 = 1, \quad h_2 = r, \quad h_3 = 1 \]  
\[ \text{div}_{r,\theta,z} \mathbf{J} = \nabla_{r,\theta,z} \cdot \mathbf{J} = \frac{1}{r} \left[ \frac{\partial (r J_r)}{\partial r} + \frac{\partial J_{\theta}}{\partial \theta} + \frac{\partial (r J_z)}{\partial z} \right] \]  
\[ = \frac{1}{r} \left[ \frac{\partial (r J_r)}{\partial r} + \frac{\partial J_{\theta}}{\partial \theta} + r \frac{\partial J_z}{\partial z} \right] \]  

In the spherical coordinates

\[ \mathbf{q} = (r, \theta, \phi) \]  
\[ h_1 = 1, \quad h_2 = r, \quad h_3 = r \sin \theta \]  
\[ \text{div}_{r,\theta,\phi} \mathbf{J} = \nabla_{r,\theta,\phi} \cdot \mathbf{J} = \frac{1}{r^2 \sin \theta} \left[ \frac{\partial (r^2 \sin \theta J_r)}{\partial r} + \frac{\partial (r \sin \theta J_\theta)}{\partial \theta} + \frac{\partial (r J_\phi)}{\partial \phi} \right] \]  
\[ = \frac{1}{r^2 \sin \theta} \left[ \sin \theta \frac{\partial (r^2 J_r)}{\partial r} + r \frac{\partial (r \sin \theta J_\theta)}{\partial \theta} + r \frac{\partial J_\phi}{\partial \phi} \right] \]  

3.3 Laplacian: ラプラシアン

We also get Laplacian \( \nabla^2 \) when we use

\[ \mathbf{J}(q_1, q_2, q_3) = \text{grad}_q f = e_1 \frac{1}{h_1} \frac{\partial f}{\partial q_1} + e_2 \frac{1}{h_2} \frac{\partial f}{\partial q_2} + e_3 \frac{1}{h_3} \frac{\partial f}{\partial q_3} \]  
\[ \text{div} \mathbf{J}(q_1, q_2, q_3) = \nabla \cdot \mathbf{J}(q_1, q_2, q_3) = \text{div} (\text{grad}_q f) = \nabla^2 f \]  
\[ \nabla^2 f = \frac{1}{h_1 h_2 h_3} \left[ \frac{\partial}{\partial q_1} \left( h_2 h_3 \frac{\partial f}{\partial q_1} \right) + \frac{\partial}{\partial q_2} \left( h_3 h_1 \frac{\partial f}{\partial q_2} \right) + \frac{\partial}{\partial q_3} \left( h_1 h_2 \frac{\partial f}{\partial q_3} \right) \right] \]  

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

\[ \frac{\partial c}{\partial t} + \text{div} \mathbf{J} = 0, \quad \mathbf{J} = -\text{grad} c \]  
\[ \frac{\partial c}{\partial t} = \text{div} (\text{grad} c) = \nabla^2 c \]  

(b) 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 cartesian coordinate

\[ \mathbf{q} = (x, y, z) \]  
\[ h_1 = 1, \quad h_2 = 1, \quad h_3 = 1 \]  
\[ \nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2} \]
In the cylindrical coordinates

\[ q = (r, \theta, z) \]  
\[ h_1 = 1, \quad h_2 = r, \quad h_3 = 1 \]  
\[ \nabla_q^2 f = \frac{1}{r} \left[ \frac{\partial}{\partial r} \left( r \frac{\partial f}{\partial r} \right) + \frac{\partial}{\partial \theta} \left( \frac{1}{r} \frac{\partial f}{\partial \theta} \right) + \frac{\partial}{\partial z} \left( \frac{r}{\partial z} \right) \right] \]

\[ = \frac{1}{r} \frac{\partial f}{\partial r} + \frac{\partial^2 f}{\partial r^2} + \frac{1}{r^2} \frac{\partial^2 f}{\partial \theta^2} + \frac{\partial^2 f}{\partial z^2} \]  

In the spherical coordinates

\[ q = (r, \theta, \phi) \]  
\[ h_1 = 1, \quad h_2 = r, \quad h_3 = r \sin \theta \]  
\[ \nabla_q^2 f = \frac{1}{r^2 \sin \theta} \left[ \frac{\partial}{\partial r} \left( r^2 \sin \theta \frac{\partial f}{\partial r} \right) + \frac{\partial}{\partial \theta} \left( \frac{r \sin \theta \partial f}{r} \right) + \frac{\partial}{\partial \phi} \left( \frac{r}{\sin \theta \partial \phi} \right) \right] \]

\[ = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial f}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( r \sin \theta \frac{\partial f}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 f}{\partial \phi^2} \]

\[ = \frac{2}{r} \frac{\partial f}{\partial r} + \frac{\partial^2 f}{\partial r^2} + \frac{1}{r^2} \frac{\partial^2 f}{\partial \theta^2} + \frac{\cos \theta}{r^2 \sin \theta} \frac{\partial f}{\partial \theta} + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 f}{\partial \phi^2} \]