## **Mathematics for Biochemistry**

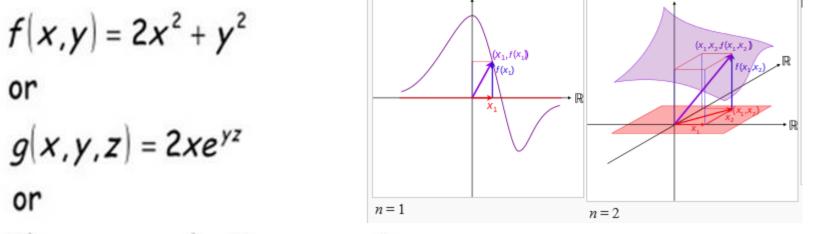
# LECTURE 13

## Functions of more variables 1

## Content:

- basic definitions and properties
- partial and total differentiation
- differential operators

Previously we have studied functions of one variable, y = f(x) in which x was the independent variable and y was the dependent variable. We are going to expand the idea of functions to include functions with more than one independent variable. For example, consider the functions below:



$$h(x_1, x_2, x_3, x_4) = 2x_1 - x_2 + 4x_3 + x_4$$

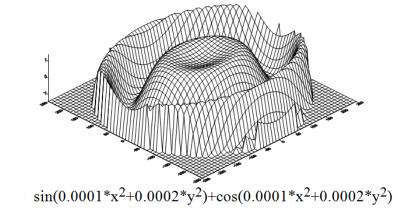
In more rigorous mathematical language:

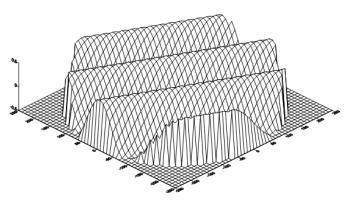
 $z: \mathbb{R}^2 \to \mathbb{R}$ z(x, y) = ax + by

where *a* and *b* are real non-zero constants

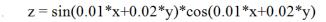
$$z: \mathbb{R}^p \to \mathbb{R}$$
  
$$z(x_1, x_2, \dots, x_p) = a_1 x_1 + a_2 x_2 + \dots + a_p x_p$$

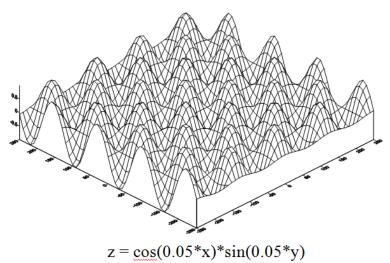
for p non-zero real constants  $a_1, a_2, ..., a_p$ 

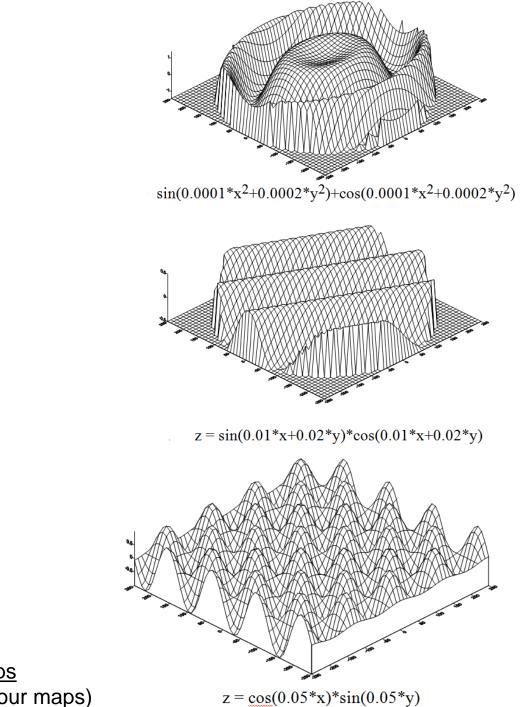


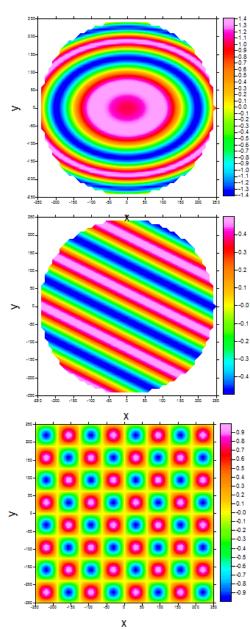


examples of graphs for f = f(x, y)

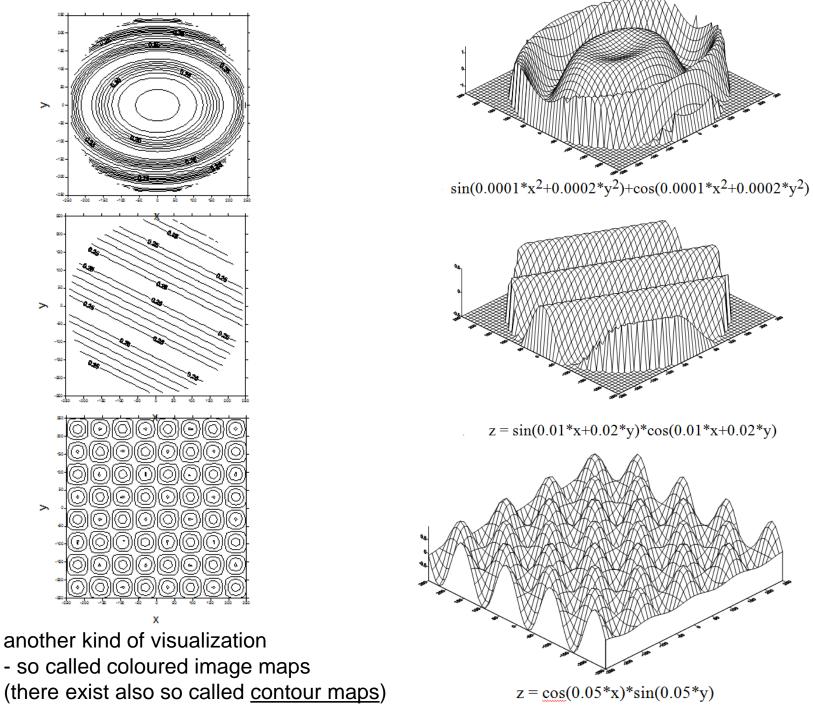








another kind of visualization - so called <u>coloured image maps</u> (there exist also so called contour maps)

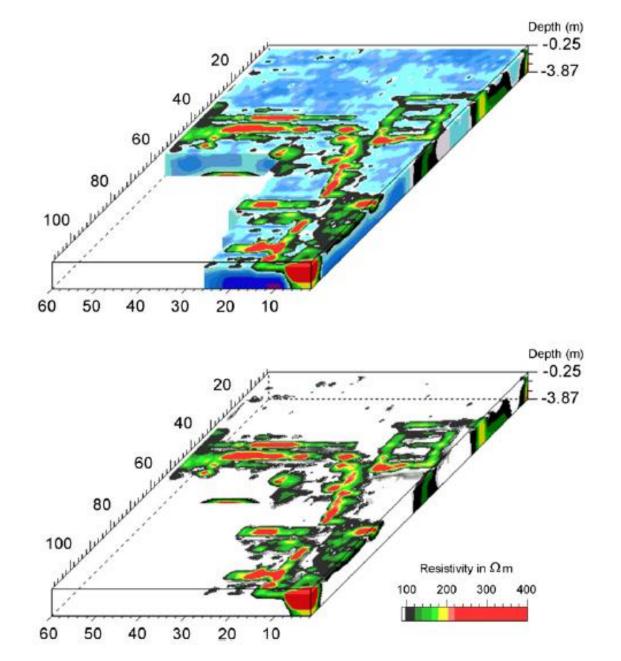


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z = cos(0.05\*x)\*sin(0.05\*y)



functions f = f(x, y, z) are often visualized in form of voxel maps

Functions of several variables are used in science for the description of various fields (physical fields, fields of properties ...).

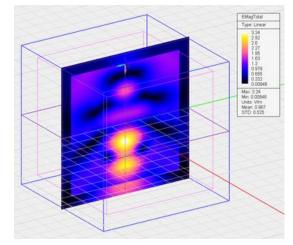
### scalar fields:

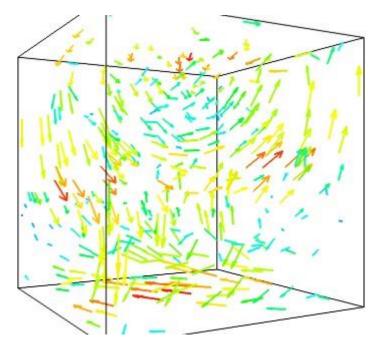
e.g. temperature, density, concentration, electric charge, ... t(x,y,z),  $\rho(x,y,z)$ , U(x,y,z),...

and also vector fields:

e.g. electrical intensity, fluid velocity, gravitational acceleration,...

$$\vec{A} = \mathbf{A} = \begin{bmatrix} A_x, A_y, A_z \end{bmatrix}$$
$$A_x = A_x (x, y, z)$$
$$A_y = A_y (x, y, z)$$
$$A_z = A_z (x, y, z)$$





Many properties are identical with the case of a function with one variable.

## Limits and Continuity

 We say that a function f(x, y) has limit L as (x, y) approaches a point (a, b) and we write

$$\lim_{(x,y)\to(a,b)}f(x,y)=L$$

if we can make the values of f(x, y) as close to L as we like by taking the point (x, y) sufficiently close to the point (a, b), but not equal to (a, b).

• We write also  $f(x, y) \rightarrow L$  as  $(x, y) \rightarrow (a, b)$  and

 $\lim_{x \to a, y \to b} f(x, y) = L$ 

Many properties are identical with the case of a function with one variable.

With the continuity is connected also the so called distance function d:

$$d(\mathbf{x}, \mathbf{y}) = d(x_1, \dots, x_n, y_1, \dots, y_n) = \sqrt{(x_1 - y_1)^2 + \dots + (x_n - y_n)^2}$$

Some properties are new (compared with a function with one variable).

#### Symmetry:

A <u>symmetric function</u> is a function f is unchanged when two variables  $x_i$  and  $x_j$  are interchanged:

$$f(\ldots, x_i, \ldots, x_j, \ldots) = f(\ldots, x_j, \ldots, x_i, \ldots)$$

where *i* and *j* are each one of 1, 2, ..., *n*.

For example:

$$f(x, y, z, t) = t^{2} - x^{2} - y^{2} - z^{2}$$

is symmetric in *x*, *y*, *z* since interchanging any pair of *x*, *y*, *z* leaves *f* unchanged, but is not symmetric in all of *x*, *y*, *z*, *t*, since interchanging *t* with *x* or *y* or *z* is a different function.

## Content:

- basic definitions and properties
- partial and total differentiation
- differential operators

Some properties are new (compared with a function with one variable).

### **Partial derivatives:**

In the case of functions of several variables, we recognize:

- a) total derivative (all variables can vary and derivatives with respect to all variables are involved)
- b) <u>partial derivative</u> (it is a derivative with respect to one of the variables with the others held constant)

$$f'_x, f_x, \partial_x f, \frac{\partial}{\partial x} f, \text{ or } \frac{\partial f}{\partial x}$$

Example, function  $f = x^2 + xy + y^2$ :

$$\frac{\partial f}{\partial x} = \frac{\partial}{\partial x} \left( x^2 + xy + y^2 \right) = 2x + y + 0 = 2x + y$$
$$\frac{\partial f}{\partial y} = \frac{\partial}{\partial y} \left( x^2 + xy + y^2 \right) = 0 + x + 2y = x + 2y$$

another tool is given in the next slide:

#### **Partial derivatives:**

For the beginner it is helpful to imagine instead of a variable (e.g. *y*) for a moment a constant (e.g. *b*).

#### Example 1

Let  $f(x,y)=y^3x^2.$  Calculate  $\frac{\partial f}{\partial x}\left(x,y\right).$ 

**Solution**: To calculate  $\frac{\partial f}{\partial x}(x, y)$ , we simply view y as being a fixed number and calculate the ordinary derivative with respect to x. The first time you do this, it might be easiest to set y = b, where b is a constant, to remind you that you should treat y as though it were number rather than a variable. Then, the partial derivative  $\frac{\partial f}{\partial x}(x, y)$  is the same as the ordinary derivative of the function  $g(x) = b^3 x^2$ . Using the rules for ordinary differentiation, we know that

$$\frac{\mathrm{d}g}{\mathrm{d}x}\left(x\right) = 2b^3x$$

Now, we remember that b = y and substitute y back in to conclude that

$$\frac{\partial f}{\partial x}\left(x,y\right) = 2y^3x.$$

## **Partial derivatives – few examples:**

Some properties are new (compared with a function with one variable).

## **Total derivative (differential):**

In the case of functions of several variables, we recognize:

- a) total derivative (all variables can vary and derivatives with respect to all variables are involved)
- b) partial derivative (it is a derivative with respect to one of the variables with the others held constant)

For a function z = f(x, y, ..., u) the total differential is defined as

$$dz = \frac{\partial z}{\partial x}dx + \frac{\partial z}{\partial y}dy + \dots + \frac{\partial z}{\partial u}du.$$

Example, function  $f = x^2 + xy + y^2$ :

$$df = \frac{\partial}{\partial x} \left( x^2 + xy + y^2 \right) dx + \frac{\partial}{\partial y} \left( x^2 + xy + y^2 \right) dy = \left( 2x + y \right) dx + \left( 2y + x \right) dy$$

There exist few special operations, which use partial derivatives and express properties of analyzed functions of several variables – so called **differential operators**:

- gradient (grad)
- divergence (div)
- rotation (rot)
- Laplacian operator (div grad)

These are used in various descriptions and derivations of basic properties of physical fields.

Gradient – show the direction and size of the greatest change of a scalar field in each point of its domain,

input of the operation: scalar field output of the operation: vector field

$$gradU = \mathbf{A} = \frac{\partial U}{\partial x}\mathbf{i} + \frac{\partial U}{\partial y}\mathbf{j} + \frac{\partial U}{\partial z}\mathbf{k}$$

where i, j, k are elementary vectors

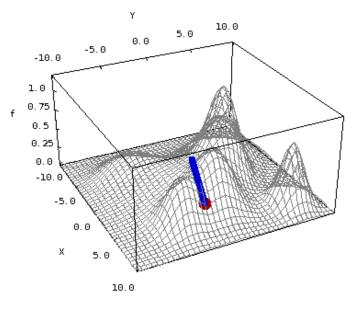
Comment to the notation:

We can write gradient using the so called nabla or del operator  $\nabla$ :

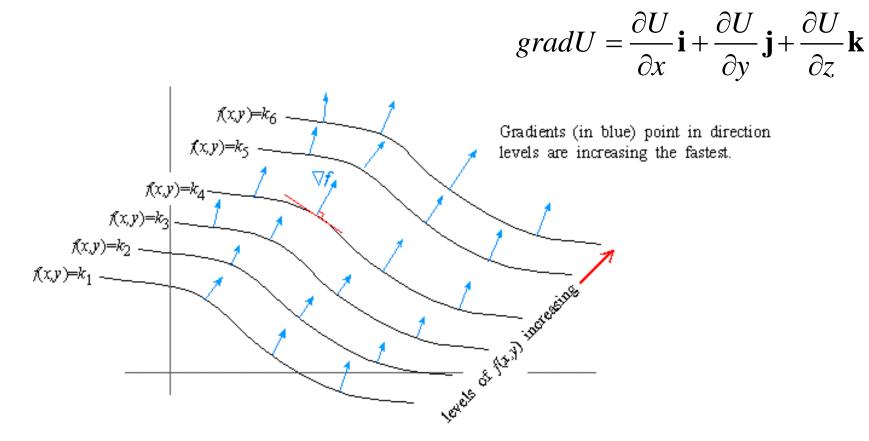
$$gradU = \nabla U$$

where

$$\nabla = \frac{\partial}{\partial x}\mathbf{i} + \frac{\partial}{\partial y}\mathbf{j} + \frac{\partial}{\partial z}\mathbf{k}$$



Gradient – show the direction and size of the greatest change of a scalar field in each point of its domain.



In physical fields, gradient is always pointing in the direction of force lines (perpendicular to equipotential lines).

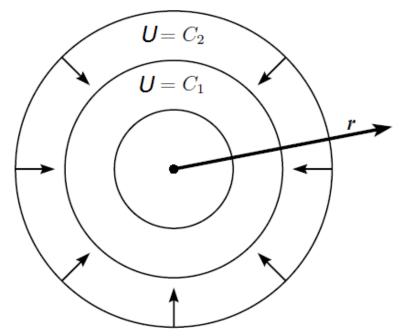
Gradient – example (field of positive electrical charge): (1/3)

Electrical potential U, caused by a positive electrical point charge (Q), situated in the origin of the coordinate system (Cartesian) can be described by means of the following equation:

$$U = \frac{1}{4\pi\varepsilon_0} \frac{Q}{r} = \frac{1}{4\pi\varepsilon_0} \frac{Q}{\sqrt{x^2 + y^2 + z^2}}$$

where  $\varepsilon_0$  is the electrical permittivity of vacuum (8.854.10<sup>-12</sup> F/m).

Equipotential surfaces of this scalar field build spherical surfaces around the origin of the coordinate system. Gradient is a vector field, which vectors point in each point of the space perpendicular to these equipotential surfaces.



Gradient – example (field of positive electrical charge): (2/3)

$$gradU = \frac{\partial U}{\partial x}\mathbf{i} + \frac{\partial U}{\partial y}\mathbf{j} + \frac{\partial U}{\partial z}\mathbf{k}$$

We will evaluate the gradient of this scalar function:

$$U = \frac{1}{4\pi\epsilon_0} \frac{Q}{r} = \frac{1}{4\pi\epsilon_0} \frac{Q}{\sqrt{x^2 + y^2 + z^2}}$$

because the field of electrical intensity (vector) is given:  $\vec{E} = -gradU$ 

First we evaluate the partial derivatives of *U* with respect to *x*, *y* and *z*.

$$\frac{\partial U}{\partial x} = \frac{Q}{4\pi\varepsilon_0} \frac{\partial}{\partial x} \left[ \left[ x^2 + y^2 + z^2 \right]^{-\frac{1}{2}} \right] = \frac{Q}{4\pi\varepsilon_0} \left( -\frac{1}{2} \right) \left[ \left[ x^2 + y^2 + z^2 \right]^{-\frac{3}{2}} 2x \right] = \frac{Q}{4\pi\varepsilon_0} \left[ \frac{x}{4\pi\varepsilon_0} \left[ \frac{x}{\left[ x^2 + y^2 + z^2 \right]^{\frac{3}{2}}} \right] = -\frac{Q}{4\pi\varepsilon_0} \left[ \frac{x}{r^3} \right]$$

Partial derivatives  $\frac{\partial U}{\partial y}$  and  $\frac{\partial U}{\partial z}$  are evaluated in a very similar way.

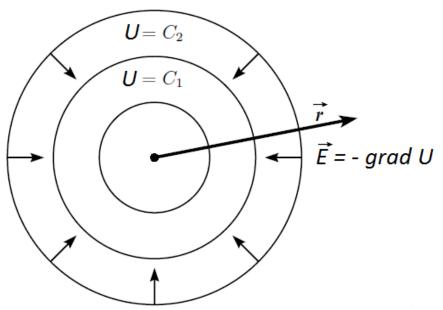
Gradient – example (field of positive electrical charge): (3/3)

$$\frac{\partial U}{\partial x} = -\frac{Q}{4\pi\varepsilon_0} \left(\frac{x}{r^3}\right), \qquad \frac{\partial U}{\partial y} = -\frac{Q}{4\pi\varepsilon_0} \left(\frac{y}{r^3}\right), \qquad \frac{\partial U}{\partial z} = -\frac{Q}{4\pi\varepsilon_0} \left(\frac{z}{r^3}\right)$$

$$\mathbf{E} = -gradU = \frac{Q}{4\pi\varepsilon_0} \left( \frac{x}{r^3} \mathbf{i} + \frac{y}{r^3} \mathbf{j} + \frac{z}{r^3} \mathbf{k} \right) = \frac{Q}{4\pi\varepsilon_0} \left( \frac{x\mathbf{i} + y\mathbf{j} + z\mathbf{k}}{r^3} \right) = \frac{Q}{4\pi\varepsilon_0} \frac{\mathbf{r}}{r^3}$$

This is a vector field, pointing in the same direction as the vector  $\vec{r}$  and having the size:

$$\left|\mathbf{E}\right| = \frac{Q}{4\pi\varepsilon_0} \frac{r}{r^3} = \frac{Q}{4\pi\varepsilon_0} \frac{1}{r^2}$$



There exist few special operations, which use partial derivatives and express properties of analyzed functions of several variables – so called **differential operators**:

- gradient (grad)
- divergence (div)
- rotation (rot)
- Laplacian operator (divgrad)

These are used in various descriptions and derivations of basic properties of physical fields.

Divergence – tells about the sources of a vector field: when the result is zero then there is no source of the field in the point. input of the operation: components of vector field output of the operation: scalar value field

$$div\mathbf{A} = \frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z}$$



where  $A_x$ ,  $A_y$ ,  $A_z$  are the components of vector  ${f A}$  .

<u>Comment</u>: Divergence depends on the changes of the size of vector components and not the change of their direction.

Comment to the notation:

We can write also divergence using the nabla or del operator  $\nabla$ :

$$div\mathbf{A} = \nabla \cdot \mathbf{A}$$
 where  $\nabla = \frac{\partial}{\partial x}\mathbf{i} + \frac{\partial}{\partial y}\mathbf{j} + \frac{\partial}{\partial z}\mathbf{k}$ 

**Divergence** – example (field of electrical charge): Field of electrical intensity (a vector field) is given by:

$$\mathbf{E} = -gradU = \frac{Q}{4\pi\varepsilon_0} \left(\frac{x\mathbf{i} + y\mathbf{j} + z\mathbf{k}}{r^3}\right) = E_x\mathbf{i} + E_y\mathbf{j} + E_z\mathbf{k}$$
$$E_x = \frac{Q}{4\pi\varepsilon_0} \left(\frac{x}{r^3}\right), \ \mathbf{E}_y = \frac{Q}{4\pi\varepsilon_0} \left(\frac{y}{r^3}\right), \ \mathbf{E}_z = \frac{Q}{4\pi\varepsilon_0} \left(\frac{z}{r^3}\right)$$

1/2)

To evaluate the divergence of this field, we need to evaluate the following derivatives:

$$\begin{aligned} \frac{\partial \mathbf{E}_{\mathbf{x}}}{\partial \mathbf{x}} &= \frac{Q}{4\pi\varepsilon_{0}} \frac{\partial}{\partial \mathbf{x}} \left( \frac{x}{r^{3}} \right) = \frac{Q}{4\pi\varepsilon_{0}} \frac{\partial}{\partial \mathbf{x}} \left( \frac{x}{\left[ x^{2} + y^{2} + z^{2} \right]^{3/2}} \right) = \frac{Q}{4\pi\varepsilon_{0}} \frac{\partial}{\partial \mathbf{x}} \left( x \left[ x^{2} + y^{2} + z^{2} \right]^{-3/2} \right) = \\ &= \frac{Q}{4\pi\varepsilon_{0}} \left( \left[ x^{2} + y^{2} + z^{2} \right]^{-3/2} + x \left( \frac{-3}{2} \right) \left[ x^{2} + y^{2} + z^{2} \right]^{-5/2} 2x \right) = \\ &= \frac{Q}{4\pi\varepsilon_{0}} \left( \left[ x^{2} + y^{2} + z^{2} \right]^{-3/2} - 3x^{2} \left[ x^{2} + y^{2} + z^{2} \right]^{-5/2} \right) \end{aligned}$$

**Divergence** – example (field of electrical charge):

For all three derivatives we get:

$$\begin{aligned} \frac{\partial E_x}{\partial x} &= \frac{Q}{4\pi\varepsilon_0} \left( \left[ x^2 + y^2 + z^2 \right]^{-3/2} - 3x^2 \left[ x^2 + y^2 + z^2 \right]^{-5/2} \right) \\ \frac{\partial E_y}{\partial y} &= \frac{Q}{4\pi\varepsilon_0} \left( \left[ x^2 + y^2 + z^2 \right]^{-3/2} - 3y^2 \left[ x^2 + y^2 + z^2 \right]^{-5/2} \right) \\ \frac{\partial E_z}{\partial z} &= \frac{Q}{4\pi\varepsilon_0} \left( \left[ x^2 + y^2 + z^2 \right]^{-3/2} - 3z^2 \left[ x^2 + y^2 + z^2 \right]^{-5/2} \right) \\ \frac{\partial E_x}{\partial x} &+ \frac{\partial E_y}{\partial y} + \frac{\partial E_z}{\partial z} = \frac{Q}{4\pi\varepsilon_0} \left( 3 \left[ x^2 + y^2 + z^2 \right]^{-3/2} - 3 \left( x^2 + y^2 + z^2 \right]^{-5/2} \right) \end{aligned}$$

$$= \frac{Q}{4\pi\varepsilon_0} \left( 3\left[x^2 + y^2 + z^2\right]^{-3/2} - 3\left[x^2 + y^2 + z^2\right]^{-3/2} \right) = 0$$

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This result is valid for all points with the exception of the coordinate system origin, where x = y = z = 0 (source area).

There exist few special operations, which use partial derivatives and express properties of analyzed functions of several variables – so called **differential operators**:

- gradient (grad)
- divergence (div)
- rotation (rot)
- Laplacian operator (divgrad)

These are used in various descriptions and derivations of basic properties of physical fields.

Rotation – tells about the existence of so called curls of the vector field (not about the sources). input of the operation: components of vector field output of the operation: vector field

$$rot\mathbf{A} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ A_x & A_y & A_z \end{vmatrix} = \mathbf{i} \left( \frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z} \right) + \mathbf{j} \left( \frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x} \right) + \mathbf{k} \left( \frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \right)$$

<u>Comment:</u> Rotation does not depend on the changes of the size of vector components (this was the role of divergence).

Comment to the notation:

We can write also divergence using the nabla or del operator  $\nabla$ :

$$rot\vec{A} = \nabla \times \mathbf{A}$$
 where  $\nabla = \frac{\partial}{\partial x}\mathbf{i} + \frac{\partial}{\partial y}\mathbf{j} + \frac{\partial}{\partial z}\mathbf{k}$ 

Rotation – example (field of electrical charge): Field of electrical intensity (a vector field) is given by:

$$\mathbf{E} = -gradU = \frac{Q}{4\pi\varepsilon_0} \left( \frac{x\mathbf{i} + y\mathbf{j} + z\mathbf{k}}{r^3} \right) = E_x\mathbf{i} + E_y\mathbf{j} + E_z\mathbf{k}$$
$$E_x = \frac{Q}{4\pi\varepsilon_0} \left( \frac{x}{r^3} \right), \ \mathbf{E}_y = \frac{Q}{4\pi\varepsilon_0} \left( \frac{y}{r^3} \right), \ \mathbf{E}_z = \frac{Q}{4\pi\varepsilon_0} \left( \frac{z}{r^3} \right)$$

(1/2)

For the rotation evaluation we need following derivatives:

$$\frac{\partial \mathbf{E}_{z}}{\partial \mathbf{y}} = \frac{Q}{4\pi\varepsilon_{0}} \frac{\partial}{\partial \mathbf{y}} \left(\frac{z}{r^{3}}\right) = \frac{Q}{4\pi\varepsilon_{0}} \frac{\partial}{\partial \mathbf{y}} \left(\frac{z}{\left[x^{2} + y^{2} + z^{2}\right]^{\frac{3}{2}}}\right) = \frac{zQ}{4\pi\varepsilon_{0}} \frac{\partial}{\partial \mathbf{y}} \left(\left[x^{2} + y^{2} + z^{2}\right]^{-\frac{3}{2}}\right) = \frac{zQ}{4\pi\varepsilon_{0}} \left(\left(\frac{-3}{2}\right)\left[x^{2} + y^{2} + z^{2}\right]^{-\frac{5}{2}} 2y\right) = \frac{-3yzQ}{4\pi\varepsilon_{0}} \left(\left[x^{2} + y^{2} + z^{2}\right]^{-\frac{5}{2}}\right)$$
$$\frac{\partial \mathbf{E}_{y}}{\partial z} = \frac{Q}{4\pi\varepsilon_{0}} \frac{\partial}{\partial z} \left(\frac{y}{\left[x^{2} + y^{2} + z^{2}\right]^{\frac{3}{2}}}\right) = \frac{-3zyQ}{4\pi\varepsilon_{0}} \left(\left[x^{2} + y^{2} + z^{2}\right]^{-\frac{5}{2}}\right)$$

Rotation – example (field of electrical charge):

From the evaluated derivatives it follows:

$$\frac{\partial \mathbf{E}_{\mathbf{z}}}{\partial \mathbf{y}} - \frac{\partial \mathbf{E}_{\mathbf{y}}}{\partial \mathbf{z}} = 0$$

In a similar way we can show:

$$\frac{\partial \mathbf{E}_{\mathbf{x}}}{\partial \mathbf{z}} - \frac{\partial \mathbf{E}_{\mathbf{z}}}{\partial \mathbf{x}} = 0 \qquad \frac{\partial \mathbf{E}_{\mathbf{y}}}{\partial \mathbf{x}} - \frac{\partial \mathbf{E}_{\mathbf{x}}}{\partial \mathbf{y}} = 0$$

... and for the rotation it is valid:

$$rot\mathbf{E} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ E_x & E_y & E_z \end{vmatrix} = \mathbf{i} \left( \frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z} \right) + \mathbf{j} \left( \frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} \right) + \mathbf{k} \left( \frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} \right) = \mathbf{0}$$

(2/2)

This result is valid for all points with the exception of the coordinate system origin, where x = y = z = 0 (source area).

There exist few special operations, which use partial derivatives and express properties of analyzed functions of several variables – so called **differential operators**:

- gradient (grad)
- divergence (div)
- rotation (rot)
- Laplacian operator (divgrad)

These are used in various descriptions and derivations of basic properties of physical fields.

Laplacian operator – in mathematical physics is often used the following (combined) differential operator, input of the operation: scalar field output of the operation: scalar field

$$div(gradU) = \frac{\partial(\partial U/\partial x)}{\partial x} + \frac{\partial(\partial U/\partial y)}{\partial y} + \frac{\partial(\partial U/\partial z)}{\partial z}$$
$$div(gradU) = \frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} + \frac{\partial^2 U}{\partial z^2}$$

Comment to the notation:

We can write gradient using the so called nabla or del operator  $\nabla$ :

$$div(gradU) = \nabla \cdot (\nabla U) = \nabla^2 U = \Delta U$$

Beside this combined operator (Laplacian), the are valid following equations:

$$rot(grad U) \equiv 0$$
$$div(rot \mathbf{A}) \equiv 0$$

These equations have important impacts on the properties of some physical fields:

- the first one tells that so called potential fields (which intensity can be expressed by means of the gradient) can not build curls,
- the second one tells us that in a curl there are no sources.

You can try to check it mathematically (make a proof) in a frame of a homework.