Physical models for micro and nanosystems

Part 2: Mathematical background

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Outline

- Review of vector analysis
- Operators (div, grad, curl) and associated theorems
- Some useful identities

Vector calculus

- Studies various differential operators defined on scalar and vector fields
- These are typically expressed in terms of the del operator, also known as nabla and represented with the symbol ∇
- In a 3D Cartesian system, del is defined as:

$$\nabla \equiv \hat{x}\frac{\partial}{\partial x} + \hat{y}\frac{\partial}{\partial y} + \hat{z}\frac{\partial}{\partial z}$$

- Note that we will be denoting unit vectors with

  $\hat{x}, \hat{y}, \hat{z}$

  and not

  $\vec{i}, \vec{j}, \vec{k}$

  or

  $\vec{e}_1, \vec{e}_2, \vec{e}_3$

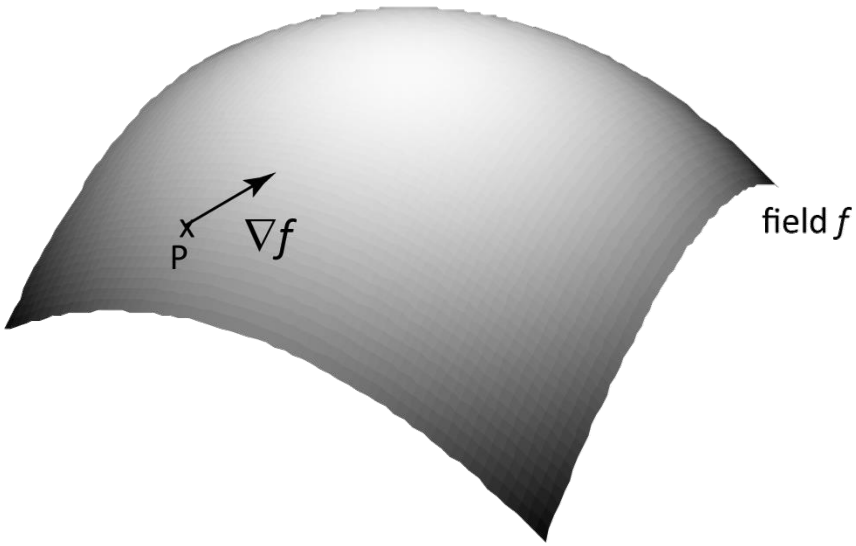
Vector calculus

- By applying the del operator to scalar or vector fields we can construct the four most important operations in vector calculus

		Operates on a:	The result is a:
Gradient	$grad(f) = \nabla f$	scalar	vector
Divergence	$div(\vec{F}) = \nabla \cdot \vec{F}$	vector	scalar
Curl (rotor)	$rot(\vec{F}) = \nabla \times \vec{F}$	vector	vector
Laplacian	$\Delta f = \nabla^2 f = \nabla \cdot \nabla f = div(grad(f))$	scalar	scalar

Gradient

- Assume that f is a scalar field.
- Its gradient is a vector field which points in the <u>direction</u> of the greatest rate of <u>increase</u> of the scalar field, and whose magnitude is the greatest rate of change.



- It is defined by the folowing expression:

$$\nabla f = \lim_{V \to 0} \frac{\int_S f d\vec{a}}{V}$$

where S is the surface enclosing volume V ar $d\vec{a}$ is normal to S and points outward

- In Cartesian coordinates:

$$\nabla f = \hat{x}\frac{\partial f}{\partial x} + \hat{y}\frac{\partial f}{\partial y} + \hat{z}\frac{\partial f}{\partial z}$$

$$\nabla \equiv \hat{x}\frac{\partial}{\partial x} + \hat{y}\frac{\partial}{\partial y} + \hat{z}\frac{\partial}{\partial z}$$

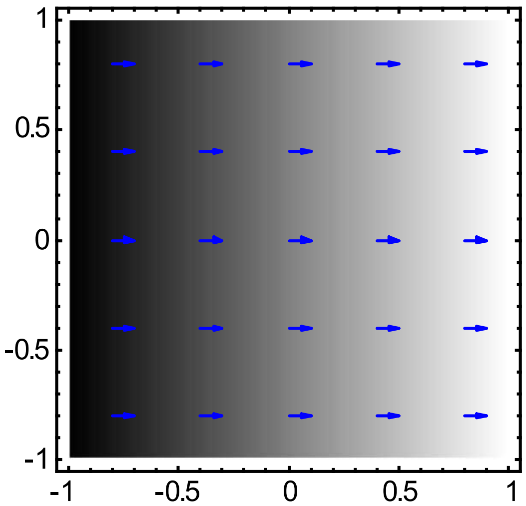
Gradient - example

- Examples:
  1. Scalar field

$$f(x,y)=5x$$

Gradient:

$$\nabla f=\hat{x}\frac{\partial f}{\partial x}+\hat{y}\frac{\partial f}{\partial y}+\hat{z}\frac{\partial f}{\partial y}=5\hat{x}$$

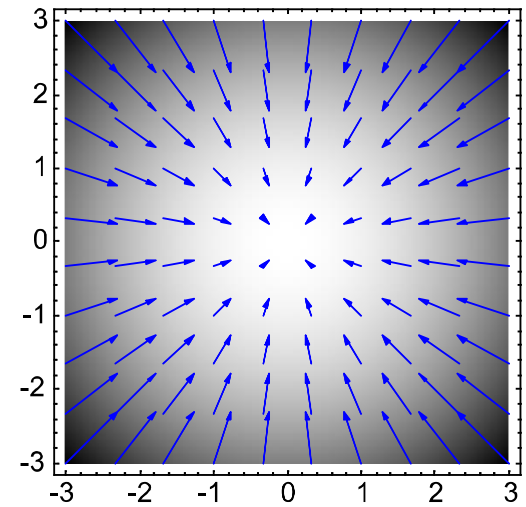


  2. Scalar field

$$f=1-(x\,^\wedge 2+y\,^\wedge 2)$$

Gradient:

$$\nabla f=-2x\hat{x}-2y\hat{y}$$



Divergence

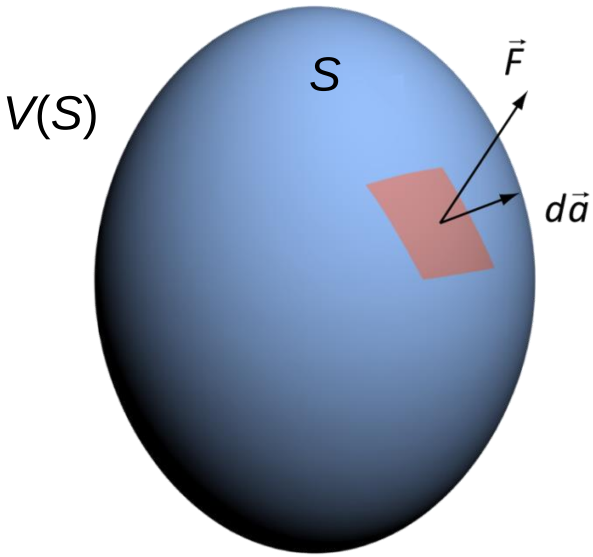
- Assume that ***F*** is a vector field. Consider a closed surface *S*, enclosing a finite volume *V*(*S*).

  The flux of field ***F*** through surface *S* is:

  $$\Phi = \int_S \vec{F} \cdot d\vec{a}$$

  The divergence of the field ***F*** is the quantity Φ / V in the limit of zero volume:

  $$\nabla \cdot \vec{F} = \lim_{V(S)\to 0} \frac{\int_S \vec{F} \cdot d\vec{a}}{V(S)}$$



- It is a scalar field with magnitude that corresponds to the local source or sink of the vector field – it can be thought of as “microscopic flow“
- In Cartesian coordinates:

$$\nabla \cdot \vec{F} = \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}$$

$$\nabla \equiv \hat{x}\frac{\partial}{\partial x} + \hat{y}\frac{\partial}{\partial y} + \hat{z}\frac{\partial}{\partial z}$$

Divergence - example

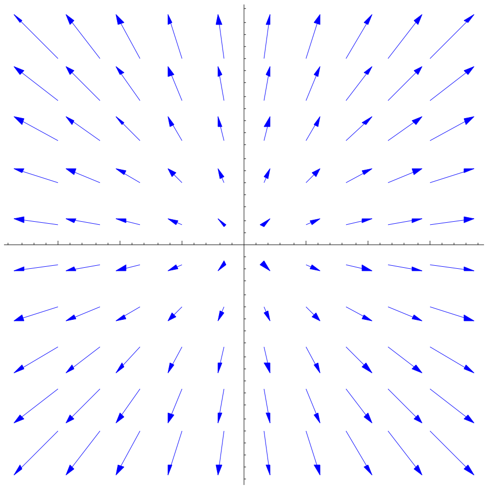
- Examples:
  1. Vector field

$$\vec{F} = x\hat{x} + y\hat{y}$$

Divergence:

$$\nabla \cdot \vec{F} = \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} =$$

$$= \frac{\partial x}{\partial x} + \frac{\partial y}{\partial y} = 2$$



div≠0

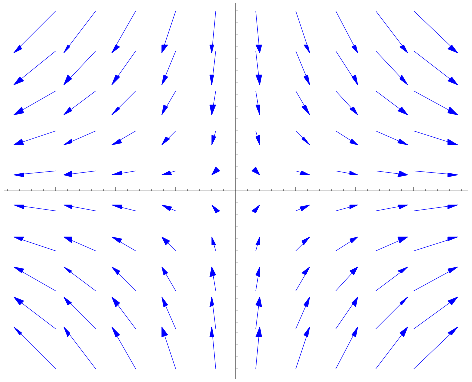
2. Field:

$$\vec{F} = x\hat{x} - y\hat{y}$$

Divergence:

$$\nabla \cdot \vec{F} = \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} =$$

$$= \frac{\partial x}{\partial x} - \frac{\partial y}{\partial y} = 0$$



div=0

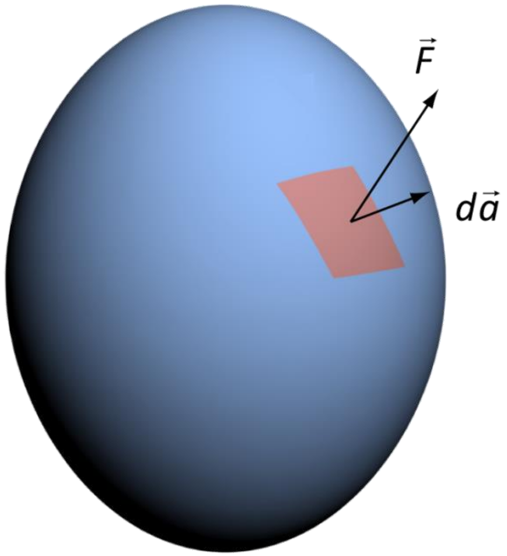
Gauss theorem (divergence theorem)

- Sometimes referred to as Ostrogradsky's theorem, Gauss-Ostrogradsky theorem, although it was first discovered by Lagrange

- Let us go back to the definition of flux and divergence:

$$\Phi = \int_S \vec{F} \cdot d\vec{a} \qquad \nabla \cdot \vec{F} = \lim_{V(S)\to 0} \frac{\int_S \vec{F} \cdot d\vec{a}}{V(S)}$$

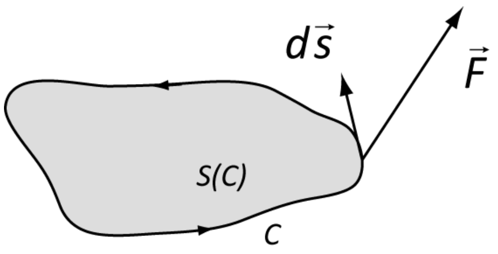
- The Gauss theorem states that the flux of the field ***F*** through a closed surface *S* is equal to the integral of the field’s divergence over the volume enclosed by *S:*



$$\int_S \vec{F} \cdot d\vec{a} = \int_{V(S)} \nabla \cdot \vec{F} dV$$

Curl (rotor)

- Assume that ***F*** is a vector field. Consider a closed path C, enclosing a finite surface *S*(C).
- The circulation Γ of field ***F*** along the path C is:



$$\Gamma = \int_C \vec{F} \cdot d\vec{s}$$

The rotation of the field *F* is the quantity Γ / S in in the limit of a small surface *S*:

$$\left(\nabla \times \vec{F}\right) \cdot \hat{n} = \lim_{S(C)\to 0} \frac{\int_C \vec{F} \cdot d\vec{s}}{S(C)}$$

Where $\hat{n}$ is a unit vector normal to the surface *S*.

- It represents the microscopic circulation of the field ***F**,* with direction following the right-hand rule

Curl in Cartesian coordinates

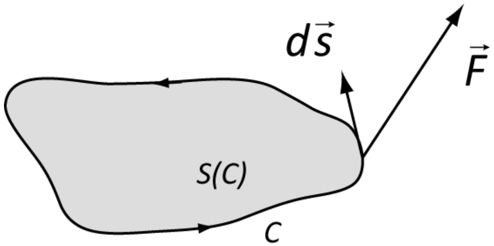
$$\nabla \times \vec{F} = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \dfrac{\partial}{\partial x} & \dfrac{\partial}{\partial y} & \dfrac{\partial}{\partial z} \\ F_x & F_y & F_z \end{vmatrix} =$$

$$= \left(\frac{\partial F_z}{\partial y} - \frac{\partial F_y}{\partial z} \right) \hat{x} + \left(\frac{\partial F_x}{\partial z} - \frac{\partial F_z}{\partial x} \right) \hat{y} + \left(\frac{\partial F_y}{\partial x} - \frac{\partial F_x}{\partial y} \right) \hat{z}$$

Stokes theorem

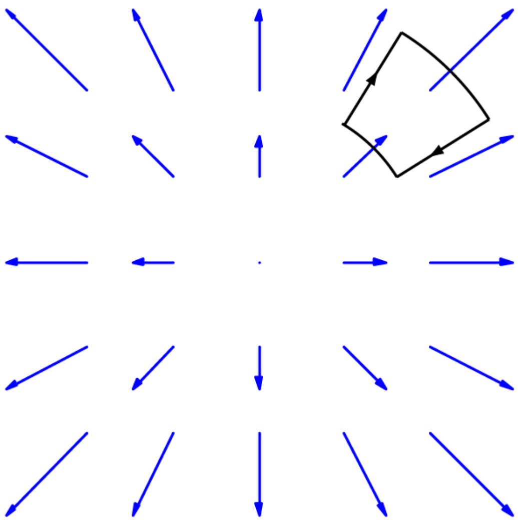
- Let us consider again the definition of circulation and rotation:

$$\Gamma = \int_C \vec{F} \cdot d\vec{s} \qquad \left(\nabla \times \vec{F}\right) \cdot \hat{n} = \lim_{S(C) \to 0} \frac{\int_C \vec{F} \cdot d\vec{s}}{S(C)}$$



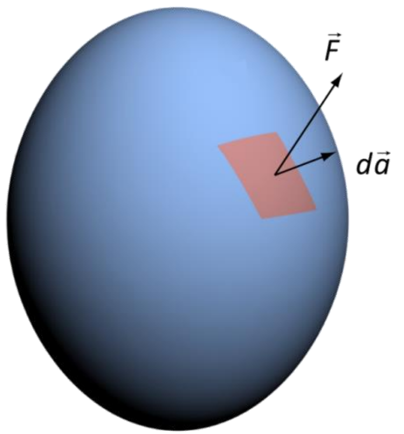
- The Stokes theorem specifies that the surface integral of the rotation over a macroscopic surface *S* is equal to the circulation around the circumference of the surface *S*:

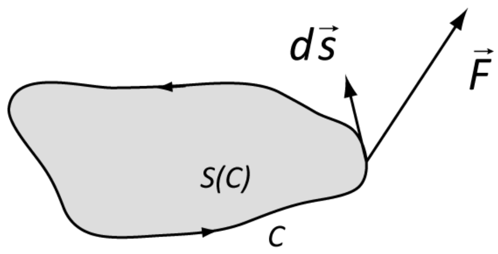
$$\int_C \vec{F} \cdot d\vec{s} = \int_{S(C)} \left(\nabla \times \vec{F}\right) \cdot d\vec{a}$$



rot=0

Gauss and Stokes theorem





Flow $\Phi = \int_S \vec{F} \cdot d\vec{a}$

Circulation $\Gamma = \int_C \vec{F} \cdot d\vec{s}$

Divergence $\nabla \cdot \vec{F} = \lim_{V(S) \to 0} \frac{\int_S \vec{F} \cdot d\vec{a}}{V(S)}$

Curl $\left(\nabla \times \vec{F}\right) \cdot \hat{n} = \lim_{S(C) \to 0} \frac{\int_C \vec{F} \cdot d\vec{s}}{S(C)}$

$$\int_S \vec{F} \cdot d\vec{a} = \int_{V(S)} \nabla \cdot \vec{F} dV$$

Gauss theorem

$$\int_C \vec{F} \cdot d\vec{s} = \int_{S(C)} \left(\nabla \times \vec{F}\right) \cdot d\vec{a}$$

Stokes theorem

Homework assignement

- **Please refresh your knowledge on the subjects of:**
  - Combination of operators

- **Test your new/old knowledge by solving the following exercise**

For the vector field $\vec{F} = 2y\hat{x} + z^2\hat{y} - xy\hat{z}$ calculate the following quantities:

a) $\nabla \cdot \vec{F}$

b) $\nabla \times \vec{F}$

c) $\nabla \cdot \left(\nabla \times \vec{F}\right)$

d) The integral $\int_S \left(\nabla \times \vec{F}\right) d\vec{A}$ for any closed surface S.

… and submit your results via moodle (exercise 1)