Modelling and Numerical Methods

Part 1
Continuum mechanics and vector/tensor calculus

Lecture 1

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Lecture Materials

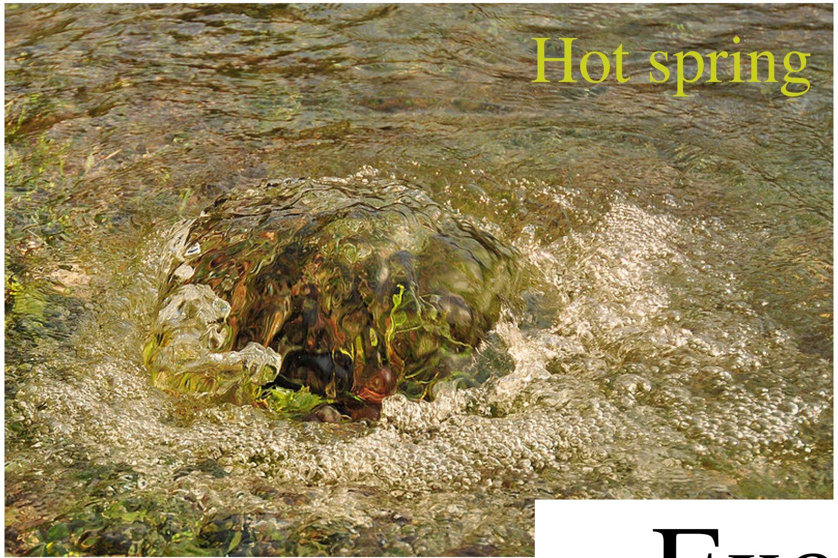
- Lecture slides
- Jupyter notebook: practical exercises
- Solutions (after workshop)

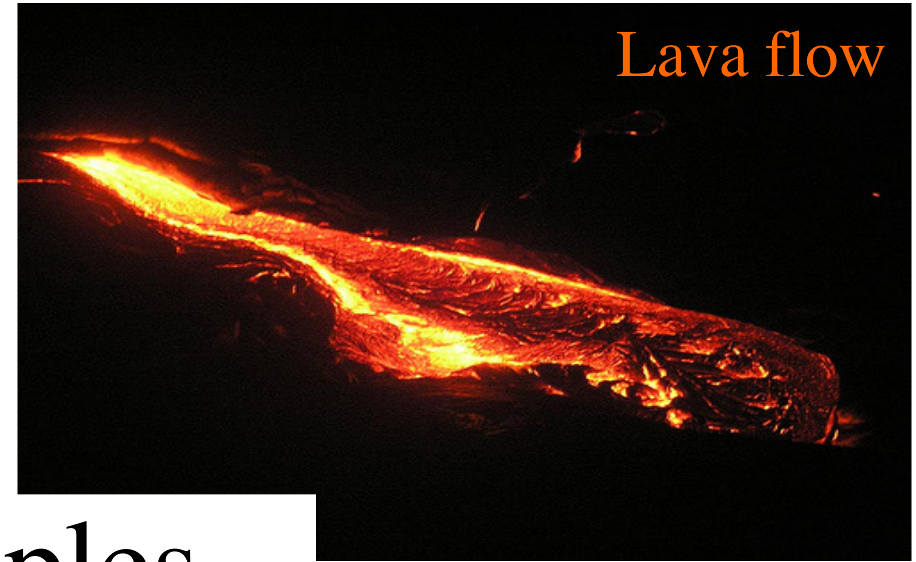
All available on GitHub

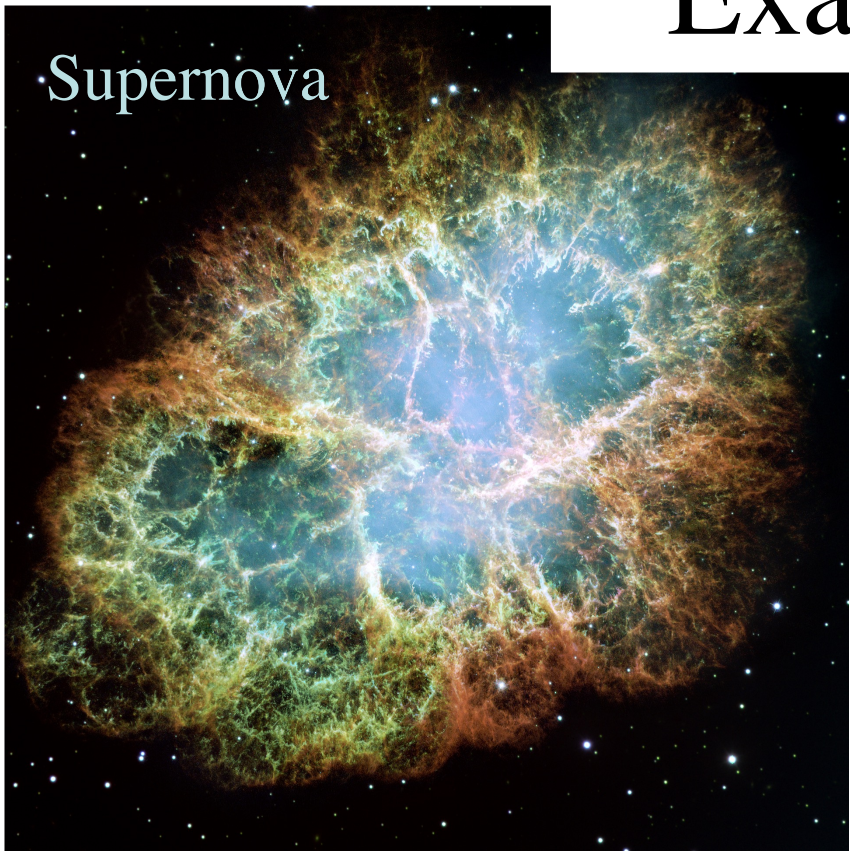
Continuum Mechanics

- *Macroscopic description* of the collective behaviour of atoms/molecules in the limit where scale >> scale of the individual components
- Treat a material, be it solid, liquid, gas, as hypothetical continuum where all quantities vary continuously so that spatial derivatives exist
- In such a treatment, we can consider infinitesimally small volumes of the material and define point quantities, like mass, velocity, stress
- Such a description has been found to be applicable in a wide range of problems in engineering and physical sciences

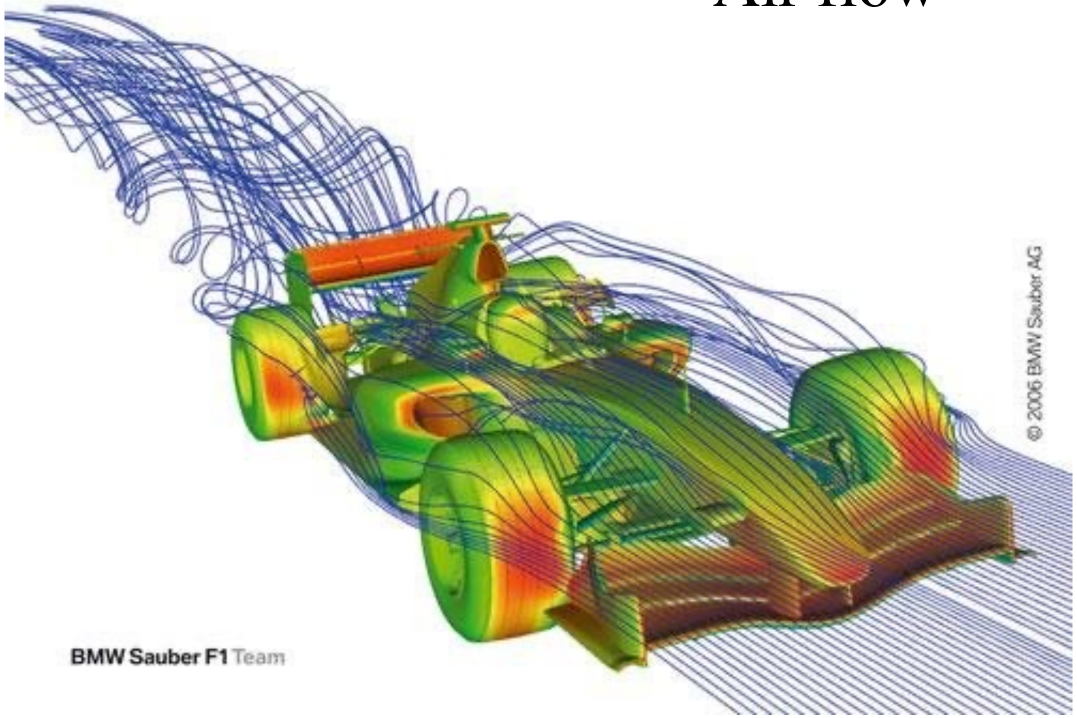
Examples



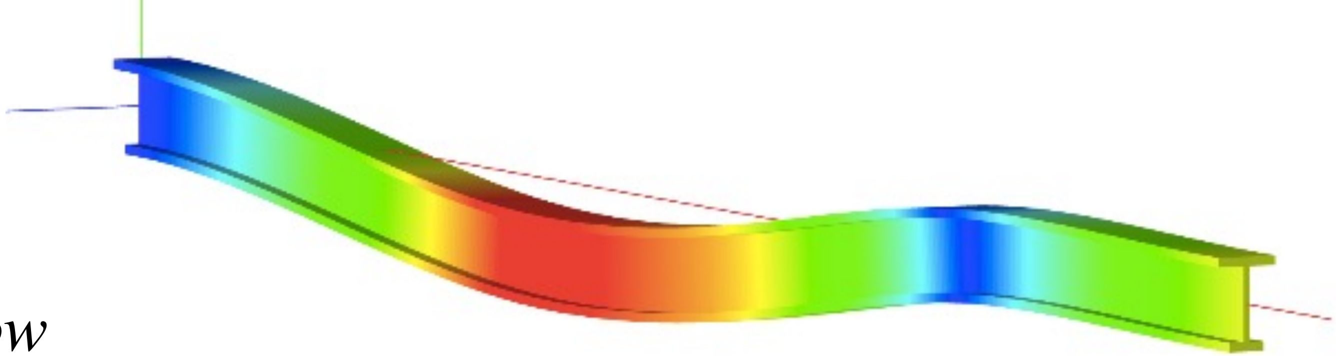




Air flow

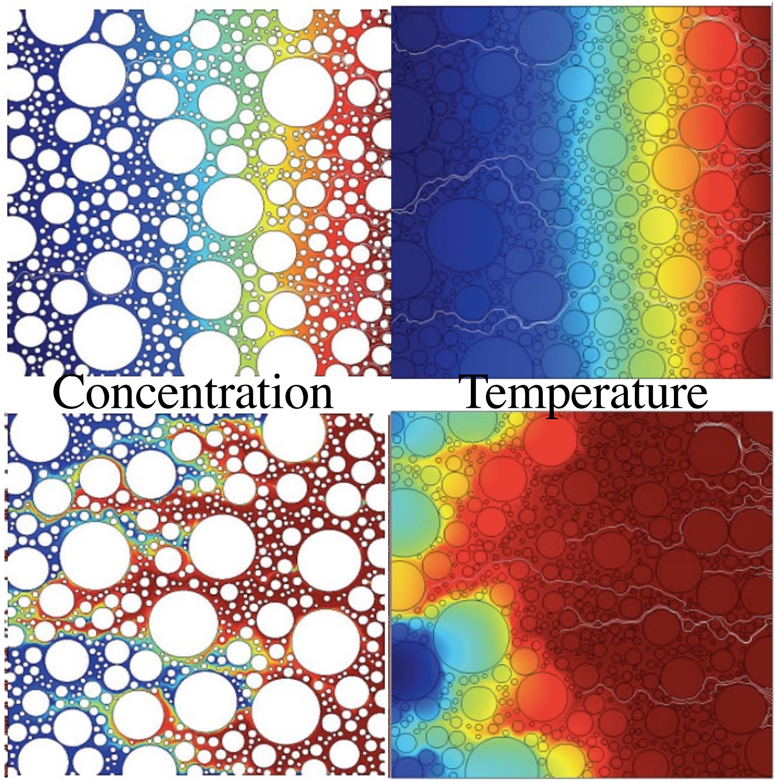


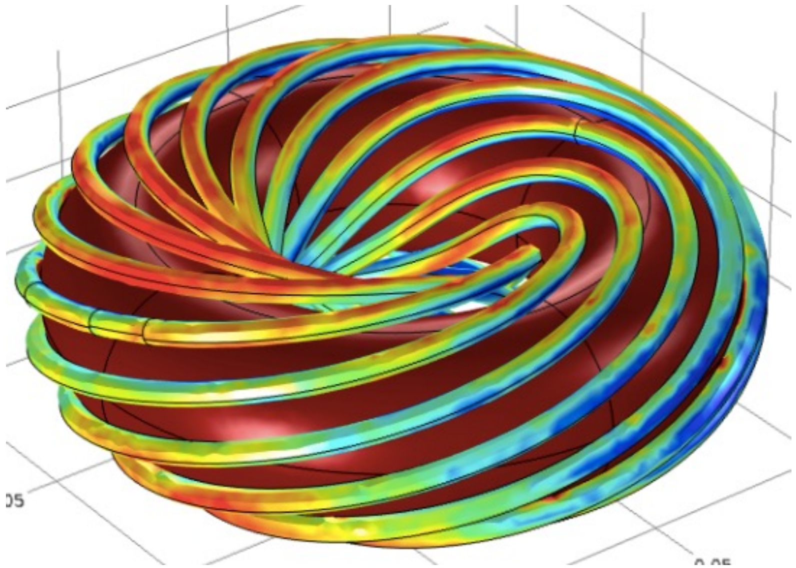
More Examples



Beam bending

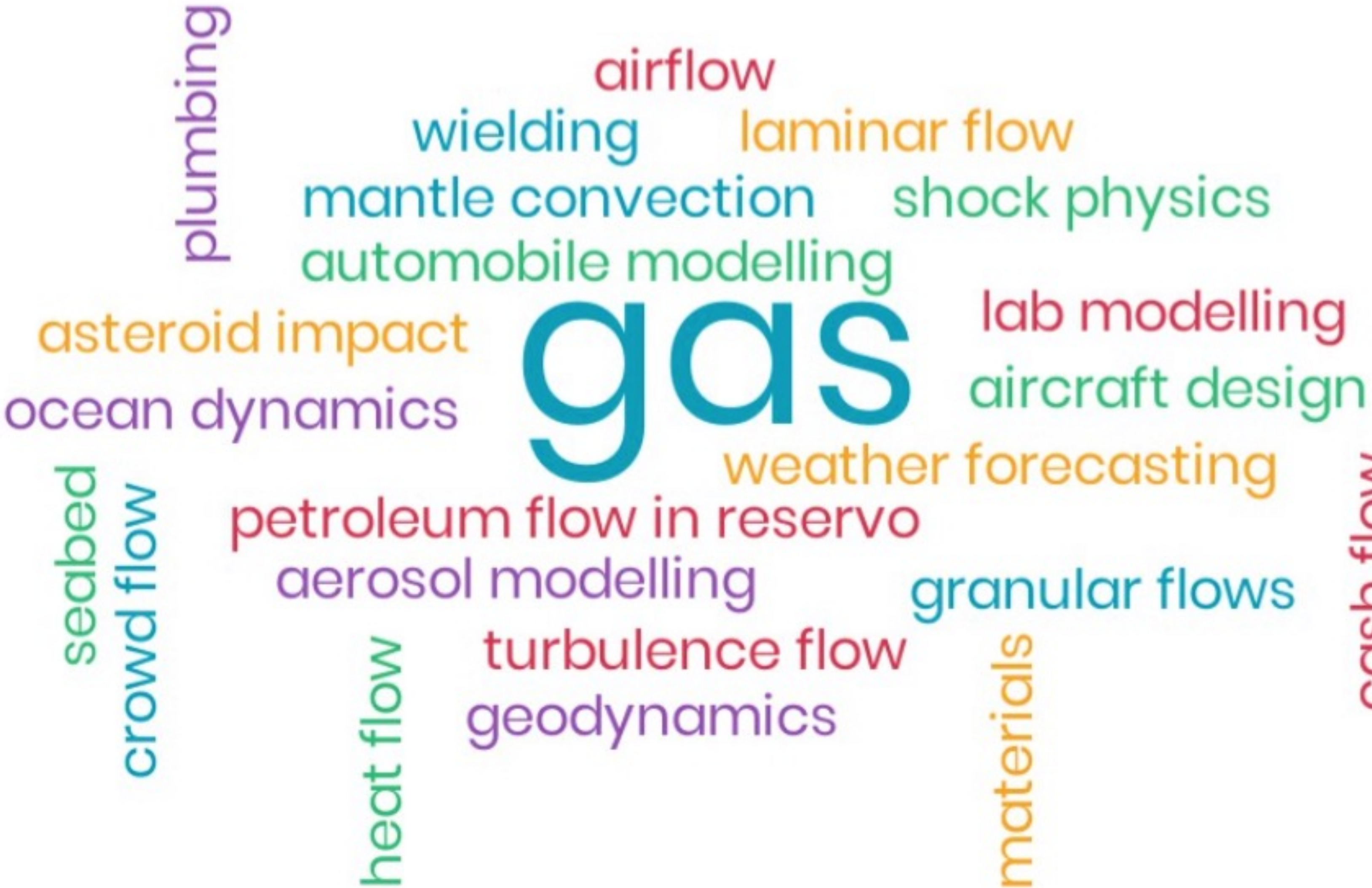
Porous flow





Electromagnetism

Other Examples?



No required text

Possible textbooks for additional background

- Introduction to Continuum Mechanics, W.M. Lai, D. Rubin, E. Krempl, 4th edition, Elsevier – available in electronic form through IC library

- An Introduction to Continuum Mechanics, J.N. Reddy, 2nd edition, Cambridge University Press, 2013

The books use similar notation as this course and cover the mathematical background for first part of this class. Different reading may be suggested for other parts of the course

Continuum Mechanics Equations

General:

1. Kinematics – describing deformation and velocity without considering forces
2. Dynamics – equations that describe force balance, conservation of linear and angular momentum
3. Thermodynamics – relations temperature, heat flux, stress, entropy

Material-specific

4. Constitutive equations – relations describing how material properties vary as a function of T,P, stress,…. Such material properties govern dynamics (e.g., density), response to stress (viscosity, elastic parameters), heat transport (thermal conductivity, diffusivity)

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$\Rightarrow$ *Yields a set of Partial Differential Equations that can be solved for displacement, velocity, temperature,…*

Partial Differential Equations

- **Ordinary Differential Equations** – describe how variables depend on a single independent parameter (e.g., time or distance).

For example: $$m\frac{d^2x}{dt^2} = F$$ *Newton's second law*

- **Partial Differential Equations** – describe how variables depend on several independent parameters (e.g., time, x,y,z coordinates)

For example: $$\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x^2}$$ *Thermal diffusion equation*

∂ - partial derivative

Today: Vectors and Tensors

chapter1.ipynb

- Revision vectors
  - Addition, linear independence
  - Orthonormal Cartesian bases, transformation
  - Multiplication
  - Derivatives, del, div, curl
- Revision/introduction tensors
  - Tensors, rank, stress tensor
  - Index notation, summation convention
  - Addition, multiplication
  - Tensor calculus: gradient, divergence, curl, ..

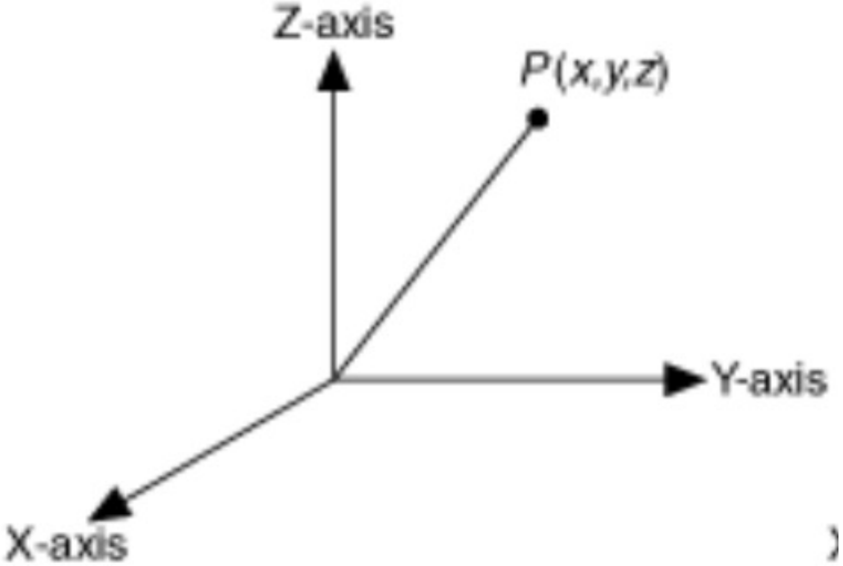
Learning Objectives

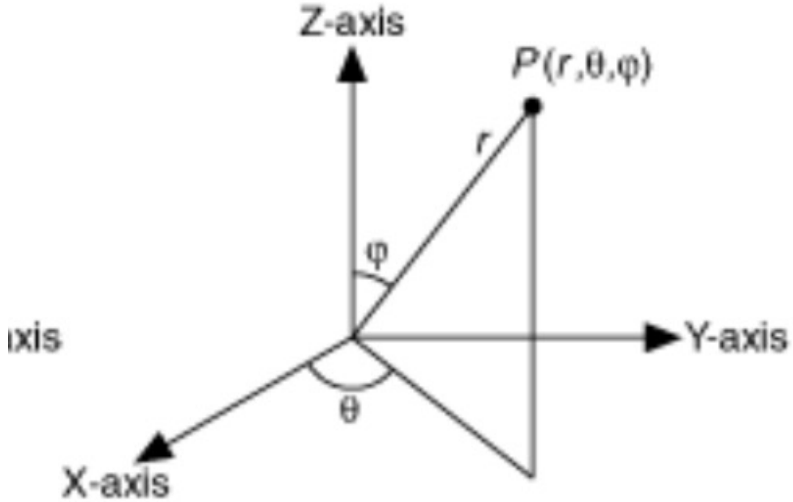
- Be able to perform vector/tensor operations (addition, multiplication) on Cartesian orthonormal bases
- Be able to do basic vector/tensor calculus (time and space derivatives, divergence, curl of a vector field) on these bases.
- Perform transformation of a vector from one Cartesian basis to another.
- Understand differences/commonalities between tensor and vector
- Familiarity with index notation and Einstein convention

Intro Vectors, Tensors

Continuum mechanics equations require vectors and tensors. E.g., velocity is a vector, with magnitude and direction in 3-D, and so are forces like gravity.

The components of a vector depend on the coordinate system chosen to represent them in. However, the actual size and orientation of the vector is not dependent on the choice of coordinate system





Key characteristics of a vector?

1. Anything that is not a scalar
2. Has three components
3. Has magnitude and direction
4. Depends on coordinate frame
5. Velocity and rotation are two examples
6. Multiplication of two vectors gives another vector

Which of these are correct?

Notation

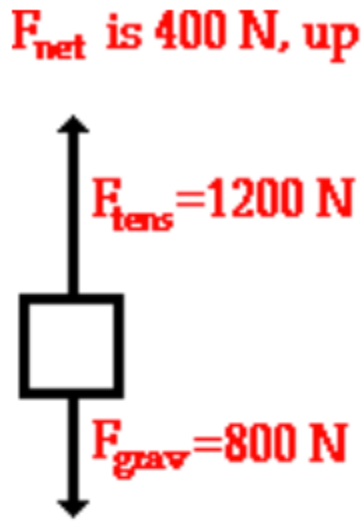
- Vectors as **v** or $\vec{v}$ or $\overline{v}$
- Length of vectors v or $|\mathbf{v}|$
- Vector in Cartesian components v_x, v_y, v_z
- Index notation v_i, $i=x,y,z$ or $i=1,2,3$
- Unit vector along direction of **v**: $\hat{\mathbf{e}}_v = \dfrac{\mathbf{v}}{|\mathbf{v}|}$

$$\mathbf{v} = \hat{\mathbf{e}}_v |\mathbf{v}|$$

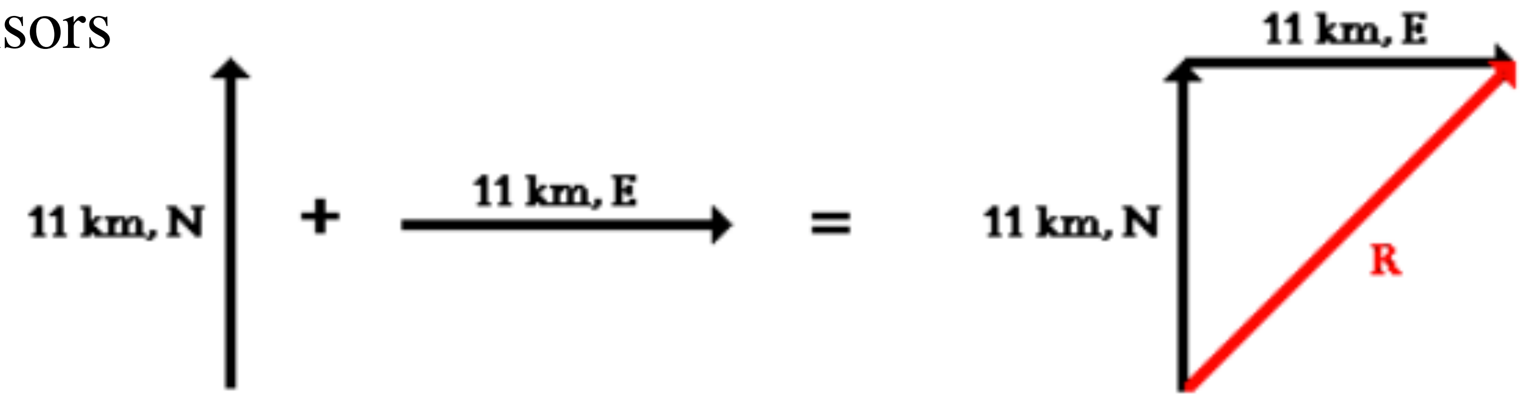
Vectors

Vectors satisfy certain rules of addition and scalar multiplication,

- $\mathbf{a}+\mathbf{b}=\mathbf{b}+\mathbf{a}$ (commutative)
- $(\mathbf{a}+\mathbf{b})+\mathbf{c}=\mathbf{a}+(\mathbf{b}+\mathbf{c})$ (associative)
- $\alpha(\mathbf{a}+\mathbf{b}) = \alpha\mathbf{a}+\alpha\mathbf{b}$ (distributive)
- $\mathbf{a}+\mathbf{0}=\mathbf{a}$ (zero vector)
- $1\cdot\mathbf{a}=\mathbf{a}\cdot 1$; $0\cdot\mathbf{a}=\mathbf{0}$

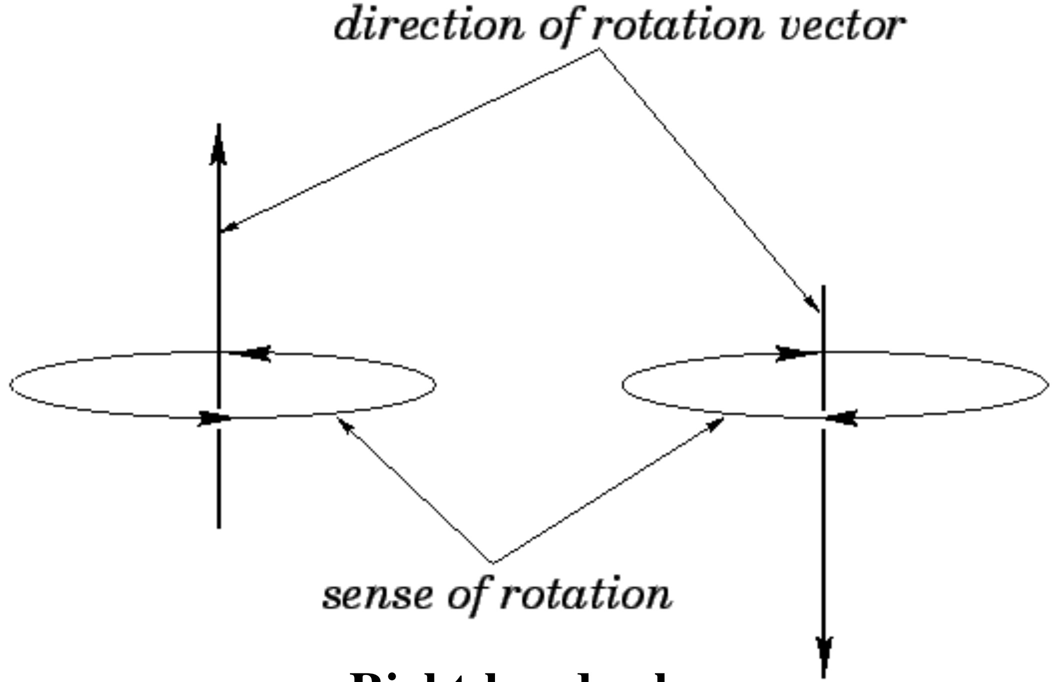


We will see that similar rules apply to tensors

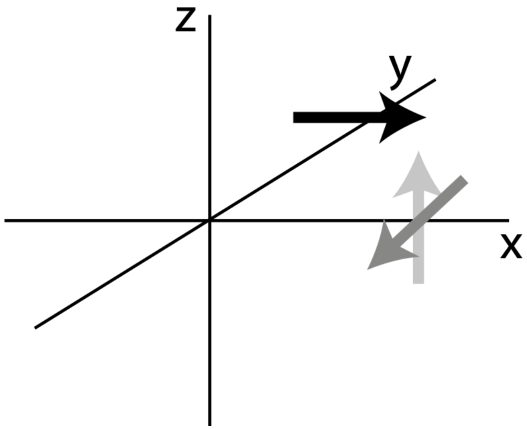


e.g. see http://mathworld.wolfram.com/Vector.html

Finite Rotation "Vector"

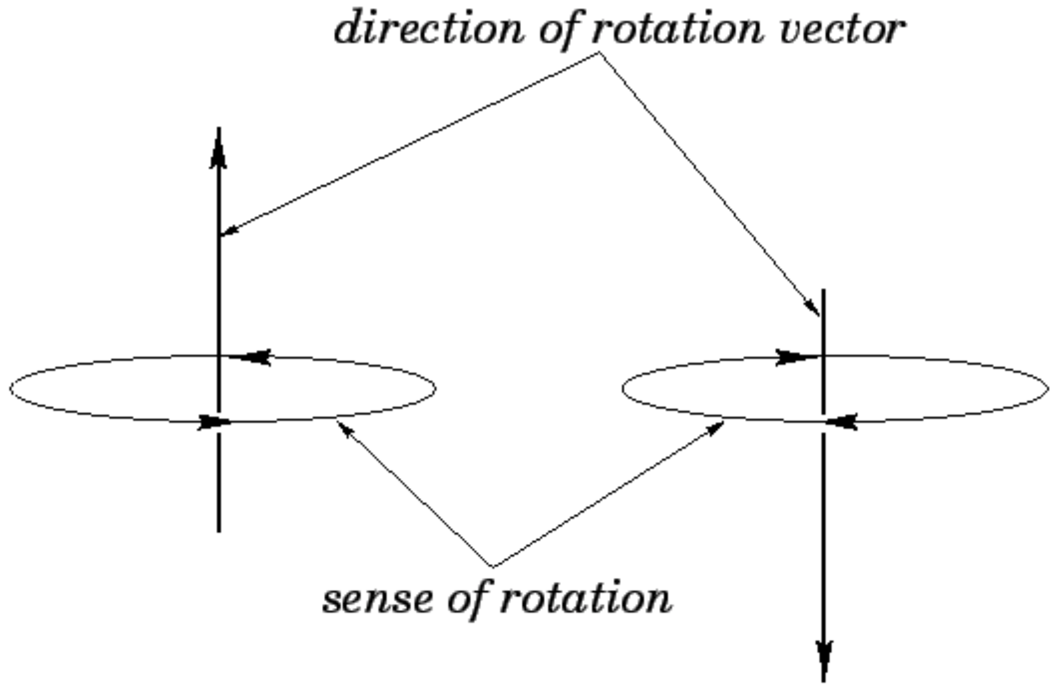


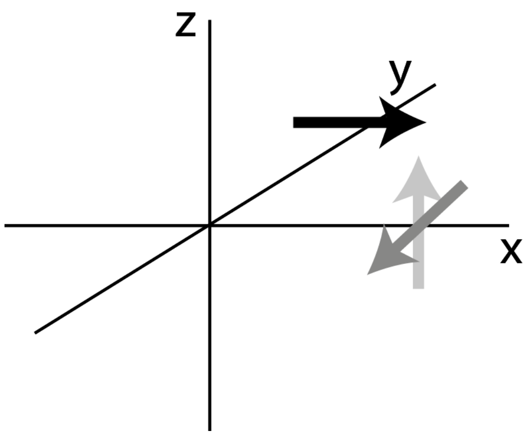
Right-hand rule



rotate 90° around **x** + 90° around **z**

Finite Rotation "Vector"





rotate 90° around **x** +
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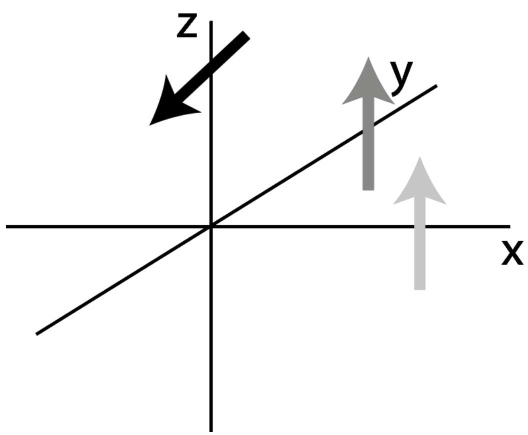


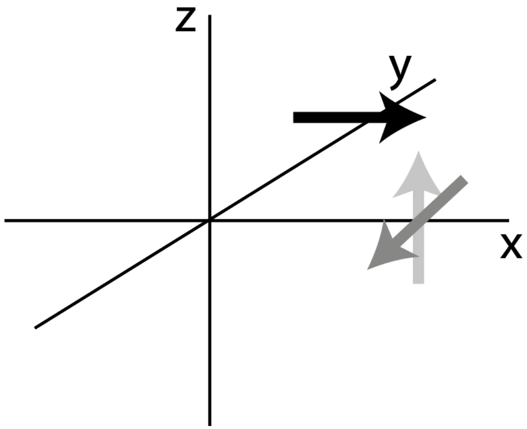
rotate 90° around **z** +
90° around **x**

Finite Rotation “Vector”

If **a** and **b** are two general vectors, then **a+b=b+a**

However, addition of two finite rotations is not commutative.

Finite rotation is pseudo-vector
Infinitesimal rotation is vector



rotate 90° around **x** +
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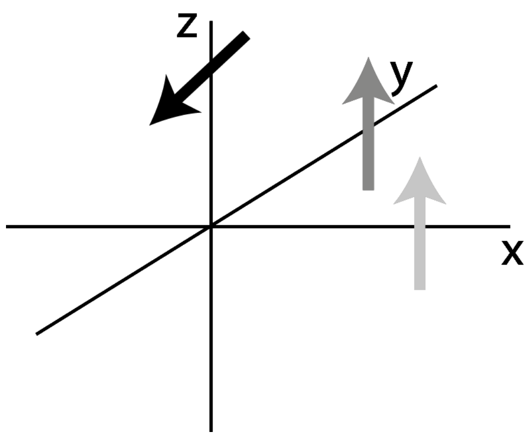


rotate 90° around **z** +
90° around **x**

Linear independence

Vectors $\mathbf{v}_1$ through $\mathbf{v}_n$ are linearly dependent if coefficients c_i can be found such that:

$$c_1\mathbf{v}_1 + c_2\mathbf{v}_2 + c_3\mathbf{v}_3 + \ldots + c_n\mathbf{v}_n = \mathbf{0}$$

where not $c_i \neq 0$

1. If two vectors are linearly dependent, they are?
2. If three vectors are all linearly dependent, they are?
3. Four or more vectors are always linearly dependent

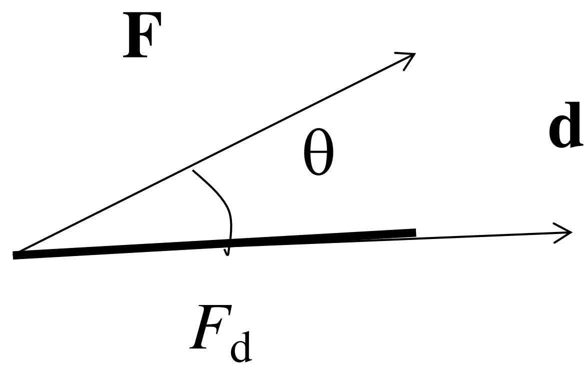
*More in **Exercise 2***

Important for defining bases, independent solutions to a problem

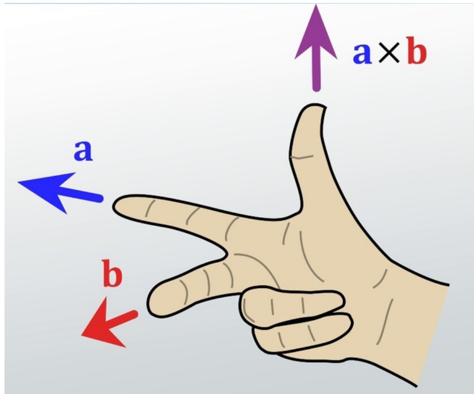
Inner product, dot product, scalar product

Geometric definition

- $\mathbf{F} \cdot \mathbf{d} = |\mathbf{F}||\mathbf{d}|\cos\theta$
  - scalar,
  - projection of **F** on **d** times |**d**|,
  - = 0 if **F** and **d** perpendicular,
  - **F·d = d·F**



- If **F** is force, **d** is displacement, then **F·d** is the work done by the force **F** for displacement **d**
- **a·a=** length(**a**)^2= $|\mathbf{a}|^2$

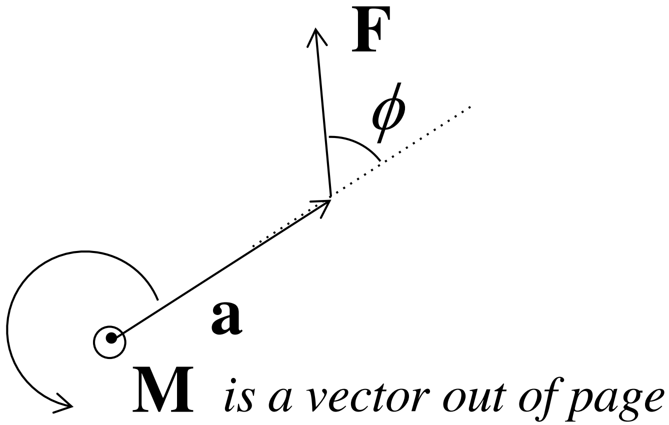


Cross product, vector product, outer product

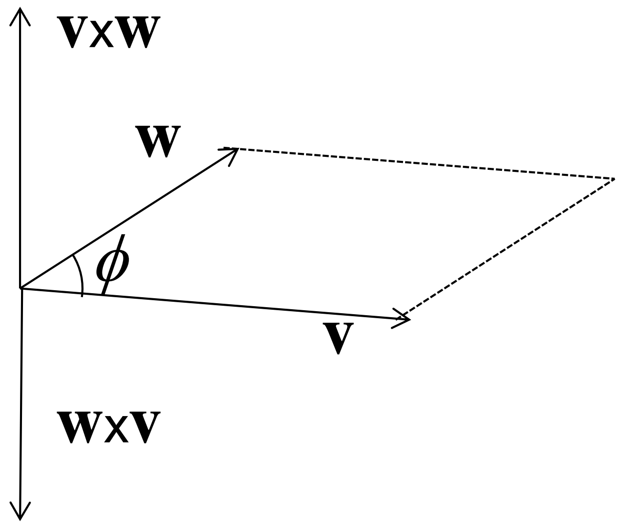
Geometric definition

- Example moment:

$$\mathbf{M} = \mathbf{a} \times \mathbf{F} = aF \sin\phi \hat{\mathbf{e}}_M$$



- Properties **vxw**
  - vector
  - magnitude = area of parallellogram spanned by **v**, **w**
  - direction is that of plane normal (right-hand rule)
  - = 0 if **v** and **w** are parallel
  - **vxw** = − **vxw**



Products of vectors

Algebraic, in rectangular Cartesian coordinates:

in 2D

$$\mathbf{v}\cdot\mathbf{w} = v_1 w_1 + v_2 w_2 \qquad \mathbf{v}\times\mathbf{w} = (v_1 w_2 - v_2 w_1)\hat{\mathbf{e}}_3$$

in 3D

$$\mathbf{v}\cdot\mathbf{w} = v_1 w_1 + v_2 w_2 + v_3 w_3$$

$$\mathbf{v}\times\mathbf{w} = \begin{pmatrix} v_2 w_3 - v_3 w_2 \\ v_3 w_1 - v_1 w_3 \\ v_1 w_2 - v_2 w_1 \end{pmatrix}$$

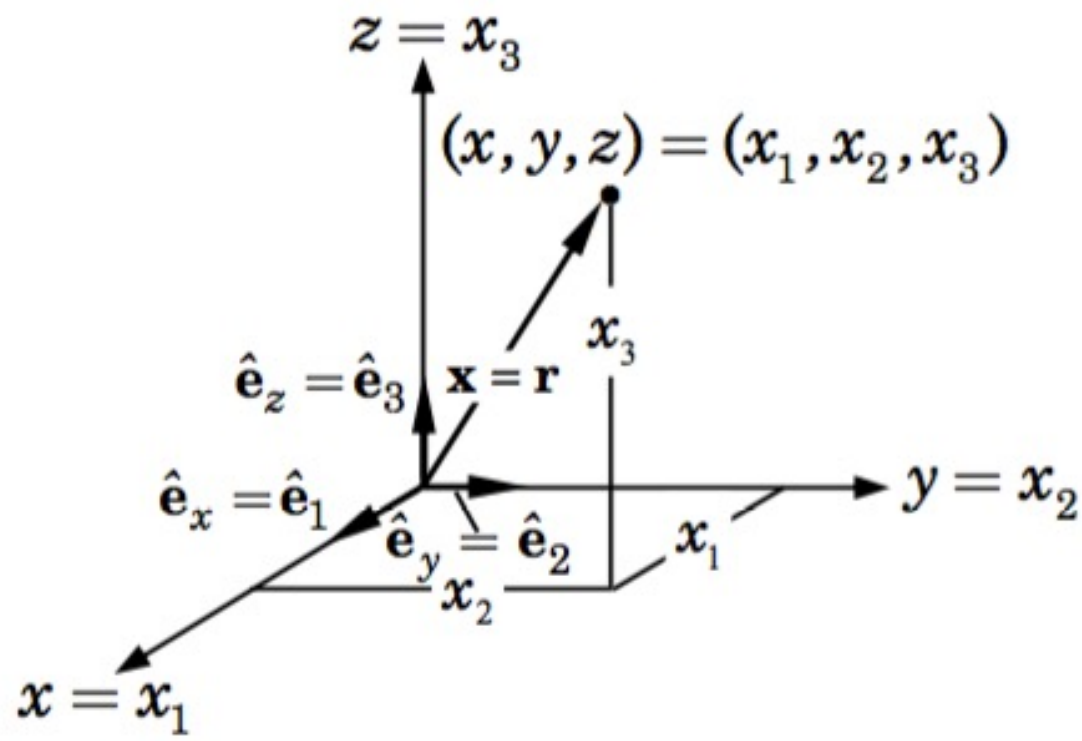
Rectangular Cartesian Coordinate System

Orthonormal basis –
Basis vectors are:
orthogonal

$\hat{\mathbf{e}}_i \cdot \hat{\mathbf{e}}_j = 0$ if i≠j

and unit length

$\hat{\mathbf{e}}_i \cdot \hat{\mathbf{e}}_i = |\hat{\mathbf{e}}_i|^2 = 1$



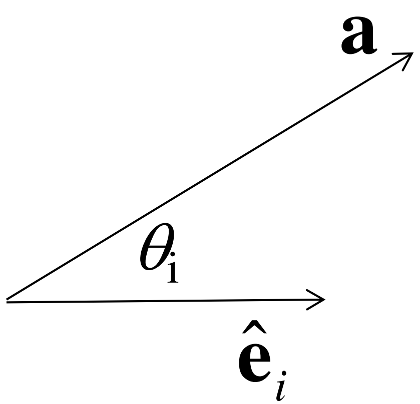
Cartesian – basis vectors with constant length and direction

In following, we will assume Cartesian orthonormal bases

Other orthonormal bases, e.g. polar or spherical, not discussed here

	Cartesian Coordinates	Cylindrical Coordinates	Spherical Coordinates
Coordinate variables	x, y, z	r, ϕ, z	R, θ, ϕ
Vector representation $\mathbf{A} =$	$\hat{\mathbf{x}}A_x + \hat{\mathbf{y}}A_y + \hat{\mathbf{z}}A_z$	$\hat{\mathbf{r}}A_r + \hat{\boldsymbol{\phi}}A_\phi + \hat{\mathbf{z}}A_z$	$\hat{\mathbf{R}}A_R + \hat{\boldsymbol{\theta}}A_\theta + \hat{\boldsymbol{\phi}}A_\phi$
Magnitude of A $\quad |\mathbf{A}| =$	$\sqrt[+]{A_x^2 + A_y^2 + A_z^2}$	$\sqrt[+]{A_r^2 + A_\phi^2 + A_z^2}$	$\sqrt[+]{A_R^2 + A_\theta^2 + A_\phi^2}$
Position vector $\quad \overrightarrow{OP_1} =$	$\hat{\mathbf{x}}x_1 + \hat{\mathbf{y}}y_1 + \hat{\mathbf{z}}z_1$, for $P(x_1, y_1, z_1)$	$\hat{\mathbf{r}}r_1 + \hat{\mathbf{z}}z_1$, for $P(r_1, \phi_1, z_1)$	$\hat{\mathbf{R}}R_1$, for $P(R_1, \theta_1, \phi_1)$
Base vectors properties	$\hat{\mathbf{x}} \cdot \hat{\mathbf{x}} = \hat{\mathbf{y}} \cdot \hat{\mathbf{y}} = \hat{\mathbf{z}} \cdot \hat{\mathbf{z}} = 1$ $\hat{\mathbf{x}} \cdot \hat{\mathbf{y}} = \hat{\mathbf{y}} \cdot \hat{\mathbf{z}} = \hat{\mathbf{z}} \cdot \hat{\mathbf{x}} = 0$ $\hat{\mathbf{x}} \times \hat{\mathbf{y}} = \hat{\mathbf{z}}$ $\hat{\mathbf{y}} \times \hat{\mathbf{z}} = \hat{\mathbf{x}}$ $\hat{\mathbf{z}} \times \hat{\mathbf{x}} = \hat{\mathbf{y}}$	$\hat{\mathbf{r}} \cdot \hat{\mathbf{r}} = \hat{\boldsymbol{\phi}} \cdot \hat{\boldsymbol{\phi}} = \hat{\mathbf{z}} \cdot \hat{\mathbf{z}} = 1$ $\hat{\mathbf{r}} \cdot \hat{\boldsymbol{\phi}} = \hat{\boldsymbol{\phi}} \cdot \hat{\mathbf{z}} = \hat{\mathbf{z}} \cdot \hat{\mathbf{r}} = 0$ $\hat{\mathbf{r}} \times \hat{\boldsymbol{\phi}} = \hat{\mathbf{z}}$ $\hat{\boldsymbol{\phi}} \times \hat{\mathbf{z}} = \hat{\mathbf{r}}$ $\hat{\mathbf{z}} \times \hat{\mathbf{r}} = \hat{\boldsymbol{\phi}}$	$\hat{\mathbf{R}} \cdot \hat{\mathbf{R}} = \hat{\boldsymbol{\theta}} \cdot \hat{\boldsymbol{\theta}} = \hat{\boldsymbol{\phi}} \cdot \hat{\boldsymbol{\phi}} = 1$ $\hat{\mathbf{R}} \cdot \hat{\boldsymbol{\theta}} = \hat{\boldsymbol{\theta}} \cdot \hat{\boldsymbol{\phi}} = \hat{\boldsymbol{\phi}} \cdot \hat{\mathbf{R}} = 0$ $\hat{\mathbf{R}} \times \hat{\boldsymbol{\theta}} = \hat{\boldsymbol{\phi}}$ $\hat{\boldsymbol{\theta}} \times \hat{\boldsymbol{\phi}} = \hat{\mathbf{R}}$ $\hat{\boldsymbol{\phi}} \times \hat{\mathbf{R}} = \hat{\boldsymbol{\theta}}$
Dot product $\quad \mathbf{A} \cdot \mathbf{B} =$	$A_x B_x + A_y B_y + A_z B_z$	$A_r B_r + A_\phi B_\phi + A_z B_z$	$A_R B_R + A_\theta B_\theta + A_\phi B_\phi$
Cross product $\quad \mathbf{A} \times \mathbf{B} =$	$\begin{vmatrix} \hat{\mathbf{x}} & \hat{\mathbf{y}} & \hat{\mathbf{z}} \\ A_x & A_y & A_z \\ B_x & B_y & B_z \end{vmatrix}$	$\begin{vmatrix} \hat{\mathbf{r}} & \hat{\boldsymbol{\phi}} & \hat{\mathbf{z}} \\ A_r & A_\phi & A_z \\ B_r & B_\phi & B_z \end{vmatrix}$	$\begin{vmatrix} \hat{\mathbf{R}} & \hat{\boldsymbol{\theta}} & \hat{\boldsymbol{\phi}} \\ A_R & A_\theta & A_\phi \\ B_R & B_\theta & B_\phi \end{vmatrix}$
Differential length $\quad d\mathbf{l} =$	$\hat{\mathbf{x}}\,dx + \hat{\mathbf{y}}\,dy + \hat{\mathbf{z}}\,dz$	$\hat{\mathbf{r}}\,dr + \hat{\boldsymbol{\phi}}r\,d\phi + \hat{\mathbf{z}}\,dz$	$\hat{\mathbf{R}}\,dR + \hat{\boldsymbol{\theta}}R\,d\theta + \hat{\boldsymbol{\phi}}R\sin\theta\,d\phi$
Differential surface areas	$d\mathbf{s}_x = \hat{\mathbf{x}}\,dy\,dz$ $d\mathbf{s}_y = \hat{\mathbf{y}}\,dx\,dz$ $d\mathbf{s}_z = \hat{\mathbf{z}}\,dx\,dy$	$d\mathbf{s}_r = \hat{\mathbf{r}}r\,d\phi\,dz$ $d\mathbf{s}_\phi = \hat{\boldsymbol{\phi}}\,dr\,dz$ $d\mathbf{s}_z = \hat{\mathbf{z}}r\,dr\,d\phi$	$d\mathbf{s}_R = \hat{\mathbf{R}}R^2\sin\theta\,d\theta\,d\phi$ $d\mathbf{s}_\theta = \hat{\boldsymbol{\theta}}R\sin\theta\,dR\,d\phi$ $d\mathbf{s}_\phi = \hat{\boldsymbol{\phi}}R\,dR\,d\theta$
Differential volume $\quad dV =$	$dx\,dy\,dz$	$r\,dr\,d\phi\,dz$	$R^2\sin\theta\,dR\,d\theta\,d\phi$

Equivalence Cartesian geometric and algebraic dot product



$$\mathbf{a} = \sum_i a_i \hat{\mathbf{e}}_i \qquad \mathbf{b} = \sum_i b_i \hat{\mathbf{e}}_i$$

$$\mathbf{a} \cdot \hat{\mathbf{e}}_i = |\mathbf{a}||\hat{\mathbf{e}}_i| \cos \vartheta_i = |\mathbf{a}| \cos \vartheta_i = a_i$$

$$\mathbf{a} \cdot \mathbf{b} = \mathbf{a} \cdot \sum_i b_i \hat{\mathbf{e}}_i = \sum_i b_i (\mathbf{a} \cdot \hat{\mathbf{e}}_i) = \sum_i b_i a_i = \sum_i a_i b_i$$

Products of vectors

Algebraic, in rectangular Cartesian coordinates:

in 2D

$$\mathbf{v} \cdot \mathbf{w} = v_1 w_1 + v_2 w_2$$

in 3D

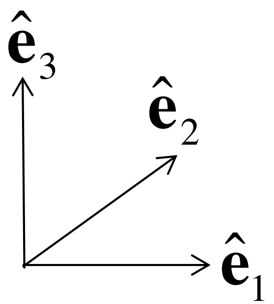
$$\mathbf{v} \cdot \mathbf{w} = v_1 w_1 + v_2 w_2 + v_3 w_3$$

Cartesian algebraic cross product

$$\hat{\mathbf{e}}_i \times \hat{\mathbf{e}}_i = 0 \qquad \begin{array}{ll} \hat{\mathbf{e}}_1 \times \hat{\mathbf{e}}_2 = \hat{\mathbf{e}}_3 & \hat{\mathbf{e}}_2 \times \hat{\mathbf{e}}_1 = -\hat{\mathbf{e}}_3 \\ \hat{\mathbf{e}}_2 \times \hat{\mathbf{e}}_3 = \hat{\mathbf{e}}_1 & \hat{\mathbf{e}}_3 \times \hat{\mathbf{e}}_2 = -\hat{\mathbf{e}}_1 \\ \hat{\mathbf{e}}_3 \times \hat{\mathbf{e}}_1 = \hat{\mathbf{e}}_2 & \hat{\mathbf{e}}_1 \times \hat{\mathbf{e}}_3 = -\hat{\mathbf{e}}_2 \end{array}$$

In 2-D:

$$\begin{aligned} \mathbf{a} \times \mathbf{b} &= (a_1\hat{\mathbf{e}}_1 + a_2\hat{\mathbf{e}}_2) \times (b_1\hat{\mathbf{e}}_1 + b_2\hat{\mathbf{e}}_2) \\ &= a_1 b_1(\hat{\mathbf{e}}_1 \times \hat{\mathbf{e}}_1) + a_1 b_2(\hat{\mathbf{e}}_1 \times \hat{\mathbf{e}}_2) \\ &\quad + a_2 b_1(\hat{\mathbf{e}}_2 \times \hat{\mathbf{e}}_1) + a_2 b_2(\hat{\mathbf{e}}_2 \times \hat{\mathbf{e}}_2) \\ &= (a_1 b_2 - a_2 b_1)\hat{\mathbf{e}}_3 \end{aligned}$$



Products of vectors

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in 3D

$$\mathbf{v}\cdot\mathbf{w} = v_1 w_1 + v_2 w_2 + v_3 w_3$$

$$\mathbf{v}\times\mathbf{w} = \begin{pmatrix} v_2 w_3 - v_3 w_2 \\ v_3 w_1 - v_1 w_3 \\ v_1 w_2 - v_2 w_1 \end{pmatrix}$$

Triple products

- $\mathbf{a}(\mathbf{b}\cdot\mathbf{c})$ – vector times scalar
- scalar triple product $\mathbf{a}\cdot(\mathbf{b}\times\mathbf{c})$

$$
\begin{aligned}
\mathbf{a}\cdot(\mathbf{b}\times\mathbf{c}) &= (\mathbf{a}\times\mathbf{b})\cdot\mathbf{c} \\
&= \mathbf{c}\cdot(\mathbf{a}\times\mathbf{b}) = \mathbf{b}\cdot(\mathbf{c}\times\mathbf{a}) \text{ (with cyclical permutation)} \\
&= -\,\mathbf{a}\cdot(\mathbf{c}\times\mathbf{b}) = -\,\mathbf{c}\cdot(\mathbf{b}\times\mathbf{a}) = -\,\mathbf{b}\cdot(\mathbf{a}\times\mathbf{c}) \\
&\qquad\qquad \text{(with order changed)} \\
&= 0 \text{ if } \mathbf{a}, \mathbf{b}, \mathbf{c} \text{ coplanar}
\end{aligned}
$$

- $\mathbf{a}\times(\mathbf{b}\times\mathbf{c})$ – lies in plane formed by $\mathbf{b} \times \mathbf{c}$; normal to $\mathbf{a}$

$$
\begin{aligned}
&\neq (\mathbf{a}\times\mathbf{b})\times\mathbf{c} \\
&= (\mathbf{a}\cdot\mathbf{c})\mathbf{b} - (\mathbf{a}\cdot\mathbf{b})\mathbf{c}
\end{aligned}
$$

Exercise 8

Covered so far

- Revision of main characteristics of a vector
- Linear independence of vectors
- Vector products: dot product, cross product
- Definition Cartesian orthonormal basis

Please take a break
then try yourself

- If the material covered so far was all familiar, please skip to **Exercise 2** in the notebook

- If you would benefit from recapping vector products, please look at **Exercise 1** first