



L5 - Classical Mechanics 1

Newton's Laws

A quick math remainder

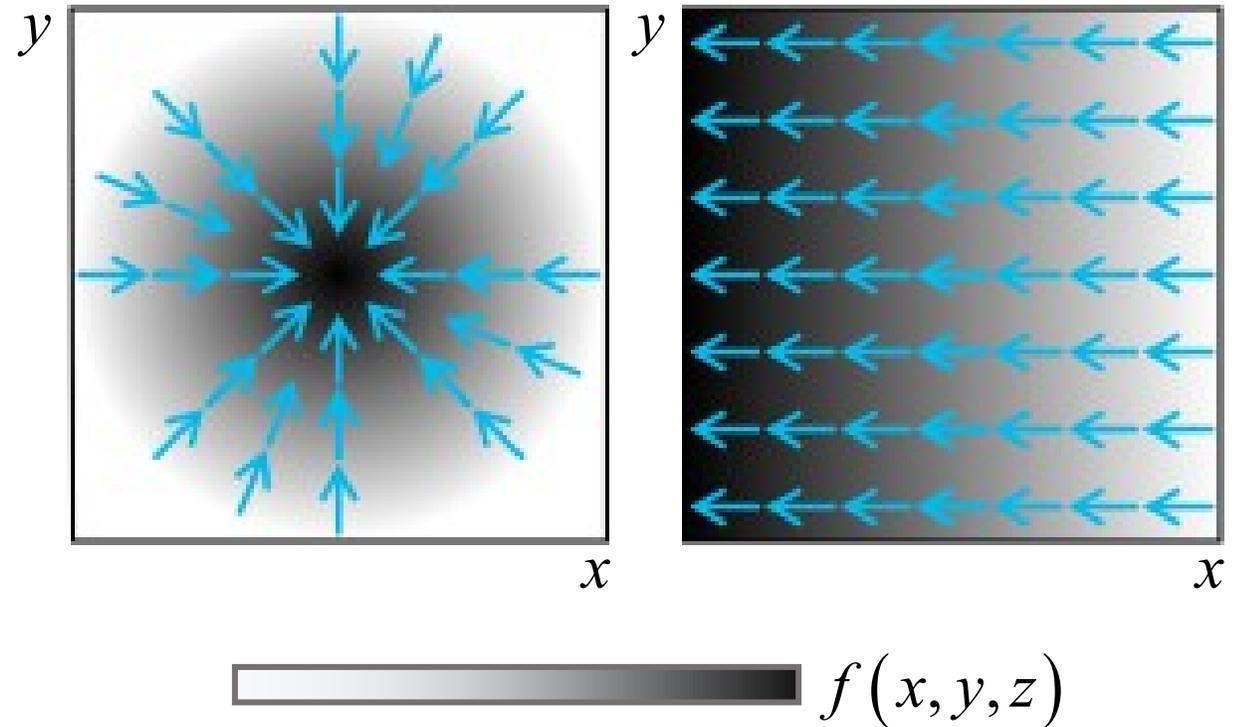
The gradient of a function

Suppose we have a scalar function

$$f(x, y, z)$$

The gradient of f is the vector

$$\nabla f(x, y, z) = \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z} \right) = \vec{\mathbf{g}}(x, y, z)$$



Example: Consider the function

$$f(x, y, z) = -\sqrt{x^2 + y^2 + z^2}$$

The gradient is

$$\nabla f = \left(-\frac{x}{\sqrt{x^2 + y^2 + z^2}}, -\frac{y}{\sqrt{x^2 + y^2 + z^2}}, -\frac{z}{\sqrt{x^2 + y^2 + z^2}} \right)$$

The cross product of two vectors

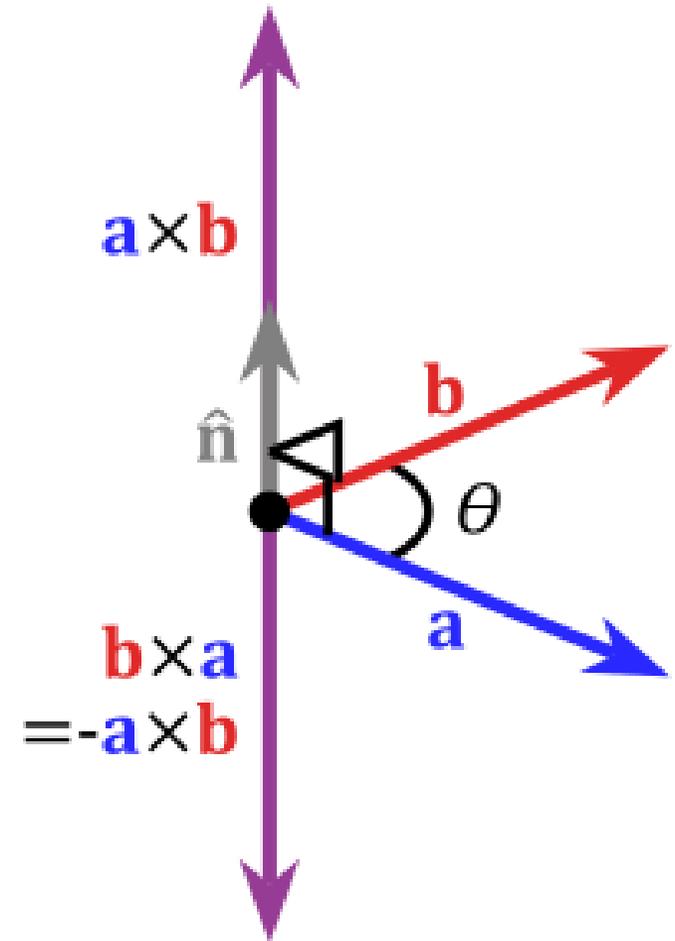
Suppose we have two vectors **a** and **b**

If their norms are

$$\|\mathbf{a}\| = \sqrt{a_x^2 + a_y^2 + a_z^2} \quad \|\mathbf{b}\| = \sqrt{b_x^2 + b_y^2 + b_z^2}$$

Their cross product is

$$\mathbf{a} \times \mathbf{b} = \|\mathbf{a}\| \|\mathbf{b}\| \sin(\theta) \hat{\mathbf{n}}$$



Mechanics of a particle

Consider a single particle with mass m and position \mathbf{r} .

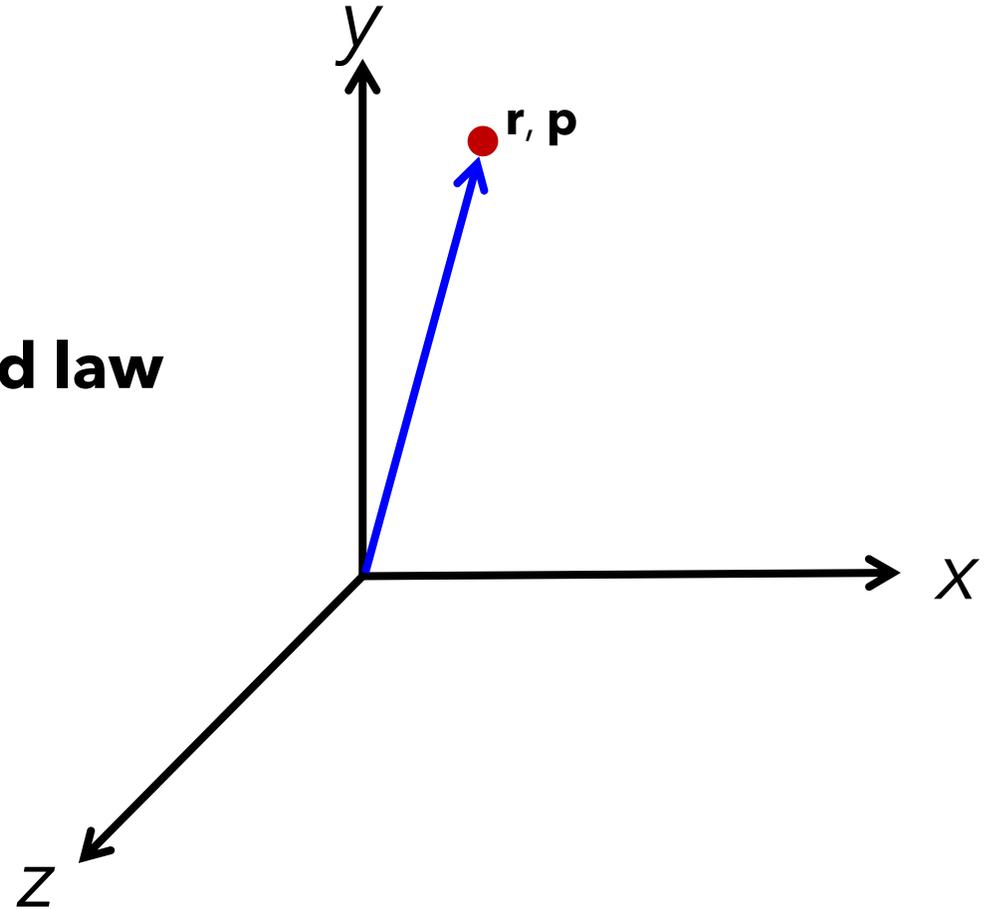
The velocity is $\mathbf{v} \equiv \frac{d\mathbf{r}}{dt}$

The linear momentum is $\mathbf{p} \equiv m\mathbf{v}$

The motion is determined by **Newton's second law**

$$\frac{d\mathbf{p}}{dt} = \mathbf{F}$$

\mathbf{F} is a force acting on the particle.



The acceleration is defined as:

$$\mathbf{a} \equiv \frac{d^2 \mathbf{r}}{dt^2}$$

If the mass is constant, Newton's second law becomes $\mathbf{F} = m\mathbf{a}$

$$\frac{d\mathbf{p}}{dt} = \mathbf{F}$$

$$\frac{d\mathbf{p}}{dt} = \frac{d(m\mathbf{v})}{dt} = m \frac{d\mathbf{v}}{dt} = m \frac{d}{dt} \left(\frac{d\mathbf{r}}{dt} \right) = m \frac{d^2 \mathbf{r}}{dt^2} = m\mathbf{a}$$

$$m\mathbf{a} = \mathbf{F}$$

Newton's second law

$$\frac{d^2 \mathbf{r}}{dt^2} = \frac{\mathbf{F}}{m}$$

Newton's second law is valid in an inertial or Galilean system.

Conservation of linear momentum of a particle

If the total force \mathbf{F} is zero, then the linear momentum \mathbf{p} is conserved

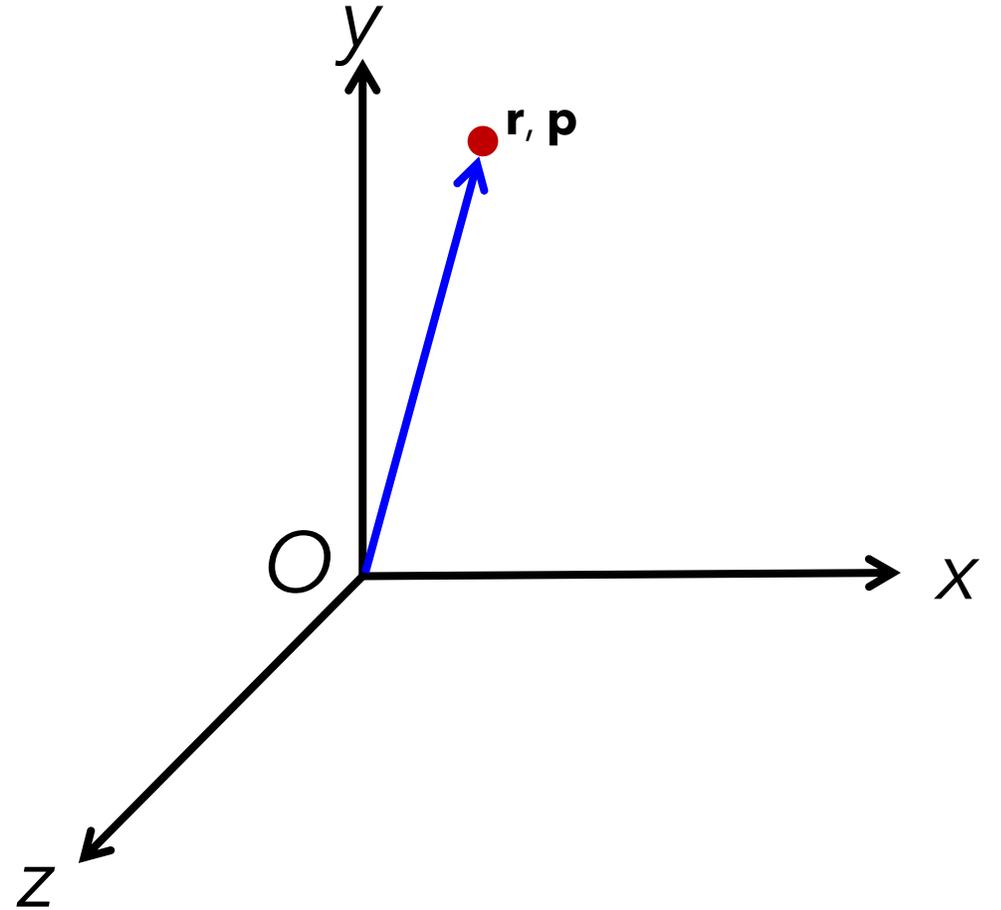
$$\frac{d\mathbf{p}}{dt} = 0 \rightarrow \mathbf{p} \text{ is a constant (Newton's first law)}$$

The angular momentum about O is

$$\mathbf{L} \equiv \mathbf{r} \times \mathbf{p}$$

The torque about O is

$$\mathbf{N} \equiv \mathbf{r} \times \mathbf{F}$$



To get the angular equation of motion

$$\frac{d(m\mathbf{v})}{dt} = \mathbf{F}$$

$$\mathbf{r} \times \frac{d(m\mathbf{v})}{dt} = \mathbf{r} \times \mathbf{F}$$

$$\frac{d(\mathbf{r} \times m\mathbf{v})}{dt} = \underbrace{\mathbf{v} \times m\mathbf{v}}_0 + \mathbf{r} \times \frac{d(m\mathbf{v})}{dt} = \mathbf{r} \times \frac{d(m\mathbf{v})}{dt}$$

$$\frac{d(\mathbf{r} \times m\mathbf{v})}{dt} = \mathbf{r} \times \mathbf{F}$$

$$\frac{d\mathbf{L}}{dt} = \mathbf{N}$$

Conservation of angular momentum of a particle

If the total torque \mathbf{N} is zero, then the angular momentum \mathbf{L} is conserved

$$\frac{d\mathbf{L}}{dt} = 0 \rightarrow \mathbf{L} \text{ is a constant}$$

The work done to move the particle from 1 to 2 along \mathbf{s} is

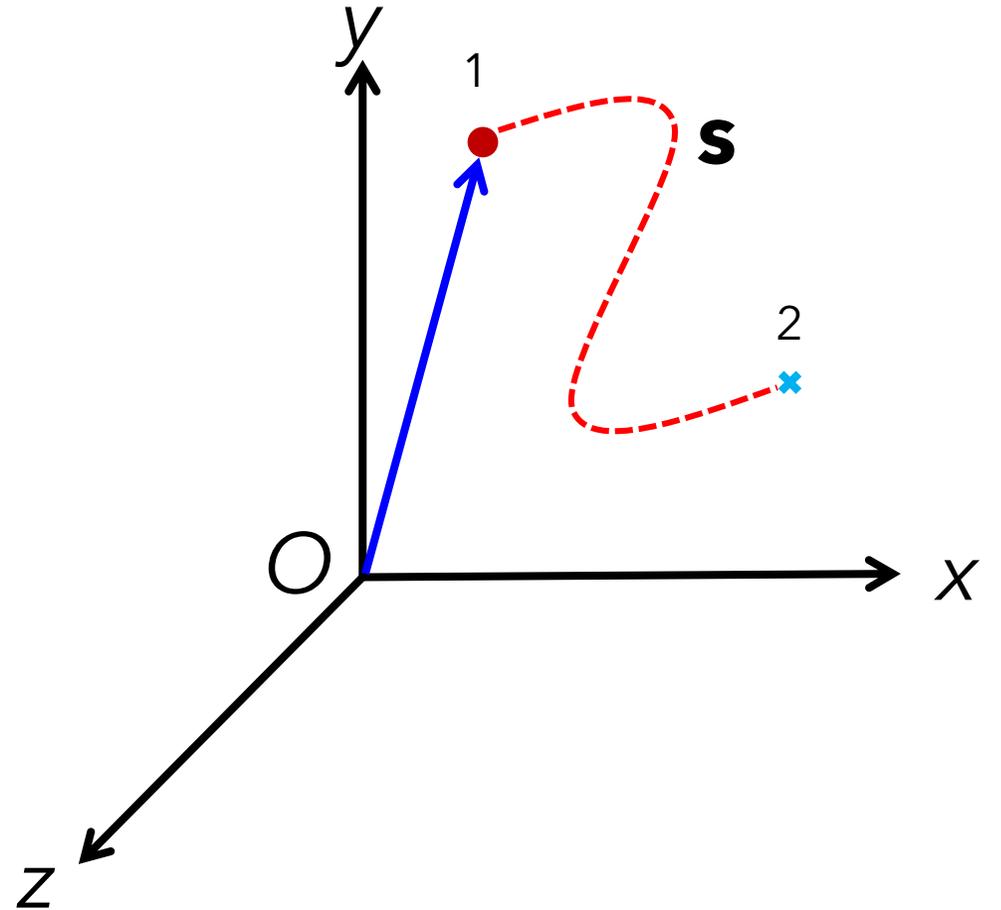
$$W_{12} \equiv \int_1^2 \mathbf{F} \cdot d\mathbf{s}$$

If the mass is constant

$$W_{12} = \int_1^2 \mathbf{F} \cdot d\mathbf{s} = m \int_1^2 \frac{d\mathbf{v}}{dt} \cdot \mathbf{v} dt$$

$$\frac{d\mathbf{v}}{dt} \cdot \mathbf{v} = \frac{1}{2} \frac{d}{dt} \mathbf{v}^2$$

$$W_{12} = \frac{1}{2} m \int_1^2 \left(\frac{d}{dt} \mathbf{v}^2 \right) dt = \frac{1}{2} m (\mathbf{v}_2^2 - \mathbf{v}_1^2)$$

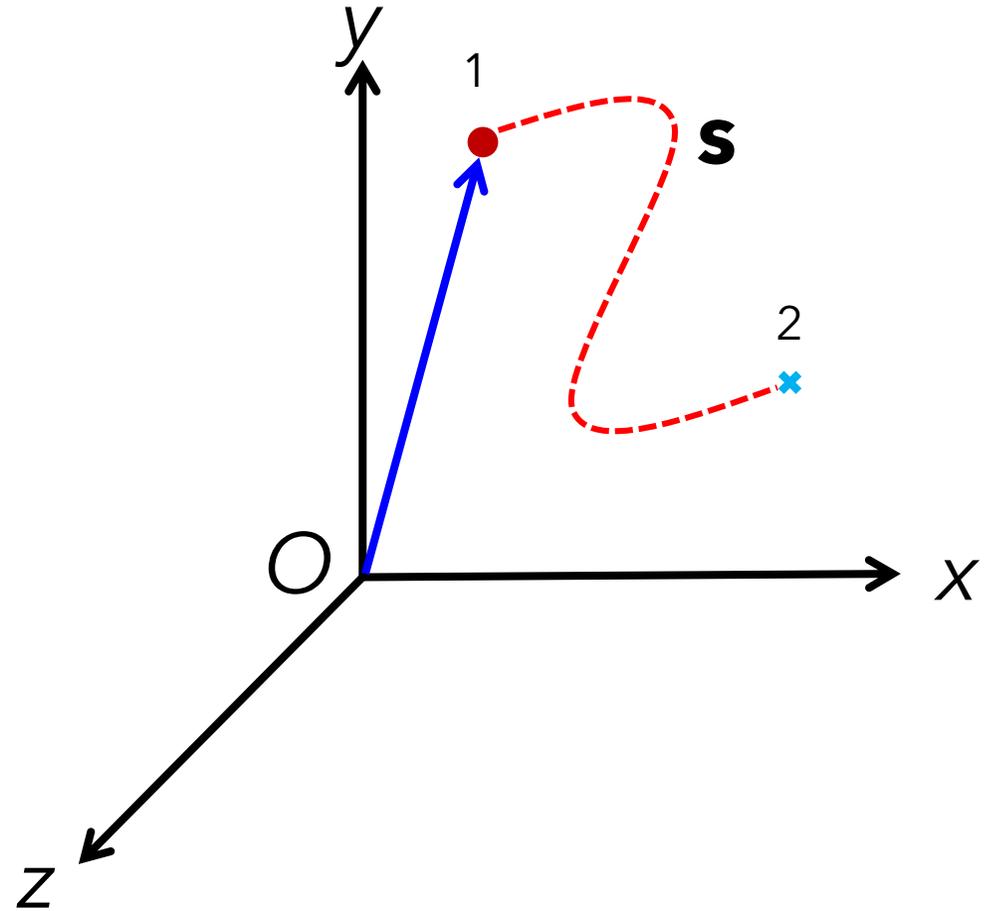


The kinetic energy is defined as

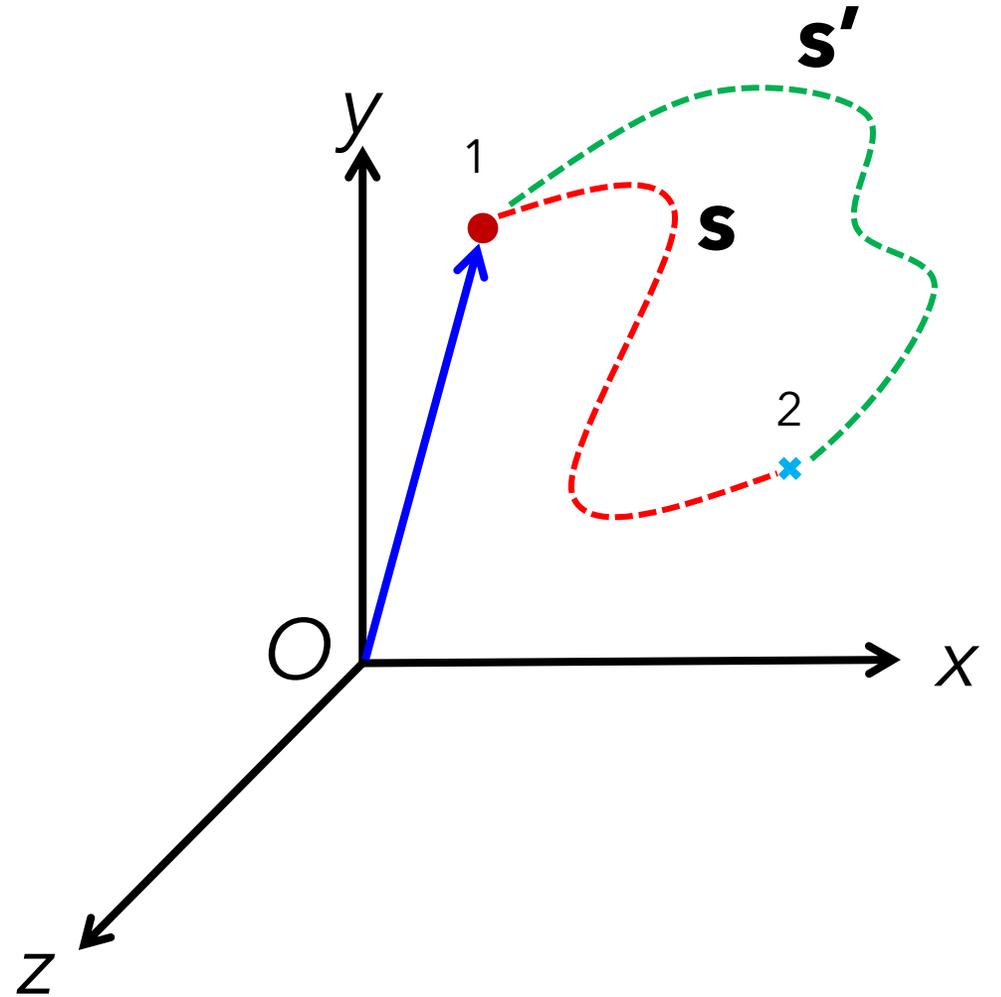
$$T \equiv \frac{1}{2} m \mathbf{v}^2$$

The work is the variation of kinetic energy

$$\begin{aligned} W_{12} &= \frac{1}{2} m (\mathbf{v}_2^2 - \mathbf{v}_1^2) \\ &= T_2 - T_1 \end{aligned}$$

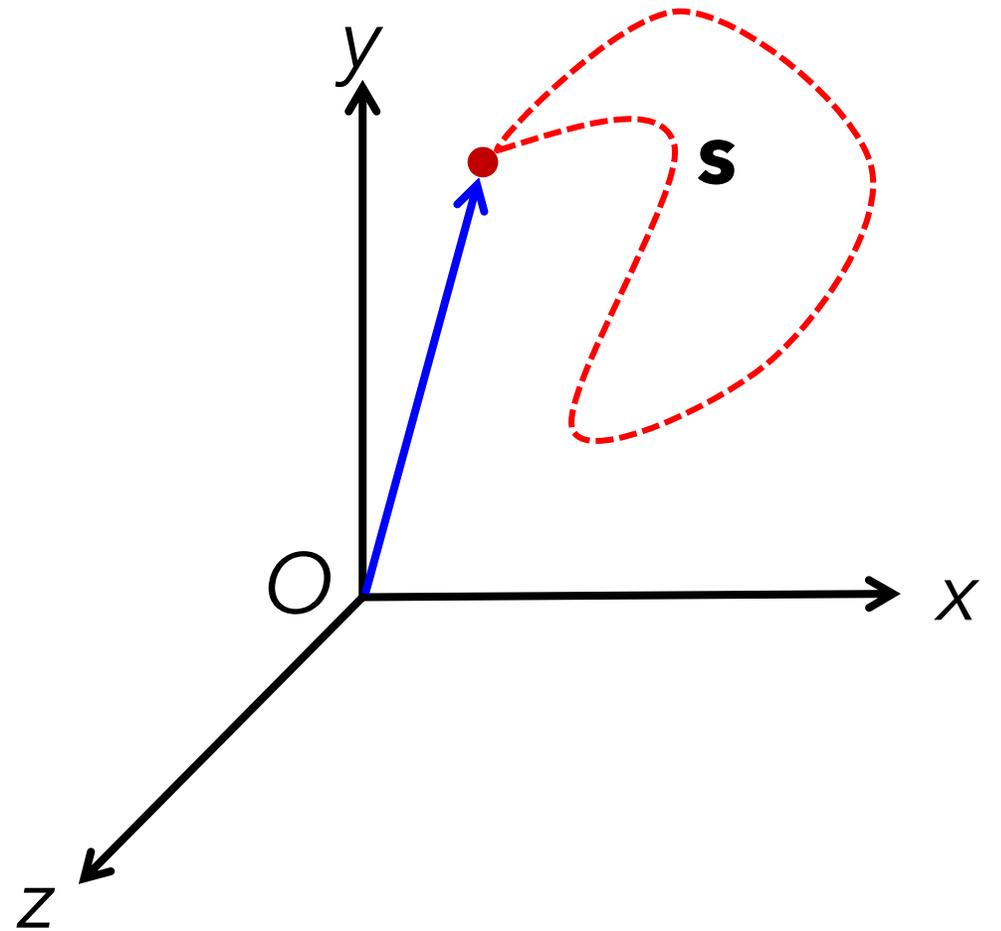


If \mathbf{F} is such that W_{12} is always the same no matter \mathbf{s} ,
 \mathbf{F} is called **conservative**.



F is conservative if

$$\oint \mathbf{F} \cdot d\mathbf{s} = 0$$



If \mathbf{F} is conservative, it can be written as the negative of the gradient of a scalar potential V that depends only on \mathbf{r} .

$$\mathbf{F} = -\nabla V(\mathbf{r})$$

The work in terms of the potential is

$$W_{12} = \int_1^2 \mathbf{F} \cdot d\mathbf{s} = -\int_1^2 \nabla V(\mathbf{r}) \cdot d\mathbf{s} = V_1 - V_2$$

We have

$$W_{12} = V_1 - V_2 = T_2 - T_1$$

Thus

$$T_1 + V_1 = T_2 + V_2$$

Energy conservation for a particle

If \mathbf{F} is conservative, then the $E = T + V$ is constant.

Mechanics of a *system* of particles

Consider a system of **2 isolated particles**

The total momentum is $\mathbf{p} = \mathbf{p}_1 + \mathbf{p}_2$

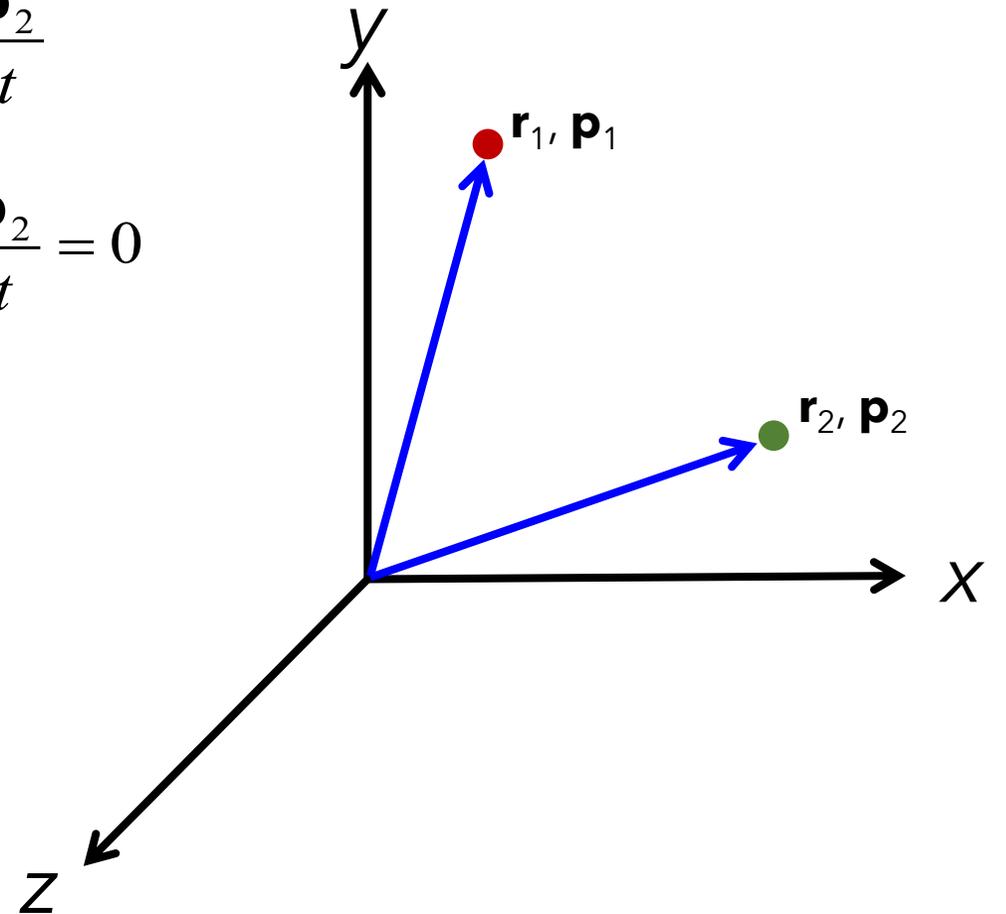
The total momentum variation is $\frac{d\mathbf{p}}{dt} = \frac{d\mathbf{p}_1}{dt} + \frac{d\mathbf{p}_2}{dt}$

If the two particles are isolated: $\frac{d\mathbf{p}}{dt} = \frac{d\mathbf{p}_1}{dt} + \frac{d\mathbf{p}_2}{dt} = 0$

Therefore, $\frac{d\mathbf{p}_1}{dt} = -\frac{d\mathbf{p}_2}{dt}$

For each body, $\frac{d\mathbf{p}_1}{dt} = \mathbf{F}_{21}$ and $\frac{d\mathbf{p}_2}{dt} = \mathbf{F}_{12}$

Thus, $\mathbf{F}_{21} = -\mathbf{F}_{12}$ (**Newton's third law**)



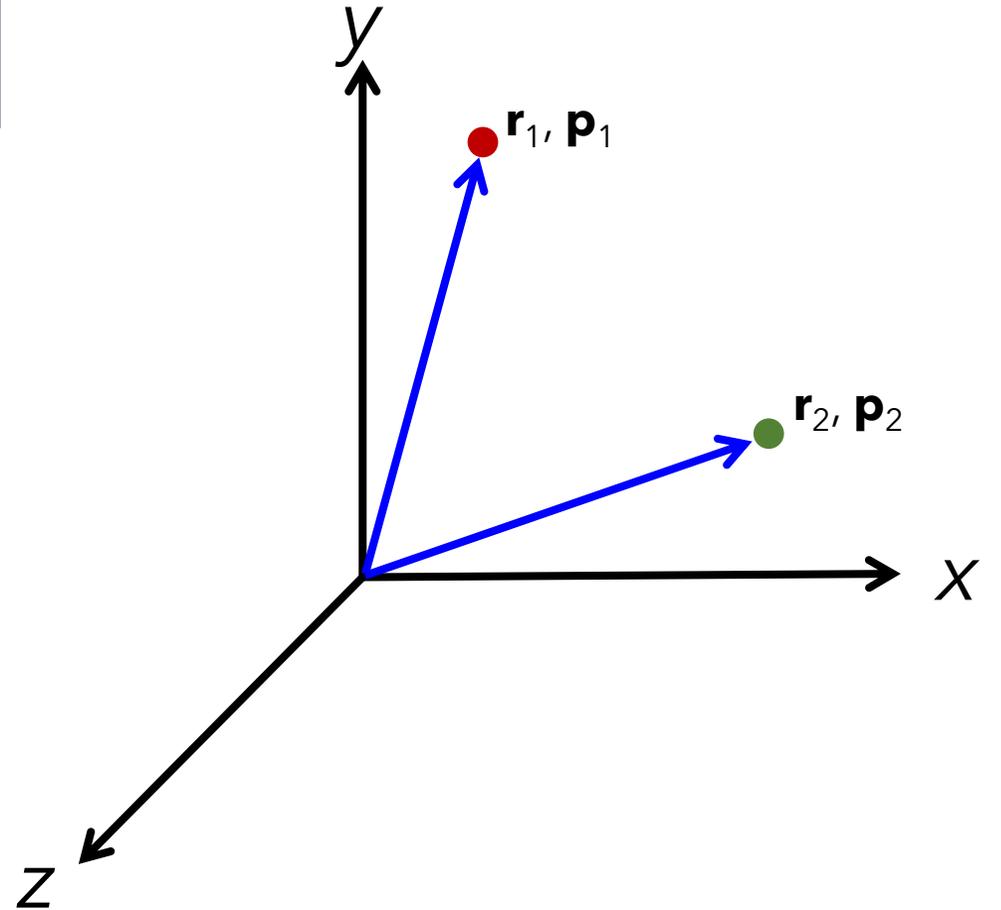
Consider a system of **N particles**

Newton's second law determines the motion of particle i

$$\frac{d\mathbf{p}_i}{dt} = \sum_{j=1(\neq i)}^N [\mathbf{F}_{ji} + \mathbf{F}_i^{(e)}]$$

\mathbf{F}_{ji} is the force on i due to j

$\mathbf{F}_i^{(e)}$ is an external force



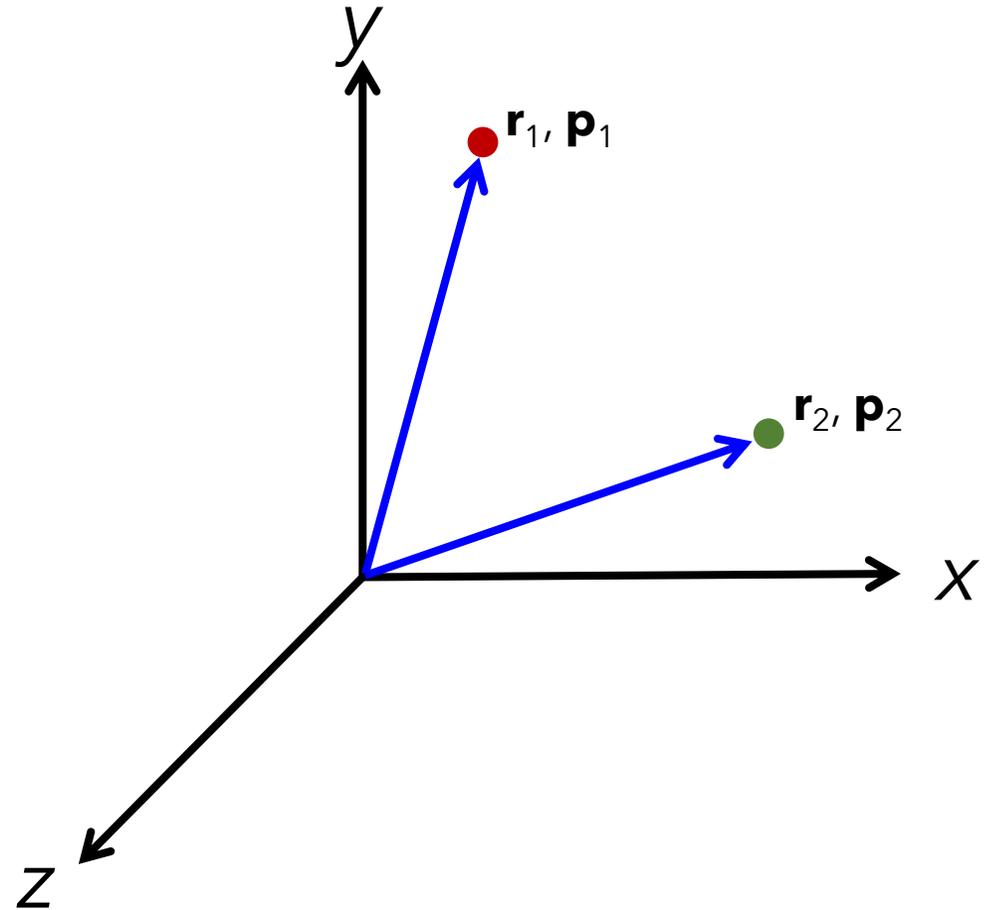
The center of mass

Sum over all particles

$$\sum_{i=1}^N m_i \frac{d^2 \mathbf{r}_i}{dt^2} = \sum_{i=1}^N \left[\sum_{j=1(\neq i)}^N \left[\mathbf{F}_{ji} + \mathbf{F}_i^{(e)} \right] \right]$$

Because $\mathbf{F}_{ji} = -\mathbf{F}_{ij}$

$$\sum_{i=1}^N m_i \frac{d^2 \mathbf{r}_i}{dt^2} = \sum_{i=1}^N \mathbf{F}_i^{(e)} = \mathbf{F}^{(e)}$$



$$\sum_{i=1}^N m_i \frac{d^2 \mathbf{r}_i}{dt^2} = \mathbf{F}^{(e)}$$

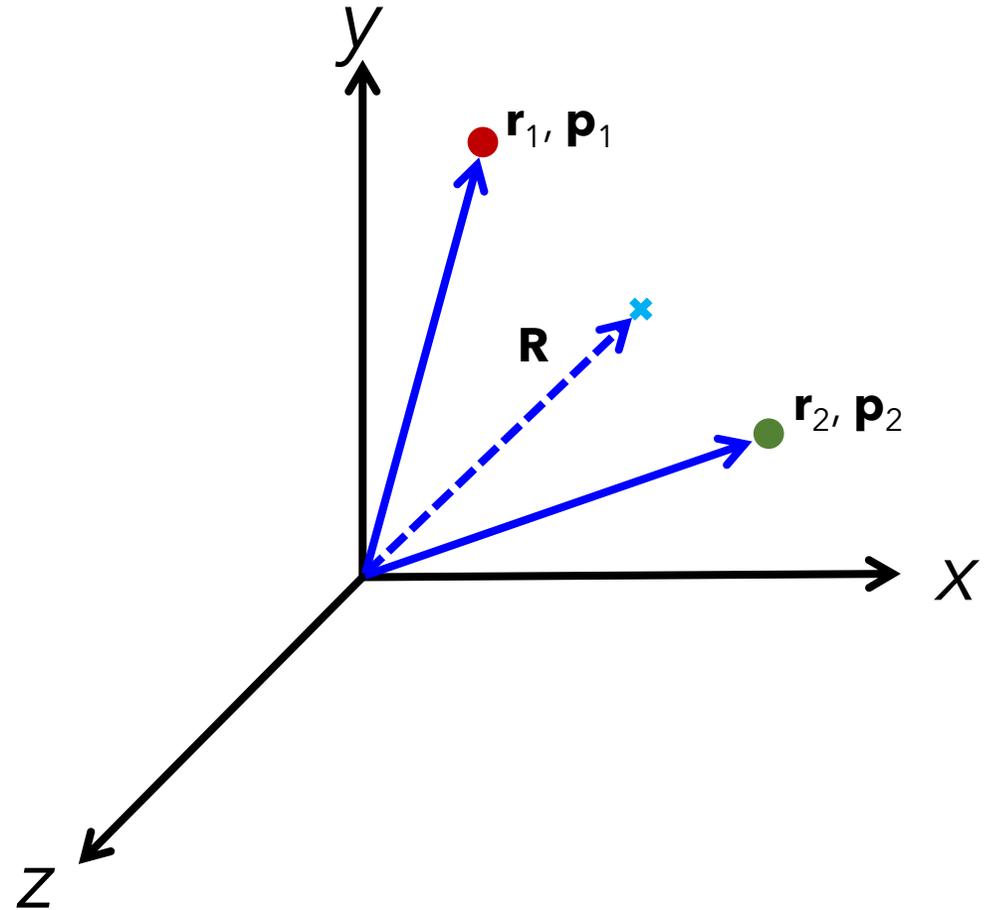
$$\sum_{i=1}^N m_i \frac{d^2 \mathbf{r}_i}{dt^2} = \frac{d^2}{dt^2} \sum_{i=1}^N m_i \mathbf{r}_i$$

$$= M \frac{d^2}{dt^2} \left(\frac{1}{M} \sum_{i=1}^N m_i \mathbf{r}_i \right) \quad M \equiv \sum_{i=1}^N m_i$$

$$= M \frac{d^2 \mathbf{R}}{dt^2}$$

Position of the center of mass

$$\mathbf{R} \equiv \frac{1}{M} \sum_{i=1}^N m_i \mathbf{r}_i$$



Using:

$$\sum_{i=1}^N m_i \frac{d^2 \mathbf{r}_i}{dt^2} = \sum_{i=1}^N \mathbf{F}_i^{(e)} = \mathbf{F}^{(e)} \quad \text{and} \quad \sum_{i=1}^N m_i \frac{d^2 \mathbf{r}_i}{dt^2} = M \frac{d^2 \mathbf{R}}{dt^2}$$

We get Newton's second law for the sum over all particles

$$M \frac{d^2 \mathbf{R}}{dt^2} = \mathbf{F}^{(e)}$$

"The center of mass moves as if the total external force were acting on the entire mass of the system concentrated at the center of mass."

Conservation of linear momentum of a system of particles

Momentum of the center of mass (total mass is constant)

$$M \frac{d^2 \mathbf{R}}{dt^2} = \mathbf{F}^{(e)}$$
$$\frac{d}{dt} \left(M \frac{d\mathbf{R}}{dt} \right) = \frac{d\mathbf{P}}{dt} = \mathbf{F}^{(e)}$$

If the total external force is zero, the total linear momentum is conserved.

$$\frac{d\mathbf{P}}{dt} = 0 \rightarrow \mathbf{P} \text{ is constant}$$

Conservation of angular momentum of a system of particles under central forces

For central forces, the total angular momentum is related to the total external torque through

$$\frac{d\mathbf{L}}{dt} = \mathbf{N}^{(e)}$$

See the demonstration in the appendix to the presentation

Therefore, if the total external torque is zero, the total angular momentum is conserved.

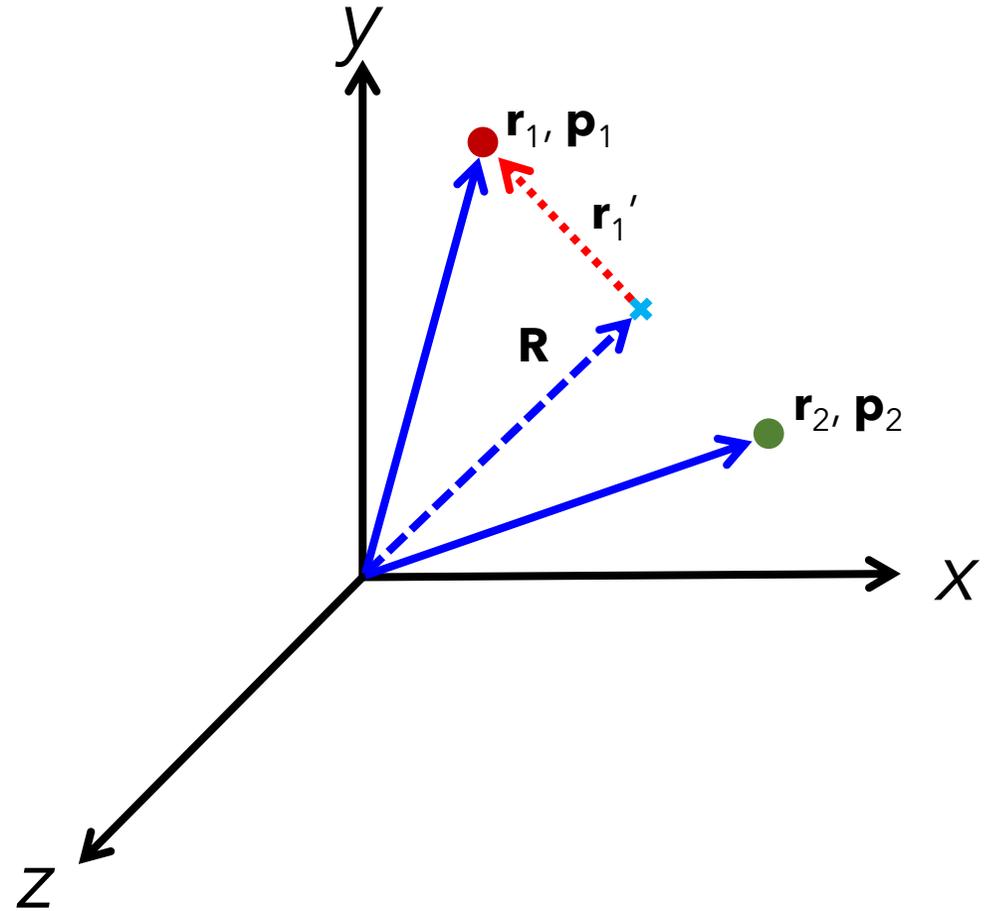
$$\frac{d\mathbf{L}}{dt} = 0 \rightarrow \mathbf{L} \text{ is constant}$$

Lab (absolute) reference and center of mass reference:

$$\mathbf{r}_i = \mathbf{r}'_i + \mathbf{R}$$

$$\frac{d\mathbf{r}_i}{dt} = \frac{d\mathbf{r}'_i}{dt} + \frac{d\mathbf{R}}{dt}$$

$$\mathbf{v}_i = \mathbf{v}'_i + \mathbf{v}$$



We can show that

$$\mathbf{L} = \sum_i \mathbf{r}'_i \times \mathbf{p}'_i + \mathbf{R} \times \mathbf{P}$$

See the demonstration
in the appendix to the
presentation

The angular momentum about point O is the angular momentum of the center of the mass plus the angular momentum of the motion about the center of mass.

If the center of mass is at rest, the total angular momentum does not depend on a reference point.

The total kinetic energy is the kinetic energy of the center of mass plus the kinetic energy about the center of mass.

$$T = \frac{1}{2} M \mathbf{v}^2 + \frac{1}{2} \sum_i m_i \mathbf{v}'_i{}^2$$

See the demonstration
in the appendix to the
presentation

The **work** of a system of particles is the variation of their **potential energy**

$$W_{12} = V_A - V_B$$

See the demonstration
in the appendix to the
presentation

But only if

1) the external forces are conservative

$$\mathbf{F}_i^{(e)} = -\nabla_i V_i$$

2) the internal forces are conservative and central

$$\mathbf{F}_{ji} = -\nabla V_{ij} (|\mathbf{r}_i - \mathbf{r}_j|)$$

The **work** of a system of particles is the variation of their **kinetic energy**

$$W_{12} = T_B - T_A$$

See the demonstration
in the appendix to the
presentation

Putting everything together

$$W_{12} = V_A - V_B = T_B - T_A$$

Thus

$$T_A + V_A = T_B + V_B$$

Energy conservation for a system of particles

If the external force is conservative and the internal forces are conservative and central, then $E = T + V$ is constant.

Another math remainder

Differential equations

A differential equation is an equation relating unknown functions and their derivatives.

Example:

$$\frac{df(x)}{dx} - f(x) = 0$$

What's $f(x)$ satisfying this equation?

Differential equations

More examples:

$$\frac{d^2 \mathbf{r}}{dt^2} = \frac{\mathbf{F}}{m} \quad \text{Newton's second law}$$

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H} \Psi \quad \text{Schrödinger equation}$$

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0} \quad \nabla \cdot \mathbf{B} = 0 \quad \text{Maxwell equations}$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \quad \nabla \times \mathbf{B} = \mu_0 \left(\epsilon_0 \frac{\partial \mathbf{E}}{\partial t} + \mathbf{J} \right)$$

Back to the simple example:

$$\frac{df(x)}{dx} - f(x) = 0$$

$$\frac{df(x)}{dx} = f(x) \quad \rightarrow \quad \frac{df(x)}{f(x)} = dx$$

$$\int_{f_0}^{f(x)} \frac{df'}{f'} = \int_{x_0}^x dx' \quad \rightarrow \quad \ln(f(x)) - \ln(f_0) = x - x_0$$

$$\ln\left(\frac{f(x)}{f_0}\right) = x - x_0$$

$$\frac{f(x)}{f_0} = e^{x-x_0}$$

$$\rightarrow f(x) = f_0 e^{x-x_0}$$

Most time, we can't get an analytical solution.
We must resort to numerical approximations.

For example

$$\frac{df(x)}{dx} = f(x) \quad \rightarrow \quad \frac{\Delta f(x)}{\Delta x} = f(x)$$

$$\frac{f(x + \Delta x) - f(x)}{\Delta x} = f(x)$$

$$f(x + \Delta x) = f(x)(1 + \Delta x)$$

$$f(x + \Delta x) = f(x)(1 + \Delta x)$$

Suppose

$$f(0) = 1$$

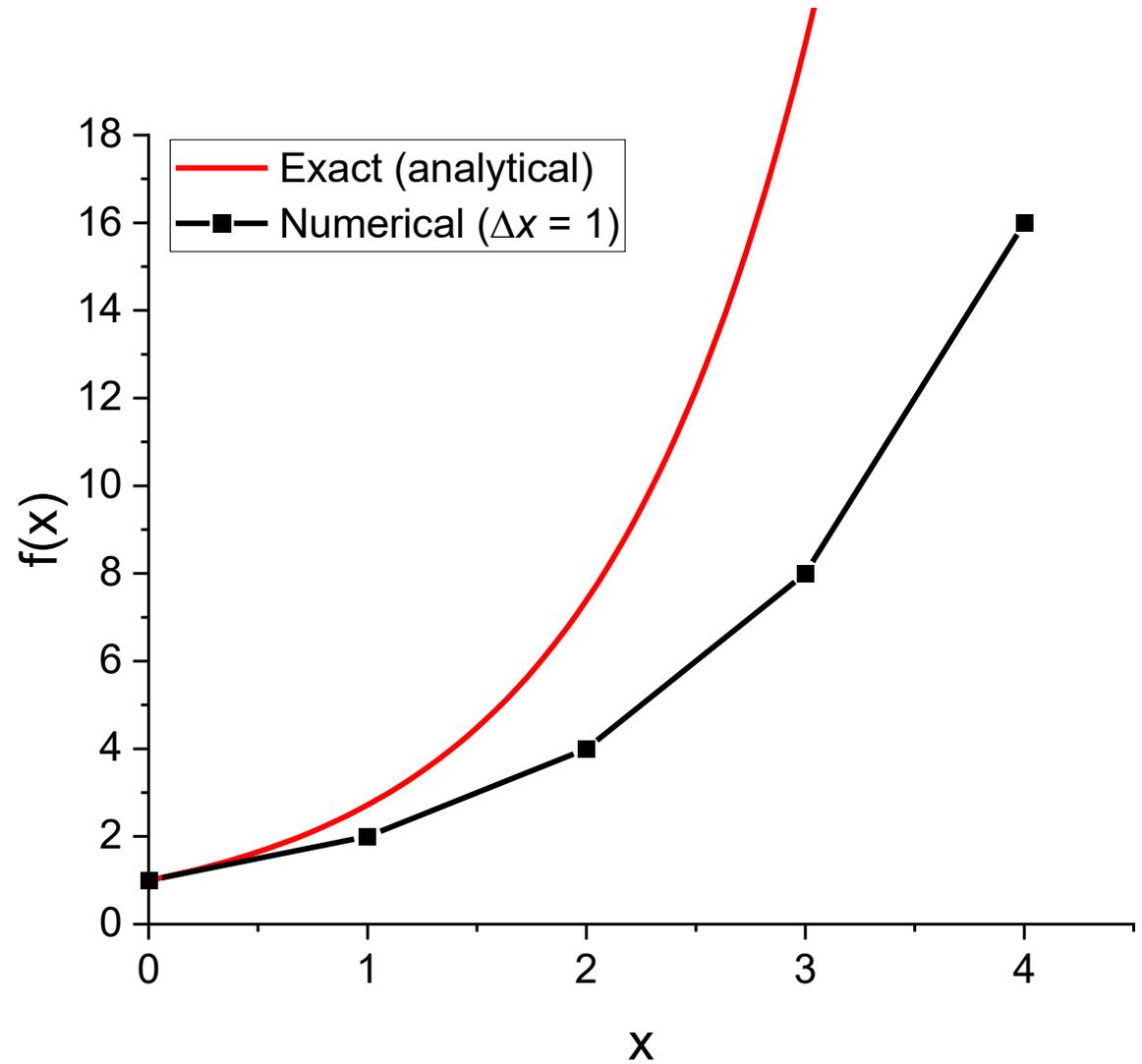
$$\Delta x = 1$$

$$f(0 + \Delta x) = f(1) = 1(1 + 1) = 2$$

$$f(1 + \Delta x) = f(2) = 2(1 + 1) = 4$$

$$f(2 + \Delta x) = f(3) = 4(1 + 1) = 8$$

$$f(3 + \Delta x) = f(4) = 8(1 + 1) = 16$$



EOM integration

Given the initial conditions \mathbf{R}_0 and \mathbf{v}_0 , we want to integrate

$$M_\alpha \frac{d^2 \mathbf{R}_\alpha}{dt^2} = \mathbf{F}_\alpha$$

where

$$\mathbf{F}_\alpha = -\nabla_\alpha E(\mathbf{R}) + \mathbf{F}^{(e)}$$

$E(\mathbf{R})$ is the Born-Oppenheimer potential energy and $\mathbf{F}^{(e)}$ are the external forces.

One of the most popular methods to integrate this differential equation is the **Velocity Verlet**.

Note that

$$M_{\alpha} \frac{d^2 \mathbf{R}_{\alpha}}{dt^2} = \mathbf{F}_{\alpha}$$

means

$$M_{\alpha} \left(\frac{d^2 x_{\alpha}}{dt^2}, \frac{d^2 y_{\alpha}}{dt^2}, \frac{d^2 z_{\alpha}}{dt^2} \right) = (F_{x,\alpha}, F_{y,\alpha}, F_{z,\alpha})$$

or yet ...

$$\begin{bmatrix} M_1 \frac{d^2 x_1}{dt^2} & M_1 \frac{d^2 y_1}{dt^2} & M_1 \frac{d^2 z_1}{dt^2} \\ M_2 \frac{d^2 x_2}{dt^2} & M_2 \frac{d^2 y_2}{dt^2} & M_2 \frac{d^2 z_2}{dt^2} \\ \vdots & \vdots & \vdots \\ M_N \frac{d^2 x_N}{dt^2} & M_N \frac{d^2 y_N}{dt^2} & M_N \frac{d^2 z_N}{dt^2} \end{bmatrix} = \begin{bmatrix} F_{1,x} & F_{1,y} & F_{1,z} \\ F_{2,x} & F_{2,y} & F_{2,z} \\ \vdots & \vdots & \vdots \\ F_{N,x} & F_{N,y} & F_{N,z} \end{bmatrix}$$

where N is the number of nuclei.

Thus, we must solve $3N$ coupled differential equations of type

$$M_\alpha \frac{d^2 x_{\alpha,i}}{dt^2} = F_{\alpha,i} \quad (x_1 = x, x_2 = y, x_3 = z)$$

Simple example

1 particle in 1 dimension

$$M \frac{d^2 x}{dt^2} = F$$

Constant force

$$F = -Mg$$

Initial conditions

$$x(0) = x_0; \quad v(0) = v_0$$

Solution

$$x(t) = x_0 + v_0 t - \frac{1}{2} g t^2$$

Velocity Verlet

For each nucleus α and coordinate $x_{\alpha i}$ ($x_{\alpha 1} = x_{\alpha}$, $x_{\alpha 2} = y_{\alpha}$, $x_{\alpha 3} = z_{\alpha}$):

$$a_{\alpha,i}(t) = -\frac{1}{M_{\alpha}} \frac{\partial E(\mathbf{R}(t))}{\partial x_{\alpha,i}}$$

$$x_{\alpha,i}(t + \Delta t) = x_{\alpha,i}(t) + v_{\alpha,i}(t)\Delta t + \frac{1}{2}a_{\alpha,i}(t)\Delta t^2$$

$$a_{\alpha,i}(t + \Delta t) = -\frac{1}{M_{\alpha}} \frac{\partial E(\mathbf{R}(t + \Delta t))}{\partial x_{\alpha,i}}$$

$$v_{\alpha,i}(t + \Delta t) = v_{\alpha,i}(t) + \frac{1}{2}(a_{\alpha,i}(t) + a_{\alpha,i}(t + \Delta t))\Delta t$$

Swope et al. J. Chem. Phys. **76**, 637 (1982)

For a recent method: Predescu et al. *Mol Phys* **2012**, 110, 967

Molecular dynamics with Velocity Verlet

Define trajectory parameters

$$\Delta t, t_{\max}, N_{at}, M_{\alpha}, \delta \mathcal{E}$$

Initialize trajectory $t = 0$

$$\mathbf{R}(0), \mathbf{v}(0)$$

$$\mathbf{a}_{\alpha}(0) = -\frac{1}{M_{\alpha}} \nabla_a E(\mathbf{R}(0))$$

$$\mathbf{R}(t + \Delta t) = \mathbf{R}(t) + \mathbf{v}(t)\Delta t + \frac{1}{2}\mathbf{a}(t)\Delta t^2$$

$$\mathbf{a}_{\alpha}(t + \Delta t) = -\frac{1}{M_{\alpha}} \nabla_a E(\mathbf{R}(t))$$

$$\mathbf{v}(t + \Delta t) = \mathbf{v}(t) + \frac{1}{2}(\mathbf{a}(t) + \mathbf{a}(t + \Delta t))\Delta t$$

$$\mathbf{a}(t) = \mathbf{a}(t - \Delta t)$$

$t + \Delta t > t_{\max} ?$

no

yes

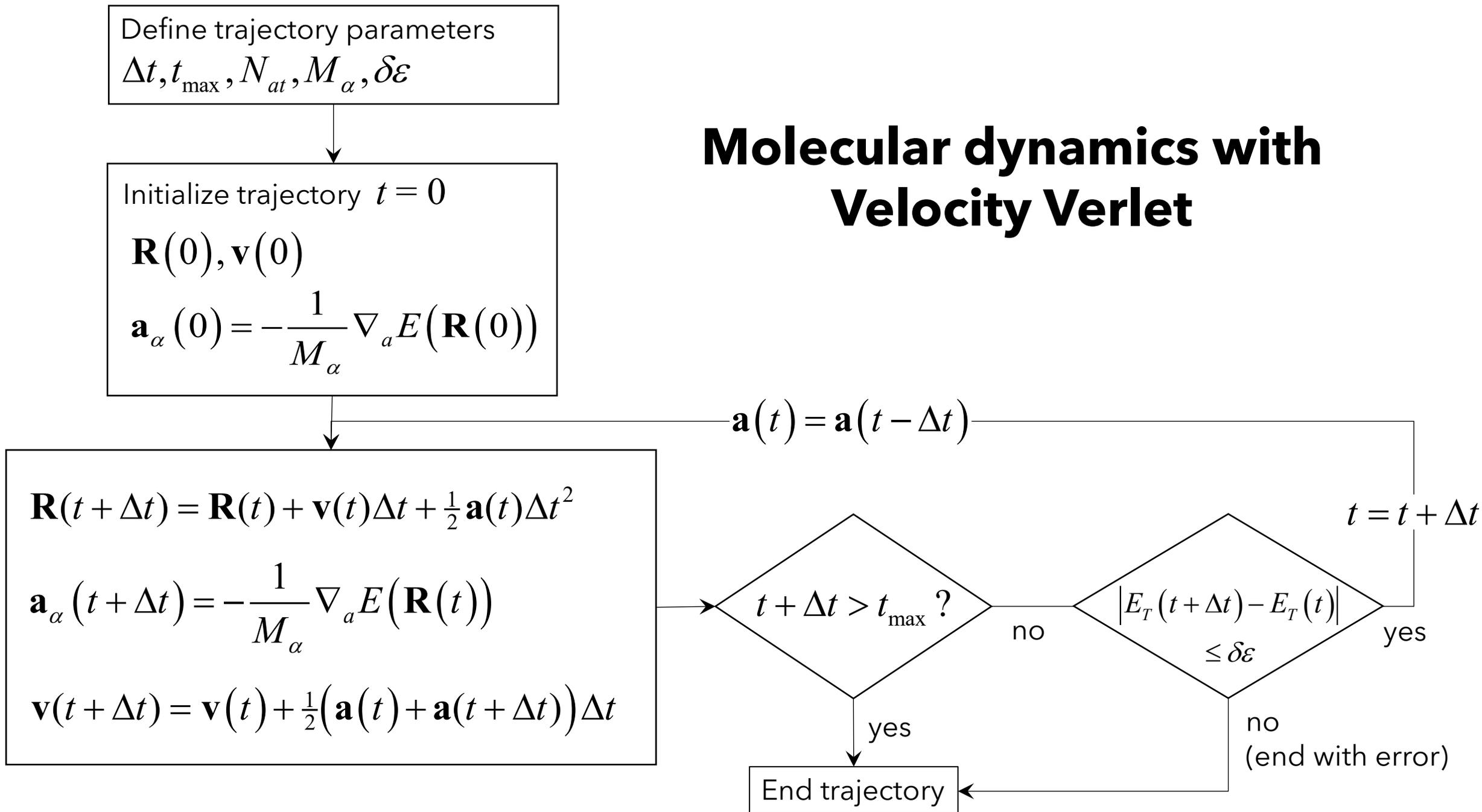
End trajectory

$|E_T(t + \Delta t) - E_T(t)| \leq \delta \mathcal{E}$

yes

no
(end with error)

$t = t + \Delta t$



Integration step size

Time-step

Table 1 Some typical vibrational modes^a

Vibrational mode	Wavelength of absorption [cm ⁻¹] (1/λ)	Absorption frequency [s ⁻¹] (ν = c/λ)	Period [fs] (1/ν)	Period/π [fs]
O–H stretch N–H stretch C–H stretch	3200–3600	1.0 × 10 ¹⁴	9.8	3.1
	3000	9.0 × 10 ¹³	11.1	3.5
	O–C–O asymmetric stretch	2400	7.2 × 10 ¹³	13.9
C≡C, C≡N stretch	2100	6.3 × 10 ¹³	15.9	5.1
C=O (carbonyl) stretch	1700	5.1 × 10 ¹³	19.6	6.2
C=C stretch				
H–O–H bend	1600	4.8 × 10 ¹³	20.8	6.4
C–N–H bend	1500	4.5 × 10 ¹³	22.2	7.1
H–N–H bend				
C=C (aromatic) stretch				
C–N stretch (amines)	1250	3.8 × 10 ¹³	26.2	8.4
Water Libration (rocking)	800	2.4 × 10 ¹³	41.7	13
O–C–O bending	700	2.1 × 10 ¹³	47.6	15
C=C–H bending (alkenes)				
C=C–H bending (aromatic)				

^aAll values are approximate; a range is associated with each motion depending on the system. The value of $c = 3.00 \times 10^{10}$ cm s⁻¹. The last column indicates the timestep limit for leap-frog stability for a harmonic oscillator: $\Delta t < 2/\omega = 2/(2\pi\nu)$.

Schlick, Barth and Mandziuk, *Annu. Rev. Biophys. Struct.* **1997**, 26, 181

Time-step

Table 1 Some typical vibrational modes^a

Vibrational mode	Wavelength of absorption [cm^{-1}] ($1/\lambda$)	Absorption frequency [s^{-1}] ($\nu = c/\lambda$)	Period [fs] ($1/\nu$)	Period/ π [fs]
{ O–H stretch N–H stretch C–H stretch	3200–3600	1.0×10^{14}	9.8	3.1
	3000	9.0×10^{13}	11.1	3.5

Time step should not be larger than 1 fs ($1/10\nu$).

$\Delta t = 0.5$ fs assures a good level of conservation of energy.

Exceptions requiring shorter steps:

- Dynamics close to a conical intersection
- Dissociation processes
- Long timescale

To know more:

- Goldstein, Classical mechanics. **1980**. Ch 1
- Verlet integrator: en.wikipedia.org/wiki/Verlet_integration
- Differential equations: youtu.be/p_di4Zn4wz4

Demonstration of equation

$$\frac{d\mathbf{L}}{dt} = \mathbf{N}^{(e)}$$

Time-derivative of the total angular momentum

$$\sum_i \frac{d\mathbf{L}_i}{dt} = \sum_i \mathbf{N}_i$$

Left side

$$\sum_i \frac{d\mathbf{L}_i}{dt} = \frac{d}{dt} \sum_i \mathbf{L}_i = \frac{d\mathbf{L}}{dt}$$

Right side

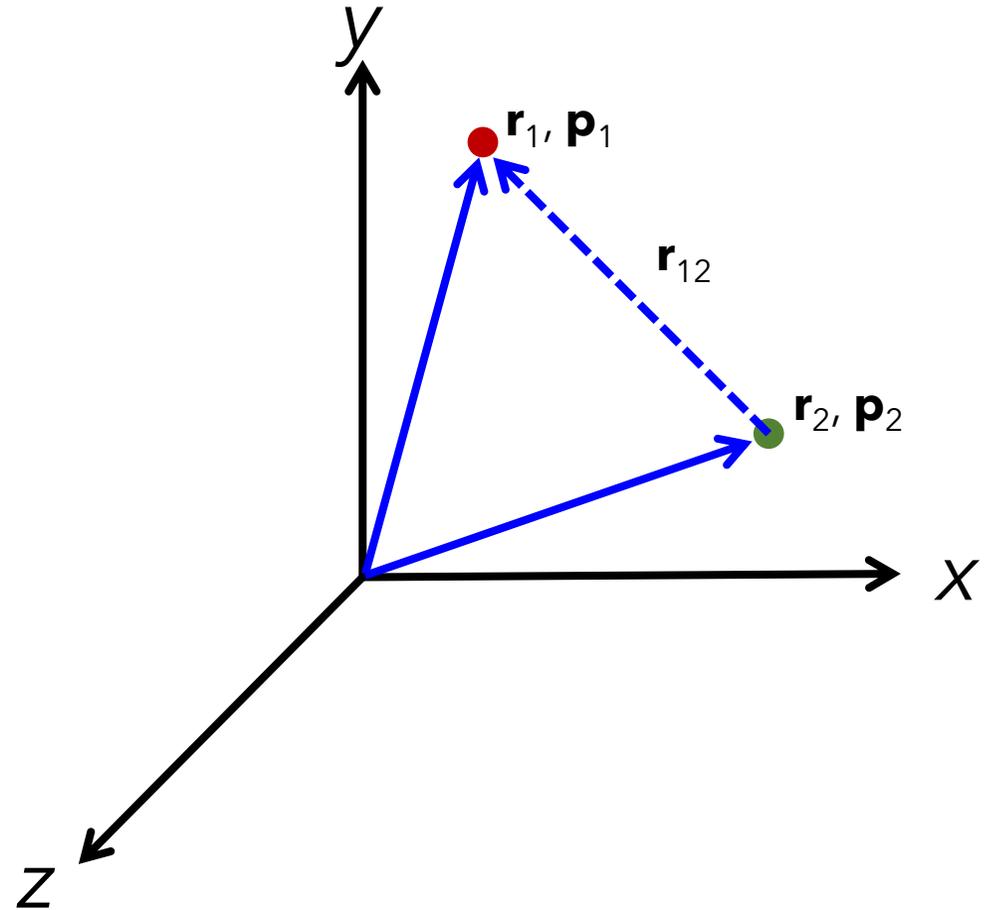
$$\begin{aligned} \sum_i \mathbf{N}_i &= \sum_i \mathbf{r}_i \times \left(\mathbf{F}_i^{(e)} + \sum_{j \neq i} \mathbf{F}_{ji} \right) \\ &= \sum_i \mathbf{r}_i \times \mathbf{F}_i^{(e)} + \underbrace{\sum_{\substack{i,j \\ j \neq i}} \mathbf{r}_i \times \mathbf{F}_{ji}} \end{aligned}$$

Example with $N = 2$

$$\begin{aligned}\sum_{\substack{i,j \\ j \neq i}} \mathbf{r}_i \times \mathbf{F}_{ji} &= \mathbf{r}_1 \times \mathbf{F}_{21} + \mathbf{r}_2 \times \mathbf{F}_{12} \\ &= \mathbf{r}_1 \times \mathbf{F}_{21} - \mathbf{r}_2 \times \mathbf{F}_{21} \\ &= (\mathbf{r}_1 - \mathbf{r}_2) \times \mathbf{F}_{21} \\ &= \mathbf{r}_{12} \times \mathbf{F}_{21}\end{aligned}$$

For central forces (forces along \mathbf{r}_{ij})

$$\sum_{\substack{i,j \\ j \neq i}} \mathbf{r}_i \times \mathbf{F}_{ji} = 0$$



Time-derivative of the total angular momentum

$$\sum_i \frac{d\mathbf{L}_i}{dt} = \sum_i \mathbf{N}_i$$

Left side

$$\sum_i \frac{d\mathbf{L}_i}{dt} = \frac{d}{dt} \sum_i \mathbf{L}_i = \frac{d\mathbf{L}}{dt}$$

Right side

$$\begin{aligned} \sum_i \mathbf{N}_i &= \sum_i \mathbf{r}_i \times \left(\mathbf{F}_i^{(e)} + \sum_{j \neq i} \mathbf{F}_{ji} \right) \\ &= \sum_i \mathbf{r}_i \times \mathbf{F}_i^{(e)} + \sum_{\substack{i,j \\ j \neq i}} \mathbf{r}_i \times \mathbf{F}_{ji} = \sum_i \mathbf{r}_i \times \mathbf{F}_i^{(e)} = \mathbf{N}^{(e)} \text{ (for central forces)} \\ &\quad \underline{\hspace{10em}} \\ &= 0 \text{ (for central forces)} \end{aligned}$$

Demonstration of equation

$$\mathbf{L} = \sum_i \mathbf{r}'_i \times \mathbf{p}'_i + \mathbf{R} \times \mathbf{P}$$

$$\mathbf{r}_i = \mathbf{r}'_i + \mathbf{R}$$

$$\frac{d\mathbf{r}_i}{dt} = \frac{d\mathbf{r}'_i}{dt} + \frac{d\mathbf{R}}{dt}$$

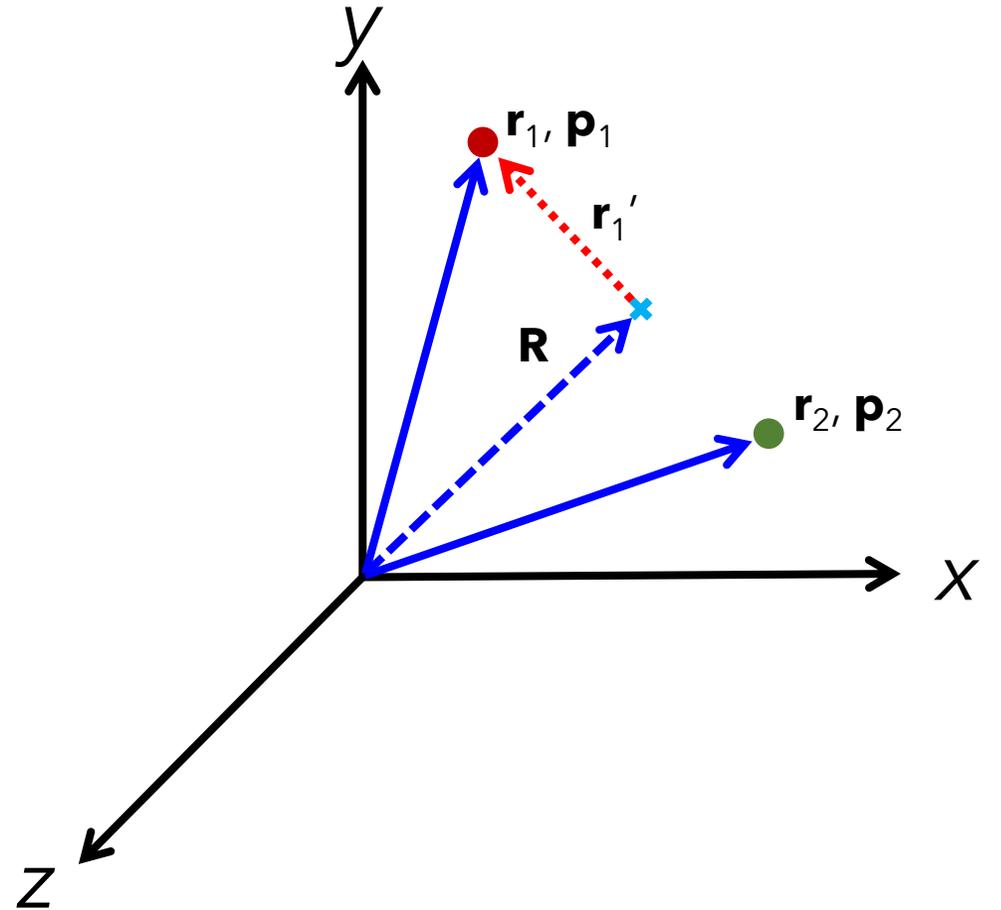
$$\mathbf{v}_i = \mathbf{v}'_i + \mathbf{v}$$

$$\mathbf{r}'_i = \mathbf{r}_i - \mathbf{R}$$

$$\sum_i m_i \mathbf{r}'_i = \sum_i m_i \mathbf{r}_i - \sum_i m_i \mathbf{R}$$

$$\sum_i m_i \mathbf{r}'_i = \sum_i m_i \mathbf{r}_i - M\mathbf{R}$$

$$= \sum_i m_i \mathbf{r}_i - M \left(\frac{1}{M} \sum_i m_i \mathbf{r}_i \right) = 0$$



$$\begin{aligned}
\mathbf{L} &= \sum_i \mathbf{r}_i \times \mathbf{p}_i \\
&= \sum_i (\mathbf{r}'_i + \mathbf{R}) \times m_i (\mathbf{v}'_i + \mathbf{v}) \\
&= \sum_i \mathbf{r}'_i \times m_i \mathbf{v}'_i + \left(\sum_i m_i \mathbf{r}'_i \right) \times \mathbf{v} + \mathbf{R} \times \left(\sum_i m_i \mathbf{v}'_i \right) + \mathbf{R} \times \left(\sum_i m_i \right) \mathbf{v} \\
&= \sum_i \mathbf{r}'_i \times m_i \mathbf{v}'_i + \left(\sum_i m_i \mathbf{r}'_i \right) \times \mathbf{v} + \mathbf{R} \times \left(\sum_i m_i \mathbf{v}'_i \right) + \mathbf{R} \times M \mathbf{v} \\
&= \sum_i \mathbf{r}'_i \times \mathbf{p}'_i + \underbrace{\left(\sum_i m_i \mathbf{r}'_i \right)}_0 \times \mathbf{v} + \mathbf{R} \times \underbrace{\left(\sum_i m_i \mathbf{v}'_i \right)}_0 + \mathbf{R} \times \mathbf{P}
\end{aligned}$$

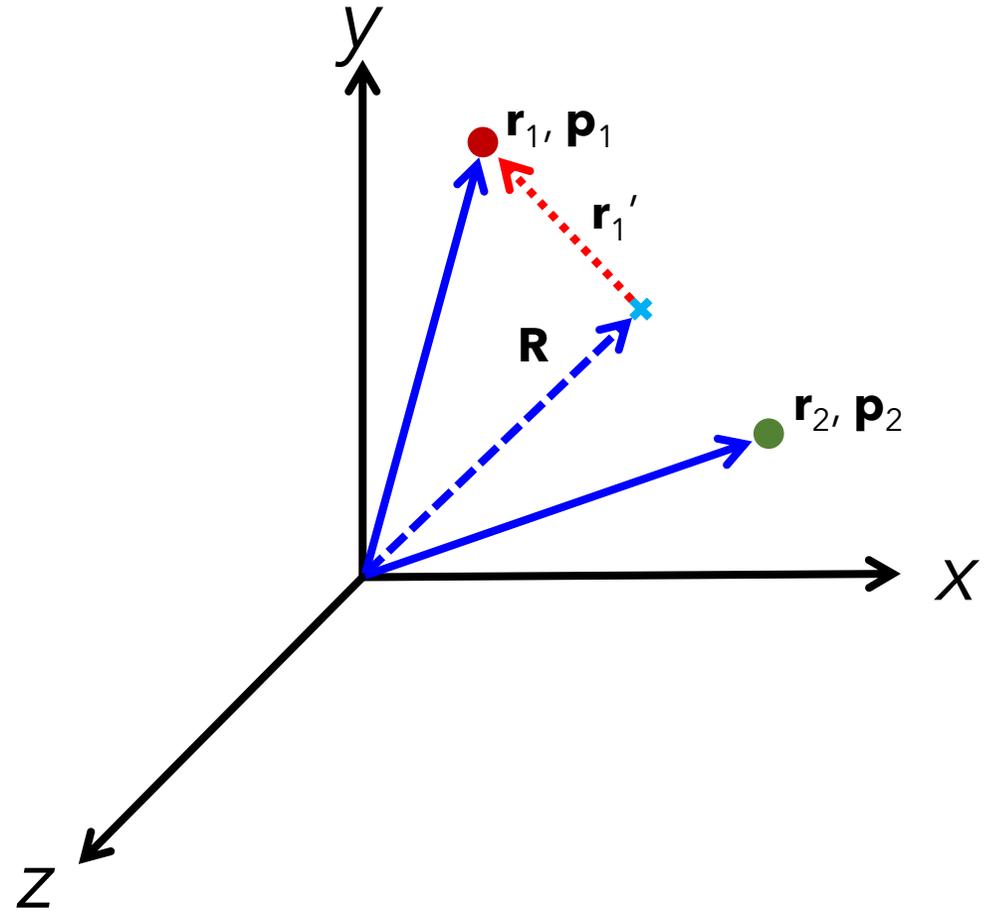
$$\mathbf{L} = \sum_i \mathbf{r}'_i \times \mathbf{p}'_i + \mathbf{R} \times \mathbf{P}$$

Demonstration of equation

$$T = \frac{1}{2} M \mathbf{v}^2 + \frac{1}{2} \sum_i m_i \mathbf{v}'_i{}^2$$

We check the total kinetic energy like we did for angular momentum:

$$\begin{aligned} T &= \sum_i \frac{1}{2} m_i \mathbf{v}_i^2 \\ &= \sum_i \frac{1}{2} m_i (\mathbf{v} + \mathbf{v}'_i)^2 \\ &= \sum_i \frac{1}{2} m_i (\mathbf{v}^2 + 2\mathbf{v} \cdot \mathbf{v}'_i + \mathbf{v}'_i{}^2) \\ &= \frac{1}{2} M \mathbf{v}^2 + \mathbf{v} \cdot \underbrace{\sum_i m_i \mathbf{v}'_i}_0 + \frac{1}{2} \sum_i m_i \mathbf{v}'_i{}^2 \\ &= \frac{1}{2} M \mathbf{v}^2 + \frac{1}{2} \sum_i m_i \mathbf{v}'_i{}^2 \end{aligned}$$



Demonstration of equations

$$W_{12} = T_B - T_A$$

$$W_{12} = V_A - V_B$$

The work of a system of particles is the variation of their kinetic energy

$$\begin{aligned}W_{AB} &= \sum_i \int_A^B \mathbf{F}_i \cdot d\mathbf{s}_i = \sum_i \int_A^B m_i \frac{d\mathbf{v}_i}{dt} \cdot \mathbf{v}_i dt \\ &= \sum_i (T_{i,B} - T_{i,A}) \\ &= T_B - T_A\end{aligned}$$

The work in terms of potential energies

$$\begin{aligned} W_{12} &= \sum_i \int_A^B \mathbf{F}_i \cdot d\mathbf{s}_i \\ &= \sum_i \int_A^B \mathbf{F}_i^{(e)} \cdot d\mathbf{s}_i + \sum_{\substack{i,j \\ j \neq i}} \int_A^B \mathbf{F}_{ji} \cdot d\mathbf{s}_i \end{aligned}$$

If the external forces are conservative

$$\sum_i \int_A^B \mathbf{F}_i^{(e)} \cdot d\mathbf{s}_i = - \sum_i \int_A^B \nabla_i V_i \cdot d\mathbf{s}_i = \sum_i (V_{i,A} - V_{i,B})$$

If the internal forces are conservative and central

$$\mathbf{F}_{ji} = -\nabla V_{ij} \left(\|\mathbf{r}_i - \mathbf{r}_j\| \right)$$

Then the work is

$$\sum_{\substack{i,j \\ j \neq i}} \int_A^B \mathbf{F}_{ji} \cdot d\mathbf{s}_i = -\sum_{\substack{i,j \\ j \neq i}} \int_A^B \nabla_i V_{ji} \cdot d\mathbf{s}_i$$

$$N = 2$$

$$\begin{aligned} -\sum_{\substack{i,j \\ j \neq i}} \int_A^B \nabla_i V_{ji} \cdot d\mathbf{s}_i &= -\int_A^B \nabla_1 V_{21} \cdot d\mathbf{s}_1 - \int_A^B \nabla_2 V_{12} \cdot d\mathbf{s}_2 & d\mathbf{s}_1 - d\mathbf{s}_2 &= d\mathbf{r}_1 - d\mathbf{r}_2 = d(\mathbf{r}_1 - \mathbf{r}_2) = d\mathbf{r}_{12} \\ & & \nabla_1 V_{12} &= -\nabla_2 V_{12} = \nabla_{12} V_{12} \\ &= -\int_A^B \nabla_{12} V_{12} \cdot d\mathbf{r}_{12} \\ &= V_{12,A} - V_{12,B} \end{aligned}$$

The work is

$$\begin{aligned} W_{12} &= \sum_i \int_A^B \mathbf{F}_i \cdot d\mathbf{s}_i \\ &= \sum_i \int_A^B \mathbf{F}_i^{(e)} \cdot d\mathbf{s}_i + \sum_{\substack{i,j \\ j \neq i}} \int_A^B \mathbf{F}_{ji} \cdot d\mathbf{s}_i \\ &= \sum_i (V_{i,A} - V_{i,B}) + \sum_{ij} (V_{ij,A} - V_{ij,B}) \\ &= V_A - V_B \end{aligned}$$