Ordinary Differential Equations

- We call **Ordinary Differential Equation** (ODE) of n-th order in the variable x, a relation of the kind:

$$\mathcal{L}\left(\frac{d^n y}{dx^n}, \frac{d^{n-1} y}{dx^{n-1}}, \ldots, \frac{dy}{dx}, y(x), x\right) = 0$$

- where $\mathcal{L}$ is an **operator**. If it is a **linear operator**, we call the equation **linear differential equation**, otherwise **non-linear differential equation**.
- The existence and uniqueness Cauchy theorem ensures that the solution exists and is unique, under appropriate conditions, only in the case of linear differential equations.

Ordinary Differential Equations

- If $\mathcal{L}$ is linear, and its coefficients are constants with respect to x, we call the equation: **linear differential equation with constant coefficients**.
- Examples:
  - 2-nd degree, linear ODE with constant coefficients:

$$\alpha \frac{d^2y}{dx^2} + \beta \frac{dy}{dx} + \gamma y(x) = \xi$$

  - 1-st degree, linear ODE with non-constant coefficients:

$$f(x)\frac{dy}{dx} + g(x)y(x) = h(x)$$

  - Non-linear ODE:

$$\alpha(x)\frac{dy}{dx} + \gamma y^2(x) = 0$$

Ordinary Differential Equations

- Ordinary differential equations are mainly distinguished into two categories:
  - Initial value problems, where the equation is represented by a single independent variable (e.g. the time) which varies along a specific direction;
  - Boundary value problems, where the equation is solved for all values of the independent variable bounded in a given domain (for example, $x \in [a, b]$)

Ordinary Differential Equations

- Example of an initial value problem:

  Newton's law for a point moving along an axis

$$\frac{d^2x(t)}{dt^2} = \frac{1}{m}F(x, v, t)$$

- Here $t > 0$ is the **independent variable**, $x(t)$ is the coordinate of the point along the axis, namely the **dependent variable**, m is the **mass** of the point and F the sum of all the **forces** acting on the point (which may depend, in turn, on time, position and speed of the point).

Ordinary Differential Equations

- Example of boundary value problems:

  Poisson's equation for the electrostatic potential generated by a spherical distribution of charges

$$\nabla^2 V(r) = \frac{1}{\epsilon}\rho(r) \qquad \Rightarrow \qquad \frac{1}{r^2}\frac{d}{dr}\left[r^2 \frac{dV(r)}{dr}\right] = \frac{1}{\epsilon}\rho(r)$$

- Here $0 \le r \le \infty$ is the **radius**, the **independent variable**, $V(r)$ is the **electrostatic potential**, the **dependent variable**, $\rho(r)$ is a known function representing the **distribution of charges** and ε the **dielectric constant**.

Ordinary Differential Equations

- The actual **difference** between an initial value problem and a boundary value problem is that for the former we need to know two (or n, if the equation is of n-th degree) **initial conditions at** $t = 0$, while for the latter we need two (or n) **boundary conditions** which can be at **one or both boundaries**!
- This makes **no difference** in the **mathematical solution** of the equation, but make indeed a **big difference** in the **numerical solution**, as we will see in next slides.

Ordinary Differential Equations

- One has to notice that $y(x)$ is a **continuous function** of the independent variable x, whilst computers deal with a **discrete subset of the real set**. Therefore a numerical solution must involve some **discretization** of the continuous function $y(x)$, representing the solution of the ODE!
- In order to solve an ODE numerically, one has to take the following fundamental steps:

Ordinary Differential Equations

1) **Limit** the independent variable x to a **well-defined, finite, interval**. For instance, for a IVP: $t \in [0, T_{\mathrm{end}}]$ or, for a BVP: $x \in [x_{\min}, x_{\max}]$

2) Discretize the given interval (e. g. the second) with a finite number N of **grid-points** x_j:

$$x_j = x_{\min} + jh, \text{ with: } j = 0, \ldots, N, ; \quad h = \frac{x_{\max} - x_{\min}}{N}$$

3) Finally, find a method to approximate in a discrete form the derivatives of the unknown function $y(x)$.

Ordinary Differential Equations

- Concerning the latter, we distinguish several methods. We will study just two:

➢ **Finite difference methods** (FDM);

➢ **Spectral methods** (SM).

- We start with the **first one**, and we will study the **second one** later, only in connection with some **special kind of boundary conditions**.

Finite Differences schemes

- The idea behind the FDM is to approximate the value of a derivative of the unknown function $y(x)$ in a generic discrete point x_j with a linear combination of the $y(x)$ function itself in points near to x_j:

$$\left.\frac{d^n y(x)}{dx^n}\right|_{x_j} = \sum_{i=-j_1}^{+j_2} a_i y(x_{j+i}) + \mathcal{E}(h^p)$$

The coefficients a_i are suitably chosen coefficients in such a way that the derivative is approximated with an **error** $\mathcal{E}$. p is the **precision** of the scheme.

Finite Differences schemes

- We notice that:

➢ If $j_1 = j_2$ we call the scheme **symmetric**, **asymmetric** in the opposite case;

➢ The precision p depends on j_1 and j_2: the higher they are, the higher is p;

➢ The coefficients a_i are determined by using the **Taylor development** of the function $y(x)$ in the points near to x_j:

Finite Differences schemes

$$y(x_{j\pm i}) = y(x_j) + \left.\frac{dy}{dx}\right|_{x_j} (x_{j\pm i} - x_j) + \left.\frac{d^2y}{dx^2}\right|_{x_j} \frac{(x_{j\pm i} - x_j)^2}{2!} +$$
$$+ \left.\frac{d^3y}{dx^3}\right|_{x_j} \frac{(x_{j\pm i} - x_j)^3}{3!} + \ldots + \left.\frac{d^ny}{dx^n}\right|_{x_j} \frac{(x_{j\pm i} - x_j)^n}{n!} + \ldots$$

- For instance, for the first derivative ($n=1$), with $j_1=0$, $j_2=1$, we have:

$$\left.\frac{dy}{dx}\right|_{x_j} = a_0 y(x_j) + a_1 y(x_{j+1}) + \mathcal{E} = a_0 y(x_j) +$$
$$+ a_1 \left[y(x_j) + y'(x_j)h + y''(x_j)\frac{h^2}{2} + O(h^3) \right] + \mathcal{E}$$

where: $h = x_{j+1} - x_j$.

Finite Differences schemes

- By re-arranging the terms:

$$\left.\frac{dy}{dx}\right|_{x_j} = (a_0 + a_1)y(x_j) + a_1 y'(x_j)h + a_1 y''(x_j)\frac{h^2}{2} + $$

$$+ a_1 O(h^3) + \mathcal{E}$$

- If this relation is to be valid, we need that:

$$\begin{cases} a_0 + a_1 = 0 \qquad \Rightarrow \qquad a_0 = -a_1 \\ a_1 = \frac{1}{h} \\ \mathcal{E} = -a_1 y''(x_j)\frac{h^2}{2} - a_1 O(h^3) = -y''(x_j)\frac{h}{2} + O(h^2) \end{cases}$$

Finite Differences schemes

- Therefore, we get an asymmetric scheme for the first derivative as:

$$\left.\frac{dy}{dx}\right|_{x_j} = \frac{y(x_{j+1}) - y(x_j)}{h} + \mathcal{E}$$

  where the error is proportional to h, so that $p=1$!

- In the same way, we can write a scheme by using: $j_1=-1$, $j_2=0$, which yields:

$$\left.\frac{dy}{dx}\right|_{x_j} = a_{-1}y(x_{j-1}) + a_0 y(x_j) + \mathcal{E} = a_{-1}\left[y(x_j) + \right.$$

$$\left. -y'(x_j)h + y''(x_j)\frac{h^2}{2} + O(h^3)\right] + a_0 y(x_j) + \mathcal{E}$$

Finite Differences schemes

Where we put: x_{j-1}-x_j = -h.

- Again, by re-arranging the formula:

$$\left.\frac{dy}{dx}\right|_{x_j} = (a_{-1}+a_0)y(x_j) - a_{-1}y'(x_j)h + a_{-1}y''(x_j)\frac{h^2}{2} +$$

$$+ a_{-1}O(h^3) + \mathcal{E}$$

$$\begin{cases} a_{-1}+a_0 = 0 \qquad \Rightarrow \qquad a_0 = -a_{-1} \\ a_{-1} = -\frac{1}{h} \\ \mathcal{E} = -a_{-1}y''(x_j)\frac{h^2}{2} - a_{-1}O(h^3) = y''(x_j)\frac{h}{2} + O(h^2) \end{cases}$$

- That is: $$\left.\frac{dy}{dx}\right|_{x_j} = \frac{y(x_j) - y(x_{j-1})}{h} + \mathcal{E}$$

Finite Differences schemes

- Also in this case, the error is proportional to h, so that the precision is: $p=1$!
- We can improve the precision by considering additional points, for instance by using the symmetric scheme with: $j_1=-1$, $j_2=+1$.
- In this case we have:

$$\left.\frac{dy}{dx}\right|_{x_j} = a_{-1}y(x_{j-1}) + a_0 y(x_j) + a_1 y(x_{j+1}) + \mathcal{E} =$$

$$= a_{-1}\left[y(x_j) - y'(x_j)h + y''(x_j)\frac{h^2}{2} - y'''(x_j)\frac{h^3}{6} + O(h^4)\right] + a_0 y(x_j) +$$

$$+ a_1\left[y(x_j) + y'(x_j)h + y''(x_j)\frac{h^2}{2} + y'''(x_j)\frac{h^3}{6} + O(h^4)\right] + \mathcal{E}$$

Finite Differences schemes

- This formula may be put under the form:

$$\left.\frac{dy}{dx}\right|_{x_j} = (a_{-1} + a_0 + a_1)y(x_j) + (-a_{-1} + a_1)y'(x_j)h +$$
$$+ (a_{-1} + a_1)y''(x_j)\frac{h^2}{2} + (-a_{-1} + a_1)y'''(x_j)\frac{h^3}{6} +$$
$$+ (-a_{-1} + a_1)O(h^4) + \mathcal{E}$$

that is:

$$\begin{cases} a_{-1} + a_0 + a_1 = 0 \quad \Rightarrow \quad a_1 = \frac{1}{2h} \\ -a_{-1} + a_1 = \frac{1}{h} \quad \Rightarrow \quad a_{-1} = -a_1 = -\frac{1}{2h} \\ a_{-1} + a_1 = 0 \quad \Rightarrow \quad a_0 = 0 \\ \mathcal{E} = -(-a_{-1} + a_1)y'''(x_j)\frac{h^3}{6} - (a_{-1} + a_1)O(h^4) = -y'''(x_j)\frac{h^2}{6} + O(h^3) \end{cases}$$

Finite Differences schemes

- The final formula for the first derivative is:

$$\left.\frac{dy}{dx}\right|_{x_j} = \frac{y(x_{j+1}) - y(x_{j-1})}{2h} + \mathcal{E}$$

where this time the error is proportional to h^2, that is this is a second order scheme ($p=2$)!

- In the same way, it is possible to have higher order schemes. For instance:

$$\left.\frac{dy}{dx}\right|_{x_j} = \frac{y(x_{j-2}) - 8y(x_{j-1}) + y(x_j) + 8y(x_{j+1}) - y(x_{j+2})}{12h} + O(h^4)$$

Finite Differences schemes

- With the same technique one can find a centered formula for the second derivative ($n=2$, $j_1=-1$, $j_2=+1$):

$$\left.\frac{dy}{dx}\right|_{x_j} = a_{-1}y(x_{j-1}) + a_0 y(x_j) + a_1 y(x_{j+1}) + \mathcal{E} =$$

$$= a_{-1}\left[y(x_j) - y'(x_j)h + y''(x_j)\frac{h^2}{2} - y'''(x_j)\frac{h^3}{3!} + y^{IV}(x_j)\frac{h^4}{4!} + O(h^5)\right] +$$

$$+ a_0 y(x_j) +$$

$$+ a_1\left[y(x_j) + y'(x_j)h + y''(x_j)\frac{h^2}{2} + y'''(x_j)\frac{h^3}{3!} + y^{IV}(x_j)\frac{h^4}{4!} + O(h^4)\right] + \mathcal{E} =$$

$$= (a_{-1} + a_0 + a_1)y(x_j) + (-a_{-1} + a_1)y'(x_j)h + (a_{-1} + a_1)y''(x_j)\frac{h^2}{2} +$$

$$+ (-a_{-1} + a_1)y'''(x_j)\frac{h^3}{6} + (a_{-1} + a_1)y^{IV}(x_j)\frac{h^4}{24} + (a_{-1} + a_1)O(h^5) + \mathcal{E}$$

Finite Differences schemes

- This gives the relations:

$$\begin{cases} a_{-1} + a_0 + a_1 = 0 \quad \Rightarrow \quad a_0 = -(a_{-1} + a_1) = -\frac{2}{h^2} \\ -a_{-1} + a_1 = 0 \quad \Rightarrow \quad a_{-1} = a_1 = \frac{1}{h^2} \\ a_{-1} + a_1 = \frac{2}{h^2} \quad \Rightarrow \quad a_1 = \frac{1}{h^2} \\ \mathcal{E} = -(-a_{-1} + a_1)y'''(x_j)\frac{h^3}{6} - (a_{-1} + a_1)y^{IV}(x_j)\frac{h^4}{24} + \\ \quad +(a_{-1} + a_1)O(h^5) = -y^{IV}(x_j)\frac{h^2}{12} + O(h^3) \end{cases}$$

that gives a second order approximation for the second derivative:

$$\left.\frac{d^2y}{dx^2}\right|_{x_j} = \frac{y(x_{j-1}) - 2y(x_j) + y(x_{j+1})}{h^2} + O(h^2)$$

Initial value problems

- Now that we have an idea about how to compute a suitable approximation for a generic derivative depending on the values of the function in the nearest points, we can afford the problem of **solving an Initial Value Problem** (IVP). Later on, we will see how to solve a Boundary Value Problem (BVP).
- Let us first consider an IVP, first order ODE:

$$\frac{dy}{dt} = F(y,t) \qquad \forall t > 0$$

with the following initial condition: $y(t=0)=y_0$.

Initial value problems

- Let us now fix a limited integration interval, for instance: $t \in [0, T_{\text{end}}]$

  and divide that interval in N equally spaced intervals, thus identifying $N+1$ discrete points in time:

$$t_n = nh, \text{ with:} \quad n = 0, \ldots, N, \quad h = \frac{T_{\text{end}}}{N}$$

- We can now write the equation on a generic discrete point in time t_n:

$$\left.\frac{dy}{dt}\right|_{t=t_n} = F(y_n, t_n)$$

Initial value problems

- Now we can write an approximation for the derivative in t_n with a Finite Difference Scheme in the form:

$$\left.\frac{dy}{dt}\right|_{t_n} = \sum_{j=-m}^{k} a_j y(t_{n+j}) + \mathcal{E} =$$

$$= \mathcal{F}(y_{n-m}, y_{n-m+1}, \ldots, y_{n+k-1}, y_{n+k}) + \mathcal{E}$$

where we write: y_m instead of $y(t_m)$ to lighten the notation.

Initial value problems

- That is, a **one-step scheme** is a relation that involves only quantities at n and $n+1$ time steps. As obvious, a **multi-step scheme** involves more time steps.
- Some **terminology**:

➢ Φ is called **increment function**;

➢ If $\Phi = \Phi\,(t_n, y_n, F_n; h)$ the scheme is said **explicit**;

➢ If Φ depends also on t_{n+1}, y_{n+1}, F_{n+1} the scheme is said **implicit**.

Initial value problems

- The quantity $\tau_{n+1}(h)$ is called **local truncation error** (LTE) and represents the error that is made in the evaluation of the solution at each time step.
- The quantity $\max_n |\tau_{n+1}|$ is called **global truncation error** (GTE).
- If $\tau_{n+1}(h) = O(h^p)$ we say that the scheme has **order** p.

Initial value problems

- We then get the relation:

$$\left.\frac{dy}{dt}\right|_{t_n} = \mathcal{F}(y_{n-m}, y_{n-m+1}, \ldots, y_{n+k-1}, y_{n+k}) + \mathcal{E} = F(y_n, t_n)$$

that is called **numerical scheme**.

- If the numerical scheme can be written in the form:

$$y_{n+1} = y_n + h\Phi(t_n, y_n, F_n, t_{n+1}, y_{n+1}, F_{n+1}; h) + h\tau_{n+1}(h)$$

we have a **one-step scheme**; if not, we have a **multi-step scheme**.

Initial value problems

- **Properties** of a numerical scheme:
  - We call a scheme **consistent** when, in the limit for h tending to zero, the **scheme reproduces the original equation**.

    That is:

$$\lim_{h\to 0} \frac{y_{n+1} - y_n}{h} = \left.\frac{dy}{dt}\right|_{t=t_n} = F(y_n, t_n) =$$

$$= \lim_{h\to 0} \Phi(t_n, y_n, F_n, t_{n+1}, y_{n+1}, F_{n+1}; h) + \lim_{h\to 0} \tau_{n+1}(h) \quad \Rightarrow$$

$$\Rightarrow \begin{cases} \lim\limits_{h\to 0} \Phi(t_n, y_n, F_n, t_{n+1}, y_{n+1}, F_{n+1}; h) = F(y_n, t_n) \\ \lim\limits_{h\to 0} \tau_{n+1}(h) = 0, \quad \text{namely: } p > 0 \end{cases}$$

Initial value problems

- **Properties** of a numerical scheme:
  - We call a scheme **convergent** when, in the limit for h tending to zero, the **numerical solution tends to the exact solution**.

    That is: $$\lim_{h \to 0} y(t_n) = y_{\text{ex}}(t_n)$$

  - We call a scheme **stable** if $\tau_{n+1}(h)$ remains finite for increasing n-s.

    That is:

    $$|\tau_{n+1}(h)| < \infty, \qquad \forall n$$

Initial value problems

- The latter means that, depending on the value of h, the **local truncation errors** may become larger and larger with increasing n.
- Notice that **convergence** property may be hardly satisfied when, that is in all practical cases, the **solution of the equation is unknown**!
- This difficulty is partially overcome thanks to **Lax equivalence theorem**, that is the **most important theorem of FDM**.

Initial value problems

- **Lax equivalence theorem**:

  A numerical scheme for a ***linear*** *differential equation is* ***convergent*** *if and only if it is* ***consistent*** *and* ***stable****.*

- The problem is now **how to ensure the stability** of a numerical scheme.

- **Von Neumann stability criterion**:

  Given an ODE in the form: $\frac{dy}{dt} = \mathcal{L}(y,t)$

  where L is a ***linear operator****, and given a one-step numerical scheme, this is stable if:*

$$A(h) = \left| \frac{y_{n+1}}{y_n} \right| \leq 1$$

Initial value problems

- This means that the scheme is **stable** if one can find some **value of h** such that the Von Neumann's stability criterion is satisfied.
- Notice that:

1) The criterion is a **necessary** condition, but **not sufficient**. This means that if the condition is satisfied, the scheme is stable, but there may exist values of h for which the conditions is **not satisfied** but the scheme is stable as well!

Initial value problems

- Notice that:

2) The stability, as well as the **convergence** depends not only on the **scheme** but also on the **equation**. That is, a scheme can be stable for an equation and unstable for another one.

3) The ODE must be **linear**, for the Theorem to be **valid**! However, in practical cases, **if a scheme is stable for the linearized version** of the equation then **it is often stable also for the non-linear equation**. This is not true all the times, unfortunately, but it works many times!

Euler's schemes

- Example:

  We can produce a simple numerical scheme by approximating the first derivative with a scheme in which *m=0, k=1*:

$$\left.\frac{dy}{dt}\right|_{t_n} = \frac{y_{n+1} - y_n}{h} + \mathcal{E} = F(y_n, t_n)$$

  where: $\mathcal{E} = -y_n'' \frac{h}{2} + O(h^2)$

- The scheme can be rewritten as:

$$y_{n+1} = y_n + hF(y_n, t_n) - h\mathcal{E}$$

Euler's schemes

- That is a one-step scheme, provided that:

$$\begin{cases} \Phi(t_n, y_n, F_n, t_{n+1}, y_{n+1}, F_{n+1}; h) = F(y_n, t_n) \\ \tau_{n+1}(h) = -\mathcal{E} = y_n'' \frac{h}{2} + O(h^2) \end{cases}$$

that means that:

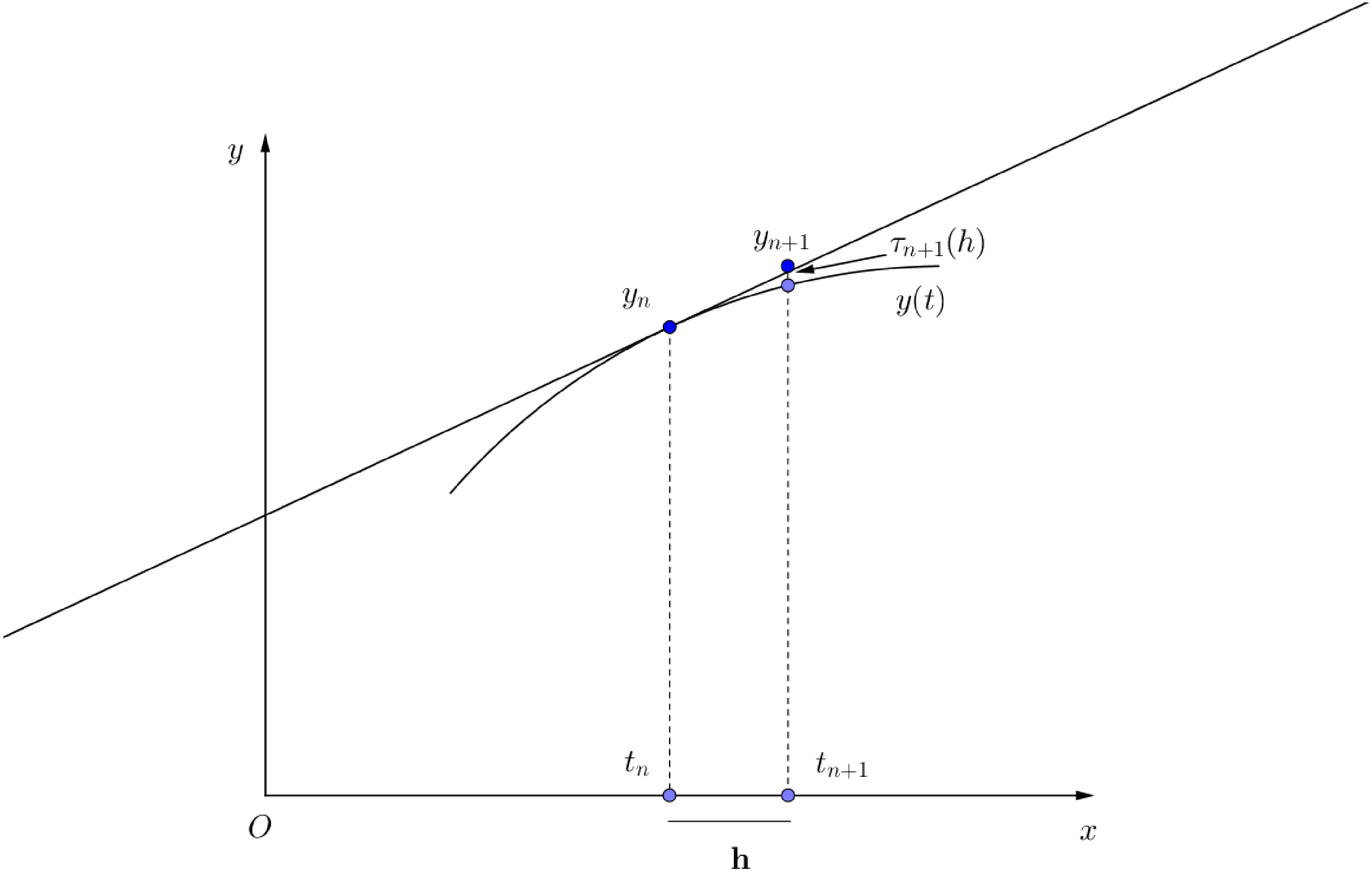
1) The scheme is **explicit** (Φ does **not** depend on quantities at t_{n+1});

2) It is a **first order scheme**, since $p=1$;

3) The scheme is **consistent**, since the **two conditions are automatically satisfied**!

Euler’s schemes

- This is the so-called **Forward Euler’s scheme.**



Euler's schemes

- Let us study briefly the **convergence and stability properties** of the scheme.
- To do this, we have to apply the scheme to some equation. As an example to start with, let us consider an **ODE with constant coefficients**.
- In this case, only two types of solutions are allowed: **exponentially increasing or decreasing functions and oscillating functions**.
- Let us start with the **first case** (exponential solutions).

Euler's schemes

- Let us consider the differential equation:

$$\frac{dy}{dt} = ky$$

with initial condition: $y(t=0) = y_0$.

- The analytical solution of this equation is an exponential function:

$$y(t) = y_0 e^{kt}$$

as it is easily shown by substituting the solution into the equation.

Euler's schemes

- In fact, given the solution, we have:

$$\frac{dy}{dt} = \frac{d}{dt}\left(y_0 e^{kt}\right) = k y_0 e^{kt} = ky$$

  that is the original equation. Therefore, the solution satisfies identically the equation.

- By using the Forward Euler's Scheme, after discretization of the integration interval $[0, T_{\text{end}}]$, we have:

$$y_{n+1} = y_n + hF(y_n, t_n) = y_n + hk\, y_n = y_n(1 + hk)$$

Euler's schemes

- This means the numerical solution is given by:

$$
\begin{aligned}
y_1 &= y_0(1+kh) && \text{for } t = t_1 \\
y_2 &= y_1(1+kh) = y_0(1+kh)^2 && \text{for } t = t_2 \\
y_3 &= y_2(1+kh) = y_0(1+kh)^3 && \text{for } t = t_3 \\
&\dots \\
y_n &= y_{n-1}(1+kh) = y_0(1+kh)^n && \text{for } t = t_n
\end{aligned}
$$

while the exact solution at the generic t=t_n is:

$$y_{\mathrm{ex}}(t = t_n) = y_0 e^{k t_n}$$

Euler's schemes

- We can now show that the scheme is indeed **convergent**, namely that:

$$\lim_{h \to 0} y_n = y_{\text{ex}}(t_n)$$

- In fact:

$$\lim_{h \to 0} y_n = \lim_{h \to 0} y_0 (1 + kh)^n = y_0 \lim_{h \to 0} (1 + kh)^n$$

$$= y_0 \lim_{h \to 0} (1 + kh)^{(kt_n)/(kh)} = y_0 \left[\lim_{h \to 0} (1 + kh)^{\frac{1}{kh}} \right]^{kt_n}$$

where we used the fact that:

$$t_n = nh \quad \Rightarrow \quad n = \frac{t_n}{h} = \frac{kt_n}{kh}$$

Euler's schemes

- By remembering that:

$$\lim_{x \to 0} (1 + x)^{\frac{1}{x}} = e$$

we finally have:

$$\lim_{h \to 0} y_n = y_0 \left[\lim_{h \to 0} (1 + kh)^{\frac{1}{kh}} \right]^{kt_n} = y_0 e^{kt_n} = y_{\text{ex}}(t_n)$$

that is, the scheme is **convergent**.

- Let us see whether it is stable.

Euler's schemes

- The scheme is: $y_{n+1} = y_n(1 + kh)$
- The Von Neumann criterion tells us that, in order to be stable, h must satisfy the relation:

$$A(h) = \left| \frac{y_{n+1}}{y_n} \right| \leq 1 \quad \Rightarrow \quad |1 + kh| \leq 1 \quad \Rightarrow$$

$$\Rightarrow \begin{cases} 1 + kh \leq 1 & \Rightarrow \quad kh \leq 0 \quad \Rightarrow \quad k \leq 0 \\ -1 \leq 1 + kh & \Rightarrow \quad -kh \leq 2 \quad \Rightarrow \quad h \leq \frac{2}{|k|} \end{cases}$$

where we used the fact that, since: $k \leq 0$

we can pose: $k = -|k|$

Euler's schemes

- Therefore, the scheme is stable only if $k < 0$ and $h < 2/|k|$. This means that:
  - the equation is **numerically solvable** only if the constant k is **negative**, that is only when **the solution is exponentially decreasing**;
  - Even for negative k-s, there is a **limit on the maximum time-step allowed** during the numerical solution of the ODE, depending on the value of k.

Euler's schemes

- It is interesting to notice the following things:

  1) Although solutions with $k > 0$ are of course **mathematically correct**, they are typically **not physically meaningful**, since a physical quantity which increases exponentially is not existing!

  2) Let us suppose that k < 0. The solution of the equation is: $y(t) = y_0 e^{-|k|t} = y_0 e^{-t/\tau}$

  where $\tau = 1/|k|$ is called **characteristic time** of the solution.

Euler's schemes

- The meaning of τ is that, after $t = \tau$ the solution has decreased of a factor about 1/3:

$$y(\tau) = y_0 e^{-\tau/\tau} = y_0 e^{-1} \sim 0.36\, y_0$$

  with respect it initial value.

- The stability condition coming from the Von Neumann's criterion thus becomes:

$$h \leq 2\tau$$

  that is, the **time step must be smaller than**, except for a given factor, **the characteristic time of the phenomenon**!

Euler's schemes

- Let us try what happens if we use another approximation for the first derivative, with *m*=-*1*, *k*=*0*:

$$\left.\frac{dy}{dt}\right|_{t_n} = \frac{y_n - y_{n-1}}{h} + \mathcal{E} = F(y_n, t_n)$$

where: $\mathcal{E} = y_n'' \frac{h}{2} + O(h^2)$

- If we multiply by h both sides, rearrange the terms and **we pass from the step *n* to *n+1***:

$$y_{n+1} = y_n + hF(y_{n+1}, t_{n+1}) - h\mathcal{E}$$

Euler's schemes

- That is a one-step scheme, provided that:

$$\begin{cases} \Phi(t_n, y_n, F_n, t_{n+1}, y_{n+1}, F_{n+1}; h) = F(y_{n+1}, t_{n+1}) \\ \tau_{n+1}(h) = -\mathcal{E} = -y_n'' \frac{h}{2} + O(h^2) \end{cases}$$

that means that:

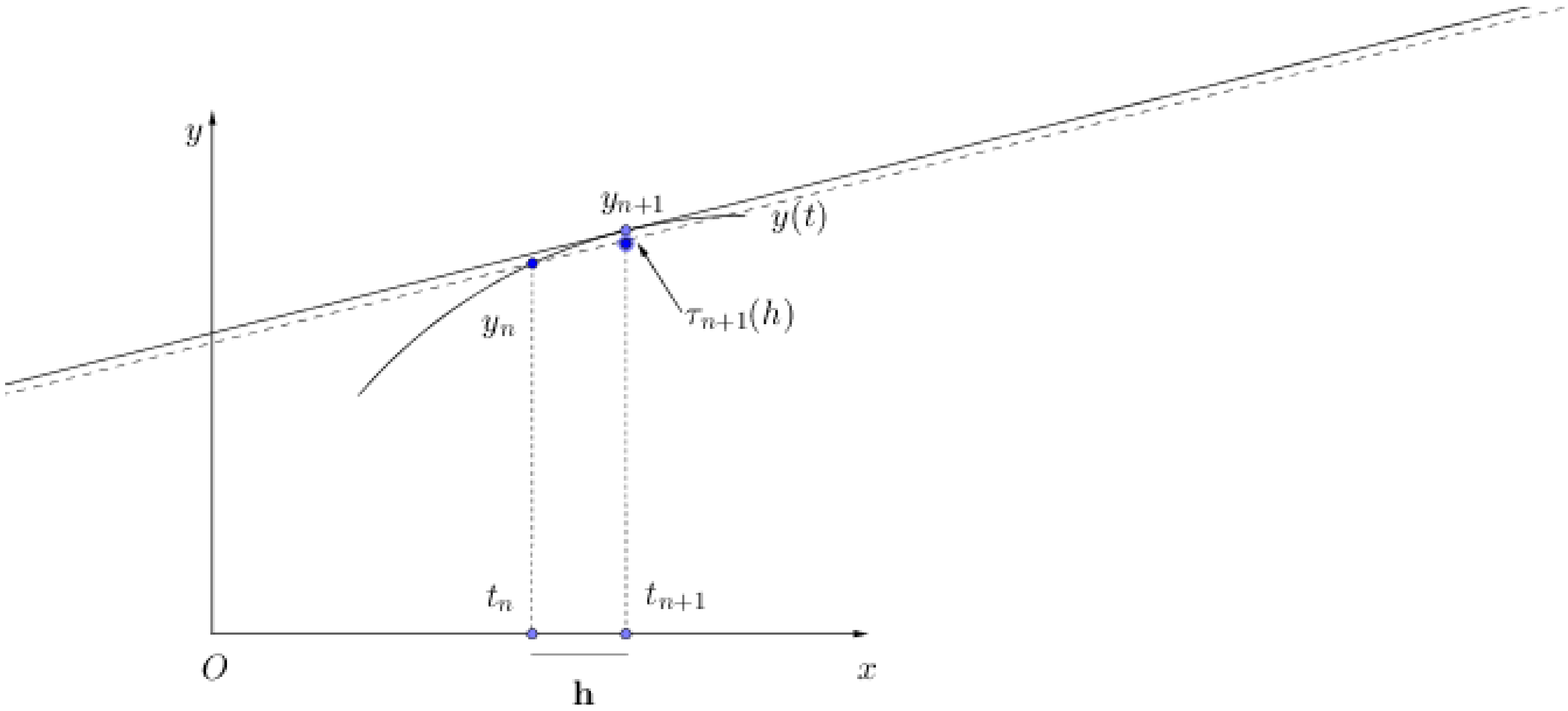
1) The scheme is **implicit** (Φ **does** depend on quantities at t_{n+1});

2) It is a **first order scheme**, since $p=1$;

3) The scheme is **consistent**, since the **two conditions are automatically satisfied** (when h tends to zero, $F(y_{n+1}, t_{n+1}) \to F(y_n, t_n)$)!

Euler's schemes

- This is the so-called **Backward Euler's scheme**:



Euler's schemes

- Let us study again the convergence and stability of the scheme when applied to the equation:

$$\frac{dy}{dt} = ky$$

with the initial condition: $y(t=0)=y_0$.

- In this case, the scheme reads:

$$y_{n+1} = y_n + hF(y_{n+1}, t_{n+1}) = y_n + hk\, y_{n+1} \Rightarrow$$

$$\Rightarrow \quad y_{n+1} = \frac{y_n}{1 - hk}$$

Euler's schemes

- The numerical solution is then:

$$y_1 = \frac{y_0}{1-kh} \qquad \text{for } t = t_1$$

$$y_2 = \frac{y_1}{1-kh} = \frac{y_0}{(1-kh)^2} \qquad \text{for } t = t_2$$

$$y_3 = \frac{y_2}{1-kh} = \frac{y_0}{(1-kh)^3} \qquad \text{for } t = t_3$$

$$\ldots$$

$$y_n = \frac{y_{n-1}}{1-kh} = \frac{y_0}{(1-kh)^n} \qquad \text{for } t = t_n$$

Euler's schemes

- To show the convergence of the scheme, we have to compute:

$$\lim_{h\to 0} y_n = \lim_{h\to 0} y_0(1-kh)^{-n} = y_0 \lim_{h\to 0}(1-kh)^{-n}$$

$$= y_0 \lim_{h\to 0}(1-kh)^{(-kt_n)/(kh)} = y_0 \left[\lim_{h\to 0}(1-kh)^{\frac{1}{kh}}\right]^{-kt_n} =$$

$$= y_0 \left[e^{-1}\right]^{-kt_n} = y_0 e^{kt_n} = y_{\mathrm{ex}}(t_n)$$

where we used the fact that: $\lim_{x\to 0}(1-x)^{\frac{1}{x}} = e^{-1}$

- That is, the scheme is **convergent**!

Euler's schemes

- Let us see whether it is stable.
- For the Von Neumann's criterion:

$$A(h) = \left|\frac{y_{n+1}}{y_n}\right| \leq 1 \quad \Rightarrow \quad \left|\frac{1}{1-kh}\right| \leq 1 \quad \Rightarrow$$

$$\Rightarrow \begin{cases} \dfrac{1}{1-kh} \leq 1 & \Rightarrow \quad 0 \leq -kh \quad \Rightarrow \quad k \leq 0 \\ -1 \leq \dfrac{1}{1-kh} & \Rightarrow \quad -1 + kh \leq 1 \quad \Rightarrow \\ & \Rightarrow -|k|h \leq 2 \quad \text{always satisfied!} \end{cases}$$

that is the scheme is **unconditionally stable**, whatever value of h we choose!

Euler's schemes

- This is a **general property** of implicit schemes:

  implicit schemes are, generally, **more stable than explicit schemes**!

- However, generally, they are also **much more difficult to implement** for **non-linear equations**!

- For instance, the non-linear equation: $\frac{dy}{dt} = k\sin(y)$

  can be solved numerically with the Backward Euler scheme as: $y_{n+1} = y_n + hk\sin(y_{n+1})$

  Finding y_{n+1} requires the solution of a non-linear, algebraic equation!

Runge-Kutta scheme

- We can improve the precision of the numerical scheme, by keeping into account that, for instance, the FD central scheme:

$$\left.\frac{dy}{dx}\right|_{x_j} = \frac{y(x_{j+1}) - y(x_{j-1})}{2h} + \mathcal{E}$$

with an error: $\mathcal{E} \propto h^2$

- We can build a one-step scheme by taking an intermediate point t^*_n which is the midpoint between t_n and t_{n+1}.

Runge-Kutta scheme

- This is equivalent to consider:

$$x_{j-1} = t_n$$

$$x_{j+1} = t_{n+1}$$

$$x_j = t_n^* = \frac{t_n + t_{n+1}}{2} = t_n + \frac{h}{2}$$

$$h \to \frac{h}{2}$$

that is, the scheme becomes:

$$\left.\frac{dy}{dt}\right|_{t_n^*} = \frac{y_{n+1} - y_n}{h} + \mathcal{E} = F(y_n^*, t_n^*) \quad \Rightarrow$$

$$\Rightarrow \quad y_{n+1} = y_n + hF(y_n^*, t_n^*) - h\mathcal{E}$$

Runge-Kutta scheme

- In order this to be useful we have to find a way to compute y^*_n and t^*_n. We can use a Forward Euler's scheme over a time-step $h/2$, to compute this:

$$y_n^* = y_n + \frac{h}{2} F(y_n, t_n)$$

- That is, the final scheme is:

$$\begin{cases} y_n^* & = y_n + \frac{h}{2} F(y_n, t_n) \\ y_{n+1} & = y_n + hF(y_n^*, t_n^*) - h\mathcal{E} \quad \text{where: } t_n^* = t_n + \frac{h}{2} \end{cases}$$

Runge-Kutta scheme

- Finally the scheme can be rewritten as:

$$y_{n+1} = y_n + hF\left(y_n + \frac{h}{2}F(y_n, t_n), t_n + \frac{h}{2}\right) - h\mathcal{E}$$

which is indeed an **explicit**, **one-step scheme**, because:

$$\Phi(y_n, t_n, F_n, y_{n+1}, t_{n+1}, F_{n+1}; h) = F\left(y_n + \frac{h}{2}F_n, t_n + \frac{h}{2}\right)$$

$$\tau_{n+1}(h) = -\mathcal{E}$$

Before concluding this is a second order scheme, however we have to show that $\mathcal{E} \propto h^2$, because the first half-step with the Euler scheme may decrease the precision!

Runge-Kutta scheme

- To show this, we re-write the two equations of the scheme by substituting the derivative of y to the RHS $F(y,t)$, from the equation:

$$y_n^* = y_n + \frac{h}{2}F(y_n, t_n) = y_n + \frac{h}{2}\left.\frac{dy}{dt}\right|_{t_n}$$

$$y_{n+1} = y_n + hF(y_n^*, t_n^*) - h\mathcal{E} = y_n + h\left.\frac{dy}{dt}\right|_{t_n^*} - h\mathcal{E} =$$

$$= y_n + h\frac{d}{dt}\left[y_n + \frac{h}{2}\left.\frac{dy}{dt}\right|_{t_n}\right] - h\mathcal{E} =$$

$$= y_n + h\frac{dy_n}{dt} + \frac{h^2}{2}\frac{d^2y_n}{dt^2} - h\mathcal{E}$$

Runge-Kutta scheme

- By comparing this relation with the Taylor's expansion of y_{n+1} as a function of y_n:

$$y_{n+1} = y_n + h\frac{dy_n}{dt} + \frac{h^2}{2!}\frac{d^2y_n}{dt^2} + \frac{h^3}{3!}\frac{d^3y_n}{dt^3} + O(h^4)$$

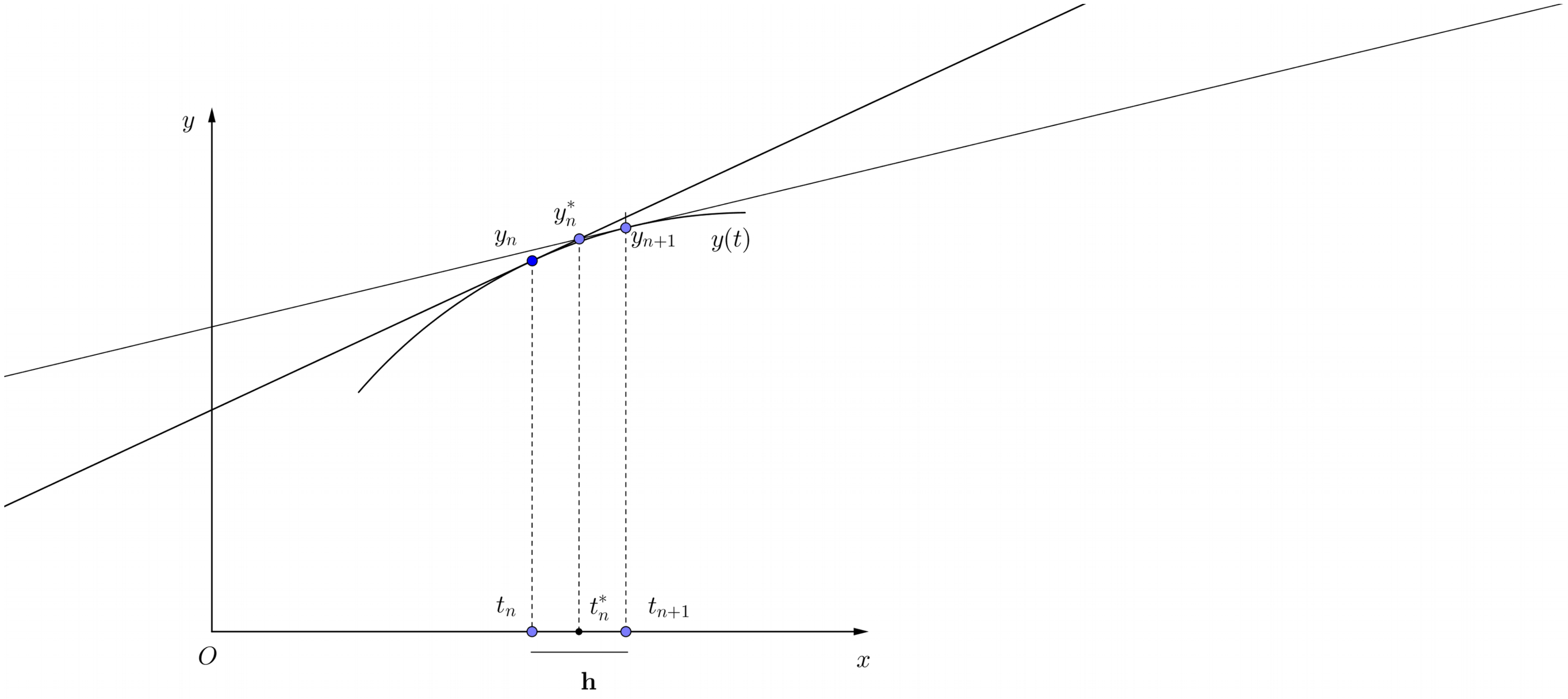
we deduce that:

$$\mathcal{E} = -\frac{h^2}{6}\frac{d^3y_n}{dt^3} + O(h^3)$$

namely the scheme is a second order scheme ($p=2$)!

Runge-Kutta scheme

- This is the so-called, **second order Runge-Kutta** scheme:



Runge-Kutta scheme

- From this, we deduce that the scheme is **consistent**, in fact:

$$\lim_{h\to 0} \Phi = \lim_{h\to 0} F\left(y_n + \frac{h}{2}, t_n + \frac{h}{2}\right) = F(y_n, t_n)$$

and: $\lim_{h\to 0} \tau_{n+1}(h) = -\mathcal{E} = 0$

- To analyze the **convergence** and **stability** properties, we have to apply it to, for instance, the usual equation...

Runge-Kutta scheme

- By considering the equation:

$$\frac{dy}{dt} = ky$$

the second-order Runge-Kutta scheme reads:

$$y_n^* = y_n + \frac{h}{2}F(y_n, t_n) = y_n + \frac{h}{2}ky_n$$

$$y_{n+1} = y_n + hF(y_n^*, t_n^*) = y_n + hky_n^* =$$

$$= y_n + hk\left(y_n + \frac{h}{2}ky_n\right) = y_n\left(1 + hk + \frac{h^2k^2}{2}\right)$$

Runge-Kutta scheme

- Therefore, the scheme can be written as:

$$y_1 = y_0 \left(1 + kh + \frac{h^2k^2}{2}\right) \qquad \text{for } t = t_1$$

$$y_2 = y_1 \left(1 + kh + \frac{h^2k^2}{2}\right) = y_0 \left(1 + kh + \frac{h^2k^2}{2}\right)^2 \qquad \text{for } t = t_2$$

$$y_3 = y_2 \left(1 + kh + \frac{h^2k^2}{2}\right) = y_0 \left(1 + kh + \frac{h^2k^2}{2}\right)^3 \qquad \text{for } t = t_3$$

$$\ldots$$

$$y_n = y_{n-1} \left(1 + kh + \frac{h^2k^2}{2}\right) = y_0 \left(1 + kh + \frac{h^2k^2}{2}\right)^n \qquad \text{for } t = t_n$$

Runge-Kutta scheme

- The convergence is trivially proven when considering that:

$$\lim_{h\to 0} y_0 \left(1 + hk + \frac{h^2k^2}{2}\right)^n \to \lim_{h\to 0} y_0(1+hk)^n$$

which is the same term appearing in the Forward Euler scheme, that is convergent, as we already showed!

- Concerning the stability, the Von Neumann's criterion gives:

$$A(h) = \left|\frac{y_{n+1}}{y_n}\right| = \left|1 + kh + \frac{h^2k^2}{2}\right| \leq 1$$

Runge-Kutta scheme

- This is equivalent to the system:

$$hk + \frac{h^2k^2}{2} \leq 0 \quad \Rightarrow \quad hk\left(1 + \frac{hk}{2}\right) \leq 0$$

$$-1 \leq 1 + hk + \frac{h^2k^2}{2} \quad \Rightarrow \quad \frac{h^2k^2}{2} + hk + 2 \geq 0$$

- The first equation has a solution:

$$hk \leq 0 \quad \Rightarrow \quad k \leq 0$$

$$1 + \frac{hk}{2} \geq 0 \quad \Rightarrow \quad 1 \geq \frac{h|k|}{2} \quad \Rightarrow \quad h \leq \frac{2}{|k|}$$

whilst the opposite case has no solution!

Runge-Kutta scheme

- The second inequality corresponds to:

$$h^2k^2 + 2hk + 4 \geq 0$$

and, posing $x=hk$, can be re-written as:

$$x^2 + 2x + 4 \geq 0$$

which is **always satisfied**, since the solutions:

$$x = \frac{-2 \pm \sqrt{4 - 16}}{2}$$

are always complex, that is the parabola has no interception with the x axis and lies in the upper part of the Cartesian plane ($y>0$).

Runge-Kutta scheme

- Finally, the stability criterion gives:

$$k \leq 0; \quad h \leq \frac{2}{|k|}$$

that is **identical** to the stability condition for the **Forward Euler's scheme**!

- The lesson we learnt so far:
  - **Explicit schemes** have more or less all the **same stability conditions**;
  - If we want **more stability**, we should use **implicit schemes**;
  - **Runge-Kutta** has however a superior precision, although it requires **two evaluations of the RHS of the equation**!

Higher order ODEs

- Till now, we studied the case of a single first order equation.
- It is possible to show that **any n-degree ODE** can be cast into the form of a **system of n first-order equations**. For instance, an ODE like:

$$\alpha_0(t)\frac{d^n y}{dt^n} + \alpha_1(t)\frac{d^{n-1} y}{dt^{n-1}} + \ldots + \alpha_{n-1}(t)\frac{dy}{dt} + \alpha_n(t)y(t) = \beta(t)$$

with initial conditions:

$$y(t=0) = y_0; \quad \left.\frac{dy}{dt}\right|_{t=0} = y_1; \quad \ldots \quad ; \left.\frac{d^{n-1}y}{dt^{n-1}}\right|_{t=0} = y_{n-1}$$

Higher order ODEs

- It can be put into the form:

$$\frac{dy}{dt} = v_1(t)$$

$$\frac{d^2y}{dt^2} = \frac{dv_1}{dt} = v_2(t)$$

$$\frac{d^3y}{dt^3} = \frac{dv_2}{dt} = v_3(t)$$

$$\cdots$$

$$\frac{d^{n-1}y}{dt^{n-1}} = \frac{dv_{n-2}}{dt} = v_{n-1}(t)$$

$$\frac{dv_{n-1}}{dt} = -\frac{1}{\alpha_0(t)}\left[\alpha_1(t)v_{n-1}(t) + \ldots + \right.$$

$$\left. + \alpha_{n-1}v_1(t) + \alpha_n y(t)\right] + \beta(t)/\alpha_0(t)$$

Higher order ODEs

- Which are a **system of n first-order ODE** with the following n initial conditions:

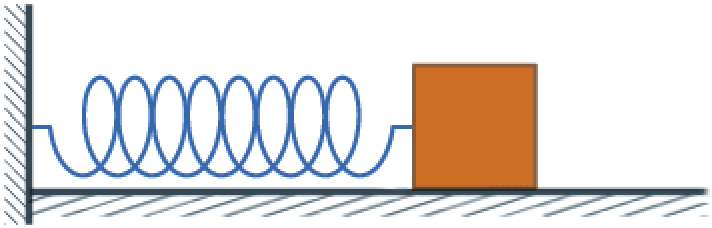
$$y(t=0)=y_0; \quad v_1(t=0)=y_1; \quad \ldots \quad ; v_{n-1}(t=0)=y_{n-1}$$

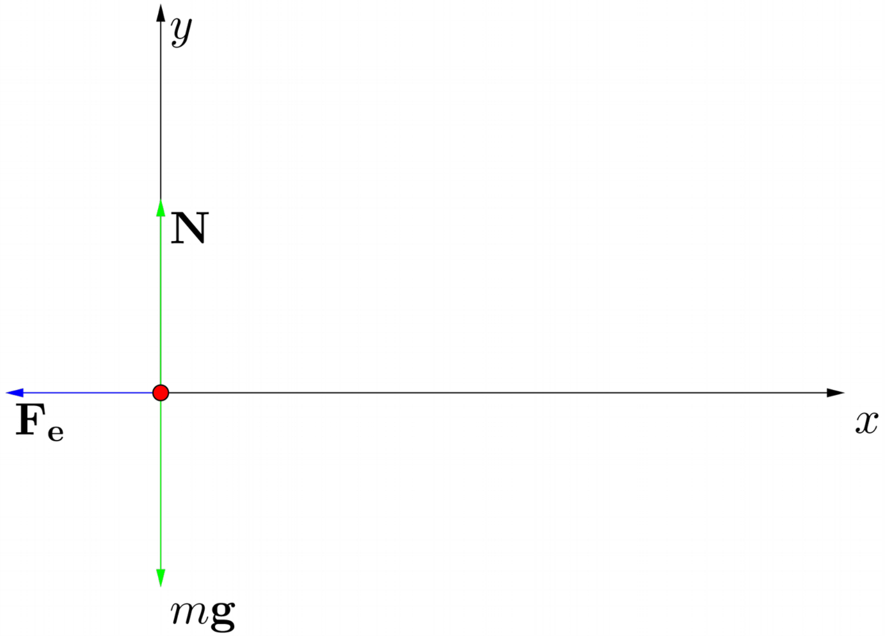
- Notice that, although this was shown in the special case above of a linear equation with non constant coefficients, **this is valid for any differential equation**.

- Therefore, the schemes we have just studied can be applied to each equation of the system, thus **finding the solution for all the unknowns** $y, v_1, v_2, \ldots, v_{n-1}$.

Harmonic oscillator

- Second example: an ODE with oscillating solutions, **the harmonic oscillator**.





$$m\mathbf{a} = \mathbf{F_e} + \mathbf{N} + m\mathbf{g}$$

$$\frac{d^2x(t)}{dt} = -\frac{k}{m}x$$

$$\frac{d^2y(t)}{dt} = -g + \frac{N}{m} = 0$$

Harmonic oscillator

- Since both k and m are both positive constants, we may assume:

$$\omega^2 = \frac{k}{m}$$

and the equation describing the motion of the body attached to the spring is:

$$\frac{d^2 x(t)}{dt^2} = -\omega^2 x(t)$$

- This is the so-called harmonic oscillator equations, which is a second order, linear, ODE, with constant coefficients.

Harmonic oscillator

- It is easy to show that any function in the form:

$$x(t) = A\sin(\omega t + \phi)$$

is a solution of such equation. In fact:

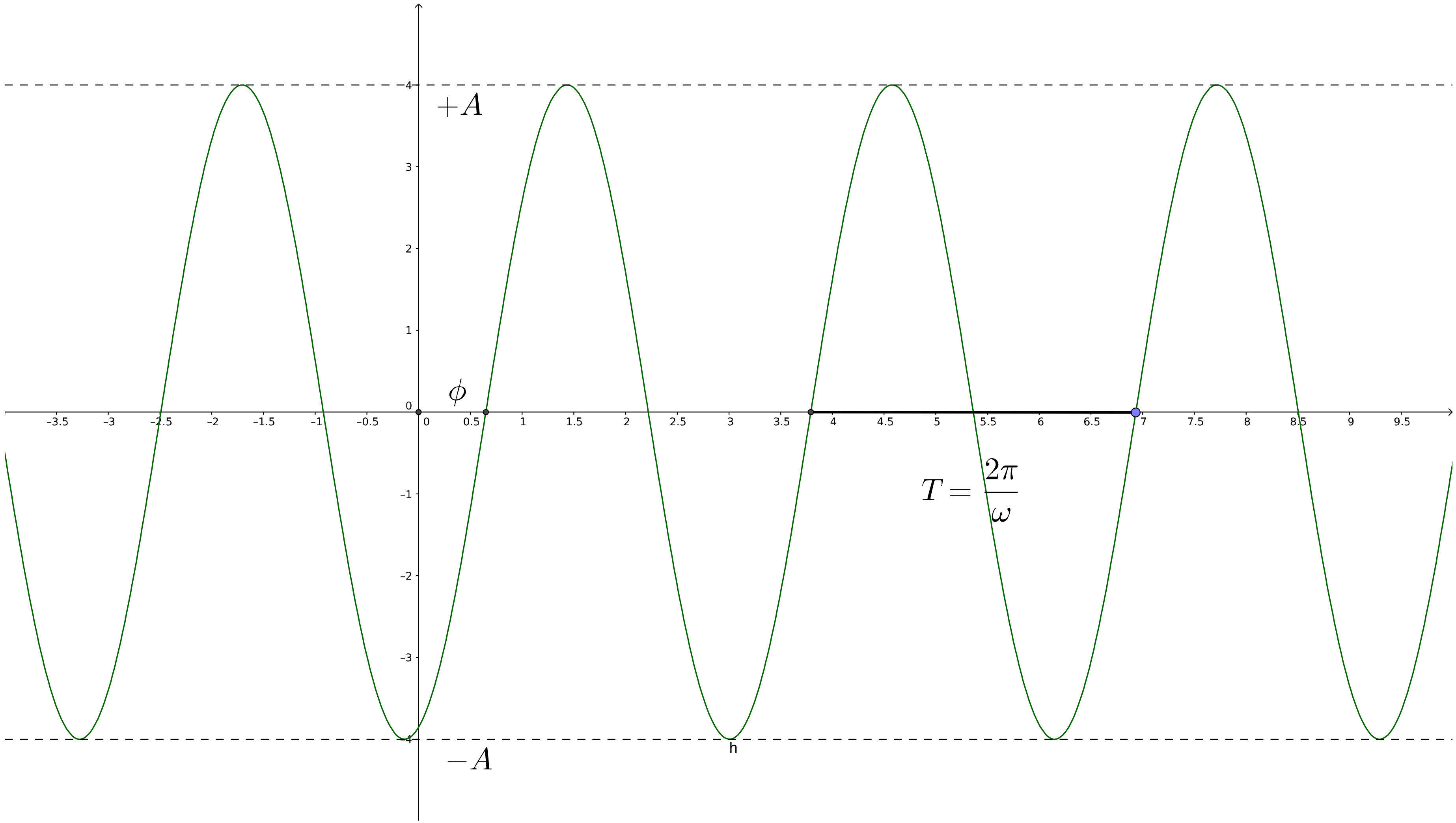
$$\frac{dx(t)}{dt} = A\omega\cos(\omega t + \phi)$$

$$\frac{d^2x(t)}{dt^2} = -A\omega^2\sin(\omega t + \phi) = -\omega^2 x(t)$$

- This represents an **oscillation** with **amplitude** A, **frequency** ω and **phase** ϕ.

Harmonic oscillator

- Representation of the solution for the harmonic oscillator.



Harmonic oscillator

- The values of A and ϕ depend on the initial conditions:

$$x(t=0) = x_0 = A\sin(\phi)$$

$$\left.\frac{dx}{dt}\right|_{t=0} = v_0 = A\omega\cos(\phi)$$

- By adding hand by hand the squares of the two equations or by dividing them, we get:

$$A = \sqrt{x_0^2 + \left(\frac{v_0}{\omega}\right)^2}; \qquad \phi = \arctan\left(\frac{x_0\omega}{v_0}\right)$$

Harmonic oscillator

- How do we proceed numerically? The original equation can be re-written as:

$$\frac{dx(t)}{dt} = v(t)$$
$$\frac{dv(t)}{dt} = -\omega^2 x(t)$$

with the initial conditions:

$$x(t=0) = x_0; \qquad v(t=0) = v_0$$

- We can now apply one of the scheme we studied, for instance Forward Euler:

Harmonic oscillator

- Fixed a total interval $[0, T_{end}]$ and subdividing into intervals of width h:

$$\frac{x_{n+1} - x_n}{h} = v_n$$
$$\frac{v_{n+1} - v_n}{h} = -\omega^2 x_n$$

- This can be written in the form:

$$x_{n+1} = x_n + h v_n$$
$$v_{n+1} = v_n - h\omega^2 x_n$$

Harmonic oscillator

- Unfortunately, a simple description like this **does not work**! The reason is that if we study the stability of such a scheme, we discover that **it is unstable for any value we choose for h**!
- Before showing this, we need to express the Von Neumann's stability criterion for a system of equations:

*Given a system of k **linear ODEs** and a one-step scheme applied to each equation of the system, the scheme is **stable** if the spectral radius of the matrix:*

Harmonic oscillator

$$\begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \dots \\ y_k \end{pmatrix}_{n+1} = A(h) \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \dots \\ y_k \end{pmatrix}_n$$

called Amplification matrix, is lesser than 1!

- The spectral radius is the maximum eigenvalue (in module) of the matrix $A(h)$.
- This can be easily applied to the simple system for the harmonic oscillator.

Harmonic oscillator

- The scheme can be written in matrix form as:

$$\begin{pmatrix} x_{n+1} \\ v_{n+1} \end{pmatrix} = \begin{pmatrix} 1 & h \\ -h\omega^2 & 1 \end{pmatrix} \begin{pmatrix} x_n \\ v_n \end{pmatrix} = A(h) \begin{pmatrix} x_n \\ v_n \end{pmatrix}$$

- We have now to find the eigenvalues of $A(h)$:

$$\det|A - \lambda\mathbb{I}| = 0 \quad \Rightarrow$$

$$\Rightarrow \quad \begin{vmatrix} 1-\lambda & h \\ -h\omega^2 & 1-\lambda \end{vmatrix} = 0 \quad \Rightarrow$$

$$\Rightarrow \quad (1-\lambda)^2 + h^2\omega^2 = 0 \quad \Rightarrow$$

$$\lambda^2 - 2\lambda + (1 + h^2\omega^2) = 0$$

Harmonic oscillator

- The solutions are:

$$\lambda = \frac{2 \pm \sqrt{4 - 4(1 + h^2\omega^2)}}{2} = 1 \pm ih\omega$$

- The modulus of this complex number is:

$$|\lambda| = \sqrt{1 + h^2\omega^2}$$

which can never be lesser than 1, that is **the scheme is never stable**, whatever value of h we choose!

Harmonic oscillator

- The interesting thing is that we obtain the same result, that is a scheme **always unstable**, even if we use **two Backward Euler schemes** for both equations:

$$\frac{x_{n+1} - x_n}{h} = v_{n+1}$$
$$\frac{v_{n+1} - v_n}{h} = -\omega^2 x_{n+1}$$

that is:

$$x_{n+1} = x_n + h v_{n+1}$$
$$v_{n+1} = v_n - h\omega^2 x_{n+1}$$

Harmonic oscillator

- This can be transformed as:

$$x_{n+1} = \frac{x_n + hv_n}{1 + h^2\omega^2}$$
$$v_{n+1} = \frac{v_n - h\omega^2 x_n}{1 + h^2\omega^2}$$

the amplification matrix reads:

$$A(h) = \begin{pmatrix} \mu & \mu h \\ -\mu h\omega^2 & \mu \end{pmatrix} \qquad \mu = \frac{1}{1 + h^2\omega^2}$$

which has always eigenvalues with modulus greater than 1.

Harmonic oscillator

- The same holds when we treat both equations with a second order Runge-Kutta scheme:

$$x_n^* = x_n + \frac{h}{2} v_n$$

$$v_n^* = v_n - \frac{h}{2}\omega^2 x_n$$

$$x_{n+1} = x_n + h v_n^*$$

$$v_{n+1} = v_n - h\omega^2 x_n^*$$

that is again always unstable...

Harmonic oscillator

- It turns out that the solution of the problem, namely a **stable scheme**, is given by considering one equation with the **Forward Euler scheme** and another with **Backward Euler**.
- For instance, by using FE for the first equation and BE for the second:

$$x_{n+1} = x_n + h v_n$$
$$v_{n+1} = v_n - h\omega^2 x_{n+1}$$

- This scheme is said **symplectic** (from Greek, "composed of different parts").

Harmonic oscillator

- The scheme can be re-written as:

$$x_{n+1} = x_n + hv_n$$

$$v_{n+1} = v_n(1 - h^2\omega^2) - h\omega^2 x_n$$

- The amplification matrix is:

$$A(h) = \begin{pmatrix} 1 & h \\ -h\omega^2 & 1 - h^2\omega^2 \end{pmatrix}$$

- The characteristic polynomial is:

$$(1-\lambda)(1 - h^2\omega^2 - \lambda) + h^2\omega^2 = 0$$

Harmonic oscillator

- It can be re-written as:

$$\lambda^2 + \lambda(h^2\omega^2 - 2) + 1 = 0$$

  whose solution is:

$$\lambda = 1 - \frac{h^2\omega^2}{2} \pm \frac{h\omega}{2}\sqrt{h^2\omega^2 - 4}$$

- We distinguish two cases:

  1) Real values for lambda: $h^2\omega^2 \geq 4 \quad \Rightarrow \quad h\omega \geq 2;$

  2) Complex conjugates root: $h^2\omega^2 < 4 \quad \Rightarrow \quad h\omega < 2.$

Harmonic oscillator

- In the first case we get:

$$|\lambda| \leq 1 \quad \Rightarrow \quad \begin{cases} 1 - \frac{h^2\omega^2}{2} \pm \frac{h\omega}{2}\sqrt{h^2\omega^2 - 4} \leq 1 \\ -1 \leq 1 - \frac{h^2\omega^2}{2} \pm \frac{h\omega}{2}\sqrt{h^2\omega^2 - 4} \end{cases}$$

- Both equations bring to the inequality:

$$\sqrt{h^2\omega^2 - 4} \leq h\omega$$

which is **always satisfied**!

- In the second case, we get complex conjugate solutions in the form:

$$\lambda = 1 - \frac{h^2\omega^2}{2} \pm \frac{ih\omega}{2}\sqrt{4 - h^2\omega^2}$$

Harmonic oscillator

- In this case we have to consider the modulus of λ:

$$|\lambda| \leq 1 \quad \Rightarrow \quad \sqrt{\left(1-\frac{h^2\omega^2}{2}\right)^2 + \frac{h^2\omega^2}{4}(4-h^2\omega^2)} \leq 1$$

  that is **always satisfied** again, because all the terms inside the square root cancel out, except one, which gives: $\sqrt{1} \leq 1$

- This means that the scheme is **unconditionally stable**. The same holds if we take FE for the second equation and BE for the first!

Higher order schemes

- We have seen the second order Runge-Kutta scheme, that can be written as:

$$y_n^* = y_n + \frac{h}{2} F(y_n, t_n)$$

$$y_{n+1} = y_n + hF(y_n^*, t_n^*)$$

- It is possible to enhance the precision of the scheme by considering further refinements of the RHS of the equation.
- A scheme often used is the fourth-order, Runge-Kutta scheme:

Higher order schemes

- Let us call: $y_n^{(0)} = y_n$, the scheme is:

$$y_n^{(1)} = y_n^{(0)} + \frac{h}{2} F(y_n^{(0)}, t_n)$$

$$y_n^{(2)} = y_n^{(0)} + \frac{h}{2} F(y_n^{(1)}, t_n^*)$$

$$y_n^{(3)} = y^{(0)} + hF(y_n^{(2)}, t_n^*)$$

$$y_{n+1} = y_n^{(0)} + \frac{h}{6} \left\{ F(y_n^{(0)}, t_n) + F(y_n^{(3)}, t_n^*) + \right.$$
$$\left. + 2 \left[F(y_n^{(1)}, t_n^*) + F(y_n^{(2)}, t_n^*) \right] \right\}$$

where, as usual: $t_n^* = t_n + \frac{h}{2}$

Higher order schemes

- The precision of the scheme **is not easy to verify in the general case**, however we can show how the scheme can be applied to the simple equation:

$$\frac{dy}{dt} = ky$$

  and we can easily verify in this **particular case** that it is indeed a fourth-order scheme.

- In this case, we have:

$$y_n^{(1)} = y_n^{(0)} + \frac{h}{2} k y_n^{(0)}$$

$$y_n^{(2)} = y_n^{(0)} + \frac{h}{2} k y_n^{(1)} = y_n^{(0)} + \frac{hk}{2} \left(y_n^{(0)} + \frac{h}{2} k y_n^{(0)} \right)$$

Higher order schemes

$$y_n^{(2)} = y_n^{(0)} + \frac{hk}{2} y_n^{(0)} + \frac{h^2k^2}{4} y_n^{(0)}$$

$$y_n^{(3)} = y_n^{(0)} + hk y_n^{(2)} = y_n^{(0)} + hk y_n^{(0)} + \frac{h^2k^2}{2} y_n^{(0)} + \frac{h^3k^3}{4} y_n^{(0)}$$

$$y_{n+1} = y_n^{(0)} + \frac{h}{6} \left\{ k y_n^{(0)} + k y_n^{(3)} + 2k y_n^{(1)} + 2k y_n^{(2)} \right\} =$$

$$= y_n^{(0)} + \frac{hk}{6} y_n^{(0)} + \frac{hk}{6} y_n^{(3)} + \frac{hk}{3} y_n^{(1)} + \frac{hk}{3} y_n^{(2)} =$$

$$= y_n^{(0)} + \frac{hk}{6} y_n^{(0)} + \frac{hk}{3} \left(y_n^{(0)} + \frac{hk}{2} y_n^{(0)} \right) +$$

$$+ \frac{hk}{3} \left(y_n^{(0)} + \frac{hk}{2} y_n^{(0)} + \frac{h^2k^2}{4} \right) +$$

$$+ \frac{hk}{6} \left(y_n^{(0)} + hk y_n^{(0)} + \frac{h^2k^2}{2} y_n^{(0)} + \frac{h^3k^3}{4} y_n^{(0)} \right)$$

Higher order schemes

- Finally, by re-arranging the terms, we have:

$$y_{n+1} = y_n^{(0)} \left(1 + hk + \frac{h^2k^2}{2} + \frac{h^3k^3}{6} + \frac{h^4k^4}{24} \right)$$

- We can notice that the exact solution is given by:

$$y(t_n) = y_0 e^{kt} \quad \Rightarrow$$

$$y(t_{n+1}) = y_0 e^{kt_{n+1}} = y_0 e^{kt_n + kh} = y_0 e^{kt_n} e^{kh} = y_n e^{kh}$$

Higher order schemes

- The Taylor's development of the function e^x about $x=0$, is:

$$e^x = e^0 + \left.\frac{de^x}{dx}\right|_{x=0} (x-0) + \left.\frac{d^2e^x}{dx^2}\right|_{x=0} \frac{(x-0)^2}{2!} +$$

$$+ \left.\frac{d^3e^x}{dx^3}\right|_{x=0} \frac{(x-0)^2}{3!} + \left.\frac{d^4e^x}{dx^2}\right|_{x=0} \frac{(x-0)^4}{4!} + O(x^5)$$

$$= 1 + x + \frac{x^2}{2} + \frac{x^3}{6} + \frac{x^4}{24} + O(x^5)$$

which corresponds to the previous formula for $x=kh$.

Higher order schemes

- This shows that the scheme represents a fourth order approximation of the exact solution!
- **Runge-Kutta scheme** can be constructed with, in principle, **any wanted precision**. Of course one must keep into account that more precise schemes require an equal amount of evaluations of the RHS of the equation, that implies **longer computational times**!
- There is a whole **“zoology” of numerical schemes**, often with very little differences among them. Just some of them:

Other One-step schemes

- **Crank-Nicolson** scheme:

$$y_{n+1} = y_n + \frac{h}{2}\left[F(y_n, t_n) + F(y_{n+1}, t_{n+1})\right]$$

this is a **second-order, implicit** scheme, rather stable a in a variety of circumstances.

- **Heun**'s scheme:

$$\tilde{y}_{n+1} = y_n + F(y_n, t_n)$$

$$y_{n+1} = y_n + \frac{h}{2}\left[F(y_n, t_n) + F(\tilde{y}_{n+1}, t_{n+1})\right]$$

that is a **second-order, explicit** scheme, a slight variant of the Crank-Nicolson scheme.

Some multi-step schemes

- **Leap-Frog** scheme:

$$y_{n+1} = y_{n-1} + 2hF(y_n, t_n)$$

this is a **second-order, explicit** scheme.

- **Adams-Bashforth** scheme:

$$y_{n+1} = y_{n-1} + \frac{h}{2}\left[3F(y_n, t_n) - F(y_{n-1}, t_{n-1})\right]$$

that is a **second-order, explicit** scheme.

- And many more...