

# Ordinary Differential Equations – IVP II



# **Numerical Methods for ODE**



- Euler's Method
- Analysis of the one-step methods
- Runge-Kutta Methods
- Multi-step Methods
  - Adams-Bashforth
  - Adams-Moulton
  - Predictor-Corrector
- Systems of ODE
- Stability
- Stiff Problems

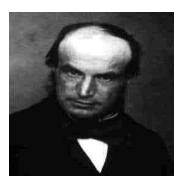


Leonhard Euler (1707-1783),

Martin Kutta Carl David Runge (1856-1927)







J.C. Adams (1819-1882)



# Some numerical one-step Methods for ODE

### $u_{n+1} \text{ depends only on } u_n \text{ for any } n$

$$u_{j+1} - u_j = h f(x_j, u_j)$$
 Forward Euler (explicit)  

$$u_{j+1} - u_j = h f(x_{j+1}, u_{j+1})$$
 Backward Euler (implicit)  

$$u_{j+1} - u_j = \frac{h}{2} [f(x_j, u_j) + f(x_{j+1}, u_{j+1})]$$
 Crank-Nicolson



# Heun's Method

Heun's method is an explicit method derived from an implicit method. Starting from the Crank-Nicolson method

$$y(x_{n} + h) - y(x_{n}) \cong \frac{h}{2} \Big[ f(x_{n}, y_{n}) + f(x_{n+1}, y_{n+1}) \Big]$$

$$\cong \frac{h}{2} \Big[ f(x_{n}, y_{n}) + f(x_{n+1}, y_{n} + hf(x_{n}, y_{n})) \Big]$$

replace the Forward Euler's method to compute  $y_{n+1}$ .

The obtained formula is called the **Heun's method**:

$$u_{n+1} - u_n = \frac{h}{2} \left[ f(x_n, u_n) + f(x_{n+1}, u_n + hf(x_n, u_n)) \right]$$



# Forward Euler's Method (explicit)

Let the initial data  $(x_0, y_0)$  be a point on the solution y(x)

The slope of y at  $(x_0,y_0)$  is y'(x) that is f(x,y) and is computed :  $f_0 = f(x_0,y_0)$ 

To determine y(x) , let consider the tangent line at  $(x_0, y_0)$  :

$$y = y_0 + (x - x_0) f(x_0, y_0)$$
  
at x<sub>1</sub>=x<sub>0</sub>+h,  $y_1 = y_0 + (x_1 - x_0) f(x_0, y_0)$   $y(x_1) \approx y_1$ 

Approximation  $y_1$  is the value of the tangent to the solution in  $(x_0, y_0)$  evaluated at  $x_1$ 

$$y_2 = y_1 + (x_2 - x_1)f(x_1, y_1)$$

Approximation  $y_2$  is the value of the tangent to the curve y at  $(x_1, y_1)$  evaluated at  $x_2$ : double error!!



# Forward Euler's Method (explicit)

$$u_{n+1} = u_n + h f(x_n, y_n)$$

$$\frac{dy}{dx} = y' = f(x, y); \quad y(x_0) = y_0$$
Linear Approximation
$$y_0$$

$$x_0 \quad h \quad x_1 \quad h \quad x_2 \quad h \quad x_3$$



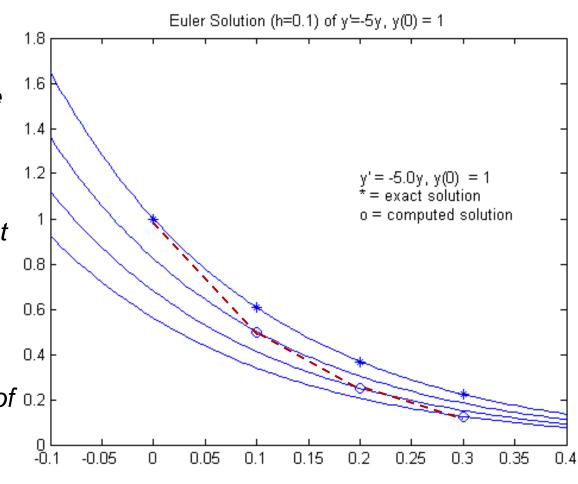
## Forward Euler's Method: example

Three steps of the forward Euler method.

The **exact solution** is the curved marked with \* on the solid line.

The **numerical values** obtained by the Euler method are circled and lie at the nodes of a broken line that interpolates them.

The **broken line** (trajectory of the approx. solution) is <sup>0.4</sup> tangential at the beginning of <sup>0.2</sup> each step to the ODE trajectory passing through <sup>-0.</sup> the corresponding node (solid lines).

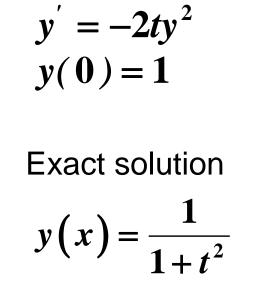


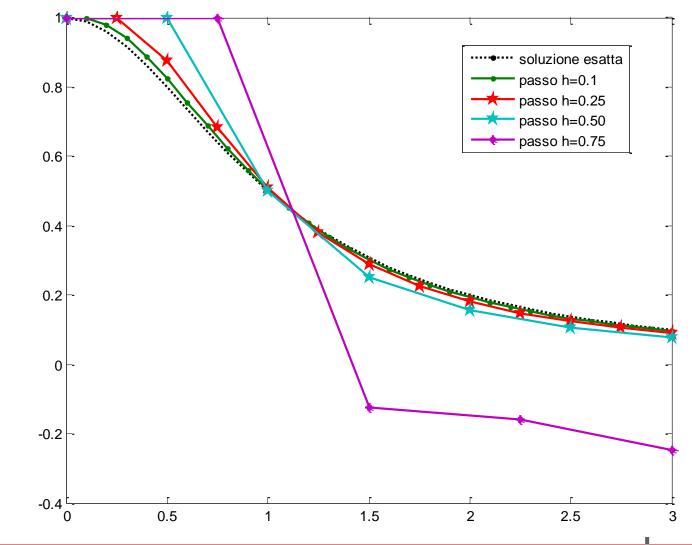


#### Forward Euler's Method : algorithm

Evaluate f at 
$$(x_n, y_n)$$
  
 $y_{n+1}$  is approximated by  $u_{n+1}$   
 $n = 0$   
for each  $x_n, n = 0, ..., N$   
 $f_n = f(x_n, u_n)$   
 $x_{n+1} = x_n + h$   
 $u_{n+1} = u_n + hf_n$   
 $n = n + 1$   
end

# Example: effect of Reduced Step Size on Euler's Method







# **Forward Euler's Method**

#### Limitations of the Forward Euler's Method:

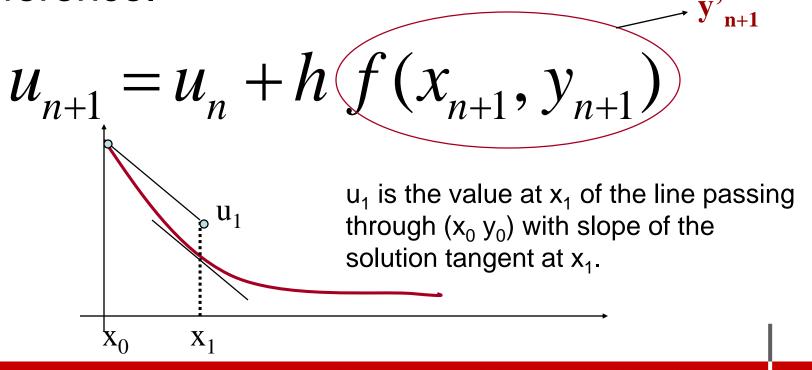
- Lack of accuracy
- Small step size

#### Explicit (vs Implicit):

- Explicit methods are significantly easier to implement,
- Carrying out an integration step is typically much faster.



It is obtained by approximating the first derivative of y at  $x_{n+1}$  with a backward finite difference.





# **Crank-Nicolson Method (implicit)**

The Crank-Nicolson method is an implicit one-step method:

$$u_{n+1} = u_n + h \left(\frac{f_n + f_{n+1}}{2}\right)$$

It uses the average slope of the slopes at the two points.

- Like other implicit methods it uses Newton's method to calculate the solution of the non-linear equation (nonlinear system), therefore it requires the derivative (Jacobian) of the function f.
- CN, Backward Euler and other implicit methods have numerical stability properties that in certain cases, make them superior to explicit methods.



# Numerical Methods for ODE

- **One-step Methods** 
  - Euler's Method

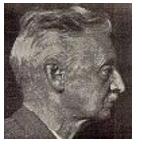


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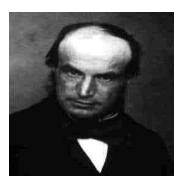


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# Analysis of the one-step methods

IVP

$$\begin{cases} y'(x) = f(x, y(x)) & \forall x \in I \equiv [a, b] \\ y(x_0) = y_0 & x_0 \in [a, b] \end{cases}$$

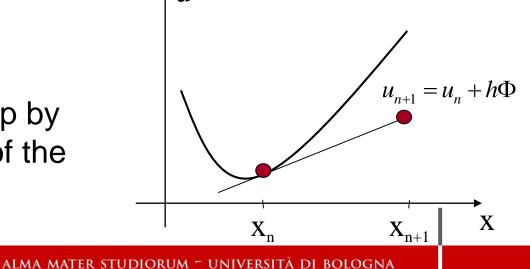
#### one-step methods

$$u_{n+1} = u_n + h\Phi(x_n, u_n, f_n; h)$$
  $0 \le n \le N_h - 1$   $u_0 = y_0$ 

 $\Phi =$  increment function or estimated slope  $\uparrow_{u}$ 

$$f_n = f(x_n, u_n)$$

This formula can be applied step by step to trace out the trajectory of the solution.

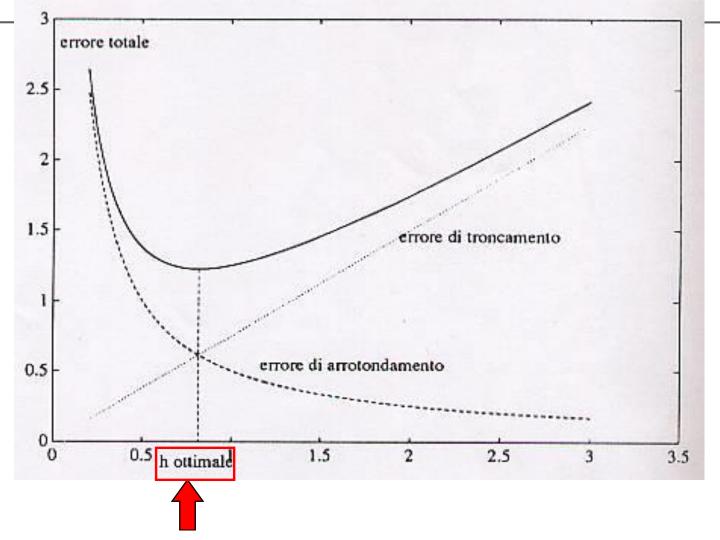




# **Total Error Analysis**

- Round-off errors caused by the limited numbers of significant digits that can be retained by a computer (roundoff error behaves like O(h<sup>-1</sup>)
- **Truncation Error**, or discretization, errors caused by the nature of the techniques employed to approximate values of y:
  - Local Truncation Error (LTE error for a single step)
  - propagated truncation error (approximations produced during the previous steps) (zero-stability)
- Absolute Stability

# **Total Error**



there exists an integration step h that balances optimally the two components of the error.



#### **One-step numerical method**

$$u_{n+1} = u_n + h\Phi(x_n, u_n, f_n; h)$$
  $0 \le n \le N_h - 1$   $u_0 = y_0$   
Exact solution Set  $y_n = y(x_n)$ 

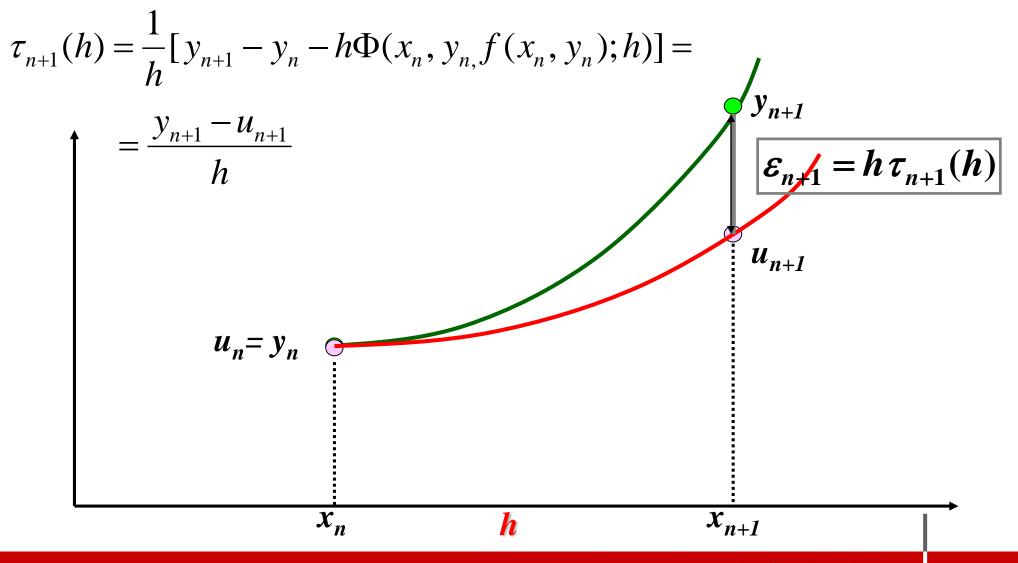
$$y_{n+1} = y_n + h\Phi(x_n, y_n, f(x_n, y_n);h) + \varepsilon_{n+1}$$
  $0 \le n \le N_h - 1$ 

 $\epsilon_{n+1}$  is the residue generated at  $x_{n+1}$  by calculating the numerical solution  $u_{n+1}$  starting from the exact solution  $y_n$  at time  $x_n$ . We rewrite the residue in the form

$$\varepsilon_{n+1} = h \tau_{n+1}(h)$$

$$\tau_{n+1}(h)$$
 LTE at  $x_{n+1}$ 

# **Local Truncation Error**





$$\tau(\mathbf{h}) = \max_{0 \le n \le N_h - 1} |\tau_{n+1}(h)| \quad \text{global truncation error}$$

Definition A one-step method is said to be consistent with the Cauchy problem

$$\begin{cases} y'(x) = f(x, y(x)) & \forall x \in I \equiv [a, b] \\ y(x_0) = y_0 & x_0 \in [a, b] \end{cases}$$

if its LTE is infinitesimal with respect to h, that is:

$$\lim_{h\to 0}\tau(h)=0$$

A method is **consistent with accurate order p**, for a suitable integer p>1, if the solution y(x) of the Cauchy problem satisfies the condition  $\tau(h) = O(h^p)$  for  $h \to 0$ 

# **Error Analysis for Euler's Method**

The method is consistent, in fact:  $\Phi = f$ 

$$\tau_{n+1}(h) = \frac{1}{h} [y_{n+1} - y_n] - f(x_n, u_n)$$

By applying a Taylor series expansion for  $y_{n+1}$ 

$$\begin{aligned} \tau_{n+1}(h) &\simeq \frac{1}{h} \left[ y(x_n) + hy'(x_n) + \frac{1}{2} h^2 y''(\eta) - y(x_n) \right] - f(x_n, u_n) \\ &\simeq \frac{1}{h} \left[ y(x_n) + hy'(x_n) + \frac{1}{2} h^2 y''(\eta) - y(x_n) \right] - y'(x_n) \\ &\simeq \frac{1}{2} h y''(\eta) \qquad x_n < \eta < x_{n+1} \end{aligned}$$

$$\begin{aligned} &= f(x_n, y(x_n)) = y'(x_n) \\ &\Rightarrow \tau_{n+1}(h) = O(h) \qquad \forall n \Rightarrow \tau(h) = O(h) \end{aligned}$$

then the Euler Method is **first order accurate** 

## Error Analysis for Crank-Nicolson Method

The method is consistent, in fact:  $\Phi = \frac{1}{2}(f_n + f_{n+1})$  $\tau_{n+1}(h) = \frac{1}{h}[y_{n+1} - y_n] - \frac{1}{2}[f(x_n, u_n) + f(x_{n+1}, u_{n+1})]$ 

By applying a Taylor series expansion for  $y_{n+1}$ 

$$\tau_{n+1}(h) = \frac{1}{h} \left[ y_n + h y'_n + \frac{1}{2} h^2 (y'_n) + O(h^3) - y_n \right] - \frac{1}{2} (f_n + f_{n+1}) \\ = \frac{1}{h} \left[ h y'_n + \frac{1}{2} h^2 \left( \frac{y'_{n+1} - y'_n}{h} + O(h) \right) + O(h^3) \right] - \frac{1}{2} (f_n + f_{n+1})$$

$$= y'_{n} + \frac{1}{2}y'_{n+1} - \frac{1}{2}y'_{n} + O(h^{2}) - \frac{1}{2}(f_{n} + f_{n+1})$$

$$= \frac{1}{2}(y'_{n} + y'_{n+1}) + O(h^{2}) - \frac{1}{2}(f_{n} + f_{n+1})$$
 Second order accurate

# Accuracy order of one-step methods

$$\begin{aligned} & \Phi(x_n, u_n, f_n; h) = f(x_n, u_n) & \text{Forward/Backward} \\ & \Phi(x_{n+1}, u_{n+1}, f_{n+1}; h) = f(x_{n+1}, u_{n+1}) & \text{Euler} \end{aligned} \\ & \Phi(x_n, u_n, f_n; h) = \frac{1}{2} \Big[ f(x_n, u_n) + f(x_n + h, u_n + hf_n) \Big] & \text{Heun} \\ & \Phi(x_n, u_n, f_n; h) = \frac{1}{2} \Big[ f(x_n, u_n) + f\left(x_{n+1}, u_{n+1}\right) \Big] & \text{Crank-Nicolson} \\ & \text{By applying Taylor series expansion, we get} & \text{Forward/Backward Euler's Method} & \text{order 1} \\ & \text{Heun's Method} & \text{order 2} \\ & \text{Crank-Nicolson Method} & \text{order 2} \end{bmatrix}$$

### Experimentally establish the order p of a method

- Let e<sub>h</sub> be the relative error with step size h, being the difference between the exact solution y and the numerical solution u<sub>h</sub> with step size h.
- If the numerical method is convergent of order p, we mean that there is a number C independent of h such that

$$e_h = |u_h - y| = Ch^p \quad C > 0$$

- Determining the order of accuracy p with known y:
  - plot  $loglog(e_h, h)$  and determine the slope of the line (p)  $\log |e_h| = \log C + p \log h$

- compute p 
$$\frac{e_h}{e_{h/2}} = \frac{Ch^p}{C(h/2)^p} = 2^p$$
  $EOC(h) := p = \log_2 \left| \frac{e_h}{e_{h/2}} \right|$ 

## Experimentally establish the order p of a method

- Determining the order of accuracy p with unknown y:
- In reality the error will not be possible to calculate since the exact solution is not known.
- look at solutions u<sub>h</sub> where h is halved successively:

$$\frac{u_h - u_{h/2}}{u_{h/2} - u_{h/4}} = \frac{Ch^p - C(h/2)^p}{C(h/2)^p - C(h/4)^p} = \frac{1 - 2^{-p}}{2^{-p} - 2^{-2p}} = 2^p$$

• Experimental Order of Convergence EOC:

$$EOC(h) := p = \log_2(\frac{u_h - u_{h/2}}{u_{h/2} - u_{h/4}})$$



# Zero-stability (roundoff errors effects)

#### Definition

A one-step numerical method for the solution of IVP

$$\begin{cases} u_{n+1} = u_n + h \Phi(x_n, u_n, f_n; h) & \forall n \\ u_0 = y_0 \\ \begin{cases} y'(x) = f(x, y(x)) & \forall x \in I \\ y(x_0) = y_0 & x_0 \in I \end{cases}$$

is said to be *zero-stable* if

$$\exists h_0 > 0, \exists C > 0 : \forall h \in (0, h_0], |z_n - u_n| < C \varepsilon \quad 0 \le n \le N_h$$

where  $z_n$ ,  $u_n$  are solutions of the problems

$$z_{n+1} = z_n + h[\Phi(x_n, z_n, f(x_n, z_n; h)) + \delta_{n+1}]$$
  
$$z_0 = y_0 + \delta_0$$

$$u_{n+1} = u_n + h\Phi(x_n, u_n, f(x_n, u_n; h))$$
  
$$u_0 = y_0$$

for  $0 \le n \le N_h - 1$ , under the assumption that  $|\delta_k| \le \varepsilon$ ,  $0 \le k \le N_h$ 



#### **Zero-stability**

#### The requirement

$$\exists h_0 > 0, \exists C > 0 : \forall h \in (0, h_0], |z_n - u_n| < C \varepsilon \quad 0 \le n \le N_h$$

guarantees that the method is not very sensitive to small perturbations.

It concerns the behavior of the numerical method in the limit case  $h \rightarrow 0$  and this justifies the name of zero-stability. It is a specific property of the numerical method and not of the Cauchy problem (which is stable, thanks to the uniform lipschitzianity of f).

Remark: the constant C is independent of h (and therefore from  $N_h$ ), but may depend on the length of the integration interval I. In fact, the formula does not exclude a priori that the constant C becomes the larger the greater the amplitude of I.





The need to formulate a request for stability for the numerical method is suggested, first of all, by the need to keep under control the inevitable errors that the finite arithmetic of each computer introduces.

If the numerical method were not zero-stable, the rounding errors introduced on  $y_0$  and propagated in the calculation of  $f(x_n, u_n)$  at each step, would in fact make the computed solution completely meaningless.



# **Theorem (Zero-stability)**

Given the generic one-step numerical method

$$u_{n+1} = u_n + h\Phi(x_n, u_n, f(x_n, u_n; h)) \qquad u_0 = y_0$$
  
for the resolution of the Cauchy problem  
$$\begin{cases} y'(x) = f(x, y(x)) & \forall x \in I \\ y(x_0) = y_0 & x_0 \in I \end{cases}$$

If the increment function  $\Phi$  is Lipschitz of constant  $\Lambda$  with respect to the second argument, uniformly with respect to h s.t.  $\exists h_0 > 0, \quad \exists \Lambda > 0 : \quad \forall h \in ]0, h_0]$  $\left| \Phi(x_n, u_n, f(x_n, u_n); h) - \Phi(x_n, z_n, f(x_n, z_n); h) \right| \le \Lambda |u_n - z_n|, \quad 0 \le n \le N_h$ then the method is **zero-stable**.





Definition: A numerical method is said to converge at the point xn if, given a subdivision of the integration interval I into Nh time steps of size h, the numerical solution tends to the exact solution of the IVP at the same point, when the number of time steps tends to infinity, this means that

$$\lim_{\substack{h\to 0\\(N_h\to\infty)}} u_n = y(x_n)$$

 We will say that the numerical method converges in the whole interval if it is convergent for each value x<sub>n</sub> in I.

$$\forall n = 0, 1, \dots, N_h, \qquad \lim_{\substack{h \to 0 \\ (N_h \to \infty)}} u_n = y(x_n)$$



## Convergence

The global error

$$\forall n = 0, 1, \dots, N_h, \quad \mathbf{e}_n = \left| u_n - y_n \right|$$

it is the result of the excessive accumulation of **local truncation errors and their propagation**, more precisely at each step a new local error is introduced and this propagates subsequently. For convergence then it is necessary that the accumulation of local errors "does not explode" when the step becomes small. This is essentially the notion of **zero-stability**.

**zero-stability** requires that the global discretization error can be made as small as desired, making the step h sufficiently small.

If, however, the problem is ill-conditioned in order to make the amplification of the error acceptable, it is necessary to take a very small step with the risk that the integration process will no longer advance.





#### Lax-Richtmyer Theorem

A consistent and zero-stable method is convergent.

consistency + zero-stability convergence

- Any one-step method considered is convergent
- Unfortunately we can have unstable computations even with a zero-stable method



# Absolute Stability (h fixed)

- Convergence is not a guarantee that the numerical method provides "acceptable" results. It is not acceptable that the step should be made very small to guarantee stability.
- Need for a new definition of stability in which one thinks the step h is fixed and requires that the error propagates in a limited way for  $N_h \to \infty$
- The form of stability now needed is something stronger than zero-stability. This property has to do with the asymptotic behavior of  $u_n$ , unlike the zero-stability in which, given a fixed interval, we study the trend of  $u_n$  as the grid is refined  $h \rightarrow 0$



# Absolute Stability (h fixed)

Consider the model problem - linear, homogeneous IVP

$$\lim_{x\to+\infty} |y(x)| = 0 \quad \text{if} \quad \operatorname{Re}(\lambda) < 0.$$

In the study of absolute stability we try to see if even the numerical solution with a given h decreases over time



# **Absolute Stability (h fixed)**

**Definition:** A numerical method for the approximation of the test IVP:

is said to be **absolutely stable** when  $|u_n| \rightarrow 0$  for  $x_n \rightarrow +\infty$ otherwise it is **unstable** 

$$\begin{cases} y'(x) = \lambda y(x) , \lambda \in \mathbf{C} \\ y(0) = 1 \end{cases}$$

#### Definition: Region of absolute stability A

Let h be the discretization step. The solution depends on h and  $\lambda$ . The region of absolute stability of the numerical method is defined as the following subset of the complex plane

$$A = \{ z = h\lambda \in C : |u_n| \to 0 \text{ per } x_n \to +\infty \}$$

Therefore A is the set of values of the product  $h\lambda$  for which the numerical method produces solutions that tend to zero when xn tends to infinity.



# Absolute Stability: Forward Euler

Euler's method

$$u_{n+1} = u_n + h f_n$$

applied to the model problem gives  $u_{n+1} = u_n + h\lambda u_n$ ,  $u_0 = 1$ Proceeding recursively with respect to n:  $u_n = (1 + h\lambda)^n u_0$ ,  $n \ge 0$ Then  $|u_n| \to 0$  when  $x_n \to +\infty$  is verified if and only if  $|1 + h\lambda| < 1$ 

That is if  $h\lambda$  belongs to the circle of unit radius and center (-1.0)

This is equivalent to

 $h\lambda \in C^{-}$  and  $0 < h < -\frac{2\operatorname{Re}(\lambda)}{|\lambda|^{2}}$  $C^{-} = \{z \in C: \operatorname{Re}(z) < 0\}$ 

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## Absolute Stability: Forward Euler Example

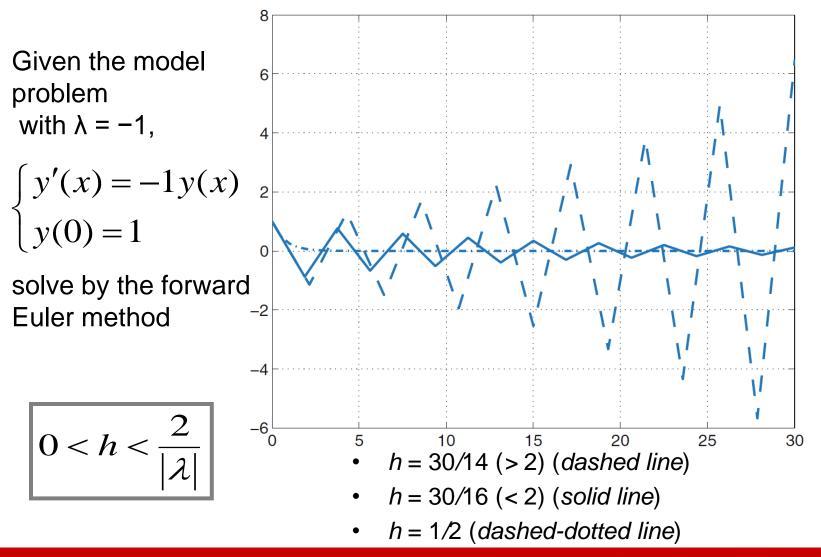
$$u_{n+1} = u_n + hf_n$$

$$y'(x) = -1y(x)$$
 per  $x > 0$  con  $y(0) = 1$ .

$$h\lambda \in C^{-} e \quad 0 < h < -\frac{2\operatorname{Re}(\lambda)}{|\lambda|^{2}}$$
$$0 < h < 2$$



### Absolute Stability: Forward Euler Example 1





# Absolute Stability: Forward Euler Example 2

Given the nonlinear scalar IVP:

$$\begin{cases} y'(x) = 1 - y^2 \\ y(0) = \frac{e - 1}{e + 1} \end{cases}$$

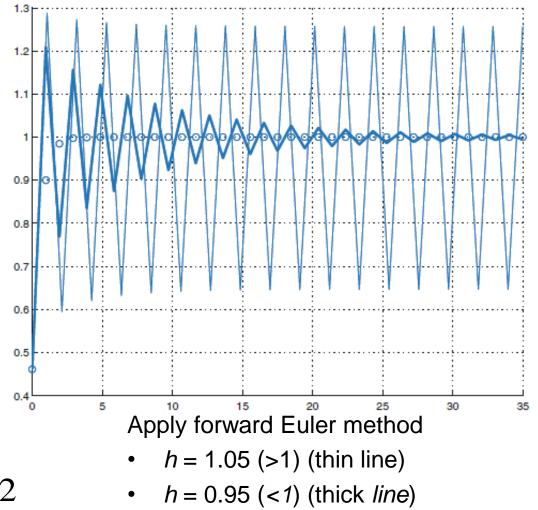
with solution:

$$y(x) = \frac{e^{2x+1} - 1}{e^{2x+1} + 1}$$

$$f_y = -2y \in (-2, -0.9)$$

Stability conditions:

$$0 < h < \frac{2}{\lambda^*} \quad \lambda^* = \max |f_y| = 2$$



• Exact solution (circles)



### Absolute Stability: Forward Euler

Given the general scalar nonlinear IVP:

$$\begin{cases} y'(x) = f(x, y(x)) \\ y(x_0) = y_0 \end{cases}$$

we can derive the same stability conclusions drawn in the linear constant  $\lambda$  case, provided the stability restriction holds:

$$0 < h < \frac{2}{\lambda^*} \tag{*}$$

• Scalar IVP  $\lambda^* = \max |f_y|$  where  $-\lambda_* < f_y = \frac{\partial f}{\partial y}(x, y) < -\lambda^* \quad \forall x, y$ 

• System IVP $\lambda^* = -\max(\rho(J_f))$  where  $\rho(J_f)$  is the spectral radius of Jacobian

we can expect that the perturbations on the forward Euler method are kept under control provided that h satisfies (\*)



# Absolute Stability: Backward Euler

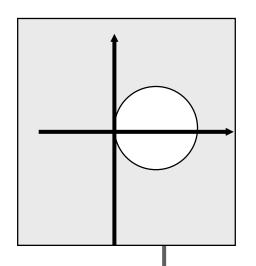
$$u_{n+1} = u_n + hf_{n+1}$$

Proceeding recursively with respect to n:

$$(1-h\lambda)u_{n+1} = u_n \qquad \Longrightarrow \qquad u_n = \frac{1}{(1-h\lambda)^n}u_0, \quad n \ge 0$$

$$\left|\frac{1}{1-h\lambda}\right| \le 1$$

The absolute stability property is satisfied by all values of  $h\lambda$  which are exterior to the circle of radius one centered in (1, 0). Backward Euler is unconditionally absolutely stable.





# Absolute Stability: Crank-Nicolson

$$u_{n+1} = u_n + \frac{h}{2} [f_n + f_{n+1}]$$

Proceeding recursively with respect to n:

$$u_{n} = \left[ \frac{\left(1 + \frac{1}{2}h\lambda\right)}{\left(1 - \frac{1}{2}h\lambda\right)} \right]^{n} u_{0}, \quad n \ge 0$$

Therefore the condition of absolute stability is verified for each

$$h\lambda \in C^{-}$$

The region A coincides with the left hand complex plane. CN is unconditionally absolutely stable.



#### Absolute Stability: Heun Method

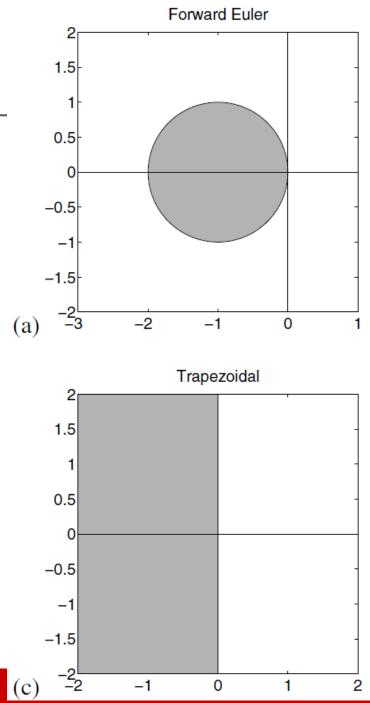
$$u_{n+1} = u_n + \frac{h}{2} [f_n + f(x_{n+1}, u_n + hf_n)]$$

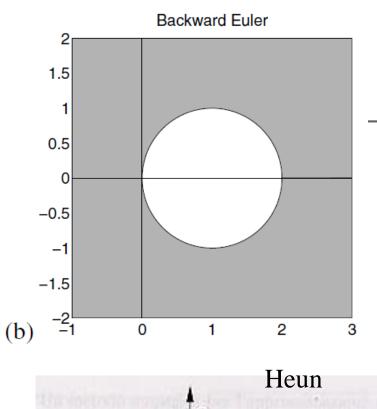
Proceeding recursively with respect to n:

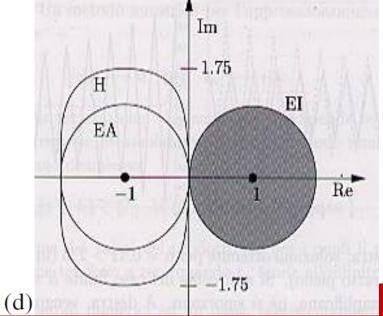
$$u_n = \left[1 + \frac{1}{2}h\lambda + \frac{(h\lambda)^2}{2}\right]^n, \quad n \ge 0$$

The region of absolute stability of the Heun method is wider than that of the forward Euler method. Only its restriction to the real axis is the same.











# **A-stable Method**

Definition. An ODE numerical method is said to be Astable if its region of absolute stability A contains the entire complex left half-plane C<sup>-</sup>

In this case the method satisfies the condition of stability  $|u_n| \rightarrow 0$  unconditionally with respect to h. Otherwise a method is called **conditionally stable**, and h should be lower than a constant depending on  $\lambda$ 

A-stable Methods:

 $CN = \frac{\left(1 + \frac{h\lambda}{2}\right)}{\left(1 - \frac{h\lambda}{2}\right)}$ 

Backward Euler  
$$r_0(h\lambda) = \frac{1}{(1-h\lambda)}$$



# **A-stable Methods**

- Forward Euler method is not A-stable: its absolute stability region coincides with the unit radius circle centered in (-1.0).
- The larger the region of absolute stability, the less restrictive the stability condition to impose on h.
- Among the explicit numerical methods, those having the region of absolute stability A very extensive or even unlimited are to be preferred.
- Many implicit methods are A-stable. This property makes implicit methods attractive in spite of being computationally more expensive than explicit methods.





#### Serena Morigi

Dipartimento di Matematica serena.morigi@unibo.it

http://www.dm.unibo.it/~morigi