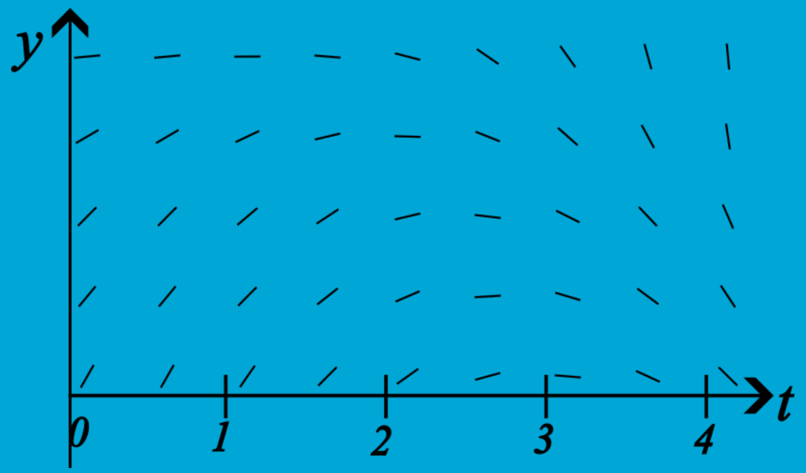
CEGM1000
Modelling, Uncertainty and Data for Engineers

Week 1.6
Numerical modelling (Beyond Fundamentals)

Jaime Arriaga

with A LOT of support from Isabel Slingerland and the rest of MUDEs' wonderful team

TU Delft



Learning objectives

At the end of this lecture, you should be able to

- Discuss the characteristics of Explicit and Implicit Numerical schemes
- Schematize numerical solutions of ODEs and PDEs
- Solve initial and boundary value problems numerically
- Solve partial differential equations

Contents

- Explicit and Implicit numerical schemes: single step
  - Initial Value Problems
- Multiple step and multi stage schemes
  -Initial Value Problems
- Second degree ODEs
  -Boundary Value Problems
- Solving PDEs: an introduction

TUDelft

Differential equations –ODEs, PDEs

Ice growth
First order ODE ➔

$$\rho_{ice}\frac{dh_{ice}}{dt} = -k_{ice}\frac{T_{water} - T_{air}}{h_{ice}}$$

Beam deformation
Second order ODE ➔

$$\frac{d^2v}{dz^2} = \frac{-1}{EI}\left(-\frac{qz^2}{2} + qLz - \frac{qL^2}{2}\right)$$

Diffusion equation 1D
Second order PDE ➔

$$\frac{du}{dt} = k\frac{d^2u}{dx^2}$$

TU Delft

How many constraints do the following equations need?

A. 1 and 1

B. 1 and 2

C. 2 and 1

D. 1 and 3

E. 3 and 1

F. 2 and 2

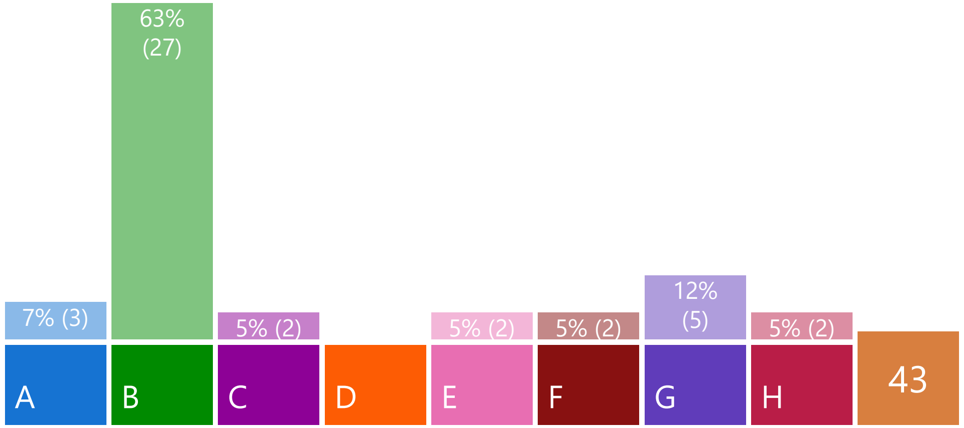
G. 2 and 3

H. 3 and 2

$$\rho_{ice}\frac{dh_{ice}}{dt} = -k_{ice}\frac{T_{water}-T_{air}}{h_{ice}}$$

and

$$\frac{d^2v}{dz^2} = \frac{-1}{EI}\left(-\frac{qz^2}{2}+qLz-\frac{qL^2}{2}\right)$$

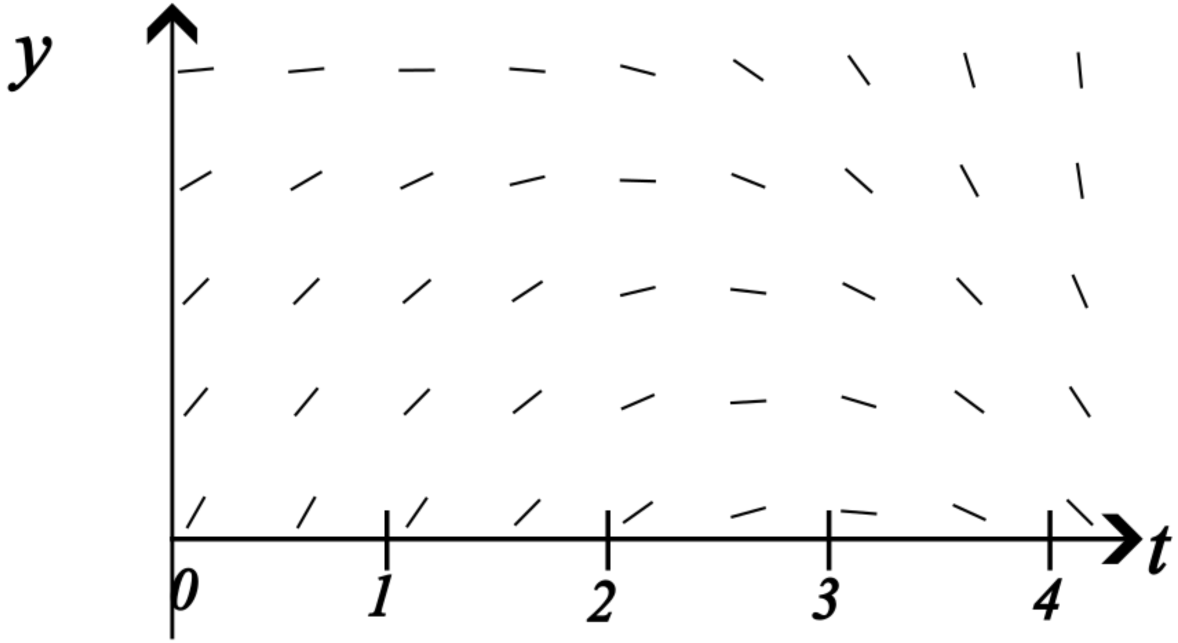


TU Delft

Initial Value Problem

$$\frac{dy}{dt} = -y + e^t$$

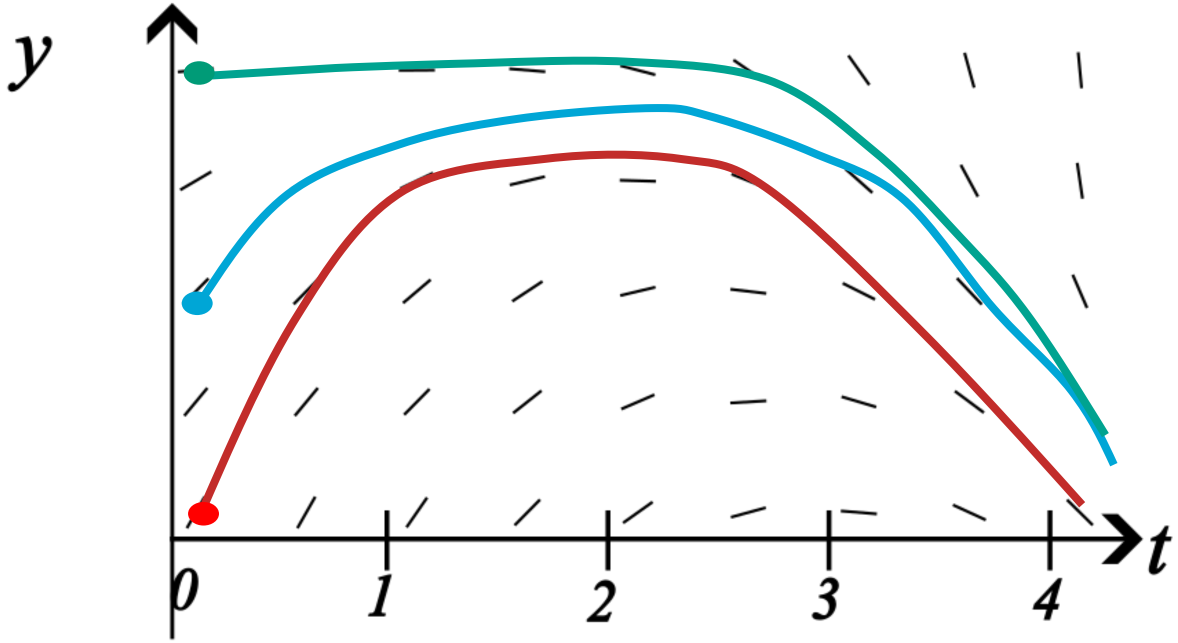
➔



Initial Value Problem

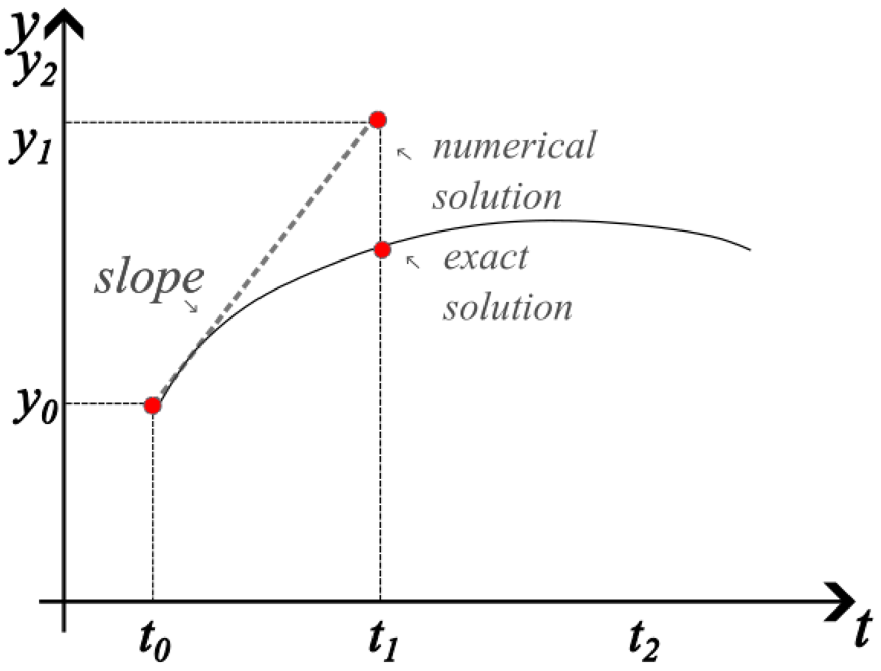
$$\frac{dy}{dt} = -y + e^t$$

➔



Any ODE, no matter the order, that has a time dependency has a solution
Completely dependent on the initial value!

Explicit Euler



$$t_{i+1} = t_i + \Delta t$$

$$y_{i+1} = y_i + \Delta t * slope_i$$

$$y_1 = y_0 + \Delta t * slope_0$$

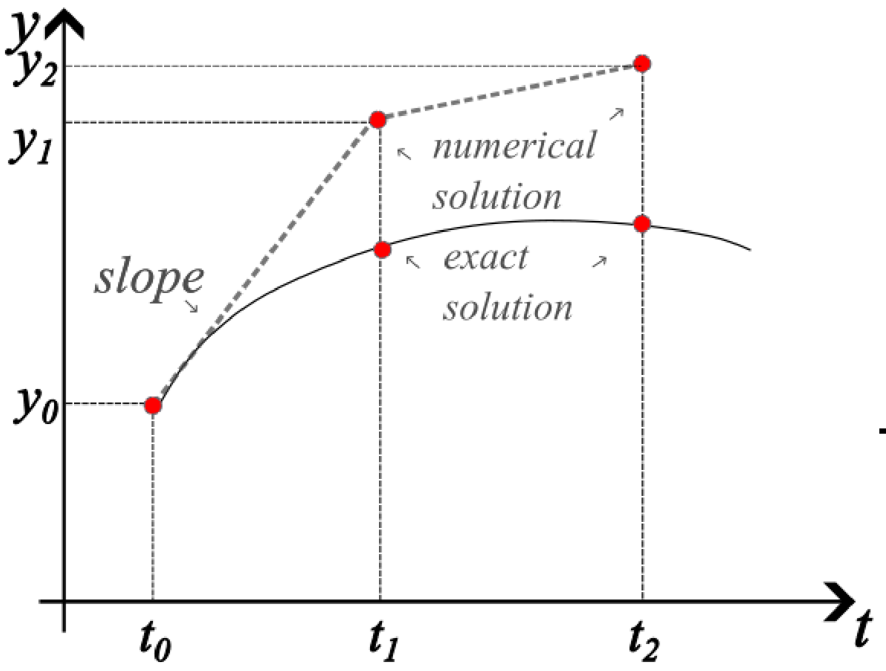
The slope is computed using the Forward Difference formula, first-order accurate.

Truncation error = $y_1^{TSE} - y_1^{FE}$

$$= y_0 + \Delta t y_0' + \frac{\Delta t^2}{2!} y''_0 + \cdots - (y_0 + \Delta t y_0')$$

$$= \frac{\Delta t^2}{2!} y''_0 + \cdots \approx O(\Delta t^2)$$

Explicit Euler



$$t_{i+1} = t_i + \Delta t$$

$$y_{i+1} = y_i + \Delta t * slope_i$$

$$y_2 = y_1 + \Delta t * slope_1$$

Total truncation error $= \sum_{i=0}^{n-1} y_{i+1}^{TSE} - y_{i+1}^{FE}$

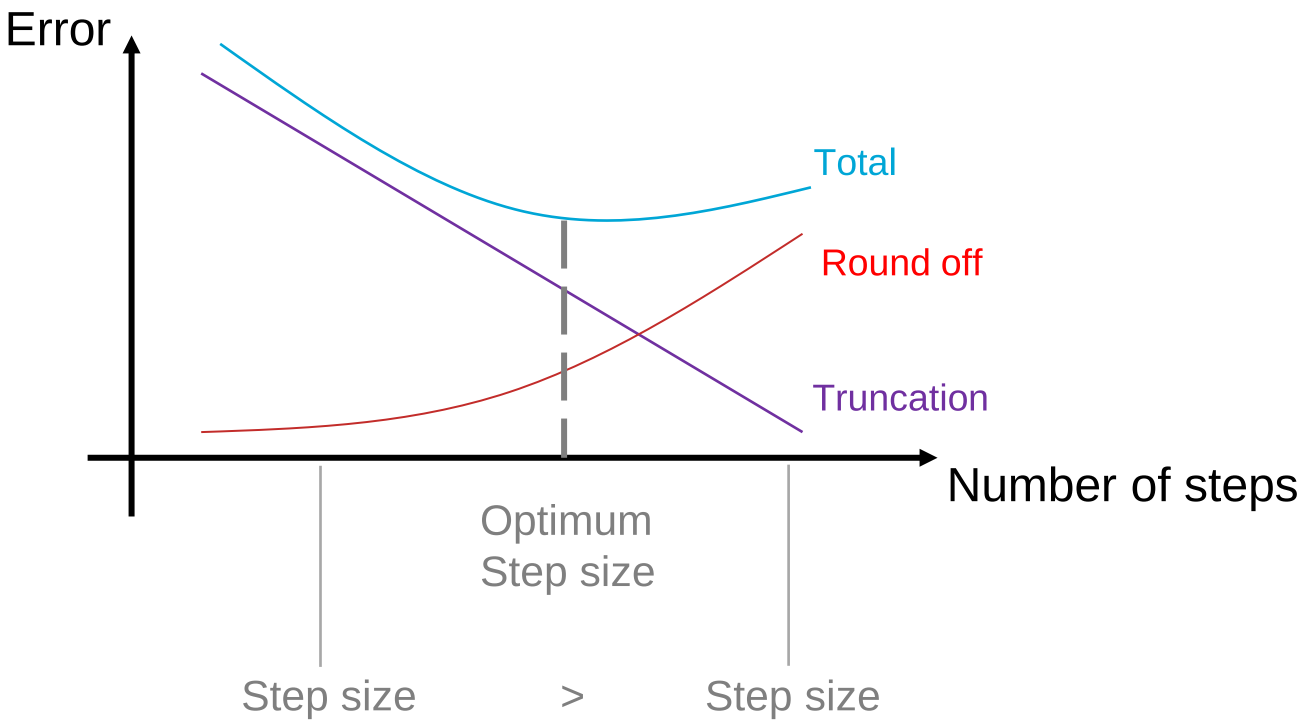
$$= \sum_{i=0}^{n-1} \frac{\Delta t^2}{2!} y''_i + \cdots \approx \frac{\Delta t^2}{2!} \frac{b-a}{\Delta t} y''_i$$

$$\approx \frac{\Delta t}{2!}(b-a)\overline{y''} \approx O(\Delta t)$$

TU Delft

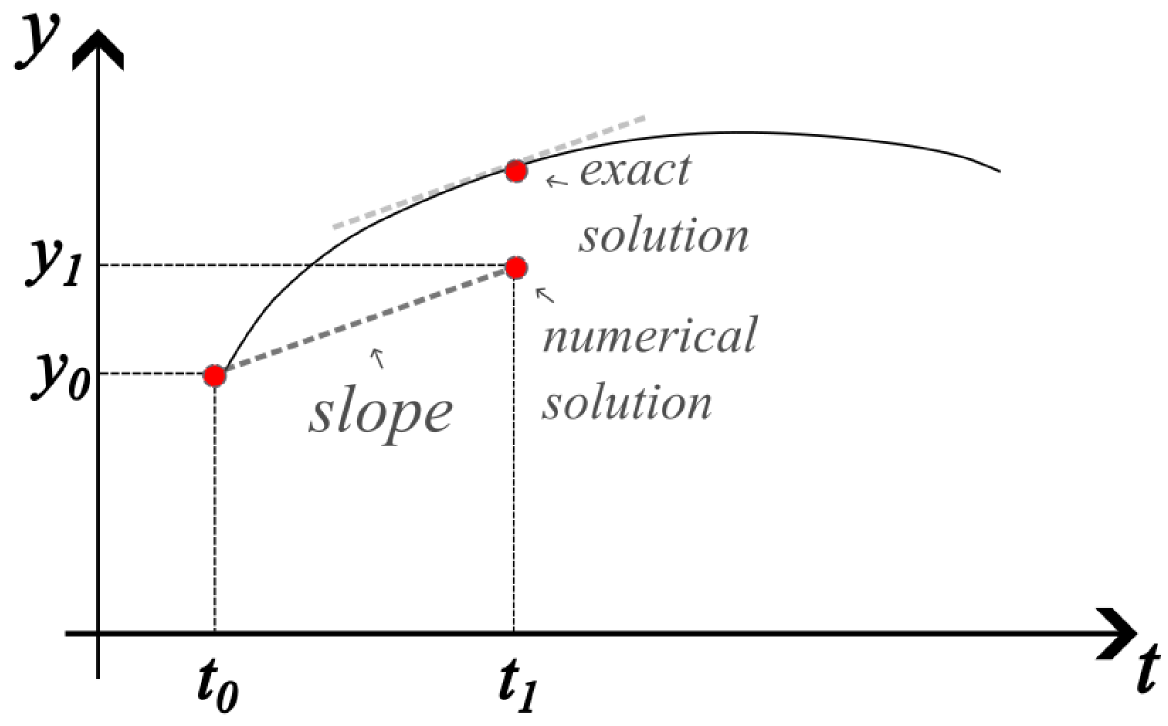
Round-off error & the better compromise

```
Error using 16 bits of memory =  -1.220703125
Error using 32 bits of memory =  -0.00022351741790771484
Error using 64 bits of memory =  2.7755575615628914e-13
```



TU Delft

Implicit Euler



$$t_{i+1} = t_i + \Delta t$$

$$y_{i+1} = y_i + \Delta t * slope_{i+1}$$

$$y_1 = y_0 + \Delta t * slope_1$$

The slope is computed using the Backward Difference formula, first-order accurate.

Total truncation error $\approx O(\Delta t)$

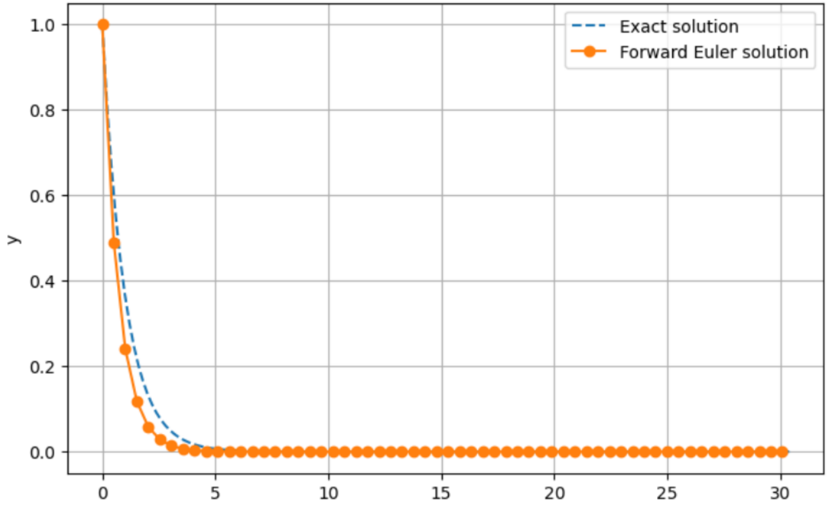
TUDelft

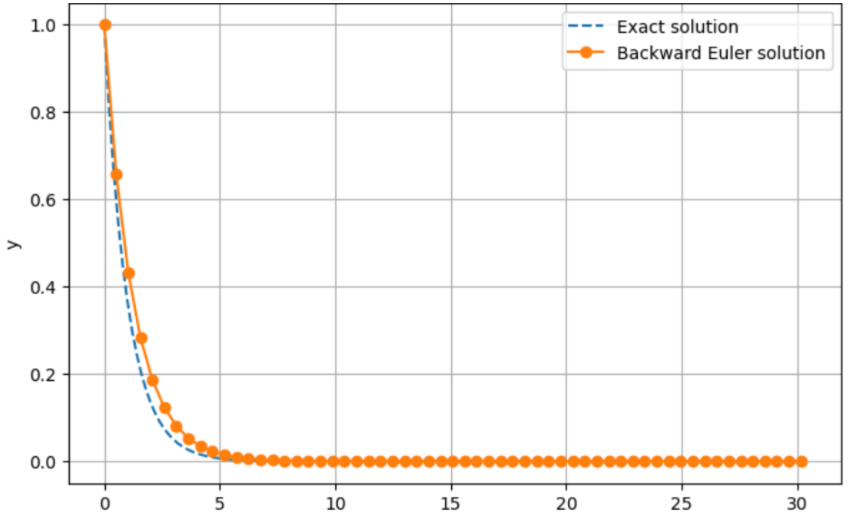
Stability

$$\frac{dy}{dt} = -\alpha y$$

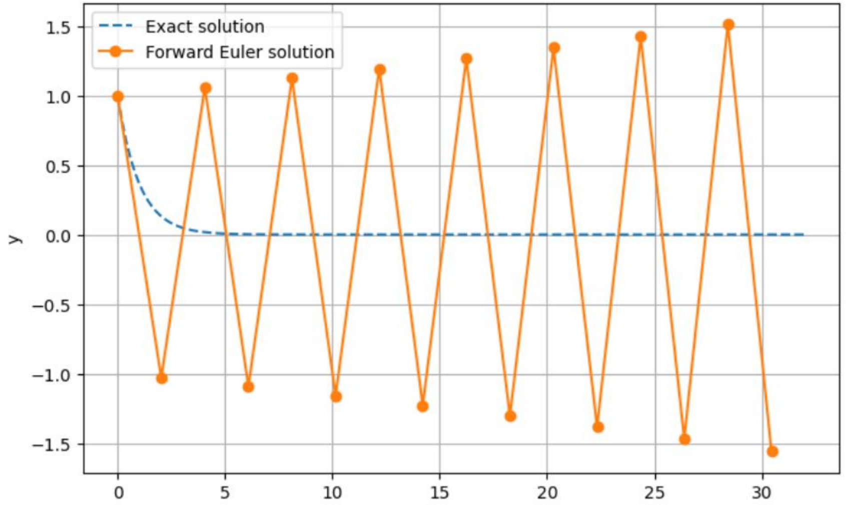
Explicit		Implicit
	← Small Step →	
	← Large Step →	

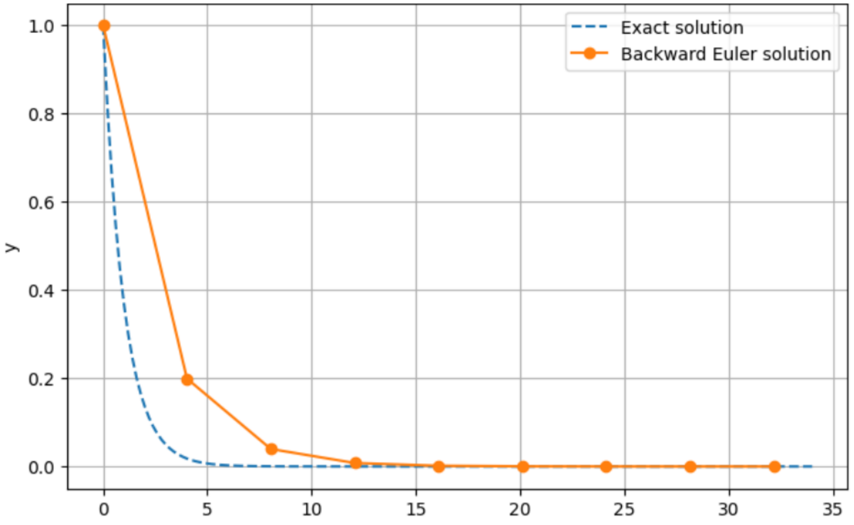
y





y





t t

TU Delft

Non-linear ODE

$$\frac{dp(t)}{dt} = -p^{3/2} + 5 \cdot p_{cst}(1 - e^{-t})$$

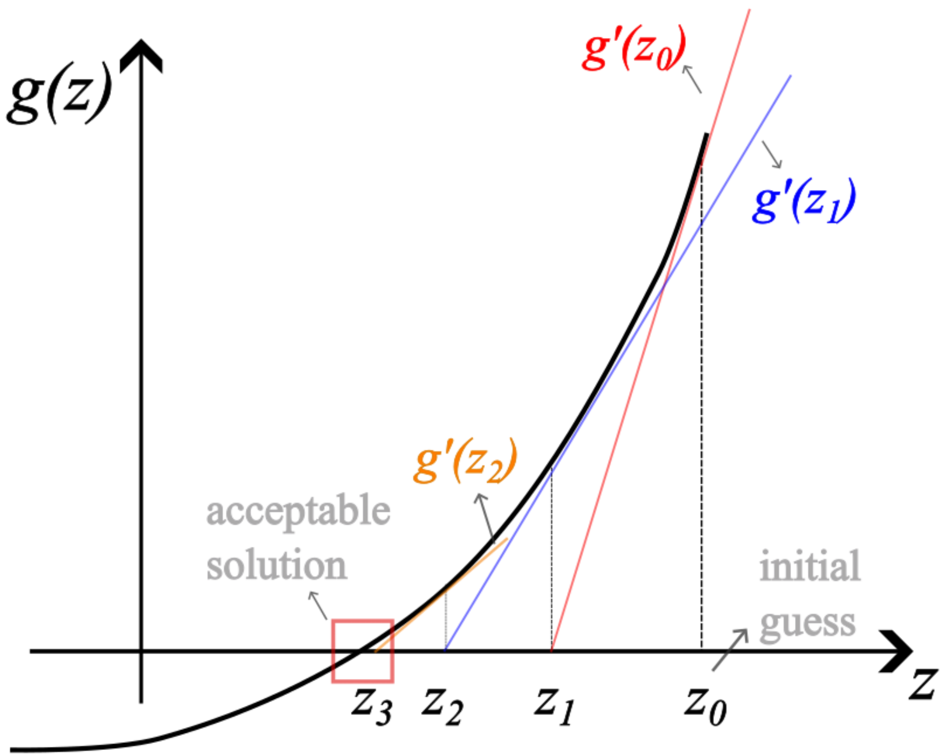
$$p_{i+1} = p_i + \Delta t \left(-p_i^{3/2} + 5p_{cst} \cdot (1 - e^{-t_i})\right)$$

Solved directly

$$p_{i+1} = p_i + \Delta t \left(-p_{i+1}^{3/2} + 5p_{cst} * (1 - e^{-t_{i+1}})\right)$$

Solved iteratively

Non-linear ODE: Newton-Rhapson (iterative) method

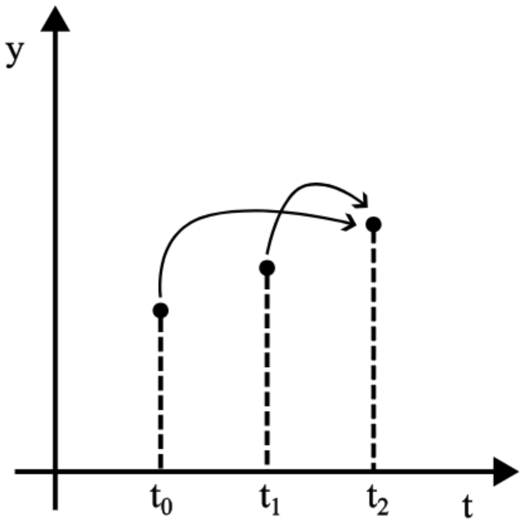


How do you increase the accuracy without compromising computational time?

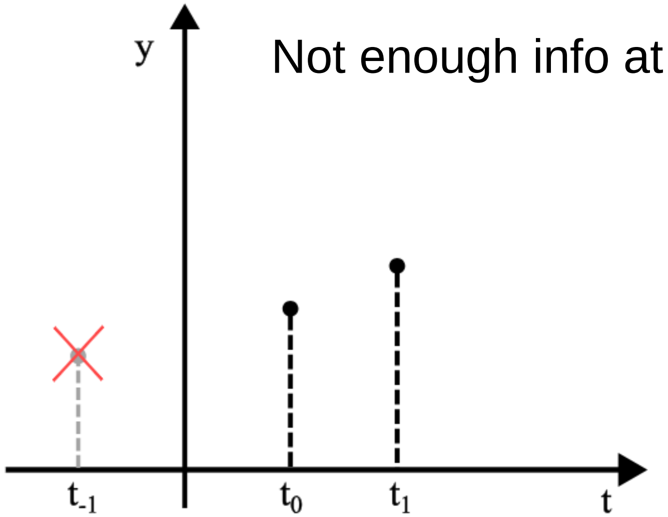
Multi-step methods

Adams-Bashfort
second order accurate

$$y_{i+1} = y_i + \frac{\Delta t}{2}(3y_i' - y'_{i-1})$$



Not enough info at t_1



- Adams-Bashfort are explicit methods of higher accuracy

- AB are not self starting!

- Adams-Moulton are implicit methods of higher accuracy

- AM are self starting but require iteration

TU Delft

Multi-stage methods

The main error of simple single step methods is assuming that the slope does not change between i and $i+1$

- Modified Euler $y_{i+1} = y_i + \Delta t\ ({y'}_i + {y'}_{i+1^*})/2$

- Midpoint $y_{i+1} = y_i + \Delta t\ {y'}_{i+\frac{1}{2}^*}$

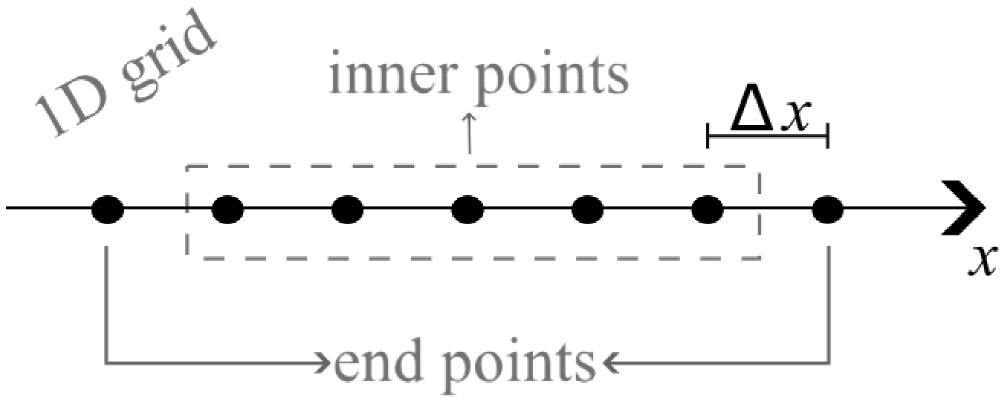
- Runge-Kutta $y_{i+1} = y_i + \Delta t\ (K_1 + K_2)$

TU Delft

Second degree ODE

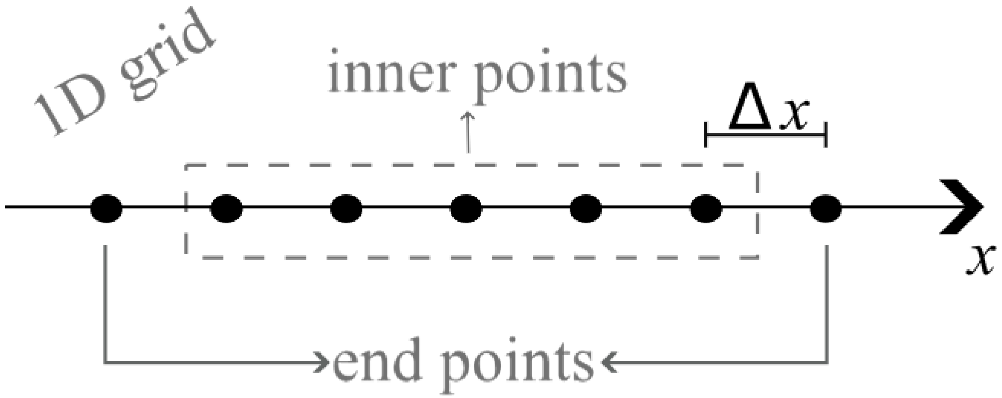
$$\frac{d^2y}{dt^2} = \frac{dy}{dt} - y + \cos t = 0$$ ➔ IVP

$$\frac{d^2T}{dx^2} - \alpha_1(T - T_s) = 0$$ ➔ BVP



Second degree ODE: Boundary Conditions

$$\frac{d^2T}{dx^2} - \alpha_1(T - T_s) = 0$$



$$\frac{d^2y}{dx^2} = g(x, y, \frac{dy}{dx})$$

- Dirichlet

$$y(x = a) = Y_a \text{ and } y(x = b) = Y_b$$

- Neumann

$$\left.\frac{dy}{dx}\right|_{x=a} = D_a \text{ and } \left.\frac{dy}{dx}\right|_{x=b} = D_b$$

- Mixed

TU Delft

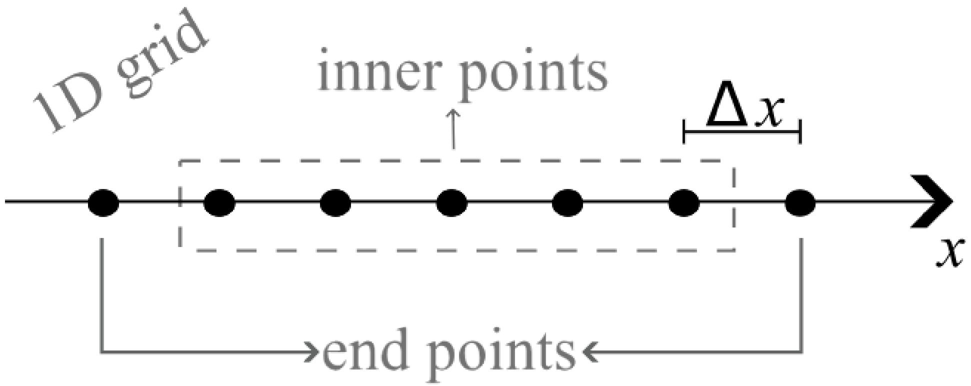
Central Difference: $f'' = \frac{f(x_i - \Delta x) - 2f(x_i) + f(x_i + \Delta x)}{\Delta x^2}$

Exercise

$$\frac{d^2T}{dx^2} - \alpha(T - Ts) = 0, \quad x \in (0, 0.1)$$

Use 5 points for your grid

$$T(0) = 473[K], \quad T(0.1) = 293[K]$$



Partial Differential Equations

1.- Discretization of the space derivative

2.- Discretization of the time derivative

3.- Parameter definition

4.- Grid creation

5.- Define initial conditions

6.- Define Boundary Conditions

7.- Build your system of equations

8.- Solve the system

9.- Update values and increment one time step

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 2xy \text{ Poisson's equation}$$

$$\frac{du}{dt} = \nu \frac{d^2 u}{dx^2} \text{ diffusion equation}$$

$$\frac{dc}{dt} + \mathrm{v}\frac{dc}{dx} = 0 \text{ convection equation}$$

TUDelft

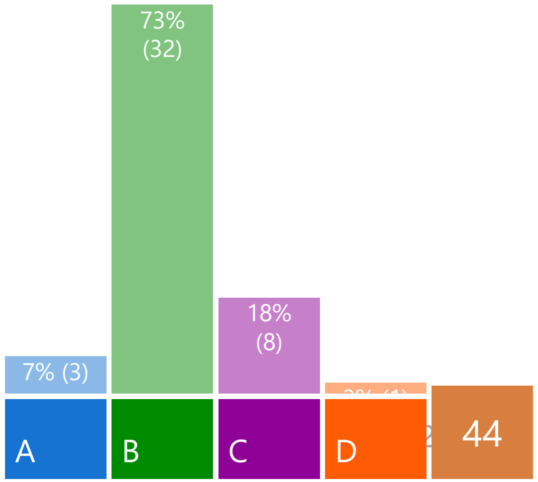
https://waves.participoll.com/

Exercise: discretize the convection equation using a central difference for space (2nd order accurate) and a forward difference for time (1st order accurate)

$$\frac{dc}{dt} + \mathrm{v}\frac{dc}{dx} = 0$$ convection equation

How many constraints are needed?

A. 1
B. 2
C. 3
D. 4



TU Delft

TU Delft

Jaime Arriaga

J.A.ArriagaGarcia@tudelft.nl