Numerical Methods in Engineering Applications

Workshop #02

Ordinary Differential Equations

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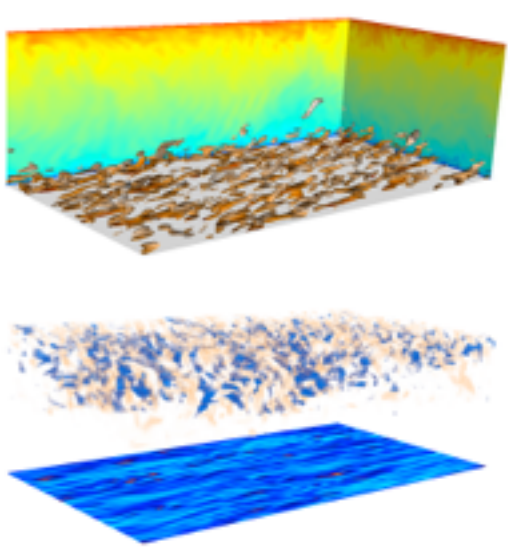
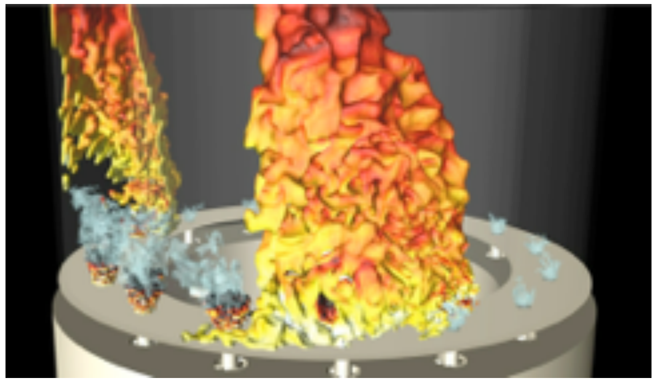
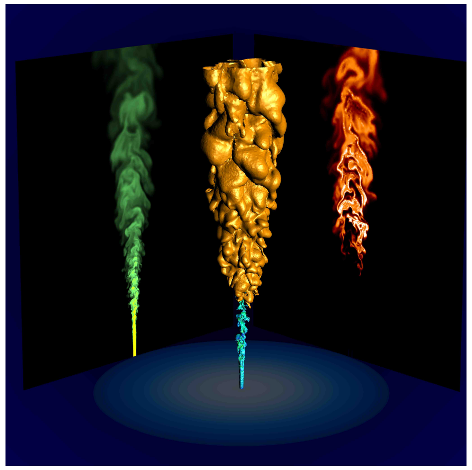
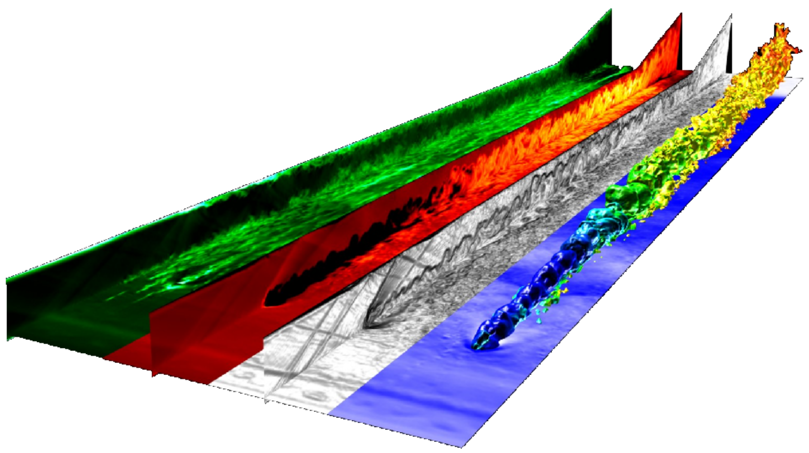
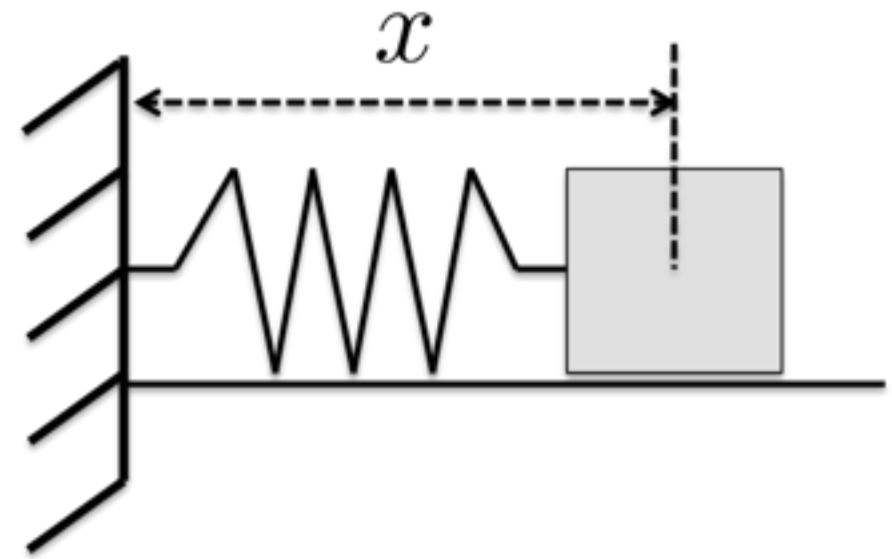





Objectives of Workshop #2

- **Solving ODE systems**
- **Using explicit methods with adequate time step**
- **Using implicit methods in full or linearised forms**

Workshop #2: harmonic oscillator



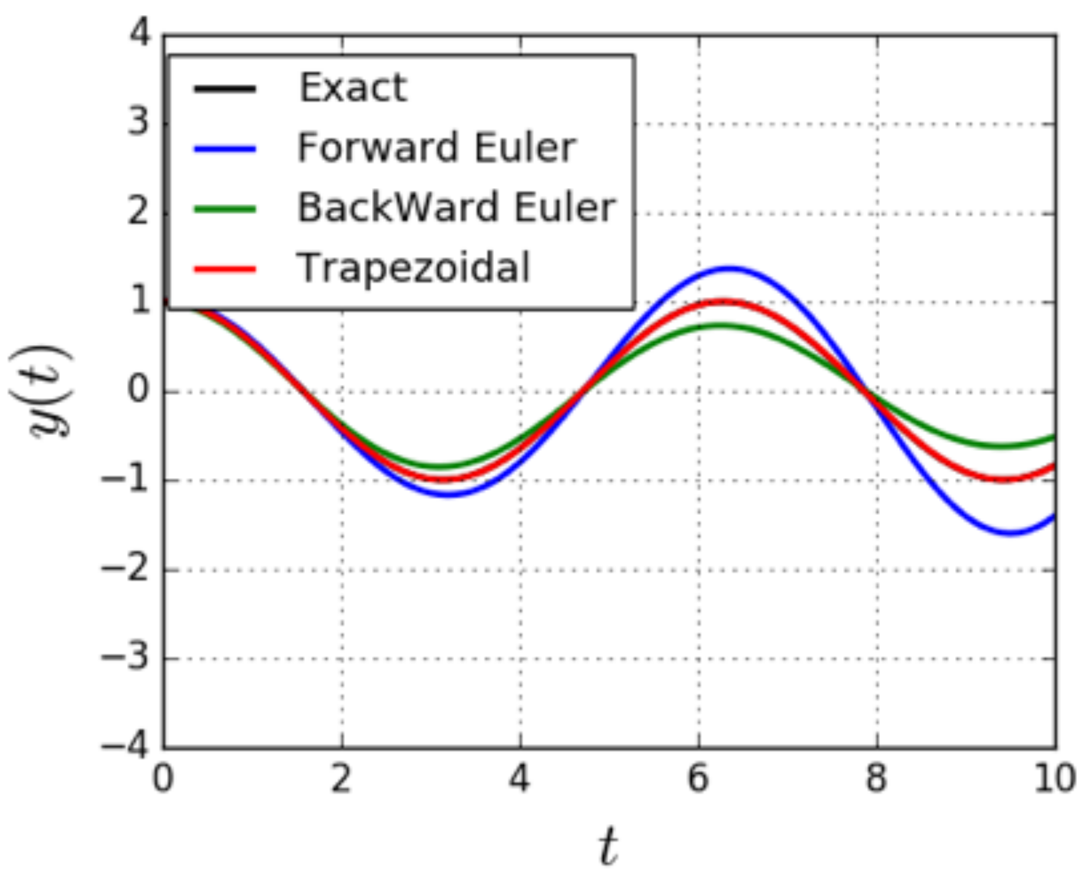
- **Example: spring-mass system**
- **Equation:**

$$\ddot{x} + \omega^2 x = 0$$

- **The analytical solution is of form:**

$$x(t) = A\cos(\omega t + \varphi)$$

- **Objectives:**
  - Implement the following methods
    - Forward Euler
    - Backward Euler
    - Trapezoidal rule
  - Compare the error with respect to the analytical solution



Workshop #2: population equation

- **Equation on P (population normalised by the maximum population**

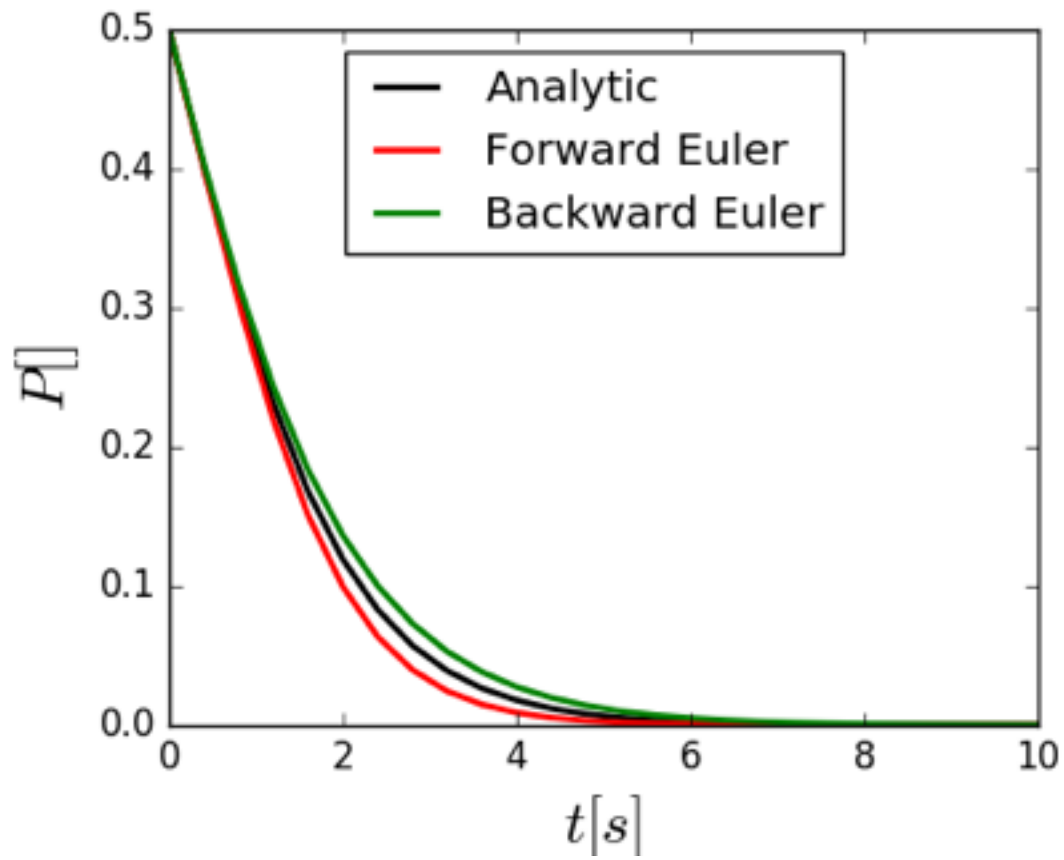
$$\dot{P} = -P(1-P)$$

- **Non-linear equation**
  - For implicit schemes, two versions: linearized and non-linearized

- **Analytical solution**

$$P(t) = \frac{1}{1 - Ae^t}$$

- **Objectives**:
  - Implement full implicit methods to a non-linear problem
  - Implement the linearized version of Backward Euler and Trapezoidal schemes
  - Compare the error of the five schemes at your disposal on this equation



Implicit schemes: linearization

- **First order Backward Euler method**

$$Y(t_{n+1}) = Y_n + \Delta t F(t_{n+1}, Y(t_{n+1}))$$

- **Two methods**

  - **Inversion of the non-linear system of equations**

$$G(Y(t_{n+1})) = Y(t_{n+1}) - Y_n - \Delta t F(t_{n+1}, Y(t_{n+1})) = 0$$

  - **Linearization**

$$F(t_{n+1}, Y(t_{n+1})) = F(t_{n+1}, Y(t_n)) + \frac{\partial F}{\partial Y}(Y(t_{n+1}) - Y(t_n))$$

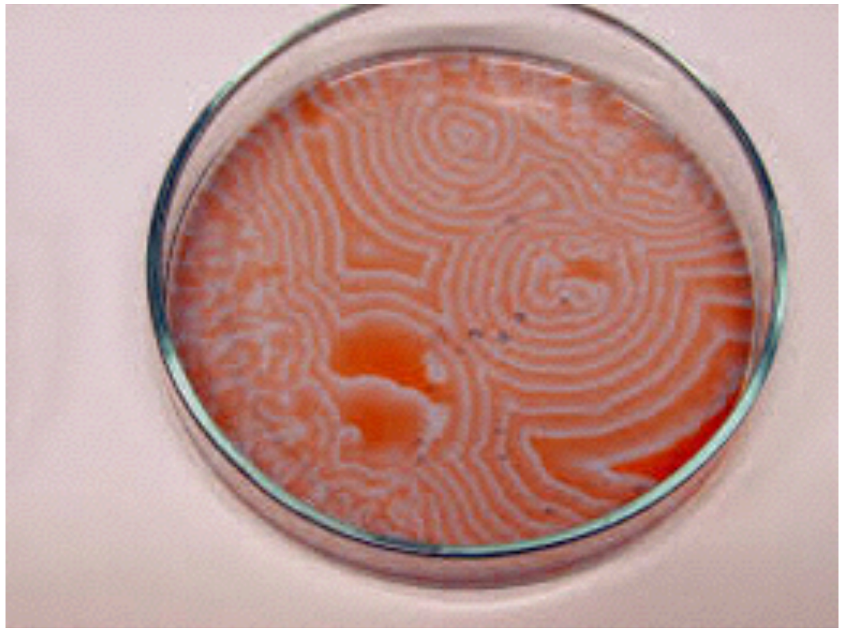
$$\left(\mathbb{1} - \Delta t \frac{\partial F}{\partial Y}\right) Y(t_{n+1}) = \left(\mathbb{1} - \Delta t \frac{\partial F}{\partial Y}\right) Y_n + \Delta t F(t_{n+1}, Y_n))$$

Project #1: The Belousov-Zhabotinskii reaction

- **Oscillating chemical system:**
  - the composition may oscillate depending on the initial concentrations

- **Belousov-Zhabotinskii reaction**
  - Oscillating equilibrium between two species:
    - reduction of Cerium(IV) in Cerium(III) by hypobromic acid
    - Oxidation of Cerium(III) into Cerium (IV) by bromate

- **Simplified system x=Cerium(IV), y=hypobromic acid**
  - two parameters: f and ϵ



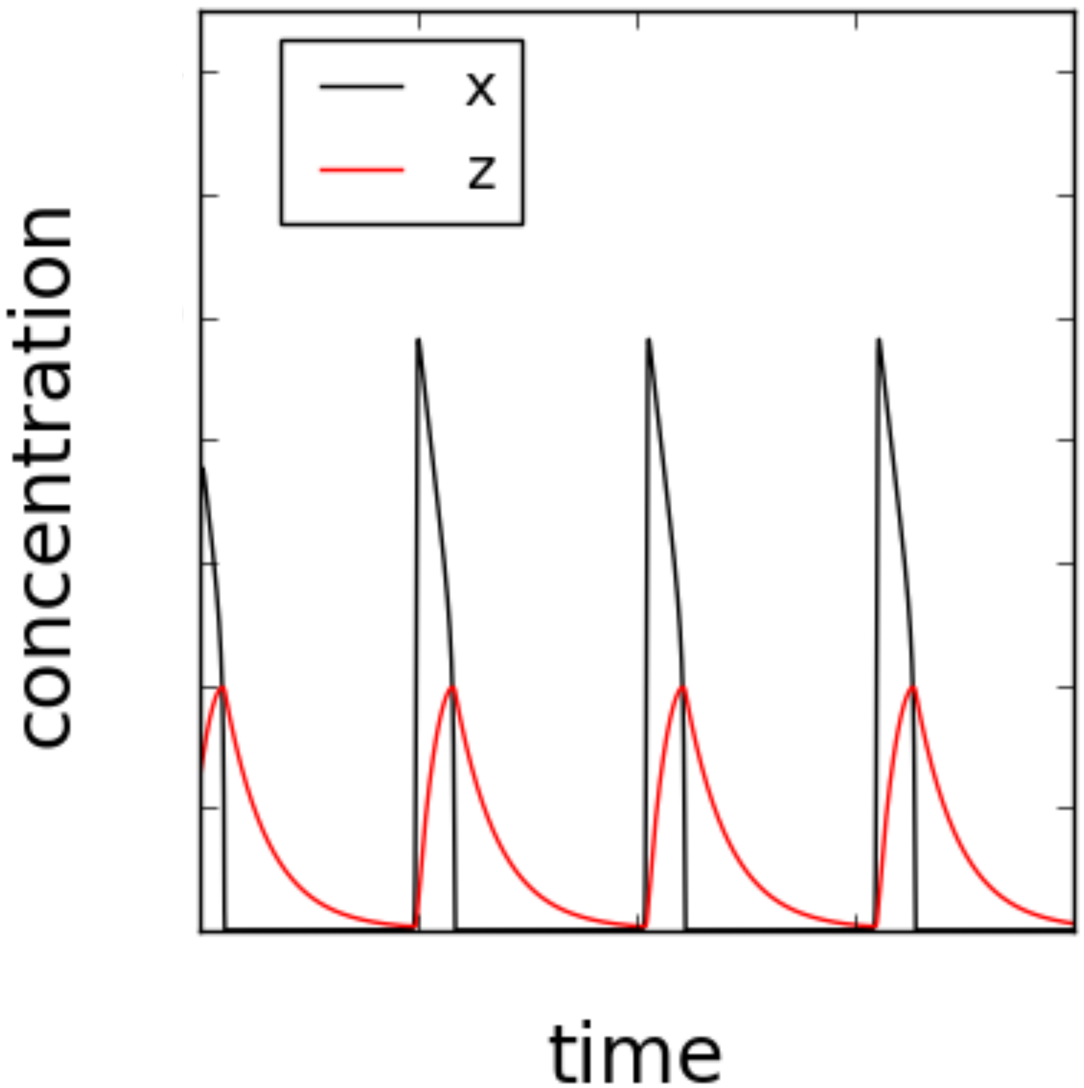
Spatial patterns in a Petri box

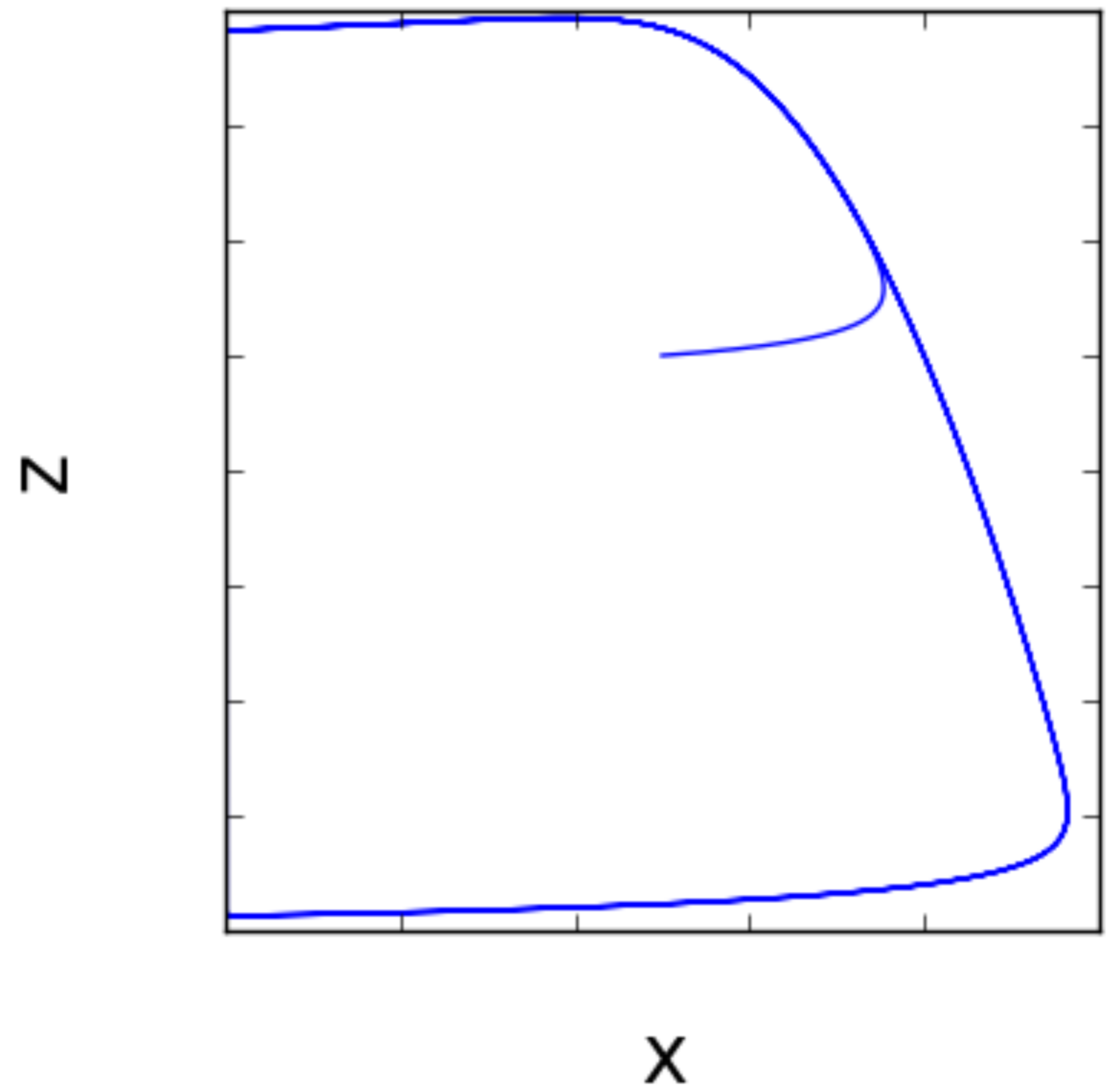
$$\epsilon \frac{\mathrm{d}x}{\mathrm{d}t} = x(1-x) + f\frac{q-x}{q+x}z$$

$$\frac{\mathrm{d}z}{\mathrm{d}t} = x - z$$

Project #1: The Belousov-Zhabotinskii reaction

axis values have been intentionally removed





- **Question: what are the minimum and maximum values of the concentration of cerium(IV) (variable z)?**

Project #1: The Belousov-Zhabotinskii reaction

Project #01 to hand out (slides in PDF) for April, 13th

Send PDF slides to ronan.vicquelin@centralesupelec.fr and aymeric.vie@centralesupelec.fr

- First slide : names (2 people)+ problem title
- Slide #2 : sum up the problem to solve
- Self-sufficient slides => clear, detailed enough, synthetic
- Explain the approach, discuss your choices
- Describe numerical method, very briefly if seen in class, specify details related to the study
- Show and analyse results
- How sure are you that your results are correct ?

- Plots :
  Readable, clear
  axis names
  units
  legend

- Last slide : highlight results and conclusions