EOSC - 213
Computational methods in geological engineering
Review of differential equations

N. Seigneur

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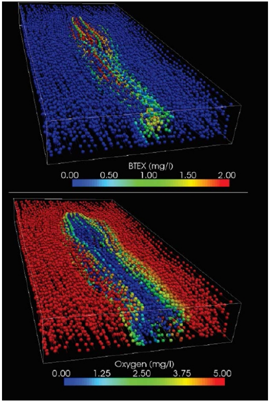
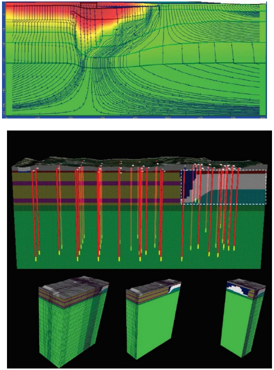
Outline

Motivation

A lot of engineering applications use computational methods

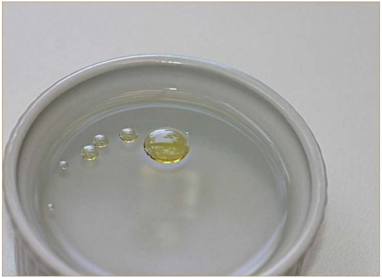


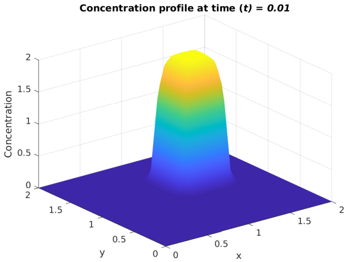


These serve multiple purposes:

1. Understanding the relevant processes (physical, chemical, ...)
2. Predict - control a process of interest

(very simple) example: diffusive migration of a contaminant in an aquifer





Our goal : that, within **4 weeks**, you are able to

1. Understand the physical-mathematical background
2. Are able to program how to solve such a problem, and make it more complicated and realistic

What is this course?

This course is

1. NOT a physics course
    - But we need some physics to describe the processes (conservation principle, ...)
2. NOT a math course
    - But we need to translate physics into mathematical concepts
3. NOT a numerical analysis course
    - but we need to translate a mathematical concept in a computer language and find numerical methods to be able to solve it
4. NOT a programming course
    - but we will use Python to apply the numerical methods.
5. a way for you to understand how these computation methods work, how you can use them, what are their limitations.

Steps towards achieving our goals

Most of the computation methods focus on solving physical problems which can be described by **partial differential equations** (PDEs). For example, the diffusion problem is described by:

$$\frac{\partial c(x,y,z,t)}{\partial t} = \mathrm{div}\left(D\vec{\nabla} c(x,y,z,t)\right) \tag{1}$$

This equation describes how the concentration of a species, described by the **function** $c(x,y,z,t)$, evolves through space and time.

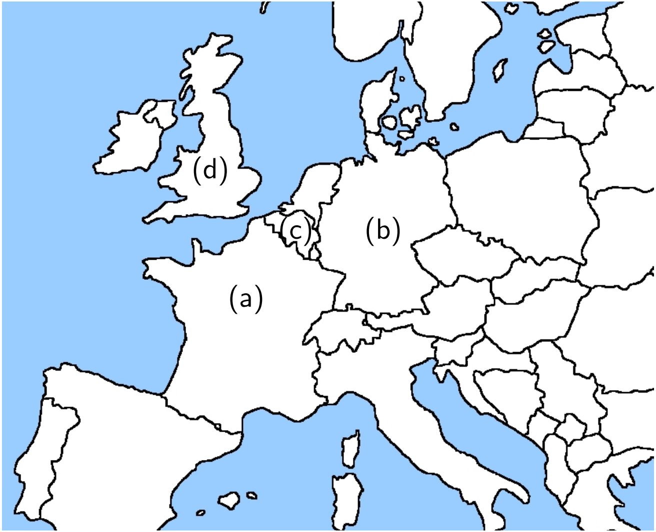
1. Physics: find out the relevant physical principle and processes
    - Mass conservation principle - diffusive movement
2. Math: PDE to describe temporal-spatial evolution of c
3. Numerics: "discretization" of time and space into timesteps and small volumes
4. Programming: solve the latter problem!

We will go slowly to reach that complexity

1. Week 3: 0D (initial condition) problem: solve an ordinary differential equation (ODE) for temporal evolution of a quantity y
   - Euler's methods, accuracy of the numerical solution, stability of the numerical approaches, ...
2. Week 4(5?): 1D/2D problem stationary/steady-state problem: add the spatial derivative complexity
   - Methods of finite difference and finite volume
   - Linear algebra
3. Week 5-6: 2D time-dependent (transient) non-homogeneous problem
4. Today, the point is to recap the fundamentals behind ODE
   - So that you don't freak out when you see one!

Quick clicker test and check

Which one of this country is Belgium?



Outline

What is a differential equation?

"Regular" vs Differential equation

$$y^2 + 6y + 5 = 0 \qquad (2)$$

- Solutions are **numbers**
- $y = -1$ and $y = -5$ are solutions of the equation

$$\begin{cases} y'' + 6y' + 5y(x) &= 0 \\ f'' + 6f' + 5f(x) &= 0 \\ \frac{d^2y}{dx^2} + 6\frac{dy}{dx} + 5y &= 0 \end{cases}$$

- Solutions are **functions** $y(x)$
- $y(x) = \exp(-1x)$ is a solution of the differential equation
- $y(x) = \exp(-5x)$ also is

Are you going to take my word for it ? Check it! Prove it!

Check if the ODE

$$y''(x) + 6y'(x) + 5y(x) = 0$$

accepts exp(-x) and exp(-5x) as solutions.

$$y_1(x) = \exp(-x)$$

$$\begin{cases} y_1' &= -y_1 \\ y_1'' &= y_1 \end{cases}$$

$$\begin{aligned} \Longrightarrow 0 &= y_1'' + 6y_1' + 5y_1(x) \\ &= y_1 - 6y_1 + 5y_1 \\ &= 0 \text{ ok!} \end{aligned}$$

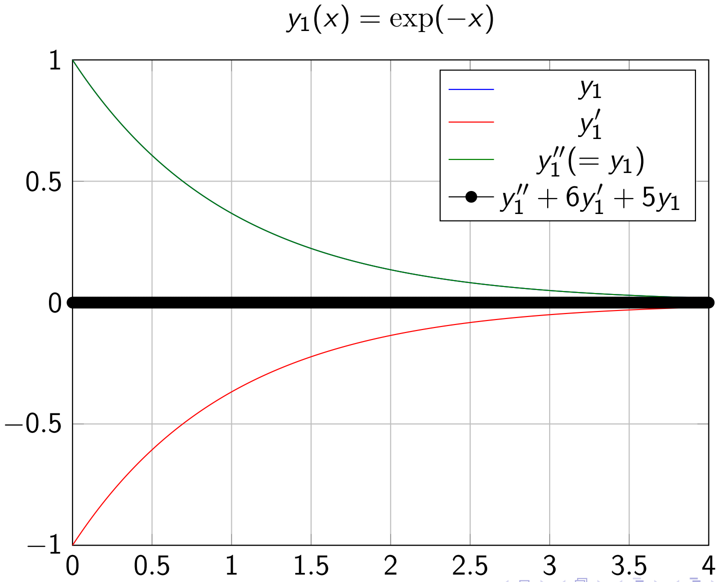
$$y_2(x) = \exp(-5x)$$

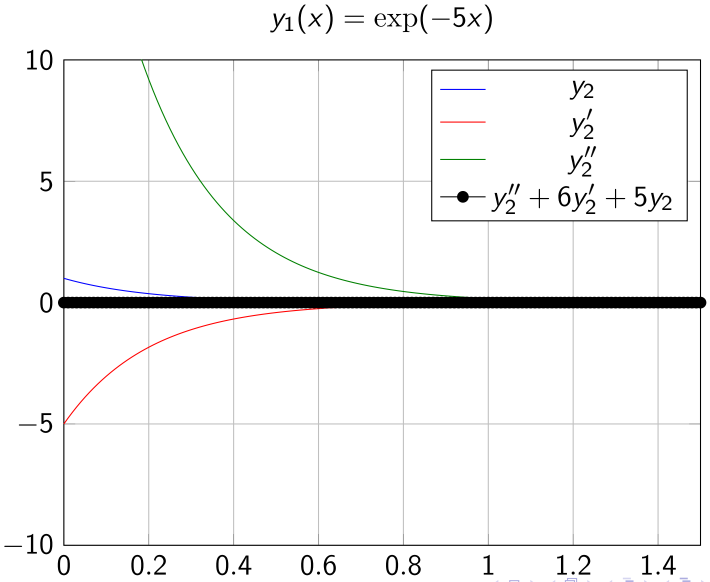
$$\begin{cases} y_2' &= -5y_2 \\ y_2'' &= 25y_2 \end{cases}$$

$$\begin{aligned} \Longrightarrow 0 &= y_2'' + 6y_2' + 5y_2(x) \\ &= 25y_2 - 30y_2 + 5y_2 \\ &= 0 \text{ ok!} \end{aligned}$$

y_1 and y_2 are solutions.

Solution




$y_1(x) = \exp(-5x)$
10
5
0
−5
−10
0
0.2
0.4
0.6
0.8
1
1.2
1.4
y_2
y_2'
y_2''
$y_2'' + 6y_2' + 5y_2$

Number of solutions

We have proven that the ODE

$$y''(x) + 6y'(x) + 5y(x) = 0$$

accepts exp(-x) and exp(-5x) as solutions.
How many other solutions are there to the ODE ?

(a) 0
(b) 2
(c) It depends
(d) There is an infinite amount of other solutions

There is an infinite amount of solutions !

Consider, with real numbers a, b ($a, b \in \mathbb{R}$) the function:

$$y(x) = ay_1(x) + by_2(x)$$

Is that function a solution of the ODE ?

$$\left\{ \begin{array}{lcl} y(x) & = & ay_1(x) + by_2(x) \\ y'(x) & = & -ay_1(x) - 5by_2(x) \\ y''(x) & = & ay_1(x) + 25by_2(x) \end{array} \right.$$

$$\Longrightarrow \left\{ \begin{array}{lcl} y'' + 6y' + 5y & = & ay_1 + 25by_2 - 6ay_1 - 30by_2 + 5ay_1 + 5by_2 \\ & = & (a - 6a + 5a)y_1 + (25b - 30b + 5b)y_2 \\ & = & 0 \text{ for all values of a,b } (\forall\, a, b \in \mathbb{R}) \end{array} \right.$$

Every linear combination of y_1 and y_2 is also a solution !

There is an infinite amount of solutions !

So how can we do physics?

Initial condition

You have actually already solved an ODE multiple times in your life. If y is the position of a moving object, how do we describe its velocity?

(a) Δy
(b) $\frac{\Delta y}{\Delta t}$
(c) $\frac{dy}{dt}$
(d) dt

If the velocity v is constant, we know the solution to this ODE:

$$\Delta y(t) = v\Delta t$$

This only represents how y changes through time. To fix it and to know the value of y at any time, we need the **initial condition**:

$$y(t) = y(t_0) + v(t - t_0)$$

For spatial problem, it will be called a **boundary condition**.

Initial - boundary condition

The **degree** of an ODE is the power of the highest derivative in the ODE. A first-order ODE will require one initial condition. It is a **fully deterministic problem**: knowing the value of y at one point in time completely describes its evolution

$$\begin{cases} \frac{dy}{dt} & = & f(y,t) \\ y(t_0) & = & y_0 \end{cases} \tag{3}$$

A second-order ODE will require two initial conditions (initial position, initial speed):

$$\begin{cases} \frac{d^2y}{dt^2} + a\frac{dy}{dt} & = & f(y,t) \\ y(t_0) & = & y_0 \\ y'(t_0) & = & y'_0 \end{cases} \tag{4}$$

Linearity

We saw that the ODE

$$y''(x) + 6y'(x) + 5y(x) = 0$$

had an infinite amount of solutions

$$y(x) = A\exp(-x) + B\exp(-5x)$$

This is because the latter ODE is linear.
What does it mean than an ODE is linear?

(a) Its only solutions are linear functions
(b) If two functions are a solution of the ODE, a linear combination of the two functions is also a solution
(c) Its only solutions are exponential functions
(d) Its solutions must tend to zero when $t \to \infty$

The latter ODE is linear because the derivative operation is linear:

$$\frac{d}{dt}(ay_1 + by_2) = a\frac{dy_1}{dt} + b\frac{dy_2}{dt}$$

This implies that any linear combination of solutions is a solution
Which of these ODE is **not** linear?

(a) $t\frac{dy}{dt} = 0$ (linear)

(b) $y\frac{dy}{dt} = 0$

(c) $\sin(t)\frac{dy}{dt} = 0$ (linear in y)

(d) $\frac{d^2y}{dt^2} + \frac{dy}{dt} = 0$ (linear)

Which of these ODE is **not** linear?

(a) $\frac{d^2y}{dt^2} + t\frac{dy}{dt} = 0$ (linear)

(b) $\frac{d^2y}{dt^2} + \frac{dy}{dt} = y$ (linear)

(c) $\frac{d^2y}{dt^2} = \sin(y)$

(d) $\frac{d^2y}{dt^2} + \frac{dy}{dt} = \sqrt{t}$ (linear in y)

Why does it matter? Because linear problems are easier to solve (computationnally as well!)
ADDENDUM: an ODE is linear with respect to y if and only if y (or its derivative) appears without a power, when they don't appear in a function (sqrt, sin, exp, ...), and when there is no cross multiplication (e.g. $y\frac{dy}{dt}$). The independant variables (x, t), however they appear, wouldn't change the linearity of the equation with respect to y.

Non Homogeneous linear ODE - general solution

Consider the following problem:

$$y''(x) + 6y'(x) + 5y(x) = 5x^2 + 2x$$

This is called **non-homogeneous** because the RHS has a $f(x)$. The associated homogeneous problem is:

$$y''(x) + 6y'(x) + 5y(x) = 0$$

whose solution $y_H(x)$ is (H stands for "homogeneous")

$$y_H(x) = A\exp(-x) + B\exp(-5x)$$

How to find that ? [No need to remember these methods]. We can obtain a **characteristic equation** $P(\lambda) = \lambda^2 + 6\lambda + 5$, whose roots are

$$\lambda_1 = -1 \qquad \lambda_2 = -5$$

So that we can write the general solution of the homogeneous problem:

$$y_H(x) = A\exp(\lambda_1 x) + B\exp(\lambda_2 x)$$

Non Homogeneous ODE - example of particular solution

Considering the non-homogeneous problem:

$$y''(x) + 6y'(x) + 5y(x) = 5x^2 + 2x$$

If you had to guess, what kind of solutions would you expect? Let us try:

$$y_p(x) = Ax^2 + Bx + C$$

Injecting the latter in the non-homogeneous problem can help determine the values of A, B and C. In this case, $y_p(x)$ (CHECK!):

$$y_p(x) = x^2 - 2x + 2$$

What happens if you combine y_p with y_H?

(a) Nothing
(b) It is a solution
(c) It is not a solution
(d) Why would you do that?

General solution

The general solution of the differential problem is a combination of

- y_H, the **solution of the associated homogeneous ODE**
- y_p which is the **particular solution**

The **general solution** to the non-homogeneous linear problem:

$$y''(x) + 6y'(x) + 5y(x) = 5x^2 + 2x$$

is

$$y(x) = A\exp(-x) + B\exp(-5x) + x^2 - 2x + 2 \tag{5}$$

Practise exercise

Consider the following problem:

$$\begin{cases} \frac{d^2y}{dt^2} + 2\frac{dy}{dt} + 2y & = & t^2 \\ y(0) & = & 0 \\ y'(0) & = & 0 \end{cases} \quad (6)$$

1. Prove/check that $y_1(t) = \exp(-t)sin(t)$ is a solution of this equation
2. Prove/check that $y_2(t) = \exp(-t)cos(t)$ is a solution of this equation
3. Prove/check that $y(t) = 1/2t^2 - t + 1/2$ is a particular solution to this equation
4. Write the general solution of that equation
5. Prove that the function which solves this problem is

$$y(t) = \frac{t^2}{2} - t + \frac{1}{2} + \frac{\exp(-t)}{2}(\sin(t) - \cos(t))$$

Variable separation

Nonlinear ODE $\neq$ unsolvable ODE! For example, the nonlinear problem:

$$\begin{cases} \frac{dy}{dx} = -\frac{\exp(-x)}{2y} \\ y(0) = 1 \end{cases}$$

can be solved through a method called variable separation.

$$\begin{array}{rlcl} & \frac{dy}{dx} & = & -\frac{\exp(-x)}{2y} \\ \iff & ydy & = & -\exp(-x)\frac{dx}{2} \\ \iff & \int ydy & = & -\int \exp(-x)\frac{dx}{2} \\ \iff & \frac{y^2}{2} + C_1 & = & \frac{1}{2}\exp(-x) + C_2 \\ \iff & y^2 & = & \exp(-x) + C_3 \\ \iff & y & = & \exp(-x/2) + C \\ \iff & C & = & 0(\mathrm{IC}) \\ \iff & y & = & \exp(-x/2) \end{array}$$

But usually, non linear ODEs cannot be solved analytically

Outline

From math to physics

A lot of mathematical methods can be used to solve such a problem:

$$\begin{cases} \dfrac{d^2y}{dt^2} + a\dfrac{dy}{dt} & = & f(y,t) \\ y(t_0) & = & y_0 \\ y'(t_0) & = & y'_0 \end{cases} \tag{7}$$

There is no limit of math problems you can create.
But here, we want these equations to represent a physical process. y can represent:

- the position of an object in a gravitational field;
- the temperature of an object;
- an amount (population, radioactive nuclei, particles, ...)

The equation has to describe something real.
The equation wants to talk to you, make sure you listen!

Moving object

Let us consider an object a certain mass m whose position in a 1D space is denoted by $y(t)$. Its velocity v is described as $v = \frac{dy}{dt}$. How would we mathematically describe its acceleration a?

(a) $a = \frac{dy}{dt}$
(b) $a = \frac{\Delta v}{\Delta t}$ (ok if speed is constant)
(c) $a = \frac{d^2y}{dt^2}$

What equation would describe the evolution of y if the object is subject to gravitation?

(a) $\frac{d^2y}{dt^2} = -g$
(b) $\frac{dy}{dt} = -gt$
(c) $\frac{d^2y}{dt^2} + \frac{dy}{dt} = 0$
(c) $\frac{dy}{dt} = v$

Moving object

You have solved the latter equations more than once, because they are easy to solve!
If you want to consider the effect of friction, air resistance, you need to add something there, which might make it more complicated to solve!
If one assumes that the force induced by friction (...) is **proportional to the square of the velocity**, how would you change the previous equation?

(a) $\frac{d^2y}{dt^2} - \lambda\left(\frac{dy}{dt}\right)^2 = -g$

(b) $\frac{d^2y}{dt^2} + \lambda\left(\frac{dy}{dt}\right) = -g$

(c) $\frac{d^2y}{dt^2} + (g - \lambda\left(\frac{dy}{dt}\right)) = 0$

(d) $\lambda\left(\frac{dy}{dt}\right)^2 = -g$

Nonlinear equation!

Example 1

We consider a process involving a physical measurable quantity y. How would you describe the evolution of this quantity if you know/assume that **the evolution of y is constant in time**?

(a) $\frac{d^2y}{dt^2} = \alpha$
(b) $\frac{dy}{dt} = \alpha$
(c) $\frac{dy}{dx} = \alpha$
(d) $\frac{d^2y}{dt^2} = \alpha t$

What physical process could that equation **not** represent?

(a) The velocity of an object travelling with a constant acceleration
(b) The position of an immobile object
(c) The growth of a bacterian population (usually exponential)
(d) The position of an object travelling with a constant speed

Example 2

How would you describe the evolution of a quantity y if you know/assume that its evolution is proportional to time?

(a) $\frac{d^2y}{dt^2} = \alpha$
(b) $\frac{dy}{dt} = \alpha t$
(c) $\frac{dy}{dx} = \alpha$
(d) $\frac{d^2y}{dt^2} = \alpha t$

What physical process could that equation **not** represent?

(a) The speed of a free-falling object in vacuum
(b) The position of an object travelling at a constant speed
(c) The heat energy generated by a constant electrical current
(d) The mass of water in an aquifer

Example 3

How would you describe the evolution of a quantity y if you know/assume that its growth is proportional to itself?

(a) $\frac{d^2y}{dt^2} = \alpha y$

(b) $\frac{dy}{dt} = \alpha y$

(c) $\frac{dy}{dt} = \alpha t$

(d) $\frac{d^2y}{dt^2} = \alpha \frac{dy}{dt}$

What physical process could that equation **not** represent?

(a) The amount of money on your savings account

(b) The amount of Uranium on the Earth

(c) The growth of a bacterial population

(d) The amount of water in an aquifer

Example 4

You put a warm(/cold) object in an infinite medium whose temperature is T_0 and is constant. How would you describe the evolution of T, the object temperature over time?

(a) $\frac{d^2T}{dt^2} = \alpha T_0$

(b) $\frac{dT}{dt} = \alpha T_0$

(c) $\frac{dT}{dt} = \alpha(T_0 - T)$

(d) $\frac{dT}{dt} = \alpha(T - T_0)$ (this would indicate that a hot object would see its temperature increase: $\frac{dT}{dt} > 0$)

Outline

Conclusions

Take away messages:

- There is a basic calculus knowledge to have (being able to verify a solution, identify a linear equation, ...)
- ODE and PDEs can be challenging to solve, particularly in the real world where there is a lot of heterogeneity
- An engineer has to understand the physical concepts underlying a certain equation: it is about understanding it, not memorizing it

What is coming next?

- Computational approach to solve ODEs
- Compare a numerical to an analytical solution
- Why are numerical approaches useful/necessary?

Clicker Question

This lecture might have been really easy for you. Unfortunately, I can't assess that on my own. So please, help me figure it out.

How easy was this lecture for you?

(a) Very easy
(b) Easy
(c) Challenging
(d) Very challenging

Thank you and see you next week!