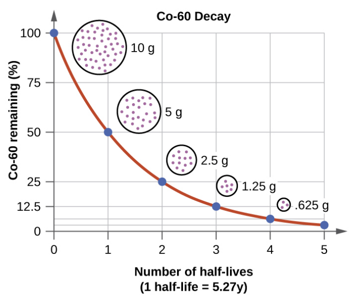
Lecture 1:

Radioactive decay

Euler's method for solving differential equations



Mathematical model & analytical solution

- Constant *fraction* of atoms decays per unit time

$$\frac{\mathrm{d}N}{N} \propto -\mathrm{d}t \rightarrow \frac{\mathrm{d}N}{\mathrm{d}t} = -\frac{N}{\tau} \equiv f(N,t)$$

  where $N(t)$ is the number of radio-active atoms at time t, and the constant τ is called mean life-time

  in this specific example, the function f does not actually depend on time t

- Analytical solution: $N(t) = N_0 \exp(-t/\tau)$
  N_0: number of radio-active atoms at $t = 0$.
  $N(t) = N_0/2$ for $\exp(-t/\tau) = 1/2$, so
  half life-time $T_{1/2} = \tau \ln(2)$.

  examples: (element, $T_{1/2}$): (U^{238}, 4.5 Gyr), (C^{14}, 5.7 kyr), (Am^{241}, 432 yr)

Numerical solution: Euler's method. (Using discretisation)

- Basic idea: replace continuous time t by discrete times t_i $_{i \in N}$.
- How does this work out?
  - Remember definition of derivative:

$$\frac{\mathrm{d}N}{\mathrm{d}t} = \lim_{\mathrm{d}t \to 0} \frac{N(t + \mathrm{d}t) - N(t)}{\mathrm{d}t}$$

  - Approximate $\mathrm{d}t \to 0$ with finite Δt which is 'small enough':

$$\frac{\mathrm{d}N}{\mathrm{d}t} \approx \frac{N(t + \Delta t) - N(t)}{\Delta t}$$

  - Approximate differential eqn by difference eqn:

$$\frac{\mathrm{d}N}{\mathrm{d}t} = -\frac{N}{\tau} \to \frac{N(t + \Delta t) - N(t)}{\Delta t} = -\frac{N(t)}{\tau} .$$

Numerical solution: Euler's method. (cont'd)

- With discrete times:

$$\begin{aligned} N(t_{i+1}) \equiv N_{i+1} &= (1 - \frac{\Delta t}{\tau})N_i \\ t_i &= i \times \Delta t \end{aligned}$$

- This is an example of Euler's method

for solving linear differential equations numerically

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{f}(\mathbf{x}, t) \rightarrow \frac{\mathbf{x}(t + \Delta t) - \mathbf{x}(t)}{\Delta t} = \mathbf{f}(\mathbf{x}(t), t)$$

in general, where $\mathbf{x}(t)$ is a vector and $\mathbf{f}$ is a given function

Euler's method: choosing the step size

- $N_{i+1} = (1 - \frac{\Delta t}{\tau})\, N_i$
  1. Requires $\Delta t < \tau$, otherwise $N_{i+1} < 0$
     method is not unconditionally stable
  2. Accuracy improves with decreasing $\Delta t/\tau$
  3. Taking Δt constant gives constant relative error per step
- In general: $f(x) \rightarrow f(x, t)$

Euler's method: error estimate

- Start with Taylor expansion,

$$x(t+\Delta t) = x(t) + \frac{\mathrm{d}x(t)}{\mathrm{d}t}\Delta t + \frac{\mathrm{d}^2 x(t)}{\mathrm{d}t^2}\frac{(\Delta t)^2}{2!} + \ldots$$

- Euler method uses first two terms, but ignores all others starting at the third one.

$$\Longrightarrow \text{Error per step: } \mathcal{O}[(\Delta t)^2]$$

- But number of steps from t_0 to $t_{\mathrm{end}} \sim 1/\Delta t$!

$$\Longrightarrow \text{Overall error: } \mathcal{O}[(\Delta t)]$$

- Take Δt small enough: compare to time-scale in the problem

  in the current problem, take $\Delta t \ll \tau$

Pseudo-code for solution

Main program

- Input initial conditions (N_0, τ) and run time parameter (final time)
- Initialise classes "Radioactive" and "DEq_Solver"
- Calculate the evolution
- Print/plot the result.

Initialisation of physics problem (in "Radioactive")

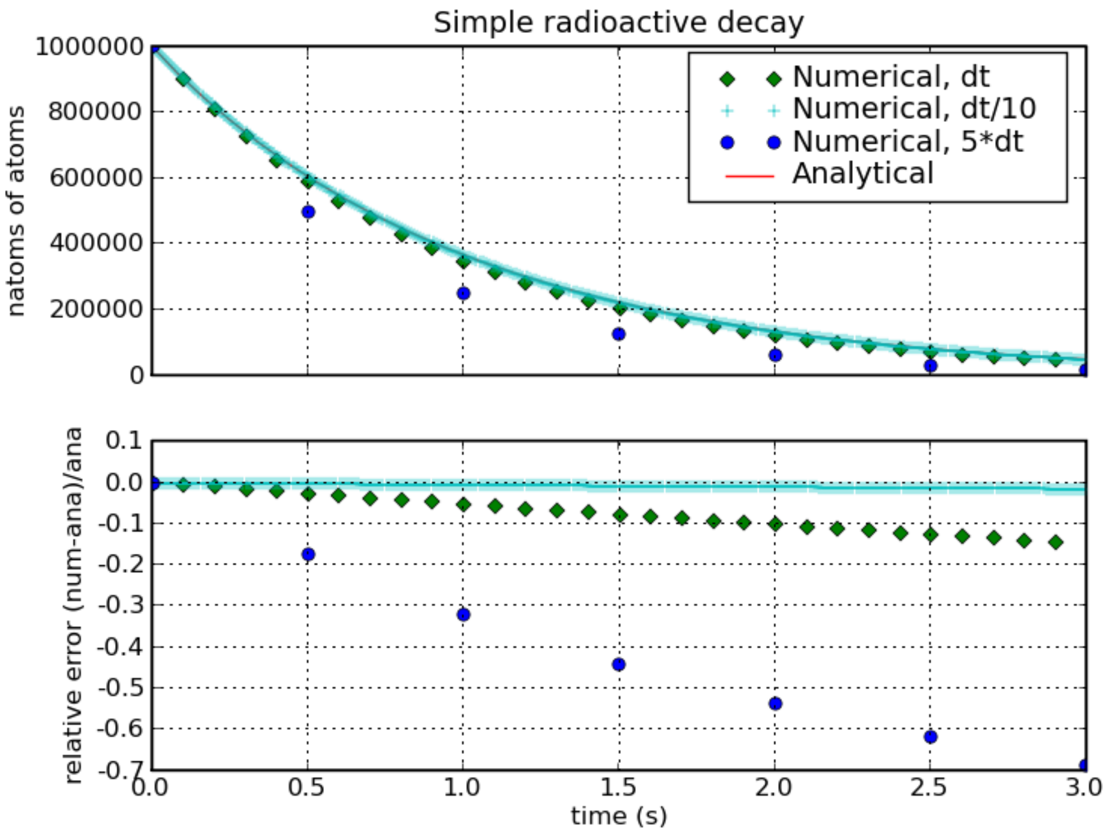
- Fix $t_0 = 0$, t_{end}, N_0, τ
- Δt part of the calculation, not the physics

Calculation (in "DEq_Solver")

- Iterate time steps until $t_i \geq t_{\mathrm{end}}$ is reached:

$$\begin{aligned} t_{i+1} &= t_i + \Delta t \\ \underline{x}(t_{i+1}) = \underline{x}_{i+1} &= \underline{x}_i + \underline{f}(\underline{x}_i)\Delta t\,. \end{aligned}$$

Example solution



Radioactive decay: a change of variables

- Original equation: $\frac{\mathrm{d}N}{\mathrm{d}t} = -\frac{N}{\tau}$
- Change of variables: $x = \ln\left(\frac{N}{N_0}\right)$ N_0 is $N(t=0)$

$$\frac{\mathrm{d}x}{\mathrm{d}t} = -\frac{1}{\tau}\,.$$

Trivial to integrate using Euler's method as well as analytically, of course
No limit on time-step!

- Even better: $t \to t' \equiv \frac{t}{\tau}$

$$\frac{\mathrm{d}x}{\mathrm{d}t'} = -1\,.$$

In the lab session/homework, we stick with the original equation to check for precision of the numerical solution

Summary

- Euler's method is work horse for solving linear differential equations
- First-order accurate
- Method is not unconditionally stable
  precision depends on discretisation step

  require $\Delta t \ll \tau$ in our example

Understanding the basics

- The function $\ln(x)$ is the *natural logarithm*. If you are unfamiliar with this concept, please read-up on it!
- Derive the relation between the half-life of a radioactive element, and the time-scale τ.
- In COVID-19 modelling, what is often report in the daily news is the current 'R' value of the infectious spread. Discuss how this is related to τ or $T_{1/2}$.
- Integrating a radio-active decay problem with a time-step Δt, we find that the numerical integration differs from the exact relation by 5 per cent. How much would you need to reduce Δt by to improve the accuracy to 2.5 per cent?