Computational Physics: Introductory Course

Assignment 6:

Differential Equations II

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What the report should contain

A report should contain:

- The py-files, with carefully commented Python code, that were used to solve the exercises. All code should start with a sentence or two describing what the code is doing. Each py-file should be embedded in the LaTeX or Word document.
- When applicable, you should include the output or plots produced by your code as part of the exercise.
- When you, as part of an exercise, are asked to draw physical conclusions it is important that these conclusions are included in the report. If you are unable to draw any conclusion you should explicitly write 'I was not able to draw any conclusion'.

Important things to keep in mind for producing a good report that adheres to the general rules in scientific writing.

- All variables in the report should be in math font, e.g. the distance was $d = 1.5$ (do not write the distance was d = 1.5, wrong).
- All units in the report should be in correct font, e.g. the acceleration is $a = 1.5\ \mathrm{ms}^{-2}$ (do not write the acceleration is $a = 1.5\, ms^{-2}$, wrong).
- Write $a = 1.5 \cdot 10^{-3}$ instead of $a = 1.5 * 10^{-3}$ (wrong, never use * in equations or text)
- If you give computed values, round them to a reasonable number of decimals.
- The font size in plots should be large enough for the axis texts and legends to be read.

Reading instructions for assignment 6

Read sections 21.1 -21.5.

Exercises

1. Consider the planetary system on page 7. Newton formulated his law of gravitation and solved the corresponding equations for planetary movement analytically. By doing this the previous astronomical observations were confirmed: the earth moves in an elliptical trajectory with the sun in the focus. This must be considered as one of the major achievements in the history of science! We will solve the equations numerically. For simplicity assume that $GM = 1$.

   (a) Solve the system of differential equations with $x(0) = 1-e$, $y(0) = 0$, $x'(0) = 0$, $y'(0) = \left(\dfrac{1+e}{1-e}\right)^{1/2}$.
   Start by formulating the differential equations as a system of equations. Use $e = 0$, 0.5 and 0.9 and plot the trajectory $(x(t), y(t))$ where t is in the interval $[0, 2\pi]$. All plots should be in the same figure. If everything goes well the trajectory should be an ellipse with the eccentricity e and period $T = 2\pi$.

(b) According to the physical preservation laws, the total kinetic and potential energy should be preserved. The kinetic energy is

$$E_{kin} = \frac{1}{2}mv^2 = \frac{1}{2}m(x'(t)^2 + y'(t)^2)$$

The potential energy in the gravitational field is

$$E_{pot} = -GMm\frac{1}{(x^2+y^2)^{1/2}}.$$

Assuming $GM = 1$ and setting $m = 1$ we get that

$$E_{kin} + E_{pot} = \frac{(x')^2 + (y')^2}{2} - \frac{1}{(x^2+y^2)^{1/2}}$$

should be preserved. In addition the angular momentum $\mathbf{L} = \mathbf{r} \times m\mathbf{v}$ should be preserved. The planetary movement is in the xy-plane and the angular momentum is a vector perpendicular to the xy-plane, i.e. $L_x = L_y = 0$. Again assuming $m = 1$, the z-component is given by

$$L_z = xy' - yx'$$

Check the conservation laws by plotting the above quantities in the time interval $[0, 2\pi]$. Note that x' and y' corresponds to column 1 and 3 of your solution from the solver. Make sure that your grid in t is dense enough.

2. Between 1908 and 1913 Hans Geiger and Ernest Marsden, under the supervision of Ernest Rutherford (Nobel Prize in Chemistry 1908), performed a series of famous experiments proving that almost all the positive charge and almost all the mass of the atom is concentrated in a very small atomic nucleus. In the experiments, they used a beam of alpha particles and directed it towards a gold foil. The scientists discovered that the alpha particles relatively often were scattered in large angles and occasionally they scattered backwards, which would be impossible if the positive charge was spread out evenly over the volume of the atom, according to the view at the time (the plum pudding model of the atom). By using Coulomb's law

$$F = K\frac{qQ}{r^2},$$

conservation of angular momentum and assuming point charges, they derived the following relation, in good agreement with observations, between the scattering angle θ and so called the impact parameter b (see figure 1):

$$\sin\frac{\theta}{2} = \frac{1}{\sqrt{1 + \frac{v^4 b^2}{(KQq)^2}}},$$

where $v = 1.53 \times 10^7$ m/s is the initial velocity of the alpha particle, $Q = 79\ e$ and $q = 2\ e$ are the elementary charges ($1\ e = 1.602 \times 10^{-19}$ C) of the gold nucleus and alpha particle, respectively, and K is a constant. In this exercise you will use an almost identical set of coupled differential equation as in exercise 1(a):

$$\begin{cases} x'' = KqQ\dfrac{x}{(x^2+y^2)^{3/2}}, \\ y'' = KqQ\dfrac{y}{(x^2+y^2)^{3/2}}, \end{cases}$$

to verify the relation above. Note that the only difference between the two sets of equations is that we replaced $-GM$ with KqQ. If all distances, including the impact factor b, are given in femtometers (fm), where 1 fm $= 1 \times 10^{-15}$ m, time is given in femtoseconds (fs), where 1 fs $= 1 \times 10^{-15}$ s, velocities are given in fm/fs (1 fm/fs = 1 m/s) and elementary charges are used, then $K = 3.477 \times 10^{13}$ fm^3 fs$^{-2}e^{-2}$.

Solve the differential equations with $x(0) = -1 \times 10^6$, $y(0) = b$, $x'(0) = v$, $y'(0) = 0$ and plot the trajectory $(x(t), y(t))$, where t is in the interval $[0, 0.1]$, for $b = 25$. In addition, estimate the numerically obtained scattering angle for $b = 0, 10, 50$ and 100, and compare with the relation above.

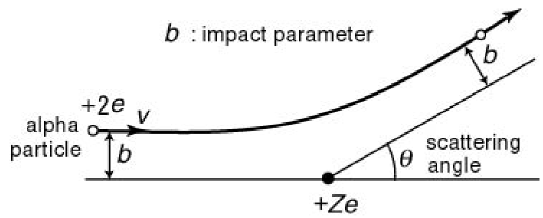

Figure 1: *Kinematics of the Rutherford experiment.*

3. We will look at a radioactive decay chain (this is an example of a compartment model). The isotope ^{210}Bi is radioactive and decays under β emission to ^{210}Po that, in turn, decays under α emission to the stable isotope ^{206}Pb. The halftime $T_{1/2}$ for the two decays are 5.01 days and 138.38 days, respectively. This corresponds to decay constants $\lambda_0 = \ln 2/5.01 \approx 0.138$ and $\lambda_1 = \ln 2/138.38 \approx 0.0050090$. Let $y_0(t)$ and $y_1(t)$ denote the amount of ^{210}Bi and ^{210}Po. We have

$$\begin{cases} \underbrace{\frac{dy_0}{dt}}_{\substack{\text{change of } y_0 \\ \text{per unit time}}} = - \underbrace{\lambda_0 y_0}_{\substack{\text{number of decays} \\ \text{of } y_0 \text{ per unit time}}} \\ \underbrace{\frac{dy_1}{dt}}_{\substack{\text{change of } y_1 \\ \text{per unit time}}} = \underbrace{\lambda_0 y_0}_{\substack{\text{number of created} \\ y_1 \text{ per unit time}}} - \underbrace{\lambda_1 y_1.}_{\substack{\text{number of decays} \\ \text{of } y_1 \text{ per unit time}}} \end{cases}$$

Suppose that we have 1 mole of ^{210}Bi and 0 mole of ^{210}Po at time $t = 0$.

(a) Solve the equation system and plot the solutions in the time interval $[0, 100]$.

(b) Determine the time for which the amount of ^{210}Po is maximal. You can determine the time graphically by zooming in the plot.

Physics background

Kepler's Laws of Planetary Motion

Johannes Kepler published three laws of planetary motion, the first two in 1609 and the third in 1619. The laws were made possible by planetary data of unprecedented accuracy collected by Tycho Brahe.

The laws were both a radical departure from the astronomical prejudices of the time and profound tools for predicting planetary motion with great accuracy. Kepler, however, was not able to describe in a significant way why the laws worked.

1st Law: Law of Ellipses

The orbit of a planet is an ellipse where one focus of the ellipse is the sun, see figure 2.

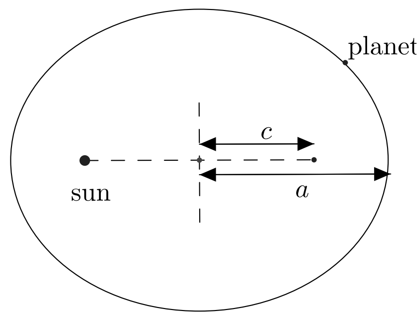

Figure 2: *The orbit of a planet is an ellipse where one focus of the ellipse is the sun. The eccentricity is equal to the distance between a focus and the center c of the ellipses divided by the semimajor axis a. That is,* $e = c/a$.

An ellipse is defined by two focii and all points for which the sum of the distances are the same. The semimajor axis a is the long distance from the center to edge of the ellipse. If r_1 and r_2 are the distances from the focii to any point on the ellipse then $r_1 + r_2 = 2a$. The short axis is called the semiminor axis. How 'elliptical' an orbit is can be described by the eccentricity e. The eccentricity is equal to the distance between a focus and the center c of the ellipses divided by the semimajor axis a. That is, $e = c/a$.

2nd Law: Law of Equal Areas

A line from the planet to the sun sweeps out equal areas in equal amounts of time, see figure 3. With elliptical orbits a planet is sometimes closer to the sun than it is at other times. The point at which it is closest is called perihelion. The point at which a planet is farthest is called aphelion. Kepler's second law basically says that the planets speed is not constant – moving slowest at aphelion and fastest at perihelion. In terms of Newtonian mechanics, developed after Kepler formulated his laws, this is explained by the fact that the total energy, kinetic plus potential, is conserved (compare exercise 1b). At perihelion the potential energy is low and the kinetic energy, and thus the speed, is high. At aphelion potential energy is high and the kinetic energy, and thus the speed, is low.

3rd Law: Law of Harmonies

The period of a planet's orbit squared is proportional to its average distance from the sun cubed. The average distance of a planet from the sun is equal to its semimajor axis (a). If the period (P) is measured in years and the semimajor axis (a) is given in astronomical units (the earth sun distance is 1 AU) then Kepler's 3rd can be written:

$$P^2 = a^3.$$

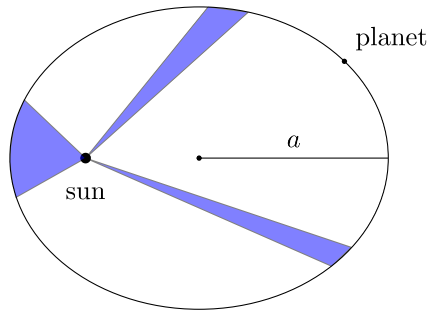

Figure 3: *A line from the planet to the sun sweeps out equal areas in equal amounts of time. The planet moves the fastest at perihelion where the potential energy is low.*

However, this equation is only good for our solar system. Isaac Newton was able to derive a more general form of the equation using his Law of Gravitation.

Newton's laws

In 1687 Isaac Newton published Philosophiae Naturalis Principia Mathematica, a work of immense and profound impact. Newton's pronounced three laws of motion and a law of universal gravitation. They were a united set of principles which applied not only to the heavens, but also to the earth in a uniform way. Their simplicity and extremely broad applicability forever changed physical science.

1st Law of Motion: Law of Inertia

A body remains at rest, or moves in a straight line (at a constant velocity), unless acted upon by a net outside force. The law of inertia did not originate with Newton, nevertheless it is integral to his system of mechanics. An object in motion will remain in motion unless something acts upon it. Because a planet is moving in an ellipse (i.e. not a straight line) this law states that there must be some 'force' acting upon the planet. If there were no force, the planet would fly off in a straight line.

2nd Law of Motion: $F = ma$

The acceleration of an object is proportional to the force acting upon it. The first law says that if no force is acting on an object, it will remain in motion. The second law tells how the motion will change when a force acts upon the object. Velocity is how fast an object is moving (speed or magnitude) and the direction it is moving. Acceleration is a change in velocity. An accelerating object can either change how fast it is moving, the direction it is moving, or both.

3rd Law: Law of Reciprocal Actions

For every action, there is an equal and opposite reaction. The law can be more fully stated as, 'Whenever one body exerts force upon a second body, the second body exerts an equal and opposite force upon the first body.' That is, when the sun pulls on a planet with the force of gravity, the planet pulls on the sun with a force of equal magnitude. But, because the sun is so much more massive than the planet, Newton's second law says that the sun will experience much less acceleration.

Law of Universal Gravitation

Every object in the Universe attracts every other object with a force directed along the line of centers for the two objects that is proportional to the product of their masses and inversely proportional to the square of the separation between the two objects. In mathematical terms the gravitational force is

$$F = G\frac{mM}{r^2}\,,$$

where G is the gravitational constant, m, M the masses and r the distance between the bodies.

Much later it was found out (Coulombs law 1785) that two charges attract or repel each other with a force

$$F = K\frac{qQ}{r^2}$$

where K is Coulomb constant and q and Q the charges of the two particles. It is interesting to note that the two basic laws in physics governing the gravitational force, e.g., between planets, and the electrostatic force, e.g., between the particles in an atom have exactly the same structure.

Planetary systems in terms of differential equations

The planets orbit the sun. Let the sun be fixed at the origin and let $(x(t), y(t))$ be the coordinates of the planet, see figure 4.

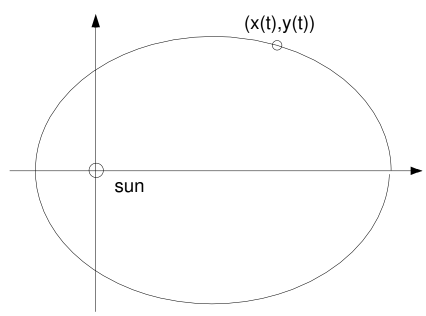

Figure 4: *Planet orbiting the sun. The system is governed by the gravitational forces.*

The planet has mass m and the sun has mass M. The gravitational force on the planet is then

$$\mathbf{F} = -\frac{GmM}{x^2+y^2}\mathbf{u}$$

where

$$\mathbf{u} = \frac{(x,y)}{\sqrt{x^2+y^2}}$$

is a unit (normed) vector, see lecture notes section 11.5, directed towards the planet. G is the gravitational constant. Using Newton's second law we get

$$\begin{cases} x'' = -GM\dfrac{x}{(x^2+y^2)^{3/2}} \\ y'' = -GM\dfrac{y}{(x^2+y^2)^{3/2}}. \end{cases}$$

To solve this in Python we write this system of two second order equations as a system of four first order equations of the variables $z_0 = x, z_1 = x', z_2 = y, z_3 = y'$ (see lecture notes example 21.6).

Compartment models

Many phenomena in physics, natural sciences and medicine can be described by compartment models. In a compartment model the system is distributed over a number of compartments. In each compartment, the system is lumped together and described by one state variable. Systems in different compartments interacts with each other in well defined ways. Read more about compartment models in wikipedia `https://en.wikipedia.org/wiki/Multi-compartment_model`.

Spread of pesticides

When spraying plants with pesticides part of the substance falls on the plants while another part falls on the soil. The pesticide is transported from the plants to the soil with the rain. Pesticides in the soil on the other hand is partly absorbed by the plants by the nutrient transportation from the roots. The amount of pesticide in the soil decrease as the substance leaks to the ground water. Denoting the amount of pesticide on the leafs by y_0 and on the ground by y_1 and the rate coefficients by a_{01}, a_{10}, a_{1g} we have the compartment model displayed in figure 5.

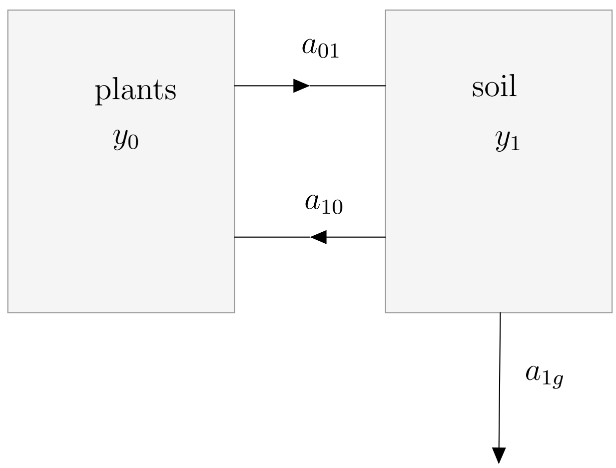

Figure 5: *A compartment model. Substance can flow between the compartments and the flow is determined by the rate coefficients* a_{01}, a_{10} *and* a_{1g}.

This translates into a system of differential equations

$$\begin{cases} y_0' = -\underbrace{a_{01}\, y_0}_{\text{flow to soil}} + \underbrace{a_{10}\, y_1}_{\text{flow from soil}} \\ y_1' = \underbrace{a_{01}\, x y_0}_{\text{flow from plants}} - \underbrace{(a_{10} + a_{1g})\, y_1}_{\substack{\text{flow to plants} \\ \text{and ground water}}} \end{cases}$$

Given values of the rate coefficients and some initial distribution of the pesticide the time development of y_0 and y_1 can be obtained.

Decay chains

Decay chains in nuclear physics are examples of compartment models. Suppose that we have an isotope 1 that decays to an isotope 2 that, in turn decays to a stable isotope. The system can be depicted as in figure 6.

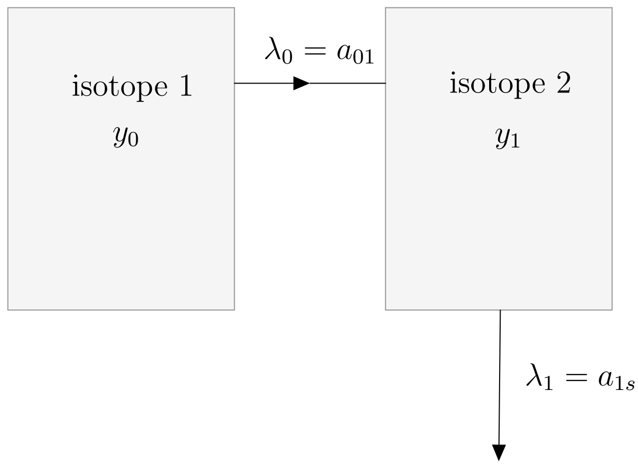

Figure 6: *A compartment model. Substance (isotopes) can flow between the compartments, and the flow is determined by the rate coefficients* $\lambda_0 = a_{01}$ *and* $\lambda_1 = a_{1s}$.

This translates into a system of differential equations

$$\begin{cases} \underbrace{\dfrac{dy_0}{dt}}_{\substack{\text{change of } y_0 \\ \text{per unit time}}} = -\underbrace{\lambda_0 y_0}_{\substack{\text{number of decays} \\ \text{of } y_0 \text{ per unit time}}} \\ \underbrace{\dfrac{dy_1}{dt}}_{\substack{\text{change of } y_1 \\ \text{per unit time}}} = \underbrace{\lambda_0 y_0}_{\substack{\text{number of created} \\ y_1 \text{ per unit time}}} - \underbrace{\lambda_1 y_1.}_{\substack{\text{number of decays} \\ \text{of } y_1 \text{ per unit time}}} \end{cases}$$

The fast carbon cycle

Compartment models can be extended to several compartments. A very interesting and important one is the fast carbon cycle. The fast carbon cycle is a compartment model that describes the movement of carbon between different compartments such as land, atmosphere, ocean, sediment etc, see for example `https://earthobservatory.nasa.gov/features/CarbonCycle` and `https://en.wikipedia.org/wiki/Carbon_cycle`. The cycle is depicted in figure 7.

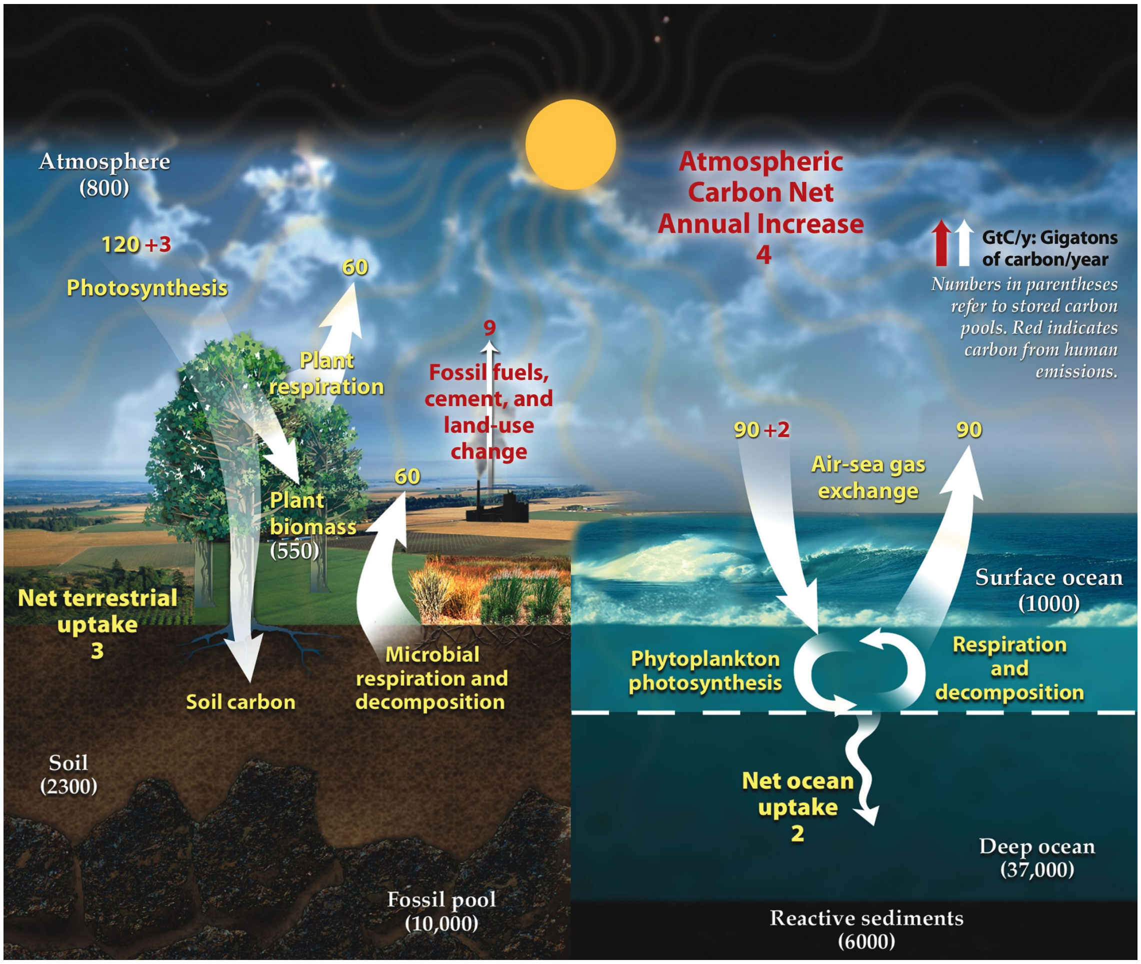

Figure 7: *Fast carbon cycle showing the movement of carbon between land, atmosphere, and oceans in gigatons per year. Yellow numbers are natural fluxes, red are human contributions, white are stored carbon. The effects of the slow carbon cycle, such as volcanic and tectonic activity are not included.*

Although, extremely complex we can set up realistic models for the fast carbon cycle. One such model is presented in *Numerical Computing with MATLAB* by Cleve Molder, `https://se.mathworks.com/content/dam/mathworks/mathworks-dot-com/moler/odes.pdf`. The model simulates the interaction of the various forms of carbon that are stored in three regimes: the atmosphere, the shallow ocean, and the deep ocean. The five principal variables in the model are all functions of time:

p, partial pressure of carbon dioxide in the atmosphere;
σ_s, total dissolved carbon concentration in the shallow ocean;
σ_d, total dissolved carbon concentration in the deep ocean;
α_s, alkalinity in the shallow ocean;
α_d, alkalinity in the deep ocean.

The rate of change of the five principal variables is given by five ordinary differential equations. The exchange between the atmosphere and the shallow ocean involves a constant characteristic transfer time d and a source term $f(t)$:

$$\frac{dp}{dt} = \frac{p_s - p}{d} + \frac{f(t)}{\mu_1}.$$

The equations describing the exchange between the shallow and deep oceans involve v_s and v_d, the volumes of the two regimes:

$$\begin{cases} \dfrac{d\sigma_s}{dt} = \dfrac{1}{v_s}\left((\sigma_d - \sigma_s)w - k_1 - \dfrac{p_s - p}{d}\mu_2\right) \\ \dfrac{d\sigma_d}{dt} = \dfrac{1}{v_d}\left(k_1 - (\sigma_d - \sigma_s)w\right) \\ \dfrac{d\alpha_s}{dt} = \dfrac{1}{v_s}\left((\alpha_d - \alpha_s)w - k_2\right) \\ \dfrac{d\alpha_d}{dt} = \dfrac{1}{v_d}\left(k_2 - (\alpha_d - \alpha_s)w\right). \end{cases}$$

Solving the differential equations with available values of the biophysical parameters using different scenarios for the carbon source term $f(t)$ (burning of fossil fuel) we get plots like the one in figure 8. These type of simulations show the timescales of the processes. We have to live with a carbon concentration in the atmosphere 4 times higher than the pre-historic concentration for thousands and thousands of years. To reduce the concentration in the atmosphere we have to rely on developing, hopefully efficient, carbon sequestration methods `https://en.wikipedia.org/wiki/Carbon_sequestration`.

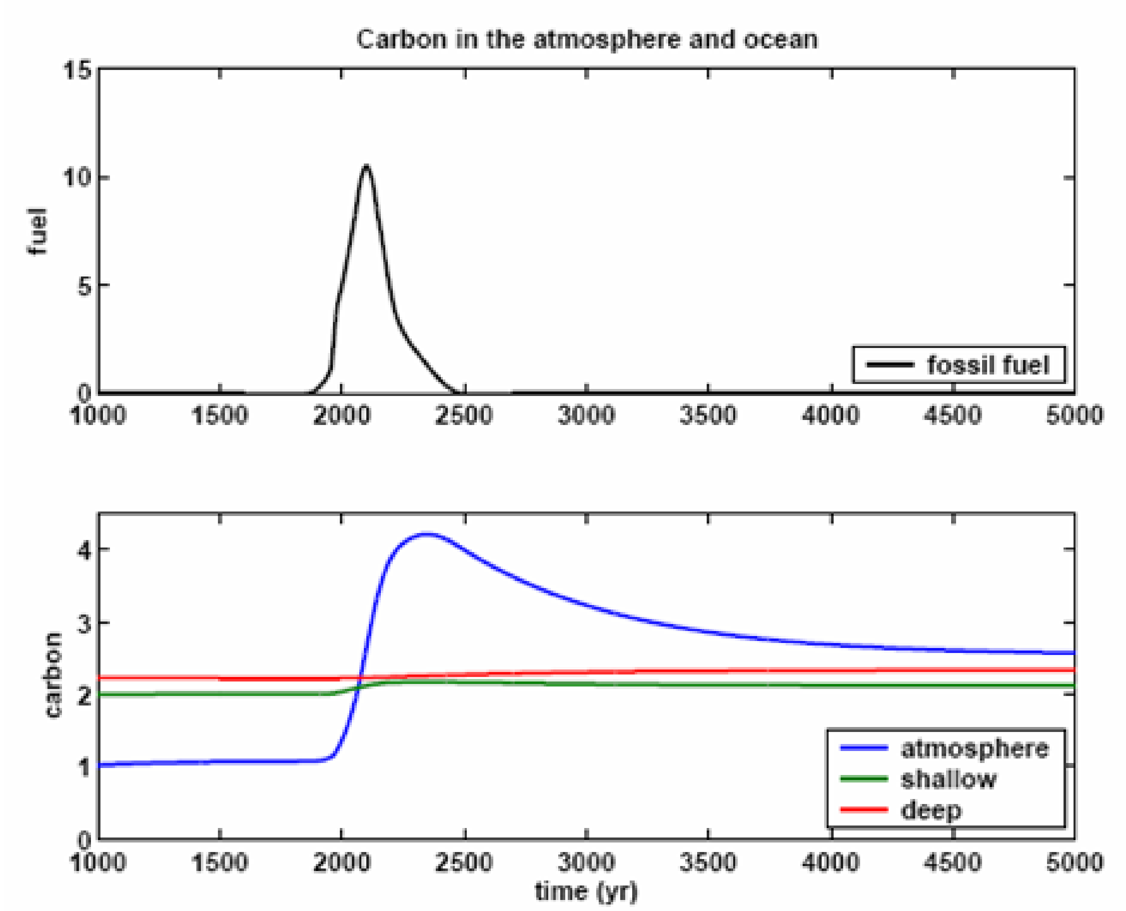

Figure 8: *Top: carbon source term $f(t)$ from burning fossil fule. Bottom: carbon in the atmosphere and ocean as a function of time.*

Summary

The concept of state variables together with the notion of lumped-element and compartment models allow us to study a very broad class of phenomena in physics, chemistry, ecology etc. in terms of systems of coupled ordinary differential equations. Python provides powerful tools to solve these equations and to visualize the solutions. Without exaggeration we may say the differential equations are at the heart of modeling and simulation.

The next step in modeling and simulation would be to try and understand and describe systems with an infinite number of state variables, and that would require continuous models formulated in terms of partial differential equations. We will touch upon these systems in assignment 8, when treating Schrödinger's equation for systems at the quantum scale.

`https://astro.unl.edu/naap/pos/pos_background2.html` `https://astro.unl.edu/naap/pos/pos_background1.html`