ModMod: Simulation environment

ModMod (modular models) is an environment that allows we to program and execute in a modular way a set of systems of ordinary differential equations (ODEs) that interact with each other, without importing that each system advances to a different time scale.

In general, ODEs systems with the following structure are considered:

$$\kappa \frac{dX}{dt} = F(\,X\,,\,I\,,\,U\,,\,\theta\,,\,t\,)$$

where κ is a constant (or function) of proportionality, X represents the vector of state variables, I the inputs of the system, U the control variables, θ are the parameters and constants and t is the time.

Equivalently we have:

$$\begin{aligned}
\kappa_1 \frac{dX_1}{dt} &= F_1(\,X\,,\,I\,,\,U\,,\,\theta\,,\,t\,) \\
&\vdots \\
\kappa_q \frac{dX_q}{dt} &= F_q(\,X\,,\,I\,,\,U\,,\,\theta\,,\,t\,)
\end{aligned}$$

where $F_1, \cdots F_q$ are the right hand sides (RHS) of the system.

The operation of ModMod is developed hierarchically. To represent an ODEs system, what is done is to build a module to describe each of its RHS, these modules are controlled by another additional module in which the structure of the EDOs system is defined. And there is a director module, which controls all modules of the ODEs systems. The figure (1) presents the structure of the ModMod simulation environment.

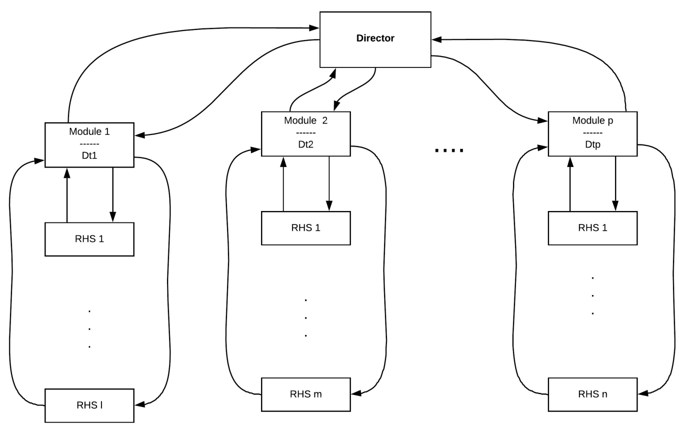

Figure 1: Structure - ModMod simulation environment

The director module contains:

- Scheduler of the order in which the modules are executed.
- Counter of the current time t and recording of the final time that it wants to reach t_f.
- Current values of the variables of each module and record of their histories.

In the ModMod simulation environment it is possible to assign the units of each of the variables and constants that are worked. A very useful tool of ModMod is that it performs a unit check, for example to verify that the units of common variables in different RHSs match or to verify the coherence between the units of a state variable and its RHS.

Additionally, it is considered a generalization that consists in assuming the structure presented in the figure (1) as a subsystem, which is part of a global system, controlled by a principal director. In this way each subsystem has a slave director, which is the one which controls only the operation of said subsystem, and is in turn controlled by the principal director. The variables are divided into global and local: the local variables are those that are only used and considered in a given subsystem, while the global variables are available for the entire system, they are controlled and stored in the principal director.

There is a lot of flexibility respect to the structures that can be built with the generalization of ModMod. For example, as illustrated in figure (2), there may be modules that are directly connected to the principal director and others that are part of a subsystem controlled by a slave director, which in turn connects with the principal director.

Examples

Example 1

We consider the ideal gas law:

$$\frac{P\,V}{T} = k \tag{1}$$

where P represents the gas pressure, V its volume, T its temperature and k is a constant.

If we assume that over time the temperature presents an exponential growth, limited by a maximum temperature, then we have:

$$\frac{dT}{dt} = (T_m - T)\lambda_T, \quad \text{with} \quad T(0) = T_0 \tag{2}$$

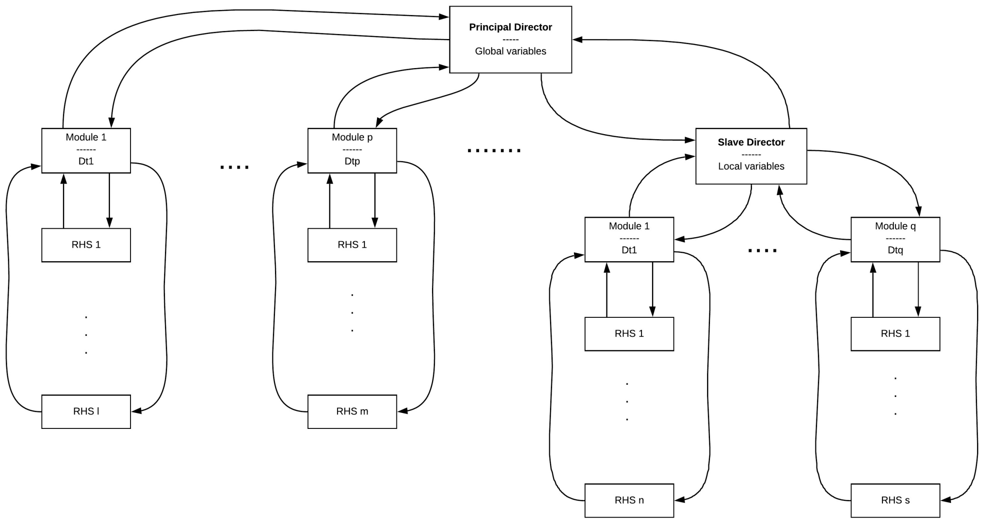

Figure 2: Structure - ModMod generalization

where T_m represents the maximun temperature and λ_T is a constant. The analytical solution of the equation (2) is:

$$T(t) = T_0 + (T_m - T_0)(1 - \exp(t\,\lambda_T)) \tag{3}$$

For this example, we only consider the change in volume with respect to pressure. We assume that this change is of exponential type, limited by a maximum volume, obtaining:

$$\frac{dV}{dP} = (V_m - V)\lambda_V, \quad \text{with} \quad V(P_0) = V_0 \tag{4}$$

where V_m represents the maximun volume and λ_V is a constant. The analytical solution of the equation (4) is:

$$V(P) = V_0 + (V_m - V_0)(1 - \exp(\lambda_V\,(P - P_0))) \tag{5}$$

Finally, the change in pressure over time is characterized by the expression (1):

$$P(t) = k\,\frac{T(t)}{V(t)}$$

This example is solved by means of 3 modules: one in which the RHS of the temperature is defined and the characteristics of how it progresses in time (in this module the pressure advance is also defined); another module that describes the RHS of the volume and its progress; and one last module in which the director which controls and executes all other modules is defined. Figure (3) presents the solution of state variables over time, setting $T_0 = 10\,C$, $P_0 = 1\,\frac{g}{cm^2}$, $V_0 = 1,000\,cm^3$, $T_m = 90\,C$, $V_m = 3,000\,cm^3$, $\lambda_T = 0.1\,\frac{1}{s}$ and $\lambda_V = \frac{1}{60}\,\frac{cm^2}{g}$.

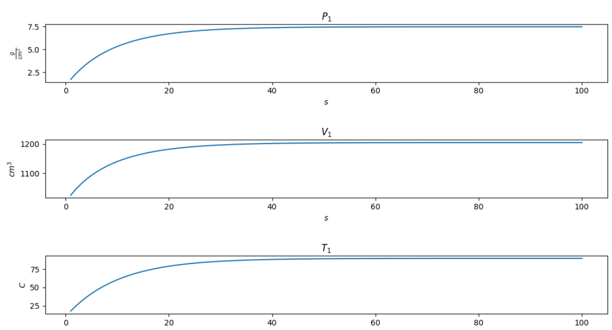

Figure 3: State variables - Example 1

Example 2

In this example, we consider again the ideal gas law, with a temperature growth over time as presented in the expression (2). Now, we will consider the change of the volume over the time, in the follow way:

$$\frac{dV}{dt} = (V_m - V)\lambda_V\,k\,\frac{(T_m - T)\lambda_T}{V}, \quad \text{with} \quad V(0) = V_0 \tag{6}$$

And, again the change in pressure over time is:

$$P(t) = k\,\frac{T(t)}{V(t)}$$

This example is solved by means of 4 modules: one in which the RHS of the temperature is presented; another that describes the RHS of the volume; another module that controls the 2 RHS and in which its advances are defined (in addition to the advance of the pressure); and one last module in which the director which controls and executes the entire system is defined. Figure (4) presents the solution of state variables over time, setting $T_0 = 10\,C$, $P_0 = 1\,\frac{g}{cm^2}$, $V_0 = 1,000\,cm^3$, $T_m = 90\,C$, $V_m = 3,000\,cm^3$, $\lambda_T = 0.1\,\frac{1}{s}$ and $\lambda_V = \frac{1}{60}\,\frac{cm^2}{g}$.

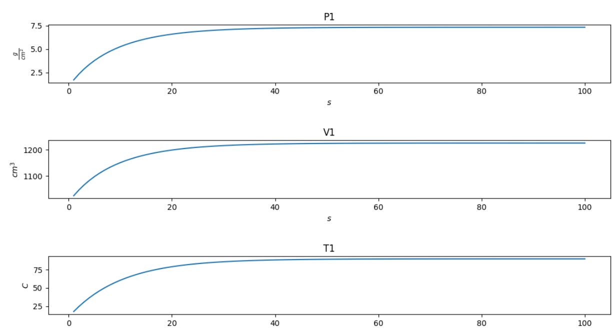

Figure 4: State variables - Example 2

Example 3

In this example we will consider the Lotka - Volterra system of equations:

$$\frac{dX}{dt} = \alpha X - \beta XY,$$

$$\frac{dY}{dt} = \delta XY - \gamma Y.$$

where X and Y represent the population at time t of the prey and predator species respectively. α, β, δ and γ are constants.

This example is solved by means of 4 modules: one in which the RHS of the prey variable is presented; another that describes the RHS of the predator variable; another module that controls the 2 RHS and in which its advances are defined; and one last module in which the director which controls and executes the entire system is defined. Figure (5) presents the solution of state variables over time, setting $X_0 = 10\,n$ (number of specimens), $Y_0 = 10\,n$, $\alpha = \frac{2}{3}\,\frac{1}{d}$, $\beta = \frac{4}{3}\,\frac{1}{nd}$, $\gamma = 1\,\frac{1}{d}$ and $\delta = 1\,\frac{1}{nd}$.

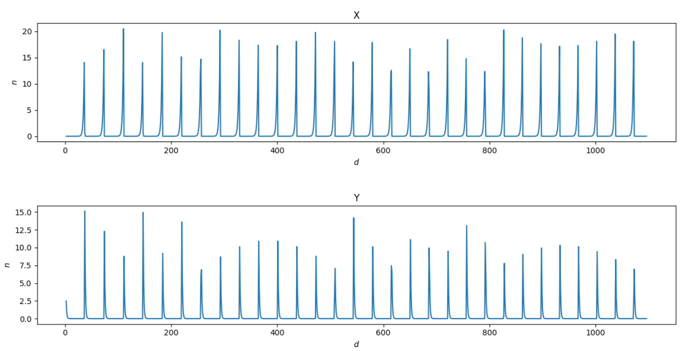

Figure 5: State variables - Example 3

Example 4

In this example we will to present a situation in which it is necessary to consider the generalized version of ModMod, think about subsystems and define local variables. We will consider the model set by Marcelis (1994), which describes the growth of fruits in a cucumber plant.

Fruit growth in a cucumber plant can be described in terms of the following stages:

$$\text{Germination} \;\rightarrow\; \text{Anthesis} \;\rightarrow\; \text{Fruit growth} \;\rightarrow\; \text{Harvest}$$

In this process, germination is the process by which an embryo develops into a plant, the anthesis is the period of flowering, the growth of the fruits is evident and the harvest is the moment where the fruit acquires the size or maturity necessary for its use. Throughout this process the vegetative parts of the plant (leaves, roots and stem) also grow in tandem and fundamentally depends on the temperature. The anthesis is a process that is carried out several times during the life of the plant and is measured in terms of the *appearance of new flowers* from time to time. It is necessary to describe the growth of the fruits individually.

Model description

The cucumber growth model is a discrete dynamic system, where the growth rate of the different elements or parts that describe the plant and its fruits is calculated day by day. The parts or elements of the plant are called SINKS and can be of the following types:

- Fruits / Flowers
- Leaves
- Stem
- Roots

In this model neither stems nor roots are taken into account, so there are two types of SINKS: the fruits / flowers that are considered individually and the leaves that are considered together and as a single SINK.

Emergence of new flowers

The appearance of flowers, which in turn will give rise to the fruits (anthesis), in this model is described by means of the daily rate TF of appearance of fruits on the main stem which is calculated as:

$$TF = \left\lfloor (-0.75 + 0.9T)(1 - \exp(-(1 + P^A)/2) \right\rfloor$$

where $\lfloor x \rfloor$ denotes the entire part of x, T is the average daily temperature measured degrees Celsius and P^A is the PAR radiation on the plant.

SINK growth

The SINK growth in this model is described by its daily growth rate, which is referred to as the " sink strength " and which we will denote for f. The " sink strength " represents the fraction of food that SINK consumes and converts to dry matter weight. For each SINK, that is, for each flower / fruit and for the vegetative part we will have a different "sink strength" that will change every day. Then, the growth rate per day twg_j of the $SINK_j$ (where j is the index of the fruit / flower or the vegetative part) is calculated as:

$$twg_j = \frac{f_j \times A}{dw_{efficiency}}$$

where A are the assimilates (or amount of "food") available in the day in grams / plant, f_j is the "sink strength" of the fruit j and $dw_{efficiency}$ is the efficiency with which the fruit converts grams of A in weight gained. Since the passage of time is one day, the weight gained that day by the fruit j is twg_j. Marcelis (1994) states that $dw_{efficiency} = 1.3$ for the fruit and $dw_{efficiency} = 1.15$ for the vegetative part.

Calculation of the sink strength

The calculation of the "sink strength" for the flowers / fruits and the vegetative part is similar and is done in terms of the following quantities:

1. The A amount of assimilates available, that is the amount of food (CHO carbohydrates) available in the day. The A amount is also called the "assimilate pool" and is calculated from the process of photosynthesis. For this model, A is considered given as a problem data.

2. Thermal age of the fruit j:

$$X_j(t) = \int_{t_j}^{t_f} (T(t) - 10)dt$$

   where t_j it is the moment when the fruit j was born. Then, if $t_f > t_j$ and $\Delta t \leq 1$:

$$X_j(t_1 + \Delta t) \approx X_j(t_1) + \Delta t \left(\frac{\int_{t_2}^{t_1+\Delta t} (T(t) - 10) dt}{t_1 + \Delta t - t_2} \right)$$

or

$$\frac{dX_j}{dt} = T - 10.$$

3. The potential growth rate for fruits:

$$Y_{pot,j} = (T - 10) \times \frac{BMe^{B(X_i - C)}}{[1 + De^{B(X_j - C)}]^{1+1/D}}$$

where $Y_{pot,j}$ is measured in units of grams $\times$ fruit / day, T is the temperature, $C = 131°C * day$ is the thermal time from the anthesis until the maximum growth rate is reached, $B = 0.017$ is a growth rate in $(°C * day)^{-1}$, $D = 0.011$ is a maximum growth rate and $M = 60.7$ grams is the maximum weight of dry matter per fruit.

4. The growth rate potential for the vegetative part is simpler and is only a function of temperature:

$$Y_{pot,0} = a + bT$$

where $a = 3.3$ and $b = 0.25$.

5. The Michaelis-Menten constant that describes the logistic growth of the fruit:

$$km_j = \begin{cases} 0.05 \left(\sum_{n=1}^{j-1} Y_{pot,n} \right) \frac{C - X_j}{C} & \text{for } X_i \le C \\ 0 & \text{for } X_i > C \end{cases}$$

where $C = 131°C$ and X_j is the thermal age of the fruit.

6. The Michaelis-Menten constant for the vegetative part is $Km_0 = 0$ since the growth rate of this part is assumed not to depend on the age of the plant.

With the above elements, the sink strength of each sink is calculated as:

$$f_j = \frac{Y_{pot,j}/(km_j + A)}{\sum_{j=0}^{N} Y_{pot,j}/(km_j + A)}$$

Climate

For this example, the climate conditions will be modeled as follows:

$$\frac{dT}{dt} = \left\{T_s + (T_m - T_s)\sin(\omega t 2\pi)^+ - T\right\} \frac{T_\lambda}{Q_0 + W(t)},$$

where T_m is the average temperature of the day, T_s is the temperature of the sky, T_λ is a constant and $W(t) = \sum Q_i(t)$ is the total weight of the all fruits that are growing (that is, they have not yet been harvested) at the time t. The variation in temperature decrease if it $W(t)$ increases.

Furthermore

$$P_i^A = \beta_i \sin(\omega t 2\pi)^+ .$$

where β_i is a parameter of radiation and depends on the position of the plant. t is measured in d days, and then $\omega = 1d^{-1}$.

Solution with ModMod

This example is solved by means of 3 modules: one in which the conditions of growth of the fruits of one plant are defined, another module in which the climatic conditions are defined, and one last module in which the director which controls and executes the entire system is defined. For each new plant the fruit growth module represents a subsystem, in which a slave director and local variables are defined. The local variables considered are: The total assimilates for plant, the weight of all fruits for plant, the historic weight of all harvested fruits for plant and the sum of all potential growths. The figure (6) presents the results of simulating 9 plants under different radiation conditions for 100 days. The results presented are: the temperature record and the average daily temperature; the total weight of the all fruits that are growing; and the historic weight of all harvested fruits.

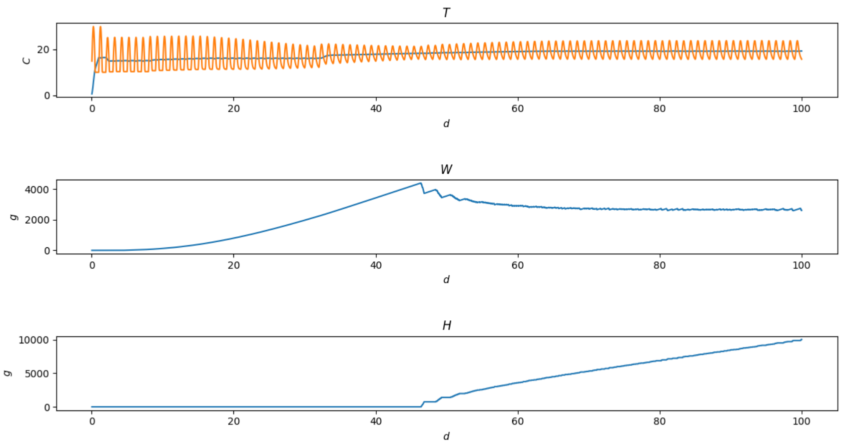

Figure 6: Results - Example 4

References

Marcelis, L. F. M. (1994). A simulation model for dry matter partitioning in cucumber. *Annals of botany*, 74(1), 43-52.