AWESCO Winter School on Numerical Optimal Control with DAE - University of Freiburg

Exercise 10: Simulation of DAE

Sébastien Gros, Moritz Diehl, Rien Quirynen, Joel Andersson, Andrea Zanelli

1 Lagrange Mechanics

1.1 Free mechanics

Consider a hanging crane, made of a cart of mass M and a hanging mass m. The mass is hanging via a spring of constant K. A unique external force u is acting on the cart. Write the dynamics of the system using Lagrange mechanics. Use as coordinates the position of the cart x and the cartesian position of the hanging mass $\mathbf{p} \in \mathbb{R}^2$.

1.2 Constrained mechanics

Consider two masses m linked together via a massless rod of length L evolving without gravity. We will select as generalized coordinates the position of the two masses $\mathbf{p}_{1,2} \in \mathbb{R}^3$ in an

inertial reference frame. The forces acting on the system are forces on the two masses given as $\mathbf{u}_{1,2} \in \mathbb{R}^3$. Write the DAE describing the evolution of the system using Lagrange.

2 Boiling glögg

We regard a pot of glögg (or glühwein) – in essence a mixture of water and ethanol – on a heating plate with constant heating power ($Q = 1$kW). We want to simulate the amount of glögg, ($n(t)$, measured in mol) and the molar concentration of ethanol ($c(t)$, unitless) in the pot. We assume that the heat of vaporization of water and ethanol are equal and both given by $h = 40$ kW/mol (this is correct up to 5%). Thus, the rate of vaporization of glögg is given by:

$$\dot{n}(t) = -Q/h$$

The boiling temperature T (in °C) will be determined by the so-called *Antoine equation*, relating the vapour pressure $p_i(T)$ of a substance i to its temperature:

$$p_i(T) = 10^{A_i - \frac{B_i}{C_i+T}}$$

The coefficients for water ($i = 1$) are given by $A_1 = 8.1$, $B_1 = 1730$ and $C_1 = 233$ and for ethanol ($i = 2$) by $A_2 = 8.2$, $B_2 = 1643$ and $C_2 = 230$, if the temperature is given in degrees Celsius, and the pressure $p_i(T)$ in mmHg. Now, the boiling temperature T of our mixture is determined by the condition that the partial vapour pressures of it components, water and alcohol, must add to the fixed air pressure in the room ($p_0 = 760$ mmHg). The partial vapour pressures result from the product of the pure vapour pressures $p_i(T)$ and the molar concentration in the mixture. Thus, the algebraic equation is given by

$$p_1(T(t))(1 - c(t)) + p_2(T(t))c(t) = p_0$$

This equation implicitly defines the algebraic variable T as a function of the state $[n, c]$.

Finally, we use mass conservation of ethanol to determine the rate of change of c. We use the fact that the molar concentration ethanol in the vapour is given by $p_2(T)/p_0$, such that the outflow of ethanol is given by $p_2(T)/p_0 \dot{n}\, c(t)$. On the other hand, the change of the amount of ethanol in the liquid is given by $d/dt(nc) = \dot{n}c + n\dot{c}$. Equating these two quantities, using $\dot{n} = -Q/h$, and dividing by n yields the second differential equation, which is given by

$$\dot{c}(t) = \frac{-Q\, c(t)}{h \cdot n(t)} \left(\frac{p_2(T(t)) \cdot c(t)}{p_0} - 1 \right).$$

We start with $n(0) = 250$ mol and a molar fraction $c(0) = 0.2$ of ethanol.

Tasks:

10.1 Find the initial temperature $T(0)$ by a root finding procedure, using $T = 100$ °C as initial guess. Does the resulting temperature make sense to you?

10.2 Simulate the evolution of n, c, T for 15 minutes (900 s). Use the solver IDAS from the SUNDIALS suite, which is available via CasADi, for this task, and formulate corresponding CasADi functions for the differential and algebraic equations.

10.3 **Extra**: Adopt the implementation of collocation (for integration) from Exercise 8 to solve the above problem. Use $M = 100$ integrator steps.