Exercises in Simulation of ODEs and DAEs

January 25, 2026

Exercises marked with (O) are mandatory assignments.

1 Simulation of ordinary differential equations

Exercise 1.1. (O) Implement the following integration methods in Matlab (or another favorite language): forward Euler, backward Euler, and the trapezoidal method. The implementation must handle y as a vector; in the implicit method a Newton method shall be used for solving the equations. Assume that both f and $\frac{df}{dy}$ are available so that you do not need to differentiate numerically in the Newton search.

a) Verify the method behavior, the stability limits, and the order of the methods on the problem

$$y' = -10y \qquad y(0) = 1$$

b) Verify the method behavior and the stability region for

$$y' = \begin{pmatrix} -1 & 0 \\ 10 & -10 \end{pmatrix} y \qquad y(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Exercise 1.2. (O) Solve the following problem by hand.

$$y' = -a(y - \cos(t)) \qquad y(0) = 0$$

Exercise 1.3. (O) Apply the three methods from Exercise 1.1 to the problem in Exercise 1.2 with $a = 10$. Investigate the stability limit and what step size is needed for the different methods to give a good approximation to the solution. Run backward Euler and the trapezoidal method with $h = 0.01$ on the problem with $a = 1000$ for $t \in [0, 2]$. Explain the behavior by pointing out properties of the problem and the method that become visible when the different solvers are applied to the problem.

Exercise 1.4. (O) Consider the problems below with tolerance 10^{-2}. Are the problems stiff? Explain why. If a problem is stiff on an interval, then identify the approximate intervals and state them.

a) $y' = -10^6 y, \quad y(0) = 1, \quad t \in [0, 10^{-6}]$

b) $y' = -10^6(y - t^2) + t, \quad y(0) = 1, \quad t \in [0, 1]$

c) $y' = -10^6(y - \sin(10^6 t)) + \cos(10^6 t), \quad y(0) = 1, \quad t \in [0, 1]$

Exercise 1.5. (O) Apply the three methods from Exercise 1.1 to the "circle drawer" where the solution should be a circle

$$y' = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} y \qquad y(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

use step size $h = 0.02$ and simulate long enough to see whether the methods produce a solution that spirals inward, outward, or traces a circle. Which property of the methods is this result linked to?

Exercise 1.6. Exercise 3.1 in Ascher, Petzold.

Exercise 1.7. (O) Consider the explicit RK methods and the choice of the parameters c_i, a_{ij}, and b_i. Describe where the conditions on the parameters come from for methods of at least orders up to 3, preferably also 4 and ideally order 5. What freedom do you have in choosing parameters for the different orders, and what choices have been made in the standard methods such as Bogacki–Shampine, Fehlberg 4(5), and Dormand–Prince 4(5)?

Exercise 1.8. Show that all explicit RK methods can be written in the form (4.11) in Ascher, Petzold, where ψ is Lipschitz continuous with respect to $\boldsymbol{y}$ if $\boldsymbol{f}$ is. (Exercise 4.2 in Ascher, Petzold.)

Exercise 1.9. Consider the following IVP

$$y' = -2\, t\, y^2, \qquad y(0) = 1$$

Determine $y(1)$ using Euler's method and using Taylor's method of third order; use step size $h = 0.1$. Compare the errors in the solutions.

Exercise 1.10. (O) Consider the following initial value problem

$$y' = \gamma \frac{y}{u(t)} \frac{du(t)}{dt}, \qquad y(-\pi) = y_0$$

$$u(t) = cos(t) + 1.1, \qquad \frac{du(t)}{dt} = -sin(t)$$

The nominal parameter values are $y_0 = 1$ and $\gamma = 1.3$ and the interesting time interval is $t \in [-\pi, \pi]$. Perform a sensitivity analysis with respect to the parameters $\phi = (y_0, \gamma)$ by both perturbing the simulation numerically and integrating the perturbation equations, then compare the solutions.

Compare the solution of the perturbation equations $P_i(t)$ with the numerical finite difference approximation

$$\frac{y_\varepsilon(t) - y(t)}{\Delta\phi_i} \tag{1}$$

where $y_\varepsilon(t)$ is the perturbed solution and $\Delta\phi_i$ is the perturbation in the parameter ϕ_i. An example of a comparison could be to plot the two quantities for different values of $\Delta\phi_i$ at $t = \pi/2$.

Comment: The exercise originates from models for cylinder pressure in an engine, and the perturbation analysis is used in connection with parameter identification.

Exercise 1.11. (O) Solve the problem below analytically and also apply the three methods from Exercise 1.1 with step size $h = 1$.

$$y' = 3y, \qquad y(0) = 1$$

Determine specifically $y(10)$ and explain the result.

Exercise 1.12. (O) Map the two tolerance parameters available in Simulink. Explain how each component in the state vector is handled and what tolerance it receives based on the parameter choices. Describe what the *auto* option means. For what magnitude of the variables (or relative magnitudes) must one be cautious about the accuracy of the variables?
Discussion points: Have you learned anything from this? What default settings for the tolerance parameters will you use in the future?

Exercise 1.13. (O) Implement an ODE solver with step size control (and possibly scaling)

a) Implement one of the options.
   1. RK45 Dormand–Prince
   2. BDF (any step size change method, preferably fixed leading coefficient)
b) Verify that the implementation works by computing $y(1)$ in Exercise 1.2.
c) Verify that the tolerance and step size control algorithm is correct.

Exercise 1.14. Exercise 5.3 in Ascher, Petzold. *(A program for computing the coefficients of a linear multistep method.)*

Exercise 1.15. Exercise 5.4 in Ascher, Petzold. *(Test the stability regions for linear multistep methods; builds on 5.3.)*

Exercise 1.16. (O) The well-known chemical Belousov–Zhabotinsky (BZ) reaction has oscillatory behavior that is well described by the "Oregonator" model. The Oregonator model can be simplified, and in its most reduced form the differential equation looks as follows

$$\begin{pmatrix} \epsilon\, x' \\ z' \end{pmatrix} = \begin{pmatrix} x\,(1-x) + f\,\frac{q-x}{q+x}\,z \\ x - z \end{pmatrix}$$

The chemical reaction and the model itself have interesting properties. The system properties change with the parameters and, among other things, one can find a Hopf bifurcation in the parameter ϵ. However, we will not look at the bifurcation but at stiffness.

Solve the initial value problems given by the differential equation above with $x(0) = z(0) = 0.4231$ on the interval $t \in [0, 15]$ s with $q = 8 \cdot 10^{-4}$ and $f = 2/3$, for two different values of ϵ, namely $4 \cdot 10^{-2}$ and $4 \cdot 10^{-3}$.

Use Matlab and solve both problems with two standard solvers that have step size control, one explicit and one for stiff systems (in one case you may use your own solver).

Study the solver runtimes and the step sizes in each step. Can you say that the problem is stiff?

Exercise 1.17. (O) Exercise 5.5 in Ascher–Petzold, with the addition of studying and discussing what happens for tolerances 1e-5, 1e-6, 1e-7, 1e-8 in the final task. *(Lorenz butterfly, with strange attractor.)*

Exercise 1.18. (O) Map the ODE solvers available in Matlab/Simulink. State the type (which family they belong to), the order of the methods, and their properties.

Exercise 1.19. Exercise 7.1 in Ascher–Petzold.

2 Simulation of differential-algebraic equations

Exercise 2.1 (O)**.**

a) Determine differential index for the differential equation

$$\dot{y} = u$$

b) Same question again for

$$\begin{aligned} \dot{x} &= u \\ y &= x \end{aligned}$$

c) Comment the results in a and b-exercises.

Exercise 2.2 (O)**.** Consider the following DAE:

$$\begin{pmatrix} 0 & 0 \\ 1 & \eta t \end{pmatrix} \begin{pmatrix} \dot{x} \\ \dot{y} \end{pmatrix} + \begin{bmatrix} 1 & \eta t \\ 0 & 1+\eta \end{bmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} q \\ 0 \end{pmatrix}$$

with $\eta > -1$ and where q is an arbitrary function of t.

a) Show that the DAE has differential index 2.

b) verify that an exact solution is given by $x(t) = q(t) + \eta t \dot{q}(t)$, $y(t) = -\dot{q}(t)$.

c) Show that the solution in b is the only solution to the differential equation.

d) Show that a direct application of backward Euler gives a solution that diverges from the exact solution for $\eta < -0.5$, regardless of step-length.

Exercise 2.3 (O)**.** The equations below corresponds to a DAE with index 3

$$\begin{aligned} x &= g(t) \\ \dot{x} - y &= 0 \\ \dot{y} - z &= 0 \end{aligned}$$

On the lecture it was outlined why a backward-Euler with variable step length does not work in this case. Show this formally.

Exercise 2.4 (O)**.** Exercise removed

Exercise 2.5 (O)**.** Exercise 9.5 i Ascher-Petzold

Exercise 2.6. For an ODE $\dot{x} = f(x)$ is all solutions at least one time differentiable, this is not generally true for DAE:s. Show a DAE where the solution contains non-differentiable solutions.

Exercise 2.7 (O)**.** Finding consistent initial conditions for a DAE can be difficult and is the topic of this exercise.

a) Write down the equations that has to be solved to find consistent initial conditions on $x(0)$, $\dot{x}(0)$, $\ddot{x}(0)$ etc. for the following two differential equations

$$\begin{cases} \dot{x} = x + y \\ 0 = x + 2y + a(t) \end{cases} \qquad \begin{cases} \dot{x}_1 = -x_1 + x_2 + a(t) \\ \dot{x}_2 = -x_2 + x_3 + b(t) \\ 0 = x_2 + c(t) \end{cases}$$

Determine how many degrees of freedom there is in the initial state.

b) Assume a general DAE

$$F(\dot{x}, x, t) = 0$$

Explain why it is not necessarily true that just because $\dot{x}(0)$ and $x(0)$ fulfills $F(\dot{x}(0), x(0), 0) = 0$ then they are valid initial conditions. Use the following model to illustrate

$$\begin{aligned} \dot{x}_1 + x_3 &= f_1 \\ \dot{x}_2 + x_1 &= f_2 \\ x_2 &= f_3 \end{aligned}$$

where f_i are arbitrary (independent from x_i) functions of t.

c) Determine the differential index for the implicit DAE

$$\begin{aligned} \dot{x}_1(t) + \dot{x}_2(t) &= u_1(t) \\ x_1(t) - x_2(t) &= u_2(t) \end{aligned}$$

where $u_i(t)$ are known functions.

d) For the implicit DAE in the c-exercise, transform into equivalent semi-explicit form by introduction of new variables and again compute the index.

Exercise 2.8. Briefly about index for a linear DAE. For this, consider the linear time-invariant DAE

$$Ax' + Bx = f$$

where $A, B \in \mathbb{R}^{m\times m}$ and f is a $\mathcal{C}^\infty$ function of t. Further, assume that the matrix pencil $\lambda A + B$ has full rank. this assumption is necessary and sufficient for the DAE to have a solution (the interested reader is welcome to prove this). To make things interesting, assume A is singular.

a) Assume there exists matrices P and Q such that

$$PAQ = \begin{bmatrix} I & 0 \\ 0 & N \end{bmatrix}, \quad PBQ = \begin{bmatrix} C & 0 \\ 0 & I \end{bmatrix}$$

where N is nilpotent of order k, i.e., $N^k = 0$ and $N^j \neq 0$ for $j < k$. Show that the index for the DAE equals k.

Brief fact: There always exists matrices P and Q like above.

b) What is the dimension of the room of consistent initial conditions?

Exercise 2.9 (O)**.** This exercise concerns sensitivity analysis for disturbances in parameters.

a) Assume a general DAE

$$F(\dot{x}, x, \theta) = 0,\; x(0) = x_0(\theta)$$

Derive a differential equation for

$$P(t) = \frac{dx(t)}{d\theta}$$

b) Consider the semi-explicit case,

$$\begin{aligned} \dot{x} &= f(x, y, \theta) \\ 0 &= h(x, y, \theta), \quad x(0) = x_0(\theta), \quad y(0) = y_0(\theta) \end{aligned}$$

Write down the sensitivity equations for the DAE and comment on the index 1 case.

c) Implement a sensitivity analysis for a DAE. Reproduce the results in Section 4.3 (Figs 7-16) in the paper Timothy Maly, Linda R. Petzold, *Numerical methods and software for sensitivity analysis of differential-algebraic systems*, Applied Numerical Mathematics Volume 20, Issues 1-2, Pages 57-79, 1996.

Unfortunately, there are typos in the model description (the plots are correct). Use the following model

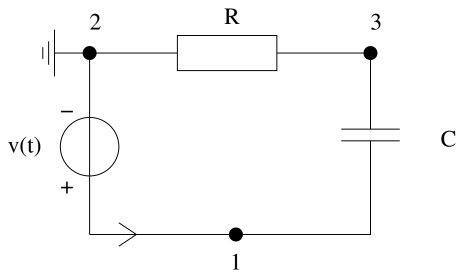
$$
\begin{aligned}
\dot{u}_1 &= -p_3u_2u_8 \\
\dot{u}_2 &= -p_1u_2u_6 + p_2u_{10} - p_3u_2u_8 \\
\dot{u}_3 &= p_3u_2u_8 + p_4u_4u_6 - p_5u_9 \\
\dot{u}_4 &= -p_4u_4u_6 + p_5u_9 \\
\dot{u}_5 &= p_1u_2u_6 - p_2u_{10} \\
\dot{u}_6 &= -p_1u_2u_6 - p_4u_4u_6 + p_2u_{10} + p_5u_9 \\
\dot{u}_7 &= -0.0131 + u_6 + u_8 + u_9 + u_{10} \\
0 &= u_8 - p_7u_1/(p_7 + u_7) \\
0 &= u_9 - p_8u_3/(p_8 + u_7) \\
0 &= u_{10} - p_6u_5/(p_6 + u_7)
\end{aligned}
$$

with initial conditions

$$
\begin{aligned}
u_1(0) &= 1.5776 \\
u_2(0) &= 8.32 \\
u_3(0) &= 0 \\
u_4(0) &= 0 \\
u_5(0) &= 0 \\
u_6(0) &= 0.0131 \\
u_7(0) &= 0.5(-p_7 + \sqrt{p_7^2 + 4p_7u_1(0)}) \\
u_8(0) &= 0.5(-p_7 + \sqrt{p_7^2 + 4p_7u_1(0)}) \\
u_9(0) &= 0 \\
u_{10}(0) &= 0
\end{aligned}
$$

Exercise 2.10 (O)**.** In a tool for simulation of equation based models, like Modelica, the tool has to automatically compute the model index. This is done by computing the, so called, *structural index.* This exercise aims to illustrate this.

a) Consider the following RC-circuit



The following equations describes the system

$$
\begin{aligned}
C(v_1' - v_3') &= i \\
-C(v_1' - v_3') + \frac{1}{R} v_3 &= 0 \\
v_1 &= v(t)
\end{aligned}
$$

What is the index of the model? Does it matter for the index if the grounding poing instead had been in point 1 or 3?

b) What is the structural index for the model? Comment!

c) Does it matter for the structural index of the grounding point had been in point 1 or 3?

d) Compute index and sthe structural index for the model

$$
\begin{aligned}
\dot{x} + \dot{y} + x + y &= \cos t \\
\dot{x} + \dot{y} + x + 2y &= t
\end{aligned}
$$

Exercise 2.11 (O)**.** Consider the DAE:n

$$
F(y, y') = y_m N y' + y = 0
$$

where $y = (y_1, \ldots, y_m)$ and N is a $m \times m$ matrix in the form

$$
N = \begin{bmatrix}
0 & 1 & 0 & 0 & \ldots & 0 \\
0 & 0 & 1 & 0 & \ldots & 0 \\
\vdots & & & \ddots & & \\
0 & 0 & 0 & \ldots & 0 & 1 \\
0 & 0 & 0 & 0 & \ldots & 0
\end{bmatrix}
$$

Compute differential index and the perturbation index.

What does this say about the realtion between the two indices?

Exercise 2.12. State and prove a necessary and sufficient condition for

$$
\begin{aligned}
\dot{x} &= f(x, y) \\
0 &= g(x, y)
\end{aligned}
$$

to have index 1.

Exercise 2.13 (O)**.** Describe how Pantelides algorithm can be used to derive the structural index for a DAE.

Exercise 2.14 (O)**.** Consider a model of an ideal pendulum, a point mass at the end of a weightless arm, in cartesian coordinates. Equations describing the motion is given by

$$
\begin{aligned}
m\,\ddot{x}(t) &= x(t)\lambda(t) \\
m\,\ddot{y}(t) &= y(t)\lambda(t) - m\,g \\
0 &= x^2(t) + y^2(t) - l^2
\end{aligned}
$$

where m is the pendulum mass, l length of the arm, and x and y pendulum position, and λ the force in the pendulum.

a) Show that the above model has index 3

b) Perform index reduction by differentiating model equations until a subset of equations become index 1. Simulate this DAE and comment on the problems that occur. Also, see if you find a simple substitution in the index reduced DAE that improves simulation performance and reduces drift.

c) Make a better index reduction to avoid the problems in b-exercise. Use either a projection method or baumgartner stabilization.

d) Write the model from the b-exercise in semi-explicit form and denote the algebraic variables with z. Add $\epsilon z'$ on the left-hand-side of the algebraic constraints and simulate using an ODE solver.

   Comment on the choice of ϵ, choice of ODE solver and the obtained numerical solution. Comment and compare with the solution from b- and c-exercise.

Exercise 2.15 (O)**.** Assume you want to use ϵ-embedding together with a Runge-Kutta method to integrate index 1 equations. Why does it only work with implicit Runge-Kutta methods?

Exercise 2.16. Assume that the original DAE

$$F(\dot{y}, y, t) = 0 \tag{2}$$

has been index reduced, by differentiations and variable substitutions, to an ODE

$$\dot{y} = f(t, y) \tag{3}$$

Assume that during index reduction, the algebraic constraints

$$g(y, t) = 0$$

has been used. One way of re-introducing the algebraic constraints is to again consider a DAE

$$\dot{y} = f(t, y) + g_y(t, y)\mu \tag{4a}$$

$$0 = g(t, y) \tag{4b}$$

Assume that $g_y(t, y)$ has fyll row rank, i.e., g does not contain any linearly dependent conditions.

a) Show that the new DAE has index 2.

b) Show that the solution set to (4) includes a solution with $\mu = 0$ and y that is a solution to (3).

c) For the interested. Assume further that g characterises solutions to (2), i.e., there is a solution y to (2) if and only if $g(y) = 0$. Now show that the solution from the b-exercise is the only solution to (4).

Exercise 2.17. *Exercise removed*

Exercise 2.18 (O)**.** The following exercise illustrates conservation of invariants. Consider the following model of a chemical reaction

$$\begin{aligned}\dot{x}_1 &= -0.04x_1 + 10^4 x_2 x_3\\ \dot{x}_2 &= 0.04x_1 - 10^4 x_2 x_3 - 3\cdot 10^7 x_2^2\\ \dot{x}_3 &= 3\cdot 10^7 x_2^2\end{aligned}$$

with the (made up) initial conditions

$$x_1(0) = 1, \quad x_2(0) = 2\cdot 10^{-4}, \quad x_3(0) = 3\cdot 10^{-1}$$

a) Show that mass conservation $x_1(t)+x_2(t)+x_3(t) = x_1(0)+x_2(0)+x_3(0) = M$ is an invariant for the model.

b) Show that the invariant is a *linear first integral*. See Hairer-Wanner for definition.

c) It is possible to show that most methods of integration, for example Runge-Kutta, conservers linear first integrals but not more complex invariants, e.g., quadratic.

   Verify by simulation that the invariant is kept by a Runge-Kutta method.

d) Verify that the invariant for the "circle drawer" is a quadratic first integral. To conserve such an invariant requires, for example, a ”symplectic Runge-Kutta”.

Exercise 2.19.

a) Exercise 2.4 in Ascher-Petzold

b) Use the sabilization method (9.40) from Ascher-Petzold on the circle drawer. Comment the simulation results and choice of γ.

Exercise 2.20. Investigate simulation time. Compare simulation time for a DAE with index 1 and the corresponding ODE. Take an example where the index reduction is easy to do by hand.

Exercise 2.21. In Matlab there are two solvers that can solve DAE:s, `ode15s` and `ode23t`, and the SUNDIALS suite (C/C++) has a solver IDA (used in OpenModelica, and scikits.odes[1] in Python)[2]. Use code and manual pages to find out the basic principles for any of the solvers.

Exercise 2.22 (O)**.** Exercise 9.11 in Ascher-Petzold

Exercise 2.23. Exercise 9.10 in Ascher-Petzold

Exercise 2.24. *Exercise removed*

[1] `https://scikits-odes.readthedocs.io/`
[2] See documentation on `https://sundials.readthedocs.io/`

Exercise 2.25. Exercise 10.4 in Ascher-Petzold

Exercise 2.26 (O)**.** Exercise 10.6 in Ascher-Petzold

Exercise 2.27. Sundials (`https://computing.llnl.gov/projects/sundials`) is a suite of high-quality nonlinear and differential/algebraic equation solvers written in C/C++.

The exercise is to write code in C/C++ that simulates a well chosen example, possibly also direct utilization of the functionality to simultaneously integrate sensitivity equations. Contact course responsible if you plan to do this exercise for further details.

Exercise 2.28. For an ODE

$$\dot{x} = f(x, t)$$

a Lipschitz condition on f is sufficient to ensure a unique solution to the initial value problem.

Find a sufficient condition, similar to a Lipschitz for an ODE, for the index 1, semi-explicit DAE

$$\begin{aligned} \dot{x} &= f(x, y) \\ 0 &= g(x, y), \quad g_y \text{ full rang} \end{aligned}$$

to have a unique solution.

Exercise 2.29 (O)**.** Consider the following DAE formulation of the pendulum equations

$$\begin{aligned} \dot{x} &= w \\ \dot{y} &= z \\ m\dot{w} &= Tx \\ m\dot{z} &= Ty - mg \\ 0 &= x^2 + y^2 - L^2 \end{aligned}$$

Implement the model in Modelica, simulate and comment the results. Prove that the potential plus kinetic energy is an invariant to the model, plot the total energy of the system and other interesting simulation results and comment.

I recommend to use OpenModelica `https://www.openmodelica.org`.

Exercise 2.30 (O)**.** Consider the same DAE formulation of the pendulum equations as in the previous exercise.

Find the system of equations to solve to find consistent initial conditions and use the dummy derivatives method to reduce the index to 1. Simulate the DAE:e and comment the result as in the previous exercise.

Also, comment on how/if your choice of dummy derivatives limits the range of the model and how you could improve your simulation model (no need to implement).

Exercise 2.31 (O)**.** Consider the scalar ODE initial value problem

$$\dot{y} + \theta y = 0, \quad y(0) = y_0$$

where θ is a parameter and let

$$G = \int_0^T y^2(t)\,dt$$

be a performance measure. Compute $dG/d\theta$ with $T = 5$, $\theta = 1$, and $y_0 = 2$. Compute the sensitivity in three different ways (which all should result in the same sensitivity)

1. exact, analytical, expression
2. forward sensitivity analysis
3. adjoint sensitivity analysis

Compare results and discuss.

Assume that you only want to compute sensitivities with respect to initial conditions. Show how the adjoint sensitivity equations simplifies.

This toy example is used to illustrate the main principles, to see how forward and adjoint sensitivity analysis could be done for larger and more complex models, I highly recommend Exercise 2.34.

Exercise 2.32. Redo exercise 2.31 where sensitivity towards θ *and* y_0 is computed by solving both forward and adjoint sensitivity equations. Discuss what changes.

Exercise 2.33. (O) This exercise aims at getting familiar with DAE simulation functionality in Matlab/Python. For this, we'll consider a common test DAE example from

Robertson, H. H. "*The solution of a set of reaction rate equations*". Numerical analysis: an introduction, (1966).

The chemical reactions are modeled by the equations

$$\begin{aligned}
\dot{y}_1 + p_1 y_1 - p_2 y_2 y_3 &= 0 \\
\dot{y}_2 - p_1 y_1 + p_2 y_2 y_3 + p_3 y_2^2 &= 0 \\
y_1 + y_2 + y_3 - 1 &= 0
\end{aligned}$$

on the interval $t \in [0, T]$, $T = 4 \cdot 10^{10}$, with initial conditions: $y_1 = 1$, $y_2 = y_3 = 0$. The reaction rates are: $p_1 = 0.04$, $p_2 = 10^4$, and $p_3 = 3 \cdot 10^7$.

Simuate the system in your system of choice and plot the solutions, with logarithmic time axis and scaled y_2 you should get solutions similar to Figure 1. Experiment with available solvers and tolerances.

Exercise 2.34. This exercise is intended to get you familiar with the C/C++ framework SUNDIALS to compute solutions and sensitivities (both forward and adjoint) of DAEs[3].

[3]This exercise requires some familiarity with C programming and compilers. It is fairly straightforward to install on your own computer. It is also pre-installed at the group computational server. If you have problems compiling, contact course responsible.

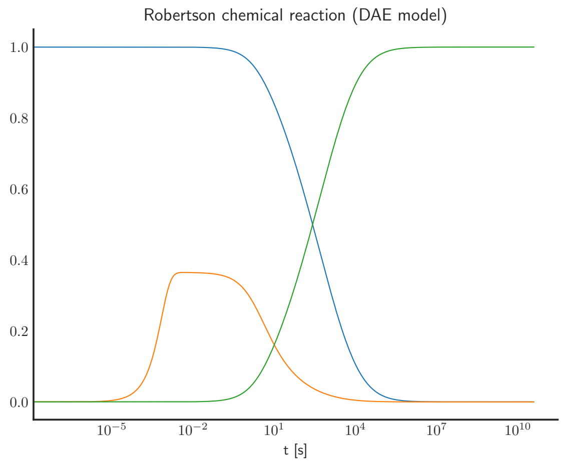


Figure 1: Solutions for the Robertson model equations.

Consider the same model as in Exercise 2.33 where we also want to compute sensitivities with respect to the problem parameters p_i of the quadrature

$$G = \int_0^T y_3(t)\, dt,$$

i.e., compute

$$\frac{dG}{dp}$$

a) Study the source file for Forward Sensitivity Analysis of the chemical reaction model in `idasRoberts_FSA_dns.c`, part of the SUNDIALS example suite[4]. To follow the steps in the code, read the documentation `https://sundials.readthedocs.io/en/latest/idas/Usage/`. In particular, see to it that you understand the functions `res`, `resS`, and `rhsQ`.

   Explain what is the difference between the *Staggered* and *Simultaneous* methods for sensitivity analysis.

   Compile, run, and experiment!

b) Compute the iteration matrix (in the SUNDIALS documentation this is referred to as the system jacobian) for forward simulation of the model

$$J = F_y + c_j F_{\dot{y}}$$

c) Now study the source file for Adjoint Sensitivity Analysis implemented in the file `idasRoberts_ASAi_dns.c`, and in particular see to it that you understand the functions `res`, `Jac`, and `rhsQ`. The solution from the b-exercise should be equivalent to the implementation in the `Jac` function.

d) Continue the study of the adjoint sensitivity simulations. Define the adjoint problem and compare with the backwards residual function `resB`.

[4]Default installation location on Linux/Mac is `/usr/local/examples/idas/serial/`.

Further, compute the iteration matrix for the adjoint problem for reverse simulation

$$J_{adj} = -F_y^T + c_j F_{\dot{y}}^T$$

and compare with the function `JacB`. Finally, explain the contents of function `rhsQB`, used to compute the sensitivity.

Simulate and compare the ouput of the the forward sensitivity example to ensure that you understand that they give equivalent outputs.

Exercise 2.35 (O)**.** Consider the following DAE[5]

$$\begin{aligned}\dot{y}_1 &= y_1 y_2^2 z^2 \\ \dot{y}_2 &= y_1^2 y_2^2 - 3y_2^2 z \\ 0 &= y_1^2 y_2 - 1\end{aligned}$$

with initial conditions $y_1(0) = y_2(0) = z(0) = 1$.

Show that the DAE has index 2 and perform exact index reduction and simulate the DAE for $t \in [0, 1]$. Verify that your solutions comply with the exact solutions

$$y_1(t) = e^t, \quad y_2(t) = e^{-2t}, \quad z(t) = e^{2t}$$

and that the algebraic constraint in the model is satisfied.

[5]Example from Section 7 in Jay, Laurent. "*Convergence of a class of Runge-Kutta methods for differential-algebraic systems of index 2*." BIT Numerical Mathematics 33.1 (1993): 137-150. (`https://doi.org/10.1007/BF01990349`)