Uppgifter i simuleringskursen

January 27, 2022

Uppgifter med (O) betecknar obligatoriska inlämningsuppgifter.

För de uppgifter som är värda extra Ladok-poäng, prata med kursledning om bedömning, omfattning och hur mycket poäng uppgiften är värd.

Alla är välkommna att föreslå egna ”mini-projekt” eller undersökningar som ni vill göra och presentera för extra Ladok-poäng.

1 Simulering av ordinära differentialekvationer

Uppgift 1.1. (O) Implementera följande integrationsmetoder i Matlab (eller ett annat favoritspråk): Euler-framåt, Euler-bakåt och trapetsmetoden. Implementationen skall klara då y är en vektor, i den implicita metoden skall en Newton metod användas för ekvationslösningen. Anta att du har både f och $\frac{df}{dy}$ tillgängliga så att du inte behöver derivera numeriskt i Newton sökningen.

a) Verifiera funtion hos metoden, stabilitetsgränserna och ordningen för metoderna på följande problem

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

b) Verifiera metodens funktion och stabilitetsområdet för

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

Uppgift 1.2. (O) Lös följande problem för hand.

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

Uppgift 1.3. (O) Applicera de tre metoderna från Uppgift 1.1 på problemet i Uppgift 1.2 med $a = 10$. Undersök stabilitetsgräns och vilken steglängd som behövs för att de olika metoderna skall ge en god approximation till lösningen. Kör Euler bakåt och trapetsmetoderna med $h = 0.01$ på problemet med $a = 1000$ för $t \in [0, 2]$. Förklara beteendet genom att peka ut egenskaper hos problemet och metoden som blir synliga när de olika lösarna appliceras på problemet.

Uppgift 1.4. (O) Betrakta nedanstående problem där toleransen är 10^{-2}. Är problemen styva? Förklara varför. Om ett problem är styvt i ett intervall identifiera då de approximativa intervallen och ange dessa.

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

Uppgift 1.5. (O) Applicera de tre metoderna från Uppgift 1.1 på "cirkelritaren" lösningen skall bli en cirkel

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

använd steglängd $h = 0.02$ simulera så lång tid att du kan se om metoderna ger en lösning som gör en spiral inåt, utåt eller om den beskriver en cirkel. Vilken egenskap hos metoderna är detta resultat kopplat till?

Uppgift 1.6. Övning 3.1 i Ascher, Petzold.

Uppgift 1.7. (O) Betrakta de explicita RK metoderna och valet av parametrarna c_i, a_{ij} och b_i. Beskriv varifrån villkoren på parametrarna kommer för metoderna av ordningar åtminstone upp till 3 och väldigt gärna även 4 och gärna även ordning 5. Vilken frihet har man att välja parametrar för de olika ordningarna och vilka val har man gjort i standardmetoderna såsom: Bogacki-Shampine, Fehlberg 4(5) och Dormand-Prince 4(5)?

Uppgift 1.8. Visa att alla explicita RK metoder kan skrivas på formen (4.11) i Ascher, Petzold, där ψ är Lipschitz kontinuerlig m.a.p. $\boldsymbol{y}$ om $\boldsymbol{f}$ är det. (Uppgift 4.2 i Ascher, Petzold.)

Uppgift 1.9. Betrakta följande IVP

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

Bestäm $y(1)$ med hjälp av Eulers metod samt med Taylors metod av tredje ordningen, använd steglängden $h = 0.1$. Jämför felen i lösningarna.

Uppgift 1.10. (O) Betrakta följande initialvärdesproblem

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

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

Nominella parametervärden är $y_0 = 1$ och $\gamma = 1.3$ och det intressanta tidsintervallet är $t \in [-\pi, \pi]$. Gör en känslighetsanalys med avseende på y_0, γ. Jämför $\frac{\bar{y}(t)-y(t)}{\phi_i}$ och $P(t)$, t.ex. genom att plotta de båda storheterna för olika värden på ϕ_i i $t = \pi/2$. (Kommentar: Uppgiften har sitt ursprung i modeller för trycket i cylindern på en motor och störningsanalysen används i samband med parameteridentifiering.)

Uppgift 1.11. (O) Lös nedanstående problem analytiskt och applicera även de tre metoderna från Uppgift 1.1 med steglängd $h = 1$.

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

Bestäm speciellt $y(10)$ och förklara resultatet.

Uppgift 1.12. (O) Kartlägg de två toleransparametrarna som finns i Simulink. Förklara hur varje enskild komponent i tillståndsvektorn hanteras och vilken tolerans den får utgående från parametervalen. Beskriv vad alternativet *auto* innebär. Vid vilken storleksordning på variablerna (eller inbördes förhållanden) måste man vara vaksam på noggrannheten i variablerna?
Diskussionspunkter: Har du dragit någon lärdom av detta? Vilken grundinställning på toleransparametrarna kommer du att ha i framtiden?

Uppgift 1.13. (O) Implementera en ODE-lösare med steglängdskontroll (och ev skalning)

a) Implementera ett av alternativen.

   1. RK45 Dormand-Prince

   2. BDF (valfri steglängdsändringsmetod, men gärna fixed leading coefficient)

b) Verifiera att implementeringen fungerar genom att beräkna $y(1)$ i uppgift 1.2.

c) Verifiera att algoritmen för tolerans och steglängdskontroll är korrekt.

Uppgift 1.14. Uppgift 5.3 i Ascher, Petzold. *(Ett program för beräkning av koefficienterna i en linjär flerstegsmetod.)*

Uppgift 1.15. Uppgift 5.4 i Ascher, Petzold. *(Testa stabilitetsområdena för linjära flerstegsmetoder, bygger på 5.3.)*

Uppgift 1.16. (O) Den välkända kemiska Belousov Zhabitinsky (BZ) reaktionen har ett oscillativt beteende som beskrivs väl av "Oregonator" modellen. Oregonator-modellens kan förenklas och i dess mest förenklade form ser differentialekvationen ut som följer

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

Den kemiska reaktionen och modellen i sig har intressanta egenskaper. Systemets egenskaper ändras med parametrarna och bland annat så kan man hitta en Hopf-bifurkation i parametern ϵ. Vi skall dock inte titta på bifurkationen utan på styvheten.

Lös initialvärdesproblemen som ges av diffekvationen ovan samt $x(0) = z(0) = 0.4231$, på intervallet $t \in [0, 15]$ s med $q = 8 \cdot 10^{-4}$ och $f = 2/3$, för två olika värden på ϵ nämligen $4 \cdot 10^{-2}$ och $4 \cdot 10^{-3}$.

Använd Matlab och lös båda problemen med två standardlösare som har steglängdskontroll, en explicit och en för styva system (i det ena fallet får du gärna använda din egen).

Studera lösarnas lösningtid samt steglängderna i varje steg. Kan man säga att problemet är styvt?

Uppgift 1.17. (O) Uppgift 5.5 i Ascher-Petzold, med tillägget att studera och diskutera vad som händer för toleranserna 1e-5, 1e-6, 1e-7, 1e-8 i sista uppgiften. *(Lorenz Buttefly, with strange attractor.)*

Uppgift 1.18. (O) Kartlägg ODE-lösarna som finns i Matlab/Simulink. Ange typ (vilken familj de tillhör), metodernas ordning och vilka egenskaper de har.

Uppgift 1.19. Övning 7.1 i Ascher-Petzold.

2 Simulation of differential-algebraic equations

Uppgift 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.

Uppgift 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.

Uppgift 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.

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

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

Uppgift 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.

Uppgift 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.

Uppgift 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?

Uppgift 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

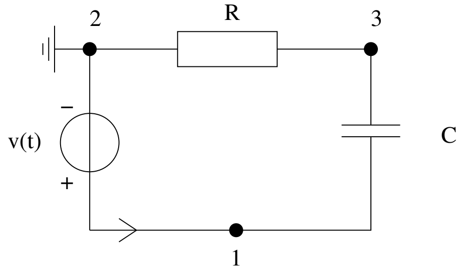
$$\begin{aligned}
\dot{u}_1 &= -p_3 u_2 u_8 \\
\dot{u}_2 &= -p_1 u_2 u_6 + p_2 u_{10} - p_3 u_2 u_8 \\
\dot{u}_3 &= p_3 u_2 u_8 + p_4 u_4 u_6 - p_5 u_9 \\
\dot{u}_4 &= -p_4 u_4 u_6 + p_5 u_9 \\
\dot{u}_5 &= p_1 u_2 u_6 - p_2 u_{10} \\
\dot{u}_6 &= -p_1 u_2 u_6 - p_4 u_4 u_6 + p_2 u_{10} + p_5 u_9 \\
\dot{u}_7 &= -0.0131 + u_6 + u_8 + u_9 + u_{10} \\
0 &= u_8 - p_7 u_1/(p_7 + u_7) \\
0 &= u_9 - p_8 u_3/(p_8 + u_7) \\
0 &= u_{10} - p_6 u_5/(p_6 + u_7)
\end{aligned}$$

with initial conditions

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

Uppgift 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

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

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

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

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

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

Compute differential index and the perturbation index.

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

Uppgift 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.

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

Uppgift 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

$$\begin{aligned} m\ddot{x} &= x\lambda \\ m\ddot{y} &= y\lambda - mg \\ 0 &= x^2 + y^2 - l^2 \end{aligned}$$

where m is the pendulum mass, l length of the arm, 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.

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.

Uppgift 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?

Uppgift 2.16. Assume that the original DAE

$$F(\dot{y}, y, t) = 0 \tag{1}$$

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

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

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

$$\dot{y} = f(t, y) + g_y(t, y)\mu \tag{3a}$$

$$0 = g(t, y) \tag{3b}$$

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 (3) includes a solution with $\mu = 0$ and y that is a solution to (2).

c) For the interested. Assume further that g characterises solutions to (1), i.e., there is a solution y to (1) if and only if $g(y) = 0$. Now show that the solution from the b-exercise is the only solution to (3).

Uppgift 2.17. *Exercise removed*

Uppgift 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".

Uppgift 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.

Uppgift 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.

Uppgift 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.

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

Uppgift 2.23. Exercise 9.10 in Ascher-Petzold

Uppgift 2.24. *Exercise removed*

Uppgift 2.25. Exercise 10.4 in Ascher-Petzold

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

Uppgift 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.

Uppgift 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.

[1] `https://scikits-odes.readthedocs.io/`

[2] See documentation on `https://sundials.readthedocs.io/`

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.

Uppgift 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`.

Uppgift 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).

Uppgift 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.

Uppgift 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.

Uppgift 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.

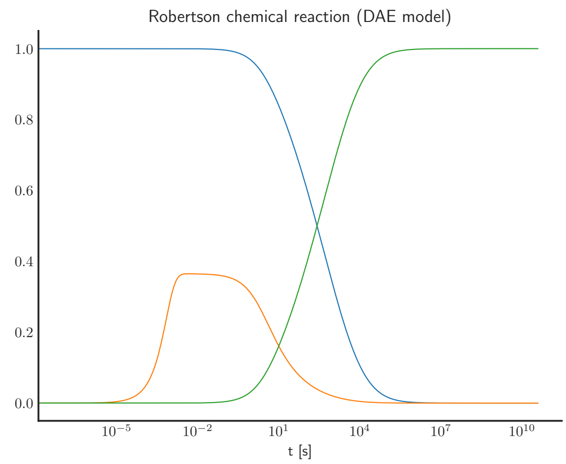


Figure 1: Solutions for the Robertson model equations.

Uppgift 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].

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`.

   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.

[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.

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