Exercises

Modelling and simulation

automation in complex systems 2022

Problem 1 (3 points)

One slow and one fast reaction are taking place in a chemical reactor. The two components c_1 and c_2 are consumed according to the kinetic equations.

$$\frac{dc_1}{dt} = -k_1 c_1 + k_{21} c_2 + b_1 u_1$$
$$\frac{dc_2}{dt} = -k_2 c_2 + b_2 u_2$$

As shown in the expressions c_1 is generated also in a reverse reaction in c_2 (indicated by the parameter k_{21}). Assume that the parameters are:

$$k_1=200,\ k_{21}=20,\ k_2=1$$

The values for b_1 and b_2 are 4 and 3. u_1 and u_2 are input signals. The system should be approximated with a difference equation on the form

$$x(t+h) \approx x(t) + hAx(t) + hBu(t)$$

where x contains the components c_1 and c_2, and A is interpreted as a consequence of this. What is the largest h that can be used if we should avoid numeric instability? (No complex calculations are needed.)

Lösningsskiss:
Egenvärdena till det diskretiserade systemet måste ligga innanför enhetscirkeln. Det diskreta systemet kan skrivas som

$$x(t+h) \approx (I + hA)\,x(t) + hBu(t) = \begin{pmatrix} 1 - hk_1 & hk_{21} \\ 0 & 1 - hk_2 \end{pmatrix} x(t) + hBu(t)$$

Vi måste alltså se till att egenvärdena för (I + hA) ligger inom enhetscirkeln (= stabilitet för diskret system)

$$-1 \le 1 - hk_i \le 1$$

vilket ger

$$0 \le hk_i \le 2$$

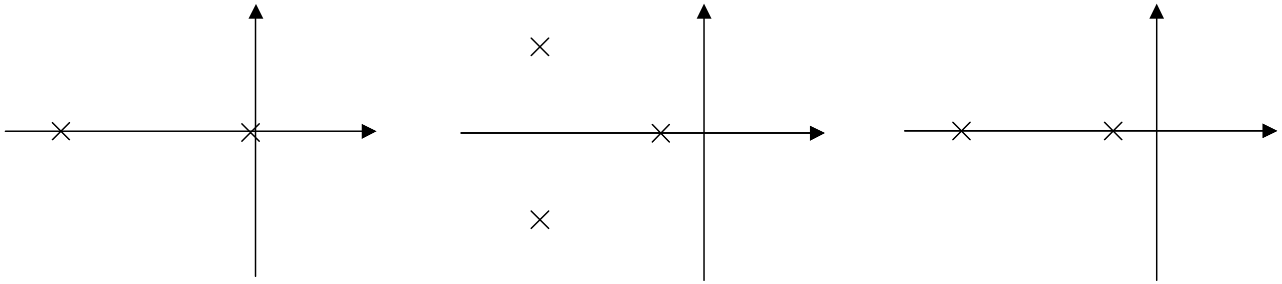
eller

$$0 \le h \le \frac{2}{k_i}$$

h måste alltså vara mindre än 2/200=0.01

Problem 1 (2 points)

a) Consider the three diagrams (a), (b) and (c) of poles of dynamical systems. Indicate if any of the systems can be considered as a stiff differential system. (1 p)



(a) (b) (c)

b) Now consider the stiff system. We wish to eliminate the fast modes and only consider the slow ones. Draw the corresponding qualitative pole diagram. (1 p)

Solution:

a) A stiff ODE has to have a large difference in time constants, or the ratio between eigenvalues is large. Thus (a) represents a stiff ODE

b) Then the fast pole is considered infinitely fast, i.e. the left pole in (a) is moved towards -infinity and only the pole close to the origin is left.

Problem 1 (5 points)
You are responsible for the development of a new modeling group (5 people full time) in your company. One of the decisions you need to make is what kind of modeling platform you are going to use. A market study has narrowed the choice down to two contenders: SuperModel and SimuFlex.

Table 1. Characteristics for two modelling/simulation platforms.

	SuperModel	SimuFlex
Library functionality	Yes	Yes, with many unit processes already developed
Object oriented	Yes	No
Index reduction	Yes	No
Solvers	DASSL (stiff solver)	DASSL, Runge-Kutta, and many more
User interface	Good with block graphics, plots and help functions, etc.	Ok with block graphics and plots but quite primitive
Optimization routine	Yes	Yes
Operating systems	Windows	Windows, Unix
Price/license and year	€ 10 000	€ 3 000

The processes you normally model are chemical processes with a wide range of time constants and many different unit operations.

a) Motivate your choice by discussing how the different features affect the choice of modeling/simulation platform *(note: there is no absolute right or wrong, it is the way you motivate your choice that matters)*. (3p)
b) Discuss other features (than those Table 1) that you would like your modeling/simulation platform to have. (2p)

Solution

a) The answer should contain:
Library function desirable, SimuFLex has the advantage since it contains developed models
Object oriented is an advantage since update and structure of model is made simple, advantage SuperModel
Index reduction: almost a must to simplify model building from libraries, advantage SuperModel
Solvers: Advantage SimuFlex since it has more solvers, both stiff and non-stiff which ensures inclusion of noise and stochastic events.
User interface: Advantage SuperModel but since the group will be full-time modelers this is not so important.
Optimization: desirable and both have it.
OS: advantage SimuFLex but no big deal since Windows dominates.
Price: Advantage SimuFlex but the difference is € 35 000 on a yearly basis with a salary cost of at least € 360 000 which means that if it is thought that the modelers will at least be 10 % more efficient using SuperModel than SimuFlex, the Supermodel has an advantage.

b) The answer could contain: data import and export off-line and in real time, linearization routines, interface to other software, possibility to import/export models to other modeling languages, report generation, etc.

Problem 5 (4 points)

The solution of a stiff system is sometimes difficult.

a) Consider the simple first order system: $dx(t)/dt = -ax,\ a > 0,\ x(0) = 1$. Motivate, using Euler backward and forward as demonstration on this system, why implicit solvers are less sensitive to long step lengths compared to explicit solvers. (2 p)

b) Unfortunately, stiff solvers cannot always be used. Discuss some important situations which are not handled well by stiff solvers. (2 p)

Solution

a) Euler backward:

$$\frac{dx(t)}{dt} \approx \frac{x(t)-x(t-h)}{h} \Rightarrow x(t) \approx \frac{1}{1+ah}x(t-h)$$

For this system to be stable

$$\left|\frac{1}{1+ah}\right| \leq 1$$

which means that

$ah \leq -2$ or $ah \geq 0$

Euler forward:

$$\frac{dx(t)}{dt} \approx \frac{x(t+h)-x(t)}{h} \Rightarrow x(t) \approx (1-ah)x(t)$$

Should be x(t-h)

For this system to be stable

$$|1-ah| \leq 1$$

which means that

$ah \leq 2$ and $ah \geq 0$

Thus, while Euler backward (implicit) has no upper limit on the step length, Euler forward (explicit) soon run into instability when the step length is increased.

b) A problem with stiff solvers is that they don't handle transient conditions well. Typical examples of these are: poor initial conditions, noise, (highly) dynamic input, discrete events.