

Lecture 1 – Simulation of differential-algebraic equations
DAE models and differential index

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Outline of the DAE module, lectures

- 1) Basic properties
 - principles
 - differences between ODE:s and DAE:s
 - differential index
- 2) Simulation methods
 - principal problems with high index problems
 - simulation of low-index problems
 - index reduction techniques
- 3) Adjoint sensitivity analysis, numerical code, and Modelica, simulation of object-oriented models
- 4) Modelica continued
 - Simulation of Modelica models, structural analysis
 - index reduction using dummy-derivatives

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Is and is not

What this part of the course is (hopefully):

- Understand what a DAE is, characteristics, and structure
- Understand why they are useful
- Understand why they are (sometimes) more difficult to simulate than an ODE
- Understand the origins of the difficulties and how to detect them
- Know how and when one can expect your favourite solver for ODE:s to work well also for DAE:s
- How to simulate models described in object oriented languages, like Modelica

What this part is not:

- detailed derivations and analysis of specific methods for simulation of DAE:s

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Outline

- *Introduction to differential-algebraic models*
- *Briefly; solution to differential-algebraic equations*
- *Illustrative example in three acts*
- *Differential index*
- *Initial conditions*
- *Simulation of DAE:s with low index*
- *Implicit and semi-explicit forms*

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ODE

A system of ordinary differential equations

$$\frac{d}{dt}x(t) = f(t, x(t)), \quad x(0) = x_0$$

where $x(t) \in \mathbb{R}^n$ and $f : \mathbb{R} \times \mathbb{R}^n \rightarrow \mathbb{R}^n$.

A mathematically, and numerically, convenient representation of a dynamical system.

DAE

A general DAE formulation instead

$$F\left(\frac{d}{dt}x(t), x(t), t\right) = 0, \quad x(0) = x_0, \dot{x}(0) = \dot{x}_0$$

where $x(t) \in \mathbb{R}^n$ and $F : \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R} \rightarrow \mathbb{R}^n$.

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Why DAE?

- Object oriented modelling
- Basic physics
- structure and numerics
- Invariants
- Simplification of an ODE, e.g., assume a physical connection is stiff instead of flexible. Can result in a DAE that is much simpler to solve than the original ODE
- Singular perturbation problems (SPP)
- Inverse problems, given $y(t)$, simulate corresponding u
- Many names: singular, implicit, descriptor, generalized state-space, non-causal, semi-state, ...

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In an ODE

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

the state is x but for a DAE

$$F(\dot{x}(t), x(t), t) = 0, \quad x(0) = x_0, \dot{x}(0) = \dot{x}_0$$

x is not exactly the state. It includes the state, but there are typically more variables than state-variables.

For that reason, it is sometimes beneficial to write a DAE as

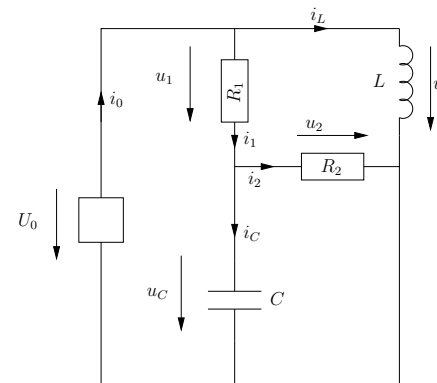
$$F(\dot{x}(t), x(t), y(t), t) = 0$$

where $x(t)$ are the dynamic variables and $y(t)$ the algebraic variables.

Again: Note that $x(t)$ not necessarily is the state here (more later).

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A simple electrical circuit



$$u_0 = f(t)$$

$$u_1 = R_1 i_1$$

$$u_2 = R_2 i_2$$

$$i_C = C \frac{du_C}{dt}$$

$$u_L = L \frac{di_L}{dt}$$

$$i_0 = i_1 + i_L$$

$$i_1 = i_2 + i_C$$

$$u_0 = u_1 + u_C$$

$$u_L = u_1 + u_2$$

$$u_C = u_2$$

10 equations in 10 unknowns

$(u_0, u_1, u_2, u_L, u_C, i_0, i_1, i_2, i_L, i_C)$

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Modelica model of the circuit

```
model Circuit
  import Modelica.Electrical.Analog.Basic.*;
  import Modelica.Electrical.Analog.Sources.*;
  Resistor R1;
  Resistor R2;
  Capacitor C;
  Inductor L;
  Ground G;
  SineVoltage src;
equation
  connect(G.p, src.n);
  connect(src.p, R1.p);
  connect(src.p, L.p);
  connect(R1.n, R2.p);
  connect(R1.n,C.p);
  connect(L.n, R2.n);
  connect(L.n, C.n);
  connect(C.n, G.p);
end Circuit;
```

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Equations generated from the Modelica model (33 eqs.)

```
R1.R * R1.i = R1.v;
R1.v = R1.p.v - R1.n.v;
0.0 = R1.p.i + R1.n.i;
R1.i = R1.p.i;
R2.R * R2.i = R2.v;
R2.v = R2.p.v - R2.n.v;
0.0 = R2.p.i + R2.n.i;
R2.i = R2.p.i;
C.i = C.C * der(C.v);
C.v = C.p.v - C.n.v;
0.0 = C.p.i + C.n.i;
C.i = C.p.i;
L.L * der(L.i) = L.v;
L.v = L.p.v - L.n.v;
0.0 = L.p.i + L.n.i;
L.i = L.p.i;
G.p.v = 0.0;

src.signalSource.y = sin();
src.v = src.signalSource.y;
src.v = src.p.v - src.n.v;
0.0 = src.p.i + src.n.i;
src.i = src.p.i;
L.n.i + R2.n.i + C.n.i + G.p.i
+ src.n.i = 0.0;
L.n.v = R2.n.v;
R2.n.v = C.n.v;
C.n.v = G.p.v;
G.p.v = src.n.v;
R1.n.i + R2.p.i + C.p.i = 0.0;
R1.n.v = R2.p.v;
R2.p.v = C.p.v;
src.p.i + R1.p.i + L.p.i = 0.0;
src.p.v = R1.p.v;
R1.p.v = L.p.v;
```

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Differential-algebraic models

A general DAE in the form

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

is kind of similar to an ODE

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

How big difference could there be?

Why not apply, e.g., an Euler-forward/backward

$$F\left(\frac{y_t - y_{t-h}}{h}, y_{t-h}, t-h\right) = 0, \quad F\left(\frac{y_t - y_{t-h}}{h}, y_t, t\right) = 0$$

and solve for y_t ?

Unfortunately, it is not that simple! (in general)(but sometimes!)

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A simple case

Assume a DAE

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

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

If you can solve for y in the second equation $y = g^{-1}(x, t)$, you'll have an ODE

$$\dot{x} = f(x, g^{-1}(x, t), t)$$

Loss of structure when transforming into an ODE (rem. the simple circuit).

As on last slide, apply Euler-backwards directly?

$$F(y_n, (y_n - y_{n-1})/h, t_n) = 0$$

But ... what happens with the mathematically well formulated model

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

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

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Differential-algebraic models

A general DAE

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

is pretty similar to an ODE

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

What is the difference? When can an ODE solver work also for DAE:s?

Answer: Sometimes

This first lecture deals with these differences, characteristics of DAE:s and when ODE methods can be directly applied

Next time more on how to simulate DAE:s and how to transform them into a form suitable for an ODE solver.

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Outline

- Introduction to differential-algebraic models
- Briefly; solution to differential-algebraic equations
- Illustrative example in three acts
- Differential index
- Initial conditions
- Simulation of DAE:s with low index
- Implicit and semi-explicit forms

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A super simple example

The DAE below can easily be transformed into an ODE

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

but for illustration, a directly applied backward Euler gives

$$\begin{aligned}\frac{x_{t+1} - x_t}{h} &= -x_{t+1} + y_{t+1} \\ 0 &= x_{t+1} + y_{t+1} - u_{t+1}\end{aligned}$$

which can be solved numerically, or analytically as

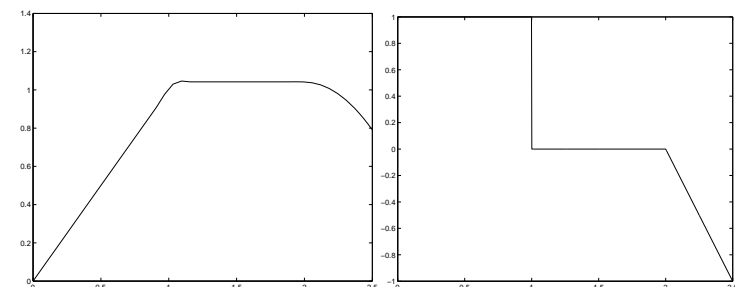
$$\begin{pmatrix} x_{t+1} \\ y_{t+1} \end{pmatrix} = \frac{1}{1+2h} \begin{pmatrix} x_t + h u_{t+1} \\ -x_t + (1+h)u_{t+1} \end{pmatrix}$$

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DAE and ODE

$$\dot{y}(t) = z(t)$$

- Integration, gives smoother solutions; differentiation gives more non-smooth solutions.
- Differentiation is "simpler" than integration analytically; numerically it is the other way around
- ODE - pure integration.
DAE - mix between integration and differentiation



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Assume a DAE

$$\begin{aligned} z_1 &= g(t) \\ \dot{z}_1 &= z_2 \end{aligned}$$

You can easily see that it is not direct to numerically derive solutions $(z_1(t), z_2(t))$ if the function $g(t)$ has discontinuities.

For ODE:s the situation is more simple

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

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Solvability/solutions

Definitions on solvability for DAE is similar to solvability for ODE:s.

Require consistency! (we will talk more about what this means)

One difference worth noting: An ODE solution is always at least once differentiable, this is not true for DAE:s and all components are not as smooth.

Consider

$$\begin{aligned} \dot{y} &= x \\ y &= v(t) \end{aligned} \Leftrightarrow \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \begin{pmatrix} \dot{x} \\ \dot{y} \end{pmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{pmatrix} x \\ y \end{pmatrix} + \begin{pmatrix} 0 \\ v(t) \end{pmatrix}$$

where $v(t) \in C^1$. Then y will be 1 time differentiable and x not differentiable.

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Different DAE formulations

Implicit ODE

$$F(y, \dot{y}, t) = 0, \quad F_{y'} \text{ invertible}$$

Linear time-invariant DAE

$$E\dot{y} = Ay, \quad E \text{ singular}$$

Semi-explicit DAE

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

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Solvability

A linear and time-invariant DAE

$$A\dot{y} + By = f(t)$$

is solvable if and only if $\lambda A + B$ has full rank for any $\lambda \in \mathbb{C}$ (think Laplace-transform) for a smooth $f(t)$.

$$(sA + B)Y(s) = F(s)$$

However, the DAE

$$\begin{bmatrix} -t & t^2 \\ -1 & t \end{bmatrix} \frac{d}{dt}y + y = 0$$

is not solvable on the interval $t > 0$ in spite of $|\lambda A(t) + B(t)| \equiv 1$.

Something to think about at home: figure out why. Hint: uniqueness.

That this is a DAE and not an (implicit) ODE is due to

$$\det A(t) \equiv 0$$

Characterizing solvability and solutions for time-variable DAE:s complex

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A semi-explicit DAE

$$\begin{aligned} \dot{x}_1 &= f_1(x_1, x_2, t) \\ 0 &= f_2(x_1, x_2, t) \end{aligned}$$

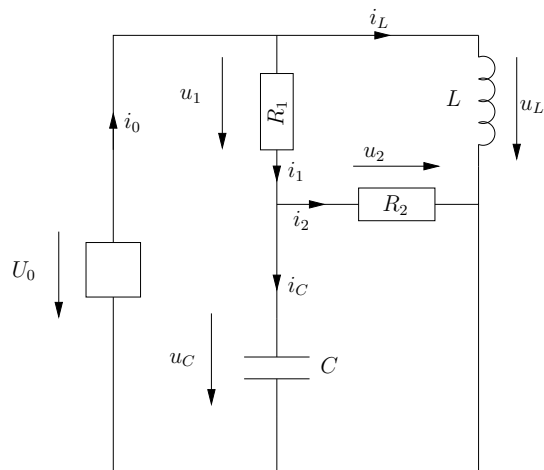
is similar to the stiff ODE (ϵ small)

$$\begin{aligned} \dot{x}_1 &= f_1(x_1, x_2, t) \\ \epsilon \dot{x}_2 &= f_2(x_1, x_2, t) \end{aligned}$$

- similarities
- differences
- when do ODE methods work for DAE:s?
- In this presentation, I will for simplicity mainly illustrate using one-step Euler-backwards

- Introduction to differential-algebraic models
- Briefly; solution to differential-algebraic equations
- Illustrative example in three acts
- Differential index
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The simple circuit model, act 1



$$x_1 = (u_C, i_L), x_2 = (u_2, i_2, u_0, u_1, u_L, i_1, i_C, i_0)$$

$$\begin{aligned} u_0 &= f(t) \\ u_1 &= R_1 i_1 \\ u_2 &= R_2 i_2 \\ i_C &= C \frac{du_C}{dt} \\ u_L &= L \frac{di_L}{dt} \\ i_0 &= i_1 + i_L \\ i_1 &= i_2 + i_C \\ u_0 &= u_1 + u_C \\ u_L &= u_1 + u_2 \\ u_C &= u_2 \end{aligned}$$

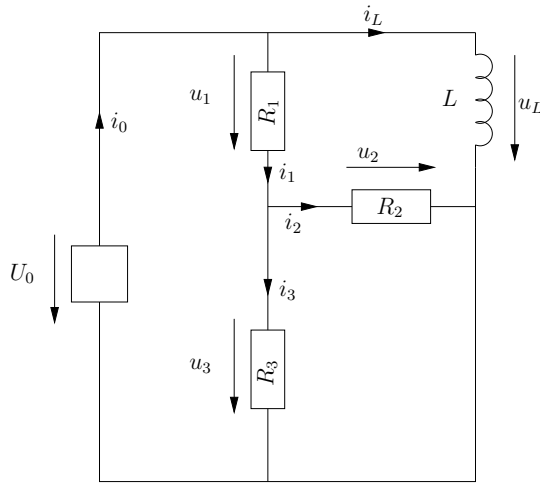
Reformulate equations into computational form

$$\begin{aligned} e_1 : u_0 &= f(t) \\ e_2 : u_1 &= R_1 i_1 \\ e_3 : u_2 &= R_2 i_2 \\ e_4 : i_C &= C \frac{du_C}{dt} \\ e_5 : u_L &= L \frac{di_L}{dt} \\ e_6 : i_0 &= i_1 + i_L \\ e_7 : i_1 &= i_2 + i_C \\ e_8 : u_0 &= u_1 + u_C \\ e_9 : u_L &= u_1 + u_2 \\ e_{10} : u_C &= u_2 \end{aligned}$$

⇒

$$\begin{aligned} e_{10} : u_2 &:= u_C \\ e_3 : i_2 &:= \frac{1}{R_2} u_2 \\ e_1 : u_0 &:= f(t) \\ e_8 : u_1 &:= u_0 - u_C \\ e_9 : u_L &:= u_1 + u_2 \\ e_2 : i_1 &:= \frac{1}{R_1} u_1 \\ e_7 : i_C &:= i_1 - i_2 \\ e_6 : i_0 &:= i_1 + i_L \\ e_4 : \frac{du_C}{dt} &= \frac{1}{C} i_C \\ e_5 : \frac{di_L}{dt} &= \frac{1}{L} u_L \end{aligned}$$

The simple circuit model, act 2 ($C \rightarrow R_3$)



$$\begin{aligned}
 u_0 &= f(t) \\
 u_1 &= R_1 i_1 \\
 u_2 &= R_2 i_2 \\
 u_3 &= R_3 i_3 \\
 u_L &= L \frac{di_L}{dt} \\
 i_0 &= i_1 + i_L \\
 i_1 &= i_2 + i_3 \\
 u_0 &= u_1 + u_3 \\
 u_L &= u_1 + u_2 \\
 u_3 &= u_2
 \end{aligned}$$

$$x_1 = i_L, x_2 = (i_3, u_2, i_2, u_0, u_1, u_L, i_1, i_C, i_0)$$

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Reformulate equations into computational form

$$\frac{di_L}{dt} = \frac{1}{L} u_L$$

$$u_0 := f(t)$$

Solve for $\{u_1, u_2, u_3, i_1, i_2, i_3\}$ in (6 unknowns, 6 equations)

$$u_1 = R_1 i_1$$

$$u_2 = R_2 i_2$$

$$u_3 = R_3 i_3$$

$$i_1 = i_2 + i_3$$

$$u_0 = u_1 + u_3$$

$$u_3 = u_2$$

$$i_0 := i_1 + i_L$$

$$u_L := u_1 + u_2$$

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Reformulate equations into computational form

$$\frac{di_L}{dt} = \frac{1}{L} u_L$$

$$u_0 := f(t)$$

Solve for $\{u_1, u_2, u_3, i_1, i_2, i_3\}$ in (6 unknowns, 6 equations)

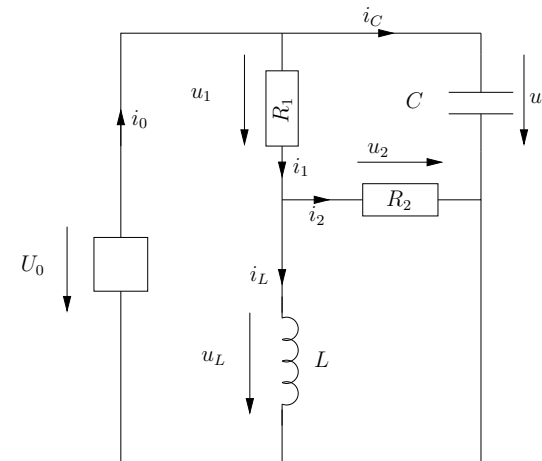
$$\begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ i_1 \\ i_2 \\ i_3 \end{pmatrix} := \frac{1}{R_1 R_2 + R_1 R_3 + R_2 R_3} \begin{pmatrix} R_1(R_2 + R_3) \\ R_2 R_3 \\ R_2 R_3 \\ R_2 + R_3 \\ R_3 \\ R_2 \end{pmatrix} u_0$$

$$i_0 := i_1 + i_L$$

$$u_L := u_1 + u_2$$

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The simple circuit model, act 3 ($C \leftrightarrow L$)



$$u_0 = f(t)$$

$$u_1 = R_1 i_1$$

$$u_2 = R_2 i_2$$

$$i_C = C \frac{du_C}{dt}$$

$$u_L = L \frac{di_L}{dt}$$

$$i_0 = i_1 + i_C$$

$$i_1 = i_2 + i_L$$

$$u_0 = u_1 + u_L$$

$$u_C = u_1 + u_2$$

$$u_L = u_2$$

$$x_1 = (u_C, i_L), x_2 = (u_2, i_2, u_0, u_1, u_L, i_1, i_C, i_0)$$

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Reformulate equations into computational form

It is not possible to, in the same way as before, to obtain a computational form. If you write the model in the form

$$\begin{aligned}\dot{x}_1 &= g(x_1, x_2) \\ 0 &= h(x_1, x_2)\end{aligned}$$

where $x_1 = (u_C, i_L)$ och $x_2 = (u_0, u_1, u_2, u_L, i_0, i_1, i_2, i_C)$. Then

$$\begin{aligned}\text{rank } h_{x_2} &= \text{rank } \frac{\partial h(x_1, x_2)}{\partial x_2} = \\ &= \text{rank } \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & -1 & -1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & -1 & -1 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & -R_1 & 0 & -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & -R_2 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \end{pmatrix} = 7 < 8\end{aligned}$$

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Transfer functions for model 1

The three models are linear, i.e., we can compute the transfer functions to show what is happening.

$$\begin{aligned}u_C &= \frac{R_2}{R_1 + R_2 + sCR_1R_2} f, & u_L &= f \\ i_L &= \frac{1}{sL} f, & i_0 &= \frac{R_1 + R_2 + s(L + CR_1R_2 + CLR_2s)}{sL(R_1 + R_2 + CR_1R_2s)} f \\ u_0 &= f, & i_1 &= \frac{1 + sCR_2}{R_1 + R_2 + sCR_1R_2} f \\ u_1 &= \frac{R_1 + sCR_1R_2}{R_1 + R_2 + sCR_1R_2} f, & i_2 &= \frac{1}{R_1 + R_2 + sCR_1R_2} f \\ u_2 &= \frac{R_2}{R_1 + R_2 + sCR_1R_2} f, & i_C &= \frac{sCR_2}{R_1 + R_2 + sCR_1R_2} f\end{aligned}$$

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Summary of the three acts

- Act 1: simple, very similar to an ODE
- Act 2: bit more difficult, took some algebra but we were OK
- Act 3: significantly more difficult

The difference between these three acts were changes in components.

Important: All three are mathematically well formed models!

A main property that separates them is: *differential index*

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Transfer functions for model 2

The three models are linear, i.e., we can compute the transfer functions to show what is happening.

$$\begin{aligned}i_L &= \frac{1}{s} f, & u_2 &= \frac{R_2R_3}{R_2R_3 + R_1(R_2 + R_3)} f \\ u_L &= f, & i_3 &= \frac{R_2}{R_2R_3 + R_1(R_2 + R_3)} f \\ i_1 &= \frac{R_2 + R_3}{R_2R_3 + R_1(R_2 + R_3)} f, & u_3 &= \frac{R_2R_3}{R_2R_3 + R_1(R_2 + R_3)} f \\ u_1 &= \frac{R_1(R_2 + R_3)}{R_2R_3 + R_1(R_2 + R_3)} f, & u_0 &= f \\ i_2 &= \frac{R_3}{R_2R_3 + R_1(R_2 + R_3)} f, & i_0 &= \frac{R_1(R_2 + R_3) + sLR_3 + R_2(R_3 + sL)}{sL(R_2R_3 + R_1(R_2 + R_3))} f\end{aligned}$$

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The three models are linear, i.e., we can compute the transfer functions to show what is happening.

$$\begin{aligned}
 u_C &= f, & u_L &= \frac{sLR_2}{R_1R_2 + sL(R_1 + R_2)} f \\
 i_L &= \frac{R_2}{R_1R_2 + sL(R_1 + R_2)} f, & i_C &= sCf \\
 u_0 &= f, & i_0 &= \frac{R_2 + sCR_2(R_1 + sL) + sL(1 + sCR_1)}{sLR_2 + R_1(R_2 + sL)} f \\
 u_1 &= \frac{R_1(R_2 + sL)}{sLR_2 + R_1(R_2 + sL)} f, & i_1 &= \frac{R_2 + sL}{sLR_2 + R_1(R_2 + sL)} f \\
 u_2 &= \frac{sLR_2}{R_1R_2 + sL(R_1 + R_2)} f, & i_2 &= \frac{sL}{R_1R_2 + sL(R_1 + R_2)} f
 \end{aligned}$$

Index, one example

A linear example that illustrates an important difference between a DAE and an ODE

$$\begin{aligned}
 \dot{x}_1 + x_2 + x_3 &= f_1 & \dot{x}_1 &= \dot{f}_2 - \ddot{f}_3 \\
 \dot{x}_2 + x_1 &= f_2 & \Rightarrow \dot{x}_2 &= -x_1 + f_2 \\
 x_2 &= f_3 & \dot{x}_3 &= x_1 - f_2 - \ddot{f}_2 + \dot{f}_1 - f_3^{(3)}
 \end{aligned}$$

- What are allowed initial conditions? For an ODE they are free
- Not the case for a DAE, there might be "hidden" algebraic constraints

$$\begin{aligned}
 x_1 &= f_2 - \dot{f}_3 \\
 x_2 &= f_3 \\
 x_3 &= f_1 - \dot{f}_2 - f_3 + \ddot{f}_3
 \end{aligned}$$

Something called (differential) *index* characterize DAE:s

- Introduction to differential-algebraic models
- Briefly; solution to differential-algebraic equations
- Illustrative example in three acts
- Differential index
- Initial conditions
- Simulation of DAE:s with low index
- Implicit and semi-explicit forms

(Differential-) Index

A DAE is almost an ODE, just need some differentiation

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

Differentiate the second equation

$$0 = g_x \dot{x} + g_y \dot{y} = g_x f + g_y \dot{y}$$

If g_y^{-1} exists we can rewrite as

$$\begin{aligned}
 \dot{x} &= f(x, y) \\
 \dot{y} &= -g_y^{-1} g_x f
 \end{aligned}$$

Comments: solutions sets, equivalence.

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

Definition

The minimum number of times the DAE has to be differentiated with respect to t to be able to determine \dot{y} as a function of t and y is called the (differential-) index of the DAE.

- index might be solution dependent, uniform index
- There are several types of index, the above is called differential index.
- Perturbation index
- variants of the above (see paper)

Anyhow: index is a measure how far from an ODE the DAE is.

Sufficient condition for index

$$\begin{aligned}
 F(y, \dot{y}) &= 0 \\
 \frac{d}{dt} F(y, \dot{y}) &= 0 \\
 &\vdots \\
 \frac{d^{j-1}}{dt^{j-1}} F(y, \dot{y}) &= 0
 \end{aligned}$$

which can be collected to $\mathbf{F}_j(t, y, \mathbf{y}_j) = 0$. Algebraically $\mathbf{F}_j(t, y, \mathbf{y}_j) = 0$ consists of n_j equations in $n_j + n$ unknown variables.

A sufficient condition for \dot{y} is a unique function (locally) if t and y is that

$$\frac{\partial \mathbf{F}_j}{\partial \mathbf{y}_j}$$

is 1-full column rank

DAE:n has index no larger than v if $\partial \mathbf{F}_{v+1} / \partial \mathbf{y}_{v+1}$ has 1-full rank and $\mathbf{F}_{v+1} = 0$ is consistent.

$$E\dot{x} = Jx + Ku$$

Then there exists a non-singular matrix P and a change of variables $z = Qx$ such that

$$\begin{pmatrix} I & 0 \\ 0 & N \end{pmatrix} \begin{pmatrix} \dot{z}_1 \\ \dot{z}_2 \end{pmatrix} = \begin{pmatrix} A & 0 \\ 0 & I \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} + \begin{pmatrix} B \\ D \end{pmatrix} u$$

Where matrix N is nilpotent, i.e., there is an integer m such that $N^i \neq 0$ for $i < m$ and $N^m = 0$.

A simple algebra exercise gives that the solution to the DAE is

$$\begin{aligned}
 \dot{z}_1 &= Az_1 + Bu \\
 z_2 &= - \sum_{i=0}^{m-1} N^i Du^{(i)}
 \end{aligned}$$

How is the degree of nilpotency m related to the index? Transfer function, how does it relate to the degrees of numerators and denominators?

1-full rank

When has the equation

$$(A_1 \quad A_2) \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = b$$

a unique solution for x_1 ?

Unique x_1 solution if and only if

$$\text{rang } A = n_1 + \text{rang } A_2$$

Example:

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = b$$

Now, back to the last slide, what does 1-full rank mean there?

- ODE

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

- Hessenberg index 1/semi-explicit index 1

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

$$0 = g(x, z, t), \quad g_z \text{ nonsingular for all } t$$

- Hessenberg index 2

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

$$0 = g(x, t), \quad g_x f_z \text{ nonsingular for all } t$$

Our index 2 equation, all algebraic variables are “index 2” variables.

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Outline

- *Introduction to differential-algebraic models*
- *Briefly; solution to differential-algebraic equations*
- *Illustrative example in three acts*
- *Differential index*
- *Initial conditions*
- *Simulation of DAE:s with low index*
- *Implicit and semi-explicit forms*

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The remainder of the lecture will introduce some important differences between ODE:s and DAE:s from a simulation perspective. We will come back to these in detail in upcoming lectures.

1 Initial conditions

2a Simulation of equations with index 0 and 1

2b Simulation of equations with index ≥ 2

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Bullet 1: Initial conditions

For the DAE

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

is it sufficient that the initial conditions $y(0)$ and $\dot{y}(0)$ satisfies

$$F(0, y(0), \dot{y}(0)) = 0?$$

Remember the model that had no degrees of freedom

$$\dot{x}_1 + x_2 + x_3 = f_1$$

$$\dot{x}_2 + x_1 = f_2$$

$$x_2 = f_3$$

- Index and “hidden” conditions
- Methods to determine consistent initial conditions
- Pantelides algorithm

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Initial conditions, cont.

What degrees of freedom do we have for the initial condition? In the equations

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

there is no freedom at all and the solution was uniquely determined (in the class of smooth functions) directly by the equations.

If we have m equations/variables, it holds that the degrees of freedom l that $0 \leq l \leq m$ and it is not trivial to find *consistent* initial conditions.

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

Pantelides algorithm

We will come back to a possible solution later

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Bullet 2a: Index 1 "as easy" as ODE

Will come back to this, but the basic principle is easily illustrated.

Assume a semi-explicit DAE in the form

$$\begin{aligned}\dot{x}_1 &= f_1(x_1, x_2, t) \\ 0 &= f_2(x_1, x_2, t)\end{aligned}$$

with index 1. Then,

$$\frac{\partial f_2}{\partial x_2}$$

has full column rank and it exists a (local) inverse w.r.t. x_2 .

The algebraic variable can then be inserted in the dynamic equation resulting in an ODE which can be solved using any standard ODE method.

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Outline

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Bullet 2a: Index 1 "as easy" as ODE, cont.

Consider an implicit index 1 DAE

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

Apply a basic implicit Euler backward

$$F\left(\frac{x_t - x_{t-1}}{h_t}, x_t, t\right) = 0$$

and solve numerically for x_t . Index 1 property ensures that a solution exists.

Important note: Procedure *no different* than implicit Euler for ODE:s.

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One conclusion: BDF and other typical implicit solvers will work approximately the same for DAE:s of index 1 as for ODE:s.

There are practical differences though, see Hairer/Wanner and the following papers for further details

- Petzold, "Differential/algebraic equations are not ODEs"
- Brenan, Campbell and Petzold Petzold, "Numerical Solution of Initial-Value Problems in Differential Algebraic Equations"

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Equations you, generally, can solve using basic ODE methodology is

- Index 1 DAE:s (more to follow)
- Linear DAE:s with constant coefficients of any index (kind of)

$$A\dot{y} + By = f$$

Will not pursue this here. More details in "ODE methods for the solution of differential/algebraic systems".

- For index > 1, direct ODE methodology does not work at all. We need new techniques and index reduction is one possibility we will discuss a lot in upcoming lectures.

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Implicit and semi-explicit forms

A fully implicit DAE

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

can always be rewritten as a semi-explicit DAE by introducing a new variable x' (algebraic, should not be confused with \dot{x})

$$\begin{aligned}\dot{x} &= x' \\ F(x', x) &= 0\end{aligned}$$

Q

Does this mean that we can forget about implicit forms and focus on semi-explicit?

A

No, not really.

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An implicit example

Consider the implicit index-1 DAE

$$e_1 : \dot{x}_1 + \dot{x}_2 = u_1$$

$$e_2 : x_1 - x_2 = u_2$$

From equations (e_1, e_2, \dot{e}_2) we can solve for the highest derivatives.

Transform the DAE into a semi-explicit DAE by introducing x'_1 and x'_2

$$e_1 : x'_1 + x'_2 = u_1$$

$$e_2 : x_1 - x_2 = u_2$$

$$e_3 : \frac{d}{dt}x_1 = x'_1$$

$$e_4 : \frac{d}{dt}x_2 = x'_2$$

Q

What is the index of this one?

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An implicit example, cont'd

Turns out that

$$e_1 : x'_1 + x'_2 = u_1$$

$$e_2 : x_1 - x_2 = u_2$$

$$e_3 : \frac{d}{dt}x_1 = x'_1$$

$$e_4 : \frac{d}{dt}x_2 = x'_2$$

has index 2.

Assignment: Verify that you need $(e_1, \dot{e}_1, e_2, \dot{e}_2, e_3, \dot{e}_3, e_4, \dot{e}_4, \ddot{e}_4)$ to be able to solve for highest derivatives.

Rule of thumb

Going from fully implicit to semi-explicit increases index by 1

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Lecture 1 – Simulation of differential-algebraic equations DAE models and differential index

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