

Lecture 3
Simulation of differential-algebraic equations

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DASSL

- DASSL is an *implementation/code* to solve systems of differential-algebraic equations of index 0 or 1
- Why am I talking about DASSL?
- Basis principle, one-step and multiple step
- A little on what it is good at
- Some principles on details
- Is available online
- Has been developed in different versions DASRT/DASKR/DASPK/...
- DASPK v3.1 latest version (v2.0 free to download)

Outline

- *DASSL - an overview*
- *Modelica*
 - *Snapshot of the language*
 - *Simulation of Modelica models*
 - *Algebraic and dynamical loops/tearing*
 - *Event functions*
- *Structural index - introduction and definition*

Basic principle

For a DAE in the form

$$\begin{aligned}F(t, y, y') &= 0 \\ y(t_0) &= y_0 \\ y'(t_0) &= y'_0\end{aligned}$$

the DASSL basic principle is not unique, replace the derivative for a difference approximation and solve the resulting system of equations with a Newton method.

Properties of the DASSL implementation:

- Variable step-length
- Variable order
- Efficient implementation, for example measured in the number of evaluations of the function F .

DASSL - first order step

Replace the derivative with a first order BDF, then

$$F(t_{n+1}, y_{n+1}, (y_{n+1} - y_n)/h_{n+1}) = 0$$

A direct Newton method to solve for y_{n+1} then becomes

$$y_{n+1}^{(m+1)} = y_{n+1}^{(m)} - \left(F_y + \frac{1}{h_{n+1}} F_{y'} \right)^{-1} F(t_{n+1}, y_{n+1}^{(m)}, (y_{n+1}^{(m)} - y_n)/h_{n+1})$$

where F_y and $F_{y'}$ is evaluated in $y_{n+1}^{(m)}$.

With a good stop condition on the iterations so this is approximately how it works. I will now briefly look at:

- higher order algorithm
- strategies for choice of order, step-length
- stop conditions for the Newton iterations

DASSL - a step of order k , cont'd.

There are y_{n-i} that approximates $y(t_{n-i})$ for $i = 0, \dots, k$. Wanted: y_{n+1} .

Prediction polynomial - $\omega_{n+1}^P(t)$, order k

$$\omega_{n+1}^P(t_{n-i}) = y_{n-i}, \quad i = 0, \dots, k$$

Prediction for y_{n+1} and y'_{n+1} is then given by

$$\begin{aligned} y_{n+1}^{(0)} &= \omega_{n+1}^P(t_{n+1}) \\ y'_{n+1}^{(0)} &= \omega'_{n+1}^P(t_{n+1}) \end{aligned}$$

Correction polynomial - $\omega_{n+1}^C(t)$, order k

$$\omega_{n+1}^C(t_{n+1} - ih_{n+1}) = \omega_{n+1}^P(t_{n+1} - ih_{n+1}), \quad i = 1, \dots, k$$

$$F(t_{n+1}, \omega_{n+1}^C(t_{n+1}), \omega'_{n+1}^C(t_{n+1})) = 0$$

i.e. $y_{n+1} = \omega_{n+1}^C(t_{n+1})$

Note: fix vs. variable step length.

DASSL - a step of order k

- 1 Compute a prediction polynomial $\omega^P(t)$ based on k previous time-points
- 2 Compute a correction polynomial $\omega^C(t)$, equal $\omega^P(t)$ on k equidistant (h_{n+1}) previous time-steps
- 3 Predict next time-step using prediction polynomial

DASSL - a step of order k , cont.

Skips a lot of notation and rather straightforward algebra,

Equations to be solved

$$\begin{aligned} \omega_{n+1}^C(t_{n+1} - ih_{n+1}) &= \omega_{n+1}^P(t_{n+1} - ih_{n+1}), \quad i = 1, \dots, k \\ F(t_{n+1}, \omega_{n+1}^C(t_{n+1}), \omega'_{n+1}^C(t_{n+1})) &= 0 \end{aligned}$$

can be written as the solution to the nonlinear equation

$$F(t_{n+1}, y_{n+1}, \alpha y_{n+1} + \beta) = 0$$

i.e. the same form that we had in the one step case (not so surprising)

$$F(t_{n+1}, y_{n+1}, (y_{n+1} - y_n)/h_{n+1}) = 0$$

but the constants α and β depends on the step length h_{n+1} , order k and y_{n-i} in a non-trivial way. Exactly how is not of main importance here.

Now solve

$$F(t, y, \alpha y + \beta) = 0$$

by

$$y^{(m+1)} = y^{(m)} - c \underbrace{(\alpha F_{y'} + F_y)^{-1}}_{\text{iteration matrix } G} F(t, y^{(m)}, \alpha y^{(m)} + \beta)$$

Each iteration is solved by $G = LU$ factorization. With $\delta^{(m)} = y^{(m+1)} - y^{(m)}$ and $r^{(m)} = cF$ then

$$Ls^{(m)} = r^{(m)}$$

$$U\delta^{(m)} = s^{(m)}$$

DASSL - stop conditions in Newton iterations

An important aspect is when to stop the Newton iterations. To directly look at $\|y^{(m+1)} - y^{(m)}\|$ is not always a good idea. Instead, define

$$d^{(m)} = \frac{\|y^{(m+1)} - y^*\|}{\|y^{(m)} - y^*\|}$$

and assume that we know an upper bound on $d^{(m)} < \rho$, direct usage of the triangle inequality gives a stop condition

$$\|y^{(m+1)} - y^*\| \leq \frac{\rho}{1 - \rho} \|y^{(m+1)} - y^{(m)}\|$$

Use, for example, the largest

$$\frac{\|y^{(m+1)} - y^{(m)}\|}{\|y^{(m)} - y^{(m-1)}\|}$$

observed so far as an estimate on ρ .

In DASSL, max 4 iterations! If $\rho > 0.9$, compute a new G . If the iteration still not converges (4 steps), reduce step length by 1/4. After 10 tries, abort.

To make an iteration, compute G and LU factorize.

$$y^{(m+1)} = y^{(m)} - cG^{-1}F(t, y^{(m)}, \alpha y^{(m)} + \beta)$$

Why is this important? Mostly to state that computation of G and the corresponding LU factorization is a main part (even dominant for large models) of the computational burden for one integration step.

If $F_{y'}$ and F_y varies slowly over the solution, reuse old already computed \hat{G} . As long as \hat{G} is sufficiently close to G we can expect on convergence.

Supervise convergence speed and compute a new G only when convergence speed is not satisfactory.

DASSL - order selection and step length

Order selection

Estimates, through some clever algebra, error of $y_{n+1} - y(t_{n+1})$ as a function of different orders

c_1 = error term of order $k - 1$

c_2 = error term of order k

c_3 = error term of order $k + 1$

c_4 = error term of order $k + 2$

The basic principle is that $c_1 > c_2 > c_3 > c_4$. Otherwise, lower the order to be more secure.

Step length

After a new order is chosen, estimate the error as if the latest k steps are taken with the same step length such that the error estimate fulfills the tolerance condition

$$ERR = M \|y_{n+1} - y_{n+1}^{(0)}\| \leq 1$$

Automatic Differentiation

An analytical expression for the iteration matrix

$$G = \frac{\partial}{\partial y_{n+1}} F(t_{n+1}, y_{n+1}, (y_{n+1} - y_n)/h_{n+1}) = F_y + F_{y'}/h_{n+1}$$

is good for efficiency and accuracy.

How do we get G ?

- Encode not only F but also G and send to DASSL.
- Difference approximations of the derivative.

Automatic Differentiation/Algorithm differentiation

- Automatically separate function F into elementary operations.
- The derivative by direct application of the chain rule
- C/C++/Fortran/Java/..., mature field with many tools
- DASPak has direct support for automatic differentiation
- Community website <http://www.autodiff.org/>
- Forward & backward operation (backprop in machine learning)

Modelica

Modelica

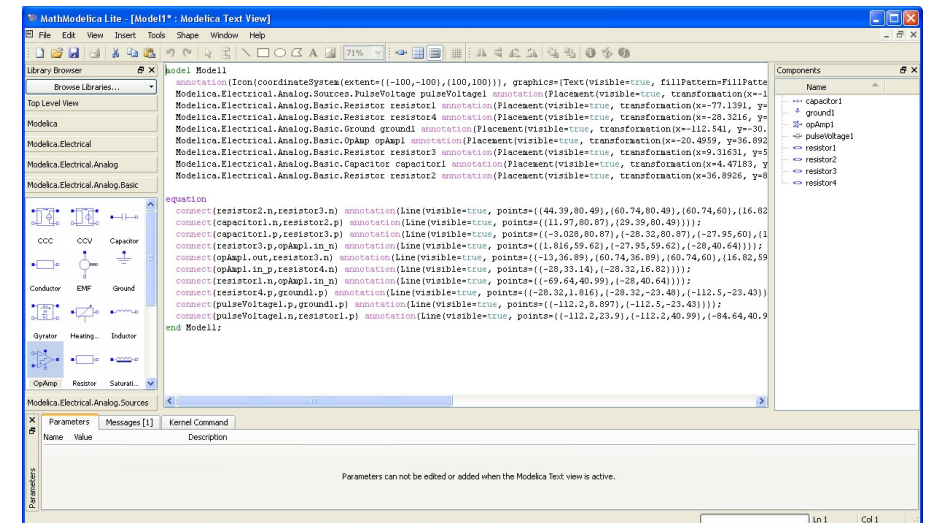
Modelica is a language for specifying mathematical models for a large class of systems.

- equation based and non-causal, equations not assignments
- declarative, not an algorithm (like Simulink)
- object oriented
- multi domain
- continuous and discrete (not time) models, hybrid systems
- mainly developed for simulation
- high index problem more “more common than not”
- Language resources <http://modelica.org/>

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- Structural index - introduction and definition

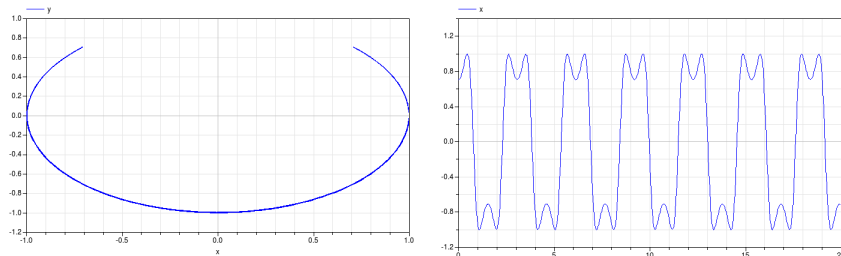
Commercial model editors



Modelica standard library v3.2.2 (2016-04-03)

- Blocks** Continuous, discrete and logical input/output blocks (Continuous, Discrete, Logical, Math, Nonlinear, Routing, Sources, Tables)
- Constants** Mathematical and physical constants (pi, eps, h, ...)
- Electrical** Electric and electronic components (Analog, Digital, Machines, MultiPhase)
- Icons** Icon definitions Math Mathematical functions for scalars and matrices (such as sin, cos, solve, eigenValues, singular values)
- Mechanics** Mechanical components (Rotational, Translational, MultiBody)
- Media** Media models for liquids and gases (about 1250 media, including high precision water model)
- SIunits** SI-unit type definitions (such as Voltage, Torque)
- StateGraph** Hierarchical state machines (similar power as Statecharts)
- Thermal** Thermal components (FluidHeatFlow, HeatTransfer)
- Utilities** Utility functions especially for scripting (Files, Streams, Strings, System)

Simulation result – pendulum example



At the end of this course, you'll understand why the solution misbehaves like this.

Modelica example

Pendulum model of index 3

```
model Pendulum
  import [Skipped some imports]
  parameter Real phi0 = 45*pi/180;
  parameter Real L = 1, M = 1, g=9.82;

  Real x(start=L*cos(phi0)), dx(start=0);
  Real y(start=L*sin(phi0)), dy(start=0);
  Real lambda;
equation
  der(x) = dx;
  der(y) = dy;
  M*der(dx) = lambda*x;
  M*der(dy) = lambda*y-M*g;
  0 = x*x+y*y-L*L;
end Pendulum;
```

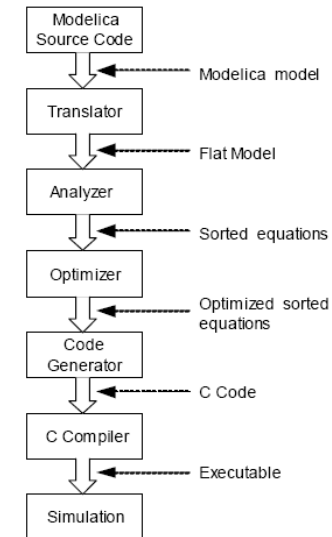
Example with components from the standard library

Electrical circuit

```
class SimpleCircuit
  Resistor R1(R=10), R2(R=100);
  Capacitor C(C=0.01);
  Inductor L(L=0.1);
  VsourceAC AC;
  Ground G;
equation
  connect(AC.p, R1.p);
  connect(R1.n, C.p);
  connect(C.n, AC.n);
  connect(R1.p, R2.p);
  connect(R2.n, L.p);
  connect(L.n, C.n);
  connect(AC.n, G.P);
end SimpleCircuit;
```

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The path from a Modelica model to C-code looks something like this



Representation of a general DAE

A DAE has the following components

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

$x(t)$ vector of dynamic variables

$y(t)$ vector of static variables

$u(t)$ vector of given input/known signals

θ model parameters

$c(t)$ Event functions (more about these later)

I have skipped discrete variables, see book by P. Fritzons for more details.

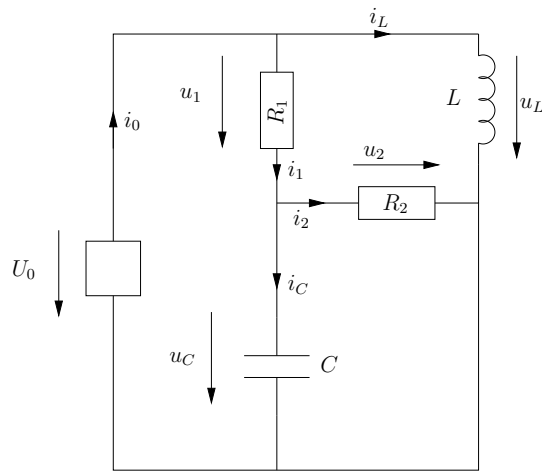
Translator

- Parse the model file into an AST (Abstract Syntax Tree), a computer representation of the model
- Flatten the model, i.e., resolve all inheritance and component equations
- Change if-expressions to if-equations

```
if (a>5.0)
  val = 10.0;
else
  val = 20.0;
end if;
```
- Change dot-notation to underbar (" \cdot " \rightarrow " $_$ ")

$$R1.p.i \rightarrow R1_p_i$$

Now we have the flattened model



```

model Circuit
  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;

```

Flattened model

```

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.p.v - src.n.v;
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;

```

Analyzer and optimizer

Main objectives

- 1 Transform the model to state space form (or index 1) through index reduction
- 2 Optimize the computation of the model (evaluation of F)

Steps

- Basic model analysis, find simple, e.g., linear, equation
- Simplify model by eliminating trivial (and some simple) equations by algebraic manipulation
- Compute index and perform index reduction
- Find algebraic loops (strong components) with respect to the most differentiated variables

Analyzer and optimizer, cont.

Three main problems I will not address further today

- compute index
- perform index reduction and transform the model equations from a high index formulation to ODE/index-1 DAE
- find consistent initial values

All these are strongly connected and the main content of the next lecture.

From now on, it is assumed the model is index 1.

Simplified; it is assumed that the model is in the form

$$F(x', x, t) = 0, \quad c_i(t), \quad i = 1, \dots, n_c$$

- The residual function $F(x', x, t)$ and event functions can now be sent directly to the numerical DAE solver (DASSL/DASRT/DASKR/...)
- This is not exactly how OpenModelica operates, it goes one step further and takes the model into an ODE. More on this later.
- On the course web site there is a (rather incomplete) document that shows by example how OpenModelica transfers a simple model to C-code. Recommended for the interested.

Flat model with index 1 to ODE, OpenModelica

$$F(x', x, y, t) = 0$$

If the model is low index, then it is possible to solve for the highest differentiated variables x' and y as

$$\begin{aligned} x' &= f(t, x, y) \\ y &= G(t, x) \end{aligned}$$

To generate code there is a need to find a computational scheme for the functions f and G , preferably as a pure substitution chain.

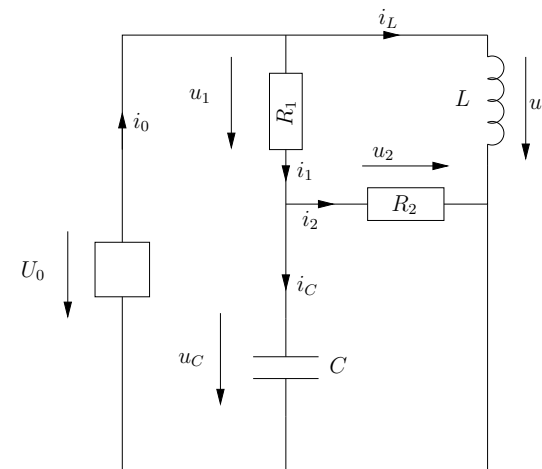
After that, OpenModelica simulates (with DASSL) x as

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

Remember the initial examples from the first DAE lecture, substitution chains not always possible.

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Remember simple circuit model



$$x_1 = (u_c, i_L), \quad x_2 = (u_2, i_2, u_0, u_1, u_L, \dot{i}_1, \dot{i}_C, \dot{i}_0)$$

$$\begin{aligned} e_1 &: u_0 = f(t) \\ e_2 &: u_1 = R_1 i_1 \\ e_3 &: u_2 = R_2 i_2 \\ e_4 &: i_C = C \frac{du_c}{dt} \\ e_5 &: u_L = L \frac{di_L}{dt} \\ e_6 &: \dot{i}_0 = i_1 + i_L \\ e_7 &: \dot{i}_1 = i_2 + i_C \\ e_8 &: u_0 = u_1 + u_C \\ e_9 &: u_L = u_1 + u_2 \\ e_{10} &: u_C = u_2 \end{aligned}$$

Algebraic and dynamic loops

An algebraic loop can, in its simplest form, look like

$$\begin{aligned}x_1 &= f_1(x_2) \\x_2 &= f_2(x_1)\end{aligned}$$

Here x_1 and x_2 has to be computed simultaneously using either analytical tools (not feasible in the general case) or a numerical solver. Two simple numerical methods are

- Newton iterations
- Fix point iterations

Tearing

For a general algebraic loop

$$f_i(x_1, \dots, x_n) = 0, \quad i = 1, \dots, n$$

it is generally a difficult problem to choose how to rewrite as a fix point iteration on the best way; requires knowledge about the analytical expressions, inversion properties, contraction properties etc.

In the course literature, there is a structural method for choosing tearing variables

Good choice of tearing variables is often based on physical insight and therefore it is possible to introduce such information in the model definition (not discussed further here)

Tearing

With fix point iterations (and contraction conditions) the loop

$$\begin{aligned}x_1 &= f_1(x_2) \\x_2 &= f_2(x_1)\end{aligned}$$

can be solved through the iteration

```
NEWx2 = INITx2
repeat
  x2 := NEWx2
  x1 := f1(x2)
  NEWx2 := f2(x1)
until converged(NEWx2-x2)
```

Here it was “clear” where to *tear* the loop due to the given causality. For a general loop

$$f_i(x_1, \dots, x_n) = 0, \quad i = 1, \dots, n$$

this is not as clear.

Tearing, example 1

Below is a system of equations, which is an algebraic loop.

$$\begin{aligned}c : & & u_3 &= R_3 i_3 \\d : & & u_1 &= u_0 - u_3 \\a : & & i_1 &= 1/R_1 u_1 \\e : & & u_2 &= u_3 \\b : & & i_2 &= 1/R_2 u_2 \\f : & & i_1 - i_2 - i_3 &= 0\end{aligned}$$

Choose i_3 as tearing variable in equation f .

Then we get an equation to solve numerically

$$f : g(i_3, i_1(i_3), i_2(i_3)) = \tilde{g}(i_3) = 0$$

For example by Newton iterations

$$i_3^{(k+1)} = i_3^{(k)} - \tilde{g}'(i_3^{(k)})^{-1} \tilde{g}(i_3^{(k)})$$

Tearing, example 2

Instead, choose i_1 in equation a as a tearing variable

$$\begin{aligned} a : & \quad u_1 - R_1 i_1 = 0 \\ b : & \quad u_2 - R_2 i_2 = 0 \\ c : & \quad u_3 - R_3 i_3 = 0 \\ d : & \quad u_1 + u_3 - u_0 = 0 \\ e : & \quad u_2 - u_3 = 0 \\ f : & \quad i_1 - i_2 - i_3 = 0 \end{aligned}$$

Then we do not get anywhere. No new variable can be computed even though i_1 is assumed known.

Tearing, conclusions

- Tearing is used to tear algebraic loops apart into smaller parts
- The objective is to rewrite a large system of equations into smaller systems of equations that can be solved numerically
- Choice of tearing variables and equations is complex, NP-hard to find a minimal set of tearing variables.

A simple heuristic

- 1 Choose an equation e that contains the most unknown variables
- 2 In equation e , for each variable v compute how many variables that can be computed by a direct substitution chain of v is assumed known.
- 3 Choose the variable that maximizes the number of new computed variables as a tearing variable and e as iteration equation.

Tearing, example 3

Now, choose a tearing variable, u_2 in equation b , then it all clears out

$$\begin{aligned} e : & \quad u_3 = u_2 \\ c : & \quad i_3 = 1/R_3 u_3 \\ d : & \quad u_1 = u_0 - u_3 \\ f : & \quad i_2 = i_1 - i_3 \end{aligned}$$

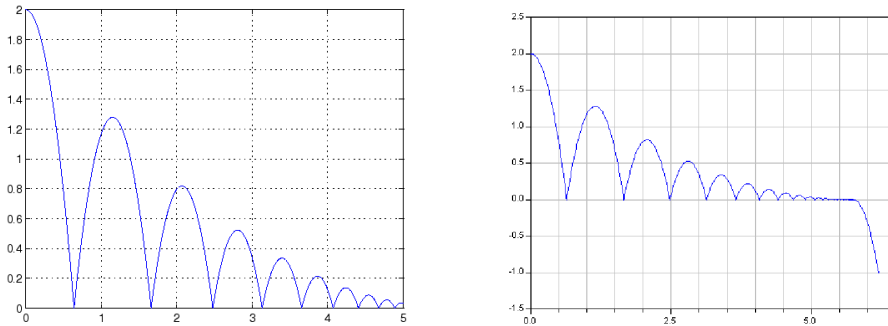
and the following two equations has to be solved, for example by Newton iterations for variables i_1 and u_2

$$\begin{aligned} a : & \quad u_1 - R_1 i_1 = 0 \\ b : & \quad u_2 - R_2 i_2 = 0 \end{aligned}$$

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Event/crossing functions



- Here it is clear that the zero-crossing is very important for the ball not to fall through the floor
- Important in many simulation problems that certain bounds not are crossed

Automatic generation of event functions

if-expression

```
y = if x>z then a else b;
```

if-equation

```
if x>z then
  y=a
else
  y=b
end if;
```

- Conditional expressions are translated into if-equations
- direct to generate event functions. In the example above we get

$$c_i(\text{vars}) = x - z$$

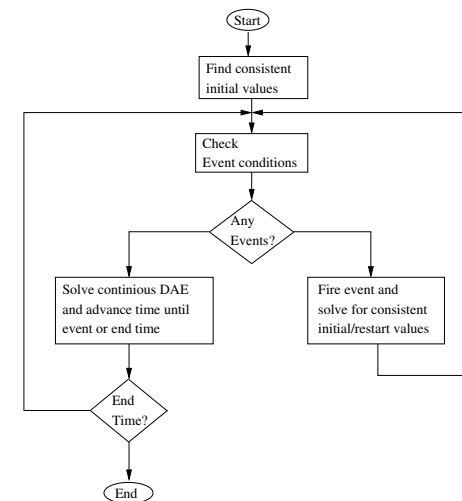
- Here it is clear that the modelling can help the compiler to, by itself, figure out important conditions that has to be monitored.

Event/crossing functions

Modelica

```
class BouncingBall
  constant Real g=10
  parameter Real c=0.9, radius=0.1
  Real y(start=1), velocity(start=0), x(start=1)
equation
  der(x)=0;
  der(y) = velocity;
  der(velocity)=-g;
  when height<=radius then
    reinit(velocity,-c*pre(velocity))
  end when;
end BouncingBall;
```

Event/crossing functions

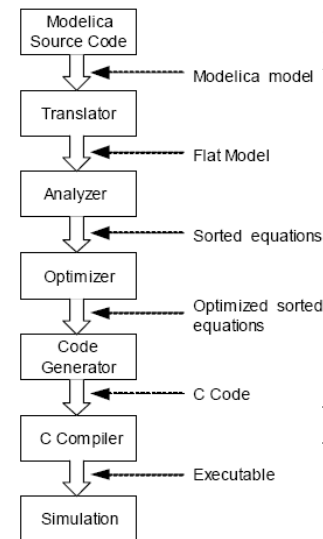


- Fits well into the framework of DASSL and other standard solvers are structured

- You may run into problems of the solution has infinitely many event detections
- Is sufficient that they are dense enough with respect to the numerical precision for this to be a problem
- For the bouncing ball, this of course happens after a while
- No general solution, logic has to be built into the model to handle the case where the ball starts to roll rather than bounce.

Reduce to ODE or DAE with index 1?

- DASSL, standard solver in Dymola/OpenModelica, why?
 - well written code, efficient
 - is it really the best?
- Implicit solvers not efficient for non-stiff problems
- Large model often exhibits stiff dynamics
- Dymola/Openmodelica reduces to ODE, is not DAE index 1 sufficient?
- "Cellier vs. Petzold"



Steps I have not yet addressed concerns the Analyzer/Optimizer steps

Earlier discussion has assumed an ODE (or low index) form

Remains to:

- compute index
- reduce index
- determine consistent initial conditions

Common, and general, solution to the above three problems has a lot in common and will be the main theme for next lecture.

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Structural index

An important step in the procedure to transfer the model to C code is to perform index reduction. Index reduction requires that you know the index of the model. As we know it is a difficult problem in general to determine index; a method based on model structure is typically used.

Structural index can be defined in many ways. One way, for the DAE

$$A\dot{x} + Bx = 0$$

the structural index is the real index the DAE has for *almost all* A and B with the same structure.

- simple to generalize to non-linear systems
- can be computed with Pantelides algorithm, which will be used also for other purposes

Structural index - introductory example

Let $x = (x_1, x_2, x_3) \in \mathbb{R}^3$

$\dot{x}_1 = x_1 + x_2 + x_3 + u$		\dot{x}_1	x_2	x_3
$0 = -2x_1 + x_2$	e_1	X	X	X
$0 = x_1 + x_2 + u$	e_2		X	
	e_3		X	

From the table on the right we see that *regardless* of which coefficient we have for the variables, the DAE has index > 1 . The DAE has a unique solution since

$$|\lambda E - A| = \lambda + 3 \neq 0, \quad (x_1, x_2, x_3) = \left(-\frac{1}{3}u, -\frac{2}{3}u, -\frac{1}{3}\dot{u}\right)$$

Turns out you can determine structural index only by looking at the tables on the right. This is also direct to automatically do for large scale models in general purpose simulation environments.

Structural index - introductory example

Let $x = (x_1, x_2) \in \mathbb{R}^2$ and consider the index 1 model

$\dot{x}_1 = x_1 + x_2 + u$		\dot{x}_1	x_2
$0 = -2x_1 + x_2$	e_1	X	X
	e_2		X

The highest differentiated variables are $x_{hd} = (\dot{x}_1, x_2)$

DAE has index 1 for almost all coefficients in front of the x variables, only when coefficients in front of \dot{x}_1 in e_1 or x_2 in e_2 is 0 we have a problem.

Conclusions: we can from the table on the right determine that this model has (structural-)index 1.

$$F(\dot{x}_1, x_1, x_2) = 0$$

has low index (locally) if

$$\frac{\partial F(\dot{x}_1, x_1, x_2)}{\partial x_{hd}} \bigg|_{\dot{x}_1 = \dot{x}_1^*, x_1 = x_1^*, x_2 = x_2^*}$$

has full rank

Structural index

Let ν and ν_{str} be the index and the structural index respectively for

$$F(t, y', y) = 0$$

What holds?

$$\begin{aligned} \nu &< \nu_{str}, & \nu &\leq \nu_{str} \\ \nu_{str} &< \nu, & \nu_{str} &\leq \nu \end{aligned}$$

What is the consequence of this for a method that relies on a structural algorithm for index reduction?

Consider the linear DAE

$$\begin{bmatrix} 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \dot{x} + x = 0$$

This DAE can be shown to have index 1 but structural index larger than 1 (exercise, what is the structural index?)

Well known that structural index can be less than the index, but the example above shows that it can also be the other way around.

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