Numerical Simulation of Dynamic Systems: Hw9 - Solution

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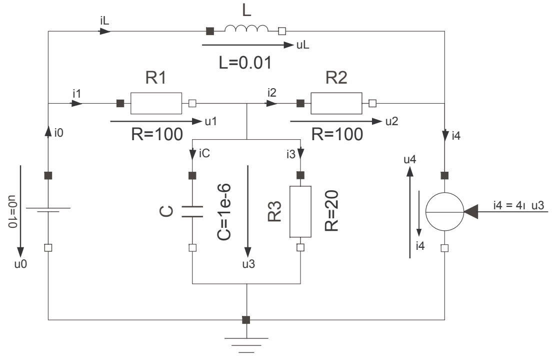
[H7.1] Electrical Circuit, Horizontal and Vertical Sorting

Given the electrical circuit:

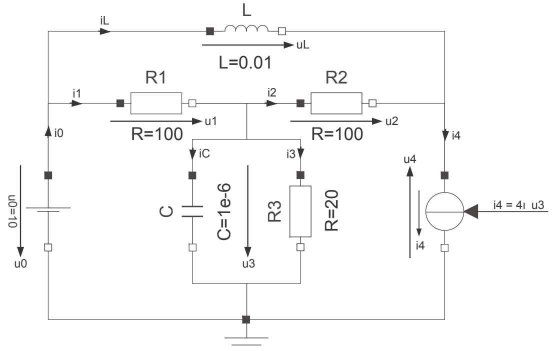


- The circuit contains a constant voltage source, u_0, and a dependent current source, i_4, that depends on the voltage across the capacitor, C, and the resistor, R_3.
- Write down the element equations for the seven circuit elements. Since the voltage u_3 is common to two circuit elements, these equations contain 13 rather than 14 unknowns. Add the voltage equations for the three meshes and the current equations for three of the four nodes.

[H7.1] Electrical Circuit, Horizontal and Vertical Sorting II

- Draw the structure digraph of the DAE system, and apply the Tarjan algorithm to sort the equations both horizontally and vertically. Write down the causal equations, i.e., the resulting ODE system.
- Simulate the ODE system across 50 μsec using RKF4/5 with Gustaffsson step-size control and with zero initial conditions on both the capacitor and the inductor.
- Plot the voltage u_3 and the current i_C, and the step size h on three separate subplots as functions of time.

[H7.1] Electrical Circuit, Horizontal and Vertical Sorting III



1: $u_0 = 10$
2: $u_1 = R_1 \cdot i_1$
3: $u_2 = R_2 \cdot i_2$
4: $u_3 = R_3 \cdot i_3$
5: $i_C = C \cdot \frac{du_3}{dt}$
6: $u_L = L \cdot \frac{di_L}{dt}$
7: $i_4 = 4 \cdot u_3$

8: $u_0 = u_1 + u_3$
9: $u_L = u_1 + u_2$
10: $u_2 = u_3 + u_4$

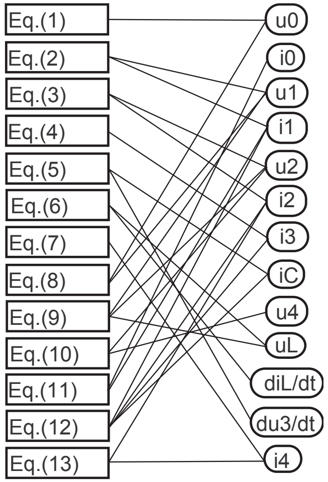
11: $i_0 = i_1 + i_L$
12: $i_1 = i_2 + i_C + i_3$
13: $i_4 = i_2 + i_L$

[H7.1] Electrical Circuit, Horizontal and Vertical Sorting IV

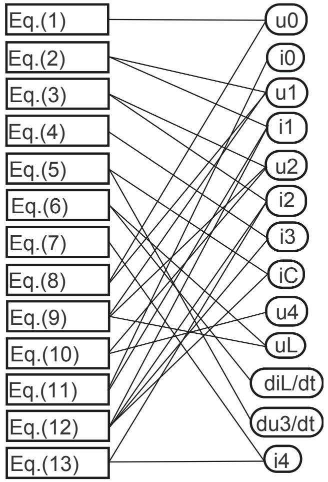
1: $u_0 = 10$
2: $u_1 = R_1 \cdot i_1$
3: $u_2 = R_2 \cdot i_2$
4: $u_3 = R_3 \cdot i_3$
5: $i_C = C \cdot \frac{du_3}{dt}$
6: $u_L = L \cdot \frac{di_L}{dt}$
7: $i_4 = 4 \cdot u_3$

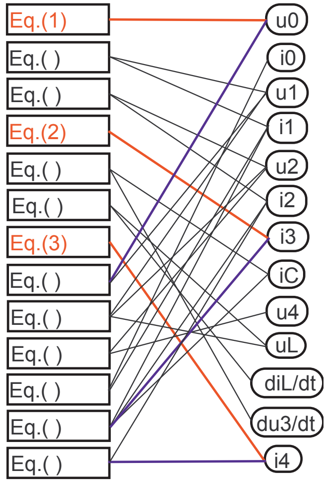
8: $u_0 = u_1 + u_3$
9: $u_L = u_1 + u_2$
10: $u_2 = u_3 + u_4$

11: $i_0 = i_1 + i_L$
12: $i_1 = i_2 + i_C + i_3$
13: $i_4 = i_2 + i_L$

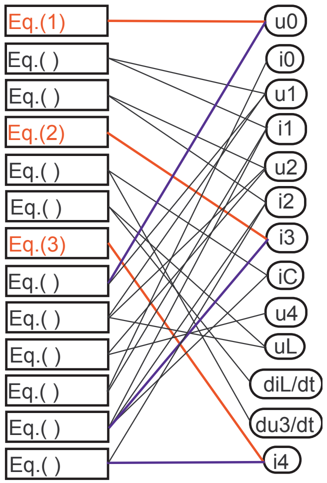


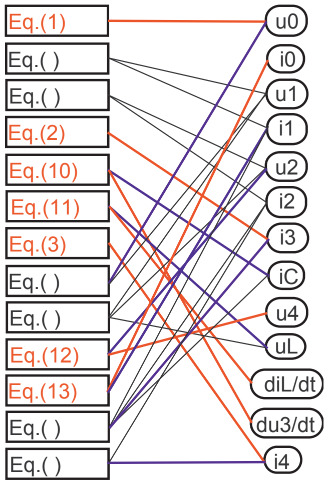
[H7.1] Electrical Circuit, Horizontal and Vertical Sorting V



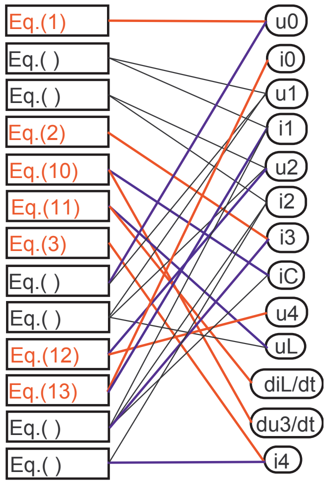


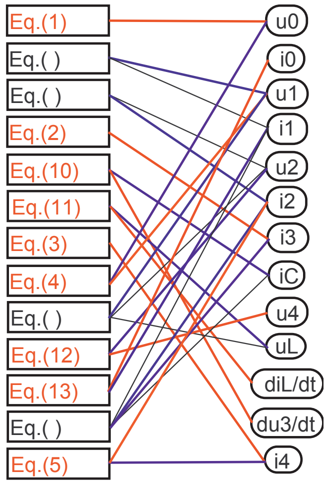
[H7.1] Electrical Circuit, Horizontal and Vertical Sorting VI



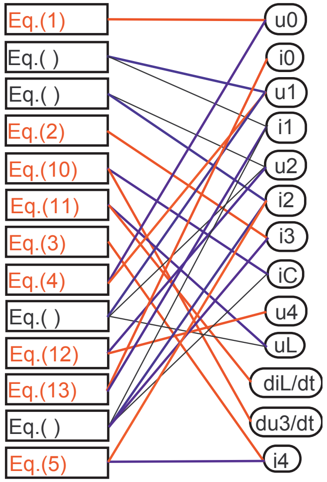


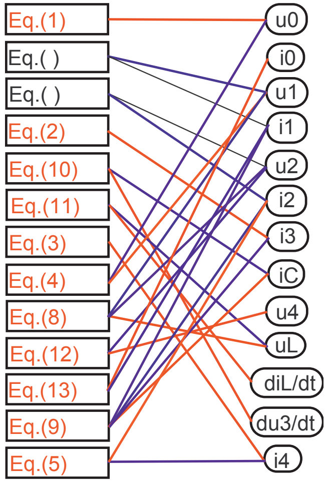
[H7.1] Electrical Circuit, Horizontal and Vertical Sorting VII



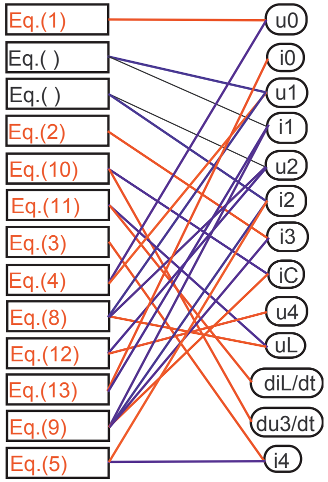


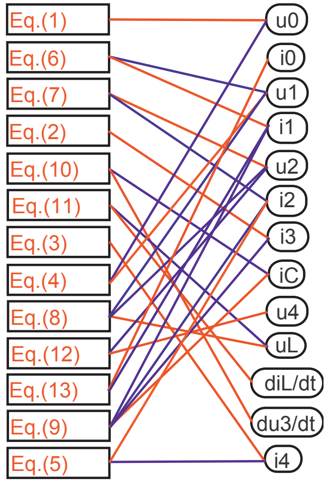
[H7.1] Electrical Circuit, Horizontal and Vertical Sorting VIII



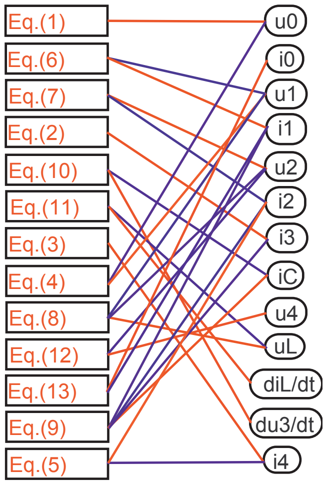


[H7.1] Electrical Circuit, Horizontal and Vertical Sorting IX





[H7.1] Electrical Circuit, Horizontal and Vertical Sorting X



$$
\begin{aligned}
1:&\quad u_0 = 10\\
6:&\quad u_1 = R_1 \cdot i_1\\
7:&\quad u_2 = R_2 \cdot i_2\\
2:&\quad u_3 = R_3 \cdot i_3\\
10:&\quad i_C = C \cdot \frac{du_3}{dt}\\
11:&\quad u_L = L \cdot \frac{di_L}{dt}\\
3:&\quad i_4 = 4 \cdot u_3\\[1em]
4:&\quad u_0 = u_1 + u_3\\
8:&\quad u_L = u_1 + u_2\\
12:&\quad u_2 = u_3 + u_4\\[1em]
13:&\quad i_0 = i_1 + i_L\\
9:&\quad i_1 = i_2 + i_C + i_3\\
5:&\quad i_4 = i_2 + i_L
\end{aligned}
$$

[H7.1] Electrical Circuit, Horizontal and Vertical Sorting XI

$$
\begin{aligned}
1:&\quad u_0 = 10\\
6:&\quad u_1 = R_1 \cdot i_1\\
7:&\quad u_2 = R_2 \cdot i_2\\
2:&\quad u_3 = R_3 \cdot i_3\\
10:&\quad i_C = C \cdot \frac{du_3}{dt}\\
11:&\quad u_L = L \cdot \frac{di_L}{dt}\\
3:&\quad i_4 = 4 \cdot u_3\\[1em]
4:&\quad u_0 = u_1 + u_3\\
8:&\quad u_L = u_1 + u_2\\
12:&\quad u_2 = u_3 + u_4\\[1em]
13:&\quad i_0 = i_1 + i_L\\
9:&\quad i_1 = i_2 + i_C + i_3\\
5:&\quad i_4 = i_2 + i_L
\end{aligned}
$$

$$
\begin{aligned}
1:&\quad u_0 = 10\\
2:&\quad i_3 = \frac{1}{R_3} \cdot u_3\\
3:&\quad i_4 = 4 \cdot u_3\\
4:&\quad u_1 = u_0 - u_3\\
5:&\quad i_2 = i_4 - i_L\\
6:&\quad i_1 = \frac{1}{R_1} \cdot u_1\\
7:&\quad u_2 = R_2 \cdot i_2\\
8:&\quad u_L = u_1 + u_2\\
9:&\quad i_C = i_1 - i_2 - i_3\\
10:&\quad \frac{du_3}{dt} = \frac{1}{C} \cdot i_C\\
11:&\quad \frac{di_L}{dt} = \frac{1}{L} \cdot u_L\\
12:&\quad u_4 = u_2 - u_3\\
13:&\quad i_0 = i_1 + i_L
\end{aligned}
$$

[H7.1] Electrical Circuit, Horizontal and Vertical Sorting XII

The model and output equations can be coded as follows:

```
function [xdot] = st_eq2(x, t)
R1 = 100;  R2 = 100;  R3 = 30;
C = 1e-6;  L = 0.01;
%
u3 = x(1);  iL = x(2);
%
u0 = 10;
i3 = u3/R3;
i4 = 4*u3;
u1 = u0 - u3;
i2 = i4 - iL;
i1 = u1/R1;
u2 = R2*i2;
uL = u1 + u2;
iC = i1 - i2 - i3;
du3 = iC/C;
diL = uL/L;
u4 = u2 - u3;
i0 = i1 + iL;
%
xdot = zeros(2, 1);
xdot(1) = du3;  xdot(2) = diL;
%
return
```

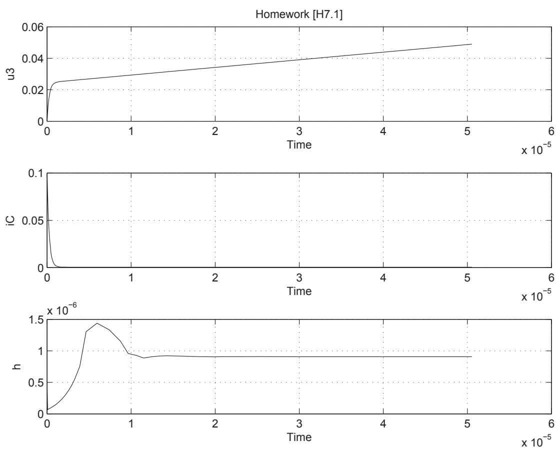
```
function [y] = out_eq2(x, t)
R1 = 100;  R2 = 100;  R3 = 30;
C = 1e-6;  L = 0.01;
%
u3 = x(1);  iL = x(2);
%
u0 = 10;
i3 = u3/R3;
i4 = 4*u3;
u1 = u0 - u3;
i2 = i4 - iL;
i1 = u1/R1;
u2 = R2*i2;
uL = u1 + u2;
iC = i1 - i2 - i3;
du3 = iC/C;
diL = uL/L;
u4 = u2 - u3;
i0 = i1 + iL;
%
y = zeros(2, 1);
y(1) = u3;  y(2) = iC;
%
return
```


[H7.1] Electrical Circuit, Horizontal and Vertical Sorting XIII

The simulation loop (with Gustafsson step-size control) can be coded as follows:

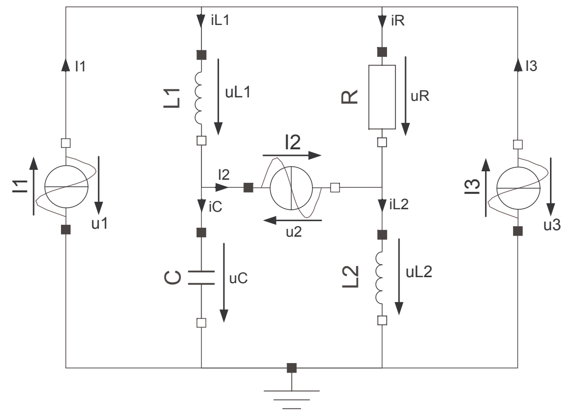
```
while t < tf,
   [x4, x5] = rkf45_step2(x, t, h);
   err = norm(x4 - x5,'inf')/max([norm(x4),norm(x5), 1.0e-10]);
   if err > tol,
      h = (0.8 * tol/err) ∧ (0.2) * h;
      errl = 0;
   else
      t = t + h;
      x = x5;
      y = out_eq2(x, t);
      tvec = [tvec, t];
      yvec = [yvec, y];
      if errl > 0,
         h = (0.8 * tol/err) ∧ (0.06) * (errl/err) ∧ (0.08) * h;
      else
         h = (0.8 * tol/err) ∧ (0.2) * h;
      end
      hvec = [hvec, h];
      errl = err;
   end
end
```


[H7.1] Electrical Circuit, Horizontal and Vertical Sorting XIV



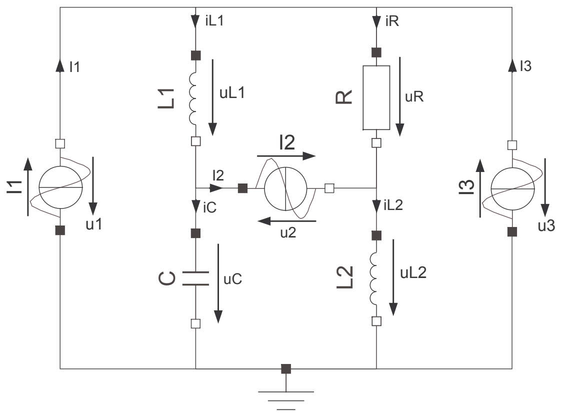
[H7.7] Electrical Circuit, Structural Singularity

Given the circuit shown below containing three sinusoidal current sources:



- Write down the complete set of equations describing this circuit. Draw the structure digraph and begin causalizing the equations. Determine a constraint equation.
- Apply the Pantelides algorithm to reduce the perturbation index to 1. Then apply the tearing algorithm with substitution to bring the perturbation index down to 0.
- Write down the structure incidence matrices of the index-1 DAE and the index-0 ODE systems, and show that they are in BLT form, and in LT form, respectively.

[H7.7] Electrical Circuit, Structural Singularity II



1: $I_1 = f_1(t)$
2: $I_2 = f_2(t)$
3: $I_3 = f_3(t)$
4: $u_R = R \cdot i_R$
5: $i_C = C \cdot \frac{du_C}{dt}$
6: $u_{L1} = L_1 \cdot \frac{di_{L1}}{dt}$
7: $u_{L2} = L_2 \cdot \frac{di_{L2}}{dt}$

8: $u_1 = u_{L1} + u_C$
9: $u_{L1} = u_R + u_2$
10: $u_{L2} = u_2 + u_C$
11: $u_3 = u_R + u_{L2}$

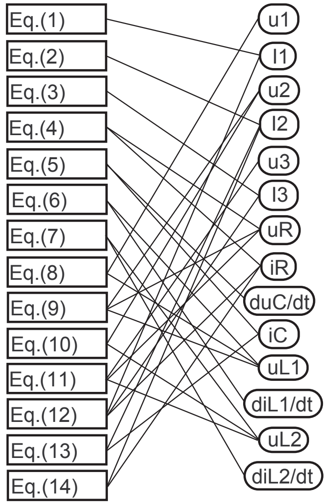
12: $I_1 + I_3 = i_{L1} + i_R$
13: $i_{L1} = I_2 + i_C$
14: $i_{L2} = I_2 + i_R$

[H7.7] Electrical Circuit, Structural Singularity III

1: $I_1 = f_1(t)$
2: $I_2 = f_2(t)$
3: $I_3 = f_3(t)$
4: $u_R = R \cdot i_R$
5: $i_C = C \cdot \frac{du_C}{dt}$
6: $u_{L1} = L_1 \cdot \frac{di_{L1}}{dt}$
7: $u_{L2} = L_2 \cdot \frac{di_{L2}}{dt}$

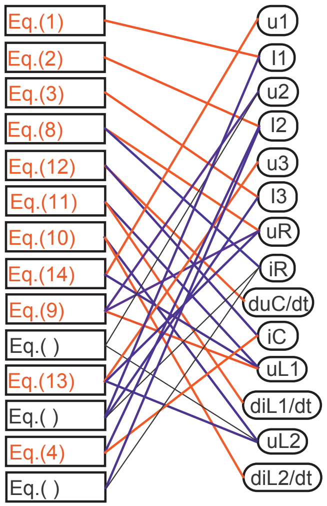
8: $u_1 = u_{L1} + u_C$
9: $u_{L1} = u_R + u_2$
10: $u_{L2} = u_2 + u_C$
11: $u_3 = u_R + u_{L2}$

12: $I_1 + I_3 = i_{L1} + i_R$
13: $i_{L1} = I_2 + i_C$
14: $i_{L2} = I_2 + i_R$



[H7.7] Electrical Circuit, Structural Singularity IV

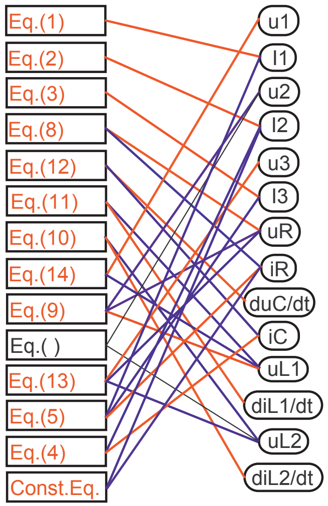
I causalized as much as I could without getting into trouble:



1: $I_1 = f_1(t)$
2: $I_2 = f_2(t)$
3: $I_3 = f_3(t)$
8: $u_R = R \cdot i_R$
12: $i_C = C \cdot \frac{du_C}{dt}$
11: $u_{L1} = L_1 \cdot \frac{di_{L1}}{dt}$
10: $u_{L2} = L_2 \cdot \frac{di_{L2}}{dt}$
14: $u_1 = u_{L1} + u_C$
9: $u_{L1} = u_R + u_2$
?: $u_{L2} = u_2 + u_C$
13: $u_3 = u_R + u_{L2}$
?: $I_1 + I_3 = i_{L1} + i_R$
4: $i_{L1} = I_2 + i_C$
?: $i_{L2} = I_2 + i_R$

[H7.7] Electrical Circuit, Structural Singularity V

Any additional causalization leads invariably to a constraint:



1: $I_1 = f_1(t)$
2: $I_2 = f_2(t)$
3: $I_3 = f_3(t)$
8: $u_R = R \cdot i_R$
12: $i_C = C \cdot \frac{du_C}{dt}$
11: $u_{L1} = L_1 \cdot \frac{di_{L1}}{dt}$
10: $u_{L2} = L_2 \cdot \frac{di_{L2}}{dt}$
14: $u_1 = u_{L1} + u_C$
9: $u_{L1} = u_R + u_2$
?: $u_{L2} = u_2 + u_C$
13: $u_3 = u_R + u_{L2}$
5: $I_1 + I_3 = i_{L1} + i_R$
4: $i_{L1} = I_2 + i_C$
const.eq.: $i_{L2} = I_2 + i_R$

[H7.7] Electrical Circuit, Structural Singularity VI

We differentiate the constraint equation and let go of the integrator for i_{L1}:

$$\begin{array}{lrcl}
1: & I_1 & = & f_1(t) \\
2: & I_2 & = & f_2(t) \\
3: & I_3 & = & f_3(t) \\
8: & u_R & = & R \cdot i_R \\
12: & i_C & = & C \cdot \frac{du_C}{dt} \\
11: & u_{L1} & = & L_1 \cdot \frac{di_{L1}}{dt} \\
10: & u_{L2} & = & L_2 \cdot \frac{di_{L2}}{dt} \\
14: & u_1 & = & u_{L1} + u_C \\
9: & u_{L1} & = & u_R + u_2 \\
?: & u_{L2} & = & u_2 + u_C \\
13: & u_3 & = & u_R + u_{L2} \\
5: & I_1 + I_3 & = & i_{L1} + i_R \\
4: & i_{L1} & = & I_2 + i_C \\
\text{const.eq.}: & i_{L2} & = & I_2 + i_R
\end{array}$$

$$\begin{array}{lrcl}
1: & I_1 & = & f_1(t) \\
2: & I_2 & = & f_2(t) \\
3: & I_3 & = & f_3(t) \\
10: & u_R & = & R \cdot i_R \\
13: & i_C & = & C \cdot \frac{du_C}{dt} \\
12: & u_{L1} & = & L_1 \cdot \frac{di_{L1}}{dt} \\
?: & u_{L2} & = & L_2 \cdot di_{L2} \\
15: & u_1 & = & u_{L1} + u_C \\
11: & u_{L1} & = & u_R + u_2 \\
?: & u_{L2} & = & u_2 + u_C \\
14: & u_3 & = & u_R + u_{L2} \\
5: & I_1 + I_3 & = & i_{L1} + i_R \\
4: & i_{L1} & = & I_2 + i_C \\
6: & i_{L2} & = & I_2 + i_R \\
?: & di_{L2} & = & dI_2 + di_R
\end{array}$$

[H7.7] Electrical Circuit, Structural Singularity VII

We introduced two new pseudo-derivatives, dI_2 and di_R:

$$\begin{array}{lrcl}
1: & I_1 & = & f_1(t) \\
2: & I_2 & = & f_2(t) \\
3: & I_3 & = & f_3(t) \\
10: & u_R & = & R \cdot i_R \\
13: & i_C & = & C \cdot \frac{du_C}{dt} \\
12: & u_{L1} & = & L_1 \cdot \frac{di_{L1}}{dt} \\
?: & u_{L2} & = & L_2 \cdot di_{L2} \\
15: & u_1 & = & u_{L1} + u_C \\
11: & u_{L1} & = & u_R + u_2 \\
?: & u_{L2} & = & u_2 + u_C \\
14: & u_3 & = & u_R + u_{L2} \\
5: & I_1 + I_3 & = & i_{L1} + i_R \\
4: & i_{L1} & = & I_2 + i_C \\
6: & i_{L2} & = & I_2 + i_R \\
?: & di_{L2} & = & dI_2 + di_R
\end{array}$$

$$\begin{array}{lrcl}
1: & I_1 & = & f_1(t) \\
2: & I_2 & = & f_2(t) \\
7: & dI_2 & = & \frac{df_2(t)}{dt} \\
3: & I_3 & = & f_3(t) \\
8: & u_R & = & R \cdot i_R \\
15: & i_C & = & C \cdot \frac{du_C}{dt} \\
?: & u_{L1} & = & L_1 \cdot \frac{di_{L1}}{dt} \\
?: & u_{L2} & = & L_2 \cdot di_{L2} \\
17: & u_1 & = & u_{L1} + u_C \\
?: & u_{L1} & = & u_R + u_2 \\
?: & u_{L2} & = & u_2 + u_C \\
16: & u_3 & = & u_R + u_{L2} \\
5: & I_1 + I_3 & = & i_{L1} + i_R \\
?: & dI_1 + dI_3 & = & \frac{di_{L1}}{dt} + di_R \\
4: & i_{L1} & = & I_2 + i_C \\
6: & i_{L2} & = & I_2 + i_R \\
?: & di_{L2} & = & dI_2 + di_R
\end{array}$$

[H7.7] Electrical Circuit, Structural Singularity VIII

Two more pseudo-derivatives, dI_1 and dI_3:

$$\begin{array}{lrcl}
1: & I_1 & = & f_1(t) \\
2: & I_2 & = & f_2(t) \\
7: & dI_2 & = & \frac{df_2(t)}{dt} \\
3: & I_3 & = & f_3(t) \\
8: & u_R & = & R \cdot i_R \\
15: & i_C & = & C \cdot \frac{du_C}{dt} \\
?: & u_{L1} & = & L_1 \cdot \frac{di_{L1}}{dt} \\
?: & u_{L2} & = & L_2 \cdot di_{L2} \\
17: & u_1 & = & u_{L1} + u_C \\
?: & u_{L1} & = & u_R + u_2 \\
?: & u_{L2} & = & u_2 + u_C \\
16: & u_3 & = & u_R + u_{L2} \\
5: & I_1 + I_3 & = & i_{L1} + i_R \\
?: & dI_1 + dI_3 & = & \frac{di_{L1}}{dt} + di_R \\
4: & i_{L1} & = & I_2 + i_C \\
6: & i_{L2} & = & I_2 + i_R \\
?: & di_{L2} & = & dI_2 + di_R
\end{array}$$

$$\begin{array}{lrcl}
1: & I_1 & = & f_1(t) \\
9: & dI_1 & = & \frac{df_1(t)}{dt} \\
2: & I_2 & = & f_2(t) \\
7: & dI_2 & = & \frac{df_2(t)}{dt} \\
3: & I_3 & = & f_3(t) \\
10: & dI_3 & = & \frac{df_3(t)}{dt} \\
8: & u_R & = & R \cdot i_R \\
17: & i_C & = & C \cdot \frac{du_C}{dt} \\
?: & u_{L1} & = & L_1 \cdot \frac{di_{L1}}{dt} \\
?: & u_{L2} & = & L_2 \cdot di_{L2} \\
19: & u_1 & = & u_{L1} + u_C \\
?: & u_{L1} & = & u_R + u_2 \\
?: & u_{L2} & = & u_2 + u_C \\
18: & u_3 & = & u_R + u_{L2} \\
5: & I_1 + I_3 & = & i_{L1} + i_R \\
?: & dI_1 + dI_3 & = & \frac{di_{L1}}{dt} + di_R \\
4: & i_{L1} & = & I_2 + i_C \\
6: & i_{L2} & = & I_2 + i_R \\
?: & di_{L2} & = & dI_2 + di_R
\end{array}$$

[H7.7] Electrical Circuit, Structural Singularity IX

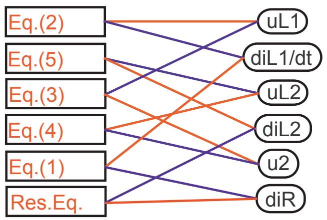
S =

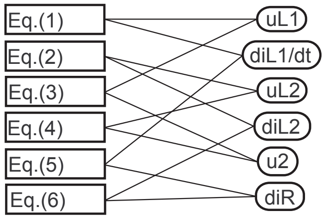
	I_1	I_2	I_3	i_C	i_R	i_{L2}	dI_2	u_R	dI_1	dI_3	u_{L1}	$\frac{di_{L1}}{dt}$	u_{L2}	di_{L2}	u_2	di_R	$\frac{du_C}{dt}$	u_3	u_1
1:	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2:	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3:	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4:	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5:	1	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6:	0	1	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0
7:	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
8:	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0
9:	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
10:	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
11:	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0
12:	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0
13:	0	0	0	0	0	0	0	1	0	0	1	0	0	0	1	0	0	0	0
14:	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0
15:	0	0	0	0	0	0	0	0	1	1	0	1	0	0	0	1	0	0	0
16:	0	0	0	0	0	0	1	0	0	0	0	0	0	1	0	1	0	0	0
17:	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
18:	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0	1	0
19:	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1

[H7.7] Electrical Circuit, Structural Singularity X

We have an algebraic loop in six equations and six unknowns:

$$
\begin{array}{lll}
?: & u_{L1} = & L_1 \cdot \frac{di_{L1}}{dt} \\
?: & u_{L2} = & L_2 \cdot di_{L2} \\
?: & u_{L1} = & u_R + u_2 \\
?: & u_{L2} = & u_2 + u_C \\
?: & dI_1 + dI_3 = & \frac{di_{L1}}{dt} + di_R \\
?: & di_{L2} = & dI_2 + di_R
\end{array}
$$





$$
\begin{array}{lll}
2: & u_{L1} = & L_1 \cdot \frac{di_{L1}}{dt} \\
5: & u_{L2} = & L_2 \cdot di_{L2} \\
3: & u_{L1} = & u_R + u_2 \\
4: & u_{L2} = & u_2 + u_C \\
1: & dI_1 + dI_3 = & \frac{di_{L1}}{dt} + di_R \\
\text{res.eq.}: & di_{L2} = & dI_2 + di_R
\end{array}
$$

[H7.7] Electrical Circuit, Structural Singularity XI

We have an algebraic loop in six equations and six unknowns:

$$
\begin{array}{lll}
2: & u_{L1} = & L_1 \cdot \frac{di_{L1}}{dt} \\
5: & u_{L2} = & L_2 \cdot di_{L2} \\
3: & u_{L1} = & u_R + u_2 \\
4: & u_{L2} = & u_2 + u_C \\
1: & dI_1 + dI_3 = & \frac{di_{L1}}{dt} + di_R \\
\text{res.eq.}: & di_{L2} = & dI_2 + di_R
\end{array}
$$

$$
\begin{array}{lll}
\text{res.eq.}: & di_R = & di_{L2} - dI_2 \\
1: & \frac{di_{L1}}{dt} = & dI_1 + dI_3 - di_R \\
2: & u_{L1} = & L_1 \cdot \frac{di_{L1}}{dt} \\
3: & u_2 = & u_{L1} - u_R \\
4: & u_{L2} = & u_2 + u_C \\
5: & di_{L2} = & \frac{1}{L_2} \cdot u_{L2}
\end{array}
$$

$$
\begin{aligned}
di_R &= di_{L2} - dI_2 \\
&= \frac{1}{L_2} \cdot u_{L2} - dI_2 \\
&= \frac{1}{L_2} \cdot u_2 + \frac{1}{L_2} \cdot u_C - dI_2 \\
&= \frac{1}{L_2} \cdot u_{L1} - \frac{1}{L_2} \cdot u_R + \frac{1}{L_2} \cdot u_C - dI_2 \\
&= \frac{L_1}{L_2} \cdot \frac{di_{L1}}{dt} - \frac{1}{L_2} \cdot u_R + \frac{1}{L_2} \cdot u_C - dI_2 \\
&= \frac{L_1}{L_2} \cdot dI_1 + \frac{L_1}{L_2} \cdot dI_3 - \frac{L_1}{L_2} \cdot di_R - \frac{1}{L_2} \cdot u_R + \frac{1}{L_2} \cdot u_C - dI_2
\end{aligned}
$$

$$
di_R = \frac{L_1 \cdot (dI_1 + dI_3) - u_R + u_C - L_2 \cdot dI_2}{L_1 + L_2}
$$

[H7.7] Electrical Circuit, Structural Singularity XII

$$
\begin{array}{lll}
1: & I_1 = & f_1(t) \\
2: & I_2 = & f_2(t) \\
3: & I_3 = & f_3(t) \\
4: & i_C = & i_{L1} - I_2 \\
5: & i_R = & I_1 + I_3 - i_{L1} \\
6: & i_{L2} = & I_2 + i_R \\
7: & dI_2 = & \frac{df_2(t)}{dt} \\
8: & u_R = & R \cdot i_R \\
9: & dI_1 = & \frac{df_1(t)}{dt} \\
10: & dI_3 = & \frac{df_3(t)}{dt} \\
11: & di_R = & \frac{L_1 \cdot (dI_1 + dI_3) - u_R + u_C - L_2 \cdot dI_2}{L_1 + L_2} \\
12: & \frac{di_{L1}}{dt} = & dI_1 + dI_3 - di_R \\
13: & u_{L1} = & L_1 \cdot \frac{di_{L1}}{dt} \\
14: & u_2 = & u_{L1} - u_R \\
15: & u_{L2} = & u_2 + u_C \\
16: & di_{L2} = & \frac{1}{L_2} \cdot u_{L2} \\
17: & \frac{du_C}{dt} = & \frac{1}{C} \cdot i_C \\
18: & u_3 = & u_R + u_{L2} \\
19: & u_1 = & u_{L1} + u_C
\end{array}
$$

[H7.7] Electrical Circuit, Structural Singularity XIII

S =

	I_1	I_2	I_3	i_C	i_R	i_{L2}	dI_2	u_R	dI_1	dI_3	di_R	$\frac{di_{L1}}{dt}$	u_{L1}	u_2	u_{L2}	di_{L2}	$\frac{du_C}{dt}$	u_3	u_1
1:	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2:	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3:	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4:	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5:	1	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6:	0	1	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0
7:	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
8:	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0
9:	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
10:	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
11:	0	0	0	0	0	0	1	1	1	1	1	0	0	0	0	0	0	0	0
12:	0	0	0	0	0	0	0	0	1	1	1	1	0	0	0	0	0	0	0
13:	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0
14:	0	0	0	0	0	0	0	1	0	0	0	0	1	1	0	0	0	0	0
15:	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0
16:	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0
17:	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
18:	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1	0	0	1	0
19:	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1

[H7.8] Chemical Reactions, Pantelides Algorithm

The following set of DAEs:

$$\begin{aligned}
\frac{dC}{dt} &= K_1(C_0 - C) - R \\
\frac{dT}{dt} &= K_1(T_0 - T) + K_2 R - K_3(T - T_C) \\
0 &= R - K_3 \exp\left(\frac{-K_4}{T}\right) C \\
0 &= C - u
\end{aligned}$$

describes a chemical isomerization reaction.

C is the reactant concentration, T is the reactant temperature, and R is the reactant rate per unit volume. C_0 is the feed reactant concentration, and T_0 is the feed reactant temperature. u is the desired concentration, and T_C is the control temperature that we need to produce u.

[H7.8] Chemical Reactions, Pantelides Algorithm II

- We want to turn the problem around (inverse model control) and determine the necessary control temperature T_C as a function of the desired concentration u. Thus, u will be an input to our model, and T_C is the output.
- Draw the structure digraph. You shall notice at once that one of the equations has no connections to it. Thus, it is a constraint equation that needs to be differentiated, while an integrator associated with the constraint equation needs to be thrown out.
- We now have five equations in five unknowns. Draw the enhanced structure digraph, and start causalizing the equations. You shall notice that a second constraint equation appears. Hence the original DAE system had been an index-3 DAE system. Differentiate that constraint equation as well, and throw out the second integrator. In the process, new pseudo-derivatives are introduced that call for additional differentiations.

[H7.8] Chemical Reactions, Pantelides Algorithm III

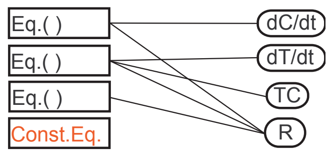
- This time around, you end up with eight equations in eight unknowns. Draw the once more enhanced structure digraph, and causalize the equations. This is an example, in which (by accident) the Pantelides algorithm reduces the perturbation index in one step from 2 to 0, i.e., the final set of equations does not contain an algebraic loop.
- Draw a block diagram that shows how the output T_C can be computed from the three inputs u, $\frac{du}{dt}$, and $\frac{d^2u}{dt^2}$.

[H7.8] Chemical Reactions, Pantelides Algorithm IV

The original equations are:

$$\begin{aligned}
?:& \quad \frac{dC}{dt} = K_1 \cdot (C_0 - C) - R \\
?:& \quad \frac{dT}{dt} = K_1 \cdot (T_0 - T) + K_2 \cdot R - K_3 \cdot (T - T_C) \\
?:& \quad 0 = R - K_3 \cdot \exp\left(\frac{-K_4}{T}\right) \cdot C \\
\text{const.eq.:}& \quad 0 = C - u
\end{aligned}$$

With the structure digraph:



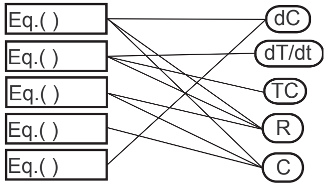
We recognize immediately a constraint equation.

[H7.8] Chemical Reactions, Pantelides Algorithm V

The enhanced equations are:

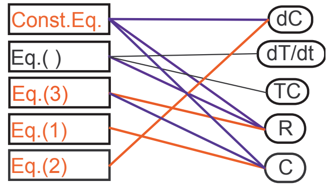
$$\begin{aligned}
?:\quad dC &= K_1 \cdot (C_0 - C) - R \\
?:\quad \frac{dT}{dt} &= K_1 \cdot (T_0 - T) + K_2 \cdot R - K_3 \cdot (T - T_C) \\
?:\quad 0 &= R - K_3 \cdot \exp\left(\frac{-K_4}{T}\right) \cdot C \\
?:\quad 0 &= C - u \\
?:\quad 0 &= dC - \frac{du}{dt}
\end{aligned}$$

With the structure digraph:



[H7.8] Chemical Reactions, Pantelides Algorithm VI

We start coloring the structure digraph and recognize soon a second constraint equation:



$$\begin{aligned}
?:\quad dC &= K_1 \cdot (C_0 - C) - R \\
?:\quad \frac{dT}{dt} &= K_1 \cdot (T_0 - T) + K_2 \cdot R - K_3 \cdot (T - T_C) \\
?:\quad 0 &= R - K_3 \cdot \exp\left(\frac{-K_4}{T}\right) \cdot C \\
?:\quad 0 &= C - u \\
?:\quad 0 &= dC - \frac{du}{dt}
\end{aligned}$$

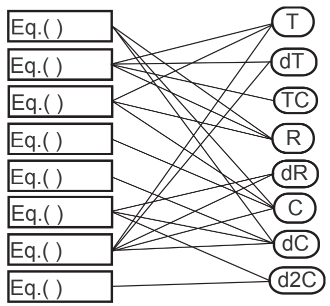
[H7.8] Chemical Reactions, Pantelides Algorithm VII

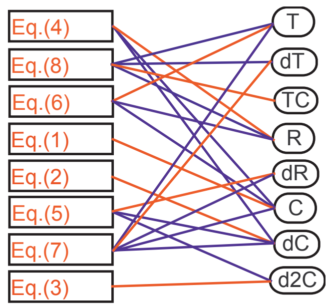
The once more enhanced equations are:

$$\begin{aligned}
?:\quad dC &= K_1 \cdot (C_0 - C) - R \\
?:\quad dT &= K_1 \cdot (T_0 - T) + K_2 \cdot R - K_3 \cdot (T - T_C) \\
?:\quad 0 &= R - K_3 \cdot \exp\left(\frac{-K_4}{T}\right) \cdot C \\
?:\quad 0 &= C - u \\
?:\quad 0 &= dC - \frac{du}{dt} \\
?:\quad d2C &= K_1 \cdot \left(\frac{dC_0}{dt} - dC\right) - dR \\
?:\quad 0 &= dR - K_3 \cdot \exp\left(\frac{-K_4}{T}\right) \cdot \left[dC + \frac{K_4 \cdot C \cdot dT}{T^2}\right] \\
?:\quad 0 &= d2C - \frac{d^2u}{dt^2}
\end{aligned}$$

[H7.8] Chemical Reactions, Pantelides Algorithm VIII

Let us color the structure digraph:





We went from index-2 directly down to index-0. This sometimes happens.

[H7.8] Chemical Reactions, Pantelides Algorithm IX

$$
\begin{aligned}
4:&\quad dC &=&\; K_1 \cdot (C_0 - C) - R \\
8:&\quad dT &=&\; K_1 \cdot (T_0 - T) + K_2 \cdot R - K_3 \cdot (T - T_C) \\
6:&\quad 0 &=&\; R - K_3 \cdot \exp\left(\frac{-K_4}{T}\right) \cdot C \\
1:&\quad 0 &=&\; C - u \\
2:&\quad 0 &=&\; dC - \frac{du}{dt} \\
5:&\quad d2C &=&\; K_1 \cdot \left(\frac{dC_0}{dt} - dC\right) - dR \\
7:&\quad 0 &=&\; dR - K_3 \cdot \exp\left(\frac{-K_4}{T}\right) \cdot \left[dC + \frac{K_4 \cdot C \cdot dT}{T^2}\right] \\
3:&\quad 0 &=&\; d2C - \frac{d^2 u}{dt^2}
\end{aligned}
$$

[H7.8] Chemical Reactions, Pantelides Algorithm X

$$
\begin{aligned}
1:&\quad C &=&\; u \\
2:&\quad dC &=&\; \frac{du}{dt} \\
3:&\quad d2C &=&\; \frac{d^2 u}{dt^2} \\
4:&\quad R &=&\; K_1 \cdot (C_0 - C) - dC \\
5:&\quad dR &=&\; K_1 \cdot \left(\frac{dC_0}{dt} - dC\right) - d2C \\
6:&\quad T &=&\; \frac{-K_4}{\log\left(\frac{R}{K_3 \cdot C}\right)} \\
7:&\quad dT &=&\; \frac{T^2}{K_3 \cdot K_4 \cdot C} \cdot \left[dR \cdot \exp\left(\frac{K_4}{T}\right) - K_3 \cdot dC\right] \\
8:&\quad T_C &=&\; \frac{dT - K_1 \cdot (T_0 - T) - K_2 \cdot R + K_3 \cdot T}{K_3}
\end{aligned}
$$

[H7.8] Chemical Reactions, Pantelides Algorithm XI