Numerical Simulation of Dynamic Systems XVII

Prof. Dr. François E. Cellier Department of Computer Science ETH Zurich

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Let us look at the DAE:

$$x - \dot{x}^2 = 0$$

Converting to ODE form, we obtain:

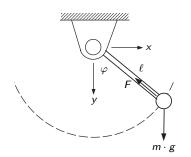
$$\dot{x} = \pm \sqrt{x}$$

- We notice that the ODE has only a real-valued solution as long as the initial value of x is positive. This constraint exists implicitly also in the DAE formulation, but it is not directly visible.
- Yet, the problem is worse, because we don't know which root to choose. If we choose the positive root, x will also be positive, and x will keep growing. However, if we choose the negative root, x is negative, and x will decrease.
- Even worse, it could be that we should choose the positive root during some period of time, and the negative root during another. Thus, at any moment in time, we obtain a potential bifurcation in the solution depending on whether we choose the positive or the negative root.

Does the solvability issue cause a real dilemma?

- Physics does not provide us with unsolvable riddles.
- Saying that a DAE is unsolvable is equivalent to saying that the phenomenon described by it is "defying causality" in the sense that the outcome of an experiment is non-deterministic, which in turn is almost equivalent to saying that the phenomenon is non-physical.
- Thus, if a DAE model contains solvability issues, this simply means that the DAE does not capture the physical phenomenon that it is supposed to describe in its full complexity. Some information is missing.
- Unfortunately, solvability issues are encountered frequently in DAE models derived from object-oriented descriptions of physical systems, and consequently, we need to deal with the consequences.

Let us look at a simple pendulum:



describable by the following set of DAEs:

$$m \cdot \frac{dv_x}{dt} = -\frac{F \cdot x}{\ell}$$

$$m \cdot \frac{dv_y}{dt} = m \cdot g - \frac{F \cdot y}{\ell}$$

$$\frac{dx}{dt} = v_x$$

$$\frac{dy}{dt} = v_y$$

$$x^2 + y^2 = \ell^2$$

Since x, y, vx, and vy are known state variables, the last equation in the set is a constraint equation.

We apply the Pantelides algorithm once:

$$m \cdot \frac{dv_x}{dt} = -\frac{F \cdot x}{\ell}$$

$$m \cdot \frac{dv_y}{dt} = m \cdot g - \frac{F \cdot y}{\ell}$$

$$dx = v_x$$

$$\frac{dy}{dt} = v_y$$

$$x^2 + y^2 = \ell^2$$

$$2 \cdot x \cdot dx + 2 \cdot y \cdot \frac{dy}{dt} = 0$$

- We decided to let go of the integrator for x, thus the six unknowns are \(\frac{dv_x}{dt}\), \(\frac{dv_y}{dt}\), \(dx\), \(\frac{dy}{dt}\), \(F\), and \(x\).
- ► Eq.(5) is no longer a constraint equation, as it can be solved for the new unknown x. Eq.(6) can be solved for the unknown dx, but this leaves Eq.(3) as a new constraint equation.
- Evidently, the original problem was an index-3 problem, and the Pantelides algorithm needs to be applied a second time.

We apply the Pantelides algorithm once more:

$$m \cdot dv_{x} = -\frac{F \cdot x}{\ell}$$

$$m \cdot \frac{dv_{y}}{dt} = m \cdot g - \frac{F \cdot y}{\ell}$$

$$dx = v_{x}$$

$$d2x = dv_{x}$$

$$\frac{dy}{dt} = v_{y}$$

$$d2y = \frac{dv_{y}}{dt}$$

$$x^{2} + y^{2} = \ell^{2}$$

$$x \cdot dx + y \cdot \frac{dy}{dt} = 0$$

$$dx^{2} + x \cdot d2x + \left(\frac{dy}{dt}\right)^{2} + y \cdot d2y = 0$$

- As additional variables were introduced in the differentiation, more equations needed to be differentiated.
- We now ended up with nine equations in the nine unknowns dv_x, x, F, dv_y/dt, dx, v_x, d2x, dy/dt, and d2y.
- Finally, another integrator had to be eliminated. We let go of the one defining the variable v_x.
- This set of equations represents an index-1 DAE problem that can be causalized using the tearing method.

Let us causalize those equations that we can:

$$m \cdot dv_{x} = -\frac{F \cdot x}{\ell}$$

$$m \cdot \frac{dv_{y}}{dt} = m \cdot g - \frac{F \cdot y}{\ell}$$

$$dx = v_{x}$$

$$d2x = dv_{x}$$

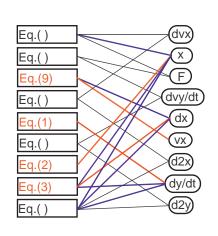
$$\frac{dy}{dt} = v_{y}$$

$$d2y = \frac{dv_{y}}{dt}$$

$$x^{2} + y^{2} = \ell^{2}$$

$$x \cdot dx + y \cdot \frac{dy}{dt} = 0$$

$$dx^{2} + x \cdot d2x + \left(\frac{dy}{dt}\right)^{2} + y \cdot d2y = 0$$

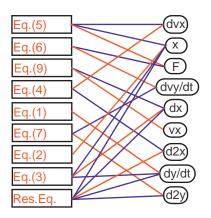


The Solvability Issue VII

- After causalizing all of the equations that we could using the Tarjan algorithm, we ended up with an algebraic loop in five equations and five unknowns.
- Since we have a choice, we decided to select a tearing variable that appears linearly in the residual equation.
- ▶ We chose d2x as our tearing variable, and the last equation as the residual equation.
- ▶ This selection allowed us to causalize all of the remaining equations.

The Solvability Issue VIII

Causalizing the remaining equations:



$$\frac{dy}{dt} = v_y$$

$$x = \pm \sqrt{\ell^2 - y^2}$$

$$dx = -\frac{y}{x} \cdot \frac{dy}{dt}$$

$$dv_x = d2x$$

$$F = -m \cdot \ell \cdot \frac{dv_x}{x}$$

$$\frac{dv_y}{dt} = g - \frac{F \cdot y}{m \cdot \ell}$$

$$d2y = \frac{dv_y}{dt}$$

$$d2x = -\frac{dx^2 + \left(\frac{dy}{dt}\right)^2 + y \cdot d2y}{x}$$

$$v_x = dx$$

The Solvability Issue IX

- ▶ The solution is formally correct. Our remaining state variables are y and v_y , and the resulting equations are thus perfectly causal except for the algebraic loop in the single tearing variable d2x that needs to be solved by Newton iteration.
- Yet, we are encountering new problems.
- First, the simulation will blow up with a division by zero, as soon as x = 0.
- Second, we seem to have a solvability issue, as we don't know which of the two roots to choose.

- Physics doesn't have a "solvability issue" with the pendulum. The problem is purely mathematical. Somehow, our model does not contain full information.
- Full information had not even been available in the original DAE model, but the conversion to ODE form using the Pantelides and Tarjan algorithms has made the problem worse.
- ▶ In the DAE formulation, x had been a state variable, and consequently, the DAE model "knew" that the pendulum cannot jump. From the ODE model, that knowledge is no longer evident. The variable x could change its sign at any point in time, making the pendulum jump instantaneously from one side to the other.
- From our physical understanding, we know that we must choose the positive root for x>0 and the negative root for x<0. We also know that the pendulum will swing through x=0, i.e., as we pass through zero, we need to switch to the other root. Yet, our mathematical description doesn't contain that information.

- One way to get around the solvability issue in the case of the pendulum system is to select another set of state variables.
- A far better choice of state variables would have been the angle φ and the angular velocity $\dot{\varphi}$.
- Unfortunately, these variables don't appear in our previous model at all.
- ► For this reason, it may be best to reformulate the original DAE model.

$$m \cdot \frac{dv_x}{dt} = -\frac{F \cdot x}{\ell}$$

$$m \cdot \frac{dv_y}{dt} = m \cdot g - \frac{F \cdot y}{\ell}$$

$$\frac{dx}{dt} = v_x$$

$$\frac{dy}{dt} = v_y$$

$$x = \ell \cdot \sin(\varphi)$$

$$y = \ell \cdot \cos(\varphi)$$

Let us apply the Pantelides algorithm to our modified DAE system:

$$m \cdot \frac{dv_x}{dt} = -\frac{F \cdot x}{\ell}$$

$$m \cdot \frac{dv_y}{dt} = m \cdot g - \frac{F \cdot y}{\ell}$$

$$\frac{dx}{dt} = v_x$$

$$dy = v_y$$

$$x = \ell \cdot \sin(\varphi)$$

$$\frac{dx}{dt} = \ell \cdot \cos(\varphi) \cdot d\varphi$$

$$y = \ell \cdot \cos(\varphi)$$

$$dy = -\ell \cdot \sin(\varphi) \cdot d\varphi$$

- The Pantelides algorithm solves Eq.(5) in the new set for φ . Consequently, Eq.(7) becomes our constraint equation that needs to be differentiated. It lets go of the integrator defining variable y in the process, i.e., $\frac{dy}{dt}$ is renamed into dy, and y is now an additional unknown.
- A new variable $d\varphi$ is introduced in the differentiation. Consequently, the equation defining φ , i.e., Eq.(5), needs to be differentiated as well.

The Solvability Issue XIII

- ▶ The Pantelides algorithm has no reason to select φ as a state variable on its own. It needs help.
- In Dymola, we can offer a choice of preferred state variables to the Pantelides algorithm.
- If we tell the algorithm that we wish to have φ as a state variable, a true state derivative, dφ/dt, will be generated in the process of differentiation in place of the algebraic variable. dφ.
- Consequently, another integrator needs to be removed, which will be the one defining variable x.

$$m \cdot \frac{dv_x}{dt} = -\frac{F \cdot x}{\ell}$$

$$m \cdot \frac{dv_y}{dt} = m \cdot g - \frac{F \cdot y}{\ell}$$

$$dx = v_x$$

$$dy = v_y$$

$$x = \ell \cdot \sin(\varphi)$$

$$dx = \ell \cdot \cos(\varphi) \cdot \frac{d\varphi}{dt}$$

$$y = \ell \cdot \cos(\varphi)$$

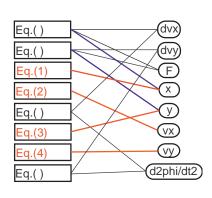
$$dy = -\ell \cdot \sin(\varphi) \cdot \frac{d\varphi}{dt}$$

- ► The resulting DAE system is still of index 2.
- Thus, the Pantelides algorithm must be applied once more.
- ▶ This time around, we shall tell Dymola to treat $\dot{\varphi}$ as an additional preferred state.
- ▶ We end up with 12 equations in 12 unknowns.

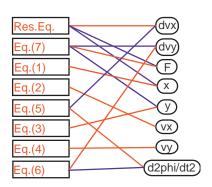
$$\begin{split} m \cdot dv_x &= -\frac{F \cdot x}{\ell} \\ m \cdot dv_y &= m \cdot g - \frac{F \cdot y}{\ell} \\ dx &= v_x \\ d2x &= dv_x \\ dy &= v_y \\ d2y &= dv_y \\ x &= \ell \cdot \sin(\varphi) \\ dx &= \ell \cdot \cos(\varphi) \cdot \frac{d\varphi}{dt} \\ d2x &= \ell \cdot \cos(\varphi) \cdot \frac{d^2\varphi}{dt^2} - \ell \cdot \sin(\varphi) \cdot \left(\frac{d\varphi}{dt}\right)^2 \\ y &= \ell \cdot \cos(\varphi) \\ dy &= -\ell \cdot \sin(\varphi) \cdot \frac{d\varphi}{dt} \\ d2y &= -\ell \cdot \sin(\varphi) \cdot \frac{d^2\varphi}{dt^2} - \ell \cdot \cos(\varphi) \cdot \left(\frac{d\varphi}{dt}\right)^2 \end{split}$$

Dymola performs one more type of symbolic preprocessing. It eliminates all trivial equations of the type a = b. Thus, we end up with eight equations in eight unknowns:

$$\begin{split} m \cdot dv_x &= -\frac{F \cdot x}{\ell} \\ m \cdot dv_y &= m \cdot g - \frac{F \cdot y}{\ell} \\ x &= \ell \cdot \sin(\varphi) \\ v_x &= \ell \cdot \cos(\varphi) \cdot \frac{d\varphi}{dt} \\ dv_x &= \ell \cdot \cos(\varphi) \cdot \frac{d^2\varphi}{dt^2} - \ell \cdot \sin(\varphi) \cdot \left(\frac{d\varphi}{dt}\right)^2 \\ y &= \ell \cdot \cos(\varphi) \\ v_y &= -\ell \cdot \sin(\varphi) \cdot \frac{d\varphi}{dt} \\ dv_y &= -\ell \cdot \sin(\varphi) \cdot \frac{d^2\varphi}{dt^2} - \ell \cdot \cos(\varphi) \cdot \left(\frac{d\varphi}{dt}\right)^2 \end{split}$$



We choose a tearing variable and a residual equation and finish causalization:



$$\begin{aligned} & x = \ell \cdot \sin(\varphi) \\ & v_x = \ell \cdot \cos(\varphi) \cdot \frac{d\varphi}{dt} \\ & y = \ell \cdot \cos(\varphi) \\ & v_y = -\ell \cdot \sin(\varphi) \cdot \frac{d\varphi}{dt} \\ & \frac{d^2\varphi}{dt^2} = \frac{dv_x}{\ell \cdot \cos(\varphi)} + \frac{\sin(\varphi)}{\cos(\varphi)} \cdot \left(\frac{d\varphi}{dt}\right)^2 \\ & dv_y = -\ell \cdot \sin(\varphi) \cdot \frac{d^2\varphi}{dt^2} - \ell \cdot \cos(\varphi) \cdot \left(\frac{d\varphi}{dt}\right)^2 \\ & F = \frac{m \cdot g \cdot \ell}{y} - \frac{m \cdot \ell \cdot dv_y}{y} \\ & dv_x = -\frac{F \cdot x}{m \cdot \ell} \end{aligned}$$

The Solvability Issue XVII

- Our remaining state variables are φ and $\frac{d\varphi}{dt}$, as desired, and the resulting equations are causal except for one algebraic loop in the single tearing variable dv_x that needs to be solved by Newton iteration.
- The former solvability issue is gone. We no longer have to choose between a positive and a negative root.
- Unfortunately, we are still facing a singularity issue. This is not a structural singularity, but rather a dynamic singularity.
- The simulation will work fine, as long as we don't let the pendulum swing beyond the horizontal position.
- ▶ Unfortunately, as y = 0, the simulation will once again blow up with a division by zero.

The Solvability Issue XVIII

- Many non-linear mechanical multi-body systems exhibit dynamic singularity issues when their dynamics are described in an object-oriented fashion by a set of DAEs.
- Dymola recognizes potential singularity issues during compilation. In such cases, Dymola will keep additional state variables in the set of equations and perform a dynamic state selection, i.e., Dymola will switch dynamically to another set of state variables on the fly as the current set approaches one of its singular points.

Conclusions

- ▶ In the previous three presentations on converting sets of DAEs to equivalent sets of ODEs, we concentrated for simplicity on *linear electric circuits* as examples, as these models are easily understandable.
- However, some issues don't show up in linear systems. In this final presentation on the symbolic preprocessing of DAE systems, we focused on precisely those remaining issues that can occur only in *non-linear systems*: the solvability issue and the dynamic singularity issue.
- ▶ Dymola recognizes *solvability issues* during compilation. To this end, Dymola avoids whenever possible to make use of state variables whose derivatives are to be solved from an equation, in which they appear in a non-linear form. Similarly, Dymola avoids to select tearing variables that appear in their residual equations in a non-linear form.

Conclusions II

▶ Dymola also recognizes dynamic singularity issues during compilation. To this end, Dymola avoids whenever possible to make use of state variables whose derivatives are multiplied by other variables in the equations from which they need to be solved, as these other variables would invariably turn up in the denominator after the symbolic manipulation. Similarly, Dymola avoids to select tearing variables that are multiplied by other variables in their residual equations. When this cannot be avoided, Dymola keeps additional state variables and/or additional tearing variables in the set of iteration variables.