The Specification of Transitions In DAE Embedded Hybrid Systems

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Introduction

Process simulation is a routinely used tool in chemical engineering and process analysis. While steady state simulation can be considered, more or less, a mature technology, dynamic models still pose challenges that increase with the incorporation of new features or formalisms that improve the capabilities of the software packages. One of the consequences of this continuously evolving and developing technology is the existence of applications with incomplete functionality, inaccurate algorithms or inefficient codes. Just to mention a decent process simulator that disappeared some years ago, SPEEDUP, notwithstanding the big claims of the comercial brochures, it was limited to index 1 differential-algebraic equations (DAEs), it was unable to correctly detect state events, support for model building (the Specify environment) was a little bit primitive and, to the surprise of the users coming from the steady-state world, one of the principal problems they have to face to run a simulation was to get initialized the model, solving a system of nonlinear algebraic equations.

Nowadays, a field in dynamic simulation where further research is needed is that of hybrid discrete/continuous systems, those exhibiting discrete and continuous state dynamics, important in many areas of science and engineering, in particular in chemical engineering. Several modeling formulations have been proposed to describe hybrid systems. In this paper we will refer to the hybrid automaton representation (Back et al., 1993; Galán & Barton, 1998) with embedded DAEs.

In the area of hybrid systems, one of the problems approached by researches in past years is that of transitions between different modes, specially when there is a discontinuity in the state variables or in the forcings. When the continuous part of the system is modeled by DAE, the solution is contained in a manifold, what imposes constraints not necessarily explicit on the variables, reducing the degrees of freedom. Only transitions leading to a consistent initialization in the new mode (consistent transitions and consistent reinitializations) are correct. Consistent initialization is related to the index of the DAE system, but the important quantity here is the dimension of the solution manifold.

Usually it is desired to keep continuity of the state variables over the transition (what is direct with ordinary differential equations, ODEs), but due to the manifold constraints several variables not known a priori may jump. Different authors have proposed methods to obtain consistent initial values in the new state after the transition when there is no explicit specification for the transfer of the states (the transition functions), leading to, e.g., the use of successive linear programming (Gopal & Biegler, 1999) or the so called natural transition functions (Barton & Lee, 2002; Reißig et al., 2002).

Unfortunately, those methods are not always applicable and are in many cases arbitrary since they exist other valid solutions. The main thrust of this paper is that there is no shortcut to the correct specification of the problem, which must include explicitly the transition functions. But the theory and software for modelling hybrid systems provides weak support for that specification.

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Hybrid Systems with Embedded DAEs

We will consider a system described by a state space $S = \bigcup_{k=1}^{n_k} S_k$ where each *mode* S_k is characterized by:

1. A set of variables $\{\dot{\mathbf{x}}^{(k)}, \mathbf{x}^{(k)}, \mathbf{y}^{(k)}, \mathbf{u}^{(k)}, \mathbf{p}, t\}$, where $\mathbf{x}^{(k)} \in \mathbf{R}^{n_x^{(k)}}$ are the differential state variables, $\mathbf{y}^{(k)} \in \mathbf{R}^{n_y^{(k)}}$ the algebraic state variables and $\mathbf{u}^{(k)} \in \mathbf{R}^{n_u^{(k)}}$ the controls. The time invariant parameters $\mathbf{p} \in \mathbf{R}^{n_p}$ and time t are independent variables. For convenience: $\mathbf{z}^{(k)} = [\mathbf{x}^{(k)}, \mathbf{y}^{(k)}]^T$.

2. A set of equations:

$$\mathbf{f}^{(k)}(\dot{\mathbf{x}}^{(k)}, \mathbf{x}^{(k)}, \mathbf{y}^{(k)}, \mathbf{u}^{(k)}, \mathbf{p}, t) = \mathbf{0} \tag{1}$$

usually a coupled system of differential and algebraic equations. In the mode S_k the specification of the parameters $\mathbf{p}$ and the controls coupled with a consistent initial condition $\mathbf{T}_k(\dot{\mathbf{x}}^{(k)}, \mathbf{x}^{(k)}, \mathbf{y}^{(k)}, \mathbf{u}^{(k)}, \mathbf{p}, t) = \mathbf{0}$ at $t = t_0^{(k)}$ determines the evolution of the system in $[t_0^{(k)}, t_f^{(k)})$.

3. A (possibly empty) set of transitions to other modes described by:

   (a) Transition conditions:

$$L_j^{(k)}(\dot{\mathbf{z}}^{(k)}, \mathbf{z}^{(k)}, \mathbf{u}^{(k)}, \mathbf{p}, t) \quad j \in J^{(k)}$$

   determining the transition times $t = t_f^{(k)}$ at which switching from mode k to mode j occurs. The transition conditions are formed by logical propositions that trigger the switching when they become true.

   (b) Transition functions:

$$\mathbf{T}_j^{(k)}(\dot{\mathbf{z}}^{(k)}, \mathbf{z}^{(k)}, \mathbf{u}^{(k)}, \dot{\mathbf{z}}^{(j)}, \mathbf{z}^{(j)}, \mathbf{u}^{(j)}, \mathbf{p}, t) \tag{2}$$

   associated with the transition conditions, relating the variables in the mode S_k and the variables in the new mode S_j at the transition time $t = t_f^{(k)}$. A special case of the transition functions is the set of initial conditions for the initial mode S_1.

In practice for many problems the transitions between modes affects only a few equations and variables and the specification of the model is concise.

Transition Functions

When the event is triggered by a transition condition the mapping between the variables in the previous mode (S_k, S_-) and the new mode (S_j, S_+) is described by the transition functions at time t_f^-:

$$\mathbf{T}_+^-(\dot{\mathbf{z}}^-, \mathbf{z}^-, \mathbf{u}^-, \dot{\mathbf{z}}^+, \mathbf{z}^+, \mathbf{u}^+, \mathbf{p}, t) = \mathbf{0} \tag{3}$$

Not all transitions functions are valid. Only transition functions that provide consistent initialization in the new mode (*consistent transitions*) are well posed. The consistency feature means that the initial state is contained in the solution manifold.

For DAEs the solution manifold is, in general, implicit, what makes difficult to specify the transition functions. In a first approach, we can consider three cases depending on the dimensions of the solution manifolds in the predecessor (δ_-) and successor (δ_+) modes at a transition:

1. If $\Delta^{\pm} = \delta_+ - \delta_- > 0$ it is compulsory to specify at least $\Delta^{\pm}$ additional transition functions, provided that it is possible to assume state continuity for the rest.

2. If $\delta_+ = \delta_-$ may be possible to assume state continuity without specify transition functions.

3. $\delta_+ - \delta_- < 0$ it is compulsory to specify δ_+ transition functions even if they are state continuity functions.

Linear Time Invariant DAEs

Let us consider the linear constant coefficient DAE:

$$\mathbf{A}\dot{\mathbf{z}} + \mathbf{B}\mathbf{z} = \mathbf{F}(t) \tag{4}$$

This system is solvable if $\lambda\mathbf{A} + \mathbf{B}$ is a regular pencil (Brenan et al., 1996). In this case, there exist nonsingular matrices $\mathbf{P}$ and $\mathbf{Q}$ such that:

$$\mathbf{z} = \mathbf{Q}\mathbf{w} \tag{5}$$

$$\mathbf{P}\mathbf{A}\mathbf{Q}\dot{\mathbf{w}} + \mathbf{P}\mathbf{B}\mathbf{Q}\mathbf{w} = \mathbf{P}\mathbf{F}(t) = \mathbf{F}'(t) \tag{6}$$

$$\mathbf{A}' = \mathbf{P}\mathbf{A}\mathbf{Q} = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{N} \end{bmatrix}, \quad \mathbf{B}' = \mathbf{P}\mathbf{B}\mathbf{Q} = \begin{bmatrix} \mathbf{C} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \tag{7}$$

where $\mathbf{N}$ is a matrix of nilpotency ν (the differential index). The dimension δ of the solution manifold $\mathbf{z}(t)$ is equal to the dimension of $\mathbf{I}$ in $\mathbf{A}'$ and the transition function to the mode cannot specify more than δ values of $\mathbf{z}$ and $\dot{\mathbf{z}}$.

The resulting system after the change of coordinates is:

$$\dot{\mathbf{w}}_1 + \mathbf{C}\mathbf{w}_1 = \mathbf{F}_1 \tag{8}$$

$$\mathbf{N}\dot{\mathbf{w}}_2 + \mathbf{w}_2 = \mathbf{F}_2 \tag{9}$$

The second equation has the only one solution, that depends on the forcing functions:

$$\mathbf{w}_2 = \sum_{i=0}^{\nu-1} (-1)^i \mathbf{N}^i \frac{\partial^i \mathbf{F}_2}{\partial t^i} \tag{10}$$

algebraic equation that defines the solution manifold:

$$\mathbf{w}_2 = \mathbf{Q}_2^{-1}\mathbf{z} \tag{11}$$

$$\text{with } \mathbf{Q}^{-1} = \begin{bmatrix} \mathbf{Q}_1^{-1} \\ \mathbf{Q}_2^{-1} \end{bmatrix} \tag{12}$$

If:

$$\mathbf{T}_+^-(\mathbf{z}^-, \mathbf{z}^+, \mathbf{u}, \mathbf{p}, t) = \mathbf{T}_+^-(\mathbf{z}^+, t) = \mathbf{0} \tag{13}$$

is the transition function from mode $-$ to $+$ a sufficient condition for it to be a well posed transition is that:

$$\mathbf{T}_+^-(\mathbf{z}^+, t_f^-) = \mathbf{0} \tag{14}$$

$$\mathbf{w}_2^+ = \mathbf{Q}_2^{-1}\mathbf{z}^+ \tag{15}$$

is a solvable system. If, additionally, transition functions are linear in $\mathbf{z}^+$, these are well posed if and only if the previous system is nonsingular.

Example: the problem

Let consider the mechanical system formed by two rotating masses used by Mattsson (1989) and whose transitions were studied later by Barton & Lee (2002). The masses, whose axis of rotation coincides, can be connected by a rigid coupling or a slip coupling. When the slip coupling is acting, the physical system can be described by the following equations:

$$I_1\dot{\omega}_1 = \tau_1 + \tau_{2,1} \tag{16}$$

$$I_2\dot{\omega}_2 = \tau_2 - \tau_{2,1} \tag{17}$$

$$\tau_{2,1} = d(\omega_2 - \omega_1) \tag{18}$$

where I_1, I_2 are the moments of inertia (subindex 1 and 2 refers to each mass), ω_1, ω_2 the angular velocities and τ_1, τ_2 the torques, known functions of time. The damping coefficient d relates the transmitted torque $\tau_{2,1}$ to the slip velocity. When the coupling is rigid, the last equation is substituted by:

$$\omega_1 - \omega_2 = 0 \tag{19}$$

Example: the specification

For this example:

$$\mathbf{F}(t) = \begin{bmatrix} \tau_1(t) \\ \tau_2(t) \\ 0 \end{bmatrix} \quad \mathbf{z} = \begin{bmatrix} \omega_1 \\ \omega_2 \\ \tau_{2,1} \end{bmatrix} \tag{20}$$

In the slipping mode:

$$\mathbf{A} = \begin{bmatrix} I_1 & 0 & 0 \\ 0 & I_2 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad \mathbf{B} = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & 1 \\ d & -d & 1 \end{bmatrix} \tag{21}$$

changing $\mathbf{B}$ when the coupling is rigid to:

$$\mathbf{B} = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & 1 \\ 1 & -1 & 0 \end{bmatrix} \tag{22}$$

The dimensions of the solution manifolds are $\delta_1 = 2$ and $\delta_2 = 1$ for each mode, being the index of the systems $\nu_1 = 1$ and $\nu_2 = 2$ respectively. Let us concentrate on the transition from mode 1 ($-$) to mode 2 ($+$). According to Eq. (11):

$$\mathbf{w}_2 = \mathbf{Q}_2^{-1}\mathbf{z} = \begin{bmatrix} -\dfrac{I_1 I_2}{I_1 + I_2} & \dfrac{I_1 I_2}{I_1 + I_2} & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \omega_1 \\ \omega_2 \\ \tau_{1,2} \end{bmatrix} \tag{23}$$

Also:

$$\mathbf{F}_2 = \mathbf{P}_2\mathbf{F} = \begin{bmatrix} 0 & 0 & -\dfrac{I_1 I_2}{I_1 + I_2} \\ -\dfrac{I_2}{I_1 + I_2} & \dfrac{I_1}{I_1 + I_2} & 0 \end{bmatrix} \begin{bmatrix} \tau_1 \\ \tau_2 \\ 0 \end{bmatrix} \tag{24}$$

and:

$$\mathbf{N} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \tag{25}$$

From Eqs. (10), (23) and (24), the solution manifold is determined by:

$$\omega_1 = \omega_2 \tag{26}$$

$$\tau_{2,1} = \frac{I_1\tau_2 - I_2\tau_1}{I_1 + I_2} \tag{27}$$

Thus, from purely mathematic arguments, there is still a degree of freedom left to specify the transition functions. If we use physical considerations, a reasonable constraint is the conservation of angular momentum:

$$I_1\omega_1^- + I_2\omega_2^- = (I_1 + I_2)\omega_1^+ \tag{28}$$

or equivalently, the energy balance taking into account the dissipated energy:

$$\frac{1}{2}I_1(\omega_1^-)^2 + \frac{1}{2}I_2(\omega_2^-)^2 = \frac{1}{2}(I_1 + I_2)(\omega_1^+)^2 + \frac{I_1 I_2(\omega_1^- - \omega_2^-)^2}{2(I_1 + I_2)} \tag{29}$$

Barton & Lee (2002) apply the theorems developed by Reißig et al. (2002), (the analysis of those theorems is out of the scope of this paper), to obtain the *natural* transition function for this case, what happens to be precisely conservation of angular momentum. This fact suggest that it is possible to implement on software packages methods to automatically derive the (natural) transition functions relieving the engineer from that task, and even that there is a physical foundation for these transition functions incorporated in the mathematics.

Revisiting the example considered, what we are dealing with could be seen as a simplified model of a clutch. Actually, it is at the transition where the complications of the phenomena occurring during engagement and disengagement are radically reduced. This is one of the reasons to use hybrid discrete-continuous models: to obtain simpler, efficient models that retain the essential characteristics of the system. But the price to pay is not so extreme simplicity, we still have degrees of freedom left to model the transitions and introduce the relevant information there. In fact, we *must* model the transition and we do it, either explicitly or relying on the program that, in the best case, will find the natural transition functions.

For the example of the clutch, a more realistic transition condition in form of energy dissipation (Howrie, 1987) is:

$$E = \frac{1}{2}\frac{I_1 I_2\left((\omega_1^-)^2 - (\omega_2^-)^2\right)}{I_1\left(1 - \dfrac{\tau_2^-}{\tau_d}\right) - I_2\left(1 - \dfrac{\tau_1^-}{\tau_d}\right)} \tag{30}$$

where τ_d is the dynamic torque clutch capacity, function of the friction coefficient and the clutch engagement force.

Conclusions

The specification of the transition functions in hybrid discrete continuous systems is a modelling issue. It is necessary the implementation of software tools in modelling and simulation environments that enforce valid transition functions, differentiating what is a mathematical requirement and what is a reasonable help.