THE SPECIFICATION OF TRANSITIONS IN DAE EMBEDDED HYBRID SYSTEMS

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Abstract

Hybrid discrete/continuous systems, those exhibiting discrete and continuous state dynamics are important in chemical engineering. The transitions between different modes, the distinctive feature of these systems, are subject to the constraints, sometimes implicit, imposed by the solution manifold and, even when the transition functions contain relevant information in a hybrid model, there is still weak support on current software packages to help the engineer formulate valid transitions. On the other hand, the theoretical developments to obtain consistent reinitializations are in some way hiding the real degrees of freedom of the modeller.

Keywords

Transitions, Hybrid discrete/continuous, Differential-algebraic equations.

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).

Brüll & Pallaske (1992) study classes of nonlinear index 1 DAEs, and in some cases are able to identify functions of the state variables that remain continuous at a discontinuity in the forcing functions, yielding fully determined consistent initialization problems. Majer et al. (1995) also study classes of nonlinear index 1 DAEs and identify subsets of state variables that remain continuous, yielding either fully or under determined consistent initialization problems.

Gopal & Biegler (1999) consider linear time invariant (LTI) DAEs of arbitrary index subject to discontinuous forcing. They argue that the dependence of an underlying ODE (UODE) of the DAE on the derivatives of the forcing functions may be employed to identify which state variables are continuous at such discontinuities. In general this yields an under determined consistent initialization problem because

the number of continuous state variables may be less than the degrees of freedom available. Barton & Galán (2000) show that in fact, for LTI DAEs of arbitrary index, this consistent initialization problem can be viewed as always fully and uniquely determined. One may conjecture that this observation extends to general nonlinear DAEs, but proof appears to be very difficult.

Rabier & Rheinboldt (1996) develop a comprehensive existence and uniqueness theory for linear DAEs with discontinuous forcing when the coefficient matrices are smooth functions of time. These authors remark that, at least in principle, there is a unique and calculable jump in the state at a discontinuity in the forcing. In closing, they develop highly tailored numerical algorithms for the index 1 and index 2 cases (only), based on the 'reduction procedure' also employed for their theoretical development.

Mosterman (2000) considers that a minimum norm approach can be applied at transitions when algebraic constraints are activated, but since in general the mapping obtained using this method is not physically sound, derives an approach based on the Kronecker Canonical Form (KCF). The result is similar to the one in (Barton & Galán, 2000) that also anticipated the use of the generalized upper triangular form of a matrix pencil, which can be computed stably, for example, with the subroutine GUPTRI (Demmel & Kågström, 1993b,a), as a practical approach to the use of KCF for transitions. The drawback is the inherent density of the matrices required for the transformation. Later, Mosterman (2003) will apply this solution.

Reißig et al. (2002) present an elegant method to compute consistent transitions for LTI DAEs, providing a relatively simple justification to the use of the Laplace transform and developing a practical method to compute the solution using LU factorization. This approach is the base for the natural transition functions mentioned in Barton & Lee (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.

To shed light on a sometimes controversial issue that paradoxically is somewhat conceptually simple, the almost classical example of the coupling/uncoupling rotating masses, used by some authors to illustrate their approaches, is revisited, showing where the border separating mathematics and physics lies. This problem is modelled by LTI DAEs, the simplest case for which the general analytical and numerical behaviour is well understood. For general nonlinear DAEs, structural methods are the common practical approach for consistent initialization in real problems: The results are valid in most of the cases.

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:

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

$$\mathbf{PAQ}\dot{\mathbf{w}} + \mathbf{PBQ}\mathbf{w} = \mathbf{PF}(t) = \mathbf{F}'(t) \tag{6}$$

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

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

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:

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

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:

$$\frac{1}{2}I_1(\omega_1^-)^2+\frac{1}{2}I_2(\omega_2^-)^2 = \frac{1}{2}(I_1+I_2)(\omega_1^+)^2+\frac{I_1I_2(\omega_1^- - \omega_2^-)^2}{2(I_1 + I_2)} \tag{29}$$

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:

$$E = \frac{1}{2}\frac{I_1I_2\left((\omega_1^-)^2 - (\omega_2^-)^2\right)}{I_1\left(1 - \frac{\tau_2^-}{\tau_d}\right) - I_2\left(1 - \frac{\tau_1^-}{\tau_d}\right)} \tag{30}$$

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.

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