A THIRD ORDER DISCRETE EVENT METHOD FOR CONTINUOUS SYSTEM SIMULATION
Part I: Theory

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***Abstract*— This paper introduces a new numerical method for integration of ordinary differential equations. Following the principles of QSS and QSS2, i.e., replacing the time discretization by state quantization, this new method performs a third order approximation allowing to achieve better accuracy than their first and second order predecessors. It is shown that the new algorithm –called QSS3– satisfies the same theoretical properties of the latter methods and also shares their main practical advantages in the numerical integration of discontinuous systems.**

***Keywords*— Hybrid systems, ODE integration, Discrete Event Systems.**

I INTRODUCTION

Numerical integration of ordinary differential equations (ODE's) is a topic which has advanced significantly with the appearance of modern computers. Based on classic methods like Euler, Runge–Kutta, Adams, etc., several variable–step and implicit ODE solver methods were developed (Hairer *et al.*, 1993; Hairer and Wanner, 1991). Simultaneously, several software simulation packages have been developed implementing these algorithms. Among them, Matlab/Simulink (Shampine and Reichelt, 1997) is probably the most popular and one of the most efficient.

In spite of the several differences between the mentioned ODE solver algorithms, all of them share a property: they are based on time discretization. This is, they give a solution obtained from a difference equation system (i.e. a discrete–time model) which is only defined in some discrete instants.

A completely different approach for ODE numerical integration started to develop since the end of the 90's, in which time discretization is replaced by state variables quantization. As a result, the simulation models are not discrete time but discrete event (in terms of the DEVS formalism (Zeigler *et al.*, 2000)).

The origin of this idea can be found in the definition of Quantized Systems (Zeigler and Lee, 1998). Quantized Systems were reformulated with the addition of hysteresis –to avoid the appearance of infinitely fast oscillations– and formalized as a numerical algorithm for ODE's in (Kofman and Junco, 2001), where the Quantized State Systems (QSS) and the QSS method were defined.

The following step was the definition of the QSS2 method (Kofman, 2002), which performs a second order approximation, and then both methods were extended to the simulation of differential algebraic equations (Kofman, 2003) and discontinuous systems (Kofman, 2004).

The discrete event nature of these methods make them particularly efficient in the last case, and a considerable reduction of computational costs with respect to the most sophisticated discrete time methods can be observed.

Despite their simplicity, the QSS and QSS2 methods satisfy some strong stability, convergence and error bound properties, and they intrinsically exploit sparsity in a very efficient fashion.

This paper continues the previous works by formulating a third order method, called QSS3, which permits improving the accuracy of QSS and QSS2 conserving their main theoretical and practical advantages. An additional advantage of QSS3 is that the choice of the quantum becomes less critical than in the lower order methods since it can be adopted in a conservative fashion without affecting considerably the number of calculations.

After a brief introduction recalling the principles of quantization based integration, the definition of the QSS3 method will be introduced. Then, we shall prove that it is *legitimate*, i.e., that it cannot produce a Zeno–like behavior, and we shall deduce the input–output relationships of the basic components of QSS3 (quantized integrators and static functions). Finally, we shall introduce a brief discussion about the theoretical properties of QSS3.

The implementation issues and practical results were included in the companion paper (Kofman, 2005). There, the mentioned input–output relationships of the elementary blocks will be expressed by the corresponding DEVS atomic models that will implement the method. Some relatively complex examples will also show that the QSS3 method is a particularly efficient algorithm for accurate simulation of strongly discontinuous systems.

II QUANTIZATION BASED INTEGRATION

A QSS–Method

Consider a time invariant ODE in its State Equation System (SES) representation:

$$\dot{x}(t) = f(x(t), u(t)) \tag{1}$$

where $x(t) \in \mathbb{R}^n$ is the state vector and $u(t) \in \mathbb{R}^m$ is an input vector, which is a known piecewise constant function.

The QSS–method (Kofman and Junco, 2001) simulates an approximate system, which is called Quantized State System:

$$\dot{x}(t) = f(q(t), u(t)) \tag{2}$$

where $q(t)$ is a vector of *quantized variables* which are quantized versions of the state variables $x(t)$. Each component of $q(t)$ is related with the corresponding component of $x(t)$ by a hysteretic quantization function, which is defined as follows:

Definition 1. *Let $Q = \{Q_0, Q_1, ..., Q_r\}$ be a set of real numbers where $Q_{k-1} < Q_k$ with $1 \leq k \leq r$. Let Ω be the set of piecewise continuous real valued trajectories and let $x_i \in \Omega$ be a continuous trajectory. Let $b : \Omega \to \Omega$ be a mapping and let $q_i = b(x_i)$ where the trajectory q_i satisfies:*

$$q_i(t) = \begin{cases} Q_m & \text{if} \quad t = t_0 \\ Q_{k+1} & \text{if} \quad x_i(t) = Q_{k+1} \wedge \\ & \qquad \wedge q_i(t^-) = Q_k \wedge k < r \\ Q_{k-1} & \text{if} \quad x_i(t) = Q_k - \varepsilon \wedge \\ & \qquad \wedge q_i(t^-) = Q_k \wedge k > 0 \\ q_i(t^-) & \qquad \text{otherwise} \end{cases} \tag{3}$$

and

$$m = \begin{cases} 0 & \text{if } x_i(t_0) < Q_0 \\ r & \text{if } x_i(t_0) \geq Q_r \\ j & \text{if } Q_j \leq x(t_0) < Q_{j+1} \end{cases}$$

Then, the map b is a hysteretic quantization function.

The discrete values Q_k are called *quantization levels* and the distance $Q_{k+1} - Q_k$ is defined as the *quantum*, which is usually constant. The width of the hysteresis window is ε and, as it was shown in (Kofman *et al.*, 2001), it is better to take it equal to the quantum.

In (Kofman and Junco, 2001) it was proven that the quantized variable trajectories $q_i(t)$ and the state derivatives $\dot{x}_i(t)$ are piecewise constant and the state variables $x_i(t)$ are piecewise linear. As a consequence, those trajectories can be represented by sequences of events and then the QSS can be simulated by a DEVS model.

The mapping of a QSS like (2) into a DEVS model can be done in several ways and one of the easiest is based on coupling principles. A generic QSS can be represented by the block diagram of Fig.1. That block diagram is composed by static functions f_i, integrators and quantizers.

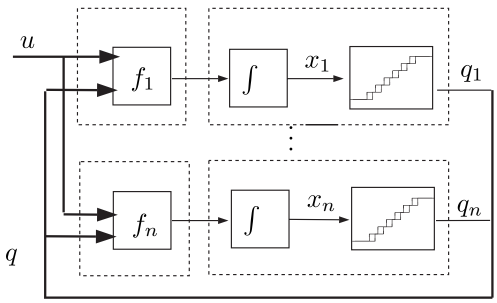

Figure 1: Block Diagram Representation of a QSS

Each pair formed by an integrator and a quantizer is called *quantized integrator* and it is equivalent to a simple DEVS model. Similarly, the static functions have DEVS equivalents and consequently, the entire block diagram has an equivalent coupled DEVS which represents it. The mentioned DEVS models can be found in (Kofman and Junco, 2001).

Some simulation programs –PowerDEVS (Pagliero and Lapadula, 2002) for instance– have libraries with DEVS blocks representing quantized integrators and static functions. Thus, the implementation of the QSS–method consists in building the block diagram in the same way that it could be done in Simulink.

B QSS2–Method

QSS only performs a first order approximation. Due to accuracy reasons, a second order method was proposed in (Kofman, 2002) which also shares the main properties and advantages of QSS.

The basic idea of the new method, (called QSS2) is the use of first–order quantization functions instead of the quantization function given by (3). Then, the simulation model can be still represented by (2) but now $q(t)$ and $x(t)$ have a different relationship. This new system is called Second Order Quantized State System or QSS2 for short.

A first–order quantization function can be seen as a function which gives a piecewise linear output trajectory, whose value and slope change when the difference between this output and the input becomes bigger than certain threshold (Fig. 2)

In that way, the quantized variable trajectories are piecewise linear and the state trajectories are piece-

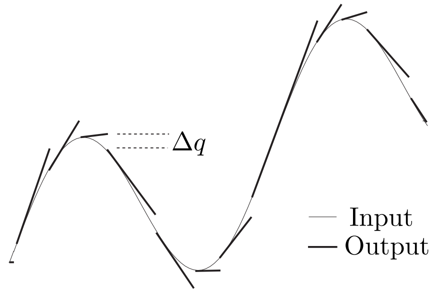

Figure 2: I/O trajectories in a *First Order* quantizer

wise parabolic[1].

As before, the system can be divided into quantized integrators and static functions like in Fig.1. However, the DEVS models of the QSS2 quantized integrators are different due to the new behavior of the quantizers. Similarly, the DEVS models of the QSS2 static functions are also different since they should take into account the slopes of the piecewise linear trajectories.

The formal definition of first order quantization functions and the DEVS models associated to the QSS2 integrators and static functions can be found in (Kofman, 2002).

Thus, the QSS2–method can be applied to ODE systems in a similar way to QSS, i.e., building a block diagram composed with the blocks representing integrators and static functions.

C Properties of QSS and QSS2

There are properties –which were proven in (Kofman and Junco, 2001) and (Kofman, 2002)– relating the solutions of Systems (1) and (2). These properties not only show theoretical features but also allow deriving rules for the choice of the quantization according to the desired accuracy.

The mentioned properties are stability, convergence and error bound and the corresponding proofs were built based on perturbation studies. In fact, defining $\Delta x(t) = q(t) - x(t)$, System (2) can be rewritten as

$$\dot{x}(t) = f(x(t) + \Delta x(t), u(t)) \qquad (4)$$

From the definition of the hysteretic and the first order quantization functions, it can be ensured that each component of Δx is bounded by the corresponding quantum adopted. Thus, the QSS and QSS2 methods simulate an approximate system which only differs from the original SES (1) due to the presence of the bounded state perturbation $\Delta x(t)$.

The Convergence Property ensures that an arbitrarily small error can be achieved by using a sufficiently small quantization. A sufficient condition which guarantees this property is that the function f is locally Lipschitz.

[1]In nonlinear systems this is only approximated.

The Stability Property relates the quantum adopted with the final error. An algorithm can be derived from the proof of this property which allows the choice of the quantum to be used in the different state variables.

Finally, the Global Error Bound is probably the most important property of quantization based methods. Given a LTI system $\dot{x}(t) = Ax(t) + Bu(t)$ where A is a Hurwitz and diagonalizable matrix, the error in the QSS or QSS2 simulation is always bounded by

$$|\tilde{\phi}(t) - \phi(t)| \leq |V||\mathbb{R}\mathrm{e}(\Lambda)^{-1}\Lambda||V^{-1}|\Delta q \qquad (5)$$

where Λ and V are the matrices of eigenvalues and eigenvectors of A (Λ is diagonal), that is, $V^{-1}AV = \Lambda$ and Δq is the vector of quantum adopted at each component[2].

Inequality (5) holds for all t, for any input trajectory and for any initial condition.

III QSS3 METHOD

In order to obtain a third order approximation, we need to consider not only the first but also the second derivative of the system trajectories. Thus, we can redefine the first order quantizer shown in Fig.2 so that the output is piecewise parabolic.

Then, given a system of state equations like (1), the QSS3 method will approximate it by (2) where x and q are related component-wise by *second order quantization functions.*

A Second order quantization

Formally, we say that the trajectories $x_i(t)$ and $q_i(t)$ are related by a second order quantization function if $q_i(t_0) = x_i(t_0)$ and

$$q_i(t) = \begin{cases} x_i(t) & \text{if } |q_i(t^-) - x_i(t^-)| = \Delta q_i, \\ q_i(t_j) + m_{i_j}(t-t_j) + p_{i_j}(t-t_j)^2 & \\ \text{otherwise,} & \end{cases} \qquad (6)$$

with $t_j \leq t < t_{j+1}$, and the sequence $t_0, \ldots, t_j, \ldots$ defined so that t_{j+1} is the minimum $t > t_j$ where

$$|x_i(t_j) + m_{i_j}(t-t_j) + p_{i_j}(t-t_j)^2 - x_i(t)| = \Delta q_i \quad (7)$$

and the slopes

$$m_{i_0} = 0, \quad m_{i_j} = \dot{x}_i(t_j^-), \quad j = 1, \cdots \qquad (8)$$

$$p_{i_0} = 0, \quad p_{i_j} = \ddot{x}_i(t_j^-), \quad j = 1, \cdots \qquad (9)$$

B Trajectories in QSS3

The basis of QSS and QSS2 are the trajectory forms that allow the discrete event representation. A crucial requirement is the legitimacy condition which requires that a finite number of events occurs in any finite interval of time.

[2]Symbol $|\cdot|$ denotes the component-wise module of a complex matrix or vector and symbol "$\leq$" in (5) also denotes a component-wise inequality.

Although the definition of a second order quantization function (6) suggests that the components of $q(t)$ are piecewise parabolic, it should be proven that the sequence t_j does not have infinite components in a finite interval of time. The following theorem gives sufficient conditions to this property.

Theorem 1. *Consider system (2). Assume that the input $u(t)$ is bounded and left differentiable and function f is continuously differentiable. Then, the components of $q(t)$ are piecewise parabolic while it remains inside any bounded set $D \subset \mathbb{R}^n$.*

Proof. Let $q_i(t)$ be an arbitrary component of $q(t)$. Taking into account (6) and the fact that $t_{j+1} > t_j$, ensuring that $q_i(t)$ is piecewise parabolic is equivalent to prove that

$$\lim_{j\to\infty} t_j = \infty$$

We shall start assuming the opposite, i.e.,

$$\lim_{j\to\infty} t_j = T \tag{10}$$

which implies that

$$\lim_{j\to\infty} (t_{j+1} - t_j) = 0$$

and then, given $\epsilon > 0$, a natural N exists so that

$$(t_{j+1} - t_j) < \epsilon \;\; \forall j > N \tag{11}$$

Continuously differentiability of f and left differentiability of $u(t)$ with the conditions $q(t) \in D$ and $\|u(t)\| < U$ imply that positive constants F_i, F_{i_q}, F_{i_u} and U_t exist so that

$$|f_i(q,u)| < F_i, \qquad \|\frac{\partial f_i}{\partial q}\| \le F_{i_q}$$
$$\|\frac{\partial f_i}{\partial u}\| \le F_{i_u}, \qquad \|\frac{du}{dt}(t^-)\| \le U_t$$

Then, from (8) it results that

$$|m_{i_j}| = |\dot{x}_i(t_j^-)| = |f_i(q,u)| < F_i \tag{12}$$

and, from (9), we have

$$\begin{aligned} |p_{i_{j+1}}| &= |\ddot{x}_i(t_{j+1}^-)| = |\frac{\partial f_i}{\partial q}\frac{dq}{dt}(t_{j+1}^-) + \frac{\partial f_i}{\partial u}\frac{du}{dt}(t_{j+1}^-)| \\ &< F_{i_q}|\frac{dq}{dt}(t_{j+1}^-)| + F_{i_u}U_t = \\ &= F_{i_q}|m_{i_j} + 2p_{i_j}(t_{j+1}-t_j)| + F_{i_u}U_t \\ &< F_{i_q}[F_i + 2|p_{i_j}|(t_{j+1}-t_j)] + F_{i_u}U_t \end{aligned}$$

Using (11) it results that, when $j > N$, it is true that

$$|p_{i_{j+1}}| < F_{i_q}(F_i + 2|p_{i_j}|\epsilon) + F_{i_u}U_t$$

Choosing $\epsilon = 1/4F_{i_q}$ we get

$$|p_{i_{j+1}}| < F_{i_q}F_i + F_{i_u}U_t + \frac{|p_{i_j}|}{2}$$

Thus, when $j > N$, the succession p_{i_j} can only grow if $|p_{i_j}| < 2(F_{i_q}F_i + F_{i_u}U_t)$. Then,

$$|p_{i_j}| < P_i \;\; \forall j \ge 0 \tag{13}$$

where

$$P_i \triangleq \max[2(F_{i_q}F_i + F_{i_u}U_t), \max_{0\le j\le N}(|p_{i_j}|)]$$

From (7) it follows that

$$\Delta q_i = |x_i(t_j) + m_{i_j}(t_{j+1}-t_j) + p_{i_j}(t_{j+1}-t_j)^2 - x_i(t_{j+1})|$$

Continuity of x_i ensures that

$$|x_i(t_j) - x_i(t_{j+1})| < F_i(t_{j+1} - t_j)$$

and then, using (12) and (13) we obtain

$$\Delta q_i < 2F_i(t_{j+1} - t_j) + P_i(t_{j+1} - t_j)^2$$

and

$$t_{j+1} - t_j > \frac{\sqrt{F_i^2 + P_i\Delta q_i} - F_i}{P_i}$$

which contradicts (10) and completes the proof. □

Corollary 1. *When f is (piecewise) linear w.r.t. x and u, and $u(t)$ is piecewise parabolic, the state derivatives $\dot{x}_i(t)$ are piecewise parabolic and the state variables $x_i(t)$ follow piecewise cubic trajectories.*

In the nonlinear cases, we cannot say anything about the form of the state trajectories. However, we can approximate function f by a piecewise linear one. Similarly, when $u(t)$ is not piecewise parabolic, we can use a piecewise parabolic approximation. Thus, we shall consider that the state trajectories and their derivatives are piecewise cubic and parabolic respectively.

Thus, as we did in QSS and QSS2, we can divide the system (2) into quantized integrators and static functions as shown in Fig.1 so that each subsystem has piecewise parabolic input and output trajectories.

C Third order quantized integrator

Quantized integrators in QSS3 will have piecewise parabolic input and output trajectories. They calculate $q_i(t)$ from $d_i(t) \triangleq \dot{x}_i(t)$. We shall deduce here the relationship between these trajectories in order to build an equivalent DEVS model. In order to simplify the notation, we shall eliminate the sub–index i.

Let $d(t)$ be a known piecewise parabolic trajectory

$$d(t) = d(\tau_k) + m_{d_k}(t - \tau_k) + p_{d_k}(t - \tau_k)^2$$

where $\tau_k \le t < \tau_{k+1}$. Notice that $d(t)$ is defined by the sequences τ_k, $d(\tau_k)$, m_{d_k} and p_{d_k}.

Let $x(t)$ be its integral, then

$$x(t) = x(\tau_k)+d(\tau_k)(t-\tau_k)+m_{d_k}\frac{(t-\tau_k)^2}{2}+p_{d_k}\frac{(t-\tau_k)^3}{3}$$

and let $q(t)$ be a second order quantized version of $x(t)$. Taking into account that it is piecewise parabolic, $q(t)$ can be written as

$$q(t) = q(t_j) + m_{q_j}(t - t_j) + p_{q_j}(t - t_j)^2$$

with $q(t_0) = x(t_0)$ (the initial condition) and $m_{q_0} = p_{q_0} = 0$. After that, the quantized variable can be calculated as

$$\begin{aligned} q(t_j) &= x(t_j) = x(\tau_k) + d(t_j)(t_j - \tau_k) + \\ &+ m_{d_k}\frac{(t_j-\tau_k)^2}{2} + p_{d_k}\frac{(t_j-\tau_k)^3}{3} \end{aligned}$$

and their first and second derivatives are

$$\begin{aligned} m_{q_j} = d(t_j) &= d(\tau_k) + m_{d_k}(t_j - \tau_k) + p_{d_k}(t_j - \tau_k)^2 \\ p_{q_j} = \dot{d}(t_j) &= m_{d_k} + 2p_{d_k}(t_j - \tau_k) \end{aligned}$$

This allows to calculate the output sequences $q(t_j)$, m_{q_j} and p_{q_j}. The time succession t_j can be calculated by

$$t_{j+1} = \min[t/|q(t^-) - x(t)| = \Delta q_i] \qquad (14)$$

with $t > t_j$. Notice that the calculation of t_{j+1} requires solving a cubic equation to determine when the difference between $q(t)$ and $x(t)$ becomes equal to the quantum.

Then, given a piecewise parabolic trajectory $d(t)$ expressed by a sequence of events carrying the values $d(\tau_k)$,m_{d_k} and p_{d_k}, we can calculate the trajectory $q(t)$, expressed as another sequence of events with values $q(t_j)$, m_{q_j} and p_{q_j}.

This behavior can be easily represented by an atomic DEVS model that we shall call *third order quantized integrator*. The mentioned DEVS model can be found in the companion paper (Kofman, 2005).

D Static functions

The right hand side of (2) is composed by n functions $f_i(q, u)$. Since q and u follow piecewise parabolic trajectories, in the linear case, the output $\dot{x}_i(t)$ will be also piecewise linear.

In order to obtain a DEVS model relating the input and output trajectories of such a function we shall consider a linear function

$$d(t) = \sum_{i=1}^{N} a_i v_i(t)$$

where

$$v_i(t) = v_i(t_{i_k}) + m_{v_i,k}(t - t_{i_k}) + p_{v_i,k}(t - t_{i_k})^2$$

so that

$$d(t) = \sum_{i=1}^{N} a_i v_i(t_{i_k})+a_i\cdot m_{v_i,k}(t-t_{i_k})+a_i\cdot p_{v_i,k}(t-t_{i_k})^2$$

This expression defines $d(t)$, and the sequences $d(\tau_k)$,m_{d_k} and p_{d_k} which allow expressing the trajectory as a sequence of events.

A DEVS model of this behavior is almost straightforward.

The nonlinear case is a bit more complicated. Here, $d(t)$ is no longer piecewise parabolic. However, we can approximate it by a piecewise parabolic trajectory, discarding the higher order terms.

We have

$$d(t) = f_i(v_1(t), \cdots, v_N(t)) = f_i(v(t))$$

where

$$v(t) = v(\tau_k) + m_{v_k}(t - \tau_k) + p_{v_k}(t - \tau_k)^2$$

Using Taylor's formulae, we have

$$\begin{aligned} d(t) &= f_i(v(\tau_k)) + \frac{\partial f_i}{\partial v}(v(t) - v(\tau_k)) + \\ &+ \frac{\partial^2 f_i}{\partial v^2}\frac{(v(t)-v(\tau_k))^2}{2!} + \cdots \end{aligned}$$

and then

$$\begin{aligned} d(t) &= f_i(v(\tau_k)) + \frac{\partial f_i}{\partial v} m_{v_k}(t - \tau_k) + \\ &+ [\frac{\partial f_i}{\partial v} p_{v_k} + \frac{\partial^2 f_i}{\partial v^2}\frac{(m_{v_k})^2}{2}](t-\tau_k)^2 + \cdots \end{aligned}$$

Discarding the higher order terms (starting from t^3), we have an expression for $d(\tau_k)$, m_{d_k} and p_{d_k}.

Notice that we need to evaluate $\frac{\partial f_i}{\partial v}$ and $\frac{\partial^2 f_i}{\partial v^2}$ at $v(\tau_k)$. When we have the expression of f_i in closed form, it can be easily done. In more general cases, we might need to evaluate it numerically.

E Theoretical properties of QSS3

From the definition of the second order quantizer – see (7)– it results that

$$|q_i(t) - x_i(t)| \leq \Delta q_i \qquad (15)$$

and then, all the properties mentioned in Sec.II.C are also satisfied by QSS3.

As in the lower order methods, the strongest property is that QSS3 has a calculateable global error bound in the simulation of LTI systems. Although this bound is the same for the three methods, in QSS3 we can use smaller quanta.

The time between successive steps on each quantized integrator is determined by the distance $t_{j+1} - t_j$ in (14). Immediately after a step, $x(t)$ and $q(t)$ have the same value and the same first and second derivatives. The only difference is in the third derivative, which is $2 \cdot p_d$ in x and 0 in q. Provided that $d(t)$ does not change between t_j and t_{j+1}, the time in which the difference between x and q becomes equal to Δq can be calculated as

$$t_{j+1} - t_j = \sqrt[3]{\frac{3\Delta q}{p_d}}$$

Thus, we can conclude that the step size in a single integrator is proportional to the cubic root of the quantum. In QSS the step size was proportional to the quantum and in QSS2 it was proportional to the square root.

For example, if we want to increase the accuracy by a factor of 1×10^6 we will have to reduce the quantum by the same factor (due to the global error bound property). In QSS it is equivalent to multiply by 1000000 the number of calculations. In QSS2 we would have to multiply it by 1000 and in QSS3 only by 100.

This fact not only permits using smaller quantization achieving better accuracy, but also makes less critical the election of the quantum since it can be chosen conservatively small without affecting considerably the computational costs.

IV CONCLUSIONS

We introduced a new numerical method called QSS3 which performs a third order discrete event approximation of ordinary differential equations.

We proved that QSS3 is *legitimate*, i.e., that it cannot produce and infinite sequence of events in a finite interval of time. In that way, the simulation with QSS3 will never be stuck at a given instant of time.

It was deduced the input–output relationship of quantized integrators and static functions so that DEVS models of these elementary blocks can be easily built.

Then, we saw that QSS3 has the same theoretical and practical properties than its lower order predecessors (QSS and QSS2). However, we showed that the reduction of the global error bound provokes a smaller increment of the computational costs.

The details of the construction of the DEVS models, its software implementation and some encouraging simulation results can be found in the companion paper (Kofman, 2005).

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