Quantization-based Integration of Ordinary Differential Equation Systems.

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Numerical Integration of ODEs Problem Formulation

We look for numerical solutions of an initial value problem given in its state-space representation:

$$\begin{aligned} \dot{x}(t) &= f(x(t), t) \\ x(t_0) &= x_0. \end{aligned} \tag{1}$$

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Here, $x \in \Re^n$ is the state vector, and x_0 is the known initial condition.

Numerical Integration of ODEs Usual Solutions

Conventional numerical methods lead to solutions of the form:

$$x(t_{k+1}) = x_{k+1} = F(x_k, t_k)$$
 (2)

or more generally

$$F(x_{k+1}, x_k, t_k) = 0$$
 (3)

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or similar expressions.

These kind of solutions explicitly or implicitly define a discrete time simulation model, where the numerical solution x_k is only defined for $t = t_1, t_2, \cdots, t_k, \cdots$.

Numerical Integration of ODEs Some Important Concepts and Problems

In order to rely on the solutions given by a method, it is important to analyze:

- Numerical stability
- Approximation accuracy

The following special cases must be treated carefully:

- Discontinuous systems
- Stiff systems
- Marginally stable systems

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Quantization-based Integration

Consider the second order LTI system

$$\dot{x}_1(t) = x_2(t)$$

 $\dot{x}_2(t) = -x_1(t)$
(4)

with initial conditions $x_1(0) = 4.5, x_2(0) = 0.5$.

Let us see what happens if instead of discretizing the time, we discretize the states in the following way:

$$\dot{x}_1(t) = \text{floor}(x_2(t)) = q_2(t)$$

 $\dot{x}_2(t) = -\text{floor}(x_1(t)) = -q_1(t)$
(5)

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Quantization-based Integration



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Quantization-based Integration



Quantization-based Integration

We can easily solve the quantized system

 $\dot{x}_1(t)=q_2(t) \ \dot{x}_2(t)=-q_1(t)$



Quantization-based Integration

We can easily solve the quantized system

 $\dot{x}_1(t) = q_2(t) \ \dot{x}_2(t) = -q_1(t)$



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Quantization-based Integration Introductory Example – Cont.

We can easily solve the quantized system

 $\dot{x}_1(t)=q_2(t) \ \dot{x}_2(t)=-q_1(t)$



Quantization-based Integration Discrete Events vs. Discrete Time

- Apparently, by replacing xk by qk on the right hand side of any ODE, we obtain a new method for simulating it.
- However, this new method does not fit the form of Eq.(2) or Eq.(3), i.e., it does not define a Discrete Time simulation model.
- Thus, we will not be able to apply this method in a standard way.

We shall see that this idea leads to a Discrete Event simulation model in terms of the DEVS formalism.

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DEVS is a formalism proposed by Bernard Zeigler to represent systems that have input and output event trajectories.



A DEVS model processes an input trajectory, specified as a series of input events, and according to these events and to its own internal state, provokes an output trajectory.

DEVS models can be coupled similarly to block diagrams.

DEVS Formalism Atomic Model Definition

$$M = (X, Y, S, \delta_{int}, \delta_{ext}, \lambda, ta)$$

•
$$X$$
 : set of input values.

- Y : set of output values.
- *S* : set of state values.
- δ_{int} : internal trans. func.
- δ_{ext} : external trans. func.
- λ : output func.
- ta : time advance func.



$$S | \underbrace{\frac{s_2 = \delta_{int}(s_1)}{s_3 = \delta_{ext}(s_2, e, x_1)}}_{Y | (x_1 = \lambda(s_1))} \underbrace{\frac{s_2 = \delta_{int}(s_1)}{s_3 = \delta_{ext}(s_2, e, x_1)}}_{Y | (x_1 = \lambda(s_1))} | \underbrace{y_2 = \lambda(s_3)}_{y_2 = \lambda(s_3)}$$



DEVS Formalism

DEVS models can be coupled in a hierarchical way. DEVS closure under coupling ensures that coupled DEVS models are equivalent to atomic DEVS models.



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DEVS Formalism

An ad-hoc computer program to simulate a DEVS model can be easily written using any programming language. However, there exist a number of software tools specifically conceived to simulate DEVS models:

- DEVS-Java (University of Arizona)
- CD++ (Carleton University)
- JDEVS (Université de Corse)
- PowerDEVS (Universidad Nacional de Rosario)
- PyDEVS (McGill University)
- etc.

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Quantized Systems and DEVS Block Diagram of the Original System



 $\dot{x}_1(t) = x_2(t)$ $\dot{x}_2(t) = -x_1(t)$

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Quantized Systems and DEVS Block Diagram of the Quantized System



 $\dot{x}_1(t) = q_2(t)$ $\dot{x}_2(t) = -q_1(t)$

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Quantized Systems and DEVS Block Diagram of the Quantized System



 $\dot{x}_1(t) = q_2(t)$ $\dot{x}_2(t) = -q_1(t)$

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Quantized Systems and DEVS Quantized Integrator



- Each change in the piecewise constant input trajectory $d_{x_i}(t)$ can be thought of as an input event.
- Each change in the piecewise constant output trajectory q_i(t) can be thought of as an output event.
- The piecewise linear state $x_i(t)$ can be treated as part of the internal DEVS state, and is updated at event times.

We can easily build a DEVS atomic model that emulates the behavior of the Quantized Integrator.

Quantized Systems and DEVS Static Function



- Each change in the piecewise constant input trajectory $q_1(t)$ can be thought of as an input event.
- Each change in the piecewise constant output trajectory $d_{x_2}(t)$ can be thought of as an output event.

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We can easily build a DEVS atomic model that emulates the behavior of this particular Static Function.

Quantized Systems and DEVS Static Function



- Each change in any of the piecewise constant input trajectories q_j(t) can be thought of as an input event.
- Each change in the piecewise constant output trajectory d_{xi}(t) can be thought of as an output event.

We can easily build a DEVS atomic model that emulates the behavior of a general Static Function.

Quantized Systems General Idea

Given a continuous system

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

the quantized system

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

is equivalent to a DEVS model and, at least in principle, can be simulated by coupling quantized integrators, static functions, and source blocks.

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Quantized Systems A Little Drawback

Let us analyze what happens with the following first order system

$$\dot{x}(t) = -x(t) - 0.5$$

and its associated Quantized System:

 $\dot{x}(t) = -floor(x(t)) - 0.5$

around the initial condition x(0) = 0.

Evidently, this idea does not work. The DEVS model is illegitimate, and the simulation will get stuck performing an infinite number of steps without advancing time.

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Outline







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Quantized State Systems Method Hysteretic Quantization Function



The basic idea to avoid infinitely fast oscillations is the use of hysteresis in the quantization.



Given an ODE in its state-space representation

$$\dot{x}_a(t) = f(x_a(t), u(t)) \tag{6}$$

with $x_a\in \Re^n$, $u\in \Re^m$ and $f: \Re^n\to \Re^n$, the QSS method approximates it by

$$\dot{x}(t) = f(q(t), u(t)) \tag{7}$$

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where q(t) y x(t) are related componentwise by hysteretic quantization functions.

The QSS of Eq.(7) is equivalent to a legitimate DEVS model.

QSS Method Block Diagram of a Generic QSS



The QSS method can be applied coupling DEVS models of hysteretic quantized integrators and static functions.

QSS Method – Properties Perturbed Representation

Defining $\Delta x(t) \triangleq q(t) - x(t)$, we can rewrite Eq.(7) as

$$\dot{x}(t) = f(x(t) + \Delta x(t), u(t)) \tag{8}$$

which is similar to Eq.(6) except for the perturbation term Δx . Notice also that

$$|\Delta x_i| \le \Delta Q_i, \quad i = 1, \dots, n \tag{9}$$

Properties related to convergence, stability, and accuracy can be studied as effects of bounded perturbations.

QSS Method – Properties Linear Time Invarying Systems

When we apply the QSS method to an LTI asymptotically stable system, defining the simulation error as $e(t) \triangleq x(t) - x_a(t)$, it results that

$$|e(t)| \le |V| \cdot |\mathbb{R}e(\Lambda)^{-1}\Lambda| \cdot |V^{-1}| \cdot \Delta Q$$
(10)

Thus,

- QSS gives always practically stable results. This property is very important taking into account that the method is fully explicit.
- We can calculate a simulation global error bound.

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QSS Method Example

The following equations represent a mass-spring-damper system.

$$egin{aligned} \dot{x}_1(t) &= x_2(t) \ \dot{x}_2(t) &= -rac{k}{m} x_1(t) - rac{b}{m} x_2(t) + rac{1}{m} F(t) \end{aligned}$$

and the QSS approximation is

$$\dot{x}_1(t) = q_2(t)$$

 $\dot{x}_2(t) = -\frac{k}{m} q_1(t) - \frac{b}{m} q_2(t) + \frac{1}{m} F(t)$

For the parameters m = b = k = 1, the simulation error bound is

$$\begin{bmatrix} |e_1(t)| \\ |e_2(t)| \end{bmatrix} \leq 2.3094 \cdot \begin{bmatrix} \Delta Q_1 + \Delta Q_2 \\ \Delta Q_1 + \Delta Q_2 \end{bmatrix}$$

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QSS Method Simulation Results



 $\Delta Q_i = 0.01$.

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QSS Method Simulation Results



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QSS Method Simulation Results

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Advantages

- Stability and Error Bound.
- Decentralization (only local calculations at each step). Sparsity exploitation
- Can reduce the number of iterations in some DAEs.
- Very efficient discontinuity handling

Disadvantages

- Problems with stiff systems.
- We have to choose the quantum.
- The number of steps grows linearly with the accuracy.

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QSS2 Method Main Features

- It follows the same idea of QSS, but the quantized trajectories are now piecewise linear instead of piecewise constant.
- Each event now must carry two numbers: the initial value and the slope of each trajectory segment.
- The quantized integrators and static functions are more complex, because they must consider and compute the slopes.
- Since the perturbations terms in Eq.(9) are still bounded by ΔQ_i , QSS2 has the same error bound as QSS.
- Now, the number of steps grows with the square root of the accuracy.

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QSS Methods Examples Conclusions

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QSS Methods and Stiff Systems Introductory example

The LTI system

$$\dot{x}_1(t) = 0.01 x_2(t)$$

$$\dot{x}_2(t) = -100 x_1(t) - 100 x_2(t) + 2020$$
(11)

has eigenvalues $\lambda_1\approx-0.01$ and $\lambda_2\approx-99.99$, so it is stiff.

The QSS method approximates this system by

 $\dot{x}_1(t) = 0.01 q_2(t)$ $\dot{x}_2(t) = -100 q_1(t) - 100 q_2(t) + 2020$ (12)

Taking initial conditions $x_1(0) = 0$, $x_2(0) = 20$, and quantization $\Delta Q_1 = \Delta Q_2 = 1$, the QSS integration does the following:

QSS Methods and Stiff Systems Introductory Example – QSS Simulation

 $\dot{x}_1(t) = 0.01 \, q_2(t)$ $\dot{x}_2(t) = -100 \, q_1(t) - 100 \, q_2(t) + 2020$

QSS Methods and Stiff Systems Introductory Example – QSS Simulation

QSS Methods and Stiff Systems Introductory Example – QSS Simulation

QSS Methods and Stiff Systems Introductory Example – QSS Simulation

QSS Methods and Stiff Systems Introductory Example – QSS Simulation

QSS Methods and Stiff Systems Introductory Example – QSS Simulation (Detail)

QSS Method and Stiff Systems

- Stiff systems provoke fast oscillations on the QSS solutions.
- Thus, the number of steps is huge. In the simulated example there were 21 changes in q_1 and 15995 in q_2 , for a final simulation time $t_f = 500$.

Evidently, the QSS method is not appropriate for the simulation of stiff systems.

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Backward QSS Basic Idea

The idea is that each quantized variable q_j has always a future value of the corresponding state x_j . This is,

- State trajectories always go to the corresponding value of q
- Although this is backward integration, it does not call for iterations, since each variable q_j can only take two values (one from below and the other from above of x_j).

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Example $\dot{x}_1(t) = 0.01 q_2(t)$ $\dot{x}_2(t) = -100 q_1(t) - 100 q_2(t) + 2020$

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 $q_2 = 19$ Prof. Dr. François E. Cellier Quantization-based Integration of ODE Systems

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 $\dot{x}_2 = -80$

20

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Backward QSS

Backward QSS Main Fatures

Advantages:

- BQSS is actually an explicit method.
- It shares the main properties of QSS (practical stability, global error bound, etc.).
- Additionally, it can deal with stiff systems.

Disadvantages:

- Like QSS, BQSS is only first order accurate.
- In some nonlinear systems, BQSS finds non existing equilibrium points.

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QSS Methods and Marginally Stable Systems Centered QSS

QSS methods have the same problems that Euler's methods have regarding marginal stability:

- Forward QSS gives unstable simulation results.
- Backward QSS gives asymptotically stable simulation results.

Forward and Backward Euler can be combined to form an F–Stable integration method (the Trapezoidal Rule). Similarly, we can blend QSS and BQSS:

- The idea that each quantized variable takes the mean value of the corresponding QSS and BQSS quantized variables, namely, $q_i = 0.5(q_{i_{OSS}} + q_{i_{BOSS}})$.
- The resulting method is called CQSS (Centered QSS).
- Unlike the trapezoidal rule, CQSS is only first order accurate.

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PowerDEVS and QSS Methods Main Features

- PowerDEVS is a general purpose DEVS simulation tool developed at the Universidad Nacional de Rosario.
- It has block libraries with Quantized Integrators, Static Functions, Hybrid and Source Blocks that implement the whole QSS family (QSS, QSS2, QSS3, BQSS and CQSS).
- PowerDEVS has a GUI that permits drawing Block Diagrams, similar to Simulink.
- It is a free tool.
- PowerDEVS can be downloaded from www.fceia.unr.edu.ar/lsd/powerdevs

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Examples Mass-Spring-Damper System

$$egin{aligned} \dot{x}_1(t) &= x_2(t) \ \dot{x}_2(t) &= -rac{k}{m} x_1(t) - rac{b}{m} x_2(t) + rac{1}{m} F(t) \end{aligned}$$

See PowerDEVS Model

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Examples Ball Bouncing Down Some Stairs

$$\dot{x} = v_x, \quad \dot{v}_x = -\frac{b_a}{m} \cdot v_x, \quad \dot{y} = v_y$$
$$\dot{v}_y = -g - \frac{b_a}{m} \cdot v_y - s_w \cdot \left[\frac{b}{m} \cdot v_y + \frac{k}{m}(y - h(x))\right]$$

where h(x) gives the height of the current stair, and $s_w(t)$ switches between 0 (ball in the air) and 1 (ball on the floor). Namely,

$$h(x) = \mathit{floor}(11-x), \hspace{1em} s_w(t) = egin{cases} 0 & ext{if } y > h(x) \ 1 & ext{otherwise} \end{cases}$$

See PowerDEVS Model

	Introduction QSS Methods Examples Conclusions		
Examples Lossless Transmission Line			

$$\dot{\phi}_1(t) = u_0(t) - u_1(t)$$

 $\dot{u}_1(t) = \phi_1(t) - \phi_2(t)$

 $\dot{\phi}_j(t) = u_{j-1}(t) - u_j(t)$ $\dot{u}_i(t) = \phi_i(t) - \phi_{i+1}(t)$

We consider an input pulse entering the line:

$$u_0(t) = egin{cases} 10 & ext{if } 0 \leq t \leq 10 \\ 0 & ext{otherwise} \end{cases}$$

and a nonlinear load:

 $g(u_n(t)) = (10000 \cdot u_n)^3$

 $\dot{\phi}_n(t) = u_{n-1}(t) - u_n(t)$ $\dot{u}_n(t) = \phi_n(t) - g(u_n(t))$

See PowerDEVS Model

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QSS Methods

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- Discretizing states instead of time, QSS methods offer a new way of simulating continuous systems.
- They have strong theoretical properties (stability and global error bound).
- QSS methods offer dense output.
- QSS methods show important advantages when handling discontinuities.
- The capability of the explicit methods BQSS and CQSS to deal with stiff and marginally stable systems represents one of the most promising results.

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- BQSS and CQSS must be extended to obtain higher order accurate methods.
- PowerDEVS only admits Block Diagram models. It is very important that the QSS methods are implemented to work with object-oriented modeling languages, such as Modelica.
- The use of uniform quantization implicitely controls the absolute error. It is better to have control over the relative error. This issue might be resolved with the usage of logarithmic quantization.
- QSS methods seem to be appropriate for parallel and also real-time simulation. However, these problems have not been studied yet in greater detail.

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