Implementation of sensitivity analysis solver for hybrid systems in DIANA simulation environment

Leonid Iakushyk
Max-Planck-Institut für Dynamik komplexer technischer Systeme
Sandtorstraße 1, 39106 Magdeburg, Germany

28.04.2010

1. Introduction

When studying physical or chemical processes, it is important to estimate the influence of parameters on solution. The studying of the solution behavior when model parameters are changing is a subject of so-called sensitivity analysis. It makes it possible to build sensitivity functions, which give important information about features of the model under the study, and can be used for optimization of models.

The possibility of sensitivity analysis has been implemented in DIANA's daspk-solver for the models with fixed structure. But many systems, particularly in chemical engineering, are hybrid and thus they contain discontinuities.

In this work the implementation of sensitivity analysis for hybrid systems in DIANA is considered. The possibility to make such analysis is added to DIANA's PetriMeta-Solver.

2. Mathematical background

The models for DIANA are generated by the process modeling tool ProMoT[1,2] and presented as linear implicit differential-algebraic system:

$$B(\underline{x}, \underline{p}, t) \cdot \dot{x} = f(\underline{x}, \underline{p}, t) \tag{1}$$

where $\underline{x}$ is state variable vector, B is square matrix, $\underline{p}$ is parameter vector, h, g are intermediates.

This work is restricted to the case, when equation system (2) can be rewritten in the semi explicit form:

$$\begin{pmatrix} B_D & \\ & 0 \end{pmatrix} \cdot \begin{pmatrix} x_D \\ 0 \end{pmatrix} = \begin{pmatrix} f_D(x,p,t) \\ f_A(x,p,t) \end{pmatrix}, \qquad x = \begin{pmatrix} x_D \\ x_A \end{pmatrix}, \tag{2}$$

where x_D is dynamical variables vector and x_A is algebraical variables vector.

In DIANA-simulation environment Petri nets are used to describe hybrid models. Each place corresponds to particular state of hybrid automaton, which is described by its equations and characteristic values of the structure parameters. Transition between two places occurs, when so called switching function (φ-function) comes from positive to negative value.

The sensitivity $s_i(t)$ is defined as the derivative of x_i by parameter ps:

$$s_i(t) = \frac{\partial x_i}{\partial p}\Big|_t \tag{3}$$

At the time when switching occurs, derivatives of dynamic state variables can have discontinuities. This leads to discontinuities of s(t)-functions.

The values of sensitivities after the switching can be recalculated using the sfollowing two formulas:

$$\frac{\partial \underline{x_D}}{\partial p}\Big|_{ts+} = \left(\frac{\partial \underline{x_D}}{\partial t}\Big|_{ts-} - \frac{\partial \underline{x_D}}{\partial t}\Big|_{ts+} \right) \cdot \frac{\partial t_s}{\partial p} + \frac{\partial \underline{x_D}}{\partial p}\Big|_{ts-} \tag{4}$$

$$\frac{\partial t_s}{\partial p} = - \frac{\frac{\partial \varphi}{\partial \underline{x}} \cdot \frac{\partial \underline{x}}{\partial p}\Big|_{ts-} + \frac{\partial \varphi}{\partial p}}{\frac{\partial \varphi}{\partial \underline{x}} \cdot \frac{\partial \underline{x}}{\partial t}\Big|_{ts-} + \frac{\partial \varphi}{\partial t_s}} \tag{5}$$

Algebraic state variables and their sensitivities after the switching also must be recalculated for consistency. x_A can be calculated from equation system (2).

$\dot{s}_D = \frac{\partial}{\partial t}\left(\frac{\partial \underline{x}_D}{\partial p}\right)$ and $s_A = \frac{\partial \underline{x}_A}{\partial p}$ are computed from:

$$\frac{\partial}{\partial p}(B\dot{\underline{x}}) = \frac{\partial f}{\partial p} + \frac{\partial f}{\partial \underline{x}} \cdot \frac{\partial \underline{x}}{\partial p} \tag{6}$$

3. Example

Let's discuss the following test model for the PetriMeta-solver (see. Fig. 1), which describes a reactor whose content may reach boiling temperature.

$$\frac{\partial x_1}{\partial t} = -a_1 x_1 + b_1 r_{reac}$$

$$\begin{cases} \dfrac{\partial x_2}{\partial t} = -a_2 x_2 + b_2 r_{reac}, onephase \\[2ex] \dfrac{\partial x_2}{\partial t} = 0, boiling \end{cases}$$

$$\begin{cases} Q = 0, onephase \\ Q = -a_2 x_2 + b_2 r_{reac} + gu, boiling \end{cases}$$

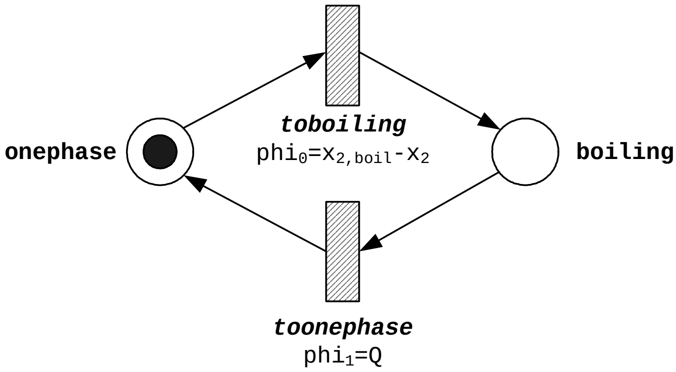

Figure 1. Equations and Petri net of two-phase reactor model

The model is described by:

x_1, x_2, Q – state variables

a_1, a_2, b_1, b_2, $x_{2,boil}$ – real parameters

$r_{reac} = (1 - x_1)e^{-\frac{E}{(1+x_2)}}$ - help variable

The system can be in one of two states: **onephase** or **boiling**. Petri net contains two transitions, ***toboiling*** and ***toonephase,*** between this states (Petri net's places). Each transition is described by an appropriate φ-function.

Template of the DIANA-script for computing the sensitivities with PetriMeta-Solver is shown below.

```
# create base model
bmodel = mmanager.CreateModel(diana.CAPE_CONTINUOUS, modelname)
bmodel.Initialize();
beso        = bmodel.GetActiveESO();
besopar     = beso.GetParameters();
besovar     = beso.GetStateVariables();

# set variables and parameters values
besovar[ "x2" ].SetValue( 0.02 );
besopar['x2boil'].SetValue( 0.06 );

# create sensitivity model based on base model
model = bmodel.GetSensitivityModel(["x2boil"],[])
model.Initialize();
...

# create the solver
```

```
solver      = sfactory.CreateSolver(diana.CAPE_DAE,model, "petri_meta");
solver.Initialize();
...

#set solver parameters
solpar      = solver.GetParameters();
solpar["Tend"].SetValue(100.0);

#run solver
solver.Solve();
```

On fig. 2 some results obtained by the simulation of two-phase reactor model are presented. There are two values of x_2 state variable computed with two near values of $x_{2,boil}$ parameter on the fig. 2a. On fig. 2b the sensitivity $s_{x2}(t)$ computed with MetaSolver (which uses daspk-solver) and sensitivity computed by approximation with finite differences are shown. The curves are close to one other that confirms correctness of results obtained using MetaSolver.

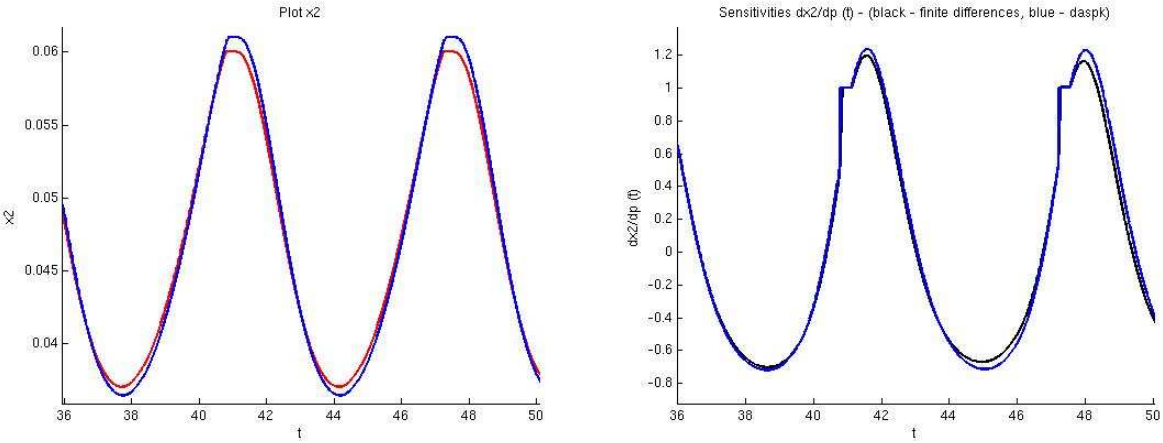

Figure 2. Simulation results for two-boiling reactor: a) $x_2(t)$ when $x_{2,boil}$=0.06 (red) and when $x_{2,boil}$=0.061 (blue); b) $s_{x2boil}(t)$

References:

[1] Krasnyk, M.; Bondareva, K.; Milokhov, O.; Teplinskiy, K.; Ginkel, M.; Kienle, A. The ProMoT / Diana simulation environment. In: W. Marquardt, C. Pantelides (Eds.), 16th European Symposium on Computer Aided Process Engineering and 9th International Symposium on Process Systems Engineering. Elsevier, 2006, pp. 445-450.

[2] M. Krasnyk. DIANA – An object oriented tool for nonlinear analysis of chemical processes. Ph.D. thesis, Otto-von-Guericke-Universität Magdeburg, 2008.

[3] G. van Rossum. Python Tutorial, URL http://www.python.org/doc/tut/tut.html