Extending System Dynamics approach to higher index DAE's.[1]

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The aim of this paper is to propose an extension of System Dynamics approach for modeling systems to systems described by higher index DAEs (Differential Algebraic Equations). Existing implementations of Forrester's methodology are commonly based on fixed step integration methods such as Euler or *n*-order explicit Runge-Kutta. The main reason for using fixed step integration schemes is their simplicity of implementation as well as the the simplicity of modeling environments based on these integration schemes. On the other hand using fixed step integration can lead to incorrect results especially when equations are stiff. The problems with adequate integration schemes can be overcome by using variable stepsize integration methods such BDF or implicit Runge-Kutta. Since these methods require jacobians of right-hand sides of equations these numerical methods must be supported by procedures for evaluating jacobians either by finite difference, or by automatic differentiation (in order to keep the simplicity of modeling environment). Once we have variable stepsize integration procedure we can attempt to extend Forrester's approach to systems described by fully implicit DAEs – the paper shows how it can be achieved.

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1. System Dynamics - mathematical overview

Traditional, System Dynamics methodology is based on well known, stocks and flows approach [2]. From the mathematical point of view, stocks are differential variables and flows are algebraic ones. Generally, modeled dynamic systems result in a system of differential-algebraic equations (DAE's) (1).

$$\begin{aligned} \frac{dx(t)}{dt} &= f(x(t), y(t), u(t), p) \\ 0 &= g(x(t), y(t), u(t), p) \end{aligned} \tag{1}$$

In (1) *x* corresponds to differential variables (stock in Forrester's approach), while *y* to algebraic variables (Inflow, Outflows, Auxiliaries in Forrester's approach). External functions of time *u* and parameters *p* must be known in advance. The above system of differential—algebraic equations is well—known in modern control theory where it is used to describe dynamical systems. If we assume that condition (2) holds

$$\det\left[\frac{\partial g(x(t), y(t), u(t), p)}{\partial y}\right] \neq 0 \tag{2}$$

then we can show that *x(t)* is uniquely determined by initial conditions *x(0)* and values of controls *u(s)* with s from the set [0,t] and parameters *p*. For that reason the variable *x* is also called the state variable.

The essential feature of System Dynamics approach is that algebraic equations in (1) can be easily eliminated and as consequence a nonlinear ordinary differential equations (ODE's) system (3) is obtained.

$$\frac{dx(t)}{dt} = f(x(t), y(t), u(t), p) \tag{3}$$

Equations (3) could then be solved numerically by using standard Euler or Runge-Kutta methods.

2. System Dynamics and the problems with using fixed integration steps

As mentioned in Section 1, most System Dynamics modeling environments implement standard integration methods like Euler (4) or n-order Runge-Kutta, e.g., 4-order RK (5). Their great advantage is the simplicity of the implementation but it is at the cost of the possibility of getting wrong numerical solutions. In both methods the user is forced to choose a value of step length *h*. The reason for using fixed step integration schemes is that these methods do not refer to jacobians of right-hand sides of differential equations – see for example Runge-Kutta scheme (4). The need for providing analytical jacobians would significantly complicate the use of simulation tools.

$$\begin{aligned} k_1 &= hf(x_n, y_n) \\ k_2 &= hf\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_1\right) \\ k_3 &= hf\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_2\right) \\ k_4 &= hf(x_n + h, y_n + k_3) \\ y_{n+1} &= y_n + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) \end{aligned} \tag{4}$$

Inappropriate step length together with the lack of understanding of stability properties of integration schemes can lead to invalid simulation results or their wrong interpretation.

Let us consider SIR epidemic model [2] illustrated in Figure 1. For model described by equations (6) let us take initial values given by (7).

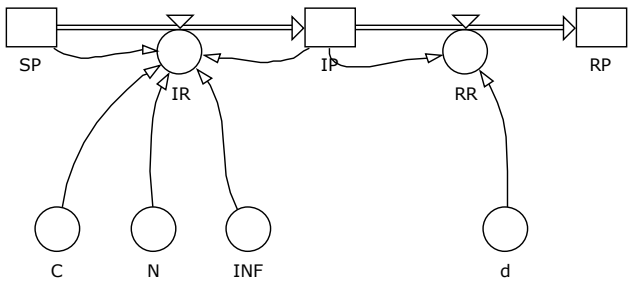

Figure 1. SIR epidemic model.

$$\begin{aligned} \frac{dSP}{dt} &= (-IR) \\ \frac{dIP}{dt} &= RR - IR \\ \frac{dRP}{dt} &= RR \\ IR &= C \cdot INF \cdot SP \cdot \left(\frac{IP}{N}\right) \\ RR &= \frac{IP}{d} \end{aligned} \tag{6}$$

$$
\begin{aligned}
SP &= 10 \\
IP &= 1 \\
RP &= 1 \\
C &= 0{,}9 \\
N &= 1 \\
INF &= 0{,}6 \\
d &= 1
\end{aligned}
\qquad (7)
$$

Having defined conditions as above it is possible to start a simulation with chosen integration method and fixed step size *h*. Figures below (2,3,4) show 4-order Runge-Kutta method with different step sizes and 10 days time horizon.

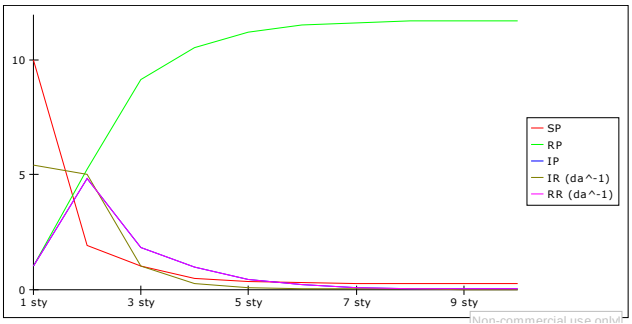

Figure 2. SIR model simulation using 4-order Runge-Kutta method with *h*=1 day (10 steps).

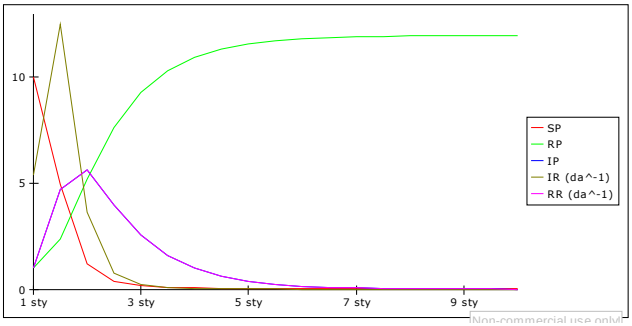

Figure 3. SIR model simulation using 4-order Runge-Kutta method with *h*=0,5 day (20 steps).

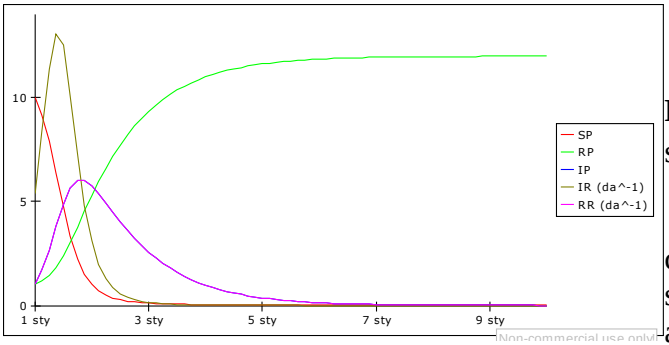

Figure 4. SIR model simulation using 4-order Runge-Kutta method with *h*=0,125 day (80 steps).

It could be observed, that during integration with 4-order Runge-Kutta method, values of variable *IR* could be difficult to interpret for either *h*=1 or *h*=0,5. Ultimately, integrating with *h*=0,125 gives results at acceptable level.

Examples above reveal that many simulation experiments with different values of integration step could be needed to be sure that numerical results are correct. However, for more complicated models than SIR we could have problems with choosing appropriate values of *h*, especially when system is described by highly nonlinear equations with sudden changes of their variables.

3. Integration methods with variables step sizes

Difficulties with choosing proper length of integration step *h* could be resolved by using advanced integration procedure with automatic step size control. The experience with variable step size integration procedures reported in this paper are based on the special written Java applet using Radau IIA integration scheme ([4]-[5]). The applet is available at http://www.optisim.org.

If the step control algorithm is enough accurate, this eliminates necessity of running simulation multiple times to verify results. It also allows, to reduce simulation costs, significantly. For considered SIR model, number of steps needed to achieve proper results is only 31. Figure 5 shows results from the example simulation.

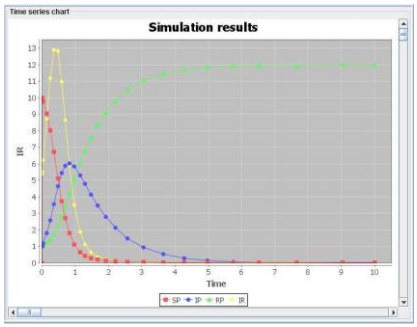

Figure 5. SIR model simulation using automatic step size control procedure (31 steps).

Points on the chart shows accepted steps and it could be observed that length of the steps are shorter when function changes rapidly (time 0 to 5) and longer when function changes are much slower (time 5-10).

However, variable stepsize integration procedures usually refer to jacobians of the right-hand sides of differential equations ([4]-[6]). In order to make modeling environments easier to use, advanced integration schemes have been abandoned.

In that way the user have not been forced to provide analytical jacobians.

If one decides to use variable stepsize integration procedure he has to rely either on:

a. finite differences schemes for gradient approximation, or on
b. tools for automatic differentiation such as ADOL-C program.

In the paper the reported results have been obtained with the help of finite differences.

4. System Dynamics tools and stiff equations

Due to the limitations of the fixed step integration procedures most of the existing System Dynamics tool are not able to cope with stiff equations. Let us consider as an example the Van der Pol's equation (8), which is said that "*is much harder than the rest…*"[2], with initial values (9).

$$\begin{aligned} \dot{y}_1 &= y_2 \\ \dot{y}_2 &= ((1-y_1^2)y_2 - y_1)/\varepsilon \end{aligned} \tag{8}$$

$$\begin{aligned} y_1 &= 2 \\ y_2 &= -0{,}66 \\ \varepsilon &= 10^{-6} \end{aligned} \tag{9}$$

System Dynamics model for this equation is illustrated in Figure 6.

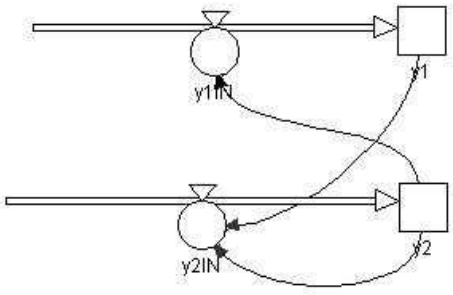

Figure 6. System Dynamics model for the Van der Pol equation.

For this equation, due to its fast trajectory changes it is hard, or even impossible, to choose fixed step length to obtain proper results on the whole time horizon. Figure 7 shows that simulation experiment fails even for fixed step h=0,00000762939453125. As presented, 4-order RK, integration method could not cope with these equations.

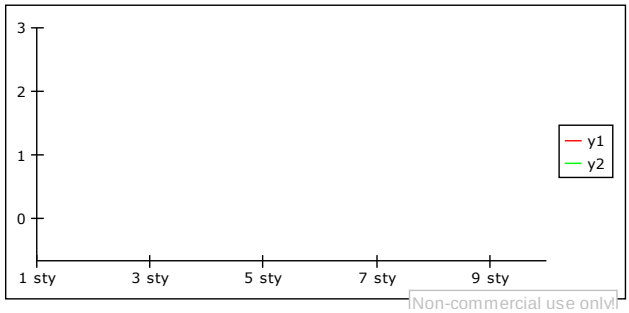

Figure 7. Simulation results for y1, y2 variable for Van der Pol equation integration with fixed step size h=0,00000762939453125.

However, when using advanced integration procedures System Dynamics approach could be easily applied to this group of equations. Figures 8-9 show results for the same model and integration procedure with automatic step size control.

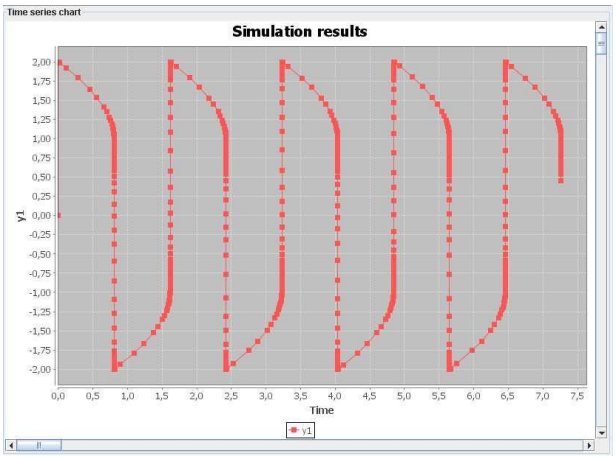

Figure 8. Simulation results for y1 variable in Van der Pol equation with automatic step size control.

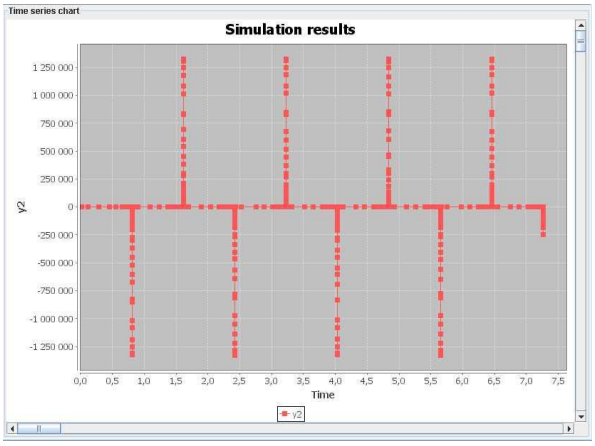

Figure 9. Simulation results for y1 variable in Van der Pol equation with automatic step size control.

[2] L.F. Shampine (1987)

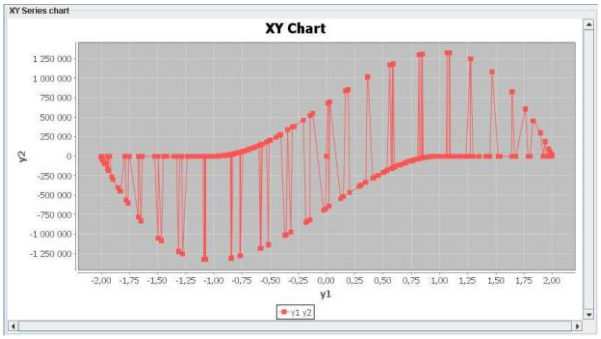

Figure 10. Trajectory for y1and y2 variables in Van der Pol equation with automatic step size control.

5. Extending System Dynamics to index-3 systems – an introduction

Once variable stepsize integration procedures are adopted within System Dynamics approach one can think to extend this approach to models described by fully implicit DAEs with possibly higher index. Such systems are described by differential-algebraic equations of the form (10).

$$F(t, y, \dot{y}) = 0 \tag{10}$$

Let us consider in Cartesian coordinates a physical pendulum illustrated in Figure 15.

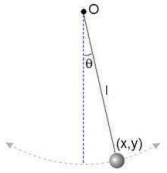

Figure 11. Physical pendulum.

In order to state equations of motion we can refer to Langrange-Hamilton principle. Let $q = [q_1, ..., q_n]^T$ be position coordinates of a system, $u_i = \dot{q}_i$ the velocities and $L=T-U$, where T is the *kinetic energy* and U the *potential energy*. The Euler equation (11) describe the movement of corresponding mechanical system.

$$\sum_{l=1}^{n} L_{\dot{q}_k \dot{q}_l} \ddot{q}_l = L_{q_k} - \sum_{l=1}^{n} L_{\dot{q}_k \dot{q}_l} \dot{q}_l \tag{11}$$

For the pendulum example with coordinate angle $\theta=q_1$, kinetic and potential energy are (12), (13) respectively.

$$T = \frac{ml^2\dot{\theta}^2}{2} \tag{12}$$

$$U = -lmg\cos\theta \tag{13}$$

Using Lagrange equation for constrained mechanical systems with constraints $g_1(q) = 0, ..., g_m(q) = 0$ (14), and replacing θ by x and y in (12), (13), for the pendulum with constraint (15) we can formulate (16).

$$L = T - U - \sum_{k=1}^{m} \lambda_k g_k(q) \tag{14}$$

$$x^2 + y^2 - l^2 = 0 \tag{15}$$

$$L = \frac{m}{2}(\dot{x}^2 + \dot{y}^2) - mgy - \lambda(x^2 + y^2 - l^2) \tag{16}$$

Applying (16) to (11), the system of following equation is obtained (17):

$$\begin{aligned} m\ddot{x} &= -2x\lambda \\ m\ddot{y} &= -mg - 2y\lambda \\ 0 &= x^2 + y^2 - l^2 \end{aligned} \tag{17}$$

where:

x,y – pendulum coordinates,
m – pendulum mass,
l – pendulum length,
λ - "Lagrange multiplier", which physical meaning is the tension in the rod, which maintains the mass point on the desired orbit.

The second derivatives of x and y in (17) can be eliminated and by making assumptions about parameters values (in order to simplify the following presentation) equations (17) can be stated as equations (18).

$$\begin{aligned} \dot{x} &= v \\ \dot{v} &= -x\lambda \\ \dot{y} &= w \\ \dot{w} &= -1 - y\lambda \\ 0 &= x^2 + y^2 - l^2 \end{aligned} \tag{18}$$

DAEs (18) have index 3.. The index of DAEs is defined as the minimal number m of differentiations

$$F(y', y) = 0, \quad \frac{dF(y', y)}{dt} = 0, ..., \frac{d^m F(y', y}{dt^m} = 0 \tag{19}$$

such that equation (19) allow us to extract by algebraic manipulation an explicit ODE system $y' = \varphi(y)$ ([7]-[9]).

One can verify that after two differentiations of the algebraic equation we come to index one DAEs.

$$\begin{aligned}
\dot{x} &= v \\
\dot{v} &= -x\lambda \\
\dot{y} &= w \\
\dot{w} &= -1 - y\lambda \\
0 &= -\lambda l^2 + v^2 + w^2
\end{aligned}$$

which can be easily transformed to ODEs by eliminating variable λ the algebraic equation. It must be mentioned that numerical integration of such obtained equations can lead to numerical instabilities. Thus it is recommended to integrate original equations (18) by using integration procedure which can cope with higher index DAEs (such as Radau IIA method).

Because of λ and algebraic constraint $0 = x^2 + y^2 - l^2$, which could not be eliminated by algebraic substitutions, a standard System Dynamics approach could not be used to simulate this system. The proposition is to add two new symbols to System Dynamics methodology:

1) triangle (Figure 12) – which represents Lagrangian multipliers- each multiplier is represented by one triangle,
2) pentagon (Figure 13) – which represents algebraic constraints – all constraints are represented by one pentagon.

Figure 12. Representation of Lagrangian multipliers

Figure 13. Representation of algebraic constraints

After such defined extensions, system from (18) could be modeled as in Figure 14.

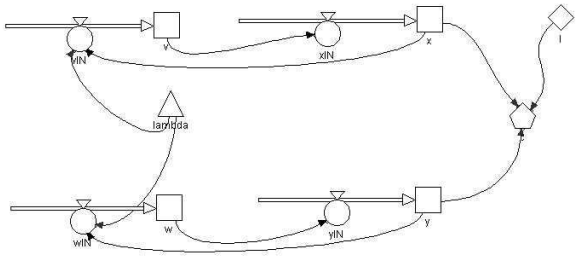

Figure 14. Extended System Dynamic model for pendulum example.

Simulation results for *x, y,* λ with initials parameters (20) are illustrated in Figure 15 and trajectory for *x* and *y* is shown in Figure 16. Equation for the model are as in (21). To write (18) in System Dynamics notation, auxiliaries variables x_{IN}, y_{IN}, v_{IN}, w_{IN}, which represents right-hand sides of differential equations from (18), were added.

$$\begin{aligned}
x &= 1, \\
y &= 0, \\
v &= 0, \\
w &= 0, \\
y &= 0, \\
l &= 1, \\
\lambda &= 0
\end{aligned} \qquad (20)$$

$$\begin{aligned}
\dot{x} &= x_{IN} \\
\dot{v} &= v_{IN} \\
\dot{y} &= y_{IN} \\
\dot{w} &= w_{IN} \\
x_{IN} &= v \\
y_{IN} &= w \\
v_{IN} &= -x\lambda \\
w_{IN} &= -1 - y\lambda \\
0 &= x^2 + y^2 - l^2
\end{aligned} \qquad (21)$$

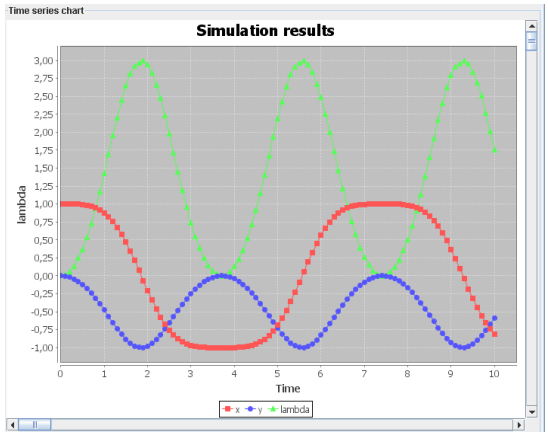

Figure 15. Simulation results for x, y, λ in pendulum example

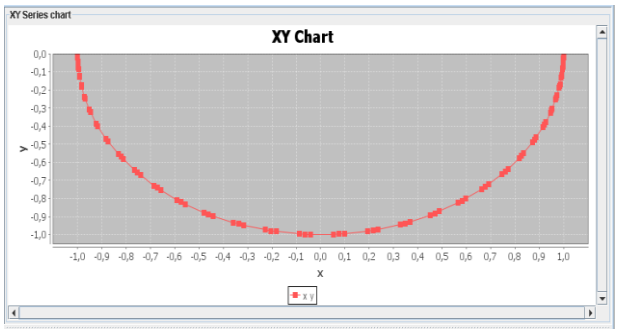

Figure 16. Trajectory for x ,y in pendulum example.

6. Extending System Dynamics to index-3 systems – the advanced case

As a more advanced example of extending System Dynamics to higher index DAE's an *"Andrews' squeezer mechanism"* illustrated in Figure 17 is considered.

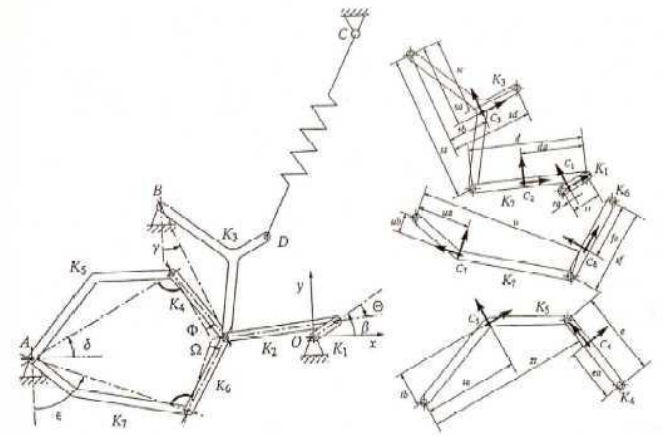

Figure 17. Andrews squeezer machnism [Gils, 1978], [Manning, 1981], [Hairer, Wanner, 1996]

The arrows in the right picture of Figure 21 indicate the positions of the centers of gravity C_1,...,C_7. Between points C and D there is a spring with coefficient c_0 and unstretched length l. The mechanism is assumed to be driven by a motor, located at O which is the coordinates origin. Coordinates of points A, B, C are as in (22).

$$\begin{bmatrix} x_a \\ y_a \end{bmatrix} = \begin{bmatrix} -0{,}06934 \\ -0{,}00277 \end{bmatrix}, \begin{bmatrix} x_b \\ y_b \end{bmatrix} = \begin{bmatrix} -0{,}03635 \\ -0{,}03273 \end{bmatrix}, \quad \begin{bmatrix} x_c \\ y_c \end{bmatrix} = \begin{bmatrix} 0{,}014 \\ 0{,}072 \end{bmatrix} \tag{22}$$

Position coordinates of the squeezer mechanism are as (23),

$$q_1 = \beta, q_2 = \Theta, q_3 = \gamma, q_4 = \Phi, \quad q_5 = \delta, q_6 = \Omega, q_7 = \varepsilon \tag{23}$$

and initial values as (24).

$$q(0) = \begin{bmatrix} -0{,}061713890014270644963589484580 01 \\ 0{,}0 \\ 0{,}455279819163070380255912382449 \\ 0{,}222668390165885884674473185609 \\ 0{,}487364979543842550225598953530 \\ -0{,}222668390165885884674473185609 \\ 1{,}230547444549821192497350155 68 \end{bmatrix} \tag{24}$$

Complete model in extended System Dynamics approach is illustrated in Figures 18, 19, 20. To make them clearer, connections between variables were deleted. The results of simulation are presented in Figures 21, 22. Equations of the model are presented in Appendix 1 but further details about the equations could be found in [3]. Generally, the model contains of:

- 14 stocks,
- 14 inflows,
- 71 auxiliaries,
- 6 Lagrange multipliers,
- 1 constraint.

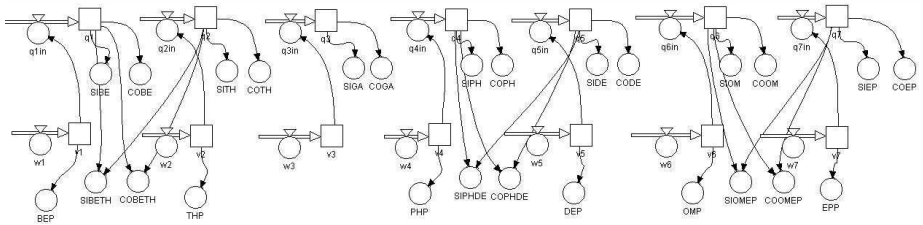

Figure 18. System Dynamics model for the Andrews' mechanism.

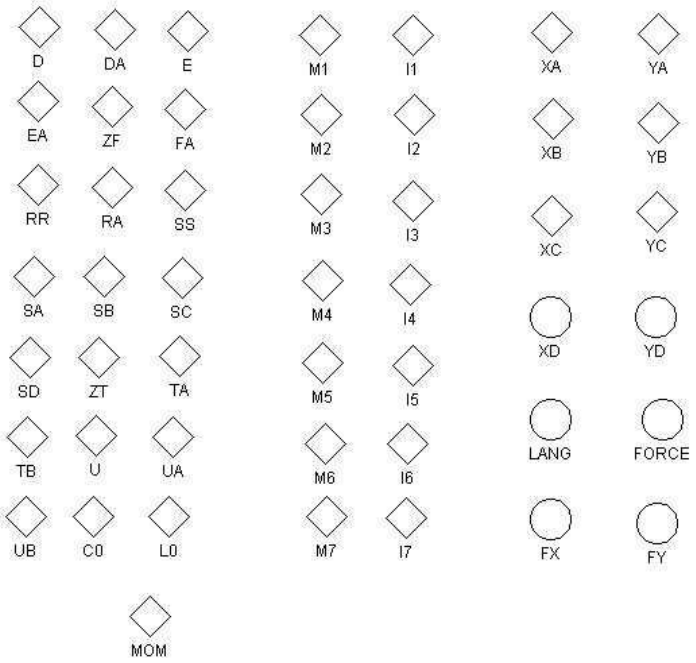

Figure 19. System Dynamics model for the Andrews' mechanism.[3]

[3] To make model clearer, connections where deleted

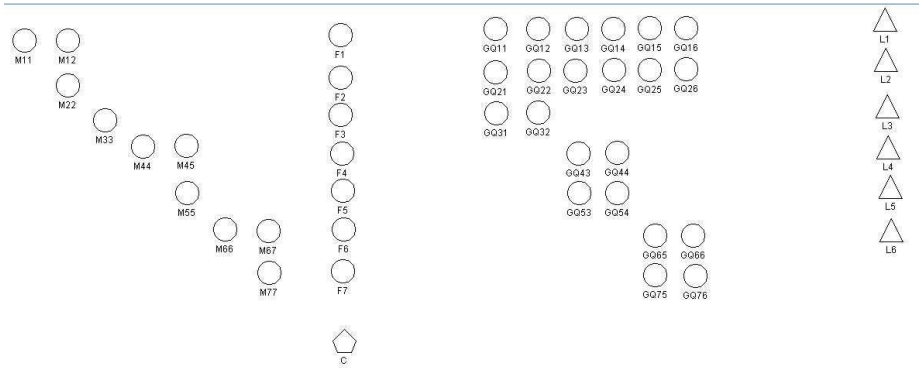

Figure 20. System Dynamics model for the Andrews' mechanism.[3]

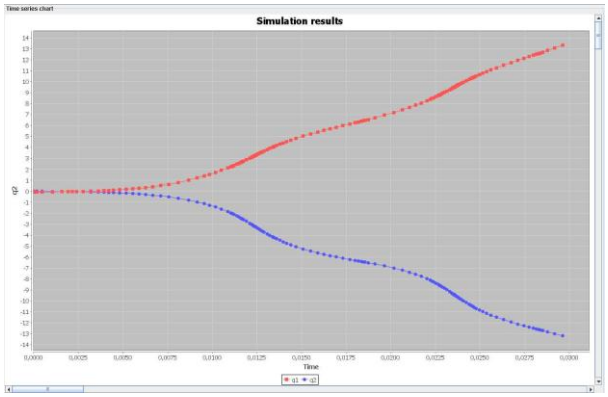

Figure 21. Simulation results for q1, q2 variables in Andrews' mechanism.

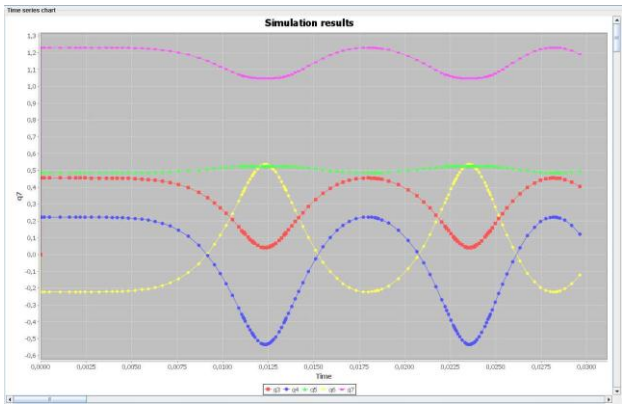

Figure 22. Simulation results for q3, q4, q5, q6, q7 variables in Andrews' mechanism.

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Appendix 1

Complete equations of the extended System Dynamics model of *"Andrews' squeezer mechanism"*.

$\dot{q}_i = q_{iIN}, i = 1,...,7$ $\dot{v}_i = w_i, i = 1,...,7$ $q_{iIN} = v_i, i = 1,...,7$	$SIBE = \sin(q_1)$ $COBE = \cos(q_1)$ $SITH = \sin(q_2)$ $COTH = \cos(q_2)$ $SIGA = \sin(q_3)$ $COGA = \cos(q_3)$ $SIPH = \sin(q_4)$ $COPH = \cos(q_4)$ $SIDE = \sin(q_5)$ $CODE = \cos(q_5)$ $SIOM = \sin(q_6)$ $COOM = \cos(q_6)$ $SIEP = \sin(q_7)$ $COEP = \cos(q_7)$	$BEP = v_1$ $SIBETH = \sin(q_1 + q_2)$ $COBETH = \cos(q_1 + q_2)$ $THP = v_2$ $PHP = v_4$ $SIPHDE = \sin(q_4 + q_5)$ $COPHDE = \cos(q_4 + q_5)$ $DEP = v_5$ $OMP = v_6$ $SIOMEP = \sin(q_6 + q_7)$ $COOMEP = \cos(q_6 + q_7)$ $EPP = v_7$	$M_1 = 0{,}4325$ $I_1 = 2{,}194 \cdot 10^{-6}$ $M_2 = 0{,}00365$ $I_2 = 4{,}410 \cdot 10^{-7}$ $M_3 = 0{,}2373$ $I_3 = 5{,}255 \cdot 10^{-6}$ $M_4 = 0{,}00706$ $I_4 = 5{,}667 \cdot 10^{-7}$ $M_5 = 0{,}7050$ $I_5 = 1{,}169 \cdot 10^{-5}$ $M_6 = 0{,}00706$ $I_6 = 5{,}667 \cdot 10^{-7}$ $M_7 = 0{,}05498$ $I_7 = 1{,}912 \cdot 10^{-5}$

$$M_{11} = M_1 \cdot RA^2 + M_2 \cdot (RR^2 - 2 \cdot DA \cdot RR \cdot COTH + DA^2) + I_1 + I_2$$
$$M_{12} = M_2 \cdot (DA^2 - DA \cdot RR \cdot COTH) + I_2$$
$$M_{22} = M_2 \cdot DA^2 + I_2$$
$$M_{33} = M_3 \cdot (SA^2 + SB^2) + I_3$$
$$M_{44} = M_4 \cdot (E - EA)^2 + I_4$$
$$M_{45} = M_4 \cdot ((E - EA)^2 + ZT \cdot (E - EA) \cdot SIPH) + I_4$$
$$M_{55} = \mathrm{M_4} \cdot (\mathrm{ZT^2} + 2 \cdot \mathrm{ZT} \cdot (\mathrm{E - EA}) \cdot \mathrm{SIPH} + (\mathrm{E - EA})^2) + \mathrm{M_5} \cdot (\mathrm{TA^2} + \mathrm{TB^2}) + \mathrm{I_4} + \mathrm{I_5}$$
$$M_{66} = \mathrm{M_6} \cdot (\mathrm{ZF - FA})^2 + \mathrm{I_6}$$
$$M_{67} = \mathrm{M_6} \cdot ((\mathrm{ZF - FA})^2 - \mathrm{U} \cdot (\mathrm{ZF - FA}) \cdot \mathrm{SIOM}) + \mathrm{I_6}$$
$$M_{77} = \mathrm{M_6} \cdot ((\mathrm{ZF - FA})^2 - 2 \cdot \mathrm{U} \cdot (\mathrm{ZF - FA}) \cdot \mathrm{SIOM} + \mathrm{U^2}) + \mathrm{M_7} * (\mathrm{UA^2} + \mathrm{UB^2}) + \mathrm{I_6} + \mathrm{I_7}$$

$$XD = SD \cdot COGA + SC \cdot SIGA + XB$$

$$YD = SD \cdot SIGA - SC \cdot COGA + YB$$

$$LANG = ((XD - XC)^2 + (YD - YC)^2)^{0.5}$$

$$FORCE = -C_0 \cdot (LANG - L_0)/LANG$$

$$FX = FORCE \cdot (XD - XC)$$

$$FY = FORCE \cdot (YD - YC)$$

$$F_1 = MOM - M_2 \cdot DA \cdot RR \cdot THP \cdot (THP + 2 \cdot BEP) \cdot SITH$$

$$F_2 = M_2 \cdot DA \cdot RR \cdot BEP^2 \cdot SITH$$

$$F_3 = FX \cdot (SC \cdot COGA - SD \cdot SIGA) + FY \cdot (SD \cdot COGA + SC \cdot SIGA)$$

$$F_4 = M4 \cdot ZT \cdot (E - EA) \cdot DEP^2 \cdot COPH$$

$$F_5 = (0 - M_4) \cdot ZT \cdot (E - EA) \cdot PHP \cdot (PHP + 2 \cdot DEP) \cdot COPH$$

$$F_6 = (0 - M_6) \cdot U \cdot (ZF - FA) \cdot EPP^2 \cdot COOM$$

$$F_7 = M_6 \cdot U \cdot (ZF - FA) \cdot OMP \cdot (OMP + 2 \cdot EPP) \cdot COOM$$

$$GQ_{11} = (0 - RR) \cdot SIBE + D \cdot SIBETH$$

$$GQ_{12} = RR \cdot COBE - D \cdot COBETH$$

$$GQ_{13} = (0 - RR) \cdot SIBE + D \cdot SIBETH$$

$$GQ_{14} = RR \cdot COBE - D \cdot COBETH$$

$$GQ_{15} = (0 - RR) \cdot SIBE + D \cdot SIBETH$$

$$GQ_{16} = RR \cdot COBE - D \cdot COBETH$$

$$GQ_{21} = D \cdot SIBETH$$

$$GQ_{22} = (0 - D) \cdot COBETH$$

$$GQ_{23} = D \cdot SIBETH$$

$$GQ_{24} = (0 - D) \cdot COBETH$$

$$GQ_{25} = D \cdot SIBETH$$

$$GQ_{26} = (0 - D) \cdot COBETH$$

$$GQ_{31} = -SS \cdot COGA$$

$$GQ_{32} = (0 - SS) \cdot SIGA$$

$$GQ_{43} = (0 - E) \cdot COPHDE$$

$$GQ_{44} = (0 - E) \cdot SIPHDE$$

$$GQ_{53} = (0 - E) \cdot COPHDE + ZT \cdot SIDE$$

$$GQ_{54} = (0 - E) \cdot SIPHDE - ZT \cdot CODE$$

$$GQ_{65} = ZF \cdot SIOMEP$$

$$GQ_{66} = (0 - ZF) \cdot COOMEP$$

$$GQ_{75} = ZF \cdot SIOMEP - U \cdot COEP$$

$$GQ_{76} = (0 - ZF) \cdot COOMEP - U \cdot SIEP$$

$L_1 = 98{,}566870396241089605765498 2170$
$L_2 = -6{,}122688344255662655031143 93122$
$L_3 = 0$
$L_4 = 0$
$L_5 = 0$
$L_6 = 0$

$D = 0{,}028$	$DA = 0{,}0115$	$E = 0{,}02$
$EA = 0{,}01421$	$ZF = 0{,}02$	$FA = 0{,}01421$
$RR = 0{,}007$	$RA = 0{,}00092$	$SS = 0{,}035$
$SA = 0{,}01874$	$SB = 0{,}01043$	$SC = 0{,}018$
$SD = 0{,}02$	$ZT = 0.04$	$TA = 0{,}02308$
$TB = 0{,}00916$	$U = 0.04$	$UA = 0{,}01228$
$UB = 0{,}00449$	$C_0 = 4530$	$L_0 = 0{,}07785$