Applications of Verified Methods for Solving Non-smooth Initial Value Problems

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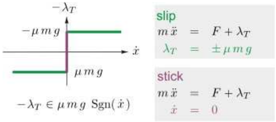
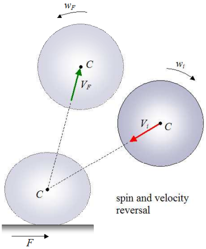
Non-smooth Models in Engineering

Friction



Contact dynamics



Besides: saturation effects, ensuring good numerical behavior, etc.

Implicitly Non-smooth Models: Traps in Code

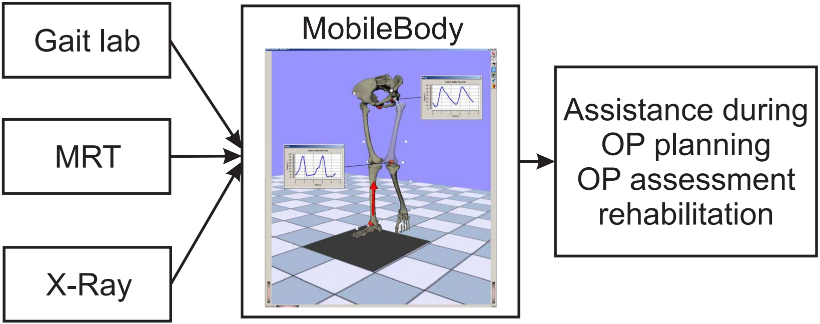
Trap	Example
`IF-THEN-ELSE`	Force: $F \leq 0$
`SWITCH`	Muscle activation function: $0 \leq a(t) = A_1 e^{-c_1(t-t_1)} + A_2 e^{-c_2(t-t_2)} \leq 1$
$\lvert x \rvert$	Hysteresis:
sgn$x$	Friction: $F(v) =$sgn$(v) \cdot F + \mu \cdot v$

Hysteresis:

$$\dot{\omega}(t) = \rho \cdot \Big(v(t) - \sigma \cdot |v(t)| \cdot |\omega(t)|^{\nu-1} \cdot \omega(t) + (\sigma - 1) \cdot v(t) \cdot |\omega(t)|^{\nu} \Big)$$

Biomechanical Context: MobileBody

Chief coordination: Prof. A. Kecskeméthy (UDE)



Our major task: Characterization of uncertain parameters
Non-smoothness in: Muscle models, stabilization of stance

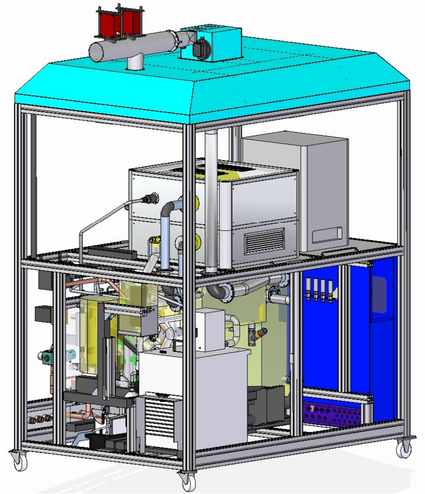
Fuel Cells Context: Development of VeriCell

Cooperation: Chair of Mechatronics, Rostock

- Gas supply
- Preheater
- SOFC stack module (30 fuel cells)

Our task: Control design, verified simulation environment

Non-smoothness: Saturation effects in reaction kinetics, etc.



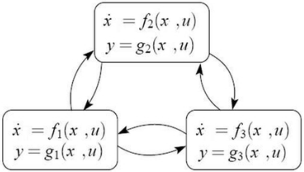
Background: Verified Methods for Non-smooth Systems

Description of a non-smooth IVP

↙ Analytical

↘ Graph-like

$$x' = \begin{cases} f^+(x), & h(x(t),t) < 0 \\ f^-(x), & h(x(t),t) > 0 \end{cases}$$



Rihm (1993), Mahmoud and Chen (2008)

Rauh (2006), Eggers (2008), Nedialkov and Mohrenschildt (2002)

Verified non-smooth optimization: Slopes, generalized gradients ...

Ratz (1995), Kearfott (2004), Schnurr (2007), ...

Problem Definition

Interval IVP: $\begin{cases} x' &= f(x), \\ x(0) &\in [x_0] \end{cases}$

where $f : \mathcal{D} \subset \mathbb{R}^n \to \mathbb{R}^n$ or $\mathcal{D} \subset \mathbb{IR}^n \to \mathbb{IR}^n$ and is given in algorithmic representation:

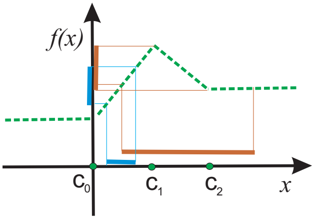
$$\begin{cases} \tau_i(x) &= g_i(x) = x_i,\ i = 1 \dots n \\ \tau_i(x) &= g_i(\tau_1(x), \dots, \tau_{i-1}(x)),\ i = n+1 \dots l, \\ g_i &\in S_{EO} \cup S_{PW} \end{cases} .$$

$S_{EO} = \{+, -, *, /, \sin, \cos, \dots\}$ and
S_{PW} are piecewise smooth functions

Definition of Piecewise Functions

$\phi_{i,\tau_\nu,c}(\tau_{i_0}(x), \ldots, \tau_{i_p}(x))$:

$$\begin{cases} \tau_{i_0}(x), & c_{-1} = -\infty < \tau_\nu(x) \leq c_0, \\ \tau_{i_1}(x), & c_0 < \tau_\nu(x) \leq c_1, \\ \ldots & \ldots \\ \tau_{i_{p-1}},(x) & c_{p-2} < \tau_\nu(x) \leq c_{p-1}, \\ \tau_{i_p}(x), & c_{p-1} < \tau_\nu(x) < c_p = +\infty \end{cases}$$



An interval extension of ϕ over X ($\phi(X)$):

$$\begin{cases} \tau_i(X), & \text{if } X \subseteq (c_{i-1}, c_i), \\ \underline{\bigcup}_{k=i+1}^{j-1} \tau_k([c_{k-1}, c_k]) \underline{\cup} \tau_i([\underline{x}, c_i]) \underline{\cup} \tau_j([c_{j-1}, \overline{x}]), & \text{if } X \subseteq (c_{i-1}, c_j) \end{cases}$$

Definition of the Derivative

An interval extension of ϕ' over X ($\phi'(X)$)

$$\begin{cases} \tau_i'(X), & \text{if } X \subseteq (c_{i-1}, c_i), \\ \underline{\bigcup}_{k=i+1}^{j-1} \tau_k'([c_{k-1}, c_k]) \underline{\cup} \tau_i'([\underline{x}, c_i]) \underline{\cup} \tau_j'([c_{j-1}, \overline{x}]) & \\ \underline{\cup}\ \mathrm{REST}, & \text{if } X \subseteq (c_{i-1}, c_j), \end{cases}$$

where REST depends on:

- how many switching points X contains,
- whether ϕ is continuous,

if we want the mean value theorem to hold.

Suppose we have a single switching point (`IF-THEN-ELSE`)

$$\phi(x) = \begin{cases} \phi_0(x), & x < c_0, \\ \phi_1(x), & x > c_0. \end{cases}$$

then REST is

- $(\phi_0'([\underline{x}, c_0]) + \phi_1'([c_0, \overline{x}])) \cdot [0, 1]$ if ϕ is continuous,
- $$\left(\frac{\phi_1(c_0) - \phi_0(c_0)}{[c_0, \overline{x}] - x_0} + (\phi_0'([\underline{x}, c_0]) + \phi_1'([c_0, \overline{x}])) \cdot [0, 1] \right)$$
  $$\underline{\cup} \left(\frac{\phi_0(c_0) - \phi_1(c_0)}{[\underline{x}, c_0] - x_0} + (\phi_0'([\underline{x}, c_0]) + \phi_1'([c_0, \overline{x}])) \cdot [0, 1] \right)$$
  if ϕ is discontinuous.

Problem: We need x_0 to avoid enclosures containing ∞ afap

Properties of $\phi'(X)$

1. If the derivative of ϕ exists for $x \in X$, then $\phi'(x) \in \phi'(X)$
2. The slope $\delta\phi(X, x_0) \subseteq \phi'(X)$
3. The mean value theorem holds:

$$\phi(x) = \phi(x_0) + \phi'(\xi)(x - x_0) \in \phi(x_0) + \phi'(X)(X - x_0)$$

4. If ϕ is continuous ($\tau_{i_j}(c_j) = \tau_{i_{j+1}}(c_j)$, $0 \leq j < p$), then $f(x)$ is continuous.

Solution Definitions

Two situations:

↙ ↘

(a) f is discontinuous only in t

$\tau_\nu(x) = t$ or

$\tau_{i_j}(c_j) = \tau_{i_{j+1}}(c_j)$

(b) f is discontinuous in t, x

Solution:

$$x(t) = x_0 + \int_0^t f(x(s))ds,\ x_0 \in [x_0]$$

Depends on the application

VALENCIA-IVP[1] For Non-smooth IVPs

General approach in VALENCIA: A posteriori

$$x(t) \in \underbrace{[x(t)]}_{\text{verified state enclosure}} := \underbrace{x_{app}(t)}_{\text{non-verified approximation}} + \underbrace{[R(t)]}_{\text{error bounds}}$$

Conditions for the right side:

1. continuous
2. Lipschitz

[1] *VAL*idation of state *ENC*losures using *I*nterval *A*rithmetic for *I*nitial *V*alue *P*roblems

VALENCIA-IVP For Non-smooth IVPs (Cont.)

The algorithm for $0 \leq t \leq T$:

1. Start with $[x^{(0)}]$, $x_{app}(t)$, $[R(0)]$
2. $k = 1 \ldots k_{max}$ or while $[\dot{R}^{(k+1)}([0,T])]!=[\dot{R}^{(k)}([0,T])]$

   Compute $[\dot{R}^{(k+1)}([0,T])] := \dot{x}_{app} + f([x^{(k)}])$, (MVT)
   where $[x^{(k)}] := [x^{(k)}([0,T])]$

   If $[\dot{R}^{(k+1)}([0,T])] \subseteq [\dot{R}^{(k)}([0,T])]$ then

$$\begin{aligned} [R^{(k+1)}([0,T])] &:= [R(0)] + [\dot{R}^{(k+1)}([0,T])][0,T] \\ [x^{(k+1)}([0,T])] &:= x_{app} + [R^{(k+1)}([0,T])] \end{aligned}$$

Differences ((non-)smooth): Derivative definition, the fixed point theorem

To-do-list: Discontinuities in x for the right side

Implementation Issues: Class pwFunc

Remarks on $f(x)$

- $f'(X)$ is obtained with pwFunc
- pwFunc uses FADBAD++ and overloads hull, d()
- $f'(X)$ encloses both left and right derivatives
- pwFunc is plugged into ValEncIA

Class declaration

```
template<class T>
class pwFunc{
public:
typedef T (*ptrFct)(const T& x);
pwFunc(const vector<interval>& p,
    const vector<ptrFct>& f);
T operator()(const T& x)
    { return getValueAtX(x);}
private:
vector< ptrFct > functions;
vector<interval> points;
vector<T> subintervals;
T getValueAtX(const T& x);
void generateSubintervals(const T& x);
};
```

Implementation Example: A Discontinuous Function

```
template <class T> T f1(const T& x){ return -1+x;}
template <class T> T f2(const T& x){ return 1+x;}
template<class T> T ff(const T& a){
    vector<INTERVAL> p; p.push_back(0);
    vector<pwFunc<T>::ptrFct> functions;
    functions.push_back(&f1<T>);functions.push_back(&f2<T>);
    pwFunc<T> fp(p, functions); return fp(a); }
ff([-1,2]);
```

Equation:

$$F_f(v) = \begin{cases} -1.0 + x & x < 0 \\ +1.0 + x & x > 0 \end{cases}$$

Result:

`[-2,3]([1,6])`

A Mechanical System with Friction and Hysteresis

$$\dot{x}(t) = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} x(t) + \begin{bmatrix} 0 \\ \frac{1}{m}\left(F_a(t) - F_f(x_2)\right) \end{bmatrix} \quad x = \begin{bmatrix} x_1 & x_2 \end{bmatrix}^T$$

Friction force:

$$F_f(x_2) = \begin{cases} -[F_s] + [\mu] \cdot x_2 & \text{for} \quad S_1 = \texttt{true} \quad \text{or} \quad S_2 = \texttt{true} \\ +[F_s] + [\mu] \cdot x_2 & \text{for} \quad S_4 = \texttt{true} \quad \text{or} \quad S_5 = \texttt{true} \end{cases}$$

with the static friction

$$F_f(x_2) \in [F_s^{max}] := \left[-\overline{F}_s \,;\, \overline{F}_s\right] \quad \text{for} \quad S_3 = \texttt{true}$$

$$S_1 = \{x < 0, \omega \geq 0\},\ S_2 = \{x < 0, \omega < 0\},\ S_3 = \{x = 0\},$$
$$S_4 = \{x > 0, \omega \geq 0\},\ S_5 = \{x < 0, \omega > 0\}$$

A Mechanical System with Friction and Hysteresis (Cont.)

Accelerating force:

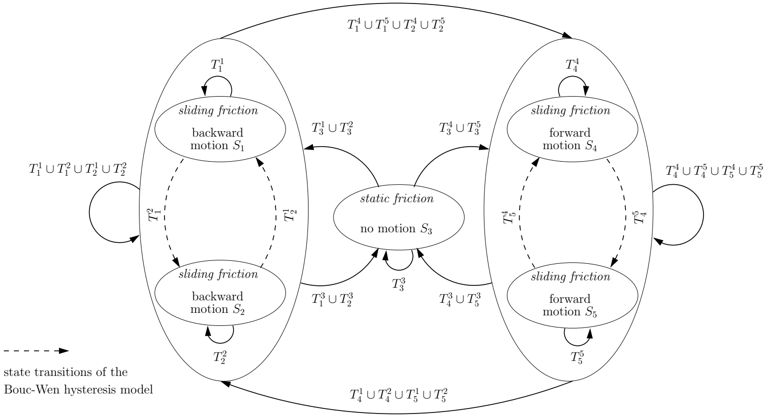
$$F_a(t) := u(t) - \phi(x_1(t), \omega(t))$$

- control variable $u(t)$ provided by an actuator
- restoring spring force $\phi(x_1(t), \omega(t)) = \kappa_x x_1 + \kappa_\omega \omega$

Restoring spring force with hysteresis (the Bouc-Wen model):

$$\begin{aligned}\dot{\omega}(t) =& \rho \cdot \Big(x_2(t) - \sigma \cdot |x_2(t)| \cdot |\omega(t)|^{\nu-1} \cdot \omega(t) \\ & + (\sigma - 1) \cdot x_2(t) \cdot |\omega(t)|^{\nu}\Big)\end{aligned}$$

Automaton-Based Method: Rauh et al.



A. Rauh, Ch. Siebert, H. Aschemann, *Verified Simulation and Optimization of Dynamic Systems with Friction and Hysteresis*, ENOC 2011, Rome, Italy, 2011

Idea of the Algorithm

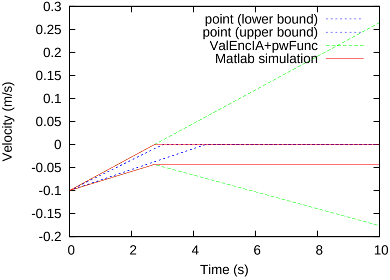
1. Detection of all possible points of time at which transition conditions $T_i^j(x, u)$ are activated
   $\Longrightarrow$ Validated enclosures of switching times as well as state variables
2. Detection of deactivation of model states
   $\Longrightarrow$ Computation of tight enclosures of state variables
3. Algorithm relying on Taylor-series method with a priori enclosures determined by the Picard iteration to detect activation of switching conditions

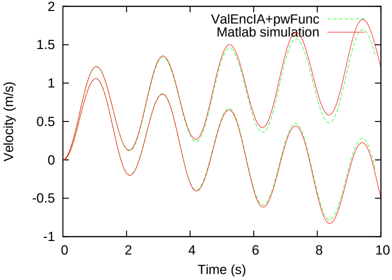
A. Rauh, M. Kletting, et al.: *Interval Methods for Simulation of Dynamical Systems with State-Dependent Switching Characteristics*, Proc. of the IEEE CCA 2006, pp. 355–360

Comparison: pwFunc+ValEncIA vs. Rauh et al.

$$\begin{aligned} \kappa_x &= 0 \\ x_1(0) &= 0 \\ x_2(0) &= -0.1 \\ \omega(0) &= -0.001 \\ u(t) &= 0.01 \end{aligned}$$

$$\begin{aligned} \kappa_x &= 0.001 \\ x_1(0) &= 0 \\ x_2(0) &= 0 \\ \omega(0) &= 0.001 \\ u(t) &= 2\sin(3t) \end{aligned}$$





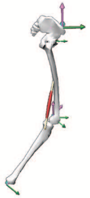
The PT Muscle Model

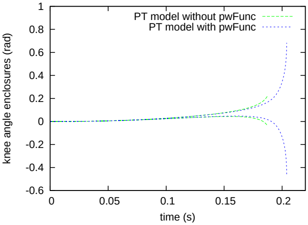
Activation function: $0 \leq a(t) = A_1 e^{-c_1(t-t_1)} + A_2 e^{-c_2(t-t_2)} \leq 1$

PT muscle force : $F \leq 0$

Thigh length: $p = 0.45 \pm 0.1\%$

Dynamics in SmartMOBILE with ValEncIA-IVP with and without piecewise functions:

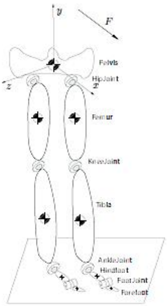




Improvement in break down times!

Stabilization of Stance*

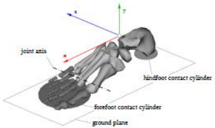
Human skeleton



⇓

Mass parameters

Foot contact



Hunt-Crossley contact

⇓

Contact parameters

Stance stabilizer

PID controller

$$Q = K_p \cdot \varphi + K_d \cdot \frac{d\varphi}{dt} + K_i \int \varphi dt$$

⇓

Force parameters

* Modeling: X. Liu, H. Albassam (UDE)

Stance Stabilization: Equations of Motion

$$M(q;t)q'' + \underbrace{b(q,q';t) = Q(q,q';t)}_{f}, \text{ dof=26}$$

Parameters of interest: m_{pelvis}, p_x, F_x, $m_{rfemur} = 10.34\text{kg}$

$$[f_1\ f_2\ f_4\ f_6] = [[0,200]\ [-940.00,-595.69]\ [-31.89,31.89]\ [-50.17,45.49]]$$

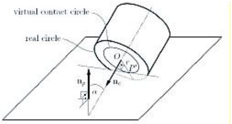
Sensitivity (interval/nominal)

	m_{pelvis}	p_x	m_{rfemur}	F_x
f_1	0.0	0.0	0.0	1
f_2	-9.8	0.0	-9.8	0.0
f_4	[-0.5,0.5]/0	0.0	0.7848	0.0
f_6	[-9.81,0.5]/-0.25	[-637.66,-343.34]/-490.5	0.5	0.0

Stance Stabilization: To-Do-List

Major challenge: Foot contact problem

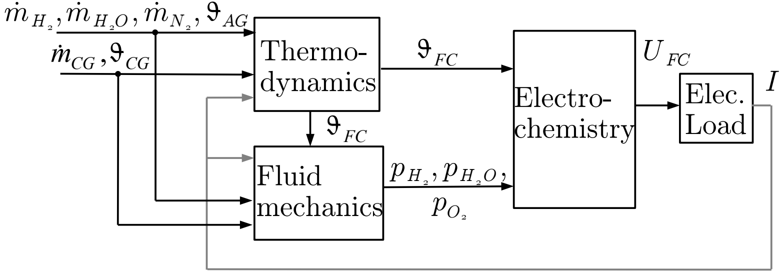
Advantages: e.g. contact area modeling with intervals



Necessary: A solver similar to Rihm's for dynamics
A solver similar to Chen's for equilibria

Outlook: Control-Oriented Modeling and Simulation for SOFC Fuel Cells

Three subprocesses:



A. Rauh, Th. Dötschel, H. Aschemann: Experimental Parameter Identification for a Control-Oriented Model of the Thermal Behavior of High-Temperature Fuel Cells MMAR 2011, accepted.

Outlook: Switchings in SOFC Modeling

- Hysteresis in the electro-chemical subsystem
  - Activation losses
  - Concentration losses
  - Storage of charge carriers in the double layer
- Detection of predominant influence factors
  - (Partial) Pressures of fuel gas and air
  - Temperatur
  - Electric load conditions
- Modeling of disturbances, especially electric load drop-off

Outlook: Switchings in SOFC Modeling (Cont.)

Locally restricted validity of system models

- Piecewise (polynomial) approximation of
    - (Specific) Heat capacity
    - Heat conductivity
    - Thermal resistances
    - Enthalpy
- Physical limitation of the range of state variables
    - Non-negativity of partial pressures
    - Temperatures
    - Volume and mass flow rates

Outlook: Switchings in SOFC Modeling (Cont.)

- Saturation in actuator dynamics
  - Gas preheaters for fuel gas and air
  - Mass flow controllers for fuel gas and air
- Introduction of hysteresis as an additional degree of freedom in controller design to reduce actuator
- Goal: Reliable detections of possible limit cycles
- Goal: Reliable prevention of limit cycles

Outlook: Switchings in SOFC Modeling (Cont.)

- General variable structure control and estimation approaches
- Nonlinear control design
  - Model predictive control with active avoidance of limit cacles
  - Sliding mode controllers
  - Sliding mode observers
- Discrete-time implementation with piecewise constant signals (control and estimated values)
- Necessity to compute derivatives of at least first order during sensitivity analysis

Conclusions

Results:

- Implementation of a simple extension for ValEncIA to work with non-smooth functions
- A proof for continuous functions
- Simulation for a system with friction and hysteresis
- Results similar to Rauh

Future work:

- Application to stance stabilization
- Application to SOFC