Nonsmooth Differential-Algebraic Equations

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Dynamic Modeling Frameworks in PSE

- Trade-off: applicability vs. ease of modeling & solving

Smooth Models
- Limited applicability
- Easy to model and solve
- Derivative information
- Strong existence & uniqueness theory

Nonsmooth Models
- Broad applicability
- Easy to model and solve
- Generalized derivative information
- (recently) Strong existence & uniqueness theory

Hybrid Models
- (near) Universal applicability
- Often challenging to model and solve
- Limited derivative information
- Pathological behaviors (hard to exclude a priori)

Smooth approximation models —— Complementarity systems
Hybrid Automaton Framework

- Simple const. $P$ flash process:
  
  \[ \dot{H}(t) = U(T_{out} - T(t)) \]
  
  \[ M = M_L(t) + M_V(t) \]
  
  \[ H(t) = Mh_V(t) - M_L(t)\Delta h_{vap}(T(t)) \]
  
  \[ h_V(t) = C_p(T(t) - T_0) \]
  
  \[ \log(P_{sat}(t)) = A - B/(T(t) + C) \]
  
  ...

- DAE embedded in hybrid automaton

Diagram:

- Mode 1:
  
  \[ M_V = 0, M_L > 0 \]
  
  \[ P \geq P_{sat}(T) \]
  
  \[ P = P_{sat}(T) \]

- Mode 2:
  
  \[ M_V, M_L > 0 \]
  
  \[ P = P_{sat}(T) \]

- Mode 3:
  
  \[ M_V > 0, M_L = 0 \]
  
  \[ P \leq P_{sat}(T) \]
Simple flash process (continued):

- Hybrid automaton formulation

- Nonsmooth DAEs formulation: continuous disjunction:

\[
0 = \text{mid} \left( M_V(t), P - P^{\text{sat}}(T(t)), -M_L(t) \right)
\]
Nonsmooth Models: Applications

- Intensive properties with flow reversals
- Flow transitions
- Thermodynamic phase changes
- Crystallization kinetics: growth vs. dissolution
- Flow control devices
- Irregularities in vessel geometry
- Dynamic flux balance analysis (DFBA) systems
  - e.g., aerobic to anaerobic switch
- Protecting domains of functions (abs)
- Piecewise properties
- etc., etc.
Flow Reversal: Intensive Properties

\[
\frac{dM_i^A}{dt}(t) = -\left(\max\left(F_{out}^A(t), 0\right)x_i^A + \min\left(F_{in}^B(t), 0\right)x_i^B\right)
\]

\[
\frac{dM_i^B}{dt}(t) = -\frac{dM_i^A}{dt}(t); \quad F_{out}^A(t) = F_{in}^B(t)
\]

\[
F_{out}^A(t) = c\frac{h^A(t) - h^B(t) + \Delta h(t)}{\sqrt{h^A(t) - h^A(t) + \Delta h(t)}} + \varepsilon
\]
Multi-component Dynamic VLE

Mass and energy balances:

\[
\begin{align*}
\frac{dM_i}{dt}(t) &= F_{in}(t)z_i(t) - F_L(t)x_i(t) - F_V(t)y_i(t) \\
\frac{dU}{dt}(t) &= F_{in}(t)h_m(t) - F_L(t)h_L(t) - F_V(t)h_V(t) + Q(t) \\
M_i(t) &= M_L(t)x_i(t) + M_V(t)y_i(t) \\
\sum_{i=1}^{n_c} M_i(t) &= M_L(t) + M_V(t) \\
H(t) &= M_L(t)h_L(t) + M_V(t)h_V(t) \\
H(t) &= U(t) + P(t)V
\end{align*}
\]

Flow control:

\[
\begin{align*}
F_V(t) &= c_v \min\left(V_{V_{\text{min}}}, V_V(t)\right) \max \left(0, \frac{P(t) - P_0}{\sqrt{|P(t) - P_0| + \varepsilon}}\right) \\
F_L(t) &= c_i \min\left(V_{L_{\text{min}}}, V_L(t)\right) \max \left(0, \frac{K_L(t)}{\sqrt{|K_L(t)| + \varepsilon}}\right) \\
K_L(t) &= g \frac{V_L(t)}{A} + \frac{P(t) - P_0}{\rho_L(t)}
\end{align*}
\]

Thermodynamic phase equilibrium:

\[
y_i(t) = k_i(t)x_i(t)
\]

0 = \min \left( \frac{M_V(t)}{M_V(t) + M_L(t)} \sum_{i=1}^{n_c} x_i(t) - \sum_{i=1}^{n_c} y_i(t), \frac{M_V(t)}{M_V(t) + M_L(t)} - 1 \right)
Multi-component Phase Change

\[ M_L = 0 \]
\[ \sum_{i=1}^{n_c} x_i(t) \leq 1 \]

\[ M_V = 0 \]
\[ \sum_{i=1}^{n_c} y_i(t) \leq 1 \]

Regularization of Nonsmooth DAEs

- Nonsmooth DAEs:
  \[
  \begin{align*}
  \dot{x}(t,p) &= f(t,p,x(t,p),y(t,p)) \\
  0 &= g(t,p,x(t,p),y(t,p)) \\
  x(t_0,p) &= f_0(p)
  \end{align*}
  \]

- \( f \) is piecewise continuous w.r.t. \( t \) and continuous w.r.t. \( p, x, y \)
- \( g \) is locally Lipschitz continuous
- “Index 1” Nonsmooth DAEs: generalized differentiation index one
- Existence, uniqueness, continuous/Lipschitz dependence on parameters, etc.

Generalized Differentiation Index

- Given locally Lipschitz continuous \( f : \mathbb{R}^n \rightarrow \mathbb{R}^m \):
  - Clarke’s Generalized Jacobian

\[
\partial f(x) := \text{conv} \left\{ H : Jf(x_j) \rightarrow H, x_j \rightarrow x, x_j \in X \setminus Z_f \right\}
\]

- Example:

\[
f(x) = |x|
\]

\[
\partial f(x) = \begin{cases} 
-1 & \text{if } f(x) = -1 \\
1 & \text{if } f(x) = 1 \\
[-1,1] & \text{if } f(0) = 0
\end{cases}
\]

- “Index-1” Nonsmooth DAE:
  - No singular matrix in the set \( \{ M : \exists [N M] \in \partial g(t,p,x(t,p),y(t,p)) \} \)
    - If \( g \) is \( C^1 \):
      \[
      \left\{ \frac{\partial g}{\partial y} (t,p,x(t,p),y(t,p)) \right\}
      \]

Clarke, Optimization and Nonsmooth Analysis, SIAM, 1990.
Dynamic Optimization in PSE

- Continuous campaign manufacturing:
  - Maximize production, minimize off-spec.
  - “Discrete” phenomena: start-up/shut-down, phase changes, crystal growth/dissolution, etc., etc.

Dynamic Optimization of DAEs

- In the smooth case:
  - Semi-explicit index-1 DAE IVP
    \[
    \begin{align*}
    \dot{x}(t,p) &= f(t,p,x(t,p),y(t,p)) \\
    0 &= g(t,p,x(t,p),y(t,p)) \\
    x(t_0,p) &= f_0(p)
    \end{align*}
    \]
  - Sensitivity DAEs
    \[
    \begin{align*}
    \frac{\partial \dot{x}}{\partial p} &= \frac{\partial f}{\partial p} + \frac{\partial f}{\partial x} \frac{\partial x}{\partial p} + \frac{\partial f}{\partial y} \frac{\partial y}{\partial p} \\
    0 &= \frac{\partial g}{\partial p} + \frac{\partial g}{\partial x} \frac{\partial x}{\partial p} + \frac{\partial g}{\partial y} \frac{\partial y}{\partial p} \\
    \frac{\partial x}{\partial p}(t_0) &= Jf_0(p_0)
    \end{align*}
    \]
- Update \( p \) via optimization
Dynamic Optimization of DAEs

- In the nonsmooth case:
  - Semi-explicit “index-1” DAE IVP
    \[
    \dot{x}(t,p) = f(t,p,x(t,p),y(t,p)) \\
    0 = g(t,p,x(t,p),y(t,p)) \\
    x(t_0,p) = f_0(p)
    \]
  - Nonsmooth sensitivity DAEs

Update \( p \) via optimization

\( x(t,p_0), y(t,p_0) \)
\( \frac{\partial x}{\partial p}, \frac{\partial y}{\partial p} \)
Sensitivities of Hybrid Automata

\[ \dot{x}^{(k)} = f^{(k)}(t,p,x^{(k)}), \quad S^{(k)} \equiv \frac{\partial x^{(k)}}{\partial p} \]

\[ S^{(k+1)} - S^{(k)} = -\left[ f^{(k+1)} - f^{(k)} \right] \frac{\partial t}{\partial p} \]

Transversality: \[ \frac{\partial g^{(k)}}{\partial x^{(k)}} \dot{x}^{(k)} \neq 0 \]

Nonsmooth DAE Sensitivities: Generalized Derivatives

- Want generalized derivative elements \( \frac{\partial x}{\partial p}(t_f, p_0), \frac{\partial y}{\partial p}(t_f, p_0) \)
  
- Nonsmooth analog of \( \frac{\partial x}{\partial p}(t_f, p_0), \frac{\partial y}{\partial p}(t_f, p_0) \)
  
- Difficult to evaluate in general (lack of sharp calculus rules, etc.)

- New tool: lexicographic directional (LD-) derivatives
  
- Nonsmooth analog to classical directional derivative
  
- Applicable to a wide class of functions (C^1, PC^1, convex, arbitrary compositions of such, etc.)
  
- Satisfies strict calculus rules (e.g. chain rule)
  
- Accurate, automatable and computationally cheap method

**LD-Derivatives**

- Given L-smooth $f$ and directions matrix $M := \begin{bmatrix} m_{(1)} \cdots m_{(k)} \end{bmatrix}$

\[
\begin{bmatrix} f'(x; M) := \begin{bmatrix} f^{(0)}_{x,M}(m_{(1)}) & f^{(1)}_{x,M}(m_{(2)}) & \cdots & f^{(k-1)}_{x,M}(m_{(k)}) \end{bmatrix} \end{bmatrix}
\]

- If $M$ is square and nonsingular:

\[
f'(x; M) = J_L f(x; M)M
\]

- If $f$ is $C^1$ at $x$:

\[
f'(x; M) = Jf(x)M
\]

- Sharp LD-derivative chain rule:

\[
\left[f \circ g \right]'(x; M) = f'(g(x); g'(x; M))
\]

Lexicographic Differentiation

- Systematically probes local derivative information

\[ f(x_1, x_2) = \max(0, \min(x_1, x_2)) \]

\[ f_{0,1}^{(2)}(d) = d_2 \]

\[ f_{0,1}^{(0)}(d) = \max(0, \min(d_1, d_2)) \]

\[ f_{0,1}^{(1)}(d) = \max(0, d_2) \]

\[ J_L f(0; I) = J f_{0,1}^{(2)}(0) \]
Given $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$

- If $m=1$ (e.g., objective function):
  - If $f$ is $\text{PC}^1$:
  - If $f$ is $\text{C}^1$:

LD-derivatives furnish gen. deriv. elements (green dots) in tractable way

---

In the nonsmooth case:

- Semi-explicit “index-1” DAE IVP
  \[
  \dot{x}(t,p) = f(t,p,x(t,p),y(t,p)) \\
  0 = g(t,p,x(t,p),y(t,p)) \\
  x(t_0,p) = f_0(p)
  \]

- Nonsmooth sensitivities DAEs
  \[
  \dot{X}(t) = [f_t]'(p_0,z(t,p_0);(M,Z(t))) \\
  0 = [g_t]'(p_0,z(t,p_0);(M,Z(t))) \\
  X(t_0) = [f_0]'(p_0;M)
  \]

where
\[
  z \equiv (x,y), \quad Z \equiv (X,Y) \equiv [z_t]'(p_0;M)
\]
Simple Flash Process: Mode Sequence

- Mode sequence varies under parametric perturbations

\[ \dot{H}(t) = U(T_{out} - T(t)) \]
\[ M = M_L(t) + M_V(t) \]
\[ H(t) = Mh_V(t) - M_L(t) \Delta h_{vap}(T(t)) \]
\[ h_V(t) = C_p(T(t) - T_0) \]
\[ \log(P^{sat}(t)) = A - B / (T(t) + C) \]
+ hybrid automaton
Simple Flash Process: Sensitivities

- Nonsmooth sensitivities:
  \[
  \dot{S}_H(t) = U(1 - S_T(t)) \\
  S_H(t) = MCpS_T(t) - \Delta h_{vap}'(T(t))S_T(t) \\
  0 = \text{mid}'\left(M_V(t), P - P_{\text{sat}}(T(t)), -M_L(t); (S_V(t), -P_{\text{sat}}'(T(t))S_T(t), -S_L(t))\right) \\
  S_V(t) = -S_L(t)
  \]
Nonsmooth DAEs

Summary of Progress:
- Possess a strong mathematical theory (recently)
  - Hence, formulate model this way if you can!
- Easy-to-use and solve and do sensitivity analysis
- Applicable to variety of operational problems:
- Numerical toolkit: amenable to computationally tractable (e.g. automatic differentiation) methods
  - See Khan and Barton, *OM&S* 30 (2015)
  - LD-derivative rules for abs, min, max, mid, 2-norm, etc.

Future Work:
- Numerical implementations
- “High-index” nonsmooth DAEs
- Adjoint sensitivities
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Crystallization Kinetics

- With the development of continuous crystallization processes, dissolution has to be considered in dynamic models of crystal size distribution:

\[
\frac{\partial (V_n)}{\partial t}(t,z) + K(t) \frac{\partial (V_n)}{\partial z}(t,z) = Q_{in}(t)n_{in}(t,z) - Q_{out}(t)n(t,z)
\]

\[
S(t) = \left( x_i(t) - x_i^{sat} \right) / x_i^{sat}, \quad K(t) = \min \left( k_D S(t) | S(t) |^{n_D - 1}, k_G | S(t) |^{n_G} \right)
\]

- With finite volume discretization of the size coordinate:

\[
\frac{dN_j}{dt}(t) + \frac{1}{\Delta z} \left( G(t) \left( N_j(t) - N_{j-1}(t) \right) + D(t) \left( N_{j+1}(t) - N_j(t) \right) \right) = Q_{in}(t)n_{j,in}(t) - Q_{out}(t)n_j(t), \quad j = 2, \ldots, m - 1
\]

\[
G(t) = \max \left( 0, k_G S(t) | S(t) |^{n_G - 1} \right)
\]

\[
D(t) = \min \left( k_D S(t) | S(t) |^{n_D - 1}, 0 \right)
\]

\[N_j \equiv Vn_j, \quad n_j - \text{density of crystals of size } (j - 1)\Delta L < L < j\Delta L\]
Crystallization Kinetics

- Switching between modes of positive and negative super-saturation:

\[ S(t) - \text{super-saturation} \]
\[ \varepsilon(t) - \text{volume fraction of solid} \]
\[ T(t) = \text{mid} \left(30, 0, -40 + | -80 + 8t | \right) \]
Flow Transitions

- Transitioning between flow regimes can be modeled using one nonsmooth equation

\[ \text{Nu}(t) = \max\left(\text{Nu}_i(t), \text{Nu}_{ir}(t)\right) \]

\[ \text{Nu}_i(t) = 14.5 \]

\[ \text{Nu}_{ir}(t) = \left(\text{Nu}_i \exp\left(\frac{(\text{Re}(t) - \text{Re}_c)}{b}\right) + \text{Nu}_c\right)^c \]

\[ \text{Nu}_i(t) = 0.023 \text{Re}(t)^{0.8} \text{Pr}^{1/3} \]

Sensitivities of Nonsmooth DAEs

- DAE Smooth vs. Nonsmooth:
  - Nonsmooth sensitivities:
    \[
    \dot{X}(t) = \left[ f_t \right]'(p_0, x(t, p_0), y(t, p_0); (M, X(t), Y(t))
    \]
    \[
    0 = \left[ g_t \right]'(p_0, x(t, p_0), y(t, p_0); (M, X(t), Y(t))
    \]
    \[
    X(t_0) = \left[ f_0 \right]'(p_0; M)
    \]
  - Nonsmooth and nonlinear DAE system
  - Unique solution and unique initialization
  - \( X \) continuous, \( Y \) discontinuous
  - Once solved, obtain generalized derivative elements (sensitivities) via linear equation solve

- Smooth sensitivities:
  \[
  \frac{\partial x}{\partial p} = \frac{\partial f}{\partial p} + \frac{\partial f}{\partial x} \frac{\partial x}{\partial p} + \frac{\partial f}{\partial y} \frac{\partial y}{\partial p}
  \]
  \[
  0 = \frac{\partial g}{\partial p} + \frac{\partial g}{\partial x} \frac{\partial x}{\partial p} + \frac{\partial g}{\partial y} \frac{\partial y}{\partial p}
  \]
  \[
  \frac{\partial x}{\partial p}(t_0) = Jf_0(p_0)
  \]
  - Linear DAE system
  - Unique soln. & init.
  - \( \frac{\partial x}{\partial p}(\cdot, p_0), \frac{\partial y}{\partial p}(\cdot, p_0) \) continuous