# NONSMOOTH DIFFERENTIAL-ALGEBRAIC EQUATIONS

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*Abstract*

A nonsmooth modeling paradigm for dynamic simulation and optimization of process operations is advocated. Nonsmooth differential-algebraic equations (DAEs) naturally model a wide range of physical systems encountered in chemical engineering conventionally viewed as exhibiting hybrid continuous/discrete behavior. Due to recent advancements in nonsmooth analysis, nonsmooth DAEs now have a suitable foundational theory regarding well-posedness and sensitivity analysis for use in, for example, dynamic optimization. Moreover, the theory is computationally relevant, allowing for implementations of numerical methods which scale efficiently for large-scale problems. State-of-the-art modeling efforts and challenges for process operations displaying hybrid behavior (e.g., hybrid automata) are highlighted as motivation for the nonsmooth DAEs approach.

*Keywords*

Dynamic simulation, Dynamic optimization, Sensitivity Analysis, Hybrid systems.

## Introduction

A variety of operational problems require dynamic simulation and optimization (e.g., for safety, quality, and economic reasons) and exhibit a mixture of continuous and discrete phenomena (Barton and Lee, 2004; Barton et al., 2006). Examples displaying such hybrid behavior include campaign continuous pharmaceutical manufacturing (Sahlodin and Barton, 2015), where "discrete" phenomena include start-up/shut-down procedures, thermodynamic phase changes, and safety devices; dynamic flux balance analysis (DFBA) modeling of microbial consortia (Höffner and Barton, 2014), where "discrete" phenomena are present because the optimal value of a linear program as a function of the constraint right-hand sides is not smooth; among others (Barton and Lee, 2002). Current prevalent modeling paradigms advocated for these applications (e.g., hybrid automata, complementarity systems, etc.) can exhibit pathological behaviors that are difficult to exclude *a priori* and lack in theoretical results needed to guarantee existence and uniqueness of solutions and their regularity with respect to parametric variation.

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The purpose of this article is to promote a nonsmooth DAE modeling approach, which captures the physical behavior of many chemical engineering systems and regularizes the mathematical properties of the models. Moreover, recent progress (Stechlinski and Barton, 2016a, In Press) has laid a strong theoretical foundation and, thanks to an extension of the vector forward mode of automatic differentiation (Khan and Barton, 2015), the approach is computationally tractable. System models that fit into the nonsmooth DAEs framework include those process operations outlined above. A very simple flash process is used to illustrate the challenges involved in the hybrid automaton framework, followed by a nonsmooth DAE reformulation of the same problem.

## Current Modeling Approaches and Challenges

Hybrid dynamic systems combine continuous and discrete dynamics and include a number of formalisms with varying degrees of abstraction (see Goebel et al. (2009); Cortes (2012); Schumacher (2004) for general overviews). Within this general framework, a hybrid automaton (Lygeros et al., 1999; Barton and Lee, 2002; Lygeros et al., 2003) is a representation applicable to a wide class of hybrid systems. It can be viewed as a di-

rected graph whose vertices represent continuous mode dynamics (e.g., using ODEs or DAEs) and whose edges represent transitions between modes. Using reachability theory, (Lygeros et al., 2003) established existence and uniqueness of executions of a hybrid automaton (see Theorem III.1); a nonblocking deterministic hybrid automaton accepts a unique infinite execution, given an initial set-up. Such an execution may be Zeno in nature (i.e., it takes an infinite number of discrete transitions in finite time). Zeno executions raise concerns both conceptually (e.g., analysis techniques such as Lyapunov methods) and computationally (e.g., possible inefficient and inaccurate simulations).

Often a consequence of modeling abstractions, the presence of Zeno executions in physical problems necessitate a remodeling of the problem or a generalized solution notion (e.g., Goebel et al. (2004)). Regularization is a possible resolution (Johansson et al., 1999), but can require intuitive knowledge of the problem on a case-by-case basis and may lead to non-unique extensions. For example, see Section 4.1 in (Johansson et al., 1999), where the authors use a temporal regularization (i.e., adding delay between switch times) and spatial regularization (i.e., adding a minimum deviation in continuous state variables for switching to occur) of a water tank problem to lead to two distinctly different extensions of the unique hybrid automaton execution.

Detailed examples of physical problems modeled as hybrid automata can be found in the following works: the design of a safe changeover operation with nonreturn valves characterizing three distinct flow regimes (i.e., zero flow, laminar/turbulent, and choked) (Barton et al., 2000; Barton and Lee, 2002); a water tank system and the classical bouncing ball example (Johansson et al., 1999); and a rocking block model for rocking and toppling motion of rigid bodies during earthquakes (Lygeros et al., 2003).

Here, a very simple flash process is used to illustrate the hybrid automaton approach, as well as the nonsmooth DAE approach in the sequel. Consider the balloon depicted in Figure 1. The dynamic model is given by the following system of equations for a single species (e.g., water) that is held at a constant pressure $P$:

$$\dot{H}(t) = hA(T_{\text{out}} - T(t)), \tag{1a}$$

$$M = M_L(t) + M_V(t), \tag{1b}$$

$$H(t) = Mh_V(t) - M_L(t)\Delta h_{\text{vap}}(T(t)), \tag{1c}$$

$$h_V(t) = \int_{T^{\text{ref}}}^{T(t)} C_p(s)\mathrm{d}s. \tag{1d}$$

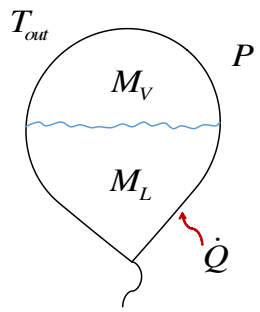


*Figure 1. A balloon with an external heat source and one species distributed between liquid and vapor phases. The heat duty at time t, $\dot{Q}(t)$, satisfies $\dot{Q}(t) = hA(T_{out} - T(t))$.*

The enthalpy of the system at time $t$, $H(t)$, changes in time according to Eq. (1a), and $T_{\text{out}}$ is the ambient temperature outside the balloon (a parameter of the model). Since there is no material flow into or out of the closed system, the total hold-up $M$ is constant in time (the liquid and vapor phase hold-ups are functions of time $M_L(t)$ and $M_V(t)$, respectively).

The governing dynamics can be completed by considering the saturation pressure, $P^{\text{sat}}(T)$, which is equal to the pressure $P$ of the system whenever both vapor and liquid phases are present:

$$\text{Liquid-only: } M_V = 0, M_L > 0, P \geq P^{\text{sat}}(T), \tag{2}$$

$$\text{Two-phase: } M_V, M_L > 0, P = P^{\text{sat}}(T), \tag{3}$$

$$\text{Vapor-only: } M_V > 0, M_L = 0, P \leq P^{\text{sat}}(T). \tag{4}$$

The basic features of a hybrid automaton are presented in the context of this physical problem, adopted from the formulations in (Galán et al., 1999; Barton and Lee, 2002). Considering the dynamics of the balloon system on a finite time horizon $[t_0, t_f] \subset \mathbb{R}$ with $t_0 < t_f$, a hybrid automaton model of this problem is described with the following characteristics: there are $n_m = 3$ modes in this model, indexed by the set $\mathcal{M} := \{1, 2, 3\}$ (corresponding to liquid-only, two-phase, and vapor-only in Eqns. (2)–(4)). The state variables, parameters, and governing equations are outlined above; each mode $m \in \mathcal{M}$ is characterized by (1), its corresponding algebraic equation (i.e., (2) or (3) or (4)), and a set of initial conditions.

The possible transitions, and possible successor modes, can be described as follows: the liquid-only and vapor-only regimes can only transition to the two-phase regime while the two-phase regime can transition to either liquid-only or vapor-only regimes. Each mode

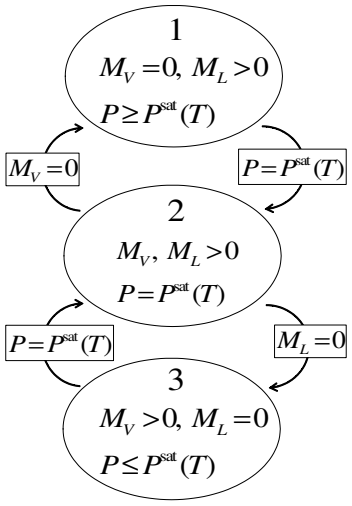


*Figure 2. A hybrid automaton representation of the balloon problem: Mode 1 (liquid-only), Mode 2 (two-phase), and Mode 3 (vapor-only).*

$m \in \mathcal{M}$ has an associated set of logical transition conditions, any of which becoming true initiates a switch between modes. Mode 1 has one transition condition, $P = P^{\text{sat}}(T)$, corresponding to a switch to Mode 2. Mode 2 has two transitions conditions, $M_V = 0$ and $M_L = 0$, corresponding to switches to Modes 1 and 3, respectively.

Furnished by the thermodynamic phase changes, an execution (simulation) comprises a sequence of $n_e \in \mathbb{N} \cup \{+\infty\}$ epochs (or switching intervals), denoted by $\{[\tau_1, \tau_1'], \ldots, [\tau_{n_e}, \tau_{n_e}']\}$, where $[\tau_i, \tau_i'] \subset [t_0, t_f]$ for all $i$. The hybrid time trajectory is finite (i.e., $n_e < +\infty$) if there are finite number of phase changes or infinite ($n_e = +\infty$) otherwise. There also exists a hybrid mode trajectory, associated with the hybrid time sequence, of modes visited. Lastly, the transition functions, which dictate how the continuous state variables evolve at switching times, are state continuity in this case. The hybrid automaton associated with (1) and (2)–(4) is illustrated in Figure 2.

Initialized in the subcooled liquid-only regime, a typical transient of the physical system may be as follows: the system transitions to the two-phase regime at the bubble point where $t = \tau_1'$ and $M_V(\tau_1') = P - P^{\text{sat}}(T(\tau_1'))$. Throughout the two-phase regime, the constant pressure is equal to the saturation pressure and the continuous dynamics continue until the dew point is reached at $t = \tau_2'$ where $P - P^{\text{sat}}(T(\tau_2')) = M_L(\tau_2')$. At this point, the system transitions to and remains in the superheated vapor-only regime.

This expected behavior does not match up with the execution of the hybrid automaton model (i.e., Figure 2): in the transition from Mode 1 to Mode 2 at $t = \tau_1'$, continuity of state variables imply that at the beginning of the next epoch (i.e., in the two-phase regime) $M_V(\tau_2) = 0$, $M_L(\tau_2) = M$, and $P = P^{\text{sat}}(T(\tau_2))$. The logical transition condition $M_V(\tau_2) = 0$ is true; the system instantaneously disengages Mode 2 and reengages Mode 1 ($\tau_2' = \tau_2 = \tau_1'$). $P = P^{\text{sat}}(T(\tau_2'))$ still holds, dictating again a mode change from 1 to 2. This behavior repeats itself ad infinitum to generate the hybrid mode sequence $\{1, 2, 1, 2, \ldots\}$ (the vapor-only regime is never reached) and hybrid time sequence $\{[t_0, \tau_1'], [\tau_1', \tau_1'], [\tau_1', \tau_1'], \ldots\}$ with $\tau_{n_e} = \tau_1' < t_f$ and $n_e = +\infty$. This is called a deadlock situation, defined roughly as the absense of motion (i.e., "stalling") in finite time, as a result of a chattering Zeno execution (as opposed to a genuine Zeno execution (Abate et al., 2009)). Clearly this pathological behavior is an unphysical representation of the physical problem, caused by the hybrid automaton model formulation.

The design and optimization of numerous process operations can be solved as open loop optimal control problems, but this relies on existence, uniqueness, and numerical solution of parametric sensitivities of the embedded dynamic system (Barton and Lee, 2002). A comprehensive theory has been developed for describing forward sensitivity functions of hybrid automata models, which provably exist and are unique (Galán et al., 1999). Efficient simulation algorithms and software for simultaneous computation of state and sensitivity trajectories of hybrid automata are in an advanced stage of development.

The sensitivity results in (Galán et al., 1999) are subject to the restriction that the sequence of modes visited by a hybrid automaton execution is unchanged by parametric variation. The theory is silent when parametric perturbations cause variations in the hybrid mode sequence, which is a major limitation since most physical systems experience transitions whose mode sequence depends on the values of the parameters (e.g., phase changes as in the balloon system) and cannot be determined *a priori* (Barton and Lee, 2002). Hence, the sensitivity analysis of (Galán et al., 1999) is applicable to certain executions of hybrid automata by recasting the problem as a multi-stage problem (i.e., with the number of epochs and mode sequence fixed). However, for many operational problems, it is desirable to address situations where the mode sequence changes as a function of

parameters (Barton and Lee, 2004).

### Nonsmooth Differential-Algebraic Equations: Theory and Implications

Considering again the model (1), the collection of disjunctive constraints

$$\begin{bmatrix} M_V(t) = 0 \\ M_L(t) > 0 \\ P \geq P^{\text{sat}}(T(t)) \end{bmatrix} \veebar \begin{bmatrix} M_V(t) > 0 \\ M_L(t) > 0 \\ P = P^{\text{sat}}(T(t)) \end{bmatrix} \veebar \begin{bmatrix} M_V(t) > 0 \\ M_L(t) = 0 \\ P \leq P^{\text{sat}}(T(t)) \end{bmatrix}$$

captures the physical behavior described above, unlike the hybrid automaton modeling framework. Include instead the following nonsmooth algebraic equation:

$$0 = \text{mid}\left(M_V(t), P - P^{\text{sat}}(T(t)), -M_L(t)\right), \tag{5}$$

where the mid function selects the middle value of its three arguments. This representation is equivalent to the disjunctive constraints above and is a form of continuous disjunction in which two relations hold simultaneously at the boundary between regions of behavior. Indeed, this is a correct and compact mathematical description of the physical behavior. Representation of the same physical behavior with the semantics of a hybrid automaton is difficult and problematic.

Equation (5) enforces different algebraic constraints based on the phase regime in the balloon model as follows: if there is only a liquid phase present at time $t$ then $M_V(t) = 0$. In this case, the first argument in the mid function is zero and the third argument is negative. Furthermore, $P \geq P^{\text{sat}}(T(t))$ yields that the middle argument is nonnegative. Hence, (5) enforces the algebraic constraint $M_V(t) = 0$ (i.e., the liquid-only regime). If there is no liquid phase present at time $t$ then $M_L(t) = 0$ so that $M_V(t) = M$ and, by similar arguments, the mid function selects the third argument in this case (i.e., (5) enforces $M_L(t) = 0$ representing the vapor-only regime). Lastly, if both phases are present, then $P = P^{\text{sat}}(T(t))$ holds and the second argument in the mid function evaluates to zero. Since $0 < M_V(t), M_L(t) < M$ in the two-phase regime, the first and third arguments are positive and negative, respectively, and the mid function selects the second argument.

This approach models dynamic transitions between the three phase regimes (i.e., vapor-only, liquid-only, and two-phase) in a continuous, nonsmooth manner and does not exhibit the pathological Zeno behavior displayed by the hybrid automaton model. Equations (1) and (5) fit into the framework of a nonsmooth (semi-explicit) DAE system, formally given by the following system:

$$\dot{\mathbf{x}}(t, \mathbf{p}) = \mathbf{f}(t, \mathbf{p}, \mathbf{x}(t, \mathbf{p}), \mathbf{y}(t, \mathbf{p})), \tag{6a}$$

$$\mathbf{0}_{n_y} = \mathbf{g}(t, \mathbf{p}, \mathbf{x}(t, \mathbf{p}), \mathbf{y}(t, \mathbf{p})), \tag{6b}$$

$$\mathbf{x}(t_0, \mathbf{p}) = \mathbf{f}_0(\mathbf{p}), \tag{6c}$$

where $t$ is the independent variable, $\mathbf{p}$ is a vector of the problem parameters, and $(\mathbf{x}, \mathbf{y})$ are the differential and algebraic state variables, respectively.

Well-posedness results for (6), when the participating functions are not necessarily continuously differentiable, are completely detailed in (Stechlinski and Barton, In Press); existence, uniqueness, continuation and parametric dependence (i.e., continuous and Lipschitzian) of "regular" solutions is resolved. Regularity here translates to a notion of generalized differentiation index 1, which is local along a solution trajectory and can be verified *a priori* in a global manner. This corresponds to the classical differentiation index 1 notion when $\mathbf{g}$ is smooth, i.e.,

$$\frac{\partial \mathbf{g}}{\partial \mathbf{y}}(t, \mathbf{p}, \mathbf{x}(t, \mathbf{p}), \mathbf{y}(t, \mathbf{p}))$$

being nonsingular for all $t \in [t_0, t_f]$ and $\mathbf{p} = \mathbf{p}_0$ (a reference parameter value).

A suitable theory (Stechlinski and Barton, 2016a) for calculating sensitivity information for (6) has recently been developed thanks to the introduction and established properties of the lexicographic directional (LD-)derivative (Khan and Barton, 2015). Crucially, the LD-derivative satisfies sharp calculus rules (i.e., the chain rule), an implicit function theorem which describes derivative information (Khan and Barton, In Press), and is practically computable, making it the ideal generalized derivative object for analyzing nonsmooth DAEs.

This theory is applicable when the participating functions $\mathbf{f}$, $\mathbf{f}_0$, and $\mathbf{g}$ are lexicographically smooth (L-smooth) (Nesterov, 2005) with respect to parameters and state variables. Roughly, L-smooth functions are locally Lipschitz continuous and have well-defined high-order directional derivatives. The class of L-smooth functions includes continuously differentiable functions, convex functions, piecewise differentiable functions, all compositions of L-smooth functions, integrals of L-smooth functions, and more.

Given a regular solution $(\mathbf{x}, \mathbf{y})$ of (6) on $[t_0, t_f]$ associated with the reference parameter value $\mathbf{p}_0$, $(\mathbf{x}, \mathbf{y})$ is L-smooth with respect to parameters near $\mathbf{p}_0$ and forward sensitivity functions can be furnished from the unique solution of an auxiliary nonsmooth DAE system

(see Eqn. (6) in Stechlinski and Barton (2016a)). Importantly, this result does not appeal to the notion of mode sequences, and applies regardless of changes in the number and/or order of nonsmooth points encountered along a solution.

More specifically, this auxiliary DAE system solution describes a generalized derivative element related to the parametric sensitivities of the differential variables $\mathbf{x}$ and algebraic variables $\mathbf{y}$, respectively, which is computationally relevant in nonsmooth equation-solving and optimization methods. If the nonsmooth DAE is embedded into a nonsmooth optimization problem, e.g.,

$$\inf_{\mathbf{p}\in P} \Phi(\mathbf{p}) \equiv \phi(t_f, \mathbf{p}, \mathbf{x}(t_f, \mathbf{p}), \mathbf{y}(t, \mathbf{p})),$$

then, according to (Stechlinski and Barton, 2016b), the auxiliary nonsmooth DAE solution can be used in a linear equation solve to furnish an element of the generalized gradient of $\Phi$ at $\mathbf{p}_0$ for use in, for example, a bundle method (Lukšan and Vlček, 1998).

The DFBA models discussed in the introduction and other flash processes (Sahlodin et al., 2016) can be modeled using (6) via a similar nonsmooth formulation. Moreover, in many instances nonsmooth DAEs correctly capture the "continuous/discrete" phenomena prevalent in a variety of chemical process models, in contrast to some efforts in the literature using more typical hybrid systems frameworks. Indeed, the authors have been surprised how the nonsmooth paradigm fundamentally alters their approach to formulating dynamic models. In general, the governing dynamics of process operations problems can involve both nonsmooth and discrete phenomena, for which a distinction has not always been made in the past (e.g., the balloon problem exhibits nonsmoothness due to phase changes with continuity in state variables and governing equations, but no true discrete phenomena).

## Conclusions

The modeling approach advocated here is appropriate for many operational processes of interest for a number of reasons: (i) pathological behaviors emanating from modeling abstractions are avoided; (ii) the model is well-posed mathematically; (iii) the framework now possesses a suitable sensitivity theory which characterizes computationally relevant derivative information; and (iv) the paradigm is amenable to numerical solution for accurate dynamic simluation and optimization in a tractable way thanks to the development of a vector forward mode of automatic differentiation (Khan and Barton, 2015). Mixed complementarity system formulations used for dynamic optimization of chemical process models (e.g., Raghunathan et al. (2004)) are a special case of nonsmooth DAEs because any complementarity system (see, e.g., Heemels et al. (2000); Schumacher (2004); Pang and Shen (2007)) can be recast as a nonsmooth DAE system using any suitable nonlinear complementarity problem (NCP) function. Other possible hybrid systems formalisms (e.g., Filippov systems under Filippov-style assumptions (Filippov, 1988; Cortes, 2012)) currently do not possess a suitable sensitivity theory and can also exhibit unpredictable pathological behaviors. Differential variational inequalities (DVIs) (Pang and Stewart, 2008), which unify a number of classes of dynamic problems (including complementarity systems), can be expressed as a class of nonsmooth DAEs by casting the variational inequality as nonsmooth equations (via the natural or normal maps).

Multi-stage systems with generalized index 1 semi-explicit nonsmooth DAEs are inherently well-behaved. Practical dynamic simulation, sensitivity analysis and optimization methods can be developed on this basis as simulation technology in this area is mature. All the necessary theoretical tools are in place, e.g., global equivalence of nonsmooth DAEs and nonsmooth ODEs (Stechlinski and Barton, In Press), for an extension of these results to "high-index" nonsmooth DAE systems with special structures, analyzing switching behavior of nonsmooth DAEs with piecewise smooth participating functions for use in developing efficient numerical methods, and adjoint sensitivities for large numbers of parameters (i.e., extending the method of adjoints for multi-stage systems in Ruban (1997)). Extending the theoretical treatment to infinite-dimensional spaces for closed loop problems to obtain optimal feedback control laws is another possible direction of future work.

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