Index Theory for Hybrid DAE Systems

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from Simulink (ODE): HS in state space form

$$\begin{cases} \dot{x} = f(x, u) \\ y = g(x, u) \end{cases}$$

the state space form depends on the context

reuse is difficult

to Modelica (DAE): HS as physical balance equations

$$\begin{cases} 0 = f(\dot{x}, x, u) \\ 0 = g(x, u) \end{cases}$$

Ohm & Kirchhoff laws, bond graphs, multi-body mechanical systems

reuse is much easier

- Modeling tools supporting DAE
 - Most modeling tools provide only a library of predefined models ready for assembly (Mathworks/Simscape, LMS/AmeSim)
 - Modelica comes with a full programming language that is a public standard https://www.modelica.org/; also Spice for EDA
- Strange outcomes for the simulations were known to occur with Simulink/Stateflow (ask Tim Bourke and Marc Pouzet for nice ones);
- Exploration of Modelica is only starting...

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- We do not claim that these tools are bad, as there are real difficulties:
 - from ODE solvers to DAE solvers
 - events of mode changes for Hybrid DAE systems
 - and the physics itself:

semiconductor, circuit breaker,

...





multibody mechanics

sliding modes

Differential Algebraic Equations systems (continuous time) may involve more constraints than specified:

$$\begin{cases} \dot{x} = f(x, u) \\ 0 = g(x) \end{cases} \xrightarrow{\text{differentiating}} \begin{cases} x = f(x, u) \\ 0 = g(x) \\ 0 = g'(x) \dot{x} \end{cases}$$

$$\begin{cases} \dot{x} = f(x, u) \\ 0 = g'_x(x) \dot{x} \end{cases}$$

$$\begin{cases} \dot{x} = f(x, u) \quad (1) \\ 0 = g(x) \quad (2) \\ 0 = g'_x(x) f(x, u) \quad (3) \end{cases}$$

(· ())

What is the effect on execution schemes? (~ constructive semantics)

difference Algebraic Equations systems (discrete time) may involve more constraints than specified:

$$\begin{cases} x^{\bullet} = f(x, u) \\ 0 = g(x) \end{cases} \stackrel{\text{shifting}}{\Longrightarrow} \begin{cases} x^{\bullet} = f(x, u) \\ 0 = g(x) \\ 0 = g(x) \end{cases}$$
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- Execution scheme (~ constructive semantics):
 - 1. Given x such that g(x) = 0
 - 2. Use (3) to evaluate *u* (constraint solver needed)
 - 3. Use (1) to evaluate x^{\bullet} , which satisfies $g(x^{\bullet}) = 0$, and repeat

Adding (3) essential in deriving the constructive semantics $x \to x^{\bullet}$

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Shifting² is useless since the second shifting introduces

- 1. eqn (4) but also
- 2. the fresh variable $x^{\bullet 2}$

Thus, adding (4) does not help getting the value of x^{\bullet}

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- Shifting² is useful since the second shifting introduces
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$$\begin{cases} \dot{x} = f(x, u) \quad (1) \\ 0 = G(x, u) \quad (2, 3) \end{cases}$$

▶ \sim ODE if we have a constraint solver getting *x* \rightarrow *u* from (2,3)



The notion of differentiation index emerged in the late 1980's in the applied mathematics community; other notions of index were proposed, see [Campbell & Gear 1995]

Research Agenda

- So-called index reduction is a front processing of models making DAE/dAE looking like known objects;
- The execution requires a constraint solver but no further deep forward exploration of runs is needed (warning: the index may be infinite)
- Unfortunately, no notion of index was mathematically defined for Hybrid DAE systems
 - it is informally claimed that
 "Hybrid DAE systems possess a mode-dependent index"
 - unfortunately this has no math basis and leads to problems at compilation: what to do at mode changes?
- This talk is about index for Hybrid DAE systems and it turns out that index for dAE systems is also interesting in itself

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Exact and Structural DAE index (linear algebra reasoning)

Structural dAE index and causality analysis

Through NonStandard semantics DAE become dAE

The index of a Hybrid DAE System is the dAE index of its NS-semantics

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Exact Differentiation/Difference Index $F(x, \dot{x}) = 0$ $F(x, x^{\bullet}) = 0$

$$\begin{bmatrix} F(x,\dot{x}) \\ \frac{d}{dt}F(x,\dot{x}) \\ \vdots \\ \frac{d^{k}}{dt^{k}}F(x,\dot{x}) \end{bmatrix} =_{def} \begin{bmatrix} F^{(0)}(x,\dot{x},w) \\ F^{(1)}(x,\dot{x},w) \\ \vdots \\ F^{(k)}(x,\dot{x},w) \end{bmatrix}, \begin{cases} v =_{def} \dot{x} \\ w =_{def} (x^{(2)},\ldots,x^{(k+1)}) \end{cases}$$

$$\begin{bmatrix} F(x,x^{\bullet}) \\ F^{\bullet}(x,x^{\bullet}) \\ \vdots \\ F^{\bullet k}(x,x^{\bullet}) \end{bmatrix} =_{def} \begin{bmatrix} F^{(0)}(x,x^{\bullet},w) \\ F^{(1)}(x,x^{\bullet},w) \\ \vdots \\ F^{(k)}(x,x^{\bullet},w) \\ \vdots \\ F^{(k)}(x,x^{\bullet},w) \end{bmatrix}, \begin{cases} v =_{def} x^{\bullet} \\ w =_{def} (x^{\bullet 2},\ldots,x^{\bullet k+1}) \\ w =_{def} (x^{\bullet 2},\ldots,x^{\bullet k+1}) \end{bmatrix}$$

$$\boxed{Index =_{def} \min k \text{ s.t. } x \to v : \exists w.F_{k}(x,v,w) = 0 \text{ is a partial function}}$$

solving $F_k = 0$ while eliminating w uniquely determines v as a partial function of x

Index $=_{def} \min k$ s.t. $x \to v : \exists w. F_k(x, v, w) = 0$ is a partial function

Whence the following questions of interest if F is smooth:

- 1. does $x \to v : \exists w.F(x, v, w) = 0$ define a partial function? \Leftrightarrow (by implicit function theorem)
- 2. does $x \rightarrow v$: $\exists w.Av + Cw + Ex = 0$ define a partial function?

where $A = F'_v$, $C = F'_w$, $E = F'_x$ are Jacobians at a solution (v_o, w_o, x_o)

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We are interested in structural properties, i.e., properties that are valid outside exceptional values for the nonzero coefficients of the matrices

Subcase Av + x = 0 with A a square matrix: A structurally invertible ⇔ ∃P permutation matrix such that PA has a nonzero diagonal

$$P = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}, A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & 0 & a_{23} \\ a_{31} & a_{32} & 0 \end{bmatrix}, PA = \begin{bmatrix} a_{21} & 0 & a_{23} \\ a_{31} & a_{32} & 0 \\ a_{11} & a_{12} & a_{13} \end{bmatrix}$$

A is structurally invertible. It may be singular for exceptional values of the nonzero coefficients of *A*, e.g., if $det(A) = a_{31}a_{12}a_{23} - a_{32}(a_{11}a_{23} - a_{21}a_{13}) = 0$.

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Finding *P* amounts to pivoting, which is a graph based algorithm:

- 1. reorder equations, and then
- 2. use the *k*th equation to eliminate v_k as a function of *x* and $\{v_i | j > k\}$

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► A similar result holds for structural properties of $x \rightarrow v : \exists w.Av + Cw + Ex = 0$

which also leads to a graph based algorithm

$$\left\{\begin{array}{rrr} 0 & = & \dot{x} - f(x, u) \\ 0 & = & g(x) \end{array} \right. \quad \text{set} \quad S(x, v) =_{\text{def}} \left[\begin{array}{r} \dot{x} - f(x, u) \\ g(x) \end{array}\right]$$

where x is the state and $v =_{def} (\dot{x}, u)$; consider the Jacobian

$$\mathcal{J} =_{def} dS/dv = \begin{bmatrix} 1 & -f'_u(x, u) \\ 0 & 0 \end{bmatrix}$$
 is structurally singular

v cannot be determined and *S* has index > 0. Set $w = (\ddot{x}, \dot{u})$ and consider

$$S_{1}(x, v, w) =_{def} \begin{bmatrix} S(x, v) \\ \frac{d}{dt}S(x, v, w) \end{bmatrix} = \begin{bmatrix} \dot{x} - f(x, u) \\ g(x) \\ \dot{x} - \frac{d}{dt}f(x, u) \end{bmatrix} \Rightarrow \begin{bmatrix} \dot{x} - f(x, u) \\ g(x) \\ g'(x)\dot{x} \end{bmatrix}$$
$$\mathcal{J}_{1} =_{def} dS_{1}/dv = \begin{bmatrix} 1 & -f'_{u}(x, u) \\ 0 & 0 \\ 1 & 0 \end{bmatrix} \Rightarrow \begin{bmatrix} 1 & -f'_{u}(x, u) \\ 1 & 0 \end{bmatrix} \text{ invertible}$$

$$\begin{cases} E_1: & 0 &= \dot{x} - f(x, u) \\ E_2: & 0 &= g(x) \\ E_3: & 0 &= g'(x) \dot{x} \end{cases}$$

 \Leftrightarrow

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structural pivoting (Pantelides algorithm)

Pantelides algorithm

searching for a consistent orientation of the incidence graph

causality analysis for constraint system

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Abstraction Principle: in F(x, u, v)=0, any of x, u, v can be turned to an output

This is a legitimate consequence of implicit function theorem if F is smooth What if F is not smooth? e.g., it involves "if-then-else" or guards

$$E(x, u, v)$$
 : $b = [x>0] \bigwedge$ if b then $v=f(u)$ else $u=g(v)$



Brute force application of the Abstraction Principle yields an incorrect abstraction

$$E(x, u, v)$$
 : $b = [x>0] \bigwedge$ if b then $v=f(u)$ else $u=g(v)$



 $\mathcal{P}_{E}(x, u, v) : x \longrightarrow b \bigwedge \text{ if } b \text{ then } u \longrightarrow v \text{ else } u \longrightarrow v$ $\vec{\mathcal{P}}_{E}(x, u, v) : x \longrightarrow b \bigwedge \text{ if } b \text{ then } u \longrightarrow v \text{ else } v \longrightarrow u$

Refined formalism: guarded equations (we consider flat guards only)

$$S = \left(\bigwedge_i A_i \ , \ \bigwedge_j E_j \right)$$
 where

- A_i = predicate over the set of guards b_j
- E_j = if b_j then $F_j(x, u, x^{\bullet})$ and Abstraction Principle applies to F

$$\mathcal{P}_{E_j} = b_j \to E_j \land \text{ if } b_j \text{ then } F_j \swarrow x_{x^{\bullet}}^{x}$$

Compute a directed covering $\vec{\mathcal{P}}_{E_i}$ of \mathcal{P}_{E_i} ensuring

- single assignment modulo assertions on guards
- circuitfreeness modulo assertions on guards

An extension of Signal clock-and-causality calculus; yields constructive semantics

Guards are not enough

$$\begin{array}{c} \text{Unilateral Constraints} \\ (\text{multi-body mechanics}) \end{array} \right\} \quad : \quad 0 \leq g(x) \\ \text{Complementarity Conditions} \\ (\text{circuits with perfect diodes}) \\ (\text{multi-body mechanics}) \end{array} \right\} \quad : \quad 0 \leq U(x) \perp V(y) \geq 0 \equiv \left\{ \begin{array}{c} U(x) \geq 0 \\ V(y) \geq 0 \\ U(x)V(y) = 0 \end{array} \right.$$

$$\begin{cases} x^{\bullet} = f(x, u) & \text{expands as} \\ 0 & \leq g(x) & \Rightarrow \end{cases} \begin{cases} E_1 : x^{\bullet} = f(x, u) \\ E_{21} : b = [0 \ge g(x)] \\ E_{22} : \text{if } b \text{ then } g(x) = 0 \end{cases}$$

- Problem: $\{E_{21}, E_{22}\}$ is a fixpoint equation in (b, x)
- Approach:
 - 1. See $E_2 = \{E_{21}, E_{22}\}$ as an atom handled like a single equation
 - 2. Assign to E_2 a set of candidate causality constraints

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Summary on dAE causality analysis

Causality analysis (from which the index follows):

- Guarded equations with assertions on guards
- Guarded causality analysis
- Atoms
 - Warning: "atom" indicates that it must be evaluated at once
 - Atoms may not be small (minimal circuits in the causality graph)

Constructive semantics and execution schemes

- Execution mode of synchronous languages, albeit
- Evaluating atoms requires dedicated constraint solvers

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Through NonStandard semantics DAE become dAE

$$\mathbb{T} =_{def} \{t_n = n\partial \mid n \in {}^{*}\mathbb{Z}\} \text{ where } \partial \text{ is an infinitesimal}$$

$$\forall t \in \mathbb{T} : {}^{\bullet}t =_{def} \max\{s \mid s \in \mathbb{T}, s < t\} = t - \partial$$

$$t^{\bullet} =_{def} \min\{s \mid s \in \mathbb{T}, s > t\} = t + \partial$$

$$\dot{x}_t =_{def} \frac{x_t \cdot - x_t}{\partial} \text{ (explicit scheme)} \left(\frac{x_t - x_{*t}}{\partial} \text{ (implicit scheme)}\right)$$

$$\begin{bmatrix} x \\ \frac{d}{dt}x \\ \frac{d}{dt^2}x \\ \vdots \end{bmatrix} = \mathcal{L} \begin{bmatrix} x \\ x^{\bullet} \\ x^{\bullet 2} \\ \vdots \end{bmatrix}, \text{ where } \mathcal{L} \text{ is an invertible lower triangular matrix}$$

Theorem: structural index of a DAE = structural index of its NS-semantics

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A conservative extension of the index

index of Hybrid DAE System $=_{def}$ dAE index of its NS-semantics

- By the previous Theorem this yields a conservative extension of
 - the index of a DAE system
 - the index of a dAE system
- Warning: the above result requires considering the structural index (not the exact one)
- The computation of the index is a byproduct of the causality analysis
- The index is a global notion (the index may be finite or infinite)
- ▶ The causality analysis is guarded, i.e., mode dependent

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A conservative extension of the index

We can perform causality analysis for the following kind of example:



A simple circuit breaker. Top: the circuit. Bottom: the mode automaton for each fuse i = 1, 2. For the ON mode, the current must stay below a threshold J_i , while in the OFF mode, the complementarity condition shown holds.

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Simulating dAE systems (discrete time)

Not much to be said:

- Guarded causality analysis yields the constructive semantics
- Not very different from synchronous languages, albeit...
- Solvers are needed to evaluate every atom (local call to solver)



This is the technique of slicing used in Zelus tool [Pouzet & Bourke]

- synchronous mode of execution: may require the use of solvers for evaluating atoms
- step: a step may have "long" duration, e.g., the solver may be stopped only at the next zero-crossing



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Difficulties with this technique of slicing :

- Can the evaluation of step consist of local calls to a solver for each block? (this holds true for for dAE)
 - No if the different blocks must interact while performing step

$$\begin{cases} \dot{x} = f(x, y) \\ \dot{y} = g(x, y) \end{cases}$$



- Yes otherwise
- Ok if "slow interactions": $f(x, y) \approx f(x, y_0)$ or $g(x, y) \approx g(x_0, y)$
- What should be considered as an event?
 - Some but not all discontinuities (next slides)

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What should be considered as an event?

Some numerical solvers ignore discontinuities (B. Caillaud at Synchron'13):



Moreau sweeping process: A cavity moves and pushes the ball



Its numerical scheme: Fixed step size; no event handler Only convex projections

This applies to unilateral constraints and complementarity conditions

Since such solvers are not bothered by discontinuities, it is subtle to decide

- which discontinuities to detect for handling as an event vs.
- which discontinuities to ignore and delegate to the solver

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Moreau sweeping process: A cavity moves and pushes the ball



Its numerical scheme: Fixed step size; no event handler Only convex projections

This applies to unilateral constraints and complementarity conditions

Since such solvers are not bothered by discontinuities, it is subtle to decide

- which discontinuities to detect for handling as an event vs.
- which discontinuities to ignore and delegate to the solver

Current status for Hybrid DAE System modeling tools

General scope tools for engineering (e.g., Modelica):

- Spurious behaviors may be encountered when handling events (cascades of)
- Discontinuities are handled as events
 - unless the engineer manually enforces the use of certain event-agnostic discretization schemes
- Causality analysis is mode-dependent
 - Still, separately compiled blocks (e.g., targeting FMU) must have an interface with static (mode-independent) causality
- No local solvers
 - unless manually enforced (e.g., for slow/fast dynamics)

Current status for Hybrid DAE System modeling tools

Solvers dedicated to nonsmooth systems (e.g., Siconos library [Acary & Brogliato])

- eventless and event based processing both supported
- global solvers
- complementarity conditions with linear coupling
- no index reduction; replaced by the evaluation of the "relative degree"

Exact and Structural DAE index (linear algebra reasoning)

Structural dAE index and causality analysis

Through NonStandard semantics DAE become dAE

The index of a Hybrid DAE System is the dAE index of its NS-semantics

Consequences for simulation

Conclusions

We have formally defined the index for Hybrid DAE

- Index of Hybrid DAE =_{def} index of its NonStandard semantics (Yet another evidence that NonStandard semantics helps...)
- Requires guarded causality analysis alike in synchronous languages (particularly Signal)
- Allows giving a mathematical semantics to more Hybrid DAE systems (of little help if the index is infinite)

dAE Systems are interesting

dAE Systems with general data types (e.g. Bool = numerics):

- Extend synchronous programming to Transition Systems where transition relations (constraints) are specified via systems of equations
- Guarded equations with atoms form an expressive syntax
- Index analysis for dAE is new (though an easy translation from DAE):
 - relies on guarded causality analysis
 - when the index is finite, index reduction identifies the look-ahead horizon that is sufficient to avoid future blocking
- Requires constraint solvers (no all purpose solver exists...)

What are dAE Systems useful for?

- model-guided testing?
- planification?

▶ ...?

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- Index-and-causality analysis is a symbolic pre-processing It does not address numerical difficulties
- Making a step is more difficult than calling an S-function
- Global vs. Distributed solvers
 - Global solver is normally used for simulation
 - Distributed solvers are used:
 - ▶ in code coupling (e.g. multi-physics)
 - in slow/fast dynamics
 - in FMI based simulation with several FMU
- What to do with events?
 - Handling every discontinuity as an event is not good
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an exciting but difficult subject