

# Simulating and Verifying Cyber-Physical Systems: Current Challenges and Novel Research Directions

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## Computer Science (Automata Theory)

Essentially **discrete**: finite set of modes with continuous evolution within modes. [Hybrid Automata, Alur et al. 1992]

## Control (Differential Equations)

Essentially **continuous**: non-smooth (discontinuous) dynamics, differential inclusions, Filippov/Utkin regularization. [Mosterman 1998, Sanfelice 2003]

Define/Describe **Reactions** to **Events**

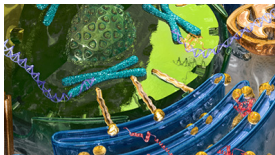
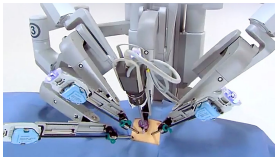
## Events

Model a simplified (often discrete) perception of the rich **environment**.

## Reactions

Model how the system is supposed to react to an event so that it respects a set of constraints which are essentially physics laws and/or predefined requirements.

# Convenient Model for a Large Class of Systems



# Modeling is Instrumental to Master Complexity

## Abstraction/Refinement Relationships

The molecular composition of the stratosphere has a minor impact on the Earth's orbit. Likewise, a galaxy is a dot in the Laniakea supercluster.

## Compositionality and Reuse

Human beings are perhaps the most extreme example of both concepts: nature builds on top of what works to create new more complex structures.



## Simulation (Time Travel)

A peek in the future (or the past) of a concrete model for a concrete initial (or final) condition. Essentially by “executing” the model step by step: only a **Local** recipe is needed.

## Verification (Time Abstraction)

Qualitative analysis of the geometry (shape) of the state space as it captures **Global** properties.

Local description defines the global properties which in turn benefit numerical approximations (eg. Geometrical Integration)

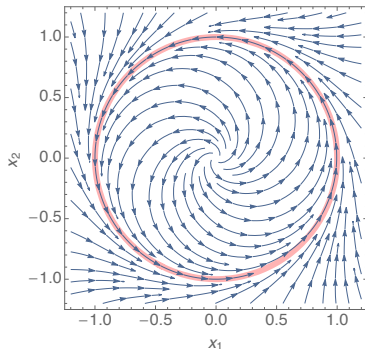
- 1 Introduction
- 2 Verification**
- 3 Simulation
- 4 Challenges

If one regards a sorting algorithm as a discrete dynamical system acting on the given set, then the sorted list is an **invariant** or fixed point. It is an **attractor** that is reached from any initial position in finite time ( $\#$  steps).



# Qualitative Analysis of Dynamical Systems

$$(\dot{x}_1, \dot{x}_2) = (x_1 - x_1^3 - x_2 - x_1 x_2^2, x_1 + x_2 - x_1^2 x_2 - x_2^3)$$

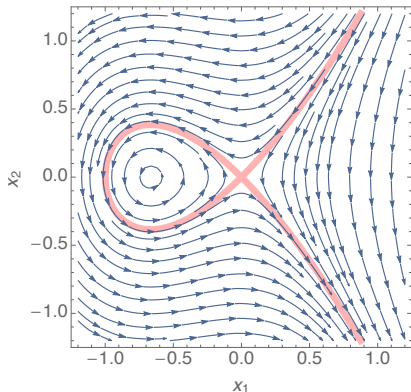


**Algebraic  
Invariant  
Equation**

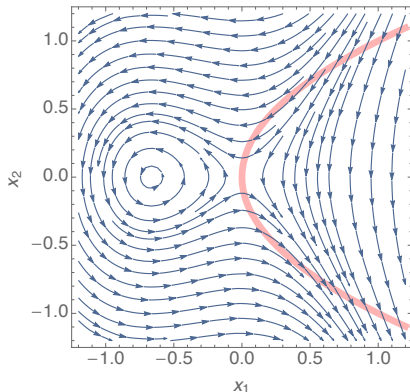
The solution for  $\mathbf{x}_0 = (1, 0)$  respects  $\boxed{x_1(t)^2 + x_2(t)^2 - 1 = 0} \quad \forall t$

## Problem I. *Checking Invariance of Algebraic Equations*

Given  $\dot{\mathbf{x}} = (-2x_2, -2x_1 - 3x_1^2)$ ,  $p(\mathbf{x}_0) = 0$ , is  $p(\mathbf{x}(t)) = 0$  for all  $t$  ?



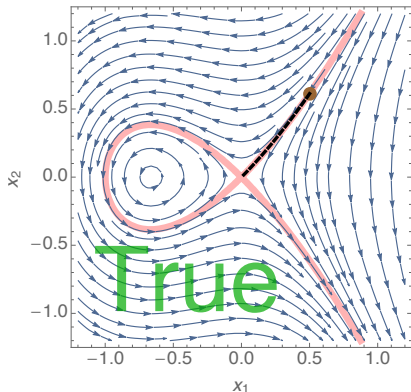
$$p(x_1, x_2) = x_1^2 + x_1^3 - x_2^2$$



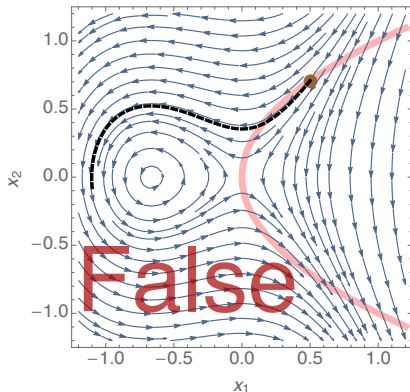
$$p(x_1, x_2) = x_1 - x_2^2$$

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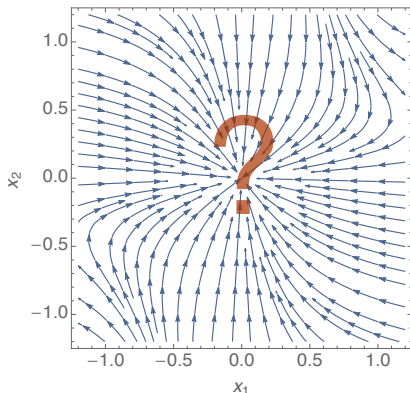
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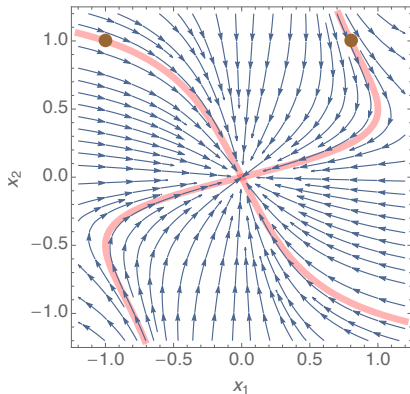
## Problem II. *Generate Algebraic Invariant Equations*

Given  $\dot{\mathbf{x}} = (-x_1 + 2x_1^2x_2, -x_2)$ , how to generate  $p$  such that  $p(\mathbf{x}(t)) = 0$  ?



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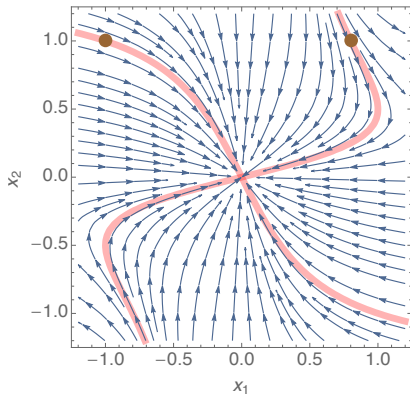


$$p_{(x_1(0), x_2(0))}(x_1, x_2) = (x_2(0) - x_1(0)x_2(0)^2)x_1 - x_1(0)(x_2 - x_1x_2^2) = 0$$



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$\frac{x_1}{x_2 - x_1x_2^2}$  is an invariant **rational function**.

**Gradient**  $\nabla p := \left( \frac{\partial p}{\partial x_1}, \dots, \frac{\partial p}{\partial x_n} \right)$

**Lie Derivation**  $\mathfrak{D}_{\mathbf{f}}(p) := \frac{dp(\mathbf{x}(t))}{dt} = \langle \nabla p, \mathbf{f} \rangle \quad (\dot{\mathbf{x}} = \mathbf{f})$

## Singular Locus

$$\text{SL}(p) := \{ \mathbf{x} \in \mathbb{R}^n \mid \nabla p = \mathbf{0} \} = \left\{ \mathbf{x} \in \mathbb{R}^n \mid \frac{\partial p}{\partial x_1} = 0 \wedge \dots \wedge \frac{\partial p}{\partial x_n} = 0 \right\}$$

$\mathbf{x} \in V_{\mathbb{R}}(p)$  ( $p(\mathbf{x}) = 0$ ) is **singular** if  $\mathbf{x} \in \text{SL}(p)$ , **regular** otherwise.

## Notation for “ $S \subseteq \mathbb{R}^n$ is invariant for $\mathbf{f}$ ”

$$S \rightarrow [\dot{\mathbf{x}} = \mathbf{f}]S$$

$\equiv$

The set  $S$  is an invariant set for  $\mathbf{f}$

$\equiv$

Starting with  $\mathbf{x}_0$  s.t  $\mathbf{x}_0 \in S$ : for all  $t > 0$ ,  $\mathbf{x}(t)$   
solution of the IVP  $(\dot{\mathbf{x}} = \mathbf{f}, \mathbf{x}(0) = \mathbf{x}_0)$  is in  $S$

N.B. Treating  $\dot{\mathbf{x}} = \mathbf{f}$  as a program, one can think of the top formula as representing the Hoare triple  $\{S\} \dot{\mathbf{x}} = \mathbf{f} \{S\}$ .

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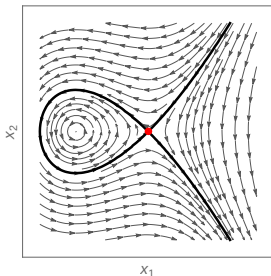
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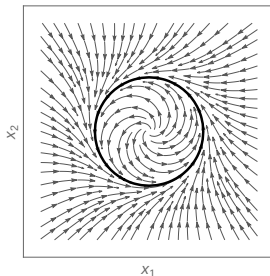
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Necessary and sufficient for smooth invariant manifolds (Lie, 1893).

$$\text{(Lie)} \frac{p = 0 \rightarrow (\mathfrak{D}_f(p) = 0 \wedge \nabla p \neq \mathbf{0})}{(p = 0) \rightarrow [\dot{\mathbf{x}} = \mathbf{f}] (p = 0)}$$



$p = 0$  non-smooth ✗



$p = 0$  smooth ✓

Handling certain **singularities** (points where  $\nabla p = \mathbf{0}$ )

No flow in the problem variables at singularities on the variety

$$(\text{Lie}^\circ) \frac{p = 0 \rightarrow (\mathcal{D}_{\mathbf{f}}(p) = 0 \wedge (\nabla p = \mathbf{0} \rightarrow \mathbf{f} = \mathbf{0}))}{(p = 0) \rightarrow [\dot{\mathbf{x}} = \mathbf{f}] \ (p = 0)}$$

Flow at singularities on the variety is directed into the variety

$$(\text{Lie}^*) \frac{p = 0 \rightarrow (\mathcal{D}_{\mathbf{f}}(p) = 0 \wedge (\nabla p = \mathbf{0} \rightarrow p(\mathbf{x} + \lambda \mathbf{f}) = 0))}{(p = 0) \rightarrow [\dot{\mathbf{x}} = \mathbf{f}] \ (p = 0)} .$$

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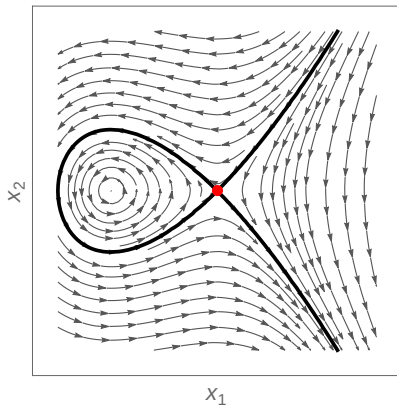
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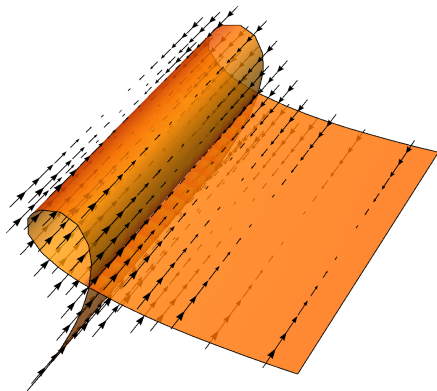


Lie ✗

$\text{Lie}^\circ$  ✓

$\text{Lie}^*$  ✓

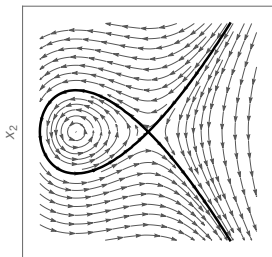
Handling certain **singularities** (points where  $\nabla p = \mathbf{0}$ )



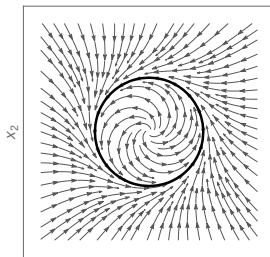
Lie **✗**   Lie<sup>o</sup> **✗**   Lie\* **✓**

Necessary and sufficient for conserved quantities (integrals of motion).

$$(FI) \frac{\mathfrak{D}_f(p) = 0}{(p = 0) \rightarrow [\dot{\mathbf{x}} = \mathbf{f}] (p = 0)}$$



$p$  conserved ✓



$p$  not conserved ✗

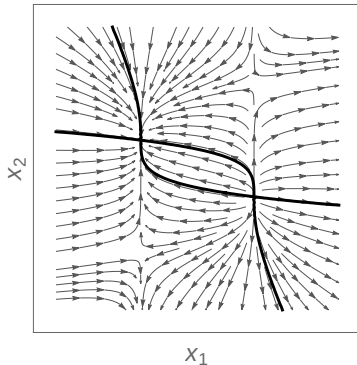
**Continuous consecutions** (C-c) and **polynomial consecutions** (P-c) are Darboux polynomials (Darboux, 1878).

$$(C-c) \frac{\exists \lambda \in \mathbb{R}, \mathcal{D}_f(p) = \lambda p}{(p = 0) \rightarrow [\dot{\mathbf{x}} = \mathbf{f}] (p = 0)},$$

$$(P-c) \frac{\exists \lambda \in \mathbb{R}[\mathbf{x}], \mathcal{D}_f(p) = \lambda p}{(p = 0) \rightarrow [\dot{\mathbf{x}} = \mathbf{f}] (p = 0)}.$$

$$\mathbf{f} = (3(x_1^2 - 4), -x_2^2 + x_1x_2 + 3), \quad p = x_2^4 + 2x_1x_2^3 + 6x_2^2 + 2x_1x_2 + x_1^2 + 3,$$

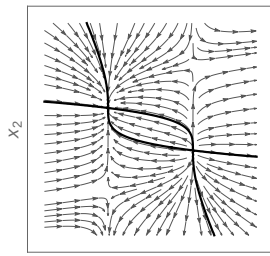
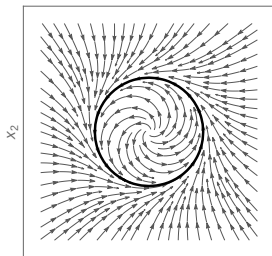
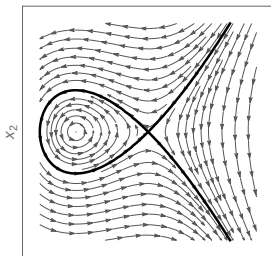
$$\mathfrak{D}_f(p) = \underbrace{(6x_1 - 4x_2)}_{\lambda} p$$



FI ✗    C-c ✗    P-c ✓

**Necessary and sufficient** for invariant varieties.

$$\text{(DRI)} \frac{p = 0 \rightarrow \bigwedge_{i=0}^{N-1} \mathfrak{D}_{\mathbf{f}}^{(i)}(p) = 0}{(p = 0) \rightarrow [\dot{\mathbf{x}} = \mathbf{f}] (p = 0)}$$



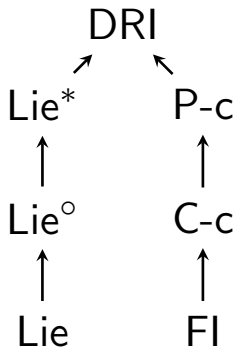
$$(R_A) \frac{A}{S_A : T_A \longrightarrow [\dot{\mathbf{x}} = \mathbf{f}] S_A : T_A} \quad (R_B) \frac{B}{S_B : T_B \longrightarrow [\dot{\mathbf{x}} = \mathbf{f}] S_B : T_B}$$

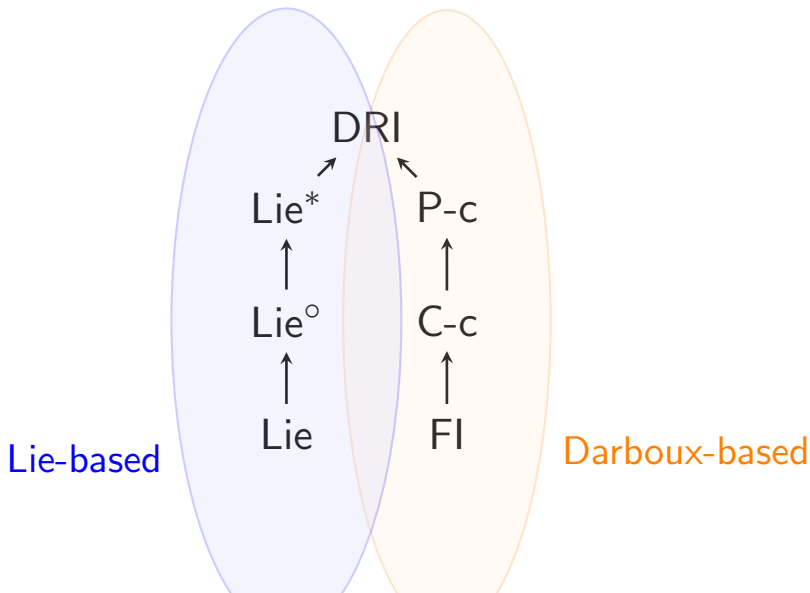
### Partial Order

$R_A \preceq R_B$  if and only if  $A \implies B$  and  $T_A$  is a “subtype” of  $T_B$ .

- $R_A \sim R_B$  ( $R_A \preceq R_B$  and  $R_A \succeq R_B$ ) **Equivalence.**
- $R_A \prec R_B$  ( $R_A \preceq R_B$  and  $R_A \not\succeq R_B$ ) **Strict increase** of deductive power







So far we have only seen **algebraic** sets:  $p = 0$

- For  $\wedge_i p_i = 0$ , we can rewrite using  $\sum_i p_i^2 = 0$
- We can do better [SAS'14]

What about **semi-algebraic** sets:

- Sets of the form  $p \leq 0$
- Closed Sets
- Arbitrary Sets: Boolean formulae with polynomial equalities and inequalities

## (Non-strict) Barrier Certificate ✓

$(\forall \mathbf{x} \in \mathbb{R}^n, \mathfrak{D}_{\mathbf{f}}(p) \leq 0) \longrightarrow p \leq 0$  is a positive invariant

## Unsound Barrier Certificate ✗

$(\forall \mathbf{x} \text{ s.t. } \mathbf{p}(\mathbf{x}) = \mathbf{0}, \mathfrak{D}_{\mathbf{f}}(p) \leq 0) \longrightarrow p \leq 0$  is a positive invariant

## Strict Barrier Certificate ✓

$(\forall \mathbf{x} \text{ s.t. } p(\mathbf{x}) = 0, \mathfrak{D}_{\mathbf{f}}(\mathbf{p}) < \mathbf{0}) \longrightarrow p \leq 0$  is a positive invariant

### Differential Invariants (DI)

$$(DI) \frac{D(S)_{\dot{\mathbf{x}}}^{\mathbf{f}}}{S \rightarrow [\dot{\mathbf{x}} = \mathbf{f}] S},$$

$D(S)_{\dot{\mathbf{x}}}^{\mathbf{f}}$ : substitute each  $\dot{x}_i$  in  $D(S)$  with  $\mathbf{f}_i(\mathbf{x})$

$$D(r) = 0 \quad \text{for numbers,}$$

$$D(x) = \dot{x} \quad \text{for variables,}$$

$$D(a + b) = D(a) + D(b),$$

$$D(a \cdot b) = D(a) \cdot b + a \cdot D(b),$$

$$D(a \leq b) \equiv D(a) \leq D(b), \quad \text{accordingly for } \geq, >, < . \text{ (BC)}$$

$$D(S_1 \wedge S_2) \equiv D(S_1) \wedge D(S_2),$$

$$D(S_1 \vee S_2) \equiv D(S_1) \wedge D(S_2), \quad (\wedge \text{ here is important for soundness})$$

## Definitions

$$\text{In}_f(S) \equiv \{\mathbf{x} \in \mathbb{R}^n \mid \exists \epsilon > 0. \forall t \in (0, \epsilon). \mathbf{x}(t) \in S\},$$

$$\text{In}_{(-f)}(S) \equiv \{\mathbf{x} \in \mathbb{R}^n \mid \exists \epsilon > 0. \forall t \in (0, \epsilon). \mathbf{x}(-t) \in S\},$$

## Characterization

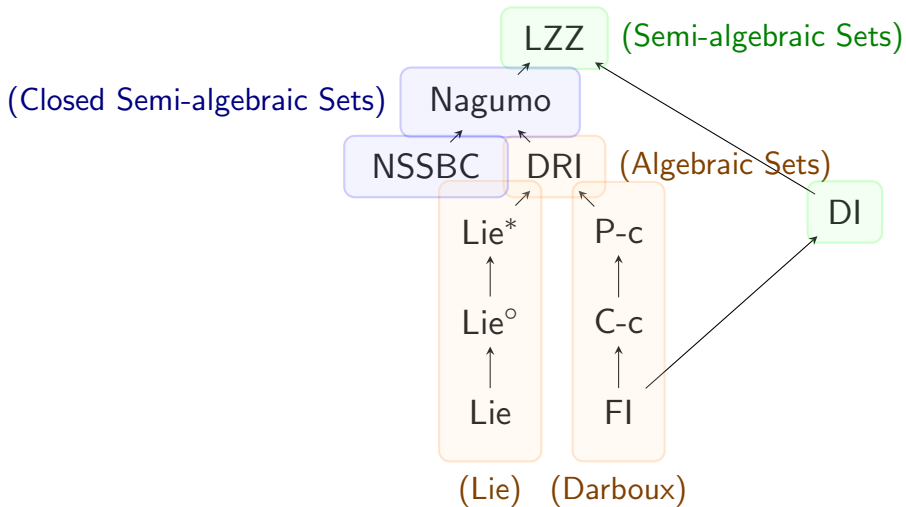
An arbitrary set  $S \subset \mathbb{R}^n$  is a positive invariant for  $\mathbf{f}$  if and only if

$$S \subseteq \text{In}_f(S) \text{ and } S^c \subseteq \text{In}_{(-f)}(S^c)$$

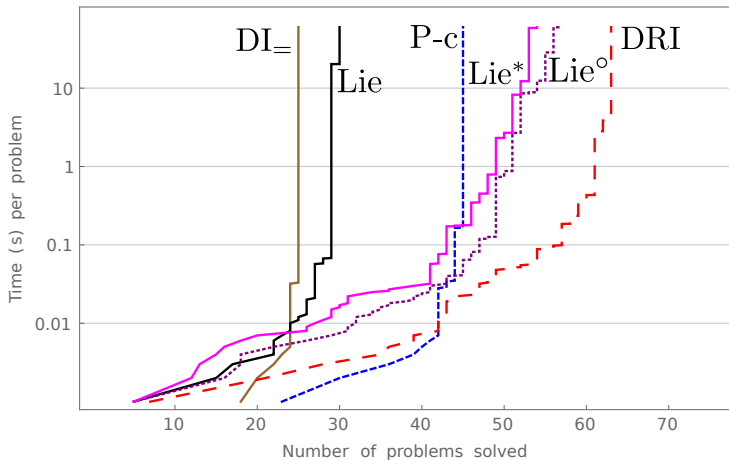
or equivalently

$$\text{In}_{(-f)}(S) \subseteq S \subseteq \text{In}_f(S)$$

- $\text{In}_f(S)$  can be computed using high-order Lie derivatives !



# Experimental Performance: Algebraic Sets





## Template-Based

- Fix a template: generic polynomials with symbolic coefficients
- Use sufficient conditions to derive constraints over the coefficients
- Solve the system
- In practice:
  - templates of the form  $p = 0$  (algebraic sets) with Darboux condition  $(\mathcal{D}_f(p) \in \langle p \rangle)$  work for  $n \leq 10$  and  $d \leq 3$ .
  - templates of the form  $p \leq 0$  relying on Barrier Certificates (SOSTools)

## Discrete Abstraction

- Discrete the space with the signs of a given set of polynomials
- Relies on sufficient conditions to remove spurious transitions
- Issue: How to populate and eventually refine the initial set of polynomials

Suppose we have a 2-dimensional ODE  $(\dot{x}_1, \dot{x}_2) = (x_1, x_2)$

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- 1 Start with parametric  $h$  of degree 1:  $h = \alpha_1 x_1 + \alpha_2 x_2 + \alpha_3$

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$$\begin{array}{rcl} (-1 + \beta)\alpha_1 & = & 0 \\ (-1 + \beta)\alpha_2 & = & 0 \\ (\beta)\alpha_3 & = & 0 \end{array} \Leftrightarrow \begin{pmatrix} -1 + \beta & 0 & 0 \\ 0 & -1 + \beta & 0 \\ 0 & 0 & \beta \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix} = 0$$

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Study the **null space** (kernel) of  $M(\beta)$



$$h = \alpha_1 x_1 + \alpha_2 x_2 + \alpha_3$$

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Study the **null space** (kernel) of  $M(\beta)$

- Max dim of ker of  $M(\beta) \rightsquigarrow$  more freedom for  $\alpha = (\alpha_1, \alpha_2, \alpha_3)$
- Increases the chances of finding **first integrals**
- Dually, minimize the rank of  $M(\beta)$

$$h = \alpha_1 x_1 + \alpha_2 x_2 + \alpha_3$$

$$\begin{aligned} (-1 + \beta)\alpha_1 &= 0 \\ (-1 + \beta)\alpha_2 &= 0 \\ (\beta)\alpha_3 &= 0 \end{aligned} \Leftrightarrow \begin{pmatrix} -1 + \beta & 0 & 0 \\ 0 & -1 + \beta & 0 \\ 0 & 0 & \beta \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix} = 0$$

Study the **null space** (kernel) of  $M(\beta)$

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$$h = x_2(0)x_1 - x_1(0)x_2$$

## Simulation (Time Travel)

A peek in the future (or the past) of a concrete model for a concrete initial (or final) condition. Essentially by “executing” the model step by step: only a **Local** recipe is needed.

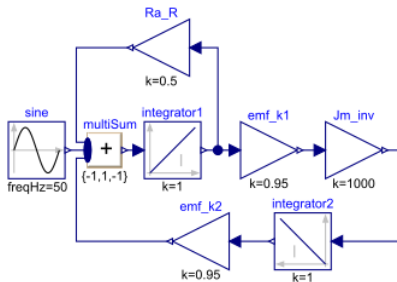
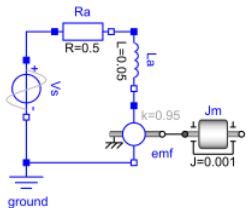
## Verification (Time Abstraction)

Qualitative analysis of the geometry (shape) of the state space as it captures **Global** properties.

Local description defines the global properties which in turn benefit numerical approximations (eg. Geometrical Integration)

- 1 Introduction
- 2 Verification
- 3 Simulation**
- 4 Challenges

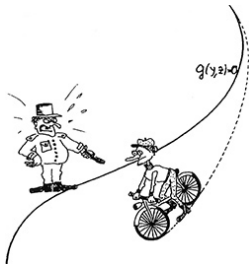
# Block Diagram vs. State Flow





- Verification and Faithful Simulation for cyber-physical systems with DAE

- Verification and Faithful Simulation for cyber-physical systems with DAE



- $\mathbf{0} = \mathbf{F}(\mathbf{x}, \dot{\mathbf{x}}, t)$
- $\begin{cases} \dot{\mathbf{x}} = \mathbf{f}(\mathbf{y}, \mathbf{x}) \\ \mathbf{0} = \mathbf{g}(\mathbf{y}, \mathbf{x}) \end{cases}$
- Compositional design
- Tools: Dymola (Dassault Systèmes), Modelica

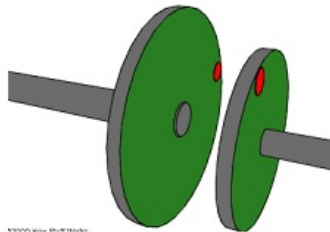
## if **Guard** do **Differential Equation**

- **Guard**: predicate in the state variables and their **time derivatives**.
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When a guard holds, its equation is enforced.



```

if t do  $J_1 \dot{\omega}_1 = \tau_1$       (e1)
if t do  $J_2 \dot{\omega}_2 = \tau_2$     (e2)
if  $\gamma$  do  $\omega_1 - \omega_2 = 0$   (e3)
if  $\gamma$  do  $\tau_1 + \tau_2 = 0$     (e4)
if  $\neg \gamma$  do  $\tau_1 = 0$         (e5)
if  $\neg \gamma$  do  $\tau_2 = 0$         (e6)
    
```

- **State Variables:** the angular velocities  $\omega_1$  and  $\omega_2$
- $\gamma$  is an input signal modelling the pedal's position

# Clutch Disengaged, $\gamma = f$

Ordinary Differential Equation

if t	do	$J_1 \dot{\omega}_1 = \tau_1$	$(e_1)$
if t	do	$J_2 \dot{\omega}_2 = \tau_2$	$(e_2)$
if $\gamma$	do	$\omega_1 - \omega_2 = 0$	$(e_3)$
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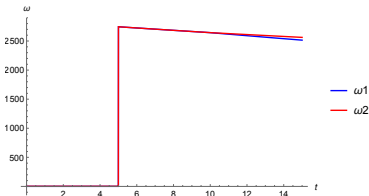
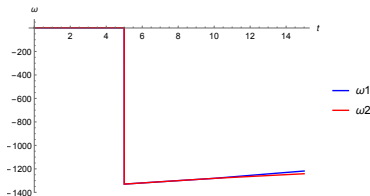
# Clutch Engaged, $\gamma = t$

## Differential Algebraic Equation

if t	do	$J_1 \dot{\omega}_1 = \tau_1$	$(e_1)$
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- Dymola **crashes** with a division by zero
- Mathematica treats resets as initializations (nondeterministic behavior)



The solution may be discontinuous when  $\gamma : f \rightarrow t$  because of the additional constraint  $\omega_1 - \omega_2 = 0$

## Problem 1 How to handle overdetermined systems ?

- The angular velocities  $\omega_1$  and  $\omega_2$  are **known**
- $\gamma$  switches to  $t$  (the driver engages the clutch)

$$\omega_1 - \omega_2 = 0 \text{ is } \mathbf{enforced}$$

- The system **becomes** overdetermined
- The solution is not smooth and even discontinuous

## Problem 2 What is the meaning of the derivatives ?

Some equations must hold for  $\gamma = t$  and  $\gamma = f$ .

$$\text{if } t \text{ do } J_1 \dot{\omega}_1 = \tau_1 \quad (e_1)$$

$$\text{if } t \text{ do } J_2 \dot{\omega}_2 = \tau_2 \quad (e_2)$$

- What is the **meaning** of derivatives when  $\gamma : f \rightarrow t$  ?
- How to compute the **reset values** ?

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$\delta \in {}^*\mathbb{R}$  is a **positive infinitesimal**

- $\delta = \langle \delta_1, \delta_2, \dots \rangle$
- $\delta_i \in \mathbb{R}$
- Not necessarily convergent
- $\langle 1, \frac{1}{2}, \frac{1}{3}, \dots \rangle$  is a (positive) infinitesimal
- $r = \langle r, r, r, \dots \rangle, r \in \mathbb{R}$
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Let  $\delta \in {}^*\mathbb{R}$  be a non zero infinitesimal.

$$\frac{x(t + \delta) - x(t)}{\delta}$$

## Proposition

A real function  $x$  is differentiable at  $t$  if and only if there exists a real number  $b$  such that

$$\frac{x(t + \epsilon) - x(t)}{\epsilon} \sim b$$

for any non zero infinitesimal  $\epsilon$ .

$\dot{x}$  is replaced by  $\frac{x(t + \delta) - x(t)}{\delta} = \frac{x^\bullet - x}{\delta}$

- **Shift forward** (when needed)
- **Formal substitution** of time derivatives into difference quotient.

if t	do	$J_1 \dot{\omega}_1 = \tau_1$	(e <sub>1</sub> )	if t	do	$J_1 \frac{\omega_1^\bullet - \omega_1}{\delta} = \tau_1$	(e <sub>1</sub> <sup>δ</sup> )
if t	do	$J_2 \dot{\omega}_2 = \tau_2$	(e <sub>2</sub> )				
if γ	do	$\omega_1 - \omega_2 = 0$	(e <sub>3</sub> )	if t	do	$J_2 \frac{\omega_2^\bullet - \omega_2}{\delta} = \tau_2$	(e <sub>2</sub> <sup>δ</sup> )
if γ	do	$\tau_1 + \tau_2 = 0$	(e <sub>4</sub> )	if γ	do	$\omega_1^\bullet - \omega_2^\bullet = 0$	(e <sub>3</sub> <sup>•</sup> )
if ¬γ	do	$\tau_1 = 0$	(e <sub>5</sub> )	if γ	do	$\tau_1 + \tau_2 = 0$	(e <sub>4</sub> )
if ¬γ	do	$\tau_2 = 0$	(e <sub>6</sub> )	if ¬γ	do	$\tau_1 = 0$	(e <sub>5</sub> )
				if ¬γ	do	$\tau_2 = 0$	(e <sub>6</sub> )

# Solving Nonstandard Systems

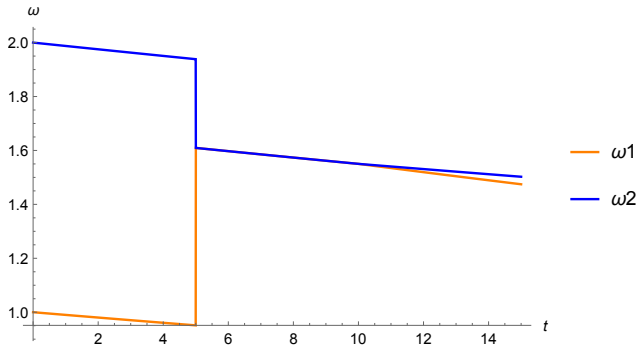
if t	do	$J_1 \frac{\omega_1^\bullet - \omega_1}{\delta} = \tau_1$	$(e_1^\delta)$
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$$\dot{\omega}_1 = \dot{\omega}_2 = \frac{J_1\omega_1 + J_2\omega_2}{J_1 + J_2}$$

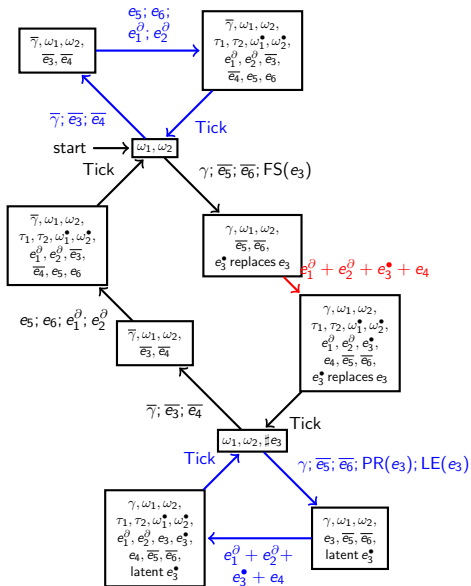
## Standardization

- Automated procedure for a class of systems
- Generalization remains a challenge

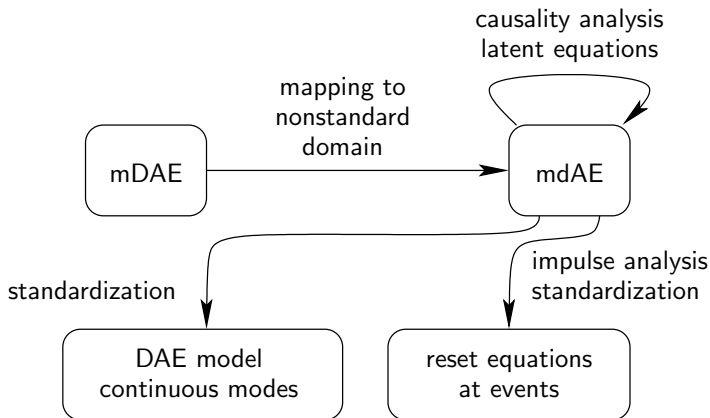
# Expected Simulation







# Unifying Discrete and Continuous Dynamics



# Challenges



# Combining Static Analysis and Symbolic Computation

## Invariants Generation

- Extends previous work (algebraic approach)
- **Approximate** exact computations to scale

## Simulation of multi-mode DAE

- Well-founded operational semantics (compilation, index reduction)
  - Preserve compositionality in presence of mode changes
  - Proper handling of zero-crossing (detection and consistent initialization)
  - Cascades of zero-crossings (sliding modes)
- ➡ Investigate the use of **static analysis** and **symbolic computation**

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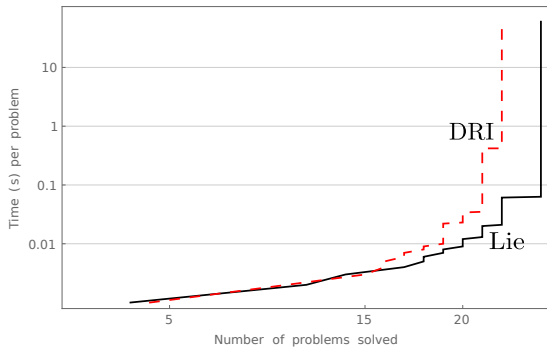
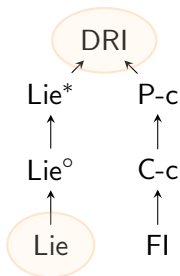
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# Thanks for your attention !



# Smooth invariant manifolds (Lie vs DRI)

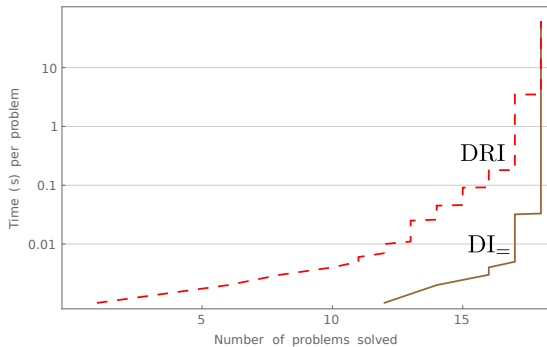
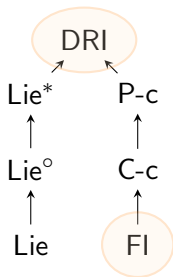
Lie and DRI **decide** invariance for **smooth invariant manifolds**.





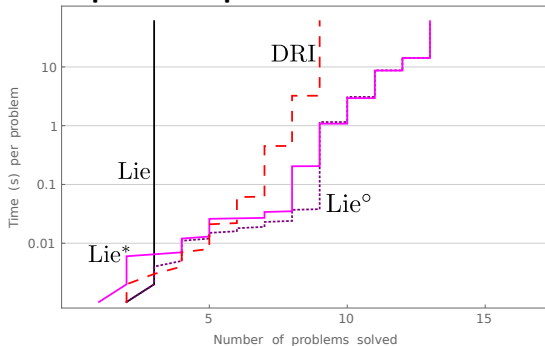
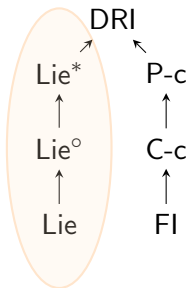
# Functional invariants (DI vs DRI)

DI<sub>=</sub> and DRI **decide** invariance of varieties of **conserved quantities**.



# Singularities at Equilibria ( $\text{Lie}$ , $\text{Lie}^\circ$ & $\text{Lie}^*$ vs DRI)

$\text{Lie}^\circ$ ,  $\text{Lie}^*$  and DRI **decide** invariance for varieties of with **singularities that are equilibrium points**.



$$\begin{aligned}
& (h_1 > \max(h_2, \dots, h_m) \rightarrow \mathfrak{D}_f(h_1) < 0) \\
\wedge \quad & (h_1 < \max(h_2, \dots, h_m) \rightarrow \mathfrak{D}_f(\max(h_2, \dots, h_m)) < 0) \\
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\end{aligned}$$

$$\begin{aligned}
& (g_1 < \min(g_2, \dots, g_m) \rightarrow \mathfrak{D}_f(g_1) < 0) \\
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\wedge \quad & (g_1 = \min(g_2, \dots, g_m) \rightarrow \mathfrak{D}_f(g_1) < 0 \vee \mathfrak{D}_f(\min(g_2, \dots, g_m)) < 0)
\end{aligned}$$