| Problem Formulation | Verification Shell | Validated Simulation | Experimental Results | Concluding Remarks |
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## Verification of Delayed Differential Dynamics Based on Validated Simulation

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Limassol, November 2016

| Problem Formulation | Verification Shell | Validated Simulation | Experimental Results | Concluding Remarks |
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# Motivation : Why Delays?

$$\begin{cases} \dot{\mathbf{x}}(t) = -\mathbf{x}(t) \\ \mathbf{x}(0) = 1 \end{cases}$$



| Problem Formulation | Verification Shell | Validated Simulation | Experimental Results<br>000 | Concluding Remarks<br>O |
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| Motivation :        | Why Delays?        |                      |                             |                         |



| Problem Formulation | Verification Shell | Validated Simulation | Experimental Results<br>000 | Concluding Remarks<br>O |
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| Motivation : \      | Why Delays?        |                      |                             |                         |

Delayed logistic equation [G. Hutchinson, 1948] :

$$\dot{N}(t) = N(t)[1 - N(t - r)]$$

| Problem Formulation | Verification Shell | Validated Simulation | Experimental Results | Concluding Remarks |
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# Motivation : Why Delays?

Delayed logistic equation [G. Hutchinson, 1948] :

$$\dot{N}(t) = N(t)[1 - N(t - r)]$$



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| Problem Formulation | Verification Shell | Validated Simulation | Experimental Results<br>000 | Concluding Remarks<br>O |
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| Outline             |                    |                      |                             |                         |

## 1 Problem Formulation

- 2 Simulation-Based Verification
- 3 Validated Simulation of Delayed Differential Dynamics
- 4 Experimental Results
- 5 Concluding Remarks

| Problem Formulation | Verification Shell | Validated Simulation | Experimental Results<br>000 | Concluding Remarks<br>O |
|---------------------|--------------------|----------------------|-----------------------------|-------------------------|
|                     |                    |                      |                             |                         |
| Outline             |                    |                      |                             |                         |

## 1 Problem Formulation

- Delayed Dynamical Systems
- Safety Verification Problem
- 2 Simulation-Based Verification
  - Basic Idea
  - Verification Algorithm
- 3 Validated Simulation of Delayed Differential Dynamics
  - Local Error Bounds
  - Simulation Algorithm
  - Solving Optimization
  - Correctness and Completeness
- 4 Experimental Results
  - Delayed Logistic Equation
  - Delayed Microbial Growth

## 5 Concluding Remarks

| Problem Formulation       | Verification Shell | Validated Simulation | Experimental Results | Concluding Remarks |
|---------------------------|--------------------|----------------------|----------------------|--------------------|
| ••                        |                    |                      |                      |                    |
| Delayed Dynamical Systems |                    |                      |                      |                    |
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# Delayed Dynamical Systems

## Delayed Dynamical Systems

$$\begin{cases} \dot{\mathbf{x}}(t) &= \boldsymbol{f}(\mathbf{x}(t), \mathbf{x}(t-r_1), \dots, \mathbf{x}(t-r_k)), \quad t \in [0, \infty) \\ \mathbf{x}(t) &\equiv \mathbf{x}_0 \in \Theta, \quad t \in [-r_{\max}, 0] \end{cases}$$

The unique *solution* (*trajectory*):  $\xi_{\mathbf{x}_0}(t) : [-r_{\max}, \infty) \mapsto \mathbb{R}^n$ .

| Problem Formulation         | Verification Shell | Validated Simulation | Experimental Results | Concluding Remarks |
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| Safety Verification Problem |                    |                      |                      |                    |
| Safety Verific              | ation Probler      | n <sup>1</sup>       |                      |                    |

Given  $T \in \mathbb{R}$ ,  $\mathcal{X}_0 \subseteq \Theta$ ,  $\mathcal{U} \subseteq \mathbb{R}^n$ , whether

$$\forall \mathbf{x}_0 \in \mathcal{X}_0: \quad \left( \bigcup_{t \leq T} \xi_{\mathbf{x}_0}(t) \right) \cap \mathcal{U} = \emptyset \quad ?$$

<sup>1.</sup> The figure is taken from [M. Althoff, 2010].

| Problem Formulation         | Verification Shell | Validated Simulation | Experimental Results | Concluding Remarks |
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| Safety Verification Problem |                    |                      |                      |                    |
| Safety Verifica             | tion Probler       | n <sup>1</sup>       |                      |                    |

Given  $T \in \mathbb{R}$ ,  $\mathcal{X}_0 \subseteq \Theta$ ,  $\mathcal{U} \subseteq \mathbb{R}^n$ , whether

$$\forall \mathbf{x}_0 \in \mathcal{X}_0: \quad \left(\bigcup_{t \leq T} \xi_{\mathbf{x}_0}(t)\right) \cap \mathcal{U} = \emptyset \quad ?$$



System is safe, if no trajectory enters the unsafe set.

1. The figure is taken from [M. Althoff, 2010].

| Problem Formulation | Verification Shell | Validated Simulation | Experimental Results | Concluding Remarks |
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## Outline

### Problem Formulation

- Delayed Dynamical Systems
- Safety Verification Problem
- 2 Simulation-Based Verification
  - Basic Idea
  - Verification Algorithm
- 3 Validated Simulation of Delayed Differential Dynamics
  - Local Error Bounds
  - Simulation Algorithm
  - Solving Optimization
  - Correctness and Completeness
- 4 Experimental Results
  - Delayed Logistic Equation
  - Delayed Microbial Growth

### 5 Concluding Remarks

| Problem Formulation     | Verification Shell | Validated Simulation | Experimental Results | Concluding Remarks |
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| Basic Idea              |                    | 0000                 | 000                  | 0                  |
| Basic Idea <sup>2</sup> |                    |                      |                      |                    |



Figure : A finite  $\epsilon$ -cover of the initial set of states.



Figure : An Over-approximation of the reachable set by bloating the simulation.

<sup>2.</sup> Figures are taken from [A. DonzDonzé & O. Maler, 2007].

| Problem Formulation    | Verification Shell | Validated Simulation | Experimental Results | Concluding Remarks |
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| Verification Algorithm |                    |                      |                      |                    |
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# Verification Algorithm

Algorithm 1: Simulation-based Verification for Delayed Dynamical Systems

input : The dynamics  $f(\mathbf{x}, \mathbf{u})$ , delay term r, initial set  $\mathcal{X}_0$ , unsafe set  $\mathcal{U}$ , time bound T, precision  $\epsilon$ . /\* initialization \*/ 1  $\mathcal{R} \leftarrow \emptyset$ ;  $\delta \leftarrow dia(\mathcal{X}_0)/2$ ;  $\tau \leftarrow \tau_0$ ; 2  $\mathcal{X} \leftarrow \delta$ -Partition $(\mathcal{X}_0)$ : while  $\mathcal{X} \neq \emptyset$  do 3 if  $\delta < \epsilon$  then 4 return (UNKNOWN, R); 5 for  $\mathcal{B}_{\delta}(\mathbf{x}_0) \in \mathcal{X}$  do 6  $\langle \mathbf{t}, \mathbf{y}, \mathbf{d} \rangle \leftarrow \text{Simulation}(\mathcal{B}_{\delta}(\mathbf{x}_0), \boldsymbol{f}(\mathbf{x}, \mathbf{u}), r, \tau, T);$ 7  $\mathcal{T} \leftarrow \bigcup_{n=0}^{N-1} \operatorname{conv}(\mathcal{B}_{\mathbf{d}_n}(\mathbf{y}_n) \cup \mathcal{B}_{\mathbf{d}_{n+1}}(\mathbf{y}_{n+1}));$ 8 if  $\mathcal{T} \cap \mathcal{U} = \emptyset$  then 9  $\mathcal{X} \leftarrow \mathcal{X} \setminus \mathcal{B}_{\delta}(\mathbf{x}_0)$ :  $\mathcal{R} \leftarrow \mathcal{R} \cup \mathcal{T}$ : 10 else if  $\exists i. \mathcal{B}_{\mathbf{d}_i}(\mathbf{y}_i) \subseteq \mathcal{U}$  then 11 return (UNSAFE, T); 12 else 13  $\mathcal{X} \leftarrow \mathcal{X} \setminus \mathcal{B}_{\delta}(\mathbf{x}_0); \ \mathcal{X} \leftarrow \mathcal{X} \cup \frac{\delta}{2}$ -Partition $(\mathcal{B}_{\delta}(\mathbf{x}_0));$ 14  $\delta \leftarrow \delta/2$ : 15 16 return (SAFE, R):

| Problem Formulation | Verification Shell | Validated Simulation | Experimental Results | Concluding Remarks |
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## Outline

## Problem Formulation

- Delayed Dynamical Systems
- Safety Verification Problem
- 2 Simulation-Based Verification
  - Basic Idea
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## 3 Validated Simulation of Delayed Differential Dynamics

- Local Error Bounds
- Simulation Algorithm
- Solving Optimization
- Correctness and Completeness

## 4 Experimental Results

- Delayed Logistic Equation
- Delayed Microbial Growth

## 5 Concluding Remarks

| Problem Formulation | Verification Shell | Validated Simulation | Experimental Results<br>000 | Concluding Remarks<br>O |
|---------------------|--------------------|----------------------|-----------------------------|-------------------------|
| Local Error Bounds  |                    |                      |                             |                         |
| Local Error B       | ounds              |                      |                             |                         |

$$\mathbf{E}(t) = \begin{cases} d_0, & \text{if } t = 0, \\ E(t_i) + (t - t_i)\mathbf{e}_{i+1}, & \text{if } t \in [t_i, t_{i+1}]. \end{cases}$$

| Problem Formulation | Verification Shell | Validated Simulation | Experimental Results | Concluding Remarks |
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| Local Error Bounds  |                    |                      |                      |                    |
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| I OCAL ELLOL R      | ounds              |                      |                      |                    |

$$\mathbf{E}(t) = \begin{cases} d_0, & \text{if } t = 0, \\ E(t_i) + (t - t_i)e_{i+1}, & \text{if } t \in [t_i, t_{i+1}]. \end{cases}$$

Validation Property :

$$\xi_{\mathbf{x}_0}(t) \in \mathcal{B}_{\textit{\textit{E}}(t)}\left(\frac{(t-t_i)\mathbf{y}_i + (t_{i+1}-t)\mathbf{y}_{i+1}}{t_{i+1}-t_i}\right), \text{for each } t \in [t_i,t_{i+1}].$$

| Problem Formulation  | Verification Shell | Validated Simulation | Experimental Results | Concluding Remarks |
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| Simulation Algorithm |                    |                      |                      |                    |
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# Simulation Algorithm

#### Algorithm 2: Simulation: a validated DDE solver producing rigorous bounds

```
input: The initial set \mathcal{B}_{\delta}(\mathbf{x}_0), dynamics f(\mathbf{x}, \mathbf{u}), delay term r, stepsize \tau, time bound T.
    output: A triple \langle t, y, d \rangle, where the components represent lists, with the same length, respectively for the
                   time points, numerical approximations (possibly multi-dimensional), and the rigorous local error
                   bounds.
     /* initializing the lists, whose indices start from -1 */
1 \mathbf{t} \leftarrow \llbracket -\tau, 0 \rrbracket; \mathbf{y} \leftarrow \llbracket \mathbf{x}_0, \mathbf{x}_0 \rrbracket; \mathbf{d} \leftarrow \llbracket 0, \delta \rrbracket;
     /* r has to be divisible by 	au (in FP numbers) */
2 n \leftarrow 0; m \leftarrow r/\tau;
3 while \mathbf{t}_{n} < T do
             t_{n+1} \leftarrow \mathbf{t}_n + \tau;
4
             /* approximating y_{n+1} using forward Euler method */
5
          y_{n+1} \leftarrow \mathbf{y}_n + f(\mathbf{y}_n, \mathbf{y}_{n-m}) * \tau;
             /* computing error slope by constrained optimization, where \sigma is a
                     positive slack constant */
              e_n \leftarrow Find minimum e s.t.
                                          \|\mathbf{f}(\mathbf{x} + t * \mathbf{f}, \mathbf{u} + t * \mathbf{g}) - \mathbf{f}(\mathbf{y}_n, \mathbf{y}_{n-m})\| \le e - \sigma, for
                                      \begin{array}{l} \underset{\mathbf{M} \in \mathcal{M}}{ \| \mathbf{J}_{\mathbf{V}_{\mathbf{C}}}(\mathbf{x}) \|} \\ \forall \mathbf{t} \in [0, \tau] \\ \forall \mathbf{x} \in \mathcal{B}_{\mathbf{d}_{n}}(\mathbf{y}) \\ \forall \mathbf{u} \in \mathcal{B}_{\mathbf{d}_{n-m}}(\mathbf{y}_{n-m}) \\ \forall \mathbf{u} \in \mathcal{B}_{\mathbf{d}_{n-m}}(\mathbf{f}(\mathbf{y}_{n}, \mathbf{y}_{n-m})) \\ \forall \mathbf{g} \in \mathcal{B}_{e_{n-m}}(\mathbf{f}(\mathbf{y}_{n-m}, \mathbf{y}_{n-2m})); \end{array} 
             d_{n+1} \leftarrow \mathbf{d}_n + \tau e_n;
             /* updating the lists by appending the extrapolation */
             \mathbf{t} \leftarrow [\![\mathbf{t}, t_{n+1}]\!]; \mathbf{y} \leftarrow [\![\mathbf{y}, y_{n+1}]\!]; \mathbf{d} \leftarrow [\![\mathbf{d}, d_{n+1}]\!];
6
              n \leftarrow n + 1:
s return \langle \mathbf{t}, \mathbf{y}, \mathbf{d} \rangle;
```

| Problem Formulation  | Verification Shell | Validated Simulation | Experimental Results<br>000 | Concluding Remarks<br>O |
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| Solving Optimization |                    |                      |                             |                         |
| Solving the C        | Optimization b     | v HvSAT-II           |                             |                         |

find min{
$$e \ge 0 \mid \forall x : \phi(x, e) \implies \psi(x, e)$$
}

| Problem Formulation                  | Verification Shell | Validated Simulation | Experimental Results | Concluding Remarks |  |
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| Solving Optimization                 |                    |                      |                      |                    |  |
| Solving the Optimization by HySAT-II |                    |                      |                      |                    |  |

find min{
$$e \ge 0 \mid \forall x : \phi(x, e) \implies \psi(x, e)$$
}

₩

find max{ $e \ge 0 \mid \exists x : \phi(x, e) \land \neg \psi(x, e)$ }

| Problem Formulation       | Verification Shell | Validated Simulation | Experimental Results | Concluding Remarks |
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| Correctness and Completen | ess                |                      |                      |                    |
| Simulation A              | laorithm           |                      |                      |                    |
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## Theorem (Correctness)

Suppose the maximum index of the lists is N, then  $\forall t \in [0, T]$  and  $\forall \mathbf{x} \in B_{\delta}(\mathbf{x}_0)$ ,

$$\xi_{\mathbf{x}}(t) \subseteq igcup_{n=0}^{N-1} \mathit{conv}(\mathcal{B}_{\mathbf{d}_n}(\mathbf{y}_n) \cup \mathcal{B}_{\mathbf{d}_{n+1}}(\mathbf{y}_{n+1})).$$

| Problem Formulation       | Verification Shell | Validated Simulation | Experimental Results | Concluding Remarks |
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| Correctness and Completen | ess                |                      |                      |                    |
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| Simulation A              | lgorithm           |                      |                      |                    |

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## Theorem (Completeness)

Suppose the function **f** is continuously differentiable in both arguments and the dynamical system is solvable for time interval [0, T], then for any  $\varepsilon > 0$ , there exists  $\delta$ ,  $\tau$  and  $\sigma$  such that the optimization problem has a solution  $\mathbf{e}_n$  for all  $\mathbf{n} \leq \frac{T}{\tau}$ , and moreover  $\mathbf{d}_n \leq \varepsilon$ .

| Problem Formulation       | Verification Shell | Validated Simulation | Experimental Results | Concluding Remarks |
|---------------------------|--------------------|----------------------|----------------------|--------------------|
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| Correctness and Completen | ess                |                      |                      |                    |
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| Simulation A              | lgorithm           |                      |                      |                    |

# Theorem (Correctness)

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Further extension to simulations with variable stepsize.

| Problem Formulation | Verification Shell | Validated Simulation | Experimental Results | Concluding Remarks |
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## Outline

## Problem Formulation

- Delayed Dynamical Systems
- Safety Verification Problem
- 2 Simulation-Based Verification
  - Basic Idea
  - Verification Algorithm
- 3 Validated Simulation of Delayed Differential Dynamics
  - Local Error Bounds
  - Simulation Algorithm
  - Solving Optimization
  - Correctness and Completeness

## 4 Experimental Results

- Delayed Logistic Equation
- Delayed Microbial Growth

### 5 Concluding Remarks

| Problem Formulation       | Verification Shell | Validated Simulation | Experimental Results<br>●○○ | Concluding Remarks<br>O |
|---------------------------|--------------------|----------------------|-----------------------------|-------------------------|
| Delayed Logistic Equation |                    |                      |                             |                         |
| Delayed Logist            | ic Equation        |                      |                             |                         |

$$\dot{N}(t) = N(t)[1 - N(t - r)]$$

| Problem Formulation       | Verification Shell | Validated Simulation | Experimental Results | Concluding Remarks |
|---------------------------|--------------------|----------------------|----------------------|--------------------|
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| Delayed Logistic Equation |                    |                      |                      |                    |
| Delaved Logis             | tic Fouation       |                      |                      |                    |

$$\dot{N}(t) = N(t)[1 - N(t - r)]$$



Figure :  $\mathcal{X}_0 = \mathcal{B}_{0.01}(1.49)$ , r = 1.3,  $\tau_0 = 0.01$ , T = 10s.

| Problem Formulation       | Verification Shell | Validated Simulation | Experimental Results | Concluding Remarks |
|---------------------------|--------------------|----------------------|----------------------|--------------------|
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| Delayed Logistic Equation |                    |                      |                      |                    |
|                           |                    |                      |                      |                    |

# Delayed Logistic Equation

 $\dot{N}(t) = N(t)[1 - N(t - r)]$ 



Figure :  $\mathcal{X}_0 = \mathcal{B}_{0.01}(1.49)$ , r = 1.3,  $\tau_0 = 0.01$ , T = 10s.



Figure : Over-approximation rigorously proving unsafe, with r = 1.7,  $\mathcal{X}_0 = \mathcal{B}_{0.025}(0.425)$ ,  $\tau_0 = 0.1$ , T = 5**s**,  $\mathcal{U} = \{N|N > 1.6\}$ .

| Problem Formulation       | Verification Shell | Validated Simulation | Experimental Results | Concluding Remarks |
|---------------------------|--------------------|----------------------|----------------------|--------------------|
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| Delayed Logistic Equation |                    |                      |                      |                    |

# **Delayed Logistic Equation**



(a) An initial over-approximaion of trajectories starting from B<sub>0.225</sub> (1.25). It overlaps with the unsafe set (s. circle). Initial set is consequently split (cf. Figs. 3b, 3c).



(b) All trajectories starting from  $\mathcal{B}_{0.125}(1.375)$ are proven safe within the time bound, as the overapproximation does not intersect with the unsafe set.



(c) Initial state set B<sub>0.125</sub>(1.125) is verified to be safe as well.



(d) B<sub>0.25</sub>(0.75) yields overlap w. unsafe; the ball is partitioned again (Figs. 3e, 3f).



(e) All trajectories originating from B<sub>0.125</sub>(0.875) are provably safe.



(f) All trajectories originating from  $B_{0.125}(0.625)$ are provably safe as well.

Fig. 3: The logistic system is proven safe through 6 rounds of simulation with base stepsize  $\tau_0 = 0.1$ . Delay r = 1.3, initial state set  $\mathcal{X}_0 = \{N | N \in [0.5, 1.5]\}$ , time bound T = 5s, unsafe set  $\{N | N > 1.6\}$ .

| Problem Formulation      | Verification Shell | Validated Simulation | Experimental Results | Concluding Remarks<br>O |
|--------------------------|--------------------|----------------------|----------------------|-------------------------|
| Delayed Microbial Growth |                    |                      |                      |                         |
| Delayed Microl           | bial Growth        |                      |                      |                         |

$$\begin{aligned} \dot{S}(t) &= 1 - S(t) - f(S(t))x(t) \\ \dot{x}(t) &= \mathbf{e}^{-r}f(S(t-r))x(t-r) - x(t) \end{aligned}$$

| Problem Formulation      | Verification Shell | Validated Simulation | Experimental Results | Concluding Remarks |
|--------------------------|--------------------|----------------------|----------------------|--------------------|
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| Delayed Microbial Growth |                    |                      |                      |                    |

# Delayed Microbial Growth

$$\begin{aligned} \hat{\mathbf{S}}(t) &= 1 - \mathbf{S}(t) - f(\mathbf{S}(t))\mathbf{x}(t) \\ \hat{\mathbf{x}}(t) &= \mathbf{e}^{-r}f(\mathbf{S}(t-r))\mathbf{x}(t-r) - \mathbf{x}(t) \end{aligned}$$



Figure : The microbial system is proven safe by 17 rounds of simulation with  $\tau_0 = 0.45$ . Here, f(S) = 2eS/(1+S), r = 0.9,  $\mathcal{X}_0 = \mathcal{B}_{0.3}((1; 0.5))$ ,  $\mathcal{U} = \{(S; x) | S + x < 0\}$ , T = 8s.

| Problem Formulation | Verification Shell | Validated Simulation | Experimental Results | Concluding Remarks |
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## Outline

## Problem Formulation

- Delayed Dynamical Systems
- Safety Verification Problem
- 2 Simulation-Based Verification
  - Basic Idea
  - Verification Algorithm
- 3 Validated Simulation of Delayed Differential Dynamics
  - Local Error Bounds
  - Simulation Algorithm
  - Solving Optimization
  - Correctness and Completeness
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  - Delayed Logistic Equation
  - Delayed Microbial Growth

## 5 Concluding Remarks

| Problem Formulation | Verification Shell | Validated Simulation | Experimental Results<br>000 | Concluding Remarks |
|---------------------|--------------------|----------------------|-----------------------------|--------------------|
| Conclusions         |                    |                      |                             |                    |
| Concluding F        | Remarks            |                      |                             |                    |

- A validated numerical solver for delay differential equations.
- A sound and robustly complete algorithm for automated formal verification of time-bounded reachability properties of a class of systems that feature delayed differential dynamics governed by DDEs with multiple delays.
- A prototypical implementation of the simulator, by which we have successfully demonstrated the method on several benchmark systems involving delayed differential dynamics.
- Forthcoming research : higher-order Runge-Kutta methods ; unbounded verification by Taylor-enclosures ; conformance testing.