Reachability for weakly nonlinear systems using Carleman linearization

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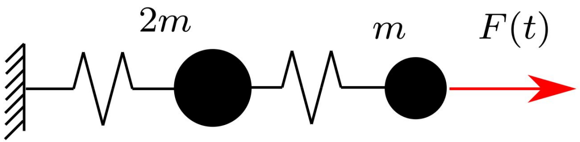
What is reachability for continuous dynamical systems?



Example (linear differential equation):

$$Mx''(t) + Cx'(t) + Kx(t) = F(t)$$

Example taken from https://github.com/JuliaReach/SetPropagation-FEM-JuliaCon21, presented at the JuliaCon'2021 Set Propagation Methods in Julia: Techniques and Applications. **Submitted to JuliaCon'21 Proceedings (extended abstract).**

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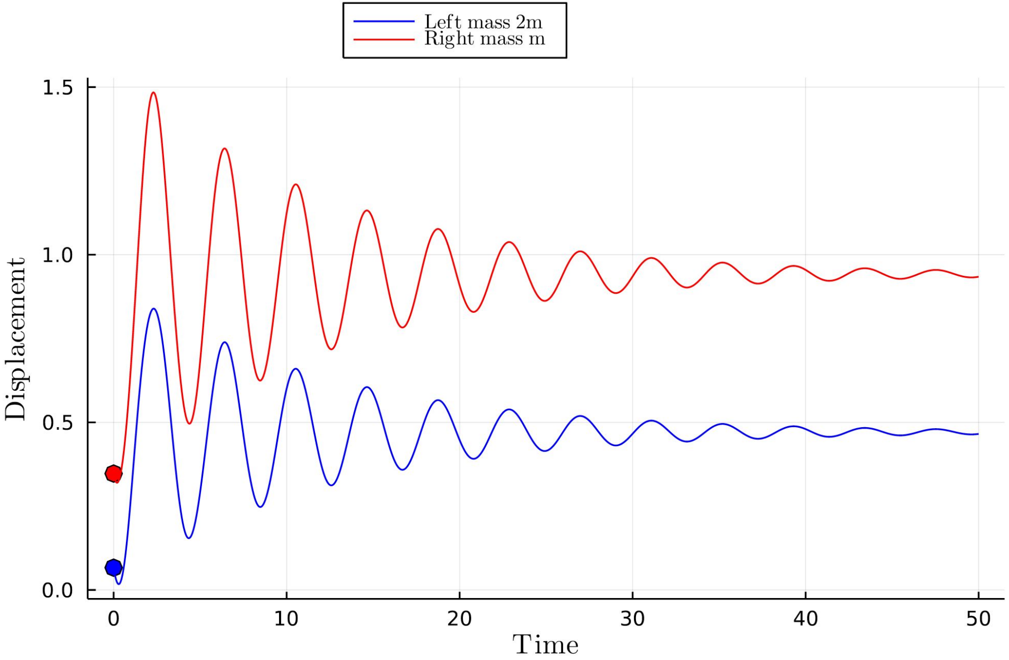

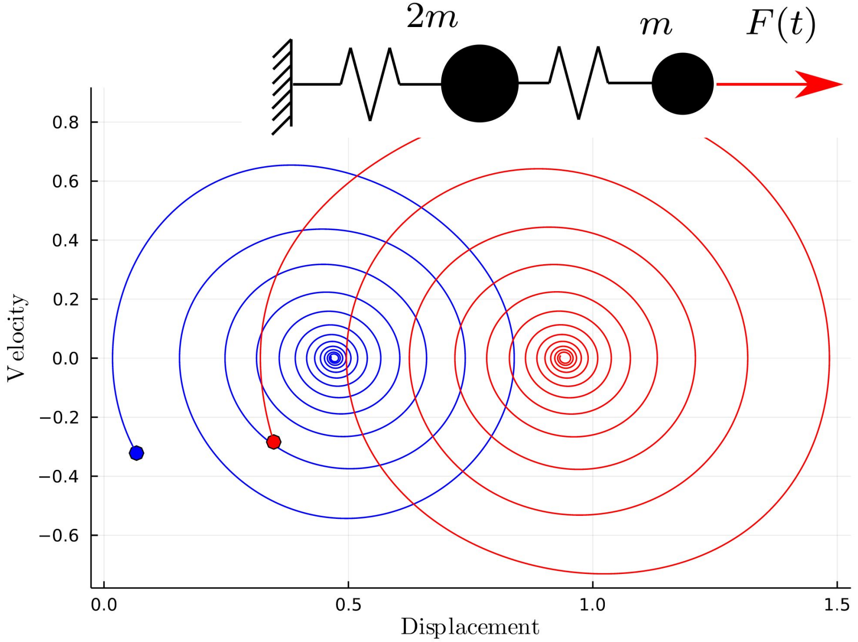

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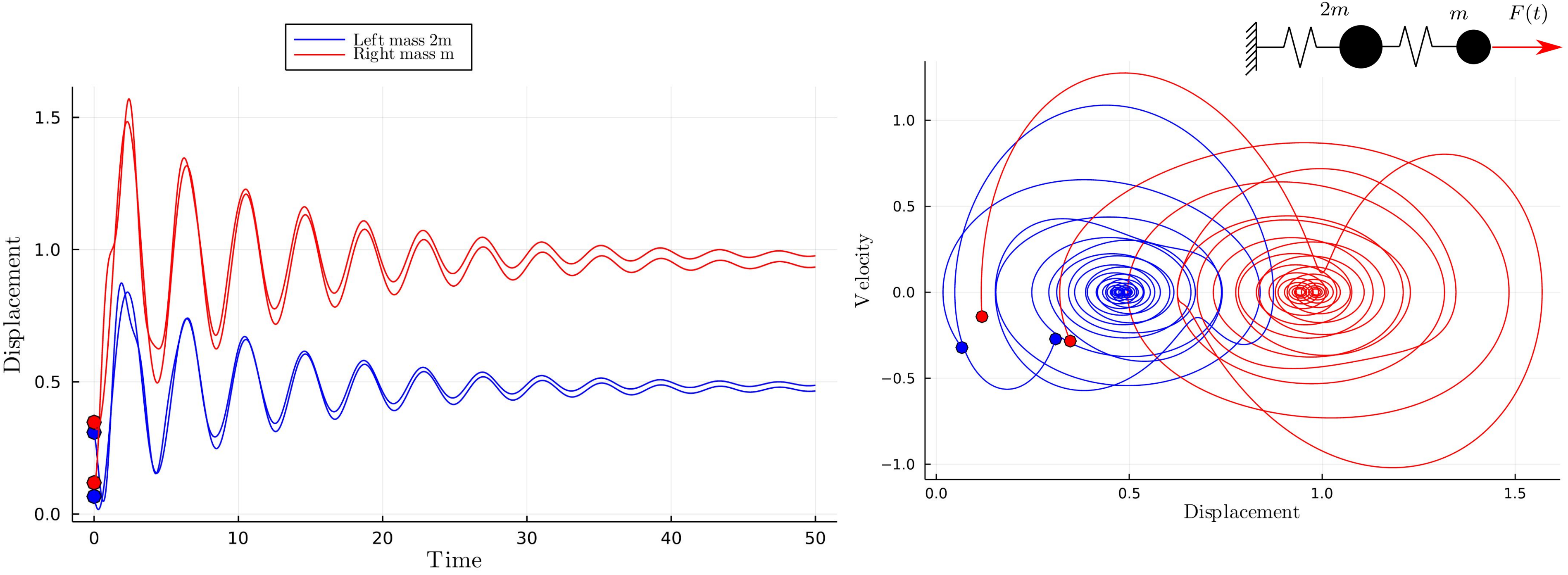

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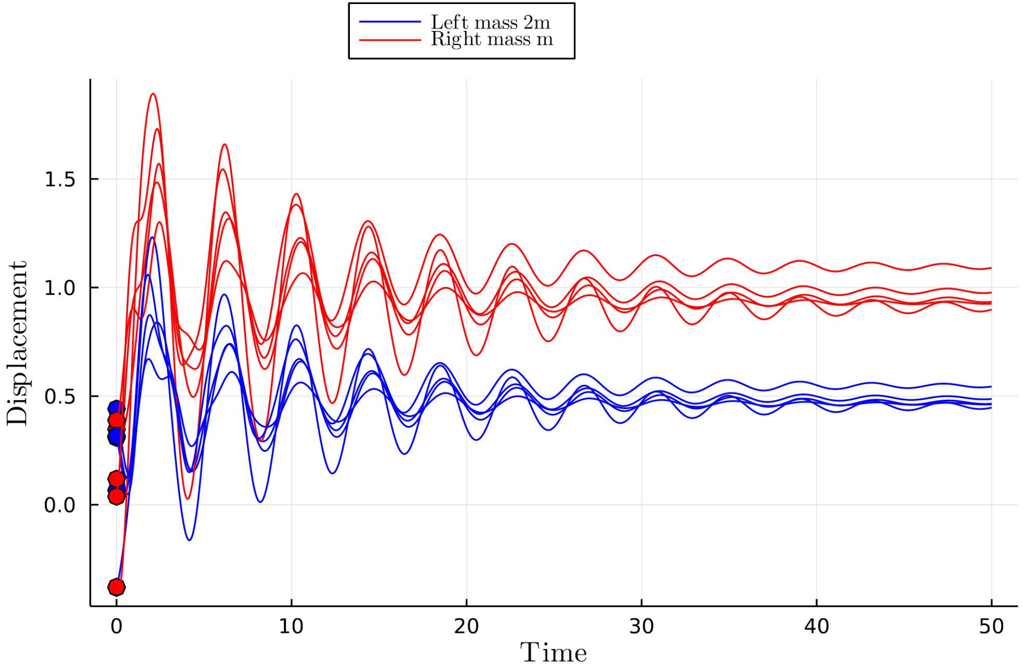

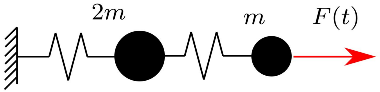

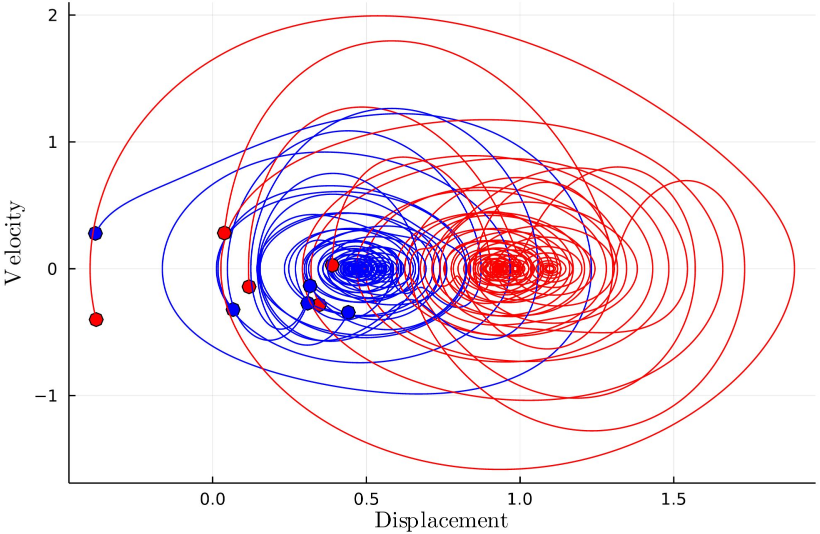

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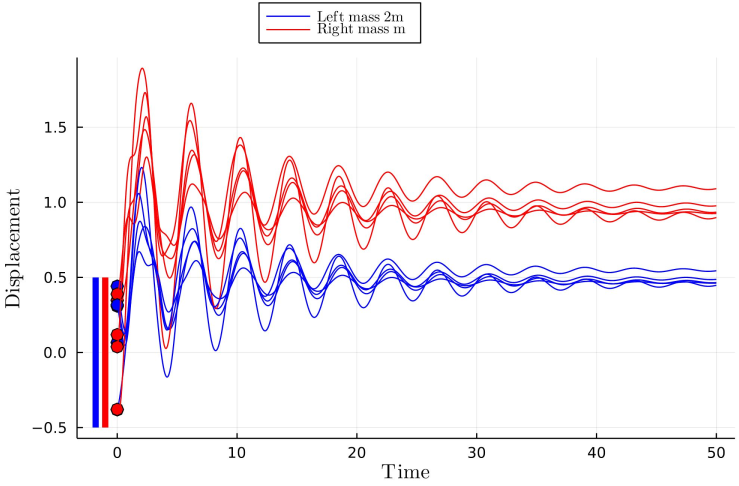

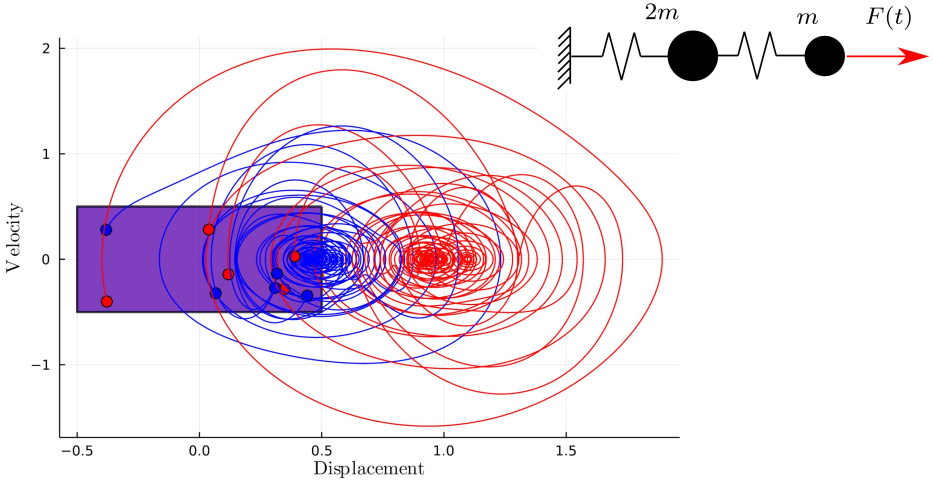

Reachability is a numerical method to compute sets of states reachable by dynamical systems for *all initial states* and all admissible *parameters* and *inputs*

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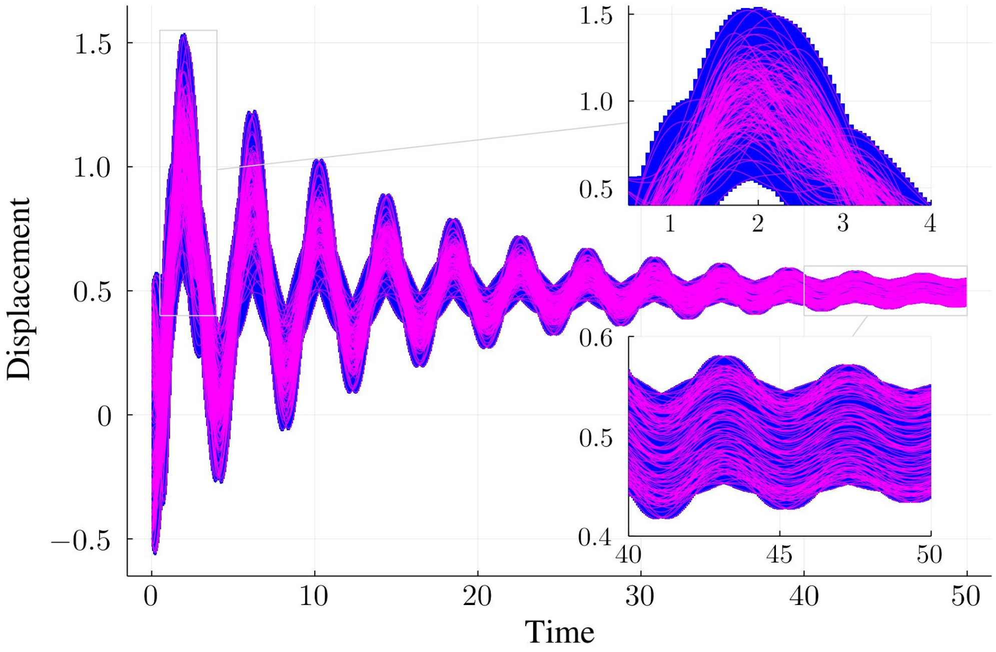


```julia
using ReachabilityAnalysis

# model parameters
m = 0.25; k = 2.0

# finite-element method assembled matrices
M = [2m 0; 0 m]; K = [2k -k; -k k]; C = (M+K)/20
F = [0.0, 1.0]; ΔF0 = Interval(0.9, 1.1)

# initial-value problem with uncertain initial conditions
U0 = BallInf(zeros(4), 0.5)
sys = SecondOrderLinearContinuousSystem(M, C, K, F)
prob = InitialValueProblem(homogeneize(sys), U0 × ΔF0)

# solve using support function method (box directions)
solA = solve(prob, 50, LGG09(δ=5e-2, dirs=:box, dim=5))
```

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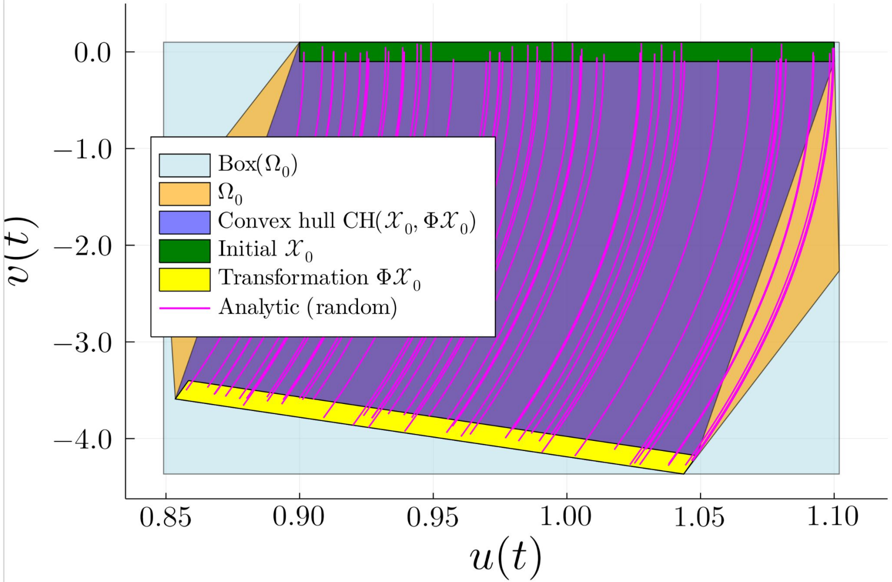
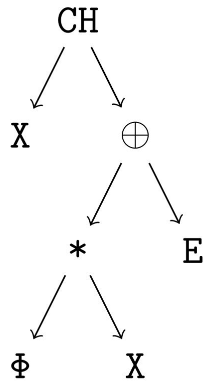
Conservative time discretization (step 1/2)



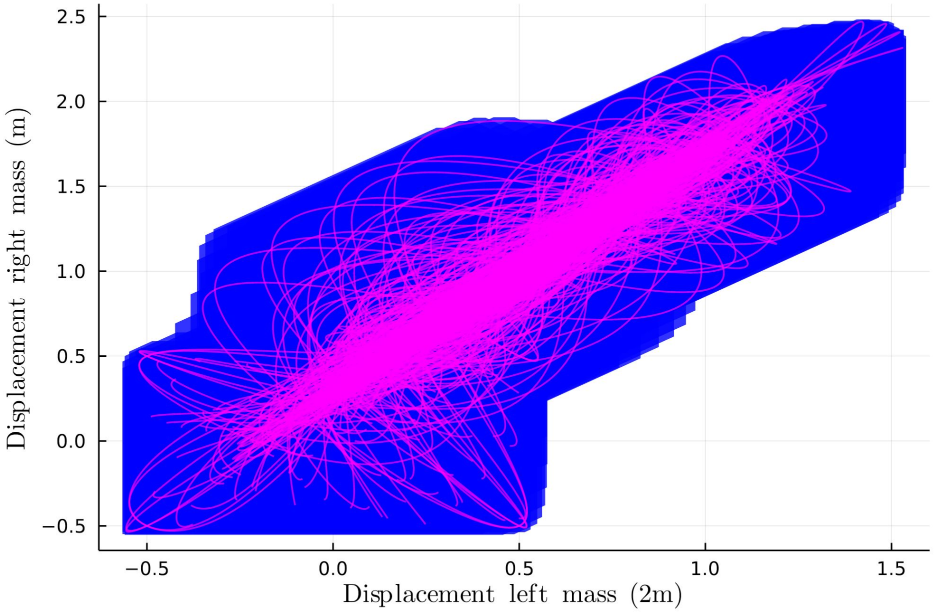

```
1  julia> Ω₀ = CH(X₀, Φ*X₀ ⊕ E₊)
```



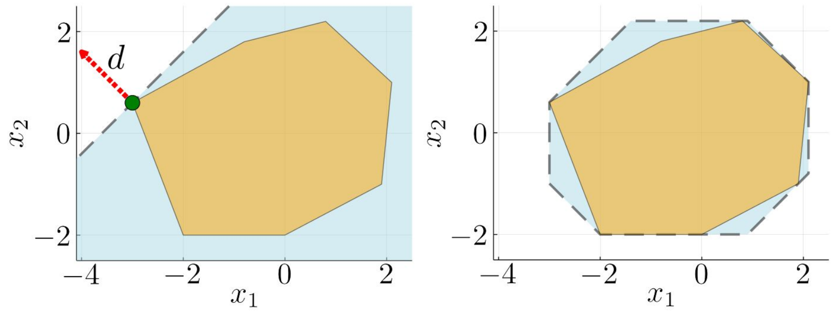
Efficient set computations require specialized algorithms based on different combinations of *set type representations* and *operations* involved.

See: *LazySets.jl: Scalable Symbolic-Numeric Set Computations.* Marcelo Forets and Christian Schilling. arXiv preprint arXiv:2110.01711 (2021). **Submitted to JuliaCon'2021 (full paper).**

Set propagation (step 2/2)




```
# solve using octagonal template directions
solB = solve(prob, 50, LGG09(δ=5e-2, dirs=:oct, dim=5))
```



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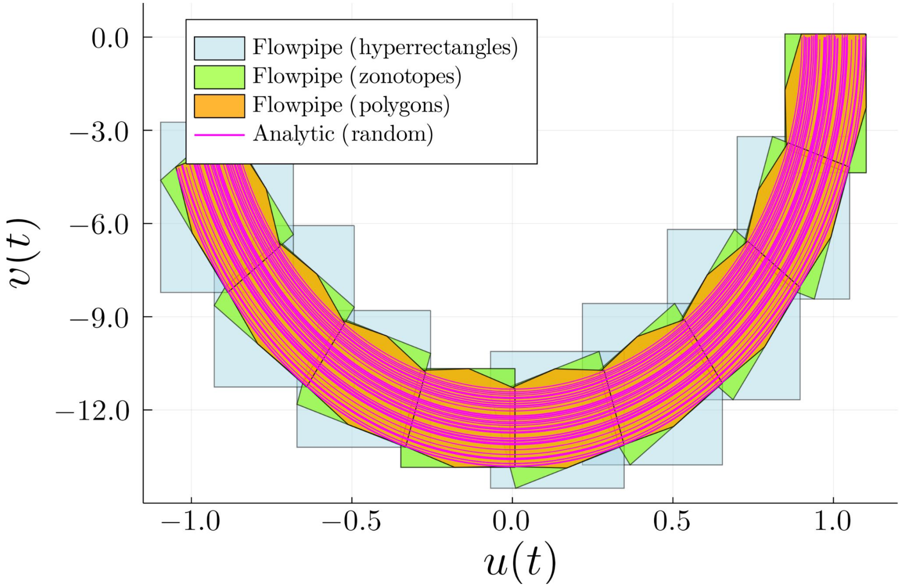

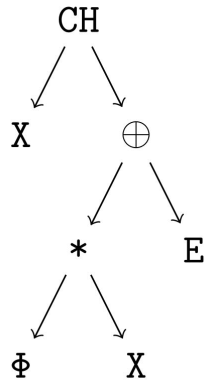

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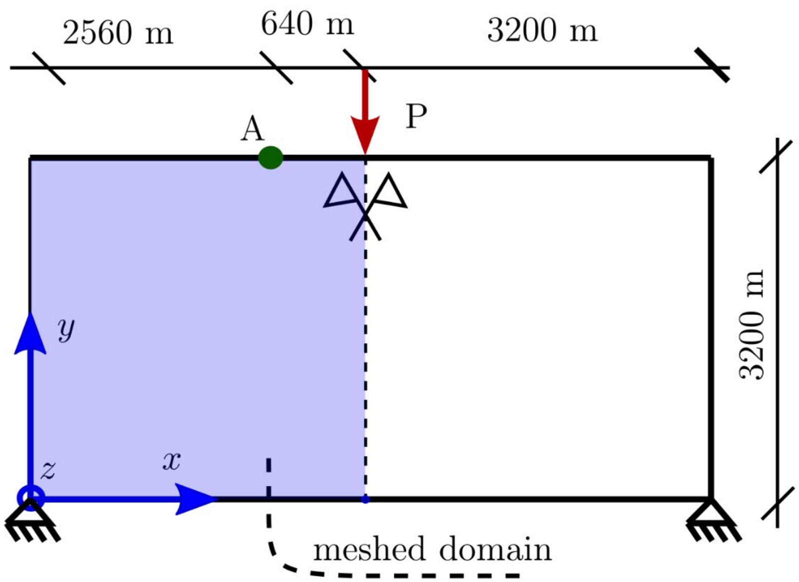
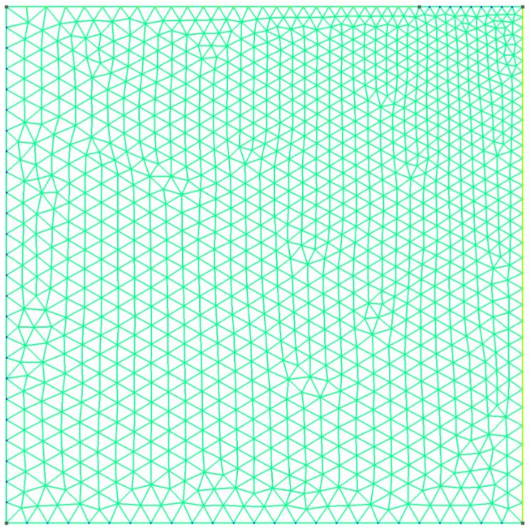
Example in higher dimensions



(a) Diagram of domain and boundary conditions considered.



(b) Finite Element Method mesh used, formed by triangular elements.

2235 linear triangular elements

1180 nodes

See: *Combining Set Propagation with Finite Element Methods for Time Integration in Transient Solid Mechanics Problems*. Forets, Marcelo, Daniel F. Caporale, and Jorge M. Pérez Zerpa. arXiv preprint arXiv:2105.05841.
Accepted in Computers & Structures Journal (2021).

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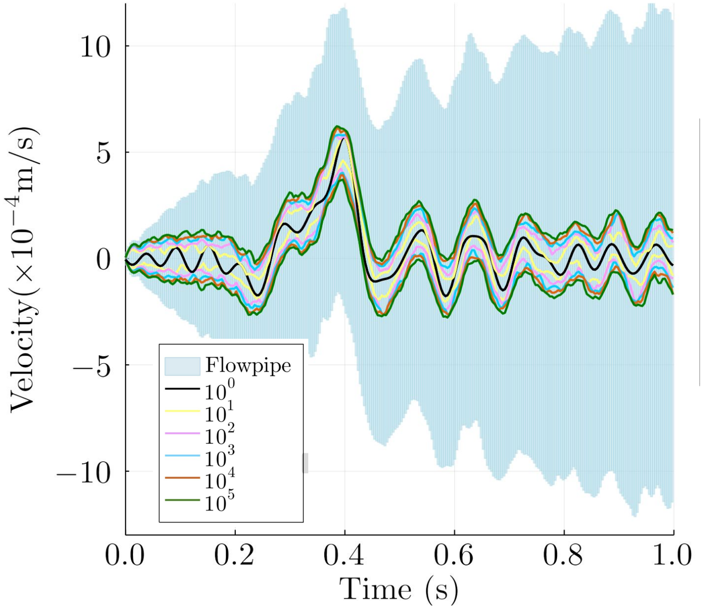

Method	# Trajectories	Time (s)	$\|v_{env}\|_{L_1}$ (10^{-5})	$\|v_{env}\|_{L_\infty}$ (10^{-5})
Newmark	1	0.3	9.27	56.98
Newmark	10	2.0	13.52	57.53
Newmark	100	17.7	16.61	57.59
Newmark	1000	175.5	18.52	58.22
Newmark	10000	1771.4	19.98	61.18
Newmark	100000	17796.1	21.42	62.21
Set Propagation	-	8.5	81.33	122.25

The initial set is propagated exponentially faster than using simulations over randomly sampled initial states

See: *Combining Set Propagation with Finite Element Methods for Time Integration in Transient Solid Mechanics Problems*. Forets, Marcelo, Daniel F. Caporale, and Jorge M. Pérez Zerpa. arXiv preprint arXiv:2105.05841 (2021).
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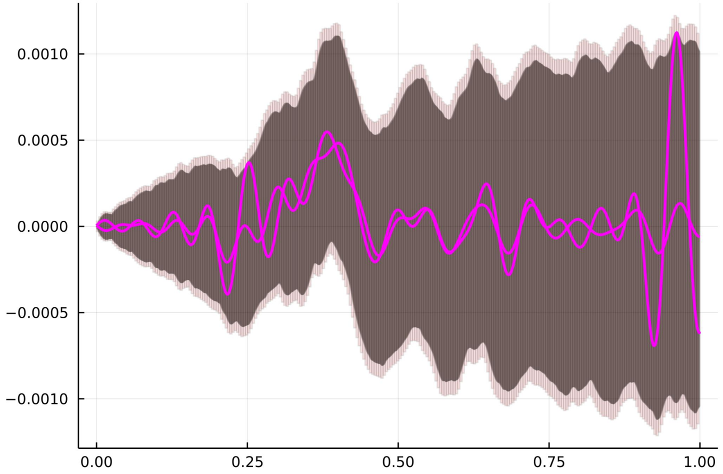
Example in higher dimensions



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The sequence of sets obtained (flowpipe) converges to the exact reachable states when the time-step decreases

See: *Combining Set Propagation with Finite Element Methods for Time Integration in Transient Solid Mechanics Problems***.**
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JuliaReach project

JuliaReach

To advance state-of-the-art working on *fundamental* problems

To build comprehensive, efficient, correct, reproducible, well documented libraries

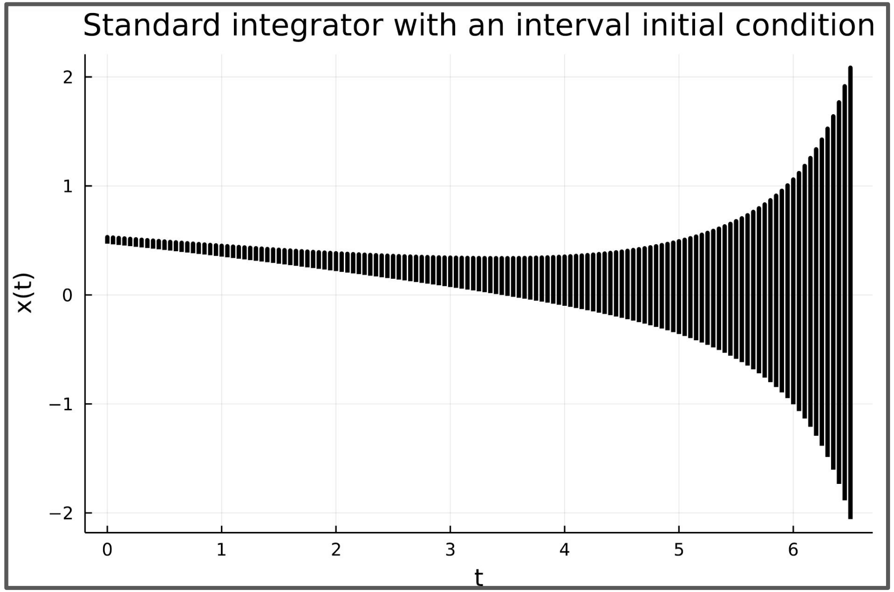
To widen the applicability of reachability analysis for scientists & engineers

Reachability for a nonlinear differential equation

$$\frac{\mathrm{d}x(t)}{\mathrm{d}t} = rx(1 - x/K)$$

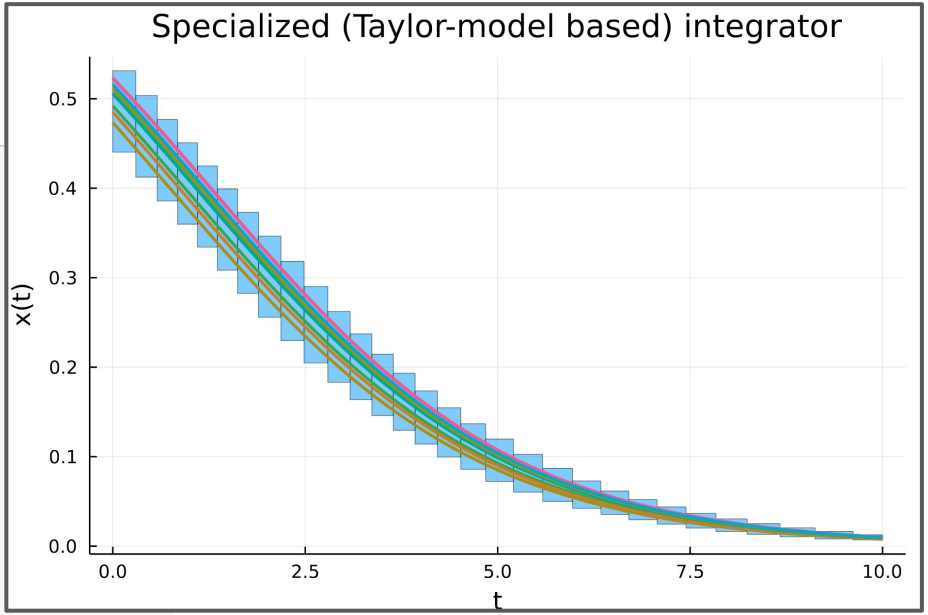
Logistic equation (population dynamics)

```
using DifferentialEquations,
      IntervalArithmetic

# define the problem
function f(dx, x, p, t)
    r = -0.5
    K = 0.8
    dx[1] = r*x[1]*(1 - x[1]/K)
end

x₀ = [0.47 .. 0.53]  # initial condition
prob = ODEProblem(f, x₀, (0.0, 6.5))
sol = solve(prob, RK4(), adaptive=false,
            dt=0.05, reltol=1e-6)
```

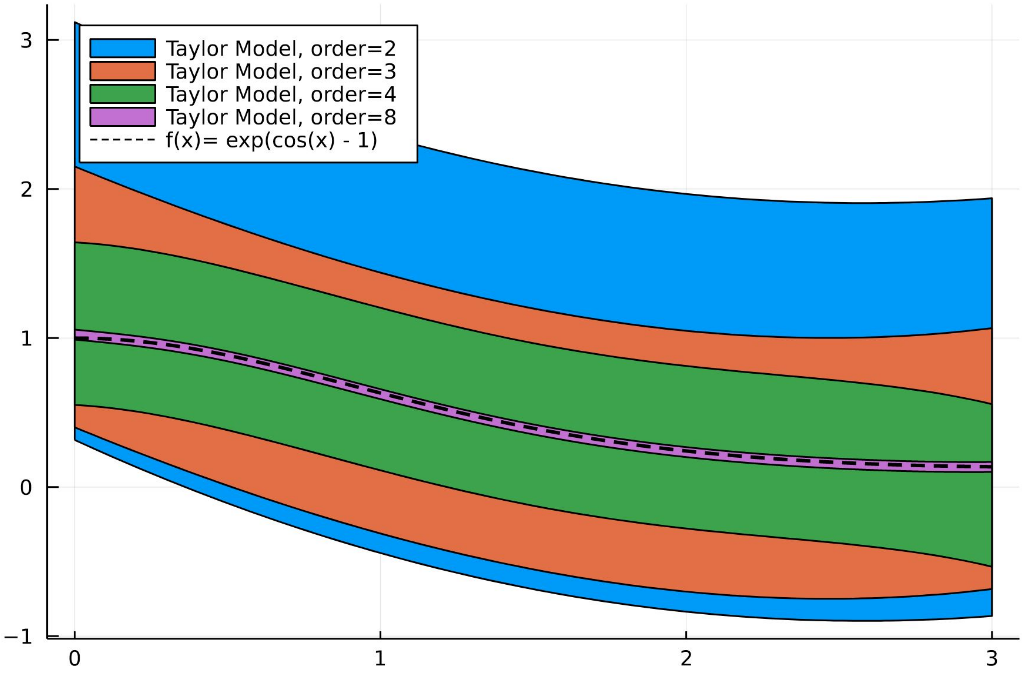


Reachability for a nonlinear differential equation

```julia
using ReachabilityAnalysis, Plots

# define the model (same as before)
function f(dx, x, p, t)
    r = -0.5
    K = 0.8
    dx[1] = r*x[1]*(1 - x[1]/K)
end

X0 = 0.47 .. 0.53 # interval initial states
# initial-value problem
prob = @ivp(x' = f(x), x(0) ∈ X0, dim=1)

# solve it
sol = solve(prob, alg=TMJets21a(abstol=1e-10), T=10.0);
```



Taylor models

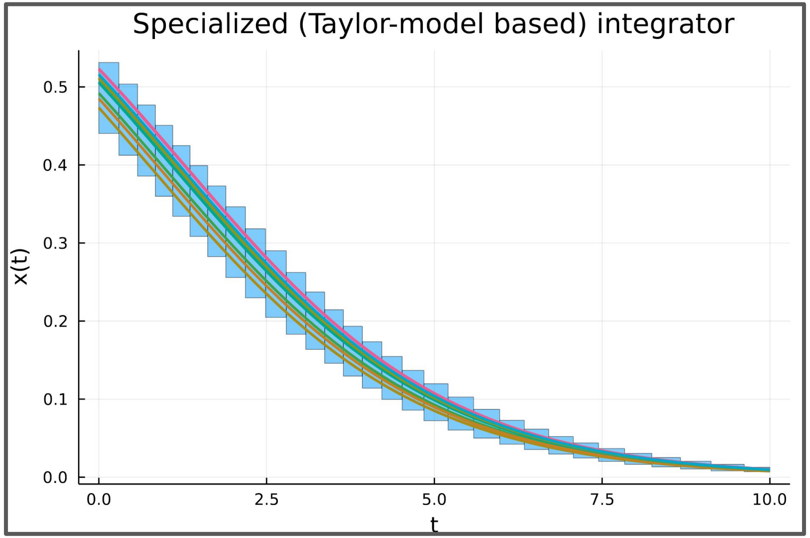


fT_3 = $0.39484468326455857 - 0.393855592043663\, t + 0.18246938526101011\, t^2 + 0.014258580485865105\, t^3 + [-0.946548, 0.803778]$

fT_8 = $0.39484468326455857 - 0.393855592043663\, t + 0.18246938526101011\, t^2 + 0.014258580485865105\, t^3 - 0.054727422711077306\, t^4 + 0.024706768559030104\, t^5 + 0.0007709727046973829\, t^6 - 0.00520692104599662\, t^7 + 0.0019470348640809945\, t^8 + [-0.0410741, 0.0258577]$

Reachability for a nonlinear differential equation

Example:
Taylor model reach-set at
the final computed interval



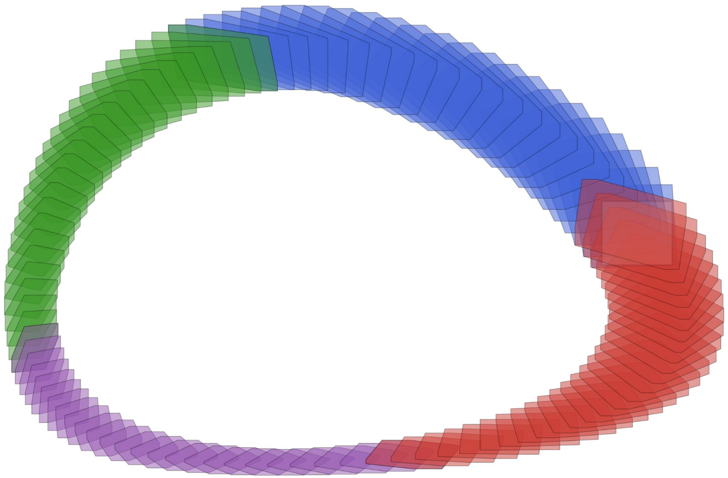

```
tspan(sol[end])
```

```
[9.61803, 10]
```

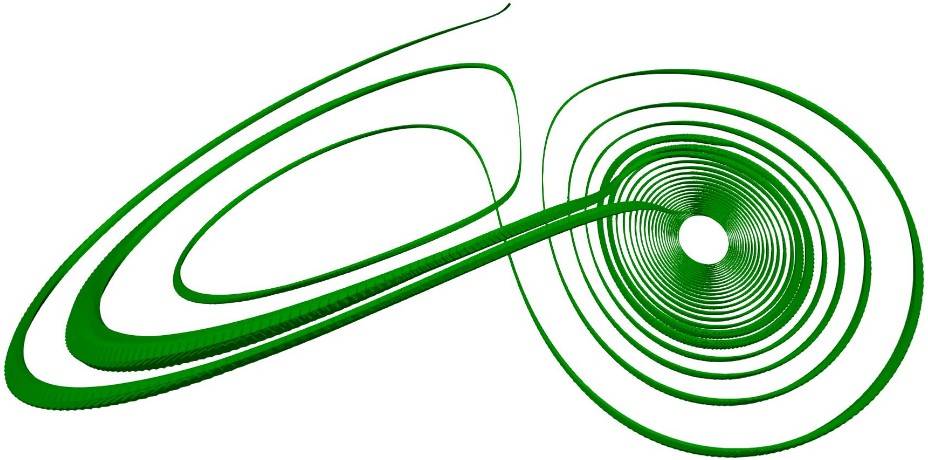
```
sol[end]
```

```
TaylorModelReachSet{Float64}(TaylorModels.TaylorModel1{TaylorN{Float64}, Float64}[  0.010728640000425796 + 0.0016935
616569102134 x₁ + 0.0001657222430356068 x₁² + ( - 0.0052923801775511875 - 0.0008240688117857138 x₁ - 7.8846059232215
5e-5 x₁²) t + ( 0.0012876075183438367 + 0.00019488963434660352 x₁ + 1.7762397657259186e-5 x₁²) t² + ( - 0.0002030100
35766464 - 2.888459368553032e-5 x₁ - 2.339217437712025e-6 x₁²) t³ + ( 2.2566088815570262e-5 + 2.752383693482914e-6 x
₁ + 1.474683203606484e-7 x₁²) t⁴ + ( - 1.7202398083315093e-6 - 1.1552580809843272e-7 x₁ + 1.1261821093858127e-8 x₁²)
t⁵ + ( 6.016969171459992e-8 - 1.413785130768101e-8 x₁ - 4.570779684951191e-9 x₁²) t⁶ + ( 6.311540762007901e-9 + 3.82
8591659395892e-9 x₁ + 7.063749944165518e-10 x₁²) t⁷ + ( - 1.4955436168686581e-9 - 4.920337196748677e-10 x₁ - 6.83032
0243727477e-11 x₁²) t⁸ + [-1.13178e-10, 1.0917e-10]], [9.61803, 10])
```

Nonlinear reachability



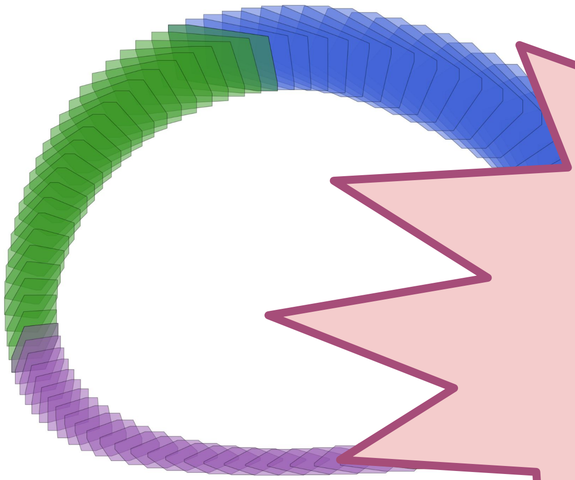
Van der pol system



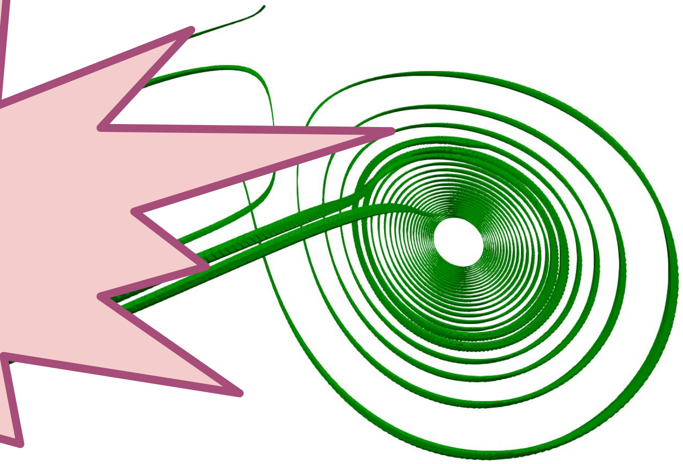
Lorenz system

Main nonlinear reachability approaches are: invariant generation, optimization based-approaches, solution-space abstractions, and state-space abstractions.

Nonlinear reachability



Open problem: nonlinear systems in high dimensions!



Van der pol system

Lorenz system

Main nonlinear reachability approaches are: invariant generation, optimization based-approaches, solution-space abstractions, and state-space abstractions.

Kronecker products, polynomial ODEs and weak nonlinearity

$$x^{\otimes 2} = x \otimes x = (x_1^2, x_1 x_2, x_2 x_1, x_2^2)^T$$

$$x^{\otimes i} := \underbrace{x \otimes \cdots \otimes x}_{i \text{ times}}, \qquad x \in \mathbb{R}^n$$

$$A \otimes B := \begin{pmatrix} a_{11}B & \dots & a_{1n}B \\ \vdots & & \vdots \\ a_{m1}B & \dots & a_{mn}B \end{pmatrix}$$

Kronecker products, polynomial ODEs and weak nonlinearity

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"linear behavior"

"nonlinear behavior"

$$\boxed{\frac{\mathrm{d}x(t)}{\mathrm{d}t} = F_1 x + F_2 x^{\otimes 2}}$$

$$\|F_2\|_2 / \|F_1\|_2$$

if this ratio is small

the system is said to be <u>weakly nonlinear</u>

Kronecker products, polynomial ODEs and weak nonlinearity

$$x^{\otimes 2} = x \otimes x = (x_1^2, x_1 x_2, x_2 x_1, x_2^2)^T$$

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"linear behavior"

"nonlinear behavior"

$$\boxed{\frac{\mathrm{d}x(t)}{\mathrm{d}t} = F_1 x + F_2 x^{\otimes 2}}$$

General for polynomial ODEs with f(0) = 0; formulation and linearization goes back to Carleman (1932)

Example: logistic equation

$$\frac{\mathrm{d}x(t)}{\mathrm{d}t} = rx(1 - x/K)$$

Bring to general quadratic form

$$x'(t) = ax(t) + bx^2(t)$$

$$a = r \text{ and } b = -r/K$$

Introduce auxiliary variables

$$\hat{y}_1' = x' = a\hat{y}_1 + b\hat{y}_2$$

$$\hat{y}_2' = 2x'x = 2a\hat{y}_2 + 2b\hat{y}_3$$

$$\hat{y}_j' = ja\hat{y}_j + jb\hat{y}_{j+1}, \qquad j \in \mathbb{N}$$

Truncate to finite order N (here: N = 4)

$$\frac{\mathrm{d}\hat{y}(t)}{\mathrm{d}t} = \begin{pmatrix} a & b & 0 & 0 \\ 0 & 2a & 2b & 0 \\ 0 & 0 & 3a & 3b \\ 0 & 0 & 0 & 4a \end{pmatrix} \hat{y}, \qquad \hat{y}(0) = \begin{pmatrix} x_0 \\ x_0^2 \\ x_0^3 \\ x_0^4 \end{pmatrix}$$

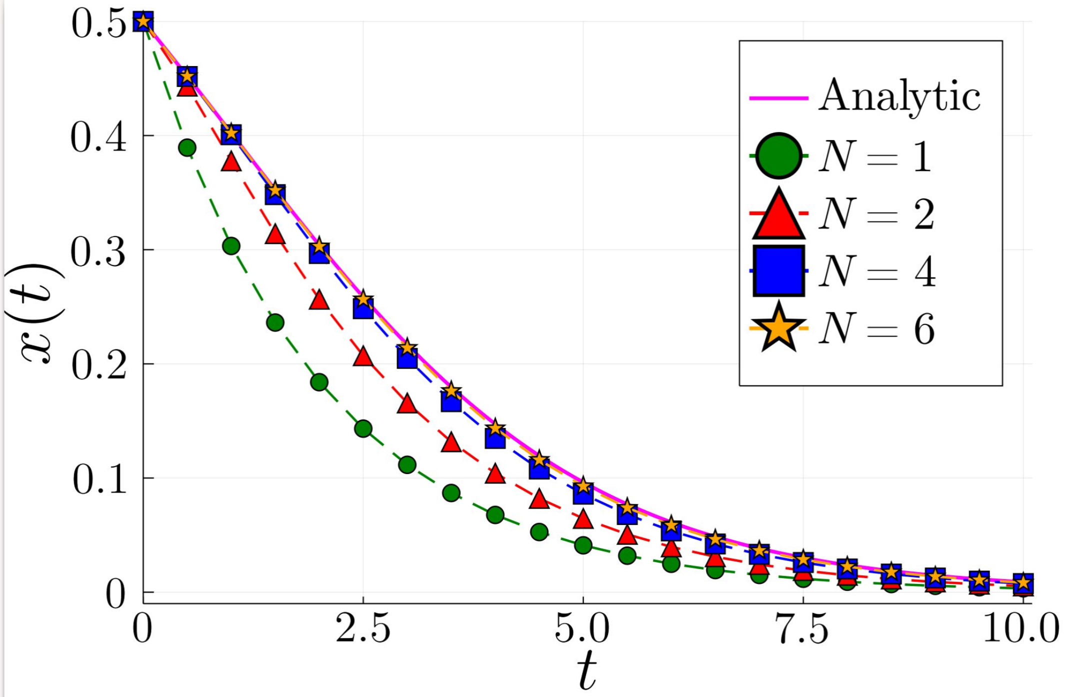
Example: logistic equation

$$\frac{\mathrm{d}\hat{y}(t)}{\mathrm{d}t} = \begin{pmatrix} a & b & 0 & 0 \\ 0 & 2a & 2b & 0 \\ 0 & 0 & 3a & 3b \\ 0 & 0 & 0 & 4a \end{pmatrix} \hat{y}, \qquad \hat{y}(0) = \begin{pmatrix} x_0 \\ x_0^2 \\ x_0^3 \\ x_0^4 \end{pmatrix}$$

The analytic solution in this case is:

$$x(t) = \frac{x_0 e^{at}}{1 + (b/a)(1 - e^{at})x_0}$$

b/a controls the "degree" of nonlinearity of the ODE



Example: logistic equation (distributed initial conditions)

$$\frac{\mathrm{d}\hat{y}(t)}{\mathrm{d}t} = \begin{pmatrix} a & b & 0 & 0 \\ 0 & 2a & 2b & 0 \\ 0 & 0 & 3a & 3b \\ 0 & 0 & 0 & 4a \end{pmatrix} \hat{y}, \qquad \hat{y}(0) = \begin{pmatrix} x_0 \\ x_0^2 \\ x_0^3 \\ x_0^4 \end{pmatrix}$$

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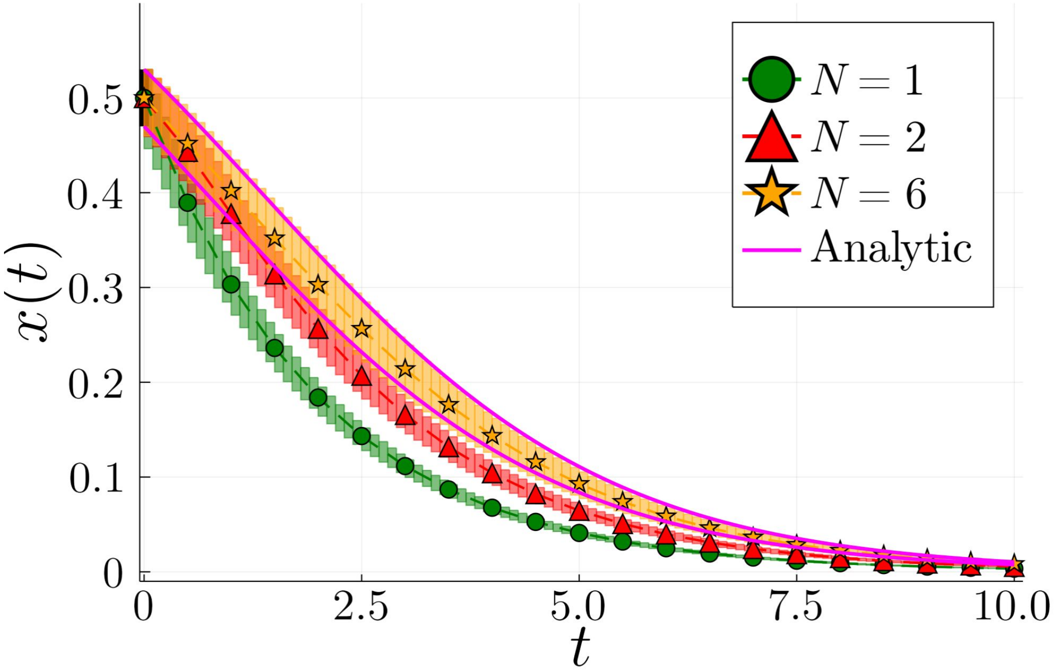


Carleman embedding: general case

$$x'(t) = f(x(t)),\ f : \mathbb{R}^n \to \mathbb{R}^n$$

Bring to general quadratic form

$$\frac{\mathrm{d}x(t)}{\mathrm{d}t} = F_1 x + F_2 x^{\otimes 2} \qquad (1)$$

Introduce auxiliary variables

$$\hat{y}_j := x^{\otimes j},\ j \in \mathbb{N}$$

Truncate to finite order N

$$A = \begin{pmatrix} A_1^1 & A_2^1 & 0 & 0 & \cdots & 0 \\ 0 & A_2^2 & A_3^2 & 0 & \cdots & 0 \\ 0 & 0 & A_3^3 & A_4^3 & 0 & \vdots \\ \vdots & \vdots & \vdots & \ddots & \ddots & 0 \\ 0 & 0 & \cdots & 0 & A_{N-1}^{N-1} & A_N^{N-1} \\ 0 & 0 & \cdots & 0 & 0 & A_N^N \end{pmatrix}$$

$$A_{i+i'-1}^i = \sum_{\nu=1}^{i} \overbrace{\mathbb{I}_n \otimes \cdots \otimes \underset{\substack{\uparrow \\ \nu\text{-th position}}}{F_{i'}} \otimes \cdots \otimes \mathbb{I}_n}^{\text{i factors}}$$

$$\boxed{\frac{\mathrm{d}\hat{y}}{\mathrm{d}t} = A\hat{y}, \qquad \hat{y}(0) = \hat{y}_0} \qquad (2)$$

Error bounds

Definition 1. *System* $\boxed{1}$ *is said to be* weakly nonlinear *if the ratio*

$$R := \frac{\|x_0\|\|F_2\|}{|\Re(\lambda_1)|} \tag{5}$$

satisfies $R < 1$.

Definition 2. *System* $\boxed{1}$ *is said to be* dissipative *if* $\Re(\lambda_1) < 0$ *(i.e., the real part of all eigenvalues is negative).*

The conditions $\Re(\lambda_1) < 0$ and $R < 1$ ensure arbitrary-time convergence.

Error bounds

Theorem 1 ([30], Corollary 1]). *Assuming that (1) is weakly nonlinear and dissipative, the error bound associated with the linearized problem (2) truncated at order N satisfies*

$$\|\eta_1(t)\| \leq \varepsilon(t) := \|x_0\| R^N (1 - e^{\Re(\lambda_1)t})^N, \tag{6}$$

with R as defined in (5). This error bound holds for all $t \geq 0$.

[30] Liu, J.P., Kolden, H.Ø., Krovi, H.K., Loureiro, N.F., Trivisa, K., Childs, A.M.:
Efficient quantum algorithm for dissipative nonlinear differential equations. Proceedings of the National Academy of Sciences 118(35) (2021)

Reachability algorithm using Carleman linearization

Algorithm 1: Reachability algorithm

Input: $\mathcal{X}_0 \subseteq \mathbb{R}^n$: hyperrectangular initial states; F_1, F_2: system matrices; N: truncation order; T: time horizon; *post*: algorithm to compute a flowpipe for linear systems

Output: flowpipe overapproximating the reachable states until T

$A, \hat{\mathcal{X}}_0 \leftarrow \mathit{linearize}(\mathcal{X}_0, F_1, F_2, N)$; // Carleman linearization

$(\mathcal{R}_0, \ldots, \mathcal{R}_m) \leftarrow \mathit{post}(y' = Ay, y(0) \in \hat{\mathcal{X}}_0)$; // flowpipe for linear system

for $j \leftarrow 0$ **to** m **do**

$\quad \varepsilon \leftarrow \mathit{error}(\mathcal{R}_j, \mathcal{X}_0, F_1, F_2, N)$; // linearization error

$\quad \mathcal{R}_j^\varepsilon \leftarrow \pi_{1:n}(\mathcal{R}_j) \oplus \mathcal{B}_\varepsilon^n$; // enlarged reach set

end

return $(\mathcal{R}_0^\varepsilon, \ldots, \mathcal{R}_m^\varepsilon)$

Numerical results: Burgers' PDE

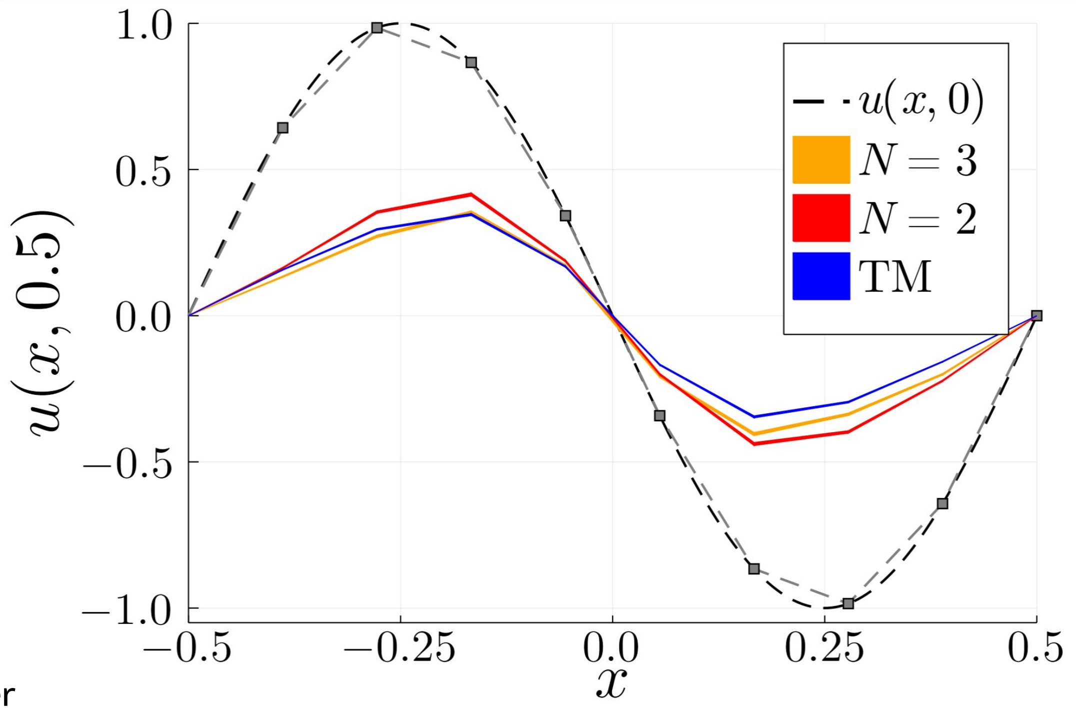
Continuous partial differential equation (space and time)

$$\partial_t u + x \partial_x u = \nu \partial_x^2 u$$

Discretize (space)

$$\partial_t u_i = \nu \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} - \frac{u_{i+1}^2 - u_{i-1}^2}{4\Delta x}$$

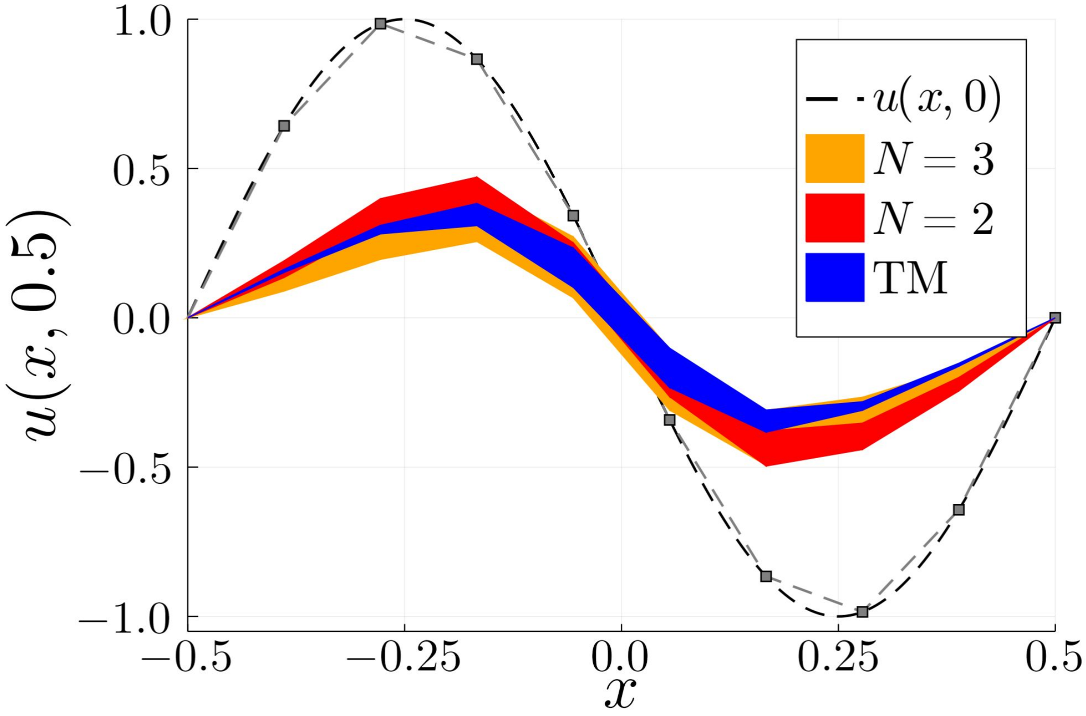
Reachability solver (integrate in time)



Numerical results: Burgers' PDE (distributed initial conditions)

$$\Re(\lambda_1) \approx -0.488 < 0$$

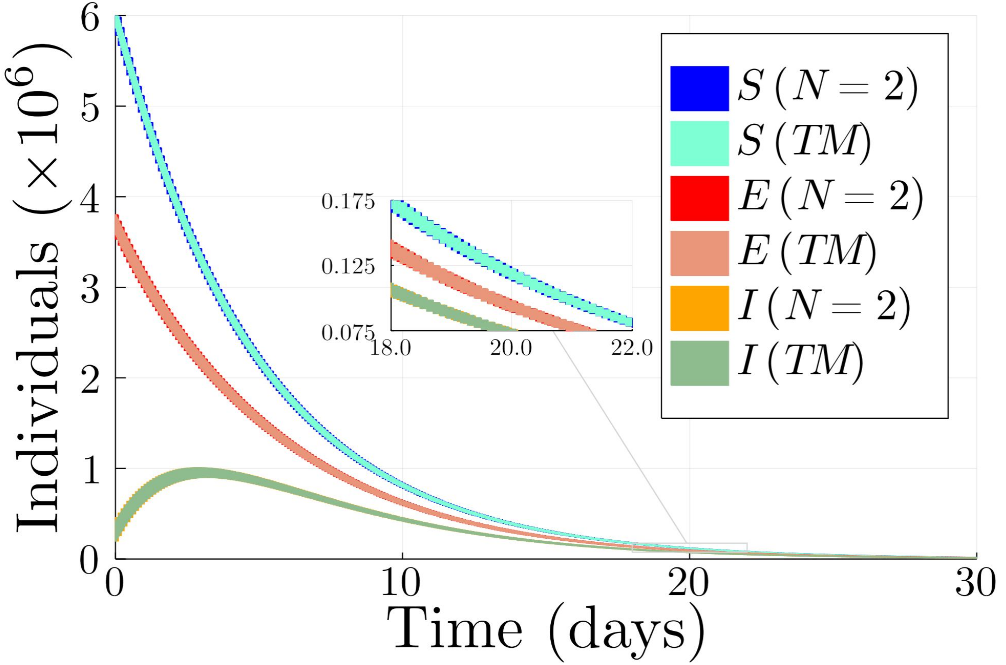
$$R \approx 18.58$$



Numerical results: Epidemic model (SEIR)

$$\frac{\mathrm{d}P_S}{\mathrm{d}t} = -\Lambda\frac{P_S}{P} - r_{\mathrm{vac}}P_S - r_{\mathrm{tra}}P_S\frac{P_I}{P} + \Lambda$$
$$\frac{\mathrm{d}P_E}{\mathrm{d}t} = -\Lambda\frac{P_E}{P} - \frac{P_E}{T_{\mathrm{lat}}} + r_{\mathrm{tra}}P_S\frac{P_I}{P}$$
$$\frac{\mathrm{d}P_I}{\mathrm{d}t} = -\Lambda\frac{P_I}{P} + \frac{P_E}{T_{\mathrm{lat}}} - \frac{P_I}{T_{\mathrm{inf}}}$$
$$\frac{\mathrm{d}P_R}{\mathrm{d}t} = -\Lambda\frac{P_R}{P} + r_{\mathrm{vac}}P_S + \frac{P_I}{T_{\mathrm{inf}}}$$

Data from the early spread of the COVID-19 disease from [P20]



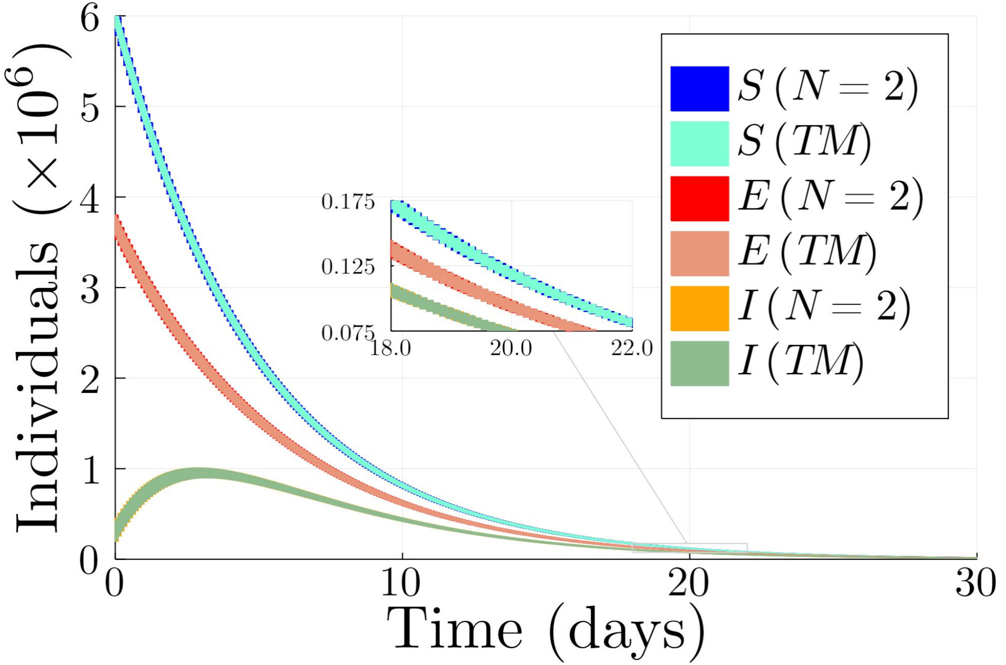
[P20] Pan, A. et al: Association of Public Health Interventions With the Epidemiology of the COVID-19 Outbreak in Wuhan, China. JAMA 323(19), 1915–1923 (2020)

Numerical results: Epidemic model (SEIR)

$$F_1 = \begin{pmatrix} -\frac{\Lambda}{P} - r_{\text{vac}} & 0 & 0 \\ 0 & -\frac{\Lambda}{P} - \frac{1}{T_{\text{lat}}} & 0 \\ 0 & \frac{1}{T_{\text{lat}}} & -\frac{\Lambda}{P} - \frac{1}{T_{\text{inf}}} \end{pmatrix}$$

$$F_2 = \begin{pmatrix} 0 & 0 & -\frac{r_{\text{tra}}}{P} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{r_{\text{tra}}}{P} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$R \approx 0.68 \text{ and } \Re(\lambda_1) \approx -0.19$$



[P20] Pan, A. et al: Association of Public Health Interventions With the Epidemiology of the COVID-19 Outbreak in Wuhan, China. JAMA 323(19), 1915–1923 (2020)

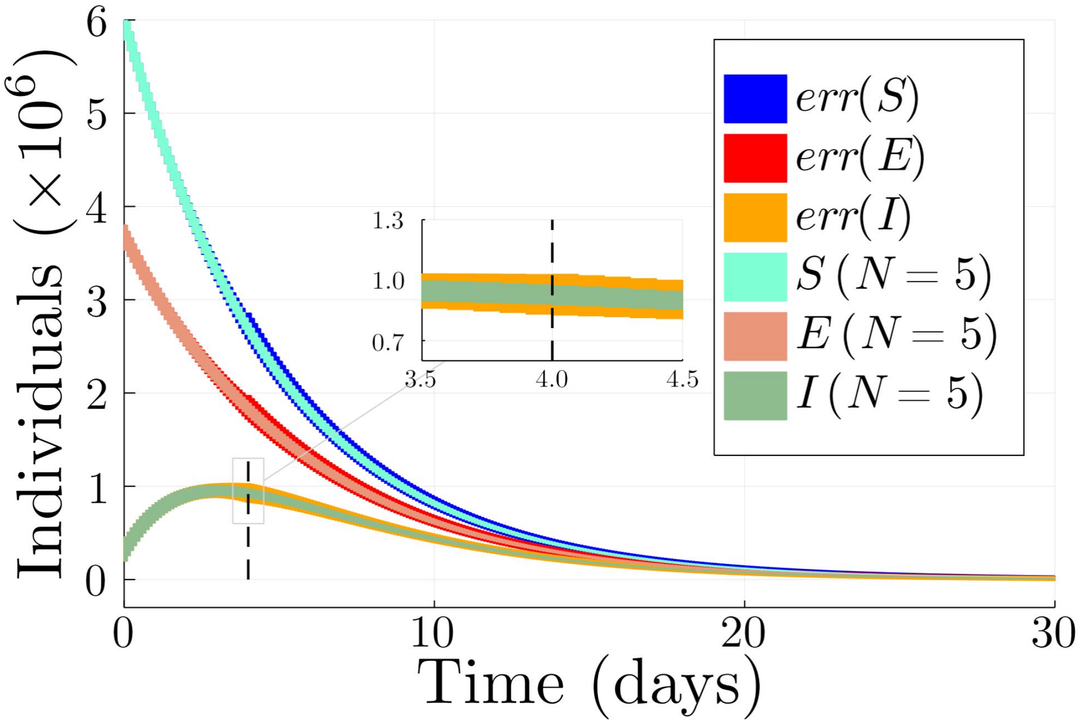
Numerical results: Run-time comparison

	SEIR model		Burgers model	
	no error bound	incl. error bound	initial point	initial set
TM	6.14 s		0.88 s	0.91 s
Carleman	$N = 2$: 0.006 s	$N = 5$: 0.185 s	$N = 2$: 0.0065 s $N = 3$: 0.24 s	$N = 2$: 0.0067 s $N = 3$: 0.29 s

Table 1: Run times for the SEIR model and the Burgers model obtained for the Taylor-model (TM) approach and the Carleman linearization with different truncation orders N.

Idea: time-triggered resets

$$\|\eta_1(t)\| \leq \varepsilon(t) := \|x_0\| R^N (1 - e^{\Re(\lambda_1)t})^N$$



Problem: correction including error term may not converge to zero, even if the true solution does

Idea: re-evaluate the error term at times t* > 0 => reduce error estimate

Question (open): Auomate / optimize when resets happen

Conclusions

We presented a novel reachability method for polynomial ODEs that can leverage established and well-optimized **high-dimensional reachability solvers**

Technique: abstract nonlinear terms into a higher-dimensional space such that the evolution is **approximately linear**

Outperforms other state-of-the-art methods in the set of examples, but requires **weak nonlinearity** and **dissipativity** (for guaranteed bounds)

Still, if the assumptions do not hold, the method returns **relatively good results** (but without guaranteed bounds)

Ideas for possible extensions

Consider time-varying matrices instead of fixed matrices.

Automation of the time-triggered process

How often and when to apply the resets?

Algorithmic specialization for Kronecker products, e.g. Krylov subspace iteration

Can we exploit the structure of the *linearized system*?

Automation and specialization of the quadratic formulation [BP21]

[BP21] Bychkov, Andrey, and Gleb Pogudin. "Optimal monomial quadratization for ODE systems." *ACM Communications in Computer Algebra* 54.3 (2021): 119-123.