Reachable Sets of Homogeneous Polynomial Dynamical Systems Using Exact Solutions

Soham Sachin Purohit, Can Chen, and Ram Vasudevan

***Abstract*—Reachability analysis is a powerful tool to analyze the behavior of dynamical systems. Typically, these tools are used to evaluate whether the dynamics of a system beginning from some initial set reaches some unsafe region of state space in a finite amount of time. To answer this question, these tools often construct over-approximations to the reachable sets of the dynamical systems, which can be overly conservative when applied to arbitrary systems. To address this challenge, this letter develops a novel technique for reachability analysis of Homogeneous Polynomial Dynamical Systems (HPDSs) by computing their exact solutions using tensor theory. In addition, this letter illustrates how to build tight over-approximations of the reachable set for HPDSs with constant control inputs. Simulation results highlight a significant improvement in the accuracy of reachable set estimates compared to established methods for HPDSs.**

***Index Terms*—Reachability analysis, outer approximation, HPDSs, exact solutions, tensor algebra.**

I. Introduction

HOMOGENEOUS polynomial dynamical systems (HPDSs) represent a special class of mathematical models that find widespread applications in scientific and engineering domains [14]. These systems are characterized by polynomial functions where all monomials have the same degree. HPDSs describe complex phenomena in systems biology, chemical reactions, and epidemiological models [8], [9]. For instance, gene regulatory networks can be modeled by a system of homogeneous polynomial equations, capturing the interactions among genes [11].

This letter is interested in determining whether a dynamical model reaches an unsafe state in a finite time when starting from a user-specified set of initial states. To assess the safety of such systems, one can apply reachability analysis, which involves determining the reachable set of a system from its initial set. Safety is guaranteed for a given initial set if no unsafe state belongs to the corresponding reachable set.

Although general methods exist for performing reachability analysis of dynamical systems [3], [4], [10], [13], they can be overly conservative. To address this issue, this letter proposes a novel method for computing a tight over-approximative reachable set for a class of Homogeneous Polynomial Dynamical Systems (HPDSs) that can be represented as orthogonally decomposable tensors. We refer to this class of systems as odeco HPDSs. We exploit properties of the exact solutions of odeco HPDSs that enable us to determine the reachable sets effectively. We demonstrate that the result can be generalized to general (non-odeco) HPDSs that can be linearly transformed to odeco HPDSs under certain conditions. We further illustrate the utility of our method by taking an example of an autocatalytic reaction, in which products of a chemical reaction catalyze the reaction. Through all our simulations, the reachable sets constructed by our method are shown to be less conservative than the results of existing tools for reachability analysis when applied to odeco HPDSs. The key contributions of this letter are listed as follows.

1) A pair of algorithms for determining the reachable sets of odeco HPDSs and odeco HPDSs with constant control, considering both axis-aligned and general initial sets.
2) An algorithm for determining the reachable sets of certain general (non-odeco) HPDSs, considering both axis-aligned and general initial sets.
3) A comparison of our algorithms with Continuous Reachability Analyzer (CORA) [3], an established tool for reachability analysis of dynamical systems.

This letter is organized as follows: Section II introduces necessary mathematical concepts and previous results. In Section III, we present the algorithms for determining the reachable sets of odeco HPDSs, odeco HPDSs with constant control, and certain general (non-odeco) HPDSs. The results of the proposed algorithms are shown in Section IV. We conclude with future directions in Section V.

II. Preliminaries

This section provides a concise overview of solutions for odeco HPDSs (without/with constant control), outer approximation techniques, and zonotope representations. Throughout this letter, scalars are represented by regular lowercase characters, vectors by bold lowercase characters, matrices by

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bold uppercase characters, and tensors by script uppercase characters.

A. Solutions of Odeco HPDSs

Here, we first introduce the idea of an odeco HPDS and its explicit solution. The properties of this solution will be exploited later in this letter to obtain reachable sets.

Every n-dimensional HPDS of degree $k-1$ can be written as tensor-vector multiplications along the first $k-1$ modes [6], [7], i.e.,

$$\dot{\mathbf{x}} = \mathcal{A} \times_1 \mathbf{x} \times_2 \cdots \times_{k-1} \mathbf{x} = \mathcal{A}\mathbf{x}^{k-1}, \quad (1)$$

where $\mathcal{A} \in \mathbb{R}^{n\times n\times\cdots\times n}$ is the dynamic tensor of order k, symmetric along the first $k-1$ modes, and $\mathbf{x} \in \mathbb{R}^n$ is the state. Here, the tensor-vector multiplication along mode r is defined as

$$(\mathcal{A} \times_r \mathbf{x})_{i_1 i_2,\ldots,i_{r-1} i_{r+1},\ldots,i_k} = \sum_{i_r=1}^{n} \mathcal{A}_{i_1 i_2,\ldots,i_k} \mathbf{x}_{i_r}. \quad (2)$$

The dynamic tensor $\mathcal{A}$ is said to be orthogonally decomposable (odeco) if it is supersymmetric (invariant under any permutation of the indices) and can be written as a sum of the outer products of orthonormal vectors, i.e.,

$$\mathcal{A} = \sum_{r=1}^{n} \lambda_r \mathbf{v}_r \circ \mathbf{v}_r \circ \cdots \circ \mathbf{v}_r, \quad (3)$$

where λ_r are the Z-eigenvalues of $\mathcal{A}$ in a descending order, and $\mathbf{v}_r$ are the corresponding Z-eigenvectors [12].

If $\mathcal{A}$ is odeco, we refer to (1) to as odeco HPDSs. In [6, Proposition 1], it was shown that given the initial condition $\mathbf{x}_0 = \sum_{r=1}^{n} \alpha_r \mathbf{v}_r$, the system has an explicit solution, which can be computed as

$$\mathbf{x}(t) = \sum_{r=1}^{n} \Big(1 - (k-2)\lambda_r \alpha_r^{k-2} t\Big)^{-\frac{1}{k-2}} \alpha_r \mathbf{v}_r. \quad (4)$$

B. Solutions of Odeco HPDSs With Constant Control

We introduce the implicit solution of an odeco HPDS with constant control. Later, we show that the properties of this solution can be used to obtain reachable sets of these systems. The odeco HPDS with constant control can be written in the form of

$$\dot{\mathbf{x}} = \mathcal{A}\mathbf{x}^{k-1} + \mathbf{b}, \quad (5)$$

where $\mathbf{b} \in \mathbb{R}^n$ is a constant vector. In [6, Proposition 4], it was shown that given the initial condition $\mathbf{x}_0 = \sum_{r=1}^{n} \alpha_r \mathbf{v}_r$, the system has a solution $\mathbf{x}(t) = \sum_{r=1}^{n} c_r(t)\mathbf{v}_r$, which can be obtained by solving the following implicit equations:

$$t = -\frac{g\Big(\frac{k-2}{k-1}, -\frac{\tilde{b}_r}{\lambda_r c_r(t)^{k-1}}\Big)}{(k-2)\lambda_r c_r(t)^{k-1}} + \frac{g\Big(\frac{k-2}{k-1}, -\frac{\tilde{b}_r}{\lambda_r \alpha_r(t)^{k-1}}\Big)}{(k-2)\lambda_r \alpha_r(t)^{k-1}}. \quad (6)$$

Here, $\tilde{b}_r$ are the rth entries of $\mathbf{V}^\top \mathbf{b}$ ($\mathbf{V}$ contains all the vectors $\mathbf{v}_r$) and $g(\cdot,\cdot)$ is the specified Gauss hypergeometric function defined as

$$g(a, z) = {}_2F_1(1, a; a+1; z) = a \sum_{m=0}^{\infty} \frac{z^m}{a+m}. \quad (7)$$

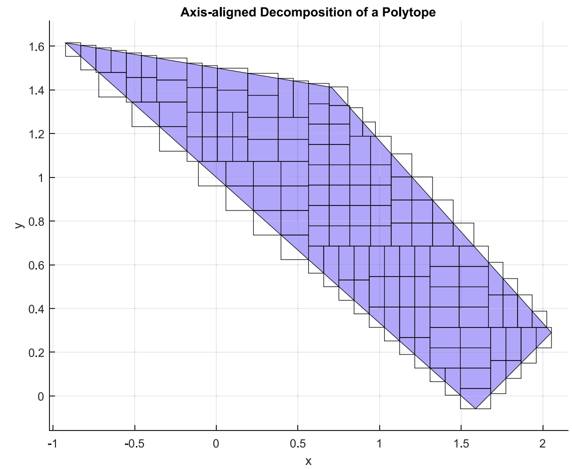

Fig. 1. Outer approximation of a polytope using axis-aligned sets. The blue region is the projection of the polytope on the X-Y plane, and the squares represent the projections of the axis-aligned boxes that over-approximate the polytope.

C. Outer Box Approximation of Polytopes

We discuss the idea of overapproximating a polytope using axis-aligned hyperboxes here. Later, we demonstrate the existence of an elegant method for determining reachable sets of axis-aligned initial sets that can be extended to general initial sets by conducting over-approximative axis-aligned decompositions of general initial sets.

We utilize the recursive algorithm [5, Algorithm 6] for computing the outer approximation of polytopes. This algorithm decomposes a polytope into axis-aligned sets with volumes below a specified threshold $\mathcal{E}$. An illustrative example is highlighted in Fig. 1.

D. Zonotope Representation of Sets

We represent all initial as well as reachable sets in this letter as zonotopes. Zonotopes provide a convenient approach for representing sets, which facilitates ease in performing operations on them [2]. A zonotope is defined as

$$Z = \{\mathbf{x} \in \mathbb{R}^n : \mathbf{x} = \mathbf{c} + \sum_{r=1}^{p} \gamma_r \mathbf{g}_r, \quad -1 \le \gamma_r \le 1\}$$

with $\mathbf{c}, \mathbf{g}_1, \mathbf{g}_2, \ldots, \mathbf{g}_p \in \mathbb{R}^n$, where $\mathbf{c}$ is known as the center of the zonotope and $\mathbf{g}_r$ are called the generators.

III. Methods

In this section, we perform the reachability analysis of HPDSs and HPDSs with constant control by leveraging their exact solutions. The code repository for the implementation of our methods can be found at [1].

A. Reachable Sets of Odeco HPDSs

We first consider an initial set that is axis-aligned with the orthonormal Z-eigenvectors $\mathbf{v}_r$ of $\mathcal{A}$. If this set is represented as a zonotope, its generators would also align with these Z-eigenvectors. Let $\mathbf{g}_r$ denote a generator along the Z-eigenvector $\mathbf{v}_r$. Suppose that all points in the zonotope can be expressed as $\mathbf{x}_0 = \sum_{r=1}^{n} \alpha_r \mathbf{v}_r$. Since the set is axis-aligned,

Algorithm 1 Reachable Sets of odeco HPDSs for Axis-Aligned Initial Sets

for each generator $\mathbf{g}_r$ **do**
  $\boldsymbol{\alpha} \leftarrow \mathbf{V}^\top(\mathbf{c}+\mathbf{g}_r)$
  $\boldsymbol{\beta} \leftarrow \mathbf{V}^\top(\mathbf{c}-\mathbf{g}_r)$
  rsbound1 $\leftarrow (1-(k-2)\lambda_r \boldsymbol{\alpha}[r]^{k-2}t)^{-\frac{1}{k-2}} \boldsymbol{\alpha}[r]$
  rsbound2 $\leftarrow (1-(k-2)\lambda_r \boldsymbol{\beta}[r]^{k-2}t)^{-\frac{1}{k-2}} \boldsymbol{\beta}[r]$
  rs_center[r] $\leftarrow 0.5\times$(rsbound1 + rsbound2)
  rs_gen[r] $\leftarrow 0.5\times$(rsbound1 − rsbound2)$\mathbf{V}^\top \mathbf{g}_r$
end for
RS $\leftarrow$ Zonotope{$\mathbf{V}\times$rs_center, $\mathbf{V}\times$rs_gen}

the maximum and minimum values of α_r over all the points in the zonotope can be computed as the rth components of $\mathbf{c}+\mathbf{g}_r$ and $\mathbf{c}-\mathbf{g}_r$, respectively, where $\mathbf{c}$ is the center of the initial set.

Lemma 1: Assume that $\mathcal{A}$ is odeco. Let $\mathbf{x}_1(t) = \sum_{r=1}^n a_r(t)\mathbf{v}_r$ be the solution of (1) for the initial condition $\mathbf{x}_0 = \sum_{r=1}^n \alpha_r \mathbf{v}_r$ and $\mathbf{x}_2(t) = \sum_{r=1}^n b_r(t)\mathbf{v}_r$ be the solution with the initial condition $\mathbf{x}_0 = \sum_{r=1}^n \beta_r \mathbf{v}_r$. If $\alpha_r > \beta_r$ for some $r \in [1, n]$, then $b_r(t) > a_r(t)$ for all t.

Proof: According to (4):

$$a_r(t) = \Big(1-(k-2)\lambda_r \alpha_r^{k-2} t\Big)^{-\frac{1}{k-2}} \alpha_r, \tag{8}$$

which can be simplified to

$$a_r(t) = (\alpha_r - (k-2)\lambda_r t)^{-\frac{1}{k-2}}. \tag{9}$$

One can apply a similar argument for $b_r(t)$. If $\alpha_r > \beta_r$, then

$$(\alpha_r - (k-2)\lambda_r t)^{-\frac{1}{k-2}} < (\beta_r - (k-2)\lambda_r t)^{-\frac{1}{k-2}}. \tag{10}$$

Therefore, $b_r(t) > a_r(t)$ for all t. ∎

According to Proposition 1, the system's state at time t is ordered based on the values of the initial state. Therefore, to compute the reachable set of an initial set with axes aligned to the Z-eigenvectors, it suffices to determine the values of the state for initial points $\mathbf{x}_0 = \mathbf{c} \pm \mathbf{g}_r$ as these values bound all other points. Given that the generators are finite, we can determine the reachable set.

We demonstrate the computation of the reachable set for an initial set represented as a zonotope and axis-aligned with the Z-eigenvectors of $\mathcal{A}$ in Algorithm 1. We assume that our reference frame is initially aligned with the axes defined by the Z-eigenvectors of $\mathcal{A}$ and subsequently reorient this frame back to the standard coordinate axes by multiplying $\mathbf{V}$ to the center and generators of the calculated reachable set. In the algorithm, $\mathbf{c}$ and $\mathbf{g}_r$ represent the center and generators of the initial zonotope, respectively. $\boldsymbol{\alpha}[r]$ and $\boldsymbol{\beta}[r]$ denote the rth component of vectors $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$, respectively. rs_center[r] and rs_gen[r] represent the rth component of the center and generator of the reachable set at time t, respectively. $\mathbf{V}$ is the matrix containing the Z-eigenvectors of $\mathcal{A}$.

By employing Algorithm 1, one can compute the reachable set for an axis-aligned initial set. One can extend this algorithm to a general initial set by performing an axis-aligned set decomposition of the initial set mentioned earlier and treating each hyperbox obtained from this decomposition as an independent axis-aligned initial set, see Algorithm 2.

Algorithm 2 Reachable Sets of odeco HPDSs for General Initial Sets

boxes $\leftarrow$ decomposition(initial set, $\mathcal{E}$)
for each b_r in boxes **do**
  box_RS[r] $\leftarrow$ reachable_set_axis-aligned(b_r)
end for
RS $\leftarrow \cup_{r=1}^M$ box_RS[r]

Here, $\mathcal{E}$ represents the volume threshold for the decomposition and M represents the total number of boxes obtained in the decomposition of the general initial set. When $\mathcal{E} \to 0$, the union of the generated axis-aligned sets tends to the original set. For our methods, choosing $\mathcal{E}$ four orders of magnitude smaller than the initial set is sufficient, as will be demonstrated in Section IV. box_RS[r] represents the reachable set of the rth hyperbox in the decomposition of the initial set. By calculating the outer-bound box approximations of sets, the union operation provides the outer approximations of the reachable sets, ensuring safety.

B. Reachable Sets of odeco HPDSs With Constant Controls

We demonstrate that the ordering properties, similar to the zero control case, persist for the solution of the constant control case. This is utilized to determine the reachable sets using a finite number of points.

Lemma 2: The following function

$$f(\alpha) = \frac{g\Big(\frac{k-2}{k-1}, \frac{-\tilde{b}}{\lambda\alpha^{k-2}}\Big)}{(k-2)\lambda\alpha^{k-2}} \tag{11}$$

is monotonic for constant $k \geq 3, \tilde{b}, \lambda$.

Proof: Consider $zg(a, z)$ with $0 < a < 1$

$$zg(a, z) = az \sum_{m=0}^{\infty} \frac{z^m}{a+m}, \tag{12}$$

and

$$\frac{\partial}{\partial z}\Big(zg(a, z)\Big) = a \sum_{m=0}^{\infty} \frac{(m+1)z^m}{a+m}. \tag{13}$$

When $z \geq 0$, the partial derivative is greater than 0 since all terms in the summation are positive. When $z < 0$, consider two successive terms in the summation

$$\frac{2k+1}{a+2k}z^{2k} + \frac{2k+2}{a+2k+1}z^{2k+1}. \tag{14}$$

We know that since $0 < a < 1$,

$$\frac{2k+1}{a+2k} > 1 \implies \frac{2k+1}{a+2k} > \frac{2k+2}{a+2k+1}. \tag{15}$$

Further, $g(a, z)$ is defined for $|z| < 1$, hence, $|z^{2k}| > |z^{2k+1}|$. Hence,

$$\left|\frac{2k+1}{a+2k}z^{2k}\right| > \left|\frac{2k+2}{a+2k+1}z^{2k+1}\right|. \tag{16}$$

This implies that every pair of terms adds to a positive number in the summation. Thus, $zg(a, z)$ increases in z.

Algorithm 3 Reachable Sets of odeco HPDSs With Constant Input for Axis-Aligned Initial Sets

for each generator $\mathbf{g}_r$ **do**
  $\boldsymbol{\alpha} \leftarrow \mathbf{V}^\top(\mathbf{c}+\mathbf{g}_r)$
  $\boldsymbol{\beta} \leftarrow \mathbf{V}^\top(\mathbf{c}-\mathbf{g}_r)$
  rsbound1 $\leftarrow$ solve for x in $t = f_r(\boldsymbol{\alpha}[r]) - f_r(x)$
  rsbound2 $\leftarrow$ solve for x in $t = f_r(\boldsymbol{\beta}[r]) - f_r(x)$
  rs_center[r] $\leftarrow$ 0.5×(rsbound1 + rsbound2)
  rs_gen[r] $\leftarrow$ 0.5×(rsbound1 - rsbound2)$\mathbf{V}^\top\mathbf{g}_r$
end for
RS $\leftarrow$ Zonotope{$\mathbf{V}$×rs_center, $\mathbf{V}$×rs_gen}

Notice that $f(\alpha)$ is $c\alpha z_1 g(a, z_1)$ where c is a constant and $z_1 = -\frac{\tilde{b}}{\lambda\alpha}$. Further, α and $z_1 g(a, z_1)$ are monotonic in α when the other variables are constant. The product of two monotonic functions is monotonic if and only if they have the same sign. Because both α and $z_1 g(az_1)$ are positive and negative in the left and right half-planes respectively, their product is monotonic. ■

Lemma 3: Let $\mathbf{x}_1(t) = \sum_{r=1}^n a_r(t)\mathbf{v}_r$ be the solution of (5) for the initial condition $\mathbf{x}_0 = \sum_{r=1}^n \alpha_r\mathbf{v}_r$ and $\mathbf{x}_2(t) = \sum_{r=1}^n b_r(t)\mathbf{v}_r$ be the solution with $\mathbf{x}_0 = \sum_{r=1}^n \beta_r\mathbf{v}_r$ as the initial condition. If $\alpha_r, \beta_r \neq 0$, $\alpha_r > \beta_r$ and $f(\alpha_r) - t, f(\beta_r) - t$ have the same sign for $t \in [0, T]$ some $r \in [1, n]$, then $a_r(t) > b_r(t)$ for all $t \in [0, T]$.

Proof: In Lemma 2, we proved that the function $f(\alpha)$ is monotonic. We can also see that $f(\alpha)$ is undefined at $\alpha = 0$. The solution to (5) can be found by solving for c for each component of the vector, the implicit equation $f(\alpha_i) - t = f(c_i)$. If the function is monotonically decreasing, then

$$\alpha_r > \beta_r \implies f(\alpha_r) - t < f(\beta_r) - t \implies f(a_r) < f(b_r) \quad (17)$$

Hence, $a_r(t) > b_r(t)$ since f is decreasing. If the function is monotonically increasing, then

$$\alpha_r > \beta_r \implies f(\alpha_r) - t > f(\beta_r) - t \implies f(a_r) > f(b_r) \quad (18)$$

Hence, $a_r(t) > b_r(t)$ using the fact that f is monotonically increasing. In both cases, $a_r(t) > b_r(t)$ for all t. ■

As outlined in Lemma 1, we establish an order among the solution values based on the initial condition values. Additionally, we introduce a criterion on $f(\alpha_r) - t$ and $f(\beta_r) - t$ having the same sign to ensure that no point in the reachable set is undefined. We can once again leverage the concept of using a rotated frame aligned with the Z-eigenvectors of $\mathcal{A}$ to evaluate the reachable set of the system, followed by a rotation of the reachable set to obtain results in our standard coordinate frame. This leads us to the following algorithm (Algorithm 3).

As before, define $\mathbf{c}$ and $\mathbf{g}_r$ as the center and generators of the initial zonotope, respectively. $\boldsymbol{\alpha}[r]$ and $\boldsymbol{\beta}[r]$ denotes the rth component of vectors $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ respectively. rs_center[r] and rs_gen[r] represent the rth component of the center and generator of the reachable set at time t, respectively. $\mathbf{V}$ is the matrix containing the Z-eigenvectors of $\mathcal{A}$. Furthermore, we define the following function:

$$f_r(x) = \frac{g\left(\frac{k-2}{k-1}, -\frac{b_r}{\lambda_r x^{k-1}}\right)}{(k-2)\lambda_r x^{k-1}}. \quad (19)$$

Algorithm 4 Reachable Sets of odeco HPDSs With Constant Input for General Initial Sets

boxes $\leftarrow$ decomposition(initial set, $\mathcal{E}$)
for each b_i in boxes **do**
  box_RS[r] $\leftarrow$ rs_axis-aligned_with_control(b_r)
end for
RS $\leftarrow \cup_{r=1}^M$ box_RS[r]

Algorithm 5 Reachable Sets of General HPDSs

IS_y $\leftarrow \mathbf{P}^{-1}$(IS)
RS_y $\leftarrow$ reachable_set_non_axis-aligned(IS_y)
RS $\leftarrow$ $\mathbf{P}$RS_y

Note that we use b_r instead of $\tilde{b}_r$ since $\tilde{b}_r$ becomes b_r in the frame with the Z-eigenvectors as the axes. Similar to the approach adopted for odeco HPDSs, we suggest employing axis-aligned box decomposition to determine the reachable sets of general initial sets and propose the following algorithm (Algorithm 4).

C. Reachable Sets of Non-odeco HPDSs

As mentioned earlier, every HPDS can be represented by a tensor $\mathcal{A}$ of order k that is symmetric along its first $k-1$ modes. These tensors are called almost symmetric and can be decomposed as

$$\mathcal{A} = \sum_{r=1}^{n} \mathbf{v}_r \circ \mathbf{v}_r \circ \cdots \circ \mathbf{v}_r \circ \mathbf{v}_r^{(f)} \quad (20)$$

It was shown in [6, Proposition 6] that if there exists an invertible linear transform $\mathbf{P}$ and diagonal matrix Λ such that $\mathbf{P}^\top\mathbf{V}$ is orthogonal and $\mathbf{P}^\top\mathbf{V} = \mathbf{P}^{-1}\mathbf{V}^{(f)}\Lambda^{-1}$, where $\mathbf{V}$ and $\mathbf{V}^{(f)}$ contain $\mathbf{v}_r$ and $\mathbf{v}_r^{(f)}$ respectively, then the non-odeco HPDS $\dot{\mathbf{x}} = \mathcal{A}\mathbf{x}^{k-1}$ can be transformed to $\dot{\mathbf{y}} = \tilde{\mathcal{A}}\mathbf{y}^{k-1}$ where $\tilde{\mathcal{A}}$ is an odeco-tensor and $\mathbf{x}(t) = \mathbf{P}\mathbf{y}(t)$.

This result is used to determine the reachable sets for general HPDSs that satisfy the above conditions. We transform the state tensor $\mathcal{A}$ to its transformed odeco HPDS $\tilde{\mathcal{A}}$ by finding the matrices $\mathbf{P}$, $\mathbf{V}$, $\mathbf{V}^{(f)}$ and Λ. We use Algorithm 5 to find the reachable sets of these systems. IS represents the initial set defined for the original system.

The linear transformation $\mathbf{P}$ does not always exist. Nevertheless, we can find an approximated tensor close to the target tensor for which $\mathbf{P}$ exists [6, Algorithm 6]. Additionally, $\mathbf{P}$ can be computed from the CANDECOMP/PARAFAC decomposition factor matrix of the approximated tensor. The CANDECOMP/PARAFAC decomposition can be achieved using nonlinear least squares, which is often efficient for small- and medium-sized tensors. However, for large-sized tensors, the computational burden can be substantial.

These algorithms enable us to over-approximate the reachable sets of odeco HPDSs both with and without constant control. The level of over-approximation can be adjusted by tuning the value of $\mathcal{E}$ in the box decompositions of non-axis-aligned initial sets, as this is the only approximation made in our algorithm. This provides us with control over the trade-off

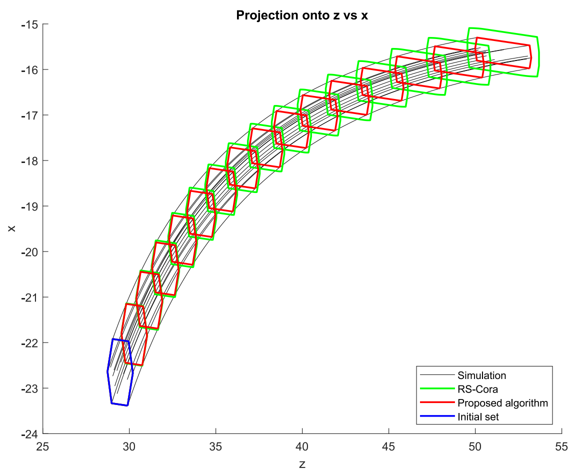

Fig. 2. Projection of the reachable sets on the X-Z plane for odeco HPDS generated by Algorithm 1 and CORA.

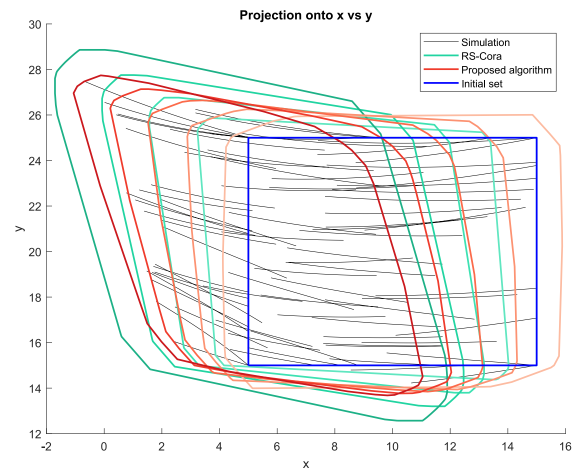

Fig. 3. Projection of the reachable sets on the X-Y plane for odeco HPDS with constant control generated by Algorithm 4 and CORA.

between the accuracy of the solution and the computational time required.

IV. Results

We simulated a variety of odeco-HPDS with and without control over a range of state-space dimensions and evolution times. For each simulation, we noted the volumes of the reachable set generated by CORA and the reachable set generated by our method. We observed a significant improvement that scaled up with both the system's dimension and the evolution time. As a proxy to the ground truth reachable set, we randomly initialized and integrated points within the initial set according to system dynamics. The accuracy of our method was validated by ensuring that the terminal states of these simulations lay within the reachable set generated by our method for all initial points.

A. Simulation Results

We demonstrate our method through the following examples. In the first example, we simulated an axis-aligned 3-dimensional odeco-HPDS with no control over 15 timesteps. As this set is already aligned with the Z-eigenvectors of the state tensor, there was no need to conduct box decomposition of the initial set, and we could directly utilize Algorithm 1. The projections of the simulation on the X-Z plane are shown in Fig. 2.

In the second example, we considered an odeco-HPDS with constant control. The initial set we considered is a $5 \times 5 \times 5$ box centered at $(10, 20, 30)$. This set is not aligned to the Z-eigenvectors of the state tensor, so we used Algorithm 4 to compute the reach set. We set a threshold of $\mathcal{E} = 0.1$ for the box decomposition of the initial set and simulated over 5 timesteps. CORA overapproximated the volume by a factor of 1.94 even with such a low-resolution box decomposition, validating our method. As mentioned in Section III-B, odeco-HPDS with constant controls have a singularity. There was a significant propagation of errors in CORA that led to a reachable set explosion, preventing us from comparing our method for longer evolution times. Results are displayed in Fig. 3.

B. Performance Comparison

We tested our methods against CORA for several high-dimensional systems and for different evolution times (represented as timesteps). CORA performs poorly on these systems, as is seen from the results in Table I. There is a significant difference in the volumes generated that increases with the dimension of the system and the timesteps. Eventually, CORA fails because the propagated errors cause the reachable set to grow unbounded, which is represented using **RSE** (reachable set explosion). CORA fails at smaller evolution times for larger dimensional systems and does not work at all for systems greater than 10 dimensions. Our methods continue to give results that closely match the random simulations.

We parallelized and ran our experiments using 8 cores of an AMD Ryzen 7 5800H processor. The simulation runtimes are reported in Table II. Algorithms 1 and 3 require less computational time than CORA. Algorithm 4 requires a nonlinear solver to find a root of (6) for each box in the decomposition, which leads to a larger computational time. In Algorithm 2, the primary contribution to the computational time is the recursive box-decomposition algorithm [5, Algorithm 6]. Based on these results, our methods often represent the sole feasible approach for determining reachable sets in systems exceeding 10 dimensions or longer evolution times.

C. Autocatalytic Reactions

Autocatalytic reactions are chemical reactions in which the product acts as a catalyst in the reaction to produce more of itself. These reactions find widespread use in the study of evolution and biochemistry. In this example, we considered a chained autocatalytic reaction in which S acts as a catalyst to convert R into S through the following reversible reaction:

$$2\mathrm{R} \rightleftharpoons \mathrm{R} + \mathrm{S} \rightleftharpoons 2\mathrm{S}.$$

The kinetics of this reaction can be represented as

$$\begin{cases} [\dot{R}] = -0.0419[R]^2 + 0.075[R][S] - 0.0915[S]^2 \\ [\dot{S}] = 0.0435[R]^2 - 0.212[R][S] + 0.1938[S]^2 \end{cases},$$

where $[R]$ and $[S]$ represent the concentrations of the species R and S, respectively.

TABLE I
VOLUMES OF REACHABLE SETS FOR SYSTEMS WITH DIFFERENT DIMENSIONS. RSE REPRESENTS FAILURE DUE TO A REACHABLE SET EXPLOSION

Dimension	5 timesteps		10 timesteps		15 Timesteps		30 Timesteps	
	Proposed Method	CORA	Proposed Method	CORA	Proposed Method	CORA	Proposed Method	CORA
3	**26.53**	51	**9.14**	24	**3.28**	12	**0.40**	2.4
5	**11.24**	58	**2.37**	27	**2.82**	51	**133**	RSE
7	**0.10**	0.32	**0.34**	RSE	**1.10**	RSE	**28**	RSE
25	**0.20**	RSE	**15.8**	RSE	**82**	RSE	**326**	RSE
50	**0.67**	RSE	**3.52**	RSE	**10.86**	RSE	**146**	RSE

TABLE II
COMPUTATIONAL TIME VS CORA IN SECONDS

	Method runtime	CORA [3]
Algorithm 1	**0.01**	2.66
Algorithm 2	28	**3.6**
Algorithm 3	**2.93**	4.07
Algorithm 4	687	**4.08**

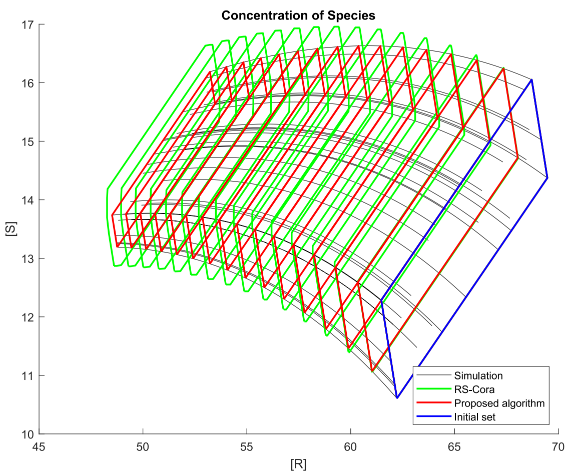

Fig. 4. Reachable sets representing chemical concentrations generated by Algorithm 5 and CORA.

We converted the HPDS into the tensor form (1) with

$$\mathcal{A}_{:1} = \begin{bmatrix} -0.042 & 0.038 \\ 0.038 & -0.092 \end{bmatrix}, \mathcal{A}_{:2} = \begin{bmatrix} 0.044 & -0.106 \\ -0.106 & 0.194 \end{bmatrix}.$$

It can be shown that $\mathcal{A}$ is not odeco, but it can be transformed into an odeco tensor using the method shown in Section III-C. We verified that this transformation can be done using

$$\mathbf{P} = \begin{bmatrix} 7 & 2 \\ 4 & -1 \end{bmatrix}, \Lambda = \begin{bmatrix} -0.5 & 0 \\ 0 & -0.2 \end{bmatrix}.$$

We simulated this system using Algorithm 5 based on an initial set over 15 time steps. Here, CORA overapproximated the reachable set by a factor of 2.7 at the final timestep. The results of the simulation are displayed in Fig. 4.

V. CONCLUSION

This letter describes how to perform the reachability analysis of odeco HPDSs and certain general HPDSs. The proposed method improves accuracy over existing methods for the reachability analysis of dynamical systems. Overly conservative estimates may lead to unnecessary design constraints, increased computational complexity, and missed opportunities for system optimization. The proposed method represents a significant step toward mitigating these challenges. To expand the applicability of this method, one could explore the possibility of approximating general HPDSs and general polynomial systems as odeco HPDSs while ensuring that the safety guarantees are not violated. Investigating the performance of this method using various set representations, such as star sets, could be explored in future work. Finally, one could explore the possibility of applying this method to other systems that have exact solutions and similar ordering properties as shown in Section III.

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