# On Global Optimization of Hybrid Systems

*Cha Kun Lee and Paul I. Barton*

*Department of Chemical Engineering*
*Massachusetts Institute of Technology*
*66-464, 77 Massachusetts Avenue*
*Cambridge, MA 02139*
*chakun@mit.edu, pib@mit.edu*

**Key words:** convex relaxations, state bounds, nonconvex outer approximation

Prepared for presentation at the 2004 Annual Meeting, Austin, TX, Nov. 7-12

# Abstract

Continuous time hybrid systems have become the modeling framework of choice for a wide variety of applications that require detailed dynamic models with embedded discontinuities. In general, these time dependent, nonlinear models exhibit model switching and state jumps as a consequence of both time and state dependent events [1]. There exist great safety, economical and environmental incentives to study the global optimization of hybrid systems as many practical problems can be formulated as dynamic optimization problems with hybrid systems embedded, for example, formal safety verification problems, and synthesis problems requiring optimal operating policies. For safety critical applications, it is crucial to locate the global solution as it often represents a counter-example to a safety specification.

A deterministic branch and bound framework has recently been developed for the global optimization of linear hybrid systems with fixed transition times and a fixed sequence of modes [2]. This work has been extended to determine the optimal mode sequence using a decomposition approach [3]. In this presentation, we address a key issue in this approach: the problem of bounding the states of a linear hybrid system with fixed transition times. It is shown via an illustrative example that a simple decomposition algorithm produces weak bounds which deteriorate as the number of epochs increases. To address this issue, a novel algorithm is proposed, based on solving families of relaxed linear programming problems, which allows the incorporation of additional constraints derived from physical insight. The remainder of this record will describe this in detail.

In addition, we will present recent progress toward handling varying transition times within a global optimization setting. The control parameterization enhancing transform (CPET) [4, 5] is used to transform the problem into one with fixed transition times. The cost of doing so is reflected by the insertion of additional nonlinearities into the resulting embedded hybrid system. To deal with these nonlinearities, a method for the global optimization of nonlinear hybrid systems with fixed transition times and a varying sequence of modes will be presented, based on a nonconvex outer approximation framework [6] utilizing novel convex relaxation techniques. Due to space constraints, this material will not be included in this presentation record; a journal article is currently in preparation.


# 1 Introduction

Many modern, general methods for deterministic global optimization in Euclidean spaces rely on the notion of a convex relaxation of a nonconvex function [7]. This is a convex function which underestimates a nonconvex function on the set of interest. The convex programs that result from convex relaxation of all nonconvex objective and constraint functions in a problem formulation can (in principle) be solved to guaranteed global optimality, which can then be used to generate rigorous lower bounds on the nonconvex problem for a branch and bound (B&B) algorithm [8].

Recently, a convexity theory has been developed that enables well known symbolic convex relaxations on Euclidean spaces [7, 9] to be harnessed in the construction of convex relaxations of general, nonconvex Bolza type functionals subject to an embedded linear time varying (LTV) hybrid system where the transition times are fixed, and the sequence of modes, $T_\mu$, is known [2]. The construction of a set enclosing the image of the parameter space under the solution of the hybrid system, $\mathcal{X}^{(i)}$, is critical for obtaining tight (accurate) convex relaxations of the participating functionals. Note that $\mathcal{X}^{(i)}$ represents the state bounds for the embedded hybrid system for all values of the parameters. The better the estimate of $\mathcal{X}^{(i)}$ is, the tighter the relaxations obtained. Consequently, tighter lower bounds are obtained, increasing the efficiency of the global optimization algorithm.

In [3], a mixed-integer reformulation is proposed to deal with the problem when $T_\mu$ is allowed to vary and becomes an optimization parameter. This results in a nonconvex mixed-integer nonlinear programming (MINLP) problem. In particular, auxiliary optimization parameters, $\mathbf{Z}$, are introduced to represent the initial conditions for each epoch. In this case, $\mathcal{X}^{(i)}$ becomes a larger set containing the image of the parameter space under the solution of the hybrid system for all possible $T_\mu$, and the bounds on $\mathbf{Z}$ are obtained from estimating $\mathcal{X}^{(i)}$ at the time events, i.e., the state bounds at the beginning of each epoch.

For analogous reasons to those presented above, it is very desirable to obtain tight bounds for $\mathbf{Z}$, as these bounds are needed to construct a convex relaxation of the nonconvex MINLP. Although the exact state bounds at the beginning of each epoch can be obtained with an explicit enumeration of all possible $T_\mu$, the cost of doing so clearly becomes prohibitive (increases exponentially) as the number of epochs increases. To deal with this problem, a decomposition algorithm for estimating valid state bounds was proposed in [3]. In the remainder of this record, we formally present the decomposition algorithm, and show that it produces weak bounds which deteriorate as the number of epochs increases. To address this issue, a novel algorithm is proposed to obtain tighter state bounds, based on solving a family of relaxations of mixed-integer linear programming (MILP) problems as LP problems.

# 2 LTV Hybrid Systems

The modeling framework of [1, 2] is used to define the LTV hybrid system of interest. The time horizon is partitioned into contiguous intervals called *epochs*. We define a *hybrid time trajectory*, $T_\tau$, as a finite sequence of epochs $\{I_i\}$ terminating with epoch $I_{n_e}$, where $n_e$ is fixed, and is the total number of epochs. Each epoch is a closed time interval $I_i = [\sigma_i, \tau_i] \subset \mathbb{R}$, $\sigma_i = \tau_{i-1}$ for $i = 2, \ldots, n_e$, $\sigma_1 \leq \tau_1$, and $\tau_{i-1} \leq \tau_i$ for all $i = 2, \ldots, n_e$. For epoch $I_i$, the system evolves continuously in time if $\sigma_i < \tau_i$, and it evolves discretely by making an instantaneous transition if $\sigma_i = \tau_i$. The continuous state subsystems are called *modes* and the corresponding sequence of modes for $T_\tau$ is called the *hybrid mode trajectory*, $T_\mu$. At the end of epoch $I_i$, a transition is made from the *predecessor* mode in $I_i$ to a *successor* mode in epoch $I_{i+1}$.

**Definition 1.** *The LTV ODE hybrid system of interest is defined by the following.*

1. *An index set of modes potentially visited along $T_\mu$, $M = \{1, \ldots, n_m\}$, and a fixed $T_\tau$ with given time events (i.e., explicit transition times) $\sigma_1, \tau_1, \tau_2, \ldots, \tau_{n_e}$. It is clear that $T_\mu = \{m_i\}$, where $m_i \in M$. Henceforth, the superscript $(m)$ will refer to any mode in $M$, while superscript $(m_i)$ will refer to the active mode in epoch $I_i$;*

2. *An invariant structure system where the number of continuous state variables is constant between modes, $V = (\mathbf{x}(\mathbf{p}, T_\mu, t), \mathbf{p})$, where $\mathbf{p} \in P \subset \mathbb{R}^{n_p}$, and $\mathbf{x}(\mathbf{p}, T_\mu, t) \in \mathbb{R}^{n_x}$ for all $(\mathbf{p}, T_\mu, t) \in P \times M^{n_e} \times I_i,\ i = 1, \ldots, n_e$;*

3. *The LTV ODE system for each mode $m \in M$, which is given by*

$$\dot{\mathbf{x}}(\mathbf{p}, T_\mu, t) = \mathbf{A}^{(m)}(t)\mathbf{x}(\mathbf{p}, T_\mu, t) + \mathbf{B}^{(m)}(t)\mathbf{p} + \mathbf{q}^{(m)}(t), \tag{1}$$

*where $\mathbf{A}^{(m)}(t)$ is continuous on $[\sigma_1, \tau_{n_e}]$, $\mathbf{B}^{(m)}(t)$ and $\mathbf{q}^{(m)}(t)$ are piecewise continuous on $[\sigma_1, \tau_{n_e}]$ and defined at any point of discontinuity, for all $m \in M$;*

4. *The transition conditions for the transitions between epochs $I_i$ and $I_{i+1}$, $i = 1, \ldots, n_e - 1$, which are explicit time events:*

$$L^{(m_i)} := (t = \tau_i), \tag{2}$$

*indicating the transition from mode $m_i$ in epoch $I_i$ to mode $m_{i+1}$ in epoch $I_{i+1}$ at time $\tau_i$;*

5. *The system of transition functions, which is given by*

$$\mathbf{x}(\mathbf{p}, T_\mu, \sigma_{i+1}) = \mathbf{D}_i\mathbf{x}(\mathbf{p}, T_\mu, \tau_i) + \mathbf{E}_i\mathbf{p} + \mathbf{k}_i, \forall\ i = 1, \ldots, n_e - 1, \tag{3}$$

*for the transition from mode $m_i$ in epoch $I_i$ to mode $m_{i+1}$ in epoch $I_{i+1}$; and*

6. *A given initial condition for mode $m_1$,*

$$\mathbf{x}(\mathbf{p}, T_\mu, \sigma_1) = \mathbf{E}_0\mathbf{p} + \mathbf{k}_0. \tag{4}$$

**Definition 2.** *Let $P$ be a nonempty compact convex subset of $\mathbb{R}^{n_p}$. Define the following sets for all $i = 1, \ldots, n_e$ where $\underline{t}$ denotes fixed $t$:*

$$\mathcal{X}^{(i)}(\underline{t}) \equiv \big\{\mathbf{x}(\mathbf{p}, T_\mu, \underline{t}) \mid \mathbf{p} \in P, T_\mu \in M^{n_e}, \underline{t}\ \in I_i\big\}, \tag{5}$$

$$\mathcal{X}^{(i)} \equiv \bigcup_{\underline{t} \in I_i} \mathcal{X}^{(i)}(\underline{t}). \tag{6}$$

# 3 The Decomposition Algorithm

Consider the following dynamic system,

$$\dot{\mathbf{x}}(\mathbf{p}, \tilde{\mathbf{z}}, t) = \mathbf{A}^{(m)}(t)\mathbf{x}(\mathbf{p}, \tilde{\mathbf{z}}, t) + \mathbf{B}^{(m)}(t)\mathbf{p} + \mathbf{q}^{(m)}(t), \tag{7}$$

$$\mathbf{x}(\mathbf{p}, \tilde{\mathbf{z}}, \sigma) = \tilde{\mathbf{z}}, \tag{8}$$

for some $m \in M$, where $\sigma < \tau, t \in T \equiv [\sigma, \tau]$, $\mathbf{p} \in P \subset \mathbb{R}^{n_p}$, $\tilde{\mathbf{z}} \in \tilde{Z} \subseteq \mathbb{R}^{n_x}$. Define the following set:

$$\mathcal{X}^a(\underline{t}) \equiv \big\{\mathbf{x}(\mathbf{p}, \tilde{\mathbf{z}}, \underline{t}) \mid \mathbf{p} \in P, \tilde{\mathbf{z}} \in \tilde{Z}, \underline{t}\ \in T\big\}. \tag{9}$$

**Theorem 1.** *[10] Given $P \equiv [\mathbf{p}^L, \mathbf{p}^U]$ and $\tilde{Z} \equiv [\tilde{\mathbf{z}}^L, \tilde{\mathbf{z}}^U]$, the set $\mathcal{X}^a(\underline{t}) \equiv [\mathbf{x}^L(\underline{t}), \mathbf{x}^U(\underline{t})]$ for $\underline{t} \in T$ can be calculated pointwise in time from the following interval equation,*

$$[\mathbf{x}](\underline{t}) = \mathbf{M}(\underline{t})[\mathbf{w}] + \mathbf{n}(\underline{t}), \tag{10}$$

*where $\mathbf{w} = (\mathbf{p}, \tilde{\mathbf{z}})$, $\mathbf{w} \in W \equiv [\mathbf{w}^L, \mathbf{w}^U]$, $\mathbf{w}^L = (\mathbf{p}^L, \tilde{\mathbf{z}}^L)$, $\mathbf{w}^U = (\mathbf{p}^U, \tilde{\mathbf{z}}^U)$, and $\mathbf{M}(t)$ and $\mathbf{n}(t)$ are given by the solution of the following LTV system,*

$$\dot{\mathbf{M}}(t) = \mathbf{A}^{(m)}(t)\mathbf{M}(t) + \mathbf{H}^{(m)}(t), \tag{11}$$

$$\dot{\mathbf{n}}(t) = \mathbf{A}^{(m)}(t)\mathbf{n}(t) + \mathbf{q}^{(m)}(t), \tag{12}$$

$$\mathbf{M}(\sigma) = \mathbf{L}, \tag{13}$$

$$\mathbf{n}(\sigma) = \mathbf{0}, \tag{14}$$

*where $\mathbf{H}^{(m)}(t) = [\mathbf{B}^{(m)}(t)\ \mathbf{0}]$, $\mathbf{L} = [\mathbf{0}\ \mathbf{I}]$, and $\mathbf{I}$ is the identity matrix of rank $n_x$.*

**Remark 1.** *The functional form of the solution of the LTV system is affine in the parameters $\mathbf{w}$,*

$$\mathbf{x}(\mathbf{w}, t) = \mathbf{M}(t)\mathbf{w} + \mathbf{n}(t). \tag{15}$$

*The entries in $\mathbf{M}(t)$ are clearly the parametric sensitivities of the dynamic system, $\frac{\partial \mathbf{x}}{\partial \mathbf{w}}(t)$. Hence,* (11) *and* (13) *are simply the forward sensitivity equations of the embedded dynamic system in* (7) *and* (8)*.*

**Remark 2.** *The bounds $\mathbf{x}^L(t)$ and $\mathbf{x}^U(t)$ from* (10) *are* exact *in the following sense. For any $i \in \{1, \ldots, n_x\}$, and any $\underline{t} \in T$, the following relationship holds,*

$$x_i(\mathbf{w}^*, \underline{t}) = x_i^L(\underline{t}) \leq x_i(\mathbf{w}, \underline{t}) \leq x_i^U(\underline{t}) = x_i(\mathbf{w}^\dagger, \underline{t}),\ \forall\ \mathbf{w} \in W, \tag{16}$$

*for some $\mathbf{w}^*, \mathbf{w}^\dagger \in W$.*

From Remark 2, we know that exact bounds for $\mathbf{x}(\tau)$ can be constructed for each sub-problem in the mixed-integer reformulation presented in [3] once the bounds for $\tilde{\mathbf{z}}$ are known. This suggests the following decomposition algorithm for estimating the bounds on $\mathbf{Z} \in Z$, where $\mathbf{z}_i$ represents the initial conditions for epoch $I_i$.

*Algorithm* 1 *(A1).*

1. Initialize $i$=1.
2. For $m = 1$ to $n_m$ do:
   (a) Integrate the following system from $\sigma_1$ to $\tau_1$, and store $\mathbf{M}_1^{(m)}(\tau_1)$ and $\mathbf{n}_1^{(m)}(\tau_1)$.

$$\dot{\mathbf{M}}_1^{(m)}(t) = \mathbf{A}^{(m)}(t)\mathbf{M}_1^{(m)}(t) + \mathbf{B}^{(m)}(t), \tag{17}$$

$$\dot{\mathbf{n}}_1^{(m)}(t) = \mathbf{A}^{(m)}(t)\mathbf{n}_1^{(m)}(t) + \mathbf{q}^{(m)}(t), \tag{18}$$

$$\mathbf{M}_1^{(m)}(\sigma_1) = \mathbf{E}_0, \tag{19}$$

$$\mathbf{n}_1^{(m)}(\sigma_1) = \mathbf{k}_0. \tag{20}$$

(b) Calculate and store $[\mathbf{x}^{(m)^L}(\sigma_2),\mathbf{x}^{(m)^U}(\sigma_2)]$ from

$$[\mathbf{x}^{(m)}](\sigma_2) = \Big(\mathbf{D}_1\mathbf{M}_1^{(m)}(\tau_1) + \mathbf{E}_1\Big)[\mathbf{p}] + \mathbf{D}_1\mathbf{n}_1^{(m)}(\tau_1) + \mathbf{k}_1. \tag{21}$$

3. For $j = 1$ to $n_x$ do:

   (a) Calculate and store the $j$th element of $[\mathbf{z}_{i+1}^L, \mathbf{z}_{i+1}^U]$ from

$$(\mathbf{z}_{i+1}^L)_j = \min_{m\in M}\ x_j^{(m)^L}(\sigma_{i+1}), \quad (\mathbf{z}_{i+1}^U)_j = \max_{m\in M}\ x_j^{(m)^U}(\sigma_{i+1}). \tag{22}$$

4. For $i = 2$ to $(n_e - 1)$ do:

   (a) For $m = 1$ to $n_m$ do:

      i. Integrate the system (11), (12), (13) and (14) from $\sigma = \sigma_i$ to $\tau = \tau_i$, and store $\mathbf{M}_i^{(m)}(\tau_i) \leftarrow \mathbf{M}(\tau)$ and $\mathbf{n}_i^{(m)}(\tau_i) \leftarrow \mathbf{n}(\tau)$.

      ii. Calculate and store $[\mathbf{x}^{(m)^L}(\sigma_{i+1}),\ \mathbf{x}^{(m)^U}(\sigma_{i+1})]$ from

$$[\mathbf{x}^{(m)}](\sigma_{i+1}) = \Big(\mathbf{D}_i\mathbf{M}_i^{(m)}(\tau_i) + \mathbf{L}_i\Big)[\mathbf{w}] + \mathbf{D}_i\mathbf{n}_i^{(m)}(\tau_i) + \mathbf{k}_i. \tag{23}$$

      where $\mathbf{w}^L = (\mathbf{p}^L, \mathbf{z}_i^L)$, $\mathbf{w}^U = (\mathbf{p}^U, \mathbf{z}_i^U)$, and $\mathbf{L}_i = [\mathbf{E}_i\ \mathbf{0}]$.

   (b) Calculate and store $[\mathbf{z}_{i+1}^L, \mathbf{z}_{i+1}^U]$ using Step 3. above.

**Remark 3.** *The staggered corrector method can be used for efficient integration of the dynamic systems [11].*

**Remark 4.** *The system* (11)*,* (12)*,* (13) *and* (14) *is independent of the parameters* $\mathbf{w}$*, hence the values of* $\mathbf{M}(\tau)$ *and* $\mathbf{n}(\tau)$ *are also independent of* $\mathbf{w}$*. Hence, if the epochs are of equal duration, i.e.,* $\tau_i - \sigma_i$ *is constant for all* $i$*, step (4ai) only needs to be executed once for* $i = 2$*.*

**Remark 5.** *Note that* $\mathbf{M}_1$ *is a* $n_x \times n_p$ *matrix, while* $\mathbf{M}_{i\neq 1}$ *is a* $n_x \times (n_p + n_x)$ *matrix.*

Although Theorem 1 guarantees exact bounds for the system (7) and (8), the bounds obtained from implementing (A1) have no guarantee of being exact for $\mathbf{Z}$ past the first epoch. This arises because bounds for different elements of $[\mathbf{z}_i^L, \mathbf{z}_i^U]$, $i > 2$, could come from different predecessor modes $I_{i-1}$, and this is illustrated in the example presented below. One way to obtain exact bounds is to solve the bounding equations (see [2] for obtaining the exact bounds for fixed $T_\mu$) for all possible combinations of $T_\mu$. This method clearly suffers from exponential complexity in the number of epochs, and an alternative algorithm for computing tighter bounds for $\mathbf{Z}$ is needed.

# 4 The Relaxed LP Algorithm

Consider the following problem.

**Problem 1 (P1($\alpha$,$\beta$)).**

$$\min_{\mathbf{p}\in P,\mathbf{Y}\in Y^b,\mathbf{Z}} \mathbf{e}_\beta^{\mathrm{T}}\mathbf{z}_{\alpha+1} \tag{24}$$

$$\textit{s.t.}\ \sum_{m=1}^{n_m} y_{mi} = 1,\ \forall\, i = 1,\ldots,\alpha, \tag{25}$$

$$\mathbf{z}_{i+1} = \sum_{m=1}^{n_m} y_{mi}\Big(\mathbf{D}_i\mathbf{x}_{mi}(\mathbf{p},\mathbf{Z},\tau_i) + \mathbf{E}_i\mathbf{p} + \mathbf{k}_i\Big), \forall\, i = 1,\ldots,\alpha, \tag{26}$$

$$\mathbf{z}_1 = \mathbf{E}_0\mathbf{p} + \mathbf{k}_0, \tag{27}$$

*where* $Y^b \equiv \{0,1\}^{n_m\times\alpha} \subset Y \equiv [0,1]^{n_m\times\alpha}$*,* $\mathbf{Z} \in \mathbb{R}^{n_x\times(\alpha+1)}$*, and the unit vector* $\mathbf{e}_\beta$ *is the* $\beta$*th column of the rank* $n_x$ *identity matrix;* $\mathbf{x}_{mi}(\mathbf{p},\mathbf{Z},t)$ *are given by the solution of the following embedded LTV ODE systems for all* $m \in M$*,* $i = 1,\ldots,\alpha$*,*

$$\dot{\mathbf{x}}_{mi}(\mathbf{p},\mathbf{Z},t) = \mathbf{A}^{(m)}(t)\mathbf{x}_{mi}(\mathbf{p},\mathbf{Z},t) + \mathbf{B}^{(m)}(t)\mathbf{p} + \mathbf{q}^{(m)}(t),\ \forall\, t \in I_i, \tag{28}$$

$$\mathbf{x}_{mi}(\mathbf{p},\mathbf{Z},\sigma_i) = \mathbf{z}_i. \tag{29}$$

Problem (P1) determines the exact lower bound for the $\beta$th component of $\mathbf{x}(\mathbf{p},T_\mu,\sigma_{\alpha+1}) = \mathbf{z}_{\alpha+1}$. We can construct a convex relaxation for (P1) by treating the bilinear terms in (26) using the exact linearizations in [12]. We can then formulate the following, equivalent, MILP.

**Problem 2 (P2($\alpha$,$\beta$)).**

$$\min_{\mathbf{p},\mathbf{Y},\mathbf{Z},\mathbf{V},\mathbf{W},\mathbf{S}} \mathbf{e}_\beta^{\mathrm{T}}\mathbf{z}_{\alpha+1} \tag{30}$$

$$\textit{s.t.}\ \sum_{m=1}^{n_m} y_{mi} = 1,\ \forall\, i = 1,\ldots,\alpha, \tag{31}$$

$$\mathbf{z}_{i+1} = \sum_{m=1}^{n_m} \mathbf{s}_{mi},\ \forall\, i = 1,\ldots,\alpha, \tag{32}$$

$$\mathbf{z}_1 = \mathbf{E}_0\mathbf{p} + \mathbf{k}_0, \tag{33}$$

$$\mathbf{v}_{mi}^U(y_{mi}-1) + \mathbf{v}_{mi} \le \mathbf{s}_{mi} \le \mathbf{v}_{mi}^L(y_{mi}-1) + \mathbf{v}_{mi},\ \forall\, m \in M, i = 1,\ldots,\alpha, \tag{34}$$

$$\mathbf{v}_{mi}^L y_{mi} \le \mathbf{s}_{mi} \le \mathbf{v}_{mi}^U y_{mi},\ \forall\, m \in M, i = 1,\ldots,\alpha, \tag{35}$$

$$\mathbf{v}_{m1} = \Big(\mathbf{D}_1\mathbf{M}_1^{(m)}(\tau_1) + \mathbf{E}_1\Big)\mathbf{p}\ + \mathbf{D}_1\mathbf{n}_1^{(m)}(\tau_1) + \mathbf{k}_1,\ \forall\, m \in M, \tag{36}$$

$$\mathbf{v}_{mi} = \Big(\mathbf{D}_i\mathbf{M}_i^{(m)}(\tau_i) + \mathbf{L}_i\Big)\mathbf{w}_i\ + \mathbf{D}_i\mathbf{n}_i^{(m)}(\tau_i) + \mathbf{k}_i,\ \forall\, m \in M, i = 2,\ldots,\alpha, \tag{37}$$

$$\mathbf{w}_i = (\mathbf{p},\mathbf{z}_i),\ \forall\, i = 2,\ldots,\alpha, \tag{38}$$

$$\mathbf{w}_1 = \mathbf{0}, \tag{39}$$

*where* $\mathbf{Y} \in Y^b \equiv \{0,1\}^{n_m\times\alpha} \subset Y \equiv [0,1]^{n_m\times\alpha}$*,* $\mathbf{Z} \in \mathbb{R}^{n_x\times(\alpha+1)}$*,* $\mathbf{V} \in V \subset \mathbb{R}^{n_x\times n_m\times\alpha}$*,* $\mathbf{W} \in \mathbb{R}^{(n_p+n_x)\times\alpha}$*,* $\mathbf{S} \in \mathbb{R}^{n_x\times n_m\times\alpha}$*, and the unit vector* $\mathbf{e}_\beta$ *is the* $\beta$*th column of a rank* $n_x$ *identity matrix;* $\mathbf{L}_i = [\mathbf{E}_i\ \mathbf{0}]$*;* $\mathbf{M}_1^{(m)}(\tau_1)$ *and* $\mathbf{n}_1^{(m)}(\tau_1)$ *are given by the solution of the system* (17)*,* (18)*,* (19) *and* (20) *from* $\sigma_1$ *to* $\tau_1$ *for* $m \in M$*; and* $\mathbf{M}_i^{(m)}(\tau_i)$ *and* $\mathbf{n}_i^{(m)}(\tau_i)$ *are given by the solution of the system* (11)*,* (12)*,* (13) *and* (14) *from* $\sigma = \sigma_i$ *to* $\tau = \tau_i$*, for* $m \in M$*,* $i = 2,\ldots,\alpha$*.*

The required bounds on the auxiliary variables $\mathbf{V}$ (see (34) and (35)) constitute the set $V$, and can be determined sequentially for each epoch (see algorithm below). The variables $\mathbf{Z}$, $\mathbf{W}$, $\mathbf{S}$ are left as free or unrestricted variables. While it is impractical to solve a family of MILPs (P2) to obtain the tightest bounds for $\mathbf{Z}$, it is much cheaper to solve (P2) on the relaxed space $\mathbf{Y} \in Y$, resulting in solving a family of relaxed LPs to provide valid (but not exact) bounds for $\mathbf{Z}$. This constitutes the following algorithm.

*Algorithm 2 (A2).*

1. Execute steps 1., 2. and 3. in (A1).
2. For $i = 2$ to $(n_e - 1)$ do:
   (a) For $m = 1$ to $n_m$ do:
      i. Integrate the system (11), (12), (13) and (14) from $\sigma = \sigma_i$ to $\tau = \tau_i$, and store $\mathbf{M}_i^{(m)}(\tau_i) \leftarrow \mathbf{M}(\tau)$ and $\mathbf{n}_i^{(m)}(\tau_i) \leftarrow \mathbf{n}(\tau)$.
      ii. Calculate and store $[\hat{\mathbf{x}}^{(m)^L}(\sigma_{i+1}), \hat{\mathbf{x}}^{(m)^U}(\sigma_{i+1})]$ from

$$[\hat{\mathbf{x}}^{(m)}](\sigma_{i+1}) = \Big(\mathbf{D}_i \mathbf{M}_i^{(m)}(\tau_i) + \mathbf{L}_i\Big)[\mathbf{w}] + \mathbf{D}_i \mathbf{n}_i^{(m)}(\tau_i) + \mathbf{k}_i. \tag{40}$$

      where $\mathbf{w}^L = (\mathbf{p}^L, \mathbf{z}_i^L)$, $\mathbf{w}^U = (\mathbf{p}^U, \mathbf{z}_i^U)$, and $\mathbf{L}_i = [\mathbf{E}_i\ \mathbf{0}]$.
   (b) For $m = 1$ to $n_m$ do:
      i. For $j = 1$ to $n_x$ do:
         A. Solve (P2($i$,$j$)), with $[\mathbf{v}_{\lambda\theta}] = [\mathbf{x}^{(\lambda)}](\sigma_{\theta+1})$, $\theta = 1, \ldots, i-1$, and $[\mathbf{v}_{\lambda i}] = [\hat{\mathbf{x}}^{(\lambda)}](\sigma_{i+1})$, for all $\lambda \in M$, on the relaxed space $Y$, with the following constraint,

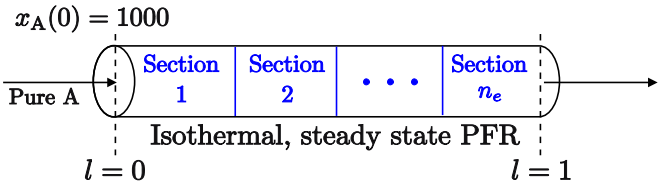
$$y_{mi} = 1, \tag{41}$$

         and store $x_j^{(m)^L}(\sigma_{i+1}) \leftarrow$ objective.
         B. Repeat step A. as a maximization problem, and store $x_j^{(m)^U}(\sigma_{i+1}) \leftarrow$ objective.
   (c) For $j = 1$ to $n_x$ do:
      i. Calculate and store the $j$th element of $[\mathbf{z}_{i+1}^L, \mathbf{z}_{i+1}^U]$ from

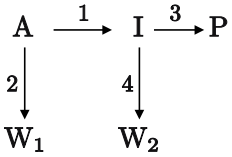
$$(\mathbf{z}_{i+1}^L)_j = \min_{m \in M}\ x_j^{(m)^L}(\sigma_{i+1}), \quad (\mathbf{z}_{i+1}^U)_j = \max_{m \in M}\ x_j^{(m)^U}(\sigma_{i+1}). \tag{42}$$

# 5 An Illustrative Example

Consider an isothermal plug flow reactor (PFR) operating at steady state, and 3 possible choices of catalyst. The reaction scheme, initial conditions and associated rate constants are shown in Fig. 1, where $x_i$ represents the molar concentration of component $i$ (mol m$^{-3}$) and $k_j$ represents the rate constant of reaction $j$ (h$^{-1}$). The PFR has a uniform cross-sectional area of 1 m$^2$,




*Reaction scheme*




*Catalyst*

| | $k_1$ | $k_2$ | $k_3$ | $k_4$ |
|---|---|---|---|---|
| 1 | 2.098 | 1.317 | 0.021 | 0.033 |
| 2 | 29.53 | 110.2 | 0.295 | 0.079 |
| 3 | 182.6 | 2325 | 1.826 | 0.143 |

*Kinetics*

$$\dot{x}_A = -(k_1 + k_2)x_A \qquad \dot{x}_I = k_1 x_A - (k_3 + k_4)x_I$$
$$\dot{x}_{W_1} = k_2 x_A \qquad \dot{x}_{W_2} = k_4 x_I$$
$$\dot{x}_P = k_3 x_I$$

Figure 1: Chemical reaction scheme and kinetics for PFR example

and a constant volumetric flow rate of 1 $m^3$ $h^{-1}$. In this example, the independent variable $t$ is the length, $l$, of the reactor. Determine the bounds on the concentration of the reactant and products at the beginning of each reactor section. Note that the choice of catalyst corresponds to the choice of the sequence of modes in a linear hybrid system with 3 modes (each mode corresponds to the choice of a different catalyst) and $n_e$ epochs (each epoch corresponds to a section of the reactor), with state continuity at the transitions.

Table 1 shows the bounds obtained for $\mathbf{z}_{15}$ when $n_e = 15$ when explicit enumeration (EE) (which obtains the exact bounds), (A1) and (A2) are used. As can be seen, (A2) produces tighter bounds than (A1). When physical information from the problem can be used, e.g., conservation of molar species, we can add the following additional constraints to (P2),

$$\sum_{j=1}^{n_x} (\mathbf{s}_{mi})_j = 1000 y_{mi}, \ \forall\, m \in M, i = 1, \ldots, \alpha. \tag{43}$$

When this physical insight is employed, it can be seen that the bounds obtained from (A2) with (43) produces tighter bounds than using (A2) alone. The reason why (A2) itself does not produce bounds which obey this conservation law is that the linearizations of the bilinear terms in (26)

Table 1: Bounds for $\mathbf{z}_{15}$ where $n_e = 15$

| Species | (EE) | | (A1) | | (A2) | | (A2) with (43) | |
|---|---|---|---|---|---|---|---|---|
| | $\mathbf{z}_{15}^L$ | $\mathbf{z}_{15}^U$ | $\mathbf{z}_{15}^L$ | $\mathbf{z}_{15}^U$ | $\mathbf{z}_{15}^L$ | $\mathbf{z}_{15}^U$ | $\mathbf{z}_{15}^L$ | $\mathbf{z}_{15}^U$ |
| A | 0.00 | 41.28 | 0.00 | 41.28 | 0.00 | 41.28 | 0.00 | 41.28 |
| $W_1$ | 369.73 | 927.18 | 78.52 | 4365.72 | 230.54 | 2030.39 | 321.03 | 981.59 |
| I | 11.60 | 567.77 | 11.60 | 815.88 | 11.60 | 567.77 | 11.60 | 567.77 |
| $W_2$ | 2.43 | 27.87 | 1.08 | 79.06 | 1.54 | 44.77 | 1.54 | 44.77 |
| P | 7.34 | 293.77 | 0.69 | 1005.21 | 1.51 | 544.39 | 1.53 | 451.06 |

are only exact on the space $Y^b$, and not on the space $Y$. Hence, we have to enforce the law with (43). Note that there is no way to incorporate additional (arbitrary) constraints within (A1). For further illustration, the upper bound computed for species $W_1$ at the beginning of each section when $n_e = 10$ is shown in Table 2.

Table 3 shows the bounds obtained for $W_1$ when the algorithms are trivially extended to calculate the bounds at $l = 1$. It can be seen that the bounds obtained from (A1) and (A2) deteriorate significantly from the exact bounds as $n_e$ increases. When physical insight (43) is employed in conjunction with (A2), much tighter bounds are obtained. All calculations were performed on an AMD 1.2 GHz, 1 GB RAM machine using CPLEX 7.5 as the LP solver, and the computation times for the algorithms are shown in Table 4, from which the exponential explosion of (EE) is clear.

Table 2: Upper bound for $W_1$ ($n_e = 10$)

| Section | (EE) | (A1) | (A2) | (A2) with (43) |
|---|---|---|---|---|
| 2 | 927.18 | 927.18 | 927.18 | 927.18 |
| 3 | 927.18 | 1586.13 | 927.18 | 927.18 |
| 4 | 927.18 | 2054.45 | 1161.34 | 932.50 |
| 5 | 927.18 | 2387.29 | 1245.91 | 945.55 |
| 6 | 927.18 | 2623.83 | 1356.05 | 954.30 |
| 7 | 927.18 | 2791.95 | 1401.19 | 961.80 |
| 8 | 927.18 | 2911.43 | 1461.41 | 967.78 |
| 9 | 927.18 | 2996.34 | 1482.13 | 972.70 |
| 10 | 927.18 | 3056.69 | 1516.14 | 976.73 |

Table 3: Upper bound for $W_1$ at $l = 1$

| $n_e$ | (EE) | (A1) | (A2) | (A2) with (43) |
|---|---|---|---|---|
| 5 | 927.18 | 1811.88 | 1094.46 | 967.02 |
| 10 | 927.18 | 3099.58 | 1523.92 | 980.04 |
| 15 | 927.18 | 4404.00 | 2052.69 | 983.43 |
| 20 | 927.18 | 5712.63 | 2605.73 | 984.89 |

Table 4: CPU times (s)

| $n_e$ | (EE) | (A1) | (A2) | (A2) with (43) |
|---|---|---|---|---|
| 5 | 0.04 | 0.04 | 1.6 | 2.3 |
| 10 | 0.4 | 0.04 | 8.3 | 12.8 |
| 15 | 135 | 0.04 | 27.1 | 45.7 |
| 20 | 44227 | 0.04 | 50.7 | 86.7 |

# References


[1] P. I. Barton and C. K. Lee. Modeling, simulation, sensitivity analysis and optimization of hybrid systems. *ACM Transactions on Modeling and Computer Simulation*, 12(4):256–289, 2002.

[2] C. K. Lee, A. B. Singer, and P. I. Barton. Global optimization of linear hybrid systems with explicit transitions. *Systems and Control Letters*, 51(5):363–375, 2004.

[3] P. I. Barton and C. K. Lee. Design of process operations using hybrid dynamic optimization. *Computers and Chemical Engineering*, 28(6-7):955–969, 2004.

[4] H.W.J. Lee, K.L. Teo, V. Rehbock, and L.S. Jennings. Control parametrization enhancing technique for time optimal control problems. *Dynamic Systems and Applications*, 6:243 – 262, 1997.

[5] K. L. Teo, L. S. Jennings, H.W.J. Lee, and V. Rehbock. The control parametrization enhancing transform for constrained optimal control problems. *Journal of the Australian Mathematical Society, Series B.*, 40:314–335, 1999.

[6] P. Kesavan, R. J. Allgor, E. P. Gatzke, and P. I. Barton. Outer approximation algorithms for separable nonconvex mixed-integer nonlinear programs. *Mathematical Programming, Series A*, 100(3):517–535, 2004.

[7] G. P. McCormick. Computability of global solutions to factorable nonconvex programs: Part I - convex underestimating problems. *Mathematical Programming*, 10:147–175, 1976.

[8] R. Horst and H. Tuy. *Global Optimization*. Springer-Verlag, Berlin, 1993.

[9] C. S. Adjiman, S. Dallwig, C. A. Floudas, and A. Neumaier. A global optimization method, $\alpha$BB, for general twice-differentiable constrained NLPs - I. Theoretical advances. *Computers and Chemical Engineering*, 22(9):1137–1158, 1998.

[10] A. B. Singer and P. I. Barton. Global solution of optimization problems with parameter-embedded linear dynamic systems. *Journal of Optimization Theory and Applications*, 121(3):613–646, 2004.

[11] W. F. Feehery, J. E. Tolsma, and P. I. Barton. Efficient sensitivity analysis of large-scale differential-algebraic systems. *Applied Numerical Mathematics*, 25(1):41–54, 1997.

[12] F. Glover. Improved linear integer programming formulations of nonlinear integer programs. *Management Science*, 22(4):455–460, 1975.