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Interval Bounds on the Solutions of Semi-Explicit Index-One DAEs. Part 2: Computation

Joseph K. Scott · **Paul I. Barton**

Abstract This article presents two methods for computing interval bounds on the solutions of nonlinear, semi-explicit, index-one differential-algebraic equations (DAEs). Part 1 presents theoretical developments, while Part 2 discusses implementation and numerical examples. The primary theoretical contributions are (1) an interval inclusion test for existence and uniqueness of a solution, and (2) sufficient conditions, in terms of differential inequalities, for two functions to describe componentwise upper and lower bounds on this solution, point-wise in the independent variable. The first proposed method applies these results sequentially in a two-phase algorithm analogous to validated integration methods for ordinary differential equations (ODEs). The second method unifies these steps to characterize bounds as the solutions of an auxiliary system of DAEs. Efficient implementations of both are described using interval computations and demonstrated on numerical examples.

1 Introduction

This work discusses the computation of guaranteed interval bounds on the solutions of nonlinear, semi-explicit index-one differential-algebraic equations (DAEs) subject to a given set of initial conditions and model parameters. In Part 1 of this article, the

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problem statement, background and necessary theoretical developments were presented. Here, two bounding methods are developed in detail and applied to numerical examples.

The first method proceeds in two-phases, as described in §3. In Phase 1, the interval inclusion test of §I-4 is applied to verify existence and uniqueness of a DAE solution, and provide a crude enclosure (throughout, I- is used to indicate references to Part 1). Unfortunately, this test is difficult to satisfy computationally because it involves implicit conditions. This challenge is addressed in §4. Using the crude enclosure from Phase 1, the second phase computes refined, time-varying bounds on the DAE solution using the results of §I-5. The implementation of Phase 2 involves numerical integration of an auxiliary system of ODEs whose solutions describe the desired bounds, and is described in §5.

The second proposed bounding method, which is described in §6, reduces the first method to a single phase based on Theorem I-5.3 in §I-5. The computation of the resulting bounds is similar to Phase 2 of the first method, only here the auxiliary system to be solved is described by semi-explicit DAEs.

The two-phase framework described above is analogous to the two-phase approach used for validated integration of ODEs [14]. Indeed, Phase 1 of this approach provides a key step toward the development of validated methods for DAEs. In Phase 2, however, we deviate from this approach by using a standard numerical integration code to compute refined bounds via the theory of differential inequalities. The resulting bounds are mathematically guaranteed, but subject to the error of numerical integration. Therefore, this method is not validated, and the same is true of the single-phase method. On the other hand, the use of state-of-the-art numerical integration codes leads to a very effective implementation. In §7, both methods are applied to numerical examples and shown to produce accurate bounds very efficiently.

2 Preliminaries

2.1 Extended interval functions

In Part 1 of this article, extensive use was made of intervals and interval-valued functions. For computational reasons, it is often convenient to extend such functions outside their domains in a regular manner. For example, it is desirable to define the behavior of an interval function taking the argument $[\mathbf{v}, \mathbf{w}]$ if, by some numerical error, we have $v_i > w_i$ for some i. There is a large literature on interval implementations that account for numerical error in a conservative manner in order to avoid these types of issues altogether. However, as we will see, the proposed methods for DAEs present unique challenges. As a particular example, we will make use of an algebraic equation solver to locate $\mathbf{v}$ and $\mathbf{w}$ such that $[\mathbf{v}, \mathbf{w}]$ satisfies an implicit interval equation. Though the solution is guaranteed to satisfy $\mathbf{v} \leq \mathbf{w}$, this may not hold for some iterate produced by the solver. If no provisions are made for this situation, the solver will be forced to abort. On the other hand, if the participating interval functions are extended onto $\mathbb{R}^n \times \mathbb{R}^n$ in a regular manner, this situation poses no problem for the solver, which may eventually converge to a solution describing a proper interval. In this section, we

compile the definitions required to address this and other similar situations that arise in the proposed computations.

Definition 2.1 Let $\square : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{IR}^n$ be defined by

$$\square(\mathbf{v}, \mathbf{w}) \equiv \left[\mathbf{v} - \max\left(\mathbf{0}, \frac{1}{2}(\mathbf{v} - \mathbf{w})\right), \mathbf{w} + \max\left(\mathbf{0}, \frac{1}{2}(\mathbf{v} - \mathbf{w})\right) \right]. \tag{1}$$

Interpretation of $\square$ is provided by the following lemma. The proof is trivial.

Lemma 2.1 *Let* $\mathbf{v}, \mathbf{w} \in \mathbb{R}^n$.

1. *If* $\mathbf{v} \le \mathbf{w}$, *then* $\square(\mathbf{v}, \mathbf{w}) = [\mathbf{v}, \mathbf{w}]$.
2. *For every i with* $v_i > w_i$, $\square(v_i, w_i)$ *is the singleton* $\{m([w_i, v_i])\}$.

The next definition extends the intersection of two intervals.

Definition 2.2 Let $\widetilde{\cap} : \mathbb{IR}^n \times \mathbb{IR}^n \to \mathbb{IR}^n$ be defined by

$$\widetilde{\cap}([\mathbf{z}^L, \mathbf{z}^U], [\hat{\mathbf{z}}^L, \hat{\mathbf{z}}^U]) \equiv [\mathrm{mid}(\mathbf{z}^L, \mathbf{z}^U, \hat{\mathbf{z}}^L), \mathrm{mid}(\mathbf{z}^L, \mathbf{z}^U, \hat{\mathbf{z}}^U)]. \tag{2}$$

Furthermore, define the standard notation $Z\widetilde{\cap}\hat{Z} \equiv \widetilde{\cap}(Z, \hat{Z}), \forall Z, \hat{Z} \in \mathbb{IR}^n$.

Lemma 2.2 *Let* $Z, \hat{Z} \in \mathbb{IR}^n$.

1. *If* $Z \cap \hat{Z} \ne \emptyset$, *then* $Z\widetilde{\cap}\hat{Z} = Z \cap \hat{Z}$.
2. *For all i such that* $Z_i \cap \hat{Z}_i = \emptyset$, $Z_i\widetilde{\cap}\hat{Z}_i$ *is either* $\{z_i^L\}$ *or* $\{z_i^U\}$.
3. $Z\widetilde{\cap}\hat{Z} \subset Z$.

The proof of the preceding lemma is straightforward and is omitted. The following two definitions modify the interval function Γ (Definition I-4.2).

Definition 2.3 Let

$$\mathcal{D}^* \equiv \{(A, B, Z) \in \mathbb{IR}^{n \times n} \times \mathbb{IR}^n \times \mathbb{IR}^n : 0 \notin A_{ii}, \forall i = 1, \ldots, n\}, \tag{3}$$

and define $\Gamma^* : \mathcal{D}^* \to \mathbb{IR}^n$ by $\Gamma^*(A, B, Z) \equiv W_1^* \times \ldots \times W_n^*$, where

$$W_i^* = \frac{1}{A_{ii}}\left(B_i - \sum_{k<i} A_{ik}W_k^* - \sum_{k>i} A_{ik}Z_k \right), \quad \forall i \in \{1, \ldots, n\}. \tag{4}$$

Definition 2.4 Define $\Gamma^+ : \mathcal{D}^* \to \mathbb{IR}^n$ by $\Gamma^+(A, B, Z) \equiv W_1^+ \times \ldots \times W_{n_y}^+$, where

$$W_i^+ = Z_i\widetilde{\cap}\frac{1}{A_{ii}}\left(B_i - \sum_{k<i} A_{ik}W_k^+ - \sum_{k>i} A_{ik}Z_k \right), \quad \forall i \in \{1, \ldots, n\}. \tag{5}$$

The functions Γ^+ and Γ^* differ from Γ in that they omit or extend the intersection with Z in the definition of Γ. We have the following properties and relationships.

Lemma 2.3 *Let* $(A, B, Z) \in \mathbb{IR}^{n \times n} \times \mathbb{IR}^n \times \mathbb{IR}^n$ *and* $(\widetilde{A}, \widetilde{B}, \widetilde{Z}) \in \mathbb{I}A \times \mathbb{I}B \times \mathbb{I}Z$.

1. *If* $(A, B, Z) \in \mathcal{D}^*$, *then* $(\widetilde{A}, \hat{B}, \hat{Z}) \in \mathcal{D}^*, \forall \hat{B}, \hat{Z} \in \mathbb{R}^n$.
2. *If* $(A, B, Z) \in \mathcal{D}^*$, *then* $\Gamma^*(\widetilde{A}, \widetilde{B}, \widetilde{Z}) \subset \Gamma^*(A, B, Z)$.

3. If $(A, B, Z) \in \mathcal{D}^*$, then $\Gamma^+(A, B, Z) \subset Z$.
4. If $(A, B, Z) \in \mathcal{D}^*$ and $\Gamma(A, B, Z) \neq \emptyset$, then $\Gamma^+(A, B, Z) = \Gamma(A, B, Z)$.
5. If $(A, B, Z) \in \mathcal{D}^*$ and $\Gamma^*(A, B, Z) \subset Z$, then $\Gamma^*(A, B, Z) = \Gamma(A, B, Z)$.
6. If $\emptyset \neq \Gamma(A, B, Z) \subset \text{int}(Z)$, then $(A, B, Z) \in \mathcal{D}^*$ and $\Gamma^*(A, B, Z) = \Gamma(A, B, Z)$.

Proof Conclusion 1 is obvious and 2 follows from inclusion monotonicity of interval arithmetic. Conclusion 3 follows from Conclusion 3 of Lemma 2.2. To show 4 and 5, suppose $(A, B, Z) \in \mathcal{D}^*$ and denote $\Gamma(A, B, Z) \equiv W_1 \times \ldots \times W_n$,

$$W_i = Z_i \cap \frac{1}{A_{ii}} \Big(B_i - \sum_{k<i} A_{ik} W_k - \sum_{k>i} A_{ik} Z_k \Big), \quad \forall i = 1, \ldots, n. \tag{6}$$

Define W_i^+ as in (5), choose any $i \in \{1, \ldots, n\}$ and assume that $W_i = W_i^+$ for all $k < i$, which is trivially true if $i = 1$. Then, comparing (6) and (5), Conclusion 1 of Lemma 2.2 implies that $W_i = W_i^+$ if $W_i \neq \emptyset$. Then, Conclusion 4 follows by finite induction.

To show 5, define W_i^* as in (4) and assume that $W_i = W_i^*$ for all $k < i$, which is again trivially true if $i = 1$. Comparing (6) and (4) yields $W_i = Z_i \cap W_i^*$. But the assumption that $\Gamma^*(A, B, Z) \subset Z$ implies that $W_i^* \subset Z_i$, and hence $W_i = W_i^*$. Therefore, Conclusion 5 also follows by finite induction.

To show 6, suppose $\emptyset \neq \Gamma(A, B, Z) \subset \text{int}(Z)$. Theorem 4.4.5 (ii) of [15] implies $(A, B, Z) \in \mathcal{D}^*$. Now denoting $\Gamma(A, B, Z) \equiv W_1 \times \ldots \times W_n$, (6) again holds. Assuming that $W_i = W_i^*$ for all $k < i$ (trivial for $i = 1$) and comparing (6) and (4) again yields $W_i = Z_i \cap W_i^*$. The assumption that $\Gamma(A, B, Z) \subset \text{int}(Z)$ implies that $W_i \subset \text{int}(Z_i)$, which is only possible if $W_i = W_i^*$. Then, Conclusion 6 follows by finite induction. $\qquad \square$

The following definition formalizes the notation $\mathcal{H}$ from Corollary I-4.1, with a slight modification to reflect the fact that, in the proposed methods, the reference point $\widetilde{\mathbf{z}}_y$ is a function of Z_y and does not need to be specified independently. Notation is also introduced for iterative application of $\mathcal{H}$, and extended forms based on Γ^+ and Γ^* are defined.

Definition 2.5 Let $\widetilde{\mathbf{z}}_y : \mathbb{ID}_y \to \mathbb{R}^{n_y}$, define $M_\Gamma : \mathbb{ID}_t \times \mathbb{ID}_p \times \mathbb{ID}_x \times \mathbb{ID}_y \times \mathbb{R}^{n_y \times n_y} \to \mathbb{R}^{n_y \times n_y} \times \mathbb{R}^{n_y} \times \mathbb{R}^{n_y}$ by

$$M_\Gamma(I, P, Z_x, Z_y, \mathbf{C}) \equiv \left(\mathbf{C} \left[\frac{\partial \mathbf{g}}{\partial \mathbf{y}} \right] (I, P, Z_x, Z_y), -\mathbf{C} [\mathbf{g}] (I, P, Z_x, \widetilde{\mathbf{z}}(Z_y)), Z_y - \widetilde{\mathbf{z}}(Z_y) \right),$$

and define the set

$$\mathcal{D}_\mathcal{H}^* \equiv \Big\{ (I, P, Z_x, Z_y, \mathbf{C}) \in \mathbb{ID}_t \times \mathbb{ID}_p \times \mathbb{ID}_x \times \mathbb{ID}_y \times \mathbb{R}^{n_y \times n_y} : M_\Gamma(I, P, Z_x, Z_y, \mathbf{C}) \in \mathcal{D}^* \Big\}.$$

For every $K \in \mathbb{N}$, let $\mathcal{H}^K : \mathbb{ID}_t \times \mathbb{ID}_p \times \mathbb{ID}_x \times \mathbb{ID}_y \times \mathbb{R}^{n_y \times n_y} \to \mathbb{R}^{n_y}$ be defined by $\mathcal{H}^K(I, P, Z_x, Z_y^0, \mathbf{C}) \equiv Z_y^K$, where $Z_y^{k+1} = \widetilde{\mathbf{z}}(Z_y^k) + \Gamma \left(M_\Gamma(I, P, Z_x, Z_y^k, \mathbf{C}) \right)$, $\forall k \in \{0, \ldots, K-1\}$. Furthermore, define $\mathcal{H}^{+,K} : \mathcal{D}_\mathcal{H}^* \to \mathbb{R}^{n_y}$ exactly as $\mathcal{H}^K$ with Γ^+ in place of Γ, and define $\mathcal{H}^* : \mathcal{D}_\mathcal{H}^* \to \mathbb{R}^{n_y}$ exactly as $\mathcal{H}^1$ with Γ^* in place of Γ. Finally, define the set

$$\mathcal{D}_\mathcal{H}^K \equiv \Big\{ (I, P, Z_x, Z_y, \mathbf{C}) \in \mathcal{D}_\mathcal{H}^* : \mathcal{H}^K(I, P, Z_x, Z_y, \mathbf{C}) \neq \emptyset \Big\}.$$

For simplicity, the superscript K on $\mathcal{H}^K$ and $\mathcal{H}^{+,K}$ will be omitted when $K = 1$. When $K > 1$, some justification for Definition 2.5 is needed. For any $k \in \{0,\ldots,K-1\}$ with $Z_y^k \in \mathbb{I}D_y$, the definition of Γ implies that $Z_y^{k+1} \subset Z_y^k$, and hence $Z_y^{k+1} \in \mathbb{I}D_y$. Then, a simple inductive argument shows that $\mathcal{H}^K$ is well-defined for any $K \in \mathbb{N}$. In the definition of $\mathcal{H}^{+,K}$, we similarly note that $(I,P,Z_x,Z_y^k,\mathbf{C}) \in \mathcal{D}_{\mathcal{H}}^*$ implies $Z_y^{k+1} \subset Z_y^k$ by Conclusion 3 of Lemma 2.3. It follows by Conclusion 1 of Lemma 2.4 below that $(I,P,Z_x,Z_y^{k+1},\mathbf{C}) \in \mathcal{D}_{\mathcal{H}}^*$, so that again induction shows that $\mathcal{H}^{+,K}$ is well-defined.

In Definition 2.5, the preconditioner $\mathbf{C}$ is allowed to be an interval matrix. This makes $\mathcal{H}^*$, $\mathcal{H}^{+,K}$ and $\mathcal{H}^K$ pure interval functions and is only done for consistency with the results on regularity of interval functions in the next section. In the proposed methods, $\mathbf{C}$ will always be a real matrix. To conform with Definition 2.5, $\mathbf{C}$ is simply identified with the corresponding degenerate element of $\mathbb{IR}^{n_y \times n_y}$.

Specific definitions for $\widetilde{\mathbf{z}}$ will be given when $\mathcal{H}^K$, $\mathcal{H}^{+,K}$ or $\mathcal{H}^*$ are used in later sections. The results in the remainder of this section are independent of this choice.

Lemma 2.4 *Let $K \in \mathbb{N}$, let $(I,P,Z_x,Z_y,\mathbf{C}) \in \mathbb{I}D_t \times \mathbb{I}D_p \times \mathbb{I}D_x \times \mathbb{I}D_y \times \mathbb{IR}^{n_y \times n_y}$ and let $(\widetilde{I},\widetilde{P},\widetilde{Z}_x,\widetilde{Z}_y,\widetilde{\mathbf{C}}) \in \mathbb{I}I \times \mathbb{I}P \times \mathbb{I}Z_x \times \mathbb{I}Z_y \times \mathbb{I}\mathbf{C}$.*

1. *If $(I,P,Z_x,Z_y,\mathbf{C}) \in \mathcal{D}_{\mathcal{H}}^*$, then $(\widetilde{I},\widetilde{P},\widetilde{Z}_x,\widetilde{Z}_y,\widetilde{\mathbf{C}}) \in \mathcal{D}_{\mathcal{H}}^*$.*
2. *If $(I,P,Z_x,Z_y,\mathbf{C}) \in \mathcal{D}_{\mathcal{H}}^*$, then $\mathcal{H}^*(\widetilde{I},\widetilde{P},\widetilde{Z}_x,\widetilde{Z}_y,\widetilde{\mathbf{C}}) \subset \mathcal{H}^*(I,P,Z_x,Z_y,\mathbf{C})$.*
3. *If $(I,P,Z_x,Z_y,\mathbf{C}) \in \mathcal{D}_{\mathcal{H}}^*$, then $\mathcal{H}^{+,K}(I,P,Z_x,Z_y,\mathbf{C}) \subset Z_y$.*
4. *If $(I,P,Z_x,Z_y,\mathbf{C}) \in \mathcal{D}_{\mathcal{H}}^K$, then $\mathcal{H}^K(I,P,Z_x,Z_y,\mathbf{C}) = \mathcal{H}^{+,K}(I,P,Z_x,Z_y,\mathbf{C})$.*
5. *If $(I,P,Z_x,Z_y,\mathbf{C}) \in \mathcal{D}_{\mathcal{H}}^*$ and $\mathcal{H}^*(I,P,Z_x,Z_y,\mathbf{C}) \subset Z_y$, then*

$$\mathcal{H}(I,P,Z_x,Z_y,\mathbf{C}) = \mathcal{H}^*(I,P,Z_x,Z_y,\mathbf{C}). \tag{7}$$

6. *If $\emptyset \neq \mathcal{H}(I,P,Z_x,Z_y,\mathbf{C}) \subset \mathrm{int}(Z_y)$, then $(I,P,Z_x,Z_y,\mathbf{C}) \in \mathcal{D}_{\mathcal{H}}^*$ and (7) holds.*
7. *If $\emptyset \neq \mathcal{H}(I,P,Z_x,Z_y,\mathbf{C}) \subset \mathrm{int}(Z_y)$, $\widetilde{\mathbf{z}}_y(Z_y) \in \mathrm{int}(Z_y)$, and $\mathbf{C}$ is degenerate, then $(\widetilde{I},\widetilde{P},\widetilde{Z}_x,Z_y,\mathbf{C}) \in \mathcal{D}_{\mathcal{H}}^K$.*

Proof Conclusions 1 and 2 follow from inclusion monotonicity of interval arithmetic and the corresponding conclusions of Lemma 2.3 (it is essential in 2 that Z_y, and not $\widetilde{Z}_y$, appears on the left, since otherwise $\widetilde{\mathbf{z}}$ will be modified and inclusion monotonicity does not apply). Conclusion 3 was argued inductively in the discussion above. Conclusion 4 follows by inductive application of Conclusion 4 in Lemma 2.3. Conclusions 5 and 6 are direct applications of the corresponding conclusions of Lemma 2.3. Assume the hypotheses of 7. By Conclusion 3 of Corollary I-4.1, to every $(t,\mathbf{p},\mathbf{z}_x) \in I \times P \times Z_x$ there corresponds some $\mathbf{z}_y \in Z_y$ satisfying $\mathbf{g}(t,\mathbf{p},\mathbf{z}_x,\mathbf{z}_y) = \mathbf{0}$. Choosing any $(t,\mathbf{p},\mathbf{z}_x) \in \widetilde{I} \times \widetilde{P} \times \widetilde{Z}_x$, Conclusion 1 of the same shows that the corresponding $\mathbf{z}_y$ must be in $\mathcal{H}^K(\widetilde{I},\widetilde{P},\widetilde{Z}_x,Z_y,\mathbf{C})$. By Conclusion 1 of the present lemma, this implies $(\widetilde{I},\widetilde{P},\widetilde{Z}_x,Z_y,\mathbf{C}) \in \mathcal{D}_{\mathcal{H}}^K$. $\square$

2.2 Regularity of interval functions

Recall the interval extensions $[\mathbf{f}]$, $[\mathbf{g}]$ and $\left[\frac{\partial \mathbf{g}}{\partial \mathbf{y}}\right]$. For certain computations required by the proposed bounding methods, it will be helpful to recognize that these mappings,

as well as others defined in the previous section, enjoy surprisingly strong regularity conditions. To maintain generality, the required regularity of $[\mathbf{f}]$, $[\mathbf{g}]$ and $\left[\frac{\partial \mathbf{g}}{\partial \mathbf{y}}\right]$ is assumed in Assumption 2.1, and it is argued in Remark 2.1 that this assumption is verifiable for natural interval extensions under very mild restrictions. Subsequently, regularity conditions for $\mathcal{H}^{+,K}$ and $\mathcal{H}^*$ are established as consequences of Assumption 2.1.

Chapter 4 in [17] introduces the class of piecewise C^1 functions, which is used below to formalize the regularity of $[\mathbf{f}]$, $[\mathbf{g}]$ and $\left[\frac{\partial \mathbf{g}}{\partial \mathbf{y}}\right]$. The formal definition of this class is not important here. Only the following known facts will be used:

Lemma 2.5 *Let $E_f \subset \mathbb{R}^n$ and $E_g \subset \mathbb{R}^m$ be open.*

1. *If $\mathbf{f} \in C^1(E_f, \mathbb{R}^m)$, then $\mathbf{f}$ is piecewise C^1 on E_f.*
2. *Let $\mathbf{f}_1, \mathbf{f}_2 : E_f \to \mathbb{R}^m$ and $\mathbf{g} : E_g \to \mathbb{R}^q$ be piecewise C^1 on E_f and E_g, respectively.*
   (a) $\mathbf{f}_1 + \mathbf{f}_2$ is piecewise C^1 on E_f.
   (b) $\mathbf{g} \circ \mathbf{f}_1$ is piecewise C^1 on the open set $E_{fg} \equiv \{\mathbf{z} \in E_f : \mathbf{f}_1(\mathbf{z}) \in E_g\}$.
   (c) If $m = 1$, then $f_1 f_2$, $\min(f_1, f_2)$ and $\max(f_1, f_2)$ are piecewise C^1 on E_f.
3. *If $\mathbf{f} : E_f \to \mathbb{R}^m$ is piecewise C^1 on E_f, then $\mathbf{f}$ is locally Lipschitz continuous on E_f.*
4. *If $\mathbf{f} : E_f \to \mathbb{R}^m$ is piecewise C^1 on E_f, then $\mathbf{f}$ is Frechet differentiable everywhere in E_f except on a subset of Lebesgue measure zero.*

Proof For Conclusions 1 and 2, see p. 92 of [17]. Conclusion 3 is Corollary 4.1.1 in [17], and Conclusion 4 follows from Theorem 3.1.1 in [5]. $\square$

The notion of a piecewise C^1 function is now extended to interval-valued mappings. It is well known that $\mathbb{IR}^n$ is a metric space when equipped with the Hausdorff metric:

$$d_H(Z, Y) = \max\left(\max_i |z_i^L - y_i^L|, \max_i |z_i^U - y_i^U|\right),$$

where $Z, Y \in \mathbb{IR}^n$, $Z \equiv [\mathbf{z}^L, \mathbf{z}^U]$ and $Y \equiv [\mathbf{y}^L, \mathbf{y}^U]$. With this metric, open and closed sets in $\mathbb{IR}^n$ are defined by the standard metric topology, and the standard definition of continuity applies to mapping to and/or from $\mathbb{IR}^n$. From the definition of d_H, it is simple to show that a mapping $\phi : E \subset \mathbb{R}^n \to \mathbb{IR}^m$ is continuous on E if and only if the real-valued functions $\phi^L, \phi^U : E \to \mathbb{R}^m$ defined by

$$[\phi^L(\mathbf{z}), \phi^U(\mathbf{z})] \equiv \phi(\mathbf{z}), \quad \forall \mathbf{z} \in E, \tag{8}$$

are continuous on E. The following definition is therefore consistent with other notions of regularity for interval-valued mappings.

Definition 2.6 Let $E \subset \mathbb{R}^n$ be open, $\phi : E \to \mathbb{IR}^m$, and let the real-valued functions $\phi^L, \phi^U : E \to \mathbb{R}^m$ be defined by (8). The mapping ϕ is called piecewise C^1 on E if ϕ^L and ϕ^U are piecewise C^1 on E.

As an example of such a function, we note the following:

Lemma 2.6 $\square$ *is piecewise C^1 on $\mathbb{R}^n \times \mathbb{R}^n$.*

Proof The result follows from Definition 2.1 and Conclusions 1 and 2 of Lemma 2.5.

From the discussion above, it follows that if ϕ is piecewise C^1 on E, then it is continuous as a mapping from E to $\mathbb{IR}^m$. This leads to the following lemma, which is required for further results to be well-posed.

Lemma 2.7 *Let $\phi : E \subset \mathbb{R}^n \to \mathbb{IR}^m$ be piecewise C^1 on E. If $\mathcal{D} \subset \mathbb{IR}^m$ is open, then*

$$E_{\mathcal{D}} \equiv \{\mathbf{z} \in E : \phi(\mathbf{z}) \in \mathcal{D}\} \tag{9}$$

is open.

Proof Since ϕ is piecewise C^1 on E, it is a continuous on E. Therefore, $E_{\mathcal{D}}$ is the inverse image in E of the open set $\mathcal{D}$ under a continuous mapping, and hence it is open with respect to E. Since E is itself open, $E_{\mathcal{D}}$ is open.

The definition of a piecewise C^1 interval-valued mapping can now be extended to mappings from $\mathbb{IR}^m$ to $\mathbb{IR}^q$ as follows.

Definition 2.7 Let $\mathcal{D} \subset \mathbb{IR}^m$ be open and let $M : \mathcal{D} \to \mathbb{IR}^q$. M is called piecewise C^1 on $\mathcal{D}$ if, for every piecewise C^1 function $\phi : E \subset \mathbb{R}^n \to \mathbb{IR}^m$, the mapping

$$E_{\mathcal{D}} \ni \mathbf{z} \longmapsto M(\phi(\mathbf{z})) \in \mathbb{IR}^q \tag{10}$$

is piecewise C^1 on the open set $E_{\mathcal{D}} \equiv \{\mathbf{z} \in E : \phi(\mathbf{z}) \in \mathcal{D}\}$.

As an example of such a function, we note the following:

Lemma 2.8 $\widetilde{\cap}$ *is piecewise C^1 on $\mathbb{IR}^n \times \mathbb{IR}^n$.*

Proof If $\mathbf{z}^L, \mathbf{z}^U \in \mathbb{R}^n$ and $\mathbf{z}^L \leq \mathbf{z}^U$, it is easily verified that $\mathrm{mid}(\mathbf{z}^L, \mathbf{z}^U, \hat{\mathbf{z}})$ is equivalent to $\max(\mathbf{z}^L, \min(\mathbf{z}^U, \hat{\mathbf{z}}))$ for all $\hat{\mathbf{z}} \in \mathbb{R}^n$. The result now follows from Definition 2.2 and Conclusion 2 of Lemma 2.5. $\square$

The following two lemmas establish some basic facts about piecewise C^1 interval functions, which will be used throughout.

Lemma 2.9 *Let $\mathcal{D} \subset \mathbb{IR}^m$. If $M : \mathcal{D} \to \mathbb{IR}^q$ is piecewise C^1 on $\mathcal{D}$, then it is continuous on $\mathcal{D}$.*

Proof Choose any $[\mathbf{v}, \mathbf{w}] \in \mathcal{D}$ and any $\epsilon > 0$. Choosing $\phi = \square$ in Definition 2.7 (see Lemma 2.6), the hypothesis on M implies that the function $M(\square(\cdot, \cdot))$ is piecewise C^1, and hence continuous, on $E_{\mathcal{D}} \equiv \{(\mathbf{v}, \mathbf{w}) \in \mathbb{R}^n \times \mathbb{R}^n : \square(\mathbf{v}, \mathbf{w}) \in \mathcal{D}\}$. Since $E_{\mathcal{D}}$ is open, $\exists \delta > 0$ such that

$$d_H(M(\square(\mathbf{v}, \mathbf{w})), M(\square(\mathbf{v}', \mathbf{w}'))) \leq \epsilon \tag{11}$$

for every $(\mathbf{v}', \mathbf{w}') \in \mathbb{R}^n \times \mathbb{R}^n$ such that $\max(\|\mathbf{v} - \mathbf{v}'\|_\infty, \|\mathbf{w} - \mathbf{w}'\|_\infty) \leq \delta$.

Now, choose any $[\mathbf{v}', \mathbf{w}'] \in \mathcal{D}$ such that $d_H([\mathbf{v}, \mathbf{w}], [\mathbf{v}', \mathbf{w}']) \leq \delta$. Noting that $\square(\mathbf{v}, \mathbf{w}) = [\mathbf{v}, \mathbf{w}]$ and $\square(\mathbf{v}', \mathbf{w}') = [\mathbf{v}', \mathbf{w}']$ by Conclusion 1 of Lemma 2.1, (11) states that

$$d_H(M([\mathbf{v}, \mathbf{w}]), M([\mathbf{v}', \mathbf{w}'])) \leq \epsilon. \tag{12}$$

Since, $[\mathbf{v}', \mathbf{w}']$ was arbitrary, M is continuous at $[\mathbf{v}, \mathbf{w}]$, and hence on $\mathcal{D}$. $\square$

Lemma 2.10 *Let $\mathcal{D}_1 \subset \mathbb{R}^m$ and $\mathcal{D}_2 \subset \mathbb{R}^k$ be open and let $M_1 : \mathcal{D}_1 \to \mathbb{R}^k$ and $M_2 : \mathcal{D}_2 \to \mathbb{R}^q$ be piecewise C^1 on $\mathcal{D}_1$ and $\mathcal{D}_2$, respectively. The set $\mathcal{D}_{12} \equiv \{Z \in \mathcal{D}_1 : M_1(Z) \in \mathcal{D}_2\}$ is open and $M_2 \circ M_1$ is piecewise C^1 on $\mathcal{D}_{12}$.*

Proof Since M_1 is piecewise C^1 on $\mathcal{D}_1$, it is continuous there. Then, the set $\mathcal{D}_{12}$ is the inverse image in $\mathcal{D}_1$ of the open set $\mathcal{D}_2$ under a continuous mapping. Therefore, $\mathcal{D}_{12}$ is open with respect to $\mathcal{D}_1$. Since $\mathcal{D}_1$ is open in $\mathbb{R}^m$, so is $\mathcal{D}_{12}$.

Choose any piecewise C^1 mapping $\phi : E \subset \mathbb{R}^n \to \mathbb{R}^m$ and define $E_{\mathcal{D}_1} \equiv \{\mathbf{z} \in E : \phi(\mathbf{z}) \in \mathcal{D}_1\}$. Now define $\phi' : E_{\mathcal{D}_1} \to \mathbb{R}^k$ by

$$\phi'(\mathbf{z}) = M_1(\phi(\mathbf{z})), \quad \forall \mathbf{z} \in E_{\mathcal{D}_1}. \tag{13}$$

Since M_1 is piecewise C^1 on $\mathcal{D}_1$, ϕ' is piecewise C^1 on $E_{\mathcal{D}_1}$. But since M_2 is piecewise C^1 on $\mathcal{D}_2$, this implies that

$$\mathbf{z} \longmapsto M_2(\phi'(\mathbf{z})) = M_2(M_1(\phi(\mathbf{z}))) \tag{14}$$

is piecewise C^1 on the set

$$\{\mathbf{z} \in E_{\mathcal{D}_1} : \phi'(\mathbf{z}) \in \mathcal{D}_2\} = \{\mathbf{z} \in E : \phi(\mathbf{z}) \in \mathcal{D}_1 \text{ and } M_1(\phi(\mathbf{z})) \in \mathcal{D}_2\}, \tag{15}$$

$$= \{\mathbf{z} \in E : \phi(\mathbf{z}) \in \mathcal{D}_{12}\}. \tag{16}$$

But ϕ was chosen arbitrarily, so $M_2 \circ M_1$ is piecewise C^1 on $\mathcal{D}_{12}$.   □

One further lemma is required, after which the fundamental assumption on the regularity of $[\mathbf{f}]$, $[\mathbf{g}]$ and $\left[\frac{\partial \mathbf{g}}{\partial \mathbf{y}}\right]$ is stated.

Lemma 2.11 *If $D \subset \mathbb{R}^n$ is open, then $\mathbb{I}D$ is open in $\mathbb{IR}^n$.*

Proof If $\mathbb{I}D$ is empty, then it is trivially open. Otherwise, choose $Z \in \mathbb{I}D$. Then, $Z \subset D$, and since D is open, $\exists \epsilon > 0$ such that $\hat{\mathbf{z}} \in D$ if $\|\hat{\mathbf{z}} - \mathbf{z}\|_\infty \leq \epsilon$ and $\mathbf{z} \in Z$ (uniformity of ϵ for every $\mathbf{z} \in Z$ results from the compactness of Z, as per Theorem 4.6 in [13]). Let $\hat{Z} \in \mathbb{IR}^n$ satisfy $d_H(Z, \hat{Z}) \leq \epsilon$. By the definition of d_H, this implies that, for any $\hat{\mathbf{z}} \in \hat{Z}$, there exists $\mathbf{z} \in Z$ such that $\|\hat{\mathbf{z}} - \mathbf{z}\|_\infty \leq \epsilon$. But this implies that $\hat{Z} \subset D$ or, equivalently, $\hat{Z} \in \mathbb{I}D$. Hence, Z is an interior point of $\mathbb{I}D$ and, since Z was chosen arbitrarily, $\mathbb{I}D$ is open.   □

Assumption 2.1 *Let $c : D_t \times D_p \times D_x \times D_y \to \mathbb{R}$ represent any of f_i, g_j or $\frac{\partial g_j}{\partial y_k}$, with indices $i \in \{1, \ldots, n_x\}$ and $j, k \in \{1, \ldots, n_y\}$. The interval extension $[c]$ is piecewise C^1 on the open set $\mathbb{I}D_t \times \mathbb{I}D_p \times \mathbb{I}D_x \times \mathbb{I}D_y$.*

Remark 2.1 When c is factorable [12,20] and $[c]$ is the natural interval extension (as it is in our implementation), Assumption 2.1 holds under minor restrictions on the factors of c. If the interval extension of each factor is piecewise C^1 on an open domain, then it follows directly from Lemma 2.10 that $[c]$ is piecewise C^1. From the rules of interval arithmetic [15], this is clearly true of the interval extensions for addition, multiplication, division, and nearly all common univariate functions (see for example the set of so-called elementary functions in Section 1.2 of [15]). Among common functions, the only problematic case is the family x^a with $0 < a < 1$ on domains containing zero.

The remaining results of this section address the regularity of $\mathcal{H}^K, \mathcal{H}^{+,K}$ and $\mathcal{H}^*$.

Lemma 2.12 $\mathcal{D}^*$ *is open and both Γ^+ and Γ^* are piecewise C^1 on $\mathcal{D}^*$.*

Proof Let $U \equiv \{(\mathbf{A}, \mathbf{b}, \mathbf{z}) \in \mathbb{R}^{n \times n} \times \mathbb{R}^n \times \mathbb{R}^n : \mathbf{A}_{ii} \neq 0, \forall i = 1, \ldots, n\}$. By definition, $\mathbb{I}U = \mathcal{D}^*$. Since U is open, $\mathcal{D}^*$ is open by Lemma 2.11. It follows from (4), the rules of interval addition, subtraction, multiplication and division (see [15]), and Conclusion 2 of Lemma 2.5 that Γ^* is piecewise C^1 on $\mathcal{D}^*$. For Γ^+, (5) leads to the same conclusion by additionally applying Lemmas 2.8 and 2.10. $\qquad\square$

Theorem 2.1 *Suppose Assumption 2.1 holds and the function $\widetilde{\mathbf{z}}_y$ in Definition 2.5 is piecewise C^1 on $\mathbb{I}D_y$. Then $\mathcal{D}^*_{\mathcal{H}}$ is open and $\mathcal{H}^{K,+}$ and $\mathcal{H}^*$ are piecewise C^1 on $\mathcal{D}^*_{\mathcal{H}}$.*

Proof Under the stated hypotheses, it follows from the rules of interval addition, subtraction and multiplication and Conclusion 2 of Lemma 2.5 that M_Γ in Definition 2.5 is piecewise C^1 on $\mathbb{I}D_t \times \mathbb{I}D_p \times \mathbb{I}D_x \times \mathbb{I}D_y \times \mathbb{R}^{n_y \times n_y}$. By Lemma 2.12, Γ^* and Γ^+ are piecewise C^1 on $\mathcal{D}^*$, which is open. Then Lemma 2.10 implies that $\mathcal{D}^*_{\mathcal{H}}$ is open and $\Gamma^* \circ M_\Gamma$ is piecewise C^1 there, so that $\mathcal{H}^*$ is piecewise C^1 on $\mathcal{D}^*_{\mathcal{H}}$ by the hypothesis on $\widetilde{\mathbf{z}}_y$ and Conclusion 2 of Lemma 2.5. For $\mathcal{H}^{+,K}$, we additionally note that $(I, P, Z_x, Z_y^k, \mathbf{C}) \in \mathcal{D}^*_{\mathcal{H}}$ for all $k \in \{0, \ldots, K-1\}$ (see discussion following Definition 2.5). Then, the result follows by K applications of Lemmas 2.10 and Lemma 2.5. $\quad\square$

3 A Generic Two-Phase Algorithm

In this section, we introduce the first bounding method of this article, which is based on a time-stepping framework outlined in Algorithm 1 below. In a generic time step j, the algorithm proceeds in two phases. The purpose of Phase 1 is to establish existence and uniqueness of a solution $(\mathbf{x}, \mathbf{y})$ of I -(1) (Equation (1) in Part 1) on $I_j \times P$, for some time interval $I_j = [t_{j-1}, t_j]$, and to determine crude enclosures $Z_{x,j}$ and $Z'_{y,j}$ satisfying

$$(\mathbf{x}(t, \mathbf{p}), \mathbf{y}(t, \mathbf{p})) \in Z_{x,j} \times Z'_{y,j}, \quad \forall (t, \mathbf{p}) \in I_j \times P. \tag{17}$$

Subsequently, Phase 2 computes refined intervals $X_j \subset Z_{x,j}$ and $Y_j \subset Z'_{y,j}$ such that

$$(\mathbf{x}(t_j, \mathbf{p}), \mathbf{y}(t_j, \mathbf{p})) \in X_j \times Y_j, \quad \forall \mathbf{p} \in P. \tag{18}$$

In contrast to $Z_{x,j}$ and $Z'_{y,j}$, the refined bounds X_j and Y_j are valid only at t_j. The method for computing these refinements is not specified in Algorithm 1. Our approach is the subject of §5.

As input, Algorithm 1 takes intervals $I = [t_0, t_f] \subset D_t$, $P \subset D_p$ and $X_0 \subset D_x$ under the assumption that $\mathbf{x}_0(P) \subset X_0$, $\forall \mathbf{p} \in P$. The final input is a vector $\hat{\mathbf{y}}_0 \in D_y$ satisfying $\mathbf{g}(t_0, \hat{\mathbf{p}}, \mathbf{x}_0(\hat{\mathbf{p}}), \hat{\mathbf{y}}_0) = \mathbf{0}$ for some $\hat{\mathbf{p}} \in P$. The purpose of this vector is to specify a particular solution of interest in case the DAE in question permits multiple regular solutions (see Example I -3.1). Phases 1 and 2 described above correspond to Steps 3 and 6, respectively. Finally, the algorithm makes use of the functions $\mathcal{H}^K$ and $\widetilde{\mathbf{z}}_y$ from Definition 2.5, and is independent of the choice of $\widetilde{\mathbf{z}}_y$. Choices for $\widetilde{\mathbf{z}}_y$ and $\mathbf{C}$ are discussed in §4.1.

Algorithm 1 (Two-phase algorithm)

1. Input: $I = [t_0, t_f]$, P, X_0, $\hat{\mathbf{y}}_0$.
2. Initialize $j := 1$, $Y_0 := [\hat{\mathbf{y}}_0, \hat{\mathbf{y}}_0]$.
3. Find $I_j = [t_{j-1}, t_j]$, $Z_{x,j}$, $Z_{y,j}$ and $\mathbf{C}_j$ satisfying

$$(I_j, P, Z_{x,j}, Z_{y,j}, \mathbf{C}_j) \in \mathbb{ID}_t \times \mathbb{ID}_p \times \mathbb{ID}_x \times \mathbb{ID}_y \times \mathbb{R}^{n_y \times n_y}, \tag{19}$$

$$Y_{j-1} \subset Z_{y,j}, \tag{20}$$

$$\widetilde{\mathbf{z}}_y(Z_{y,j}) \in \operatorname{int}(Z_{y,j}), \tag{21}$$

$$\emptyset \neq Z'_{y,j} \equiv \mathcal{H}(I_j, P, Z_{x,j}, Z_{y,j}, \mathbf{C}_j) \subset \operatorname{int}(Z_{y,j}), \tag{22}$$

$$X_{j-1} + [0, t_j - t_{j-1}][\mathbf{f}](I_j, P, Z_{x,j}, Z'_{y,j}) \subset Z_{x,j}. \tag{23}$$

4. Set $X_j := Z_{x,j}$ and $Y_j := Z'_{y,j}$. If $j = 1$, set $Y_0 := Z'_{y,j}$.
5. If $j = 1$, refine Y_0 (see §5).
6. Refine X_j and Y_j (see §5).
7. If $t_j \geq t_f$, terminate. Otherwise, set $j := j + 1$ and go to 3.

The behavior of Algorithm 1 is formalized in Corollary 3.1 below. Of course, this depends on the refinement procedures in Steps 5 and 6, which have not yet been specified. Therefore, we assume the following:

Assumption 3.1 *Consider an iteration $J \in \mathbb{N}$ of Algorithm 1 and suppose that Steps 3-4 are complete. Let $(\mathbf{x}, \mathbf{y})$ be a regular solution of I-(1) on $[t_0, t_J] \times P$ satisfying (17) for all $j \in \{1, \ldots, J\}$. If $J = 1$, the refinement to Y_0 computed in Step 5 satisfies (18) with $j = 0$. Suppose that Step 5 is complete. If $(\mathbf{x}, \mathbf{y})$ additionally satisfies (18) for all $j \in \{0, \ldots, J-1\}$, then Step 6 produces X_J and Y_J satisfying (18) with $j = J$.*

Corollary 3.1 *Let $(I, P, X_0, \hat{\mathbf{y}}_0) \in \mathbb{ID}_t \times \mathbb{ID}_p \times \mathbb{ID}_x \times D_y$ satisfy $\mathbf{x}_0(\mathbf{p}) \in X_0$, $\forall \mathbf{p} \in P$, and $\mathbf{g}(t_0, \hat{\mathbf{p}}, \mathbf{x}_0(\hat{\mathbf{p}}), \hat{\mathbf{y}}_0) = \mathbf{0}$ for some $\hat{\mathbf{p}} \in P$. Suppose that Algorithm 1 has completed J iterations, furnishing the intervals Y_0 and*

$$I_j, Z_{x,j}, Z_{y,j}, Z'_{y,j}, X_j, Y_j, \quad j = 1, \ldots, J. \tag{24}$$

Then there exists a regular solution $(\mathbf{x}, \mathbf{y})$ of I-(1) on $[t_0, t_J] \times P$ with $\mathbf{y}(t_0, \hat{\mathbf{p}}) = \hat{\mathbf{y}}_0$, satisfying (17) for every $j \in \{1, \ldots, J\}$ and (18) for every $j \in \{0, \ldots, J\}$. Furthermore, for any $\widetilde{I} = [t_0, \widetilde{t}] \subset [t_0, t_J]$, any connected $\widetilde{P} \subset P$, and any solution $(\mathbf{x}^*, \mathbf{y}^*)$ of I-(1) on $\widetilde{I} \times \widetilde{P}$, either $(\mathbf{x}^*, \mathbf{y}^*) = (\mathbf{x}, \mathbf{y})$ on $\widetilde{I} \times \widetilde{P}$, or $\mathbf{y}^*(t_0, \mathbf{p}) \notin Z_{y,1}$, $\forall \mathbf{p} \in \widetilde{P}$.

Proof Define $(\mathbf{x}^*, \mathbf{y}^*)$ as above and suppose that $\mathbf{y}^*(t_0, \mathbf{p}) \in Z_{y,1}$ for at least one $\mathbf{p} \in \widetilde{P}$. Consider the following inductive hypotheses for $k \in \{1, \ldots, J\}$:

1. There exists a regular solution $(\mathbf{x}, \mathbf{y})$ of I-(1) on $[t_0, t_k] \times P$,
2. $(\mathbf{x}, \mathbf{y}) = (\mathbf{x}^*, \mathbf{y}^*)$ on $[t_0, \min(t_k, \widetilde{t})] \times \widetilde{P}$,
3. (17) holds for $j \in \{1, \ldots, k\}$,
4. $\mathbf{y}(t_0, \hat{\mathbf{p}}) = \hat{\mathbf{y}}_0$,
5. (18) holds for $j \in \{0, \ldots, k\}$.

It suffices to show that these hypotheses hold with $k = J$.

Let $k = 1$. Since (19)-(23) hold with $j = 1$, Theorem I-4.2 establishes Hypotheses 1-3. Because $\hat{\mathbf{y}}_0$ is a zero of $\mathbf{g}(t_0, \hat{\mathbf{p}}, \mathbf{x}_0(\hat{\mathbf{p}}), \cdot)$ and $\hat{\mathbf{y}}_0 \in Z_{y,1}$ by (20), Hypothesis 4 follows

from Conclusion 3 of Corollary I-4.1. Applying Assumption 3.1 with $J = 1$ proves Hypothesis 5.

Choose any $k \in \{1, \ldots, J-1\}$ and assume Hypotheses 1-5. Since $\mathbf{x}(t_k, P) \subset X_k$ and (19)-(23) hold with $j = k+1$, Theorem I-4.2 furnishes a regular solution of I-(1a) on $I_{k+1} \times P$, $(\hat{\mathbf{x}}, \hat{\mathbf{y}}) \in C^1(I_{k+1} \times P, Z_{x,k+1}) \times C^1(I_{k+1} \times P, Z'_{y,k+1})$, satisfying $\hat{\mathbf{x}}(t_k, \mathbf{p}) = \mathbf{x}(t_k, \mathbf{p})$, $\forall \mathbf{p} \in P$. Noting that both $\mathbf{y}(t_k, \mathbf{p})$ and $\hat{\mathbf{y}}(t_k, \mathbf{p})$ are zeros of $\mathbf{g}(t_k, \mathbf{p}, \mathbf{x}(t_k, \mathbf{p}), \cdot)$ and $\mathbf{y}(t_k, \mathbf{p}) \in Y_k \subset Z_{y,k+1}$ by (20), it follows from Conclusion 3 of Corollary I-4.1 that $\mathbf{y}(t_k, \mathbf{p}) = \hat{\mathbf{y}}(t_k, \mathbf{p})$, $\forall \mathbf{p} \in P$. If $\widetilde{t} \geq t_k$, Hypothesis 2 implies that we also have $\hat{\mathbf{x}}(t_k, \mathbf{p}) = \mathbf{x}^*(t_k, \mathbf{p})$ and $\hat{\mathbf{y}}(t_k, \mathbf{p}) = \mathbf{y}^*(t_k, \mathbf{p})$, $\forall \mathbf{p} \in \widetilde{P}$, so that $(\hat{\mathbf{x}}, \hat{\mathbf{y}}) = (\mathbf{x}^*, \mathbf{y}^*)$ on $[t_k, \min(t_{k+1}, \widetilde{t})] \times \widetilde{P}$ by Theorem I-4.2.

From the arguments above, $(\hat{\mathbf{x}}, \hat{\mathbf{y}})$ extends $(\mathbf{x}, \mathbf{y})$ onto all of $[t_0, t_{k+1}] \times P$, and this extension satisfies Hypothesis 1-4 with $k := k+1$. Applying Assumption 3.1 with $J = k+1$ establishes Hypotheses 5, and finite induction completes the proof. $\square$

From Corollary 3.1, it is clear that Algorithm 1 produces bounds on a single, isolated solution of I-(1) specified by the input $\hat{\mathbf{y}}_0$. This input can be ignored by omitting (20) when $j = 1$. However, the algorithm still produces bounds on a unique solution dictated by the interval $Z_{y,1}$ found in the first time step. If one is interested in bounds on all solutions, then Algorithm 1 would need to be applied to each solution in turn, though it has no provisions for exhaustively enumerating solutions. This problem is not pursued in this article, though a good starting point is provided by Theorem I-5.1. On the other hand, if there is a particular solution of interest, then Algorithm 1 avoids any unnecessary conservatism that would result from bounding other solutions as well.

4 Satisfying the existence and uniqueness test computationally (Phase 1)

In this section, the execution of Step 3 in a single time step J of Algorithm 1 is considered. Based on the previous time step, it is assumed that there exists a regular solution $(\mathbf{x}, \mathbf{y})$ of I-(1) on $[t_0, t_{J-1}] \times P$ satisfying $\mathbf{y}(t_0, \hat{\mathbf{p}}) = \hat{\mathbf{y}}_0$ and $\mathbf{x}(t_{J-1}, P) \subset X_{J-1}$. The objective is to derive an automatic computational procedure for finding intervals I_J, $Z_{x,J}$, $Z_{y,J}$ and $\mathbf{C}_J$ satisfying (19)-(23). Though we present an effective method for this task, it is generally impossible to guarantee that such intervals can be found. This seems to be an inherent complication owing to the implicit nature of nonlinear DAEs, and hence of the inclusion (22), and it appears in much the same form in both of the methods in [16] and [10]. However, it is important to note that the validity of any intervals provided by Step 3 is guaranteed, regardless of the method used to find them. The proposed procedure will either succeed in satisfying (19)-(23), and hence (17) with $j = J$, or it will fail and report an error, forcing Algorithm 1 to terminate prematurely.

Since the implicit conditions (22) and (23) are the most challenging, they are addressed first. The key insight used to satisfy these conditions is that, once some putative $\mathbf{C}_J$ and t_J have been chosen, intervals $Z_{x,J}$ and $Z_{y,J}$ satisfying (22) and (23) are related to solutions of a square system of real-valued algebraic equations that can be solved by standard methods with a few caveats. This approach is developed

below. A complete algorithm for satisfying all of the conditions (19)-(23) is presented in §4.2.

Lemma 4.1 *The conditions* (19) *and* (22), *with* $j = J$, *are equivalent to*

$$(I_J, P, Z_{x,J}, Z_{y,J}, \mathbf{C}_J) \in \mathcal{D}_{\mathcal{H}}^*, \tag{25}$$

$$\mathcal{H}^*(I_J, P, Z_{x,J}, Z_{y,J}, \mathbf{C}_J) \subset \mathrm{int}(Z_{y,J}), \tag{26}$$

provided that $\mathbf{C}_J$ *is degenerate (i.e., a singleton).*

Proof The result is a direct application of Conclusions 5 and 6 of Lemma 2.4. □

For the following result, denote $[\mathbf{x}_{J-1}^L, \mathbf{x}_{J-1}^U] \equiv X_{J-1}$ and

$$[\mathcal{H}^{*,L}(I, P, Z_x, Z_y, \mathbf{C}), \mathcal{H}^{*,U}(I, P, Z_x, Z_y, \mathbf{C})] \equiv \mathcal{H}^*(I, P, Z_x, Z_y, \mathbf{C}). \tag{27}$$

Lemma 4.2 *Let* $I_J \equiv [t_{J-1}, t_J] \in \mathbb{ID}_t$, $P \in \mathbb{ID}_p$, $\mathbf{C}_J \in \mathbb{R}^{n_y \times n_y}$ *and* $\gamma > 0$. *If the vectors* $\mathbf{z}_x^L, \mathbf{z}_x^U \in \mathbb{R}^{n_x}$ *and* $\mathbf{z}_y^L, \mathbf{z}_y^U \in \mathbb{R}^{n_y}$ *satisfy*

$$(I_J, P, \square(\mathbf{z}_x^L, \mathbf{z}_x^U), \square(\mathbf{z}_y^L, \mathbf{z}_y^U), \mathbf{C}_J) \in \mathcal{D}_{\mathcal{H}}^*, \tag{28}$$

$$\mathbf{z}_y'^L := \mathcal{H}^{*,L}(I_J, P, \square(\mathbf{z}_x^L, \mathbf{z}_x^U), \square(\mathbf{z}_y^L, \mathbf{z}_y^U), \mathbf{C}_J), \tag{29}$$

$$\mathbf{z}_y'^U := \mathcal{H}^{*,U}(I_J, P, \square(\mathbf{z}_x^L, \mathbf{z}_x^U), \square(\mathbf{z}_y^L, \mathbf{z}_y^U), \mathbf{C}_J), \tag{30}$$

$$\mathbf{0} = \mathbf{z}_y^L - \mathbf{z}_y'^L + \mathbf{1}\gamma, \tag{31}$$

$$\mathbf{0} = -\mathbf{z}_y^U + \mathbf{z}_y'^U + \mathbf{1}\gamma, \tag{32}$$

$$\mathbf{0} = \mathbf{z}_x^L - \mathbf{x}_{J-1}^L - [0, t_J - t_{J-1}][\mathbf{f}]^L(I_J, P, \square(\mathbf{z}_x^L, \mathbf{z}_x^U), \square(\mathbf{z}_y'^L, \mathbf{z}_y'^U)) + \mathbf{1}\gamma, \tag{33}$$

$$\mathbf{0} = -\mathbf{z}_x^U + \mathbf{x}_{J-1}^U + [0, t_J - t_{J-1}][\mathbf{f}]^U(I_J, P, \square(\mathbf{z}_x^L, \mathbf{z}_x^U), \square(\mathbf{z}_y'^L, \mathbf{z}_y'^U)) + \mathbf{1}\gamma, \tag{34}$$

then $\mathbf{z}_x^L < \mathbf{z}_x^U$ *and* $\mathbf{z}_y^L < \mathbf{z}_y^U$, *and* $Z_{x,J} \equiv [\mathbf{z}_x^L, \mathbf{z}_x^U]$ *and* $Z_{y,J} \equiv [\mathbf{z}_y^L, \mathbf{z}_y^U]$ *satisfy* (19), (22) *and* (23) *with* $j = J$. *Furthermore, these conclusions remain true if the right-hand sides of* (31)-(34) *are componentwise less than* γ.

Proof It suffices to prove the case where the right-hand sides of (31)-(34) are componentwise less than γ. Since $\mathcal{H}^*$ returns an interval, $\mathbf{z}_y'^L \le \mathbf{z}_y'^U$ and hence

$$\mathbf{z}_y^L < \mathbf{z}_y'^L \le \mathbf{z}_y'^U < \mathbf{z}_y^U. \tag{35}$$

An analogous argument shows that $\mathbf{z}_x^L < \mathbf{z}_x^U$.

Let $Z_{x,J}$ and $Z_{y,J}$ be as in the statement of the lemma, and let $Z_y' = [\mathbf{z}_y'^L, \mathbf{z}_y'^U]$. Then, (28) implies (25) and (35) implies (26). Then, (19) and (22) follow from Lemma 4.1. Again, an argument analogous to (35) shows that $X_{J-1} + [0, t_J - t_{J-1}][\mathbf{f}](I_J, P, Z_{x,J}, Z_{y,J}') \subset \mathrm{int}(Z_{x,J})$, which implies (23). □

Equations (31)-(34) form a system of nonlinear algebraic equations of the general form

$$\mathbf{L}(\mathbf{z}) = \mathbf{0}, \tag{36}$$

where $\mathbf{z}$ is a concatenation of the vectors $\mathbf{z}_x^L$, $\mathbf{z}_x^U$, $\mathbf{z}_y^L$ and $\mathbf{z}_y^U$, and the domain of $\mathbf{L}$ is specified by (28). To compute intervals satisfying the existence and uniqueness conditions (19), (22) and (23), (36) is solved using a Newton-type iteration of the form

$$\mathbf{z}^{k+1} := \mathbf{z}^k - \widetilde{\mathbf{J}}^{-1}(\mathbf{z}^k)\mathbf{L}(\mathbf{z}^k) \tag{37}$$

(this should not be confused with the interval Newton method used to derive $\mathcal{H}^*$, and hence equations (31) and (32)). During this iteration, we may terminate whenever $\mathbf{L}(\mathbf{z}^k) < \mathbf{1}\gamma$ for some iterate, and Lemma 4.2 ensures that $\mathbf{z}^k$ furnishes the desired intervals. Using the definition of $\mathcal{H}^*$ and the rules of interval arithmetic, it is in principle possible to write out explicit expressions for the functions $\mathbf{L}$, though they may be very cumbersome. Then, the only complication with this approach is that $\mathbf{L}$ is in general nonsmooth owing to the rules of interval arithmetic. Even so, the developments of §2.2 imply sufficient regularity of $\mathbf{L}$ for a Newton-type method to be well motivated.

Lemma 4.3 *Let $I_J \equiv [t_{J-1}, t_J] \in \mathbb{ID}_t$, $P \in \mathbb{ID}_p$, $\mathbf{C}_J \in \mathbb{R}^{n_y \times n_y}$ and $\gamma > 0$. Suppose Assumption 2.1 holds and the function $\widetilde{\mathbf{z}}_y$ in Definition 2.5 is piecewise C^1 on $\mathbb{ID}_y$. Then the set*

$$E_{\mathcal{H}}^* \equiv \left\{ (\mathbf{z}_x^L, \mathbf{z}_x^U, \mathbf{z}_y^L, \mathbf{z}_y^U) \in \mathbb{R}^{2(n_x+n_y)} : (I_J, P, \square(\mathbf{z}_x^L, \mathbf{z}_x^U), \square(\mathbf{z}_y^L, \mathbf{z}_y^U), \mathbf{C}_J) \in \mathcal{D}_{\mathcal{H}}^* \right\} \tag{38}$$

is open and $\mathbf{L}$ is Frechet differentiable a.e. in $E_{\mathcal{H}}^*$.

Proof Define $\phi : \mathbb{R}^{2(n_x+n_y)} \to \mathbb{IR} \times \mathbb{IR}^{n_p} \times \mathbb{IR}^{n_x} \times \mathbb{IR}^{n_y} \times \mathbb{IR}^{n_y \times n_y}$ by

$$\phi(\mathbf{z}_x^L, \mathbf{z}_x^U, \mathbf{z}_y^L, \mathbf{z}_y^U) \equiv (I_J, P, \square(\mathbf{z}_x^L, \mathbf{z}_x^U), \square(\mathbf{z}_y^L, \mathbf{z}_y^U), \mathbf{C}_J). \tag{39}$$

By Lemma 2.6, ϕ is piecewise C^1 on $\mathbb{R}^{2(n_x+n_y)}$. By Theorem 2.1, $\mathcal{D}_{\mathcal{H}}^*$ is open and $\mathcal{H}^*$ is piecewise C^1 there. Then Lemma 2.7 shows that $E_{\mathcal{H}}^*$ is open by and it follows from Definition 2.7 that the right-hand sides of (31) and (32) are piecewise C^1 on $E_{\mathcal{H}}^*$. From Assumption 2.1, the same holds for (33) and (34). Then, Conclusion 4 of Lemma 2.5 implies differentiability a.e. in $E_{\mathcal{H}}^*$. $\qquad\square$

To implement (37), the matrix $\widetilde{\mathbf{J}}(\mathbf{z}^k)$ is computed by forward automatic differentiation [7]. Automatic differentiation (AD) provides exact derivative evaluations for factorable functions by propagating derivatives through the sequence of factors by repeated application of the addition, multiplication and chain rules of differentiation. As mentioned above, the right-hand sides of (31)-(34) may involve nonsmooth operations resulting from the rules of interval arithmetic. If these operations are piecewise C^1, as we have assumed, then AD can be easily extended to handle them as well. For example, consider the operation

$$c(\mathbf{z}) = \min(a(\mathbf{z}), b(\mathbf{z})), \tag{40}$$

which is ubiquitous in interval computations. To propagate derivatives through this operation, we simply let $\partial c / \partial \mathbf{z}$ equal $\partial a / \partial \mathbf{z}$ when $a(\mathbf{z}) \leq b(\mathbf{z})$, and $\partial b / \partial \mathbf{z}$ when $a(\mathbf{z}) > b(\mathbf{z})$. The value assigned to the derivative when $a(\mathbf{z}) = b(\mathbf{z})$ is arbitrary. Extending

this approach to other simple piecewise C^1 functions, an in house C++ library has been developed that uses operator overloading to both do interval computations and compute such pseudo-derivatives of the resulting bounds. During the differentiation of $\mathbf{L}$ at some point $\mathbf{z}$, the evaluation of any operation at a nondifferentiable point (e.g., when $a(\mathbf{z}) = b(\mathbf{z})$ above) implies that $\mathbf{z}$ is a member of the set of measure zero in Lemma 4.3. For all other points, this scheme results in the true Jacobian.

A thorough survey of methods for solving nonsmooth equations is given in [5]. Among these, the *semi-smooth Newton methods*, which are based on the set-valued *generalized Jacobian*, provide the most satisfactory convergence properties, similar to those of a standard Newton iteration. Unfortunately, there is little work on computing an element of the generalized Jacobian. It is known that the directional derivatives of piecewise C^1 functions obey a chain rule, from which it follows that the forward mode of AD will give correct directional derivatives [6,17]. On the other hand, the matrix formed by computing the directional derivatives in all coordinate directions is not necessarily an element of the generalized Jacobian [11]. From this, it follows that $\widetilde{\mathbf{J}}$, as computed above, will not necessarily be an element of the generalized Jacobian, and hence (37) may not enjoy the properties of semi-smooth Newton methods. However, [11] also presents a modified forward mode AD algorithm that is guaranteed to generate an element of the generalized Jacobian for functions where the nonsmoothness arises from the absolute value function. Further work is underway to extend this method to a much broader class of functions. Thus, the prospects for improving the iteration (37) in the future are promising. Finally, we emphasize again that the use of this iteration is still valid. It will either succeed in satisfying (19)-(23), or it will fail and report an error. Under no circumstances will Algorithm 1 proceed with invalid bounds computed through the use of this iteration.

Remark 4.1 During the search for a computational means of satisfying (22), we did a significant amount of experimentation with methods that, modulo various heuristics, centered around the iteration

$$Z_{y,J} := \mathcal{H}^*(I_J, P, Z_{x,J}, Z_{y,J}, \mathbf{C}_J) + [-\mathbf{1}\gamma, \mathbf{1}\gamma] \tag{41}$$

(here, $Z_{x,J}$ is fixed, having been selected earlier by other means). Though this avoids evaluation and inversion of $\widetilde{\mathbf{J}}$, we had only limited success. In hindsight, this approach can be viewed as an attempt to solve the system of equations (31)-(32) using a successive substitution algorithm. Even for the best heuristics found, our results were exactly what one should expect in light of this observation: slow convergence for some systems and disastrous divergence for others. In comparison, the iteration (37) is much more robust.

4.1 Specification of $\mathbf{C}_J$ and $\widetilde{\mathbf{z}}_y$

In the Phase 1 implementation below, $\mathcal{H}^*$ is implemented with

$$\widetilde{\mathbf{z}}_y(Z_y) \equiv m(Z_y), \quad \forall Z_y \in \mathbb{IR}^{n_y}. \tag{42}$$

Note in particular that this guarantees (21) for any $Z_{y,J}$ with nonempty interior.

In practice, the choice of preconditioner can have a large impact on the sharpness of the bounds $Z_{x,J}$ and $Z_{y,J}$, and even the ability to satisfy (22) and (23) at all. A good preconditioner for evaluating $\mathcal{H}^*(I,P,Z_x,Z_y,\mathbf{C})$ is the midpoint inverse

$$\mathbf{C} \equiv \left(m\left(\left[\frac{\partial \mathbf{g}}{\partial \mathbf{y}} \right](I,P,Z_x,Z_y) \right) \right)^{-1}. \tag{43}$$

For efficiency reasons, however, it is desirable to compute a preconditioner only once per time step of Algorithm 1. Therefore, the definition

$$\mathbf{C}_J \equiv \left(m\left(\left[\frac{\partial \mathbf{g}}{\partial \mathbf{y}} \right]([t_{J-1},t_{J-1}],P,X_{J-1},Y_{J-1}) \right) \right)^{-1} \tag{44}$$

is used instead. Thus, $\mathbf{C}_J$ is constant throughout the iteration (37). For $J > 1$, X_{J-1} and Y_{J-1} are subsets of $Z_{x,J-1}$ and $Z_{y,J-1}$, and these intervals will have satisfied (19)-(23) with $j = J - 1$ in the previous time step. It follows that the inverse in (44) exists because $\left[\frac{\partial \mathbf{g}}{\partial \mathbf{y}} \right]([t_{J-2},t_{J-1}],P,Z_{x,J-1},Z_{y,J-1})$ cannot contain any singular matrices (Corollary I-4.1). If invertibility fails for $J = 1$, then the inverse of $\frac{\partial \mathbf{g}}{\partial \mathbf{y}}(t_0,\hat{\mathbf{p}},\mathbf{x}(\hat{\mathbf{p}}),\hat{\mathbf{y}}_0)$ is used instead. If this matrix is singular, then the corresponding solution of I-(1) is not regular and the method does not apply.

4.2 Phase 1 algorithm

Algorithm 2 below describes the complete implementation of Step 3 of Algorithm 1. Algorithm 2 terminates with flag $= 0$ when (19)-(23) have been satisfied successfully, and returns flag $= -1$ otherwise. For the examples in §7, Algorithm 2 is implemented with $\gamma = 10^{-4}$, H_MAX $= 1$, H_MIN $= 10^{-6}$ and PH1_MAX_ITER $= 10$.

Algorithm 2 (Phase 1)

1. Input: $[t_0,t_f]$, P, γ, t_{J-1}, X_{J-1}, Y_{J-1}, Δt_{J-1}.
2. Assign $\Delta t_J := \min(2\Delta t_{J-1}, \text{H\_MAX}, t_f - t_{J-1} + \text{H\_MIN})$ and $t_J := t_{J-1} + \Delta t_J$.
3. Assign $\mathbf{z}_x^L := \mathbf{x}_{J-1}^L - \mathbf{1}\gamma$, $\mathbf{z}_x^U := \mathbf{x}_{J-1}^U + \mathbf{1}\gamma$, $\mathbf{z}_y^L := \mathbf{y}_{J-1}^L - \mathbf{1}\gamma$, $\mathbf{z}_y^U := \mathbf{y}_{J-1}^U + \mathbf{1}\gamma$.
4. With initial guesses from 3, apply the iteration (37) described above.
   (a) If PH1_MAX_ITER iterations are taken without success, go to 6.
   (b) If any iterate violates (28), go to 6.
   (c) If $(\mathbf{z}_x^L, \mathbf{z}_x^U, \mathbf{z}_y^L, \mathbf{z}_y^U)$ is found such that the right-hand sides of (31)-(34) are componentwise less than γ, set $Z_{x,J} := [\mathbf{z}_x^L, \mathbf{z}_x^U]$ and $Z_{y,J} := [\mathbf{z}_y^L, \mathbf{z}_y^U]$ and go to 5.
5. If $Y_{J-1} \subset Z_{y,J}$, terminate with flag $= 0$. Otherwise, go to 6.
6. Assign $\Delta t_J := \Delta t_J/2$ and $t_J := t_{J-1} + \Delta t_J$. If $\Delta t_J \geq$ H_MIN go to 3. Otherwise, terminate with flag $= -1$.

Suppose that Algorithm 2 returns 0. By Step 4 and Lemma 4.2, (19), (22) and (23) are satisfied. Since (22) implies that $Z_{y,J}$ has nonempty interior, (21) is guaranteed by the choice of $\widetilde{\mathbf{z}}_y$ in §4.1. Finally, (20) is verified by Step 5. Then, Phase 1 is complete. The only way Algorithm 2 can fail is if Δt_J is reduced below H_MIN by repeated failure in Step 4 or 5. To avoid many such failures, Δt_J is bounded by $2\Delta t_{J-1}$.

In practice, Step 4 succeeds reliably when the intervals I_J and P are narrow, and becomes less reliable as they are widened. This is natural given that (17) follows from (19)-(23). When I_J and P are narrow, (19)-(23) can potentially be satisfied by narrower intervals $Z_{x,J}$ and $Z_{y,J}$. Working with narrower intervals in turn reduces the overestimation incurred through interval computations, and reduces the likelihood of violating (19). Both of these factors make Step 4 more likely to succeed.

When Step 4 fails, the recourse is to half Δt_J and try again. On the other hand, Algorithm 2 does not resort to partitioning P. Though algorithms for bisecting P and propagating bounds valid on each partition element separately are easily conceivable, computational efficiency will be lost if many partitions are required, so this strategy is avoided. With P fixed, one can create pathological problems for which it is impossible to satisfy (22), and therefore there is no theoretical guarantee that Step 4 will succeed. This happens, for example, if the algebraic equations permit multiple solution branches on $[t_{J-1}, t_{J-1}] \times P \times X_{J-1}$ and it is geometrically impossible to enclose one uniquely by an interval (see Corollary I-4.1).

Though the condition (20) is checked in Step 5 of Algorithm 2, no special attempt is made to guarantee it. The condition (20) is merely a provision for the case where I-(1) permits multiple regular solutions. Its purpose is to ensure that the interval $Z_{y,J}$ computed in Step 4 encloses the solution of I-(1) that is consistent with the input $\hat{\mathbf{y}}_0$ in Algorithm 1, rather than jumping to some other solution (see the proof of Corollary 3.1). Since the initial guesses specified in Step 3 are in the vicinity of the solution of interest, (20) is likely to hold whenever Step 4 succeeds.

4.3 Phase 1 refinement

Before moving on to Phase 2 of Algorithm 1, $Z_{x,J}$ and $Z_{y,J}$ may be refined by iteratively assigning

$$Z_{x,J} := \Big(X_{J-1} + [0, t_J - t_{J-1}][\mathbf{f}](I_J, P, Z_{x,J}, Z_{y,J})\Big) \cap Z_{x,J}, \qquad (45)$$

$$Z_{y,J} := \mathcal{H}(I_J, P, Z_{x,J}, Z_{y,J}, \mathbf{C}_J). \qquad (46)$$

By (18), it is clear that

$$\mathbf{x}(t, \mathbf{p}) = \mathbf{x}(t_{J-1}, \mathbf{p}) + \int_{t_{J-1}}^{t} \mathbf{f}(s, \mathbf{p}, \mathbf{x}(s, \mathbf{p}), \mathbf{y}(s, \mathbf{p})) ds, \qquad (47)$$

$$\in X_{J-1} + [0, t - t_{J-1}][\mathbf{f}](I_J, P, Z_{x,J}, Z_{y,J}), \qquad (48)$$

for all $(t, \mathbf{p}) \in I_J \times P$. Therefore, (17) remains valid after the assignment (45). By Conclusion 1 of Corollary I-4.1, the same is true of the assignment (46). Note that these refinements are distinct from the refinements X_J and Y_J detailed in §5 in that (17) remains true. That is, the refined intervals still provide bounds on all of $I_J \times P$, rather than only at t_J, as in (18). For the examples in §7, (45) and (46) are applied with a maximum of 50 iterations, terminating early if the absolute or relative change between each bound in successive iterates is less that 10^{-8}.

5 Computing Refined Enclosures Using Differential Inequalities (Phase 2)

In this section, we consider the implementation of Step 6 in a single time step J of Algorithm 1. It is assumed that a solution $(\mathbf{x}, \mathbf{y})$ of I-(1) exists on $[t_0, t_J] \times P$, and that Y_0 and $(I_j, Z_{x,j}, Z_{y,j}, Z'_{y,j}, \mathbf{C}_j, X_j, Y_j)$ are available and satisfy (17) and (19)-(23) for all $j \in \{1, \ldots, J\}$ and (18) for all $j \in \{0, \ldots, J-1\}$. The present task is to compute refined intervals $X_J \subset Z_{x,J}$ and $Y_J \subset Z'_{y,J}$ satisfying (18) with $j = J$.

By the assumption that (19)-(23) hold with $j = J$, Corollary I-4.1 guarantees that $\exists \mathbf{H} \in C^1(I_J \times P \times Z_{x,J}, Z'_{y,J})$ such that, for every $(t, \mathbf{p}, \mathbf{z}_x) \in I_J \times P \times Z_{x,J}$, $\mathbf{z}_y = \mathbf{H}(t, \mathbf{p}, \mathbf{z}_x)$ is the unique element of $Z_{y,J}$ satisfying $\mathbf{g}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y) = \mathbf{0}$. Therefore, we aim to apply Theorem I-5.2 to derive time-varying bounds on $(\mathbf{x}, \mathbf{y})$ over I_J.

Choose any $K \in \mathbb{N}$ and, for every $i \in \{1, \ldots, n_x\}$, define

$$\phi_i^L, \phi_i^U : \mathbb{R} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} \to \mathbb{IR} \times \mathbb{IR}^{n_p} \times \mathbb{IR}^{n_x} \times \mathbb{IR}^{n_y} \times \mathbb{IR}^{n_y \times n_y}, \tag{49}$$

$$\mathcal{Y}_i^L, \mathcal{Y}_i^U : \mathbb{R} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} \to \mathbb{IR}^{n_y}, \tag{50}$$

$$\psi_i^L, \psi_i^U : \mathbb{R} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} \to \mathbb{IR} \times \mathbb{IR}^{n_p} \times \mathbb{IR}^{n_x} \times \mathbb{IR}^{n_y}, \tag{51}$$

by

$$\phi_i^L(t, \mathbf{v}, \mathbf{w}) \equiv \left(I_J \widetilde{\cap} [t, t], P, \mathcal{B}_i^L(Z_{x,J} \widetilde{\cap} \square(\mathbf{v}, \mathbf{w})), Z'_{y,J}, \mathbf{C}_J \right), \tag{52}$$

$$\phi_i^U(t, \mathbf{v}, \mathbf{w}) \equiv \left(I_J \widetilde{\cap} [t, t], P, \mathcal{B}_i^U(Z_{x,J} \widetilde{\cap} \square(\mathbf{v}, \mathbf{w})), Z'_{y,J}, \mathbf{C}_J \right), \tag{53}$$

$$\mathcal{Y}_i^L(t, \mathbf{v}, \mathbf{w}) \equiv \mathcal{H}^{+,K}(\phi_i^L(t, \mathbf{v}, \mathbf{w})), \tag{54}$$

$$\mathcal{Y}_i^U(t, \mathbf{v}, \mathbf{w}) \equiv \mathcal{H}^{+,K}(\phi_i^U(t, \mathbf{v}, \mathbf{w})), \tag{55}$$

$$\psi_i^L(t, \mathbf{v}, \mathbf{w}) \equiv \left(I_J \widetilde{\cap} [t, t], P, \mathcal{B}_i^L(Z_{x,J} \widetilde{\cap} \square(\mathbf{v}, \mathbf{w})), \mathcal{Y}_i^L(t, \mathbf{v}, \mathbf{w}) \right), \tag{56}$$

$$\psi_i^U(t, \mathbf{v}, \mathbf{w}) \equiv \left(I_J \widetilde{\cap} [t, t], P, \mathcal{B}_i^U(Z_{x,J} \widetilde{\cap} \square(\mathbf{v}, \mathbf{w})), \mathcal{Y}_i^U(t, \mathbf{v}, \mathbf{w}), \right). \tag{57}$$

Now, consider the initial value problem in ODEs

$$\dot{v}_i(t) = [f_i]^L (\psi_i^L(t, \mathbf{v}(t), \mathbf{w}(t))), \tag{58}$$

$$\dot{w}_i(t) = [f_i]^U (\psi_i^U(t, \mathbf{v}(t), \mathbf{w}(t))), \tag{59}$$

for all $i = 1, \ldots, n_x$, with initial conditions

$$[\mathbf{v}(t_{J-1}), \mathbf{w}(t_{J-1})] = X_{J-1}. \tag{60}$$

The following results show that these ODEs are well-defined and have a unique solution describing the desired bounds. It is assumed throughout that Assumption 2.1 holds and $\widetilde{\mathbf{z}}_y$ is the midpoint, as in §4.1.

Corollary 5.1 *When viewed as functions of $(t, \mathbf{v}, \mathbf{w})$, the right-hand sides of (58) and (59) are defined and piecewise C^1 on $\mathbb{R} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x}$. Furthermore,*

$$\mathcal{Y}_i^L(t, \mathbf{v}, \mathbf{w}) = \mathcal{H}^K \left(\phi_i^L(t, \mathbf{v}, \mathbf{w}) \right) \quad and \quad \mathcal{Y}_i^U(t, \mathbf{v}, \mathbf{w}) = \mathcal{H}^K \left(\phi_i^U(t, \mathbf{v}, \mathbf{w}) \right), \tag{61}$$

for all $(t, \mathbf{v}, \mathbf{w}) \in \mathbb{R} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x}$ and every $i = 1, \ldots, n_x$.

Proof Choose any $i \in \{1, \ldots, n_x\}$ and any $(t, \mathbf{v}, \mathbf{w}) \in \mathbb{R} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x}$. By Conclusion 3 of Lemma 2.2, $\phi_i^L(t, \mathbf{v}, \mathbf{w}) \subset (I_J, P, Z_{x,J}, Z_{y,J}, \mathbf{C}_J)$. Using (19), (21) and (22), Conclusion 7 of Lemma 2.4 implies that $\phi_i^L(t, \mathbf{v}, \mathbf{w}) \in \mathcal{D}_{\mathcal{H}}^K$. Then, $\mathcal{Y}_i^L(t, \mathbf{v}, \mathbf{w})$ is well-defined and Conclusion 4 of Lemma 2.4 shows (61) (an analogous argument holds for $\mathcal{Y}_i^U$).

Now (61) implies that $\mathcal{Y}_i^L(t, \mathbf{v}, \mathbf{w}) \subset Z_{y,J}'$. It follows that $\psi_i^L(t, \mathbf{v}, \mathbf{w})$ is in $\mathbb{ID}_t \times \mathbb{ID}_p \times \mathbb{ID}_x \times \mathbb{ID}_y$. Then, the right-hand side of (58) is defined on $\mathbb{R} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x}$.

By Lemmas 2.6 and 2.8 and Definition I-5.1, it is clear that ϕ_i^L is piecewise C^1 on $\mathbb{R} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x}$, which is open. Theorem 2.1 shows that $\mathcal{H}^{+,K}$, and hence $\mathcal{Y}_i^L = \mathcal{H}^{+,K} \circ \phi_i^L$, is also piecewise C^1 on $\mathbb{R} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x}$. It follows that ψ_i^L is piecewise C^1 on $\mathbb{R} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x}$. Finally, Assumption 2.1 implies that $[f_i]^L \circ \psi_i^L$ is piecewise C^1 on $\mathbb{R} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x}$, which is the desired result (an analogous argument holds for $[f_i]^U \circ \psi_i^U$). $\qquad\square$

Lemma 5.1 *There exist* $\mathbf{v}, \mathbf{w} \in C^1(I_J, \mathbb{R}^{n_x})$ *satisfying the ODEs* (58)-(60). *Moreover, this solution is unique and satisfies* $\mathbf{v}(t) \leq \mathbf{w}(t)$ *and* $[\mathbf{v}(t), \mathbf{w}(t)] \cap Z_{x,J} \neq \emptyset, \forall t \in I_J$.

Proof Consider the ODEs

$$\dot{s}(t) = 1, \tag{62}$$

$$\dot{v}_i(t) = [f_i]^L(\psi_i^L(s(t), \mathbf{v}(t), \mathbf{w}(t))), \tag{63}$$

$$\dot{w}_i(t) = [f_i]^U(\psi_i^U(s(t), \mathbf{v}(t), \mathbf{w}(t))), \tag{64}$$

with initial conditions (60) and $s(t_0) = t_0$. This system simply describes the bounding ODEs (58) and (59) in autonomous form.

By Corollary 5.1 and Conclusion 3 of Lemma 2.5, the right-hand sides of (62)-(64) are locally Lipschitz continuous on $\mathbb{R} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x}$. Moreover, ψ^L and ψ^U are easily seen to map into subsets of $(I_J, P, Z_{x,J}, Z_{y,J})$. Thus, the right-hand sides of (62)-(64) are also bounded on $\mathbb{R} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x}$ by

$$\max\left(1, \left|[f_i]^L(I_J, P, Z_{x,J}, Z_{y,J})\right|, \left|[f_i]^U(I_J, P, Z_{x,J}, Z_{y,J})\right|\right). \tag{65}$$

For any $(\hat{s}, \hat{\mathbf{v}}, \hat{\mathbf{w}}) \in \mathbb{R} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x}$ and any $i \in \{1, \ldots, n_x\}$, the definitions of $\square$ and $\widetilde{\cap}$ guarantee that

$$\hat{v}_i = \hat{w}_i \implies (Z_{x,J})_i \widetilde{\cap} \square(\hat{v}_i, \hat{w}_i) \text{ is a singleton}, \tag{66}$$

$$\implies \mathcal{B}_i^L(Z_{x,J} \widetilde{\cap} \square(\hat{\mathbf{v}}, \hat{\mathbf{w}})) = \mathcal{B}_i^U(Z_{x,J} \widetilde{\cap} \square(\hat{\mathbf{v}}, \hat{\mathbf{w}})), \tag{67}$$

$$\implies \mathcal{Y}_i^L(\hat{s}, \hat{\mathbf{v}}, \hat{\mathbf{w}}) = \mathcal{Y}_i^U(\hat{s}, \hat{\mathbf{v}}, \hat{\mathbf{w}}), \tag{68}$$

$$\implies [f_i]^L(\psi_i^L(\hat{s}, \hat{\mathbf{v}}, \hat{\mathbf{w}})) \leq [f_i]^U(\psi_i^U(\hat{s}, \hat{\mathbf{v}}, \hat{\mathbf{w}})). \tag{69}$$

This implies that $\mathcal{K} \equiv \{(\hat{s}, \hat{\mathbf{v}}, \hat{\mathbf{w}}) \in \mathbb{R} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} : \hat{\mathbf{v}} \leq \hat{\mathbf{w}}\}$ is a viability domain for the ODEs (62)-(64) (Definition 1.1.5 in [1]). Combining this with continuity and boundedness of the right-hand sides, Nagumo's Theorem implies that there exist $s \in C^1(I_J, \mathbb{R}^n)$ and $\mathbf{v}, \mathbf{w} \in C^1(I_J, \mathbb{R}^{n_x})$ satisfying (62)-(64) and satisfying $(s(t), \mathbf{v}(t), \mathbf{w}(t)) \in \mathcal{K}$, and hence $\mathbf{v}(t) \leq \mathbf{w}(t), \forall t \in I_J$ (see Theorem 1.2.4 in [1]). Clearly, this $\mathbf{v}, \mathbf{w}$ also satisfies (58)-(60). Due to the local Lipschitz continuity of the ODE right-hand side

functions on $\mathbb{R} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x}$, uniqueness follows by a standard application of Gronwall's inequality.

Let $[x_{J-1,i}^L, x_{J-1,i}^U]$ and $[z'^L_{y,J,i}, z'^U_{y,J,i}]$ denote the ith components of X_{J-1} and $Z'_{y,J}$, respectively. By (23) and the integral form of (58),

$$v_i(t) = v_i(t_{J-1}) + \int_{t_{J-1}}^t [f_i]^L(\psi_i^L(s, \mathbf{v}(s), \mathbf{w}(s)))ds, \tag{70}$$

$$\geq x_{J-1,i}^L + \int_{t_{J-1}}^t [f_i]^L(I_J, P, Z_{x,J}, Z'_{y,J}), \tag{71}$$

$$\geq x_{J-1,i}^L + [0, t_J - t_{J-1}][f_i]^L(I_J, P, Z_{x,J}, Z'_{y,J}) \geq z_{x,J,i}^L, \quad \forall t \in I_J. \tag{72}$$

Using an analogous argument for w_i, it follows that $[\mathbf{v}(t), \mathbf{w}(t)] \subset Z_{x,J}, \forall t \in I_J$. □

Corollary 5.2 *Let* $\mathbf{v}, \mathbf{w} \in C^1(I_J, \mathbb{R}^{n_x})$ *be the unique solutions of* (58)-(60). *Then*

$$\mathbf{x}(t, \mathbf{p}) \in [\mathbf{v}(t), \mathbf{w}(t)], \tag{73}$$

$$\mathbf{y}(t, \mathbf{p}) \in \mathcal{Y}(t, \mathbf{v}(t), \mathbf{w}(t)) \equiv \mathcal{H}^q\left([t, t], P, Z_{x,J} \cap [\mathbf{v}(t), \mathbf{w}(t)], Z_{y,J}\right), \tag{74}$$

for all $(t, \mathbf{p}) \in I_J \times P$ *and any* $q \in \mathbb{N}$.

Proof To show (73), it suffices to establish the hypotheses of Theorem I-5.2 with $(I, Z_x, Z'_y) = (I_J, Z_{x,J}, Z'_{y,J})$, $t_f = t_J$, $t_0 = t_{J-1}$ and $\mathbf{x}_0 = \mathbf{x}_{J-1} \equiv \mathbf{x}(t_{J-1}, \cdot)$. By (19)-(23) and Corollary I-4.1, there exists $\mathbf{H} \in C^1(I_J \times P \times Z_{x,J}, Z'_{y,J})$ such that, for every $(t, \mathbf{p}, \mathbf{z}_x) \in I_J \times P \times Z_{x,J}$, $\mathbf{z}_y = \mathbf{H}(t, \mathbf{p}, \mathbf{z}_x)$ is the unique element of $Z_{y,J}$ satisfying $\mathbf{g}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y) = \mathbf{0}$. Then, it only remains to satisfy the hypotheses (EX), (IC) and (RHS). (EX) holds by Lemma 5.1. By (60) and (18) with $j = J - 1$, (IC) is clearly satisfied. Choose any $t \in I_J$. If there exists $(\mathbf{p}, \mathbf{z}_x, \mathbf{z}_y) \in P \times Z_{x,J} \times Z'_{y,J}$ such that $\mathbf{g}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y) = \mathbf{0}$ and $\mathbf{z}_x \in \mathcal{B}_i^L(Z_{x,J} \cap [\mathbf{v}(t), \mathbf{w}(t)])$, then (61) and Conclusion 1 of Corollary I-4.1 ensure that $\mathbf{z}_y \in \mathcal{Y}_i^L(t, \mathbf{v}(t), \mathbf{w}(t))$. It follows that

$$f_i(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y) \in [f_i]([t, t], P, \mathcal{B}_i^L(Z_{x,J} \cap [\mathbf{v}(t), \mathbf{w}(t)]), \mathcal{Y}_i^L(t, \mathbf{v}(t), \mathbf{w}(t))), \tag{75}$$

$$= [f_i](\psi_i^L(t, \mathbf{v}(t), \mathbf{w}(t))), \tag{76}$$

and hence (58) ensures that (RHS).1 is satisfied. Proof of (RHS).2 is analogous. Then, (73) holds, and (74) follows from Conclusion 1 of Corollary I-4.1. □

According to Corollary 5.2, Step 6 of Algorithm 1 can be accomplished by solving (58)-(60) on I_J and assigning $X_J := [\mathbf{v}(t_J), \mathbf{w}(t_J)]$ and $Y_J := \mathcal{Y}(t_J, \mathbf{v}(t_J), \mathbf{w}(t_J))$. Provided that numerical error is not a crucial concern, these ODEs can be solved numerically using any state of the art code. In the examples in §7, we use CVODE [2] with absolute and relative tolerances of 10^{-5}. The evaluation of $\mathcal{Y}_i^L$ and $\mathcal{Y}_i^U$ for each i can make evaluating the right-hand sides of (58)-(59) costly, so K should be small (see §6.1). On the other hand, q can be fairly large, because $\mathcal{Y}$ is evaluated after numerical integration is complete rather than within the right-hand sides of (58) and (59). Moreover, $\mathcal{Y}$ need only be evaluated at select points of interest in I_J, since only the value at t_J, which defines Y_J, will effect the next time step of Algorithm 1. In §7, we choose $K = 5$ and evaluate $\mathcal{Y}$ with $q = 50$ at all points shown in the plots there.

6 A single-phase method

In this section, a single-phase method is presented which essentially combines the two phases of the previous approach. In short, time-varying bounds for both the differential and the algebraic state variables will be computed by satisfying the hypotheses of Theorem I-5.3. As before, let $I = [t_0, t_f] \subset D_t$, $P \subset D_p$ and $X_0 \subset D_x$ be intervals and suppose that $\mathbf{x}_0(P) \subset X_0$.

For every $i \in \{1, \ldots, n_x\}$, let

$$\eta : \mathbb{R} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_y} \times \mathbb{R}^{n_y} \to \mathbb{IR} \times \mathbb{IR}^{n_p} \times \mathbb{IR}^{n_x} \times \mathbb{IR}^{n_y} \tag{77}$$

$$\mathbf{C} : E_{\text{inv}} \to \mathbb{IR}^{n_y \times n_y}, \tag{78}$$

$$\phi, \phi_i^L, \phi_i^U : E_{\text{inv}} \to \mathbb{IR} \times \mathbb{IR}^{n_p} \times \mathbb{IR}^{n_x} \times \mathbb{IR}^{n_y} \times \mathbb{IR}^{n_y \times n_y}, \tag{79}$$

$$\mathcal{Y}_i^L, \mathcal{Y}_i^U : E_{\mathcal{H}}^* \to \mathbb{IR}^{n_y}, \tag{80}$$

$$\psi_i^L, \psi_i^U : E_{\mathcal{H}}^* \to \mathbb{IR} \times \mathbb{IR}^{n_p} \times \mathbb{IR}^{n_x} \times \mathbb{IR}^{n_y}, \tag{81}$$

where

$$E_{\mathbb{ID}} \equiv \left\{ (t, \mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U) \in \mathbb{R} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_y} \times \mathbb{R}^{n_y} : \tag{82}$$

$$\eta(t, \mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U) \in \mathbb{ID}_t \times \mathbb{ID}_p \times \mathbb{ID}_x \times \mathbb{ID}_y \right\}, \tag{83}$$

$$\mathcal{D}_{\text{inv}} \equiv \{ Q \in \mathbb{IR}^{n_y \times n_y} : \det(m(Q)) \neq 0 \}, \tag{84}$$

$$E_{\text{inv}} \equiv \left\{ (t, \mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U) \in E_{\mathbb{ID}} : \left[\frac{\partial \mathbf{g}}{\partial \mathbf{y}} \right] (\eta(t, \mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U)) \in \mathcal{D}_{\text{inv}} \right\}, \tag{85}$$

$$E_{\mathcal{H}}^* \equiv \left\{ (t, \mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U) \in E_{\text{inv}} : \phi(t, \mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U) \in \mathcal{D}_{\mathcal{H}}^* \right\}. \tag{86}$$

Choosing any $K \in \mathbb{N}$, define the functions in (77)-(81) by

$$\eta(t, \mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U) \equiv \left(I \widetilde{\cap} [t, t], P, \square(\mathbf{v}, \mathbf{w}), \square(\mathbf{z}_y^L, \mathbf{z}_y^U) \right), \tag{87}$$

$$\mathbf{C}(t, \mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U) \equiv m \left(\left[\frac{\partial \mathbf{g}}{\partial \mathbf{y}} \right] (\eta(t, \mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U)) \right)^{-1}, \tag{88}$$

$$\phi(t, \mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U) \equiv \left(I \widetilde{\cap} [t, t], P, \square(\mathbf{v}, \mathbf{w}), \square(\mathbf{z}_y^L, \mathbf{z}_y^U), \mathbf{C}(t, \mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U) \right), \tag{89}$$

$$\phi_i^L(t, \mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U) \equiv \left(I \widetilde{\cap} [t, t], P, \mathcal{B}_i^L(\square(\mathbf{v}, \mathbf{w})), \square(\mathbf{z}_y^L, \mathbf{z}_y^U), \mathbf{C}(t, \mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U) \right), \tag{90}$$

$$\phi_i^U(t, \mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U) \equiv \left(I \widetilde{\cap} [t, t], P, \mathcal{B}_i^U(\square(\mathbf{v}, \mathbf{w})), \square(\mathbf{z}_y^L, \mathbf{z}_y^U), \mathbf{C}(t, \mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U) \right), \tag{91}$$

$$\mathcal{Y}_i^L(t, \mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U) \equiv \mathcal{H}^{+,K}(\phi_i^L(t, \mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U)), \tag{92}$$

$$\mathcal{Y}_i^U(t, \mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U) \equiv \mathcal{H}^{+,K}(\phi_i^U(t, \mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U)), \tag{93}$$

$$\psi_i^L(t, \mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U) \equiv \left(I \widetilde{\cap} [t, t], P, \mathcal{B}_i^L(\square(\mathbf{v}, \mathbf{w})), \mathcal{Y}_i^L(t, \mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U) \right), \tag{94}$$

$$\psi_i^U(t, \mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U) \equiv \left(I \widetilde{\cap} [t, t], P, \mathcal{B}_i^U(\square(\mathbf{v}, \mathbf{w})), \mathcal{Y}_i^U(t, \mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U) \right). \tag{95}$$

For any continuous and pointwise positive $\gamma : I \to \mathbb{R}$, consider the initial value problem in DAEs

$$\dot{v}_i(t) = [f_i]^L (\psi_i^L(t, \mathbf{v}(t), \mathbf{w}(t), \mathbf{z}_y^L(t), \mathbf{z}_y^U(t))), \tag{96}$$

$$\dot{w}_i(t) = [f_i]^U (\psi_i^U(t, \mathbf{v}(t), \mathbf{w}(t), \mathbf{z}_y^L(t), \mathbf{z}_y^U(t))), \tag{97}$$

$$\mathbf{0} = \mathbf{z}_y^L(t) - \mathcal{H}^{*,L}(\phi(t, \mathbf{v}(t), \mathbf{w}(t), \mathbf{z}_y^L(t), \mathbf{z}_y^U(t))) + \mathbf{1}\gamma(t), \tag{98}$$

$$\mathbf{0} = -\mathbf{z}_y^U(t) + \mathcal{H}^{*,U}(\phi(t, \mathbf{v}(t), \mathbf{w}(t), \mathbf{z}_y^L(t), \mathbf{z}_y^U(t))) + \mathbf{1}\gamma(t), \tag{99}$$

for all $i = 1, \ldots, n_x$, with initial conditions

$$[\mathbf{v}(t_0), \mathbf{w}(t_0)] = X_0. \tag{100}$$

In the following results, it will be shown that the solutions of these DAEs describe the desired bounds. It is assumed thoughout that Assumption 2.1 holds and $\widetilde{\mathbf{z}}_y$ is the midpoint, as in §4.1.

Corollary 6.1 $E_{\mathcal{H}}^*$ is open and, when viewed as functions of $(t, \mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U)$, the right-hand sides of (96)-(99) are defined and piecewise C^1 on $E_{\mathcal{H}}^*$.

Proof By Lemmas 2.6 and 2.8, η is piecewise C^1 on $\mathbb{ID}_t \times \mathbb{ID}_p \times \mathbb{ID}_x \times \mathbb{ID}_y$. Since this set is open, $E_{\mathbb{ID}}$ is open by Lemma 2.7. Moreover, the set of nonsingular matrices is open. Then, since $m(\cdot)$ is clearly a continuous function from $\mathbb{R}^{n_y \times n_y}$ to $\mathbb{R}^{n_y \times n_y}$, $\mathcal{D}_{\mathrm{inv}}$ is the inverse image of an open set under a continuous mapping, and is hence open. By Assumption 2.1, $\left[\frac{\partial \mathbf{g}}{\partial \mathbf{y}}\right] \circ \eta$ is piecewise C^1 on $E_{\mathbb{ID}}$. Then, another application of Lemma 2.7 now shows that E_{inv} is open. The fact that $\mathbf{C}$ is piecewise C^1 on E_{inv} now follows from the definition of $m(\cdot)$ and the fact that the inverse of a matrix is a differentiable function of its elements. Combining this with Lemmas 2.6 and 2.8 shows that ϕ, ϕ_i^L and ϕ_i^U are piecewise C^1 on E_{inv}, so that openness of $\mathcal{D}_{\mathcal{H}}^*$ and a final application of Lemma 2.7 show that $E_{\mathcal{H}}^*$ is open.

Choose any $i \in \{1, \ldots, n_x\}$. By the definition of $E_{\mathcal{H}}^*$ and Conclusion 1 of Lemma 2.4,

$$\phi_i^L(t, \mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U) \in \mathcal{D}_{\mathcal{H}}^*, \quad \forall (t, \mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U) \in E_{\mathcal{H}}^*. \tag{101}$$

Theorem 2.1 shows that $\mathcal{H}^*$ and $\mathcal{H}^{+,K}$ are piecewise C^1 on $\mathcal{D}_{\mathcal{H}}^*$, and hence $\mathcal{H}^* \circ \phi$ and $\mathcal{Y}_i^L = \mathcal{H}^{+,K} \circ \phi_i^L$ are piecewise C^1 on $E_{\mathcal{H}}^*$. It follows that the right-hand side of (98) and ψ_i^L are piecewise C^1 on $E_{\mathcal{H}}^*$. For any $(t, \mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U) \in E_{\mathcal{H}}^*$, the definition of $\mathcal{H}^{+,K}$ implies that $\mathcal{Y}_i^L(t, \mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U) \subset \square(\mathbf{z}_y^L, \mathbf{z}_y^U)$, and hence

$$\psi_i^L(t, \mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U) \subset \eta(t, \mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U) \subset D_t \times D_p \times D_x \times D_y. \tag{102}$$

Then, Assumption 2.1 implies that $[f_i]^L \circ \psi_i^L$ is piecewise C^1 on $E_{\mathcal{H}}^*$. Analogous arguments hold for the right-hand sides of (99) and (97). $\square$

In contrast to the analysis of the Phase 2 bounding ODEs in §5, existence and uniqueness of a solution of (96)-(100) does not follow from standard results because the participating functions are only piecewise C^1, rather than C^1. However, such a result seems quite plausible. From a variant of the implicit function theorem in [17], one can write an invertibility condition for the right-hand sides of (98)-(99) which guarantees the existence of a piecewise C^1 implicit function locally around a consistent initial condition. By Conclusion 3 of Lemma 2.5, this would imply that $\mathbf{v}$ and $\mathbf{w}$ are, locally, described by ODEs with locally Lipschitz continuous right-hand sides. Combining this with standard results for Lipschitz ODEs then implies that there exists a solution in a neighborhood of t_0 with $\mathbf{v}$ and $\mathbf{w}$ continuously differentiable and $\mathbf{z}_y^L$ and $\mathbf{z}_y^U$ piecewise C^1. We do not pursue this development formally here. Instead, we will assume that such a solution exists on an open set I_0 containing I and demonstrate that it must describe the desired bounds.

Lemma 6.1 *Let $(\mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U)$ be a solution of (96)-(100). Then $\mathbf{v}(t) \leq \mathbf{w}(t)$ and $\mathbf{z}_y^L(t) < \mathbf{z}_y^U(t)$ for all $t \in I$.*

Proof Arguing as in Lemma 4.2, it is clear from (98) and (99) that any solution must satisfy $\mathbf{z}_y^L(t) < \mathbf{z}_y^U(t)$ for all $t \in I$.

For a contradiction, suppose that $\{t \in I : v_i(t) > w_i(t) \text{ for at least one } i\}$ is nonempty and let $t_1 < t_f$ denote its infimum. Because t_1 is a lower bound, $\mathbf{v}(t) \leq \mathbf{w}(t), \forall t \in [t_0, t_1]$. Because t_1 is the greatest lower bound, it follows that $v_i(t) > w_i(t)$ for at least one i for t arbitrarily close to the right of t_1.

Now, treating $\mathbf{z}_y^L$ and $\mathbf{z}_y^U$ as known functions, consider the ODEs

$$\dot{s}(t) = 1, \tag{103}$$

$$\dot{v}_i^*(t) = [f_i]^L (\psi_i^L(s(t), \mathbf{v}^*(t), \mathbf{w}^*(t), \mathbf{z}_y^L(s(t)), \mathbf{z}_y^U(s(t)))), \tag{104}$$

$$\dot{w}_i^*(t) = [f_i]^U (\psi_i^U(s(t), \mathbf{v}^*(t), \mathbf{w}^*(t), \mathbf{z}_y^L(s(t)), \mathbf{z}_y^U(s(t)))), \tag{105}$$

for all $i = 1, \ldots, n_x$. Corollary 6.1 implies that the right-hand sides of these ODEs are piecewise C^1, and hence locally Lipschitz continuous, on the set

$$Q \equiv \left\{ (\hat{s}, \hat{\mathbf{v}}, \hat{\mathbf{w}}) \in I_0 \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} : (\hat{s}, \hat{\mathbf{v}}, \hat{\mathbf{w}}, \mathbf{z}_y^L(\hat{s}), \mathbf{z}_y^U(\hat{s})) \in E_{\mathcal{H}}^* \right\}. \tag{106}$$

We refer to these ODEs as the reduced ODEs and consider them with initial conditions $(s(t_1), \mathbf{v}^*(t_1), \mathbf{w}^*(t_1)) = (t_1, \mathbf{v}(t_1), \mathbf{w}(t_1))$. Clearly, for any solution $(s, \mathbf{v}^*, \mathbf{w}^*)$ of the reduced ODEs on $[t_t, t_1 + \delta]$, $(s, \mathbf{v}, \mathbf{w})$ is also a solution.

For any $(\hat{s}, \hat{\mathbf{v}}, \hat{\mathbf{w}}) \in Q$ and any $i \in \{1, \ldots, n_x\}$,

$$\hat{v}_i = \hat{w}_i \implies \mathcal{B}_i^L(\Box(\hat{\mathbf{v}}, \hat{\mathbf{w}})) = \mathcal{B}_i^U(\Box(\hat{\mathbf{v}}, \hat{\mathbf{w}})), \tag{107}$$

$$\implies \mathcal{Y}_i^L(\hat{s}, \hat{\mathbf{v}}, \hat{\mathbf{w}}, \mathbf{z}_y^L(\hat{s}), \mathbf{z}_y^U(\hat{s})) = \mathcal{Y}_i^U(\hat{s}, \hat{\mathbf{v}}, \hat{\mathbf{w}}, \mathbf{z}_y^L(\hat{s}), \mathbf{z}_y^U(\hat{s})), \tag{108}$$

$$\implies [f_i]^L (\psi_i^L(\hat{s}, \hat{\mathbf{v}}, \hat{\mathbf{w}}, \mathbf{z}_y^L(\hat{s}), \mathbf{z}_y^U(\hat{s}))) \leq [f_i]^U (\psi_i^U(\hat{s}, \hat{\mathbf{v}}, \hat{\mathbf{w}}, \mathbf{z}_y^L(\hat{s}), \mathbf{z}_y^U(\hat{s}))). \tag{109}$$

This implies that $\mathcal{K} \equiv \{(\hat{s}, \hat{\mathbf{v}}, \hat{\mathbf{w}}) \in I \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} : \hat{\mathbf{v}} \leq \hat{\mathbf{w}}\}$ is a viability domain for the reduced ODEs (Definition 1.1.5 in [1]). Combining this with continuity the right-hand sides, Nagumo's Theorem implies that there exist $\delta > 0$ $s \in C^1([t_1, t_1 + \delta], \mathbb{R})$ and

$\mathbf{v}^*, \mathbf{w}^* \in C^1([t_1, t_1 + \delta], \mathbb{R}^{n_x})$ satisfying the reduced ODEs and satisfying $(s(t), \mathbf{v}^*(t), \mathbf{w}^*(t)) \in \mathcal{K}$, and hence $\mathbf{v}^*(t) \leq \mathbf{w}^*(t), \forall t \in [t_1, t_1 + \delta]$ (see Theorem 1.2.3 in [1]). But by the definition of t_1, $(s, \mathbf{v}, \mathbf{w})$ leaves $\mathcal{K}$ immediately to the right of t_1. Therefore, $(s, \mathbf{v}, \mathbf{w}) \neq (s, \mathbf{v}^*, \mathbf{w}^*)$ on $[t_1, t_1 + \delta]$. But it has been shown above that the right-hand sides of the reduced ODEs are locally Lipschitz continuous, so a standard application of Gronwall's inequality yields a contradiction. $\qquad\square$

Corollary 6.2 *Let* $(\mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U)$ *be a solution of* (96)-(100) *on* I. *Then any regular solution* $(\mathbf{x}, \mathbf{y})$ *of* I-(1) *on* $I \times P$ *satisfying* $\mathbf{y}(t_0, \widetilde{\mathbf{p}}) \in [\mathbf{z}_y^L(t_0), \mathbf{z}_y^U(t_0)]$ *for at least one* $\widetilde{\mathbf{p}} \in P$ *also satisfies*

$$\mathbf{x}(t, \mathbf{p}) \in [\mathbf{v}(t), \mathbf{w}(t)], \tag{110}$$

$$\mathbf{y}(t, \mathbf{p}) \in \mathcal{Y}(t, \mathbf{v}(t), \mathbf{w}(t), \mathbf{z}_y^L(t), \mathbf{z}_y^U(t)) \equiv \mathcal{H}^q\left(\phi\left(t, \mathbf{v}(t), \mathbf{w}(t), \mathbf{z}_y^L(t), \mathbf{z}_y^U(t)\right)\right), \tag{111}$$

for all $(t, \mathbf{p}) \in I \times P$ *and any* $q \in \mathbb{N}$.

Proof Consider Hypothesis I-5.1. By Lemma 6.1, the condition (EX) holds. Since $(\mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U)$ satisfy (98)-(99) on I, we must have $(t, \mathbf{v}(t), \mathbf{w}(t), \mathbf{z}_y^L(t), \mathbf{z}_y^U(t)) \in E_{\mathcal{H}}^*, \forall t \in I$. Then, by (98), (99) and Conclusion 5 of Lemma 2.4, the condition (ALG) in Hypothesis I-5.1 also holds. Now, it suffices to establish Hypotheses (IC) and (RHS) of Theorem I-5.3. (IC) holds by (100). To show (RHS).1, choose any $t \in I$ and suppose $\exists (\hat{\mathbf{p}}, \hat{\mathbf{z}}_x, \hat{\mathbf{z}}_y) \in P \times D_x \times [\mathbf{z}_y^L(t), \mathbf{z}_y^U(t)]$ such that $\mathbf{g}(t, \hat{\mathbf{p}}, \hat{\mathbf{z}}_x, \hat{\mathbf{z}}_y) = \mathbf{0}$ and $\hat{\mathbf{z}}_x \in \mathcal{B}_i^L([\mathbf{v}(t), \mathbf{w}(t)])$. By definition,

$$\phi_i^L(t, \mathbf{v}(t), \mathbf{w}(t), \mathbf{z}_y^L(t), \mathbf{z}_y^U(t)) \subset \phi(t, \mathbf{v}(t), \mathbf{w}(t), \mathbf{z}_y^L(t), \mathbf{z}_y^U(t)). \tag{112}$$

Then, by Conclusions 5 and 7 of Lemma 2.4, satisfaction of (98) and (99) implies that $\phi_i^L(t, \mathbf{v}(t), \mathbf{w}(t), \mathbf{z}_y^L(t), \mathbf{z}_y^U(t)) \in \mathcal{D}_{\mathcal{H}}^K$. By Conclusion 4 of the same,

$$\mathcal{Y}_i^L(t, \mathbf{v}(t), \mathbf{w}(t), \mathbf{z}_y^L(t), \mathbf{z}_y^U(t)) = \mathcal{H}^K(\phi_i^L(t, \mathbf{v}(t), \mathbf{w}(t), \mathbf{z}_y^L(t), \mathbf{z}_y^U(t))). \tag{113}$$

Then, Conclusion 1 of Corollary I-4.1 ensures that $\hat{\mathbf{z}}_y \in \mathcal{Y}_i^L(t, \mathbf{v}(t), \mathbf{w}(t), \mathbf{z}_y^L(t), \mathbf{z}_y^U(t))$. It follows that

$$f_i(t, \hat{\mathbf{p}}, \hat{\mathbf{z}}_x, \hat{\mathbf{z}}_y) \in [f_i]([t, t], P, \mathcal{B}_i^L([\mathbf{v}(t), \mathbf{w}(t)]), \mathcal{Y}_i^L(t, \mathbf{v}(t), \mathbf{w}(t), \mathbf{z}_y^L(t), \mathbf{z}_y^U(t))), \tag{114}$$

$$= [f_i](\psi_i^L(t, \mathbf{v}(t), \mathbf{w}(t), \mathbf{z}_y^L(t), \mathbf{z}_y^U(t))), \tag{115}$$

and hence (96) ensures that (RHS).1 is satisfied. Proof of (RHS).2 is analogous. $\quad\square$

A primary distinction between the two-phase and single-phase methods thus far is that the former is able to verify existence of a solution, while this has been assumed for the latter. It is shown below that the conditions of Corollary 6.2 are in fact sufficient to assert existence as well.

Theorem 6.1 *Let* $(\mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U)$ *be a solution of* (96)-(100) *on* I. *Then there exists a regular solution* $(\mathbf{x}, \mathbf{y})$ *of* I-(1) *on* $I \times P$ *satisfying* (110) *and* (111) *for all* $(t, \mathbf{p}) \in I \times P$ *and any* $q \in \mathbb{N}$.

Proof Let A be the set of points $(\hat{t}, \hat{\mathbf{v}}, \hat{\mathbf{w}}, \hat{\mathbf{z}}_y^L, \hat{\mathbf{z}}_y^U) \in E_{\mathcal{H}}^*$ such that

$$\mathcal{H}^{*,L}(\phi(\hat{t}, \hat{\mathbf{v}}, \hat{\mathbf{w}}, \hat{\mathbf{z}}_y^L, \hat{\mathbf{z}}_y^U)) > \hat{\mathbf{z}}_y^L \quad \text{and} \quad \mathcal{H}^{*,U}(\phi(\hat{t}, \hat{\mathbf{v}}, \hat{\mathbf{w}}, \hat{\mathbf{z}}_y^L, \hat{\mathbf{z}}_y^U)) < \hat{\mathbf{z}}_y^U. \tag{116}$$

By Theorem (6.1), A is open. Furthermore, $A \supset A_\phi$, where A_ϕ is the image of I under $\phi(\cdot, \mathbf{v}(\cdot), \mathbf{w}(\cdot), \mathbf{z}_y^L(\cdot), \mathbf{z}_y^U(\cdot))$ because $(\mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U)$ satisfy (98)-(99). Because A_ϕ is compact, $\exists \delta > 0$ such that $\mathbf{q} \in A_\phi$ and $\|\mathbf{q} - \mathbf{q}'\|_\infty \leq \delta$ implies $\mathbf{q}' \in A$. As a special case, this implies that (116) holds with $(\hat{t}, \hat{\mathbf{v}}, \hat{\mathbf{w}}, \hat{\mathbf{z}}_y^L, \hat{\mathbf{z}}_y^U) = (t, \mathbf{v}(t) - \mathbf{1}\delta, \mathbf{w}(t) + \mathbf{1}\delta, \mathbf{z}_y^L(t), \mathbf{z}_y^U(t))$ for every $t \in I$. Arguing as in Corollary 6.2, this implies that Hypothesis I-5.1 is satisfied with $[\mathbf{v}(t) - \mathbf{1}\delta, \mathbf{w}(t) + \mathbf{1}\delta]$ in place of $[\mathbf{v}(t), \mathbf{w}(t)]$.

Define

$$V_\delta \equiv \{(t, \mathbf{p}, \mathbf{z}_x) \in I \times P \times D_x : \mathbf{z}_x \in [\mathbf{v}(t) - \mathbf{1}\delta, \mathbf{w}(t) + \mathbf{1}\delta]\}. \tag{117}$$

By Lemma I-5.4, $\exists \mathbf{H}_\delta \in C^1(V_\delta, D_y)$ such that, for every $(t, \mathbf{p}, \mathbf{z}_x) \in V_\delta$, $\mathbf{z}_y = \mathbf{H}_\delta(t, \mathbf{p}, \mathbf{z}_x)$ is an element of $Z_y'(t)$ and satisfies $\mathbf{g}(t, \mathbf{p}, \mathbf{z}_x, \mathbf{z}_y) = \mathbf{0}$ uniquely among elements of $Z_y(t)$.

Now consider the system of ODEs

$$\dot{\mathbf{x}}(t, \mathbf{p}) = \mathbf{f}(t, \mathbf{p}, \mathbf{x}(t, \mathbf{p}), \mathbf{H}_\delta(t, \mathbf{p}, \mathbf{x}(t, \mathbf{p}))), \quad \mathbf{x}(t_0, \mathbf{p}) = \mathbf{x}_0(\mathbf{p}). \tag{118}$$

By the definition of C^1 functions (see §I-2), the right-hand side above is defined and C^1 on an open set $\widetilde{V} \supset V_\delta$. Fixing any $\mathbf{p} \in P$, it follows that there exists a unique solution of (118), $\mathbf{x}(\cdot, \mathbf{p}) \in C^1([t_0, \widetilde{t}], D_x)$, for some sufficiently small $\widetilde{t} \in (t_0, t_f]$ (see [8], Ch. II, Thm. 1.1). Furthermore, this solution can be extended to a maximal interval of existence $[t_0, t^*)$ such that $(t, \mathbf{p}, \mathbf{x}(t, \mathbf{p})) \to \partial \widetilde{V}$ as $t \to t^*$ (see [8], Ch. II, Thm. 3.1). Formally, this means that, for any compact $\Omega \subset \widetilde{V}$, there exists $\hat{t} \in (t_0, t^*)$ with $(\hat{t}, \mathbf{p}, \mathbf{x}(\hat{t}, \mathbf{p})) \notin \Omega$.

Note that V_δ is compact and suppose that $t^* \leq t_f$. Then, since $(t_0, \mathbf{p}, \mathbf{x}_0(\mathbf{p})) \in V_\delta$, continuity ensures that $\exists t' \in (t_0, t_f)$ with $(t, \mathbf{p}, \mathbf{x}(t, \mathbf{p})) \in V_\delta$, $\forall t \in [t_0, t']$, and $\mathbf{x}(t', \mathbf{p}) \notin [\mathbf{v}(t'), \mathbf{w}(t')]$. Define $\mathbf{y}(t, \mathbf{p}) \equiv \mathbf{H}_\delta(t, \mathbf{p}, \mathbf{x}(t, \mathbf{p}))$, $\forall t \in [t_0, t']$. It follows from the properties of $\mathbf{H}_\delta$ on V_δ that $(\mathbf{x}, \mathbf{y})$ is a solution of I-(1) on $[t_0, t'] \times \{\mathbf{p}\}$. It further follows that $\mathbf{y}(t, \mathbf{p}) \in Z_y(t)$, $\forall t \in [t_0, t']$. Then, Conclusion 3 of Corollary I-4.1 shows that this solution is regular. By Corollary 6.2, this implies that $\mathbf{x}(t', \mathbf{p}) \in [\mathbf{v}(t'), \mathbf{w}(t')]$, which is a contradiction. Therefore, $t^* > t_f$.

Since $\mathbf{p} \in P$ was arbitrary, the previous construction defines $(\mathbf{x}, \mathbf{y}) \in C^1(I \times P, D_x \times D_y)$, which is C^1 because $\mathbf{f}$ and $\mathbf{H}_\delta$ are. Arguing as above, this is a regular solution of I-(1) on $I \times P$ and satisfies (110) and (111) for all $(t, \mathbf{p}) \in I \times P$ and any $q \in \mathbb{N}$. $\square$

In light of Theorem 6.1, the single-phase bounding method is simply to solve the DAEs (96)-(100). Provided that numerical error is not a critical concern, this can be done using any state-of-the-art DAE solver. In the case studies in §7 we use `IDA` [9] with absolute and relative tolerances of 10^{-5}. Furthermore, we choose $K = 4$ and $\gamma(t) = 10^{-4}$, $\forall t \in I$. In addition to the function evaluators, IDA is provided with an additional routine to compute the system Jacobian. This is done using the forward mode AD scheme discussed in §4, with the exception that the contribution to the Jacobian owing to the dependence of $\mathbf{C}$ on $(\mathbf{v}, \mathbf{w}, \mathbf{z}_y^L, \mathbf{z}_y^U)$ is ignored.

Table 1 Computational complexity of evaluating the right-hand sides of (96)-(99). The left portion shows the sequence of computations, from top to bottom, using the definitions (87)-(95). The right portion shows the complexity of evaluating each function on the left, assuming that values for all previous computations (i.e. all quantities directly above the function on the left portion of the table) are given. For functions with subscript i, the tabulated complexities are for all $i = 1, \ldots, n_x$ evaluations.

η			$n_x + n_y$		
C			$mn_y^2 + n_y^3$		
ϕ	ϕ_i^L	ϕ_i^U	1	n_x	n_x
$\mathcal{H}^* \circ \phi$	$\mathcal{Y}_i^L$	$\mathcal{Y}_i^U$	$mn_y^2 + n_y^3$	$n_x K\left(mn_y^2 + n_y^3\right)$	$n_x K\left(mn_y^2 + n_y^3\right)$
	ψ_i^L	ψ_i^U		0	0
	$[f_i]^L \circ \psi_i^L$	$[f_i]^U \circ \psi_i^U$		$n_x m$	$n_x m$

6.1 Computational complexity of the single-phase and two-phase methods

Suppose that the cost of evaluating any of the functions $[f_i]$, $[g_j]$ or $[\frac{\partial g_j}{\partial y_k}]$ is $O(m)$, where m can be interpreted as the number of bits required to store the longest code list describing one of these functions. Then complexity of a single evaluation of the right-hand sides of (96)-(99) is $O\left(n_x K\left(mn_y^2 + n_y^3\right)\right)$. The contributions to this figure are described in Table 1. From the table, it can be seen that the cost of a right-hand side evaluation is dominated by the evaluation of $\mathcal{Y}_i^{L/U}$ and hence $\mathcal{H}^{+,K}$. The complexity of this step derives from the $O(mn_y^2)$ evaluation of $[\frac{\partial g}{\partial y}]$ and the $O(n_y^3)$ multiplication $\mathbf{C}[\frac{\partial g}{\partial y}]$. In addition to right-hand side evaluations, numerical integration of (96)-(100) will require $O((n_x + n_y)^3)$ operations due to matrix factorization in the corrector iteration.

The complexity of the two-phase method is the same as that of the single-phase method. By a similar analysis, evaluation of the right-hand sides of (58) and (59) is $O\left(n_x K\left(mn_y^2 + n_y^3\right)\right)$, while numerical integration requires $O\left(n_x^3\right)$ operations. Phase 1 is dominated by Step 4 of Algorithm 2, which requires the $O((n_y + n_x)^3)$ factorization of $\widetilde{\mathbf{J}}$. In practice, we find that the single-phase method is significantly more efficient than the two-phase method (see §7).

Table 1 suggests some target areas for efficiency gains in the single-phase method, and similar considerations also apply to the two-phase method. An approach that removes a factor of n_x from the entries in the last two columns of the fourth row is to replace each $\mathcal{Y}_i^L$ and $\mathcal{Y}_i^U$ by $\mathcal{Y}(t, \mathbf{v}, \mathbf{w}) \equiv \mathcal{H}^{+,K}(\phi(t, \mathbf{v}, \mathbf{w}))$. It is not difficult to show that Corollary 6.2 remains true, and because $\mathcal{Y}$ is used for all i, $\mathcal{H}^{+,K}$ only needs to be evaluated once in order to compute the right-hand sides of the entire system. However, the resulting bounds are weaker, and our experience suggests that the original implementation is well worth the effort. Another approach is to eliminate the n_y^3 terms in the second and fourth rows of Table 1 by using a different preconditioning scheme and/or exploiting sparsity of $\partial \mathbf{g}/\partial \mathbf{y}$. For larger systems, this will become important not only for efficiency, but also because computing $\mathbf{C}$ by direct matrix inversion will become numerically unstable. We leave these considerations for future work.

7 Case Studies

The computations presented in this section were performed on a Dell Precision T3400 workstation with a 2.83 GHz Intel Core2 Quad CPU. All experiments had one core and 512 MB of memory dedicated to the job. All interval computations and differentiation of interval equations was done using an in house C++ library based on operator overloading.

7.1 Example 1: A simple DAE with a singularity

Consider the semi-explicit DAEs

$$\dot{x}(t,p) = -px(t,p) - 0.1y(t,p), \tag{119}$$

$$0 = y(t,p) - \frac{\sin(p)}{\sqrt{y(t,p)}} - 25x(t,p),$$

with initial condition $x_0 = 1$ at $t_0 = 0$ and $p \in P \equiv [0.5, 4.0]$. We note that the solutions $y(t, \mathbf{p})$ approach 0 for all $\mathbf{p} \in P$ (Figure 2). Since the algebraic equation is not defined at $y = 0$, this poses an interesting challenge for bounding because even slight conservatism in the bounds for y will eventually enclose 0 and cause the methods to fail.

The results of applying the two proposed bounding approaches are shown in Figures 1 and 2. Note that the refined time-varying bounds computed in Phase 2 of the two-phase method are not shown because they are indistinguishable from those computed by the single-phase method (scrutiny shows that the latter are slightly sharper). The bounds produced by both methods are very sharp until roughly $t = 0.25$, where some slight overestimation becomes apparent. Computational times and other performace statistics are shown in Table 3 for various values of t_f (see also Table 2).

With $t_f = 0.25$, neither method has any significant difficulty and both produce bounds very efficiently. As t_f is increased to 0.30 and 0.33, the effort required of both methods increases significantly, with the increase for the two-phase method being more pronounced. For both methods, failure occurs around $t = 0.3313$ and bounds cannot be propagated further. For the single-phase method, IDA terminates after the corrector iteration fails to converge with minimum step size. Similarly for the two-phase method, repeated failures in Step 4 of Algorithm 2 cause the time step to be reduced below H_MIN (via Step 6). Indeed, the time steps taken by Algorithm 1 are evident from the staircase structure of the Phase 1 bounds in Figures 1 and 2, and are seen to shrink dramatically as t approaches 0.3313.

The ultimate cause of failure is that the inclusion (22), and analogously the equations (98)-(99), becomes difficult to satisfy. For the two-phase approach, the statistic STP in Table 3 shows that the relative number of failed time steps is increasing with increasing final time. These correspond to failures in Step 4 of Algorithm 2, which are split evenly between cases (a) and (b), with (b) occurring because $0 \in \square(z_y^L, z_y^U)$ for some iterate. In the single-phase approach, the corrector iteration in IDA encounters the same problems. Table 3 shows disproportionate increases in both the number of

Table 2 Definition of algorithm statistics presented in Tables 3 and 4.

CPU(s)	Both methods: Computational time for the complete bounding algorithm.
Ph1(s)	Two-phase method: Time spent in Phase 1 (Step 3 of Algorithm 1 as in §4).
Ph2(s)	Two-phase method: Time spent in Phase 2 (Step 6 of Algorithm 1 as in §5).
STP	Two-phase method: Number of time steps taken by Algorithm 1 over the number of attempted steps (the difference is the number of visits to Step 6 in Algorithm 2). Single-phase method: Number of times steps required by IDA [9] to solve (96)-(100).
CRI	Single-phase method: Cumulative number of corrector iterations during solution of (96)-(100) by IDA [9].

Table 3 Algorithm statistics for Example 1. Columns represents single experiments, which vary in the specified value of t_f.

t_f	0.25	0.30	0.33
Two-Phase Method Statistics			
CPU(s)	0.0026	0.0055	0.0500
Ph1(s)	0.0007	0.0020	0.0280
Ph2(s)	0.0019	0.0034	0.0212
STP	4/5	11/25	100/214
Single-Phase Method Statistics			
CPU(s)	0.0020	0.0024	0.0089
STP	40	45	84
CRI	58	73	268

time steps and the number of corrector iterations required by IDA as t_f is increased, indicating that the solver is having trouble satisfying (98)-(99). Despite their eventual failures, both methods produce bounds over a longer time horizon than any other approaches tried (see Remark 4.1).

On the whole, the two bounding methods fail at nearly the same time and produce nearly identical bounds where they are successful. In cases where the two-phase method reaches the final time with few, large time steps, the CPU time is nearly equivalent to that of the single phase method. On the other hand, the single-phase method is significantly faster in the difficult experiments where t_f approaches the failure time of 0.3313.

7.2 Example 2: Simple distillation

Consider the simple distillation of a Benzene/ Toluene mixture. Following the analysis in [3], this process can be described by the system of semi-explicit index-one
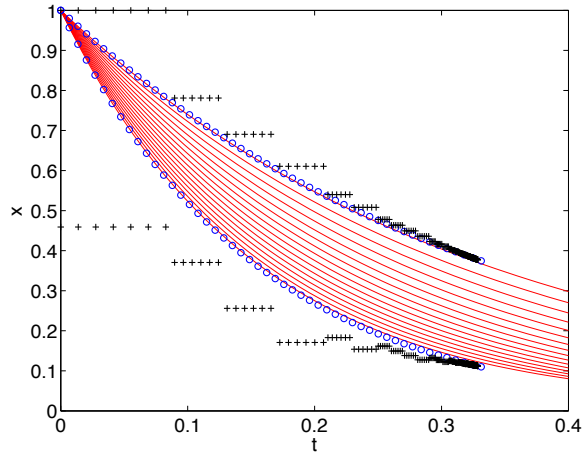
Fig. 1 Solutions $x(t, p)$ of (119) for 16 values of $p \in [0.5, 4.0]$ (solid curves), along with bounds from the single-phase method (circles) and bounds from Phase 1 of the two-phase method (crosses). Bounds from Phase 2 of the two-phase method are indistinguishable from the single-phase bounds and are not shown.
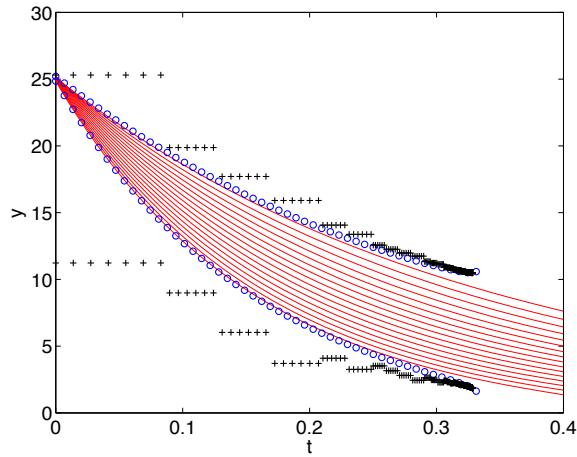
Fig. 2 Solutions $y(t, p)$ of (119) for 16 values of $p \in [0.5, 4.0]$ (solid curves), along with bounds from the single-phase method (circles) and bounds from Phase 1 of the two-phase method (crosses). Bounds from Phase 2 of the two-phase method are indistinguishable from the single-phase bounds and are not shown.

DAEs

$$\frac{d\phi_B}{d\xi} = \phi_B - \psi_B, \tag{120}$$

$$0 = \phi_B + \phi_T - 1,$$

$$0 = \psi_B + \psi_T - 1,$$

$$0 = \mathcal{P}\psi_B - \mathcal{P}_B^{sat}(T)\phi_B,$$

$$0 = \mathcal{P}\psi_T - \mathcal{P}_T^{sat}(T)\phi_T,$$

where the subscripts B and T denote Benzene and Toluene, respectively, ϕ is a liquid phase mole fraction, ψ is a vapor phase mole fraction, T denotes temperature, $\mathcal{P}$ denotes pressure, and the vapor pressures $\mathcal{P}_{\mathrm{B}}^{\mathrm{sat}}(T)$ and $\mathcal{P}_{\mathrm{T}}^{\mathrm{sat}}(T)$ are given by the Antoine expression

$$\log_{10} \mathcal{P}_i^{\mathrm{sat}}(T) = A_i - \frac{B_i}{T + C_i}, \quad i \in \{\mathrm{B}, \mathrm{T}\}. \tag{121}$$

The independent variable ξ is a dimensionless *warped time* (see [3]). The last two equations in (120) are derived assuming that Benzene/ Toluene is an ideal mixture. Nominal values of the Antoine coefficients in (121) are given for temperature in degrees C and pressures in mm HG in [4] as: $A_{\mathrm{B}} = 6.87987$, $B_{\mathrm{B}} = 1196.76$, $C_{\mathrm{B}} = 219.161$, $A_{\mathrm{T}} = 6.95087$, $B_{\mathrm{T}} = 1342.31$ and $C_{\mathrm{T}} = 219.187$. With $\mathcal{P} = 759.81$ mm Hg constant, we consider bounding the solutions of (120), $\mathbf{x} = \phi_{\mathrm{B}}$ and $\mathbf{y} = (\phi_{\mathrm{T}}, \psi_{\mathrm{B}}, \psi_{\mathrm{T}}, T)$, over the interval $\xi \in [0, 6]$, while considering various combinations of the Antoine coefficients as uncertain parameters. Computational times and algorithm statistics are presented in Table 4, where the first row indicates the Antoine coefficients which are considered to be uncertain, and the second row describes the interval P as a percent deviation around the nominal values of these coefficients. Though the uncertainty ranges considered may seem small, they describe a wide range of solution behavior because the corresponding parameters appear inside of an exponential in the model equations. Indeed, within a 6% deviation from the nominal value of A_{B} alone, the most volatile component can switch from Benzene to Toluene.
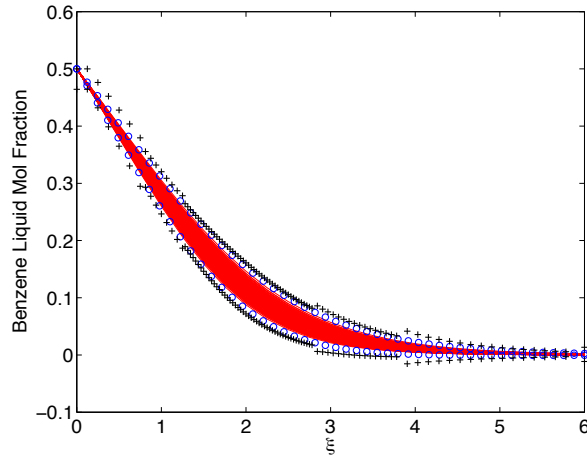
In the case where $\mathbf{p} = (A_{\mathrm{B}}, B_{\mathrm{B}}, A_{\mathrm{T}}, B_{\mathrm{T}})$ and the deviation is $\pm 0.2\%$, the results of both bounding methods are shown for $\phi_{\mathrm{B}}, \psi_{\mathrm{B}}$ and T in Figures 3, 4 and 5, respectively. Again, the time-varying bounds computed in Phase 2 of the two-phase method are not shown because they are indistinguishable from the single-phase bounds. Both methods provide very tight bounds on ϕ_{B} throughout the ξ interval of interest, and very reasonable bounds on ψ_{B} and T, with tight bounds at the beginning and end of the integration time.

In contrast to the simple example of the previous section, Algorithm 1 is forced to take relatively small time steps here. In Figures 3, 4 and 5, every cross plotted marks the end of a single such step. For experiments requiring many time steps of Algorithm 1, most are taken between ξ values of about 1.2 and 2.6. Within this interval, it is difficult to satisfy the inclusions of Step 3 and the step must be restricted often. In Figures 4 and 5, sharp jumps in the Phase 1 bounds can be observed at values of ξ where a relatively large step has been achieved after a difficult period through which the step size has been kept small. These jumps reflect the fact that wider $Z_{x,j}$ and $Z_{y,j}$ are required to satisfy (22) and (23) over large steps. For the single-phase method, one similarly observes that IDA takes more time steps for $\xi \in [1.2, 2.6]$, where it is difficult to satisfy (98)-(99). When the parameter interval P is sufficiently wide, neither algorithm is able to produce bounds through the difficult region between $\xi = 1.2$ and $\xi = 2.6$ (see Table 4). For example, when all six Antoine coefficients are considered as unknown with a $\pm 0.2\%$ deviation, both algorithms fail near $\xi = 1.53$.

As in the first example, the two bounding methods are equally robust and produce nearly identical bounds. However, the single-phase method is faster than the two-phase method in every experiment, with a factor varying between 3.5 to 7.

Table 4 Algorithm statistics for Example 2. Each column represents a single experiment. The first row indicates the model parameters considered as uncertain, and the second row indicates the percent deviation considered around the nominal parameter values. The symbol † indicates that the algorithm terminated unsuccessfully before $\xi = 6.0$.

	$[A_B\ B_T]$		$[A_B\ B_B\ A_T\ B_T]$		$[A_B\ B_B\ C_B\ A_T\ B_T\ C_T]$	
	±0.2%	±0.4%	±0.2%	±0.3%†	±0.1%	±0.2%†
ξ	6.0	6.0	6.0	1.090	6.0	1.534
	Two-Phase Method Statistics					
CPU(s)	0.073	0.1610	0.1637	0.24	0.0929	0.22
Ph1(s)	0.0315	0.0746	0.0800	0.16	0.0413	0.15
Ph2(s)	0.0412	0.0862	0.0835	0.08	0.0516	0.07
STP	44/88	93/187	96/193	100/214	55/110	100/209
	Single-Phase Method Statistics					
CPU(s)	0.0204	0.0229	0.0241	0.06	0.0185	0.06
STP	77	83	103	89	77	91
CRI	110	132	160	259	103	244

Fig. 3 Solutions $\phi_B(\xi, \mathbf{p})$ of (120) for $\mathbf{p} = (A_B, B_B, A_T, B_T)$ uniformly sampled within a ±0.2% deviation from nominal values (solid curves), along with bounds from the single-phase method (circles) and bounds from Phase 1 of the two-phase method (crosses). Bounds from Phase 2 of the two-phase method are indistinguishable from the single-phase bounds and are not shown.

8 Conclusions and Future Work

Two methods have been proposed for computing interval bounds on the solutions of semi-explicit index-one DAEs over a range of initial conditions and problem parameters. The first method is a two-phase approach using an interval existence and uniqueness test in Phase 1 and a refinement procedure based on differential inequalities in Phase 2. Efficient implementations for both phases were presented using interval computations and a state-of-the-art ODE solver. The second method combines the two phases of the first method and requires numerical solution of a system of semi-
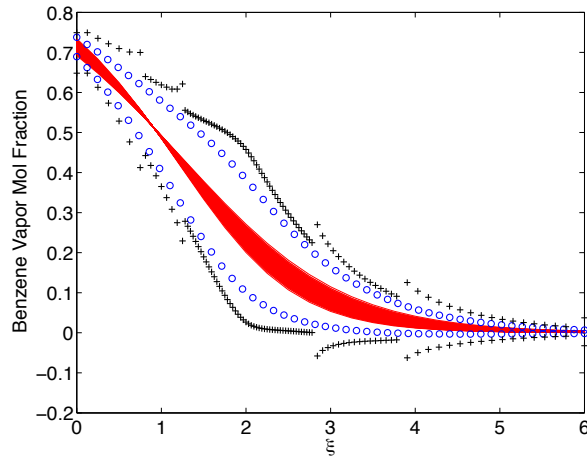
Fig. 4 Solutions $\psi_B(\xi, \mathbf{p})$ of (120) for $\mathbf{p} = (A_B, B_B, A_T, B_T)$ uniformly sampled within a $\pm 0.2\%$ deviation from nominal values (solid curves), along with bounds from the single-phase method (circles) and bounds from Phase 1 of the two-phase method (crosses). Bounds from Phase 2 of the two-phase method are indistinguishable from the single-phase bounds and are not shown.

explicit DAEs. Two case studies were considered, demonstrating that both methods produce sharp bounds very efficiently, with the single-phase method being consistently faster.

Several potential improvements to the presented algorithms remain to be explored. In the case of ODEs, it has been shown that problem specific physical information can often be incorporated into bounding methods based on differential inequalities to achieve significantly sharper bounds [18,19]. The use of such information is being explored for sharpening the results in Theorems I-4.2, I-5.1, I-5.2 and I-5.3. In addition to interval bounds, methods have been developed for ODEs which provide nonlinear convex and concave (with respect to parameters $\mathbf{p}$) bounds on the ODE solutions, pointwise in the independent variable [20]. Bounds of this type are often sharper than interval bounds and are more appropriate for certain applications, such as global dynamic optimization. Extending these methods to semi-explicit DAEs is currently under investigation. Finally, extensions to fully-implicit and high-index DAEs are being pursued.

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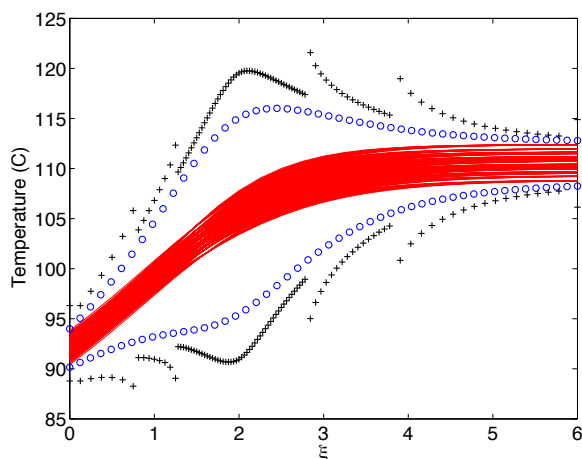
Fig. 5 Solutions $T(\xi, \mathbf{p})$ of (120) for $\mathbf{p} = (A_B, B_B, A_T, B_T)$ uniformly sampled within a $\pm 0.2\%$ deviation from nominal values (solid curves), along with bounds from the single-phase method (circles) and bounds from Phase 1 of the two-phase method (crosses). Bounds from Phase 2 of the two-phase method are indistinguishable from the single-phase bounds and are not shown.

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