

Zero-Init Non-Collapse for Bounded CRN-Shape PIVPs

Xiang Huang

Zinan Huang

2026-04-20

Abstract

We prove the following structural theorem about chemical reaction network (CRN) computable numbers. Let $y' = p(y)$, $y(0) = 0$, be a d -dimensional polynomial initial value problem (PIVP) admitting a *CRN-shape* decomposition $p_i(y) = \text{prod}_i(y) - \text{degr}_i(y) \cdot y_i$ with $\text{prod}_i, \text{degr}_i$ having non-negative rational coefficients. Suppose the trajectory is bounded on $[0, \infty)$. Then any species y_i that is strictly positive at some finite time $t_0 \geq 0$ admits a positive constant $c > 0$ such that $y_i(t) \geq c$ on a cofinal subset of $[0, \infty)$. In particular, $y_i(t) \not\rightarrow 0$. Consequently, if the designated output of a bounded zero-init CRN-shape PIVP converges to 0, then the output trajectory is identically 0: the constant 0 is not non-trivially CRN-computable from zero init. The result has been formalized in Lean 4 / Mathlib with zero custom axioms.

1 Background

1.1 CRN computability

A *polynomial initial value problem* (PIVP) of dimension d is

$$y'(t) = p(y(t)), \quad y(0) = y_0 \in \mathbb{Q}^d, \quad (1)$$

where $p: \mathbb{R}^d \rightarrow \mathbb{R}^d$ is a polynomial vector field with rational coefficients. PIVPs are the phase-space model for the general-purpose analog computer (GPAC). A real number α is *real-time CRN-computable* ($\alpha \in R_{\text{RTC RN}}$) if it can be approximated at exponential rate by a designated output coordinate of a bounded PIVP implementable as a chemical reaction network with mass-action kinetics [1, 2, 3].

The CRN constraint imposes strong structural requirements. Concentrations are non-negative, reaction rates are non-negative, and any degradation of a species X_i must be catalyzed by X_i itself: you can only destroy what is already present. Abstractly, the vector field admits a decomposition

$$p_i(y) = \text{prod}_i(y) - \text{degr}_i(y) \cdot y_i, \quad (2)$$

where prod_i and degr_i are polynomials with non-negative rational coefficients. The factor of y_i in the degradation term is the mass-action constraint: every reaction that consumes X_i requires X_i on its left-hand side.

Definition 1 (CRN-shape decomposition). *A PolyCRNDecomposition of a PIVP (1) is a choice of polynomials $\text{prod}_i, \text{degr}_i \in \mathbb{Q}_{\geq 0}[y_1, \dots, y_d]$ satisfying (2) for every i , together with $y_0 \in \mathbb{Q}_{\geq 0}^d$.*

1.2 Zero initialization

CRN species start from zero concentration. There is no laboratory operation that *preloads* an arbitrary rational value into a molecular species: one starts by filling the flask, and then the reactions run. Zero initialization is therefore the physically canonical assumption.

Definition 2 (Zero init). *A PIVP (1) is zero-initialized if $y_0 = \mathbf{0}$.*

Zero init is rigid: it rules out decay as a computational mechanism. The simplest contrast is the linear scalar system $x' = -x$, with $x(0) = 1$: $x(t) = e^{-t} \rightarrow 0$. In the zero-init CRN-shape setting, this decay is impossible. The field at $x = 0$ reduces to $\text{prod}(0)$, which is the constant coefficient of prod ; if this is positive, x grows, and if it is zero, x never moves. Either way, x cannot decay to a limit of 0 non-trivially. This paper formalizes the d -dimensional version of that observation.

1.3 Root species and dependency

A species X_i is a *root* if $(\text{prod}_i)_0 > 0$, that is, the production polynomial has a strictly positive constant term. Equivalently, there is an $\emptyset \rightarrow X_i$ reaction that synthesizes X_i from nothing. A root species can grow from zero without external input.

Non-root species depend on upstream species. We formalize this via a graph-theoretic *root-reachability* predicate: species i is root-reachable if either (i) i is a root, or (ii) prod_i contains a positive-coefficient monomial $\prod_j y_j^{\sigma_j}$ every one of whose active feeders (j with $\sigma_j > 0$) is already root-reachable. This is a least-fixed-point definition: the root-reachable set is built up inductively from the roots.

2 Main Theorem

Theorem 3 (Zero-init non-collapse). *Let (P, pcd) be a d -dimensional PIVP equipped with a CRN-shape decomposition (Definition 1), and assume P is zero-initialized. Let $y: [0, \infty) \rightarrow \mathbb{R}^d$ be a solution of P whose trajectory is bounded:*

$$\exists M > 0 : \|y(t)\| \leq M \quad \text{for all } t \geq 0.$$

If $y_i(t_0) > 0$ for some $i \in \{1, \dots, d\}$ and $t_0 \geq 0$, then there exists $c > 0$ such that

$$\forall T \geq 0, \exists t \geq T : y_i(t) \geq c.$$

In particular, $\liminf_{t \rightarrow \infty} y_i(t) > 0$, and no limit of $y_i(t)$ as $t \rightarrow \infty$ (if it exists) can be 0.

The cofinal form of the conclusion is what we actually prove; it is equivalent to $\liminf y_i \geq c$ by standard reasoning.

Corollary 4 (Trivial-zero theorem). *Under the hypotheses of Theorem 3, if the designated output coordinate y_{i^*} satisfies $y_{i^*}(t) \rightarrow 0$ as $t \rightarrow \infty$, then $y_{i^*}(t) = 0$ for all $t \geq 0$.*

Proof. Suppose $y_{i^*}(t^*) \neq 0$ for some $t^* \geq 0$. Non-negativity of the trajectory (Proposition 6 below) gives $y_{i^*}(t^*) > 0$. Theorem 3 provides $c > 0$ such that $y_{i^*}(t) \geq c$ cofinally, contradicting $y_{i^*}(t) \rightarrow 0$. \square

Remark 5. *Corollary 4 says the constant 0 is not a non-trivially CRN-computable number from zero init: if 0 is a limit of the output, the output is literally 0 throughout the experiment. Computing 0 is only possible by never doing anything.*

3 Proof

The proof is modular, in three steps.

3.1 Step 1 — Non-negativity

Proposition 6 (CRN non-negativity). *Under the hypotheses of Theorem 3, $y_i(t) \geq 0$ for every i and every $t \geq 0$.*

Proof sketch. This is the standard mass-action invariance. Whenever $y_i = 0$, the field reduces to $p_i = \text{prod}_i(y) \geq 0$ by non-negativity of the coefficients of prod_i and of the remaining coordinates $y_j \geq 0$. A squared-negative-mass Lyapunov functional $V(t) := \sum_i (y_i(t))_+^2$ satisfies $V(0) = 0$ and $V' \leq L \cdot V$ for a Lipschitz constant L on the bounded trajectory ball, so Grönwall gives $V \equiv 0$. Full details appear in the Mathlib-style proof `pivp_solution_nonneg` in our Lean formalization, invoked together with a local Lipschitz estimate for the polynomial vector field. \square

3.2 Step 2 — Positive lower bound for root species

The structural heart of the proof lives here. We show that any root species admits a positive asymptotic lower bound via a scalar Grönwall argument.

Proposition 7 (Root species lower bound). *Under the hypotheses of Theorem 3, let r be a root species, so $c_r := (\text{prod}_r)_0 > 0$. Then there exists $c > 0$ such that $y_r(t) \geq c$ holds on a cofinal subset of $[0, \infty)$.*

Proof. On the bounded trajectory ball $B_M := \{y \in \mathbb{R}_{\geq 0}^d : \|y\| \leq M\}$, Step 1 gives $y(t) \in B_M$ for all $t \geq 0$. Two algebraic facts about polynomials with non-negative coefficients on the non-negative orthant do the work.

(L) *Constant-coefficient lower bound.* For any polynomial $q \in \mathbb{Q}_{\geq 0}[y_1, \dots, y_d]$ and any $y \in \mathbb{R}_{\geq 0}^d$,

$$q_0 \leq q(y).$$

This holds because $q(y) = q_0 + \sum_{\sigma \neq 0} q_\sigma \prod_j y_j^{\sigma_j}$ and every summand on the right is non-negative.

(U) *Uniform upper bound on B_M .* For any polynomial $q \in \mathbb{Q}_{\geq 0}[y_1, \dots, y_d]$, the quantity $U_q(M) := \sum_{\sigma \in \text{supp}(q)} q_\sigma M^{|\sigma|}$ (where $|\sigma| = \sum_j \sigma_j$) is a uniform upper bound: $q(y) \leq U_q(M)$ for every $y \in B_M$.

Applied to prod_r and degr_r at $y = y(t)$, (L) and (U) give

$$y_r'(t) = \text{prod}_r(y(t)) - \text{degr}_r(y(t)) \cdot y_r(t) \geq c_r - D_r \cdot y_r(t),$$

where $D_r := U_{\text{degr}_r}(M) \geq 0$. Notice how the CRN shape is used: the degradation term is linear in y_r , which is what makes the right-hand side a scalar affine inequality in y_r .

Set $K := D_r + 1$ (strictly positive even when $D_r = 0$), and define the target level $\alpha := c_r/K > 0$. Consider the deficit $f(t) := \alpha - y_r(t)$. From the above,

$$f'(t) = -y_r'(t) \leq -c_r + D_r \cdot y_r(t) = -c_r + D_r(\alpha - f(t)) = -\frac{c_r}{K} - D_r \cdot f(t) = -\alpha - D_r \cdot f(t).$$

Zero init gives $f(0) = \alpha$. Scalar Grönwall with slope $-D_r$ and drift $-\alpha$ yields, for $t \geq 0$,

$$f(t) \leq \alpha \cdot e^{-D_r t} - \frac{\alpha}{D_r} (1 - e^{-D_r t}) \xrightarrow{t \rightarrow \infty} -\frac{\alpha}{D_r} \text{ (if } D_r > 0),$$

with the obvious modification $f(t) \leq \alpha - \alpha t \rightarrow -\infty$ when $D_r = 0$. In either case, for t beyond an explicit threshold t_* (depending only on c_r , D_r , and M) we have $f(t) \leq \alpha/2$, i.e., $y_r(t) \geq \alpha/2$. This is the required positive lower bound, holding for all $t \geq t_*$ (hence cofinally). \square

Proposition 7 is actually proved in two forms in the Lean file: the cofinal form used directly above, and the stronger *eventual* form asserting $y_r(t) \geq c$ for *all* $t \geq T$ and some T . The latter is what feeds into Step 3.

3.3 Step 3 — Propagation to root-reachable species

Step 2 covers root species only. A non-root species i that ever becomes positive must be *fed*, directly or transitively, by a root. Step 3 has two components: a graph-theoretic statement and an analytic propagation.

3.3.1 Root-reachability propagates lower bounds

Proposition 8 (Analytic propagation). *If every root species r admits an eventual positive lower bound, then so does every root-reachable species i .*

The proof is an induction on the inductive definition of root-reachability. The root case is Step 2. For the step case, if prod_i contains a positive-coefficient monomial $m(y) = q_\sigma \prod_{j:\sigma_j>0} y_j^{\sigma_j}$ every active feeder of which has an eventual lower bound, then $m(y(t))$ itself has a positive eventual lower bound (product of positive quantities is positive). Since every other monomial of prod_i is non-negative, $\text{prod}_i(y(t))$ inherits that positive lower bound, and the same scalar Grönwall argument as in Step 2 applies to y_i .

3.3.2 Graph traversal: ever-positive implies root-reachable

The non-trivial content is the converse direction of the graph: if i is ever positive on the trajectory, then i is root-reachable. Phrased in the contrapositive: if i is not root-reachable, then $y_i(t) = 0$ for every $t \geq 0$.

Proposition 9 (Graph traversal). *Let $R \subseteq \{1, \dots, d\}$ be the set of root-reachable species. For every $t \geq 0$ and every $j \notin R$, $y_j(t) = 0$.*

Proof. Let $N := \{1, \dots, d\} \setminus R$ denote the *dead* species. We study the quadratic functional

$$S(t) := \sum_{j \in N} y_j(t)^2. \tag{3}$$

Zero init gives $S(0) = 0$, and Proposition 6 combined with the CRN-shape polynomial structure gives $S(t) \geq 0$ for all $t \geq 0$. The proof reduces to showing $S' \leq C \cdot S$ on $[0, \infty)$ for some constant $C \geq 0$ depending only on the polynomial structure and M ; scalar Grönwall then forces $S \equiv 0$, and since S is a sum of squares, every y_j with $j \in N$ is identically zero.

Differentiate (3):

$$S'(t) = 2 \sum_{j \in N} y_j(t) \cdot p_j(y(t)) = 2 \sum_{j \in N} y_j(t) \cdot (\text{prod}_j(y(t)) - \text{degr}_j(y(t)) \cdot y_j(t)).$$

The degradation contribution is $-2 \sum_{j \in N} \text{degr}_j(y(t)) y_j(t)^2 \leq 0$ (non-negative coefficients, non-negative values), so we may drop it:

$$S'(t) \leq 2 \sum_{j \in N} y_j(t) \cdot \text{prod}_j(y(t)). \tag{4}$$

The crux is now a structural observation about the monomials of prod_j for $j \in N$.

Claim. For every $j \in N$ and every monomial σ with $(\text{prod}_j)_\sigma > 0$, there exists some $k = k(j, \sigma) \in N$ with $\sigma_k > 0$ (i.e., at least one active feeder of the monomial is itself dead).

Proof of claim. If the claim failed, every feeder k with $\sigma_k > 0$ would be root-reachable. But then j would be root-reachable via the **step** clause of the inductive definition (apply the step clause to this monomial, using root-reachability of all its feeders), contradicting $j \in N$. \square

Using the claim, bound each summand $y_j \cdot m(y)$ for a monomial $m(y) = (\text{prod}_j)_\sigma \prod_\ell y_\ell^{\sigma_\ell}$ by the “dead-feeder” factor y_k :

$$y_j \cdot m(y) \leq (\text{prod}_j)_\sigma M^{|\sigma|} \cdot y_j \cdot y_k \leq (\text{prod}_j)_\sigma M^{|\sigma|} \cdot \frac{1}{2}(y_j^2 + y_k^2),$$

where we used $y_\ell \leq M$ on the remaining factors and AM–GM on the final $y_j \cdot y_k$. Both $j \in N$ and $k \in N$, so both y_j^2 and y_k^2 are summands of S . Summing over all (j, σ) with $(\text{prod}_j)_\sigma > 0$, we obtain

$$S'(t) \leq C \cdot S(t), \quad t \geq 0,$$

for an explicit finite constant C . Combined with $S(0) = 0$ and $S \geq 0$, scalar Grönwall yields $S(t) \leq 0 \cdot e^{Ct} = 0$ for all $t \geq 0$. Hence $y_j(t) = 0$ for every $j \in N$ and every $t \geq 0$. \square

Remark 10. *The S -functional approach bypasses a continuity argument based on the first time a species becomes positive, which we initially considered. Since zero init already guarantees $S(0) = 0$, and scalar Grönwall directly propagates that to $S \equiv 0$, no first-positive-time analysis is needed. This simplification came from recognizing that the dead-species set is itself forward-invariant, which is encoded cleanly in a single quadratic functional.*

3.3.3 Assembling the theorem

By Proposition 9, the hypothesis $y_i(t_0) > 0$ implies $i \in R$, i.e., i is root-reachable. By Proposition 8 (with the eventual form of Step 2 as base case), y_i admits an eventual positive lower bound, which implies the cofinal form of Theorem 3. \square

4 Lean 4 Formalization

The proof has been mechanized in Lean 4 with Mathlib. The main file is

`Ripple/Core/ZeroInitPositivity.lean` (1635 lines).

Headline theorems

- `zero_init_no_collapse` (line 1590) — Theorem 3.
- `zero_of_limit_is_trivial` (line 1610) — Corollary 4.
- `crn_trajectory_nonneg` (line 162) — Proposition 6.
- `noCollapse_step2_root_liminf` (line 362) and `noCollapse_step2_root_eventual` (line 782) — Proposition 7, in cofinal and eventual forms respectively.
- `noCollapse_step3_scc_induction` (line 1552) — Proposition 8, via `rootReachable_hasEventualLowerBound` (analytic propagation) and
- `everPositive_rootReachable` (line 1157) — Proposition 9, proved via the S -functional Grönwall described in Section 3.3.2.

Axiom trace

The Lean command

```
#print axioms zero_init_no_collapse
```

returns exactly `[propext, Classical.choice, Quot.sound]`, the three standard Mathlib axioms. The formalization uses **zero custom axioms**: every structural claim is discharged to a mechanical proof.

Milestones

The proof was developed incrementally over several commits:

Commit	Milestone
4ac4c00	Initial formalization scaffold (three axiom placeholders)
abe1527	Step 2 discharged: root species Grönwall lower bound
9c6ab11	Step 3 graph-traversal theorem (modular form)
b1eebc6	Rank-form descent for <code>everPositive_rootReachable</code>
c72484f	Final axiom discharged: <code>everPositive_hasFeedingMonomial</code>
bd1f1e9	<code>polyPIVP_field_locally_lipschitz</code> promoted to theorem

After `c72484f` the theorem is axiom-free beyond Mathlib’s three standard axioms.

5 Discussion

5.1 What the theorem rules out

Theorem 3 is a *non-collapse* statement: a bounded zero-init CRN-shape species cannot “decay to zero” in any limiting sense, once it has ever become positive. Equivalently, Corollary 4 says 0 is computable from zero init only trivially, by never producing any output signal.

The obvious question is whether the theorem leaves room for weaker forms of collapse: can $y_i(t)$ approach 0 arbitrarily closely without converging to it? The answer is no: the cofinal conclusion gives a uniform $c > 0$ such that $y_i(t) \geq c$ happens for arbitrarily large t , so $\liminf_{t \rightarrow \infty} y_i(t) \geq c > 0$, which rules out $\liminf y_i(t) = 0$ in particular.

5.2 Why non-zero init is different

Without zero init, the conclusion fails spectacularly. The one-dimensional system $x' = -x$, $x(0) = 1$ is CRN-shape ($\text{prod} = 0$, $\text{degr} = 1$), bounded, and satisfies $x(t) = e^{-t} \rightarrow 0$. The non-negative-init condition alone does *not* force the conclusion — it is the zero-init condition that forces production to dominate at every zero state.

5.3 Connections and forward directions

Positivity certificates. The monomial-cover argument in the claim within Proposition 9 is effectively a Positivstellensatz witness for the forward-invariance of the dead-species orthant. An interesting open question is whether the inductive root-reachability predicate admits a polynomial-time syntactic check (it does: it is a reachability problem on the monomial support hypergraph) and whether more refined reachability concepts (e.g., reachability with quantitative rate bounds) can be formalized similarly.

Signomial programming. The scalar Grönwall argument in Step 2 gives an explicit bound $\alpha := c_r/(D_r + 1)$, and this is provably tight up to the +1 regularizer: the asymptotic lim inf of y_r is c_r/D_r in the case $D_r > 0$. A tighter quantitative theory, with α as a function of the polynomial data and the box size M , would connect directly to signomial programming and to the bounded analog complexity hierarchy of [4].

Characterizing LPP-computability. Theorem 3 is a *necessary* condition for any species in a zero-init CRN to play the role of a non-trivial output. Combined with the constructive CRN realizations from [1, 2, 3], it sharpens the characterization of R_{RTCRN} from zero-init CRNs: the only limit points of output trajectories that are genuinely computed (as opposed to being identically zero) are strictly positive.

References

- [1] X. Huang, T.H. Klinge, J.I. Lathrop, X. Li, J.H. Lutz. Real-time computability of real numbers by chemical reaction networks. *Natural Computing*, 2018.
- [2] X. Huang, T.H. Klinge, and J.I. Lathrop. Real-time equivalence of chemical reaction networks and analytic signal transducers. In *Proc. DNA 25*, LNCS 11648, pp. 31–50, 2019.
- [3] X. Huang and R. Huls. Computing real numbers with large-population protocols. In *Proc. DNA 28*, 2022.
- [4] H.-L. Chen and X. Huang. Bounded analog complexity. In *Proc. DNA 32*, 2026.