

# Comparing Discrete and Piecewise Affine Differential Equation Models of Gene Regulatory Networks (Long Version)

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## Abstract

Mathematical modeling often helps to provide a systems perspective on gene regulatory networks. In particular, qualitative approaches are useful when detailed kinetic information is lacking. Multiple methods have been developed that implement qualitative information in different ways, e.g., in purely discrete or hybrid discrete/continuous models. In this paper, we compare the discrete asynchronous logical modeling formalism for gene regulatory networks due to R. Thomas with piecewise affine differential equation models. We provide a local characterization of the qualitative dynamics of a piecewise affine differential equation model using the discrete dynamics of a corresponding Thomas model. Based on this result, we investigate the consistency of higher-level dynamical properties such as attractor characteristics and reachability. We show that although the two approaches are based on equivalent information, the resulting qualitative dynamics are different. In particular, the dynamics of the piecewise affine differential equation model is not a simple refinement of the dynamics of the Thomas model

*Keywords:* Gene regulatory networks, mathematical modeling, discrete models, piecewise affine models

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## 1. Introduction

Gene regulation is the result of a complex interplay of molecular components forming large interaction networks. Mathematical modeling of gene regulatory networks gives insights into the underlying structure and dynamics of various biological systems. If information on kinetic parameters is lacking, *qualitative formalisms* offer a well-established alternative to the more traditionally used differential equation models. Using only qualitative information on the network

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structure and the interactions between the components, these approaches allow obtaining an abstract description of the system's dynamics.

The discrete formalism of Thomas (1973) (Thomas and D'Ari, 1990) is a qualitative method describing a gene regulatory network by a discrete function. Each network component is represented by a variable that takes integer values representing the different levels of gene activity. The information on how the behavior of one component is governed by the values of the other components is captured in a discrete function. The component functions then constitute the coordinate functions of the update function of the network. To derive the dynamics of the system, Thomas introduced the asynchronous update method where only one variable changes per discrete time step, and only by a unit value. Since the state space is finite, the dynamics can be represented by a directed graph, the so-called asynchronous *state transition graph* (STG).

The particularities of the asynchronous update method result in a close correspondence of the discrete model to certain differential equation systems (Snoussi, 1989). Differential equation models consisting of step functions retain a continuous time evolution, yet can be seen as qualitative due to the close relation of step and discrete functions. Such piecewise affine differential equation (PADE) models approximate certain ordinary differential equation models (Glass and Kauffman, 1972, 1973). De Jong et al. (2004) have shown that they can essentially be captured by a discrete representation which abstracts the continuous solution trajectories of the differential equations into transitions between different regions of the phase space. Again, the resulting dynamics can be represented by a directed graph, the *qualitative transition graph* (QTG).

In this paper, we aim at clarifying the relation between Thomas and PADE models by comparing the respective graphs capturing the dynamical behavior. Several results in this direction already exist. For example, attractors, including steady states and certain limit cycles, are related (Glass and Kauffman, 1972; Snoussi, 1989; Snoussi and Thomas, 1993; Chaves et al., 2010; Wittmann et al., 2009). Our goal here is to present a comprehensive comparison between the STG and the QTG.

The paper is organized as follows. Sect. 2 presents a discrete modeling approach based on the Thomas formalism. PADE systems and the qualitative analysis developed by de Jong et al. (2004) are introduced in Sect. 3. In Sect. 4, we start comparing the two formalisms. Sect. 5 describes our main result characterizing transitions in the QTG using edges originating in corresponding vertices in the STG. We illustrate the application of this result with examples of relations between paths and attractors in the two graphs. The conclusion and perspectives for future work are given in Sect. 6.

This paper is the full version of an extended abstract included in the proceedings of IPCAT 2012 (Jamshidi et al., 2012).

## 2. Discrete formalism

Consider a gene network with  $n$  regulatory components. In the discrete modeling approach, the activity level of a component  $i$  is modeled by a dis-

crete variable  $q_i$ , which takes its values in a finite set of natural numbers  $Q_i = \{0, \dots, p_i\}, p_i \geq 1$ . The *state space* of the discrete model is  $Q = Q_1 \times \dots \times Q_n$ , and the regulatory interactions are captured by a discrete *update function*  $f = (f_1, \dots, f_n) : Q \rightarrow Q$ . The function  $f$  uniquely determines the *state transition graph*  $STG(f) = (Q, E)$ , a directed graph with node set  $Q$  and edge set  $E \subset Q \times Q$ . For any  $j \in \{1, \dots, n\}$ ,  $q \in Q$  with  $f_j(q) \neq q_j$ , there is an edge  $(q, q') \in E$ , where  $q'_j = q_j + \text{sgn}(f_j(q) - q_j)$  and  $q'_i = q_i$ , for all  $i \in \{1, \dots, n\} \setminus \{j\}$ . Here,  $\text{sgn} : \mathbb{R} \rightarrow \{-1, 0, 1\}$  denotes the sign function. If  $f(q) = q$ , then  $(q, q) \in E$  and  $q$  is called a *fixpoint*.

Unless  $f$  is Boolean, it is not possible to recover  $f$  from  $G = STG(f)$ . However, we may obtain from  $G$  a *unitary update function*  $f^G : Q \rightarrow Q$  by setting

$$f_j^G(q) = q_j + \sum_{q' \in AS(q)} (q'_j - q_j), \text{ for } j \in \{1, \dots, n\}.$$

Here  $AS(q) := \{q' \in Q \mid (q, q') \in E\}$  denotes the set of *asynchronous successors* of  $q$  in  $G$ .

**Lemma 1.** *Let  $f : Q \rightarrow Q$  be an update function and  $G = STG(f)$ . Then*

$$STG(f) = STG(f^G).$$

*Proof.* Let  $j \in \{1, \dots, n\}$  and  $q \in Q$ . By definition of  $AS(q)$ , there exists at most one  $q' \in AS(q)$  such that  $|q'_j - q_j| = 1$ . This implies  $\text{sgn}(f_j(q) - q_j) = q'_j - q_j$ . Therefore,  $\text{sgn}(f_j(q) - q_j) = \sum_{q' \in AS(q)} (q'_j - q_j)$ , and the result follows.  $\square$

The unitary update function  $f^G$  captures the information from the original update function  $f$  contained in  $G = STG(f)$ . If  $f$  is Boolean,  $f$  and  $f^G$  are the same.

**Example 1.** For  $Q = \{0, 1\} \times \{0, 1, 2\}$  and the update function  $f : Q \rightarrow Q$

$q$	00	01	02	10	11	12
$f(q)$	12	12	11	00	10	11

the state transition graph  $STG(f)$  is displayed on the left of Fig. 2(a).

### 3. Piecewise affine differential equations

Next we discuss piecewise affine differential equations (PADE) and the qualitative modeling approach introduced by de Jong et al. (2004). While a number of refinements have been proposed (Batt et al., 2008), we use here the original approach for the comparison with the Thomas formalism. The focus of this section is the *qualitative dynamics* associated with a system of PADEs, i.e., the discrete representation of all possible solution trajectories of the PADEs satisfying certain parameter constraints.

Consider an  $n$ -dimensional phase space  $\Omega = \Omega_1 \times \dots \times \Omega_n \subset \mathbb{R}_{\geq 0}^n$ , where  $\Omega_i = \{x_i \in \mathbb{R} \mid 0 \leq x_i \leq \max_i\}$ , and  $\max_i \in \mathbb{R}_{> 0}$ . For every continuous variable  $x_i \in \Omega_i$  we assume  $p_i \in \mathbb{N}$  thresholds  $\theta_i^1, \dots, \theta_i^{p_i}$  satisfying the ordering

$$0 < \theta_i^1 < \dots < \theta_i^{p_i} < \max_i, \quad \text{for all } i \in \{1, \dots, n\}. \quad (1)$$

In the comparison with the discrete formalism in Sect. 2, the value  $p_i$  chosen here corresponds to the maximal value  $p_i$  of the component range  $Q_i$  of a discrete model. The union of the threshold hyperplanes is denoted by  $\Theta := \bigcup_{i \in \{1, \dots, n\}, j_i \in \{1, \dots, p_i\}} \{x \in \Omega \mid x_i = \theta_i^{j_i}\}$ . We consider a set of PADEs in  $\Omega \setminus \Theta$  of the form

$$\dot{x}_i = F_i(x) - G_i(x)x_i, \quad i \in \{1, \dots, n\}, \quad (2)$$

where the functions  $G_i : \Omega \setminus \Theta \rightarrow \mathbb{R}_{> 0}$  and  $F_i : \Omega \setminus \Theta \rightarrow \mathbb{R}_{\geq 0}$  are linear combinations of products of step functions  $S^+(x_l, \theta_l^k) = \begin{cases} 0 & \text{if } x_l < \theta_l^k, \\ 1 & \text{if } x_l > \theta_l^k, \end{cases}$  and  $S^-(x_l, \theta_l^k) = 1 - S^+(x_l, \theta_l^k)$  for  $l \in \{1, \dots, n\}$ .

To obtain a discrete representation of the PADE system, the state space is partitioned into a set of domains.

**Definition 1.** Consider a set of PADEs of the form (2) with phase space  $\Omega$  and thresholds  $\theta_i^j$ . The  $(n-1)$ -dimensional hyperplanes corresponding to the equations  $x_i = \theta_i^j$ ,  $j \in \{1, \dots, p_i\}$ , divide  $\Omega$  into hyper-rectangular regions called domains. A domain  $D \subset \Omega$  is defined by  $D = D_1 \times \dots \times D_n$  where every  $D_i$  is given by one of the following equations

$$\begin{aligned} D_i &= \{x_i \mid 0 \leq x_i < \theta_i^1\}, \\ D_i &= \{x_i \mid \theta_i^k < x_i < \theta_i^{k+1}\} \text{ for } k \in \{1, \dots, p_i - 1\}, \\ D_i &= \{x_i \mid \theta_i^{p_i} < x_i \leq \max_i\}, \\ D_i &= \{x_i \mid x_i = \theta_i^k\} \text{ for } k \in \{1, \dots, p_i\}. \end{aligned}$$

By  $\mathcal{D}$  we denote the set of all domains in  $\Omega$ . A domain  $D \in \mathcal{D}$  is called a *singular domain*, if there exists  $i \in \{1, \dots, n\}$  such that  $D_i = \{x_i \mid x_i = \theta_i^k\}$  for some  $k \in \{1, \dots, p_i\}$ . The variable  $x_i$  is then called *singular variable*. The *order* of a singular domain is the number of its singular variables. A domain  $D \in \mathcal{D}$  is called a *regular domain*, if it is not a singular domain. The set of regular and singular domains are denoted by  $\mathcal{D}_r$  and  $\mathcal{D}_s$  respectively.

It follows immediately that for any regular domain  $D \in \mathcal{D}_r$ , the functions  $F_i(x)$  and  $G_i(x)$  are constant on  $D$ . Thus (2) can be written as a linear system  $\dot{x} = F^D - G^D x$ , for all  $x \in D$ , where  $G^D = \text{diag}(G_1^D, \dots, G_n^D)$  is a diagonal matrix with strictly positive entries and  $F^D = (F_1^D, \dots, F_n^D)$  a positive vector. It is easy to see that solutions of (2) starting in a regular domain  $D$  converge monotonically towards the so-called *focal point*  $\phi(D) := (G^D)^{-1}F^D$ .

In agreement with de Jong et al. (2004), we will assume that all focal points lie in a regular domain. By definition of the regular domains, we can then encode

the position of each focal point by strict inequalities involving the threshold values and the components of the focal point. We call these constraints *ordering constraints*.

To define a suitable dynamics of (2) on singular domains, the differential equations can be extended to differential inclusions, and methods presented in (Filippov, 1988; Gouzé and Sari, 2002; de Jong et al., 2004) give us so-called Filippov solutions of the differential inclusions. However, our focus here is on the qualitative dynamics, which does not depend on the particularities of the Filippov extension. The qualitative analysis of the dynamics on the singular domains requires the following notions.

**Definition 2.** Consider a set of PADEs of the form (2) with domain set  $\mathcal{D}$ . For every  $D \in \mathcal{D}_s$  of order  $k$ , let  $\text{supp}(D)$  be the  $(n - k)$ -dimensional hyperplane in  $\Omega$  containing  $D$ . If  $D \in \mathcal{D}_r$ , let  $\text{supp}(D) = \Omega$ . The *boundary* of  $D$  in  $\text{supp}(D)$  is the set  $\partial D$  of all points  $x \in \text{supp}(D)$ , such that each ball  $B_D(x, \epsilon)$  in  $\text{supp}(D)$  of center  $x$  and radius  $\epsilon > 0$  intersects both  $D$  and  $\text{supp}(D) \setminus D$ . For all  $D \in \mathcal{D}_s$ , we define the set

$$R(D) = \{D' \in \mathcal{D}_r \mid D \subset \partial D'\}.$$

So  $R(D)$  is the set of all regular domains that have  $D$  in their boundary. With this relation of singular domains to multiple regular domains we can extend the dynamics of the regular domains to the singular domains.

**Definition 3.** Consider a set of PADEs with domain set  $\mathcal{D}$ . We define the *focal set*  $\Psi(D)$  for every domain  $D$  as follows:

$$\Psi(D) := \begin{cases} \{\phi(D)\} & \text{if } D \in \mathcal{D}_r, \\ \text{supp}(D) \cap \overline{\text{rect}}(\{\phi(D') \mid D' \in R(D)\}) & \text{if } D \in \mathcal{D}_s, \end{cases}$$

where  $\phi(D) := (G^D)^{-1}F^D$  is the focal point of  $D$  for  $D \in \mathcal{D}_r$  and  $\overline{\text{rect}}(P)$  is the smallest closed hyperrectangular set that contains  $P \subset \Omega$ .

As noted before, the solutions of (2) starting in a regular domain  $D$  converge monotonically towards  $\phi(D)$ . Applying the Filippov extensions, the behavior of the system in singular domains can be described in relation to the focal points of adjacent regular domains. Using a hyperrectangular set in defining  $\Psi(D)$  for singular domains results in an overapproximation of the PADE behavior by the qualitative dynamics we introduce below. The consequences of this overapproximation and the convergence properties of the focal set are discussed in detail in (de Jong et al., 2004).

Because we focus on the qualitative dynamics, the possible behaviors in a domain  $D$  can be determined by the relative position of the focal set  $\Psi(D)$  with respect to the domain  $D$ .

**Definition 4.** Consider a set of PADEs of the form (2). Let  $D \in \mathcal{D}$  and  $e \in \Omega$ . We call the mapping  $v : \mathcal{D} \times \Omega \rightarrow \{-1, 0, 1\}^n$  the *relative position vector* and define it as follows

$$v_i(D, e) = \begin{cases} -1 & \text{if } e_i < x_i, \text{ for all } x \in D, \\ 0 & \text{if } e_i = x_i, \text{ for some } x \in D, \\ +1 & \text{if } e_i > x_i, \text{ for all } x \in D. \end{cases}$$

Let  $E \subset \Omega$  be a non-empty set of points. The set  $V(D, E)$  is defined as

$$V(D, E) := \{v(D, e) \mid e \in E\}.$$

Taking into account the above considerations about the behavior of the system with respect to the focal points, we can interpret the  $i$ -th component of  $\nu \in V(D, \Psi(D))$  as a command for the variable  $x_i$  to increase ( $\nu_i = 1$ ), to decrease ( $\nu_i = -1$ ), or to remain steady ( $\nu_i = 0$ ) in domain  $D$ . Note that the definition of the domains in  $\mathcal{D}$  ensures that  $V(D, D')$  is a singleton for all  $D, D' \in \mathcal{D}$ .

With this idea in mind, we define the qualitative dynamics via transitions between domains.

**Definition 5.** Consider a set of PADEs of the form (2). Let  $D, D' \in \mathcal{D}$  such that  $D' \subset \partial D$ .

1. There is a *transition*  $(D, D')$  from  $D$  to  $D'$  if
  - (a)  $\Psi(D) \neq \emptyset$ , and
  - (b) for  $V(D, D') = \{w\}$  there exists  $\nu \in V(D, \Psi(D))$  such that  $\nu_i w_i = 1$  for every  $x_i, i \in \{1, \dots, n\}$  that is a singular variable in  $D'$  but not in  $D$ .
2. There is a *transition*  $(D', D)$  from  $D'$  to  $D$  if
  - (a)  $\Psi(D) \neq \emptyset$ , and
  - (b) for  $V(D', D) = \{w'\}$  there exists  $\nu \in V(D, \Psi(D))$  such that  $\nu_i w'_i \neq -1$  for every  $x_i, i \in \{1, \dots, n\}$  that is a singular variable in  $D'$  but not in  $D$ .

Definition 5 has been extracted from Propositions 6.4 and 6.5 of de Jong et al. (2004), which relates the purely qualitative conditions to a definition for transitions between adjacent domains based on the existence of suitable solution trajectories of (2).

Following the idea of the discrete state transition graph, we represent the qualitative dynamics of a PADE system again by a directed graph.

**Definition 6.** Let  $\mathcal{A}$  be a system of PADEs of the form (2). The *qualitative transition graph*  $QTG(\mathcal{A}) = (\mathcal{D}, \mathcal{T})$  is a directed graph with  $\mathcal{D}$  being the set of domains and  $\mathcal{T}$  the set of transitions between domains.

As shown in (de Jong et al., 2004), all systems in the class of PADEs satisfying the same ordering constraints have the same qualitative transition graph (QTG). Transitions in the QTG represent possible trajectories of the PADE system. However, the QTG is an overapproximation of the dynamics of the PADE, as discussed in (de Jong et al., 2004).

From Def. 5, we can easily see that we do not need the full information inherent in the ordering constraints to determine the outgoing transitions for a given domain  $D$ . Similar to the sufficiency of the unitary update function for the construction of the state transition graph, we can utilize just the set

$V(D, \Psi(D))$  for all  $D \in \mathcal{D}$  to determine the QTG. For a regular domain  $D$  we have

$$V(D, \Psi(D)) = \{v(D, \phi(D))\},$$

by Def. 3. For a singular domain  $D$ , the situation is not as clear-cut. However, Propositions 6.2 and 6.3 in (de Jong et al., 2004) characterize the set  $V(D, \Psi(D))$  also for singular domains. The characterization is rooted in the overapproximation of the set of focal points of adjacent regular domains by a hyperrectangle. The results in (de Jong et al., 2004) are not formulated in terms of relative position vectors, but they can easily be rephrased. Thus, we derive the following proposition.

**Proposition 2.** *Consider a set of PADEs of the form (2) and let  $D \in \mathcal{D}_s$ . We have  $\Psi(D) \neq \emptyset$  if and only if for all singular variables  $x_i$  in  $D$  we have*

$$\min_{D' \in R(D)} v_i(D, \phi(D')) = -1 \text{ and } \max_{D' \in R(D)} v_i(D, \phi(D')) = 1. \quad (3)$$

Let  $D \in \mathcal{D}_s$  and  $\Psi(D) \neq \emptyset$ . Define  $V_i(D, \Psi(D)) := \{\nu_i \mid \nu \in V(D, \Psi(D))\}$ . Then, for all  $i \in \{1, \dots, n\}$ , if  $x_i$  is a singular variable,  $V_i(D, \Psi(D)) = \{0\}$ , and if  $x_i$  is a non-singular variable

$$V_i(D, \Psi(D)) = [\min_{D' \in R(D)} v_i(D', \phi(D')), \max_{D' \in R(D)} v_i(D', \phi(D'))], \quad (4)$$

where  $[a, b] = \{a, a+1, \dots, b-1, b\}$  denotes the discrete interval for  $a \leq b \in \mathbb{N}$ .

To determine the transitions of the QTG, we only need to know the set  $V(D, \Psi(D))$  for all domains  $D$ . Obviously, we can derive this set immediately from  $v(D, \phi(D))$  for regular domains  $D$ . Easy calculation using Prop. 2 and the definition of  $\Psi(D')$  for singular domains show that the information inherent in the set  $\{v(D, \phi(D)) \mid D \in \mathcal{D}_r\}$  is sufficient to derive  $V(D', \Psi(D'))$  for a singular domain  $D'$ . We summarize these observations in the following lemma.

**Lemma 3.** *Let  $\mathcal{A}$  be a set of PADEs. The positions of the focal points in relation to their corresponding regular domains, i.e.,  $\{v(D, \phi(D)) \mid D \in \mathcal{D}_r\}$ , is sufficient to calculate  $QTG(\mathcal{A}) = (\mathcal{D}, \mathcal{T})$ .*

Conversely, it is easy to see from the definitions that we can derive the relative position vectors  $v(D, \phi(D))$  for regular domains from the QTG.

**Example 2.** Consider the system of PADEs

$$\begin{aligned} \dot{x}_1 &= \alpha_1 + \beta_1 S^+(x_1, \theta_1^1) S^-(x_2, \theta_2^1) - \lambda_1 x_1, \\ \dot{x}_2 &= \alpha_2 + \beta_2 S^+(x_1, \theta_1^1) S^-(x_2, \theta_2^2) + \gamma_2 S^-(x_1, \theta_1^1) S^-(x_2, \theta_2^2) - \lambda_2 x_2. \end{aligned}$$

The system has six regular domains with corresponding focal points, e.g., the focal point of  $D = [0, \theta_1^1] \times [0, \theta_2^1]$  being  $(\alpha_1/\lambda_1, (\alpha_2 + \gamma_2)/\lambda_2)$ . We impose the ordering constraints  $0 < (\alpha_1 + \beta_1)/\lambda_1 < \theta_1^1 < \alpha_1/\lambda_1 < \max_1$  and  $0 < (\alpha_2 + \beta_2)/\lambda_2 < \theta_2^1 < \alpha_2/\lambda_2 < \theta_2^2 < (\alpha_2 + \gamma_2)/\lambda_2 < \max_2$ . The resulting QTG is given on the right of Fig. 2(a).

#### 4. Relating the discrete and the PADE formalism

In this section, we show that the PADE and the discrete formalism contain the same information in the sense that we can transform a PADE system with given ordering constraints into a discrete update function and vice versa.

To obtain a discrete update function from a PADE system we can use a straightforward method originally proposed by Snoussi (1989). First, we discretize the continuous phase space of the PADE system according to its threshold values.

**Definition 7.** Let  $\mathcal{A}$  be a set of PADEs as in (2), where each variable  $x_i$  has  $p_i$  ordered threshold values. Let  $Q := Q_1 \times \dots \times Q_n$ , where  $Q_i := \{0, 1, \dots, p_i\}$ ,  $i \in \{1, \dots, n\}$ . Define the bijective mapping  $d^{\mathcal{A}} : \mathcal{D}_r \rightarrow Q$ , where

$$d_i^{\mathcal{A}}(D) := \begin{cases} 0 & \text{if } D_i = \{x \in \mathbb{R} \mid 0 \leq x < \theta_i^1\}, \\ q & \text{if } D_i = \{x \in \mathbb{R} \mid \theta_i^q < x < \theta_i^{q+1}\}, \\ p_i & \text{if } D_i = \{x \in \mathbb{R} \mid \theta_i^{p_i} < x \leq \max_i\}. \end{cases} \quad (5)$$

Second, we exploit the localization of the focal points in the regular domains in order to construct an update function on the discretized state space  $Q$  that shares the dynamical properties of the PADE system  $\mathcal{A}$ . Note that in general such a focal point may lie on a threshold plane, which by definition has no corresponding value in  $Q$ . As in the previous section, we exclude the comparatively small set of PADE systems with focal points on a threshold plane.

**Definition 8.** Let  $\mathcal{A}$  be a set of PADEs as in (2) such that all focal points lie in regular domains and let  $d = d^{\mathcal{A}}$  be the mapping in (5). Define an update function  $f^{\mathcal{A}} : Q \rightarrow Q$  by

$$q \mapsto d(D_{\phi((d^{-1}(q)))}),$$

where  $D_{\phi(D')}$  denotes the regular domain containing the focal point  $\phi(D')$  of the regular domain  $D'$ .

The function  $f^{\mathcal{A}}$  is uniquely determined by the ordering constraints for  $\mathcal{A}$ . Consequently, the set of PADE systems  $\mathcal{A}$  satisfying given ordering constraints can be associated with a single discrete update function  $f^{\mathcal{A}}$ . Conversely, a discrete update function can easily be transformed into a PADE system that shares the same qualitative dynamics.

**Definition 9.** Let  $f : Q \rightarrow Q$  be an update function. We denote by  $PADE(f)$  the system of PADEs on  $\Omega := \prod_{i=1}^n [0, \max_i]$ ,  $\max_i \in \mathbb{R}_{>0}$  for all  $i \in \{1, \dots, n\}$ , of the form  $\dot{x}_i = F_i(x) - x_i$ ,  $i \in \{1, \dots, n\}$ , where

$$F_i(x) = \sum_{q \in Q} f_i(q) \prod_{j=1}^n S(x_j, q_j), \text{ with}$$

$$S(x_j, q_j) = \begin{cases} S^+(x_j, \theta_j^{q_j}) S^-(x_j, \theta_j^{q_j+1}) & \text{if } q_j \in \{1, \dots, p_j - 1\}, \\ S^-(x_j, \theta_j^1) & \text{if } q_j = 0, \\ S^+(x_j, \theta_j^{p_j}) & \text{if } q_j = p_j, \end{cases}$$



and  $\theta_j^k = k - 1/2$  for  $j \in \{1, \dots, n\}$ ,  $k \in \{1, \dots, p_j\}$ .

The choice of threshold values is generic, ensuring an obvious correspondence between the values  $0, 1, \dots, p_i$  in  $Q_i$ ,  $i \in \{1, \dots, n\}$ , and the intervals  $[0, \theta_i^1)$ ,  $(\theta_i^k, \theta_i^{k+1})$  for  $k \in \{1, \dots, p_i - 1\}$ , and  $(\theta_i^{p_i}, \max_i]$ . If we calculate the regular domains according to the threshold values and their focal points, we have  $\phi(D) = F(x) = f(d(D))$  for all  $x \in D$ , where  $d := d^{PADE(f)}$  and  $D \in \mathcal{D}_r$ . Equivalently, it holds that  $\phi(d^{-1}(q)) \in d^{-1}(f(q))$  for  $q \in Q$ , which immediately implies that the focal points of  $PADE(f)$  satisfy the set of corresponding ordering constraints. Therefore we can apply Def. 8 to  $PADE(f)$  and by construction we then have  $f^{PADE(f)} = f$ .

In contrast, we generally do not have equality of the PADE systems  $\mathcal{A}$  and  $PADE(f^{\mathcal{A}})$  due to the normalized form of  $PADE(f^{\mathcal{A}})$ . However, threshold order and relative focal point positions obviously coincide, i.e.,  $\mathcal{A}$  and  $PADE(f^{\mathcal{A}})$  satisfy the same ordering constraints. In consequence, the two corresponding qualitative transition graphs are isomorphic, and only differ in the specific set of real vectors contained in corresponding domains, i.e., the designation of the vertices of the QTGs. We summarize the preceding observations in the following proposition.

**Proposition 4.** *Let  $f : Q \rightarrow Q$  be an update function and  $\mathcal{A}$  be a PADE such that all focal points lie in regular domains. We then have*

$$f^{PADE(f)} = f \text{ and therefore } STG(f^{PADE(f)}) = STG(f).$$

and

$$QTG(\mathcal{A}) \cong QTG(PADE(f^{\mathcal{A}})),$$

where ' $\cong$ ' denotes graph isomorphism.

Using these two transformations, we can associate a class of PADE systems characterized by their ordering constraints with a unique discrete update function, and vice versa. In other words, the information necessary for constructing the STG resp. QTG is inherent in both representations. In that sense, we can identify every STG with a QTG and vice versa. However, this does not imply that the resulting qualitative dynamics are the same. In the following, we analyze differences and similarities between the STG and QTG of a discrete function resp. the corresponding set of PADE systems.

**Example 3.** Our update function  $f$  from Ex. 1 generates  $PADE(f)$  whose parameter values satisfy the ordering constraints of the PADE system  $\mathcal{A}$  introduced in Ex. 2. Therefore  $PADE(f)$  belongs to the class of PADEs represented by  $\mathcal{A}$ . Similarly, if we discretize  $\mathcal{A}$  using Snoussi's method, we obtain the update function  $f$  from Ex. 1.

## 5. Comparing the dynamics

Throughout this section we consider an update function  $f : Q \rightarrow Q$  and the PADE system  $\mathcal{A} := PADE(f)$  representing the class of PADE systems corresponding to  $f$  according to the preceding section. In particular, discretization

of  $\mathcal{A}$  via the function  $d := d^A$  yields  $f$ . The aim of this section is the comparison of  $STG(f) = (Q, E)$  and  $QTG(\mathcal{A}) = (\mathcal{D}, \mathcal{T})$ .

In the multi-valued other than in the Boolean setting, the state transition graph  $STG(f)$  generally does not carry enough information to reconstruct  $f$ . However, by definition it is possible to derive the unitary update function  $\tilde{f} := f^{STG(f)}$ . We have already seen that  $\tilde{f}(q) - q_j = \text{sgn}(f_j(q) - q_j)$  for all  $q \in Q$ ,  $j \in \{1, \dots, n\}$ . Furthermore, we know from the preceding section that  $\phi(d^{-1}(q)) \in d^{-1}(f(q))$ . Applying the definition for the relative position vector  $v_j(d^{-1}(q), \phi(d^{-1}(q)))$  we immediately obtain the following lemma.

**Lemma 5.** *For all  $q \in Q$  and  $j \in \{1, \dots, n\}$ , we have*

$$v_j(d^{-1}(q), \phi(d^{-1}(q))) = \tilde{f}_j(q) - q_j, \quad (6)$$

and similarly

$$v_j(D, \phi(D)) = \tilde{f}_j(d(D)) - d_j(D)$$

for all  $D \in \mathcal{D}_r$ .

Given the right hand side of (6), we are able to reconstruct  $STG(f)$  by definition of the state transition graph, while Lemma 3 ensures that we can build  $QTG(\mathcal{A})$  knowing the relative position vectors given by the left hand side of the equation. In addition, given  $STG(f)$  and  $QTG(\mathcal{A})$ , we can extract the unitary update function and the relative position vectors for regular domains. Consequently, we can construct  $STG(f)$  given  $QTG(\mathcal{A})$  and vice versa. In the following we will see that despite this correspondence of  $STG(f)$  and  $QTG(\mathcal{A})$  it is difficult to relate the dynamical behaviors that the different graphs represent.

### 5.1. Edges

The discretization in Sect. 4 implies that the vertices of  $STG(f)$  correspond to the regular domain vertices of  $QTG(\mathcal{A})$ . However, there is no representation of the singular domains in the purely discrete setting. To overcome this problem we associate with every singular domain  $D$  the set  $H(D) \subset Q$  corresponding to the discretization of those regular domains that have  $D$  in their boundary. We thus introduce the mapping  $H : \mathcal{D} \rightarrow 2^Q$

$$H(D) := \begin{cases} \{d(D)\}, & \text{if } D \in \mathcal{D}_r, \\ \{d(D') \in Q \mid D' \in R(D)\} & \text{if } D \in \mathcal{D}_s. \end{cases}$$

For example, for a singular domain  $D'$  of order one,  $H(D')$  constitutes the set  $\{d(D), d(\tilde{D})\}$  for the two regular domains  $D, \tilde{D}$  adjacent to  $D'$ . With this definition, we are able to state our main result on the correspondences between edges in  $QTG(\mathcal{A}) = (\mathcal{D}, \mathcal{T})$  and  $STG(f) = (Q, E)$ .

**Theorem 6.** *Let  $D \in \mathcal{D}$  and  $D' \subset \partial D$ . Denote by  $I$  (resp.  $I'$ ) the index set of singular variables in  $D$  (resp.  $D'$ ). Then we have:*

- (1)  $\Psi(D) \neq 0$  if and only if for all  $i \in I$  one of the following conditions holds (where  $e^i = (0, \dots, 1, \dots, 0)$  denotes the  $i$ -th unit vector in  $\mathbb{R}^n$ ):

- (a) there exist  $q, q' \in H(D)$  with  $q' = q + e^i$  such that  $(q, q') \in E$  and  $(q', q) \in E$ .
  - (b) there exist  $q, q' \in H(D)$  with  $q' = q + e^i$  such that  $(q, q') \notin E$  and  $(q', q) \notin E$ .
  - (c) there exist  $q, q' \in H(D)$  and  $\tilde{q}, \tilde{q}' \in H(D)$  with  $q' = q + e^i, \tilde{q}' = \tilde{q} + e^i$  such that both  $(q, q') \in E, (q', q) \notin E$ , and  $(\tilde{q}', \tilde{q}) \in E, (\tilde{q}, \tilde{q}') \notin E$ .
- (2)  $(D, D') \in \mathcal{T}$  if and only if  $\Psi(D) \neq \emptyset$  and for all  $i \in I' \setminus I$  there exists  $q \in H(D)$  and  $q' \in H(D') \setminus H(D)$  with  $q_i \neq q'_i$  and  $(q, q') \in E$ .
- (3)  $(D', D) \in \mathcal{T}$  if and only if  $\Psi(D) \neq \emptyset$  and for all  $i \in I' \setminus I$  there exists  $q \in H(D)$  and  $q' \in H(D') \setminus H(D)$  such that  $q_i \neq q'_i, q'_j = q_j$  for all  $j \neq i$  and  $(q, q') \notin E$ .

*Proof.* The conditions for the existence of transitions in  $QTG(A)$  are basically the two conditions given in Def. 5 reformulated in the context of edges of  $STG(f)$ .

We start by showing that the condition  $\Psi(D) \neq \emptyset$  is equivalent to condition (1) in the theorem. If  $D$  is a regular domain, then  $\Psi(D) \neq \emptyset$  by definition and condition (1) is true by default since  $I$  is empty. Therefore, we now assume  $D \in \mathcal{D}_s$ . We observe  $|q_i - q'_i| \leq 1$  for all  $q, q' \in H(D)$  and  $i \in \{1, \dots, n\}$  by definition of  $H(D)$ . In particular,  $1 + \min_{\tilde{q} \in H(D)} \tilde{q}_i = \max_{\tilde{q} \in H(D)} \tilde{q}_i$  for all  $i \in I$ .

First, we want to transform the condition  $\Psi(D) \neq \emptyset$  into a condition expressed in terms of the unitary update function  $\tilde{f}$ . Suppose  $D_i = \{x_i \mid x_i = \theta_i^k\}$  for some  $i \in I$ . By Prop. 2, a domain  $D \in \mathcal{D}_s$  has a non-empty focal set, i.e.,  $\Psi(D) \neq \emptyset$ , if for all  $i \in I$  there exist  $D', D'' \in R(D)$  such  $v_i(D, \phi(D')) = -1$  and  $v_i(D, \phi(D'')) = 1$ .

We now look at the condition  $v_i(D, \phi(\tilde{D})) = 1$  and what it is equivalent to in terms of the update function. For fixed  $i \in I$  and due to the adjacency of each  $\tilde{D} \in R(D)$  to  $D$ , we have for all  $\tilde{D} \in R(D)$  that  $v_i(D, \phi(\tilde{D})) = 1$  is equivalent to

$$v_i(\tilde{D}, \phi(\tilde{D})) \in \begin{cases} \{1\} & \text{if } w_i = -1 \\ \{0, 1\} & \text{if } w_i = 1 \end{cases}, \quad (7)$$

where  $V(D, \tilde{D}) = \{w\}$ . That is if  $\tilde{D} \in R(D)$  is below the threshold  $\theta_i^k$  and  $v_i(D, \phi(\tilde{D})) = 1$ , then its focal point is definitely above  $\theta_i^k$  and hence  $v_i(\tilde{D}, \phi(\tilde{D})) = 1$ . If however  $\tilde{D}$  is above  $\theta_i^k$  and  $v_i(D, \phi(\tilde{D})) = 1$ , then its focal point is either within or above  $\tilde{D}_i$ , that is  $v_i(\tilde{D}, \phi(\tilde{D})) \in \{0, 1\}$ . Applying Lemma 5 and the definition of  $H(D)$ , (7) can be reformulated such that for all  $\tilde{D} \in R(D)$ , the condition  $v_i(D, \phi(\tilde{D})) = 1$  is equivalent to

$$\tilde{f}_i(d(\tilde{D})) - d_i(\tilde{D}) \in \begin{cases} \{1\} & \text{if } d_i(\tilde{D}) = \min_{\tilde{q} \in H(D)} \tilde{q}_i \\ \{0, 1\} & \text{if } d_i(\tilde{D}) = \max_{\tilde{q} \in H(D)} \tilde{q}_i \end{cases}. \quad (8)$$

Analogously, we can derive for all  $\tilde{D} \in R(D)$  that the condition  $v_i(D, \phi(\tilde{D})) = -1$  is equivalent to

$$\tilde{f}_i(d(\tilde{D})) - d_i(\tilde{D}) \in \begin{cases} \{-1, 0\} & \text{if } d_i(\tilde{D}) = \min_{\tilde{q} \in H(D)} \tilde{q}_i \\ \{-1\} & \text{if } d_i(\tilde{D}) = \max_{\tilde{q} \in H(D)} \tilde{q}_i \end{cases}. \quad (9)$$

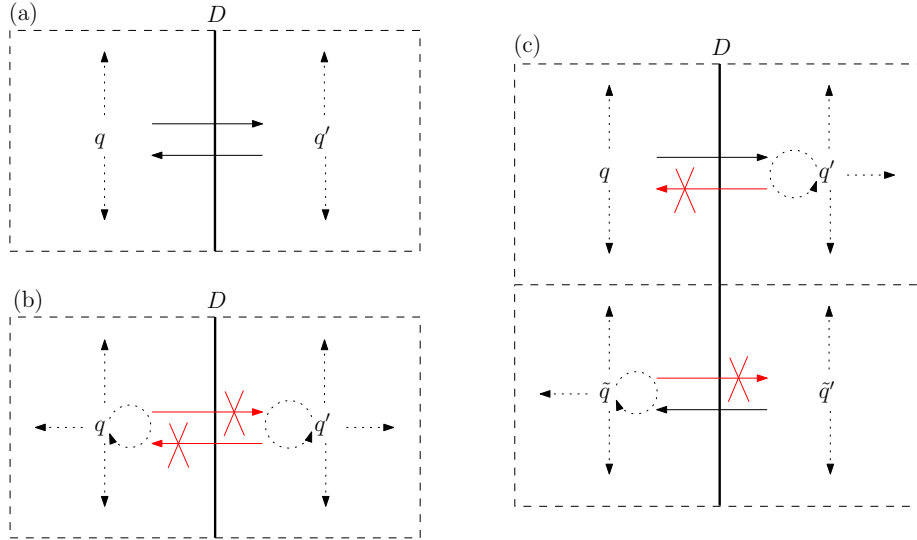


Figure 1: Illustration of the condition (1) of Theorem 6 for a singular domain  $D$ . The property  $\Psi(D) \neq \emptyset$  translates to edge constraints for outgoing edges of discrete states in  $H(D)$ . Here are the three cases in (1) of Theorem 6, where the vertical line denotes the threshold of a singular variable of  $D$  separating either two (in (a) and (b)) or four (in (c)) regular domains. Permissible edges are depicted as dotted lines, mandatory edges are depicted as solid lines and the edges that are not allowed are depicted as red lines.

We next show that there exists  $\tilde{D} \in R(D)$  with  $v_i(D, \phi(\tilde{D})) = 1$  iff there exist  $q, q' \in H(D)$  with  $q' = q + e^i$  such that  $(q, q') \in E$  or  $(q', q) \notin E$ . Suppose  $\tilde{D} \in R(D)$  with  $v_i(D, \phi(\tilde{D})) = 1$ . If  $d_i(\tilde{D}) = \min_{\tilde{q} \in H(D)} \tilde{q}_i$ , let  $q = d(\tilde{D})$ . Then  $\tilde{f}_i(q) - q_i = 1$ , i.e., for  $q' = q + e^i$ , we get  $(q, q') \in E$ . If  $d_i(\tilde{D}) = \max_{\tilde{q} \in H(D)} \tilde{q}_i$ , let  $q' = d(\tilde{D})$ . Then  $\tilde{f}_i(q') - q'_i \neq -1$ , i.e., for  $q = q' - e^i$ , we have  $(q', q) \notin E$ . The reverse direction uses the same arguments. Analogous arguments imply that there exists  $\tilde{D} \in R(D)$  with  $v_i(D, \phi(\tilde{D})) = -1$  iff there exist  $q, q' \in H(D)$  with  $q' = q + e^i$  such that  $(q, q') \notin E$  or  $(q', q) \in E$ .

As stated before, we have  $\Psi(D) \neq \emptyset$  iff there exist  $D', D'' \in R(D)$  such  $v_i(D, \phi(D')) = -1$  and  $v_i(D, \phi(D'')) = 1$ . Logical reformulation leads to the three cases (a), (b), (c) in condition (1) of the theorem, cf. Fig. 1 for illustration.

Next, we consider conditions (2) and (3) of the theorem, provided that condition (1), and thus  $\Psi(D) \neq \emptyset$ , holds. Condition 1(b) of Def. 5 states that there exists  $\nu \in V(D, \Psi(D))$  such that  $\nu_i w_i = 1$  for every  $i \in I' \setminus I$ , where  $V(D, D') = \{w\}$ . Let us first remark that  $w_i \neq 0$  iff  $i \in I' \setminus I$ . Moreover,  $w_i = q'_i - q_i$  for all  $q \in H(D)$ ,  $q' \in H(D') \setminus H(D)$  for  $i \in I' \setminus I$ . Now, let  $i \in I' \setminus I$ , i.e.,  $w_i \neq 0$ , and choose  $q \in H(D)$ ,  $q' \in H(D') \setminus H(D)$  with  $(q, q') \in E$  and  $q_i \neq q'_i$  according to condition (2) of the theorem. Let us assume that  $w_i = 1$ , the case  $w_i = -1$  can be treated analogously. Then  $1 = w_i = q'_i - q_i$ , i.e.,  $q'_i > q_i$ . It follows that  $\tilde{f}_i(q) > q_i$ , and thus  $\max_{\tilde{q} \in H(D)} \tilde{f}_i(\tilde{q}) - \tilde{q}_i = 1$ . If  $D$  is

a regular domain, then  $v_i(D, \phi(D)) = 1$  by Lemma 5. If  $D$  is a singular domain, then  $1 \in [\min_{\tilde{q} \in H(D)} \tilde{f}_i(\tilde{q}) - \tilde{q}_i, \max_{\tilde{q} \in H(D)} \tilde{f}_i(\tilde{q}) - \tilde{q}_i] = V_i(D, \Psi(D))$  according to Prop. 2 and Lemma 5. In both cases, there exists  $\nu_i \in V(D, \Psi(D))$  with  $\nu_i w_i = 1$ . Since the definition of  $V(D, \Psi(D))$  for regular domains and Prop. 2 allow for a componentwise argument, the existence of a vector  $\nu \in V(D, \Psi(D))$  with  $\nu_i w_i = 1$  for all  $i \in I' \setminus I$  follows.

To show the reverse statement, assume that there exists  $\nu \in V(D, \Psi(D))$  with  $\nu_i w_i = 1$  for all  $i \in I' \setminus I$ , and choose  $i \in I' \setminus I$ . Again we restrict ourselves to the exemplary case  $w_i = 1$ . Then  $\nu_i = 1$ , and therefore there exists  $q \in H(D)$  with  $\tilde{f}_i(q) - q_i = 1$  according to Lemma 5 and Prop. 2. In particular,  $(q, q') \in E$  for  $q' \in Q$  with  $q'_i = q_i + 1$  and  $q'_j = q_j$  for all  $j \neq i$ . Then  $q' \notin H(D)$ , since  $q'_i \neq q_i$  and  $i \notin I$ , but  $q' \in H(D')$ , since  $q'_i = q_i + w_i$ . Thus, condition (2) of the theorem holds.

Lastly, we show equivalence of the condition (3) of the theorem and condition 2(b) in Def. 5. Suppose there exists  $\nu \in V(D, \Psi(D))$  with  $\nu_i w_i \neq -1$  for all  $i \in I' \setminus I$ . Let  $i \in I' \setminus I$ , then  $w_i \neq 0$ . Again, we only show the exemplary proof for the case  $w_i = 1$ . Then  $\nu_i \neq -1$ , and thus  $\max_{\tilde{q} \in H(D)} \tilde{f}_i(\tilde{q}) - \tilde{q}_i \geq 0$  according to Prop. 2 and Lemma 5. Then there exists  $q \in H(D)$  with  $q_i \leq \tilde{f}_i(q)$ , which yields  $q_i \leq p_i$  for all asynchronous successors  $p \in AS(q)$ . Now, let  $q' \in H(D') \setminus H(D)$  with  $q'_i \neq q_i$  and  $q'_j = q_j$  for all  $j \neq i$ . Since  $w_i = 1$ , we have  $q'_i < q_i$ . In particular,  $q'$  cannot be an asynchronous successor of  $q$ , i.e.,  $(q, q') \notin E$ .

Conversely, given  $i \in I' \setminus I$  and  $q, q'$  according to condition (3) of the theorem, i.e.,  $q \in H(D)$ ,  $q' \in H(D') \setminus H(D)$  with  $q_i \neq q'_i$ ,  $q_j = q'_j$  for all  $j \neq i$ , and  $(q, q') \notin E$ , then  $w_i = q_i - q'_i$ . Again, let us just focus on the case  $w_i = 1$ , i.e.,  $q_i > q'_i$ . Since  $(q, q') \notin E$ , we have  $p_i \geq q_i$  for all  $p \in AS(q)$ , i.e.,  $\tilde{f}_i(q) - q_i \in \{0, 1\}$ . It follows from Prop. 2 and Lemma 5 that  $\max_{\tilde{D} \in R(D)} v_i(\tilde{D}, \phi(\tilde{D})) \geq 0$ . Thus we can find  $\nu \in V(D, \Psi(D))$  with  $\nu_i \neq -1$ , and in particular  $\nu_i w_i \neq -1$ . Again, the definition of  $V(D, \Psi(D))$  for regular domains and Prop. 2 allow for a componentwise argument, and we can fulfill condition 2(b) of Def. 5.  $\square$

**Example 4.** Using Theorem 6 we can determine in our running example (see Fig. 2a)) whether the focal set of the singular domain  $D' := [\theta_1^1] \times [\theta_2^1]$  of order two is empty or not, by looking at the edges within  $H(D') := \{00, 01, 10, 11\}$ . For the second variable the edges (00, 01) and (11, 10) satisfy 1(c) of Theorem 6, while for the first variable the edges (00, 10) and (10, 00) satisfy 1(a), which means that  $D'$  has a non-empty focal set. The edges (00, 10) and (10, 00) also mean that the singular domain  $D := [\theta_1^1] \times [0, \theta_2^1]$  of order one has a non-empty focal set. Thus transitions between  $D$  and  $D'$  can be determined from the edges between the states  $H(D) = \{00, 10\}$  and  $H(D') \setminus H(D) = \{01, 11\}$ . From the conditions (2) and (3) of Theorem 6, we have that (00, 01)  $\in E$  corresponds to  $(D, D') \in \mathcal{T}$  and (10, 11)  $\notin E$  corresponds to  $(D', D) \in \mathcal{T}$  respectively.

In the same example the singular domain  $\tilde{D} := [0, \theta_1^1] \times [\theta_2^2]$  of order one has a non-empty focal set as reflected by the edges (01, 02) and (02, 01), which also imply that 1(a) is satisfied for the second variable of  $\tilde{D}' := [\theta_1^1] \times [\theta_2^2]$ . For the first variable, however, we have that the edges (01, 11) and (02, 12) do not satisfy any subcase in (1) of Theorem 6, which means that  $\tilde{D}'$  has an empty focal

set. We see that either  $(01, 11) \in E$  or  $(02, 12) \in E$  corresponds to  $(\tilde{D}, \tilde{D}') \in \mathcal{T}$  by (2) of Theorem 6. However, both edges  $(01, 11)$  and  $(02, 12)$  correspond to  $(\tilde{D}', \tilde{D}) \notin \mathcal{T}$  because (3) of Theorem 6 is not satisfied.

Looking at the simplest case of the theorem we can see how edges (or missing edges) between two nodes  $q, q' \in Q$ ,  $q \neq q'$ , in  $STG(f) = (Q, E)$  always correspond to edges in  $QTG(\mathcal{A}) = (\mathcal{D}, \mathcal{T})$  for the singular domain  $D'$  of order one with  $H(D') = \{q, q'\}$ .

**Corollary 7.** *Let  $D \in \mathcal{D}_r$ , and let  $D' \subset \partial D$  be a singular domain of order one. Set  $q := d(D)$  and denote by  $q'$  the unique element in the set  $H(D') \setminus H(D)$ . Then  $(D, D') \in \mathcal{T}$  if and only if  $(q, q') \in E$ , and  $(D', D) \in \mathcal{T}$  if and only if  $(q, q') \notin E$ .*

This statement agrees with the observations of Chaves et al. (2010) for boolean discrete models and with Gouzé and Sari (2002). Thus the basic correspondences of edges known from the literature is also incorporated in our result. Moreover, Theorem 6 provides the basis for elucidating the correspondences between more complex structures, such as paths or attractors. On the one hand, it can be used for proof building on local considerations concerning the edges involved. On the other hand, it provides ideas for the construction of counterexamples. In the following, we illustrate both uses of the theorem.

## 5.2. Paths and Attractors

We start by considering reachability properties. In simple cases, we can find conditions ensuring the existence of corresponding paths. The following statement applies Cor. 7 repeatedly to show the paths that correspond in the two graphs.

**Proposition 8.** *There exists a path  $(D^1, \dots, D^{2k+1})$  in  $QTG(\mathcal{A})$  with  $D^i \in \mathcal{D}_r$  for  $i \in \{1, \dots, 2k+1\}$  odd and  $D^i$  a singular domain of order one for  $i \in \{1, \dots, 2k+1\}$  even, if and only if  $(q^0, q^1, \dots, q^k)$  is a path in  $STG(f)$  such that  $(q^j, q^{j-1}) \notin E$  for all  $j \in \{1, \dots, k\}$  and  $q^i = d(D^{2i+1})$  for all  $i \in \{0, \dots, k\}$ .*

In spite of Prop. 8, we are able to construct examples of paths that do not correspond in the two graphs.

**Example 5.** We see in Fig. 2(a) that state (0,2) is reachable from (1,0) in the STG via the path indicated in gray. In contrast, all paths starting in the regular domain corresponding to (1,0) and all adjacent singular domains do not cross the first threshold plane of the second component. In Fig. 2(b), we see by considering reachability of state (1,1) from (0,0) that reachability properties of the QTG are also not conserved in the corresponding STG.

These two examples illustrate that in general reachability properties are not conserved between the two graphs. A further important characteristic of  $QTG(\mathcal{A})$  and  $STG(f)$  are their respective attractors. The next definition introduces our terminology.

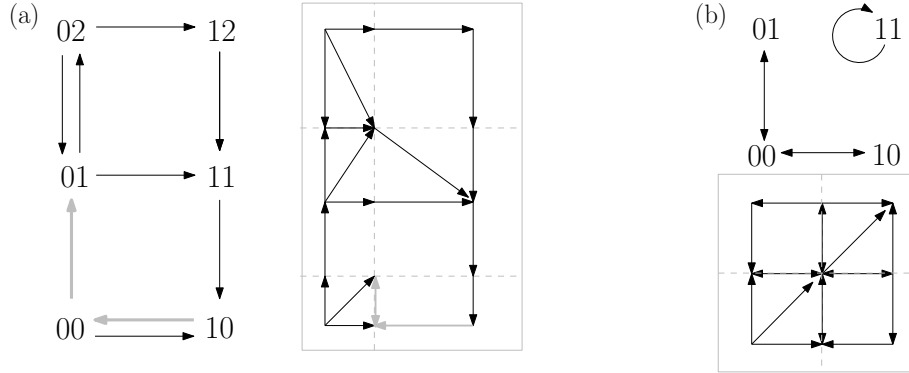


Figure 2: Corresponding STGs and QTGs. The partitioned phase space of a corresponding PADE underlying a QTG is shown in fine gray lines (dashed for threshold planes) underneath the QTG and allows identification of nodes representing singular resp. regular domains. In (a), STG of Ex. 1 and QTG of Ex. 2. In (b), the STG of a two component Boolean network with the corresponding QTG right. Heavier gray edges illustrate reachability properties discussed in the text.

**Definition 10.** Let  $G$  be a directed graph and  $S$  a subset of the nodes of  $G$ . The set  $S$  is *strongly connected* if any two nodes in  $S$  are connected by a path in  $S$ . The set  $S$  is a *trap set* if there is no path leaving  $S$ . An *attractor* of a graph is a strongly connected trap set. A *steady state* is an attractor consisting of a single node. A *simple cycle* is an attractor of cardinality greater than one where every node has only one outgoing edge. A *complex attractor* is an attractor that has at least one node which has two or more outgoing edges.

Note that we consider each node set of cardinality one to be strongly connected by default, i.e., not depending on the existence of a loop on the respective node. The steady states in a discrete state transition graph correspond to the fixed points of the update function  $f$ , and by definition there exists an edge  $(q, q)$  for each fixed point  $q$ . In contrast, the steady states of the QTG are, by definition of the transitions, nodes without outgoing edges. Note that here a steady state is simply a singleton terminal strongly connected component in a graph. There is no implicit statement about the stability of such a steady state included, i.e., it does not necessarily correspond to an asymptotically stable steady state in a PADE system (see e.g. Snoussi, 1989).

Attractors of cardinality greater than one are often called *cyclic*. Both complex attractors and simple cycles are then cyclic attractors. We often denote a simple cycle  $\{s^1, \dots, s^k\}$  by the path  $(s^1, \dots, s^k, s^1)$  traversing the cycle. Similar to the reachability properties we are able to find correspondences between attractors of  $STG(f)$  and  $QTG(\mathcal{A})$ .

**Proposition 9.** *The following relations hold for attractors in  $QTG(\mathcal{A})$  and  $STG(f)$ .*

1. A regular domain  $D$  is a steady state in  $QTG(\mathcal{A})$  if and only if  $d(D)$  is

a steady state in  $STG(f)$ . A singular domain  $D$  of order one is a steady state in  $QTG(\mathcal{A})$  if and only if  $H(D)$  is a simple cycle in  $STG(f)$ .

2. There is a simple cycle  $(D^1, D^2, \dots, D^{2m}, D^1)$  with  $D^{2j} \in \mathcal{D}_r$  for  $j \in \{1, \dots, m\}$  in  $QTG(\mathcal{A})$ , if and only if  $(d(D^2), d(D^4), \dots, d(D^{2m}), d(D^2))$  is a simple cycle in  $STG(f)$ .

*Proof.* 1. The first statement immediately follows from Lemma 5, where a regular domain  $D$  is a steady state if and only if  $v(D, \phi(D)) = 0$ , which is equivalent to  $f(d(D)) = d(D)$ . Now, let  $\{\tilde{q}, \tilde{q}'\}$  be a simple cycle in  $STG(f)$  and  $D$  be the singular domain of order one with  $H(D) = \{\tilde{q}, \tilde{q}'\}$ . According to Theorem 6, if there exists an edge from  $D$  to a singular domain  $D'$  of higher order, then we could find  $q \in H(D)$ ,  $q' \in H(D') \setminus H(D)$ , i.e.,  $q \in \{\tilde{q}, \tilde{q}'\}$  and  $q' \notin \{\tilde{q}, \tilde{q}'\}$ , with  $(q, q') \in E$ , which would be contradictory to  $H(D)$  being a simple cycle. If there exists an edge from  $D$  to a regular domain  $\tilde{D}$ , then, since  $H(D) \setminus H(\tilde{D}) = \{q\}$  and  $H(\tilde{D}) = \{q'\}$  for some  $q, q' \in H(D)$  with  $q \neq q'$ , we would have  $(q', q) \notin E$  according to Theorem 6, which contradicts  $\{\tilde{q}, \tilde{q}'\}$  being a simple cycle. In summary,  $D$  has no outgoing edges and is a steady state.

If  $H(D) = \{q, q'\}$  is not a simple cycle, then either one of the edges  $(q, q')$ ,  $(q', q)$  is missing in  $STG(f)$  or there exists an edge leaving  $H(D)$ . In the first case, there exists a transition from  $D$  to a regular domain, as we can see immediately from Theorem 6. If  $(q, q'), (q', q) \in E$ , then condition 1(a) of Theorem 6 holds for  $D$ , i.e.  $\Psi(D) \neq \emptyset$ . If we find an additional edge leaving  $H(D)$ , then condition (2) of Theorem 6 holds as well, and we find an edge from  $D$  to some singular domain. In any case  $D$  is not a steady state.

2. If there is a simple cycle  $(D^1, D^2, \dots, D^{2m}, D^1)$  in  $QTG(\mathcal{A})$ , then  $(d(D^2), d(D^4), \dots, d(D^{2m}), d(D^2))$  is a simple cycle in  $STG(f)$  according to Cor. 7. If, on the other hand,  $(d(D^2), d(D^4), \dots, d(D^{2m}), d(D^2))$  is a simple cycle in  $STG(f)$ , then, again according to Cor. 7, each regular domain  $D^{2j}$  has only one outgoing edge, namely  $(D^{2j}, D^{2j+1})$ , where  $2m+1$  is identified with index 1. For the singular domains  $D^{2j+1}$  in the cycle, we can derive the existence of only one outgoing edge, namely  $(D^{2j+1}, D^{2j+2})$ , from condition (3) of Theorem 6.  $\square$

In spite of the findings in Prop. 9 the number of attractors is not necessarily preserved in general.

**Example 6.** While in Fig. 2(a) both systems have one attractor, the STG in Fig. 2(b) exhibits two attractors, a fixed point and a cyclic attractor. However, the corresponding QTG has only one attractor, namely a steady state in the upper right node. In Fig. 3(a), the STG has fewer attractors than the corresponding QTG.

In addition, the relation between the attractor structure is not clear-cut. While the cyclic attractor of the STG in Fig. 2(a) comprises all nodes of the STG and contains nodes with multiple outgoing edges, the cyclic attractor in the QTG is a simple cycle consisting only of two nodes joined by the heavier gray double edge in the lower part of the graph. In Fig. 2(b) the cyclic attractor in the STG vanishes in the corresponding QTG. The same happens in Fig. 3(b), but here an additional steady state can be observed in a singular node.



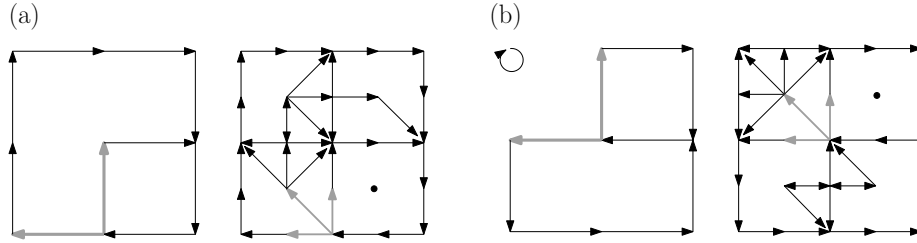


Figure 3: Two examples for networks with two components and three activity levels for each component. In each case, the STG is depicted on the left, the corresponding QTG on the right. Depiction of the graphs corresponds to that in Fig. 2, only the explicit labeling of the STG nodes is omitted. In (a), the STG consists of a single cyclic attractor, while the QTG has an additional steady state at the lower right singular node depicted by a fat dot. In (b), both STG and QTG have a steady state in the upper left node, but the STG has an additional cyclic attractor. The QTG has no cyclic attractor, but an additional singular steady state at the upper right singular node depicted by a fat dot.

Let us also consider a singular domain  $D$  of order greater than 1 which is a steady state in the QTG. Translating the condition of  $D$  having no outgoing edges obviously imposes constraints on a corresponding STG via Theorem 6. However, these constraints are generally not strong enough to link  $D$  to some unique structure in the STG.

**Example 7.** In Fig. 4, we see two examples, where both QTGs contain a singular domain of order two, which is a steady state. However, the corresponding STGs differ, the one in (a) consisting of a complex attractor and the one in (b) consisting of a simple cycle.

So, in general the number, structure and uniqueness of the corresponding attractors cannot be assured. Nevertheless, we are able to narrow down the locations of attractors by observing the trap sets. In particular we can show that hyper-rectangular trap sets correspond in the two graphs.

**Proposition 10.** *Let  $\mathcal{R} := R_1 \times \dots \times R_n \subset Q$  be a discrete hyperrectangle, i.e.,  $R_i$  is an integer interval  $[a_i, b_i] \subset Q_i$  for all  $i \in \{1, \dots, n\}$ . Then  $\mathcal{R}$  is a trap set in  $STG(f)$  if and only if  $U := \{D \mid H(D) \subset \mathcal{R}\}$  is a trap set in  $QTG(\mathcal{A})$ .*

*Proof.* Let  $U$  be a trap set in  $QTG(\mathcal{A})$ . Let  $q \in \mathcal{R}$  and  $q' \in Q$  with  $(q, q') \in E$ . Then Theorem 6 ensures that there exists  $D' \subset \partial D$ ,  $D := d^{-1}(q)$ , with  $(D, D') \in \mathcal{T}$  and  $H(D') = \{q, q'\}$ . Since  $U$  is a trap set, we have  $D' \in U$ . Then, by definition,  $H(D') \in \mathcal{R}$ , i.e.,  $q' \in \mathcal{R}$ .

Now, let  $\mathcal{R}$  be a trap set in  $STG(f)$ . Let  $D \in U$  and  $D' \in \mathcal{D}$  with  $(D, D') \in \mathcal{T}$ . If  $D \subset \partial D'$ , then  $H(D') \subset H(D) \subset \mathcal{R}$ , and therefore, by definition,  $D' \in U$ . If  $D' \subset \partial D$ , then condition (2) of Theorem 6 yields the existence of an edge  $(q, q') \in E$  such that  $q \in H(D)$ , i.e.,  $q \in \mathcal{R}$ , and  $q' \in H(D') \setminus H(D)$  with  $q_i \neq q'_i$  for all indices  $i$  indicating singular variables of  $D'$  but not of  $D$ . Since  $\mathcal{R}$  is a hyperrectangle, we then have  $H(D') \subset \mathcal{R}$ , that is,  $D' \in U$ .  $\square$

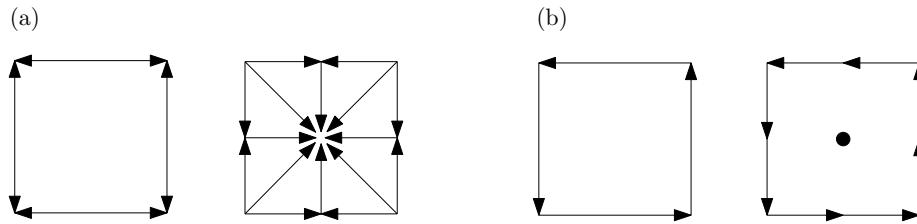


Figure 4: STGs and QTGs for networks with two components and two activity levels for each component, the STG shown on the left, the corresponding QTG on the right of each figure. Both the QTGs in (a) and (b) have a steady state in the singular domain of order two.

The above proposition may be helpful in elucidating the correspondences of attractors in the STG and the QTG further. Since a trap set always contains at least one attractor, we can relate attractors that we can separate using hyperrectangles.

Overall, we see that the relations between attractors in corresponding STGs and QTGs are not clear-cut. The examples illustrate that, in general, neither number nor character of attractors are preserved.

## 6. Discussion and perspectives

In summary, the information inherent in the STG of the discrete update function is sufficient to derive the QTG of the corresponding PADE system and vice versa. However, despite this correspondence, basic structures between the two graphs are not preserved. This implies that, contrary to what might be expected, the QTG of the PADE system is not a straightforward refinement of the STG of the Thomas model.

Motivated by these findings, there are several directions for future work. First, we would like to better understand and characterize the network properties that lead to substantial differences, e.g., in the number of attractors in the dynamics of the Thomas and the PADE model. Second, we plan to extend the analysis to closely related formalisms like the refined qualitative representation of PADE systems (Batt et al., 2008) as well as piecewise multi-affine models (Kloetzer and Belta, 2009). Also, there exist approaches that allow the integration of threshold values directly into the Thomas formalism (Thomas et al., 1995; Richard et al., 2005). Clarifying the relation between the different approaches may allow one to transfer available results and analysis methods from one formalism to the other. Furthermore, progress in this direction may be helpful when deciding on the most suitable and efficient modeling framework in a concrete application.

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