Compositional Definitions of Minimal Flows in Petri Nets

Michael Pedersen

LFCS, School of Informatics, University of Edinburgh

Abstract. This paper gives algebraic definitions for obtaining the minimal transition and place flows of a modular Petri net from the minimal transition and place flows of its components. The notion of modularity employed is based on place sharing. It is shown that transition and place flows are *not* dual in a modular sense under place sharing alone, but that the duality arises when also considering transition sharing. As an application, the modular definitions are used to give compositional definitions of transition and place flows of models in a subset of the Calculus of Biochemical Systems.

Keywords: Petri nets, minimal flows, minimal invariants, modularity, the Calculus of Biochemical Systems.

1 Introduction

Since their introduction in the early sixties, Petri nets have been used to model concurrent systems in a wide variety of fields [1]. They have long been recognised as a suitable modelling formalism for systems biology; see e.g. [2–4] for basic ideas and surveys, [5–10] for applications to metabolic pathways, [10–14] for applications to signalling pathways and [15, 16] for applications to gene regulatory networks. Applications in model-driven synthetic biology are also starting to emerge [17]. Petri nets are appealing because of their intuitive visual representation as bipartite graphs over *places* and *transitions*, which corresponds well to that of informal biological pathway diagrams: places represent species, transitions represent reactions, and weighted edges represent stoichiometries (see Figure 1 for an example). In addition to their visual appeal, they have a formally defined structure and behaviour and are supported by a large body of simulation and analysis techniques.

High-level extensions of Petri nets enable complex models to be expressed more concisely and at higher levels of abstraction, e.g. as in coloured Petri nets [18]. A key feature of many such extensions is the notion of *modularity*, meaning that a complex model can be composed from modules representing its parts. This is a clear advantage from a modelling point of view as demonstrated in e.g. [19, 20] for the yeast pheromone pathway. But modularity can also give rise to modular analysis, potentially reducing computational complexity dramatically, enabling parallel computation, and allowing analysis results to be reused in different contexts.

This paper investigates modular analysis in the specific case of Petri net *flows* (also known as *invariants*). Intuitively, a *transition flow* (or T-flow) is a vector representing reaction counts which, when the reactions occur together, have no net effect on species populations. They hence correspond to a notion of cyclic pathways. A *place flow* (or P-flow) is a vector representing species weights for which the weighted sum of species populations is always constant. They hence correspond to chemical conservation relations. More precisely, T and P-flows are natural-number solutions to the equations $Wx = 0$ and $xW = 0$, respectively, where W is the flow matrix of a Petri net which corresponds to the stoichiometry matrix of a biological reaction network. These equations generally have infinitely many solutions, but one can always find finite sets of *minimal* flows which can be combined to generate all other flows. Algorithms for obtaining minimal flows are computationally expensive and the exact algorithmic performance is difficult to estimate [21].

Flow analysis has proven an important tool in biological model validation: the modeller should be able to give biological justification to each minimal flow, otherwise it is likely that the model is incorrect for the intended purpose [10, 13]. Flows are also closely related to the notion of *elementary modes* [22] from metabolic pathway analysis.

The main contributions of this paper are the algebraic definitions of minimal T and P-flows of a Petri net given the minimal T and P-flows of its components (Sections 4 and 5, respectively). We employ a notion of modularity where two modules are composed by merging their shared places/species, also known as *place fusion*. As a second contribution we show that, perhaps contrary to expectation, P and T-flows are *not* dual in a modular sense under place sharing alone, but that the duality arises when also considering composition based on shared transitions/reactions (also known as *transition fusion*, Section 3). Finally, as an application we use our modular definitions to derive compositional definitions of minimal flows in a subset of the Calculus of Biochemical Systems (CBS) [19, 23] in Section 6.

Previous efforts have been made towards modular definitions of P-flows in particular, and related work will be discussed in Section 7 before concluding. Detailed proofs of all results can be found in [24] and selected proofs are given in Appendix A. Although the work in this paper is motivated by biological applications, the results are equally applicable outside of biology and flows play an important role in the general analysis of Petri nets; for example, P-flows can be used for determining boundedness of a net, and T-flows can be used for investigating liveness [25].

2 Preliminaries

2.1 Petri Nets

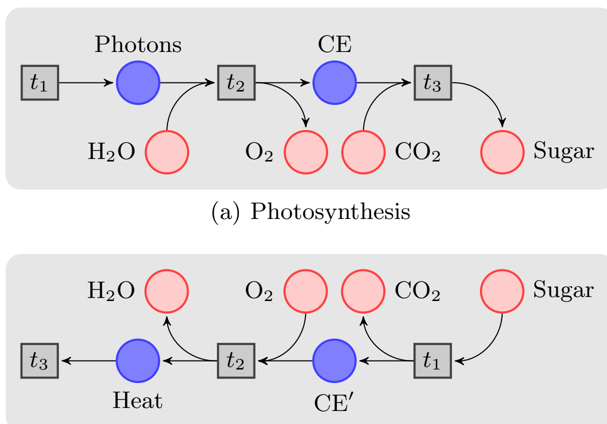
We start with the formal definition of Petri nets.

Definition 1 (Petri net). *A* Petri net $\mathcal{P}$ *is a tuple* $(S, T, W^{\text{in}}, W^{\text{out}})$ *where*

– S *is a finite set of* places.
– T *is a finite set of* transitions.
– $W^{\text{in}} : S \times T \to \mathbb{N}$ *is the* flow-in *function.*
– $W^{\text{out}} : S \times T \to \mathbb{N}$ *is the* flow-out *function.*

Define also the derived flow *function* $W(s,t) \triangleq W^{\text{out}}(s,t) - W^{\text{in}}(s,t)$.

Given a Petri net $\mathcal{P}$, we shall often write $S_{\mathcal{P}}$ for the places of $\mathcal{P}$ and similarly for the transitions and flow functions. As a running example we shall consider simple Petri net models of the foundations of life itself, namely photosynthesis and respiration.



(a) Photosynthesis

(b) Respiration

Fig. 1. Two Petri net models of respectively photosynthesis and respiration, with a distinct shading used for shared places.

Example 1. Photosynthesis is the process by which plants produce sugar and oxygen from water, carbon dioxide and sun light (photons). This is modelled by the Petri net in Figure 1(a); places are circles, transitions are squares and arcs (all with the weight 1 omitted) represent the flow function. The first transition provides an unlimited amount of photons. The second converts photons and water into chemical energy (CE) and oxygen, and the third converts chemical energy and carbon dioxide into sugar.

Respiration is the converse process by which e.g. humans use oxygen to break down sugar while producing carbon dioxide and water. This is modelled by the Petri net in Figure 1(b). The first transition breaks down sugar into carbon dioxide and chemical energy CE′, distinct from the chemical energy used in photosynthesis. The second transition utilises this chemical energy and oxygen to make e.g. muscles move, and in the process producing water and heat; the heat is finally removed. Note that both models are strongly simplified and not chemically correct.

If for a Petri net $\mathcal{P}$ we assume some arbitrary but fixed strict total orderings $\prec_{\mathrm{s}} \subsetneq S_{\mathcal{P}} \times S_{\mathcal{P}}$ on places and $\prec_{\mathrm{t}} \subsetneq T_{\mathcal{P}} \times T_{\mathcal{P}}$ on transitions, we can write $S_{\mathcal{P}} = (s_1, \ldots, s_m)$ and $T_{\mathcal{P}} = (t_1, \ldots, t_n)$ and view the flow functions of $\mathcal{P}$ as $m \times n$ matrices thus:

$$(W^{\mathrm{in}}_{\mathcal{P}})_{i,j} \stackrel{\Delta}{=} W^{\mathrm{in}}_{\mathcal{P}}(s_i, t_j) \qquad (W^{\mathrm{out}}_{\mathcal{P}})_{i,j} \stackrel{\Delta}{=} W^{\mathrm{out}}_{\mathcal{P}}(s_i, t_j) \qquad W_{\mathcal{P}} \stackrel{\Delta}{=} W^{\mathrm{out}}_{\mathcal{P}} - W^{\mathrm{in}}_{\mathcal{P}}$$

This will allow us to take advantage of matrix operations. Row $(W^{\mathrm{in}}_{\mathcal{P}})_{(i,\cdot)}$ represents the number of tokens *consumed* from place s_i by the respective transitions, and row $(W^{\mathrm{out}}_{\mathcal{P}})_{(i,\cdot)}$ represents the number of tokens *produced* in place s_i by the respective transitions. Row $(W_{\mathcal{P}})_{(i,\cdot)}$ then represents the net effect of transitions on place s_i. The behaviour of Petri nets is defined in the following. Here, and throughout the paper, we use $(\cdot)^{\mathbf{T}}$ to denote vector/matrix transposition.

Definition 2 (Behaviour). *Let* $\mathcal{P} = (S, T, W^{\mathrm{in}}, W^{\mathrm{out}})$ *be a Petri net. Let* $\mathcal{M}(\mathcal{P}) \stackrel{\Delta}{=} \mathbb{N}^{|S|}$ *be the set of markings of* $\mathcal{P}$*. Then the* transition relation $\rightarrow \subseteq \mathcal{M}(\mathcal{P}) \times (\mathbb{N}^{|T|})^{\mathbf{T}} \times \mathcal{M}(\mathcal{P})$ *is defined as follows:* $M \xrightarrow{x} M'$ *if*

1. $M \geq W^{\mathrm{in}} x$
2. $M' = M + W^{\mathrm{out}} x - W^{\mathrm{in}} x = M + Wx$

So in order for a transition count vector x to fire, the marking M must contain enough tokens in each place to supply the inputs of all transitions in x. The marking M' results from removing the tokens consumed by x and adding the tokens produced. The marking of a Petri net then evolves from an initial marking by playing this "token game". But since we consider structural properties only, we shall generally not be concerned with initial markings.

2.2 Petri Net Flows

Transition flows represent transitions which, after they fire, have no net effect on any markings of a Petri net. Place flows represent weights for which the weighted sum of places is constant in any marking reachable from the initial marking. Hence flows give rise to invariance relations. Here is the formal definition:

Definition 3 (T and P-flows). *Let* $\mathcal{P} = (S, T, W^{\mathrm{in}}, W^{\mathrm{out}})$ *be a Petri net. Define*

$$\mathrm{TF}(\mathcal{P}) = \mathrm{TF}(W) \stackrel{\Delta}{=} \{x \in (\mathbb{N}^{|T|})^{\mathbf{T}} \mid Wx = 0 \wedge x \neq 0\}$$
$$\mathrm{PF}(\mathcal{P}) = \mathrm{PF}(W) \stackrel{\Delta}{=} \{y \in \mathbb{N}^{|S|} \mid yW = 0 \wedge y \neq 0\}$$

The elements of $\mathrm{TF}(\mathcal{P})$ *and* $\mathrm{PF}(\mathcal{P})$ *are called* transition flows *(or* T-flows*) and* place flow *(or* P-flows*), respectively.*

Observe that T and P-flows are dual in the following sense:

$$x \in \mathrm{TF}(\mathcal{P}) \Leftrightarrow Wx = 0 \Leftrightarrow x^{\mathbf{T}} W^{\mathbf{T}} = 0 \Leftrightarrow x^{\mathbf{T}} \in \mathrm{PF}(\mathcal{P}^{\mathcal{D}})$$

where the Petri net duality operator $(\cdot)^{\mathcal{D}}$ swaps around the places and transitions in a Petri net and reverses arcs (see [1] for details).

A Petri net generally has infinitely many flows. But it is possible to obtain a finite set of *minimal flows* which can be combined to form all other flows. In the following we shall consider the structure of flows irrespective of whether they are T or P flows. We hence use $\mathrm{F}(\mathcal{P})$ and $\mathrm{MF}(\mathcal{P})$ to denote the set of either type of flows and minimal flows of $\mathcal{P}$, respectively.

Definition 4 (Support). *The support of a vector $x \in \mathbb{N}^*$, denoted by $\sup(x)$, is the set of indices of non-zero entries in x:* $\sup(x) \triangleq \{i \mid x_i \neq 0\}$.

Definition 5 (Minimal flows). *A flow $x \in \mathrm{F}(\mathcal{P})$ is* minimal *if*

1. *x is* canonical*, i.e. the greatest common divisor of non-zero entries of x, written $\gcd(x)$, is 1 and*
2. *x has* minimal support*, i.e. there are no other flows $x' \in \mathrm{F}(\mathcal{P})$ with $\sup(x') \subsetneq \sup(x)$.*

We denote by $\mathrm{MTF}(\mathcal{P})$ (or $\mathrm{MTF}(W_{\mathcal{P}})$) and $\mathrm{MPF}(\mathcal{P})$ (or $\mathrm{MPF}(W_{\mathcal{P}})$) the sets of minimal T and P-flows of $\mathcal{P}$, respectively.

Example 2. Let us find the minimal flows for the photosynthesis and respiration Petri nets introduced in Example 1. We will do so informally without writing out the flow matrices and full vectors, and instead simply listing the places and transitions which have non-zero entries in the flows.

There are three minimal place flows in the photosynthesis Petri net determined by the places (H_2O, O_2), (CO_2, Sugar) and $(\mathrm{CE}, H_2O, \mathrm{Sugar})$. Symmetrically, there are three minimal place flows in the respiration Petri net determined by the places (H_2O, O_2), (CO_2, Sugar) and $(H_2O, \mathrm{Sugar}, \mathrm{CE}')$. However, neither Petri net has any transition flows.

The following two theorems are adapted from [21]. They state that $\mathrm{MTF}(\mathcal{P})$ and $\mathrm{MPF}(\mathcal{P})$ are well-defined, and that any flow can be generated from minimal flows by natural-number linear combinations followed by a division.

Theorem 1. $\mathrm{MTF}(\mathcal{P})$ *and* $\mathrm{MPF}(\mathcal{P})$ *are finite and unique.*

Theorem 2. *For any flow $x \in \mathrm{F}(\mathcal{P})$ there are $a, \alpha_1, \ldots, \alpha_k \in \mathbb{N}$ and minimal flows $x_1, \ldots, x_k \in \mathrm{MF}(\mathcal{P})$ s.t. $x = \frac{1}{a}(\alpha_1 x_1 + \cdots + \alpha_k x_k)$*

We shall also need the following theorem, adapted from [26], which states that any two flows with the same minimal support are multiples of each other.

Theorem 3. *Let $x, y \in \mathrm{F}(\mathcal{P})$. If they both have the same minimal support, i.e. there are no other flows $z \in \mathrm{F}(\mathcal{P})$ with $\sup(z) \subsetneq \sup(x) = \sup(y)$, then there is $n \in \mathbb{N}$ s.t. either $x = ny$ or $y = nx$.*

Given a set of flows we shall need to filter out the non-minimal ones as in the following definition.

Definition 6 (Minimisation). *Let X be a set of flows. Define minimisation thus:*

$$\min(X) \triangleq \{\frac{x}{\gcd(x)} \mid x \in X \wedge \forall x' \in X.\text{sup}(x') \subsetneq \text{sup}(x)\}$$

There is a less common definition of minimality which dispenses with the notion of support and defines a flow to be minimal if it cannot be written as the sum of two other flows. This yields a unique set of minimal flows which contains, possibly strictly, the set of minimal flows defined above [21]. The results in this paper are proven valid for both definitions of minimality, and the details can be found in [24].

3 Composition of Petri Nets

In this section we consider how, given two Petri nets $\mathcal{P}_1$ and $\mathcal{P}_2$, these can be composed to form a *parallel* Petri net $\mathcal{P}_1 \mid_{\text{p}} \mathcal{P}_2$. In order for this to be interesting, $\mathcal{P}_1$ and $\mathcal{P}_2$ must have some means of interacting. Two common such means are via *shared places* and *shared transitions*. We will focus on shared places since this appears to be the natural interpretation in the context of chemical reactions. We also see that P and T-flows are *not* dual in a modular sense when considering place sharing alone, but that the duality arises when also considering transition sharing. This allows our results for place sharing to be easily adapted to transition sharing.

3.1 Composition Based on Place Sharing

Following [23] we let the shared places of two Petri nets be determined by syntactic equality of place names rather than introducing explicit place fusion sets. So if two Petri nets $\mathcal{P}_1$ and $\mathcal{P}_2$ both have a place named s, this will be merged to a single place in the composite net $\mathcal{P}_1 \mid_{\text{p}} \mathcal{P}_2$. When modelling large systems one may wish to identify places with different syntactic names, but this can be handled at a higher level of abstraction as in e.g. the Language for Biochemical Systems [19].

In order to ensure that there is no transition sharing, the parallel composition operation will implicitly rename the transitions of parallel component. This is achieved in a notationally convenient manner by assuming that transitions are strings over the binary alphabet, and prefixing 0 to the transitions of $\mathcal{P}_1$ and 1 to the transitions of $\mathcal{P}_2$.

Definition 7. *Let* $\mathcal{P}_1 = (S_1, T_1, W_1^{\text{in}}, W_1^{\text{out}})$ *and* $\mathcal{P}_2 = (S_2, T_2, W_2^{\text{in}}, W_2^{\text{out}})$ *be two petri nets with* $T_1, T_2 \subsetneq \{0,1\}^*$. *Then define* $\mathcal{P}_1 \mid_{\text{p}} \mathcal{P}_2 \triangleq (S, T, W^{\text{in}}, W^{\text{out}})$ *where* $S \triangleq S_1 \cup S_2$, $T \triangleq \{0t \mid t \in T_1\} \cup \{1t \mid t \in T_2\}$ *and for* $\text{io} \in \{\text{in}, \text{out}\}$, $b \in \{0,1\}$ *we define* $W^{\text{io}} : S \times T \to \mathbb{N}$ *as follows:*

$$W^{\text{io}}(s, bt) \triangleq \begin{cases} W_1^{\text{io}}(s,t) & \text{if } s \in S_1 \wedge b = 0 \\ W_2^{\text{io}}(s,t) & \text{if } s \in S_2 \wedge b = 1 \\ 0 & \text{otherwise} \end{cases}$$

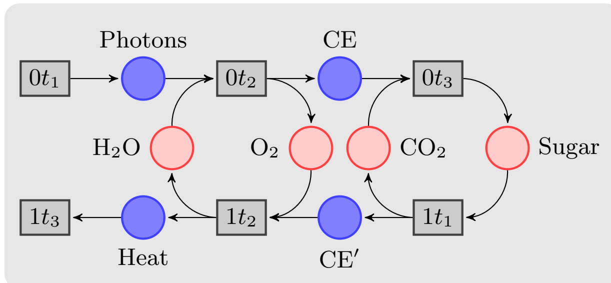


Fig. 2. Photosynthesis and respiration combined into a single Petri net by merging shared places.

Example 3. Let $\mathcal{P}_1$ and $\mathcal{P}_2$ be the Petri nets shown in Figure 1. Then $\mathcal{P} = \mathcal{P}_1 \mid_{\mathrm{p}} \mathcal{P}_2$ is shown in Figure 2.

Let us consider the structure of the full flow matrix W arising from the composition of $\mathcal{P}_1$ and $\mathcal{P}_2$ with flow matrices W_1 and W_2. For notational convenience we will assume that all shared places are ordered *after* the non-shared places in $\mathcal{P}_1$, and *before* the non-shared places in $\mathcal{P}_2$. More precisely we assume for $\Delta S = S_{\mathcal{P}_1} \cap S_{\mathcal{P}_2}$ and all $s_1 \in S_{\mathcal{P}_1} \setminus \Delta S$, $s \in \Delta S$ and $s_2 \in S_{\mathcal{P}_2} \setminus \Delta S$ that $s_1 \prec_{\mathrm{s}} s$ and $s \prec_{\mathrm{s}} s_2$. In the running example we could for example order the places as Photons, CE, H_2O, O_2, CO_2, Sugar, CE′, Heat. Then W_1, W_2 and W can be partitioned as follows where, for $i \in \{1, 2\}$, W_i^{s} consists of the rows from W_i which represent shared places, and W_i^- are the remaining rows for non-shared places.

$$W_1 = \begin{bmatrix} W_1^- \\ W_1^{\mathrm{s}} \end{bmatrix},\ W_2 = \begin{bmatrix} W_2^{\mathrm{s}} \\ W_2^- \end{bmatrix},\ W = \begin{bmatrix} W_1^- & 0 \\ W_1^{\mathrm{s}} & W_2^{\mathrm{s}} \\ 0 & W_2^- \end{bmatrix}$$

When considering parallel compositions in the remainder of the paper, we shall write W_1^-, W_1^{s}, W_2^-, W_2^{s} and W with the above meaning in mind. We shall furthermore write W_1^+ and W_2^+ to denote respectively the left and right partition of W, i.e. the extensions of W_1 and W_2 with 0-entries for non-shared places from the parallel counterpart. W^- will denote W without the rows $W_1^{\mathrm{s}} W_2^{\mathrm{s}}$ for shared places.

3.2 Modular Duality: Composition Based on Transition Sharing

We have seen that T-flows and P-flows are duals. A natural question then arises of whether this duality holds in the *modular* sense that $\mathrm{PF}(\mathcal{P}_1 \mid_{\mathrm{p}} \mathcal{P}_2) = \mathrm{TF}((\mathcal{P}_1 \mid_{\mathrm{p}} \mathcal{P}_2)^{\mathcal{D}}) = \mathrm{TF}(\mathcal{P}_1^{\mathcal{D}} \mid_{\mathrm{p}} \mathcal{P}_2^{\mathcal{D}})$. The answer is *no*. To see why, let us assume that $T_{\mathcal{P}_1} \cap T_{\mathcal{P}_2} = \emptyset$ and write out the flow matrices $W^{\mathbf{T}}$ of $(\mathcal{P}_1 \mid_{\mathrm{p}} \mathcal{P}_2)^{\mathcal{D}}$ and W' of $(\mathcal{P}_1^{\mathcal{D}} \mid_{\mathrm{p}} \mathcal{P}_2^{\mathcal{D}})$:

$$W^{\mathbf{T}} = \begin{bmatrix} W_1^{-\mathbf{T}} & W_1^{s\mathbf{T}} & 0 \\ 0 & W_2^{s\mathbf{T}} & W_2^{-\mathbf{T}} \end{bmatrix} \quad W' = \begin{bmatrix} W_1^{-\mathbf{T}} & W_1^{s\mathbf{T}} & 0 & 0 \\ 0 & 0 & W_2^{s\mathbf{T}} & W_2^{-\mathbf{T}} \end{bmatrix}$$

The two matrices do not generally have the same dimensions because the dual nets $\mathcal{P}_1^{\mathcal{D}}$ and $\mathcal{P}_2^{\mathcal{D}}$ share transitions rather than places. Hence the modular duality suggested above clearly does not hold in general.

However, we can define the *transition-based* composition operation where transitions (rather than places) of a parallel net are merged based on name equality, and where places are strings over the binary alphabet for the sake of convenient renaming:

Definition 8. *Let $\mathcal{P}_1 = (S_1, T_1, W_1^{\text{in}}, W_1^{\text{out}})$ and $\mathcal{P}_2 = (S_2, T_2, W_2^{\text{in}}, W_2^{\text{out}})$ be two Petri nets with $S_1, S_2 \subsetneq \{0,1\}^*$. Then define $\mathcal{P}_1 \mid_{\text{t}} \mathcal{P}_2 \triangleq (S, T, W^{\text{in}}, W^{\text{out}})$ where $S \triangleq \{0s \mid s \in S_1\} \cup \{1s \mid s \in S_2\}$, $T \triangleq T_1 \cup T_2$, and for $\text{io} \in \{\text{in}, \text{out}\}$, $b \in \{0,1\}$ we define $W^{\text{io}} : S \times T \to \mathbb{N}$ as follows:*

$$W^{\text{io}}(bs, t) \triangleq \begin{cases} W_1^{\text{io}}(s,t) & \text{if } t \in T_1 \wedge b = 0 \\ W_2^{\text{io}}(s,t) & \text{if } t \in T_2 \wedge b = 1 \\ 0 & \text{otherwise} \end{cases}$$

Then the *P-flows* of a parallel net under *transition sharing* are the same as the *T-flows* of the parallel dual nets under *place sharing*, and symmetrically for T-flows under transition sharing:

Theorem 4. *Let $\mathcal{P}_1$ and $\mathcal{P}_2$ be Petri nets. Then*

1. $\text{TF}(\mathcal{P}_1 \mid_t \mathcal{P}_2) = \text{PF}(\mathcal{P}_1^{\mathcal{D}} \mid_{\text{p}} \mathcal{P}_2^{\mathcal{D}})$.
2. $\text{PF}(\mathcal{P}_1 \mid_t \mathcal{P}_2) = \text{TF}(\mathcal{P}_1^{\mathcal{D}} \mid_{\text{p}} \mathcal{P}_2^{\mathcal{D}})$.

The proof relies on a partitioning of flow matrices similar to the partitioning in the previous subsection, but for shared transitions rather than places. It follows from Theorem 4 that the results for modular flows under place sharing, to be given in the following sections, can be easily adapted to (dual) modular flows under transition sharing.

4 Minimal Transition Flows

We start with an example of how T-flows arise through parallel composition.

Example 4. As noted in Example 2, neither of the photosynthesis and respiration Petri nets has any T-flows. But observe that the composite net in Figure 2 *does* have a single T-flow determined by the transitions $(0t_1, 0t_2, 0t_3, 1t_1, 1t_2, 1t_3)$. How did this flow arise from the parallel composition? To answer this, we need to look at *potential* T-flows of the two nets rather than the *actual* T-flows of which there are none. The potential T-flows are the ones arising from restricting individual components to private places only, i.e. by disregarding the shared places. If we do so, the photosynthesis Petri net has a single T-flow determined by $(0t_1, 0t_2, 0t_3)$, and the respiration net has a single T-flow determined by $(1t_1, 1t_2, 1t_3)$. The T-flow in the parallel net is composed from these two, because the transitions from the two nets operating on shared places cancel each other out.

The general case is slightly more complicated, because there may be many potential T-flows of each parallel component. These T-flows can then be combined by natural-number linear combinations in such a way that the resulting flow has no net effect on shared places. The weights of this natural-number linear combination must be minimal in some sense in order for there to be any hope of minimality of the composite flow in the composite net. A formal definition is given below, where we use the conventions on flow matrix partitioning introduced in Section 3.1; by $[\mathrm{MTF}(W_i^-)]$ we mean the matrix consisting of the column vectors in $\mathrm{MTF}(W_i^-)$ in some arbitrary order.

Definition 9. *Let $\mathcal{P}_1$ and $\mathcal{P}_2$ be Petri nets and let $X_1 = \left[\mathrm{MTF}(W_1^-)\right]$, $X_2 = \left[\mathrm{MTF}(W_2^-)\right]$ and W^{s} be given. Define the following:*

1. $X \triangleq \begin{bmatrix} X_1 & 0 \\ 0 & X_2 \end{bmatrix}$
2. $C \triangleq W^{\mathrm{s}} X$.
3. $Z \triangleq \{X\alpha \mid \alpha \in \mathrm{MTF}(C)\}$.

We then define $\mathrm{MTF}^{\mathrm{Par}}(X_1, X_2, W^{\mathrm{s}}) \triangleq \min(Z)$.

To elaborate on this definition, let $m_1 = |T_{\mathcal{P}_1}|$, $m_2 = |T_{\mathcal{P}_2}|$, $n_1 = |\mathrm{MTF}(W_1^-)|$ and $n_2 = |\mathrm{MTF}(W_2^-)|$. Then X_1 and X_2 are $m_1 \times n_1$ and $m_2 \times n_2$ matrices with the transition flows of respectively $\mathcal{P}_1$ and $\mathcal{P}_2$ *without their shared places*, i.e. of W_1^- and W_2^-. Also,

1. X is an $(m_1 + m_2) \times (n_1 + n_2)$ matrix with columns representing minimal T-flows of W^-.
2. C is an $(|S_{\mathcal{P}_1} \cap S_{\mathcal{P}_2}|) \times (n_1 + n_2)$ matrix with each column c_i representing the effect of the corresponding minimal T-flow x_i on the shared places.
3. Z is a set of linear combinations of the minimal T-flow-columns in X. These linear combinations are chosen in such a way that they have no net effect on the shared species. Note that the set Z is well-defined because $\mathrm{MTF}(C)$ is finite and unique by Theorem 1.

Remarks regarding the use of minimisation are made towards the end of the section. The following results state that Definition 9 is sound and complete. Soundness is split into two lemmas, the first of which is needed to prove completeness.

Lemma 1 (Soundness part 1). *Let Z be as given in Definition 9. Then*

1. $Z \subsetneq \mathrm{TF}(\mathcal{P}_1 \mid_{\mathrm{p}} \mathcal{P}_2)$.
2. $\min(Z) \subsetneq \mathrm{TF}(\mathcal{P}_1 \mid_{\mathrm{p}} \mathcal{P}_2)$.

The proof uses the definition of C to show that any $X\alpha \in Z$ is a T-flow of W^{s}. Since X consists of minimal T-flows of W^-, $X\alpha$ is also a T-flow of W^-. Together these give that $X\alpha$ is a T-flow of W and hence of $\mathcal{P}_1 \mid_{\mathrm{p}} \mathcal{P}_2$.

Lemma 2 (Completeness). *Let $\mathcal{P}_1$, $\mathcal{P}_2$, X_1, X_2 and W^{s} be as given in Definition 9. Then* $\mathrm{MTF}(\mathcal{P}_1 \mid_{\mathrm{p}} \mathcal{P}_2) \subseteq \mathrm{MTF}^{\mathrm{Par}}(X_1, X_2, W^{\mathrm{s}})$.

The proof starts by showing that any $x \in \mathrm{MTF}(\mathcal{P}_1 \mid_{\mathrm{p}} \mathcal{P}_2)$ can be written $x = \frac{1}{a}X\alpha$ where $\alpha \in \mathrm{TF}(C)$ and $a \in \mathbb{N}$ (uses Theorem 2 and the definition of C). Using Euclid's lemma and that x is canonical, we show that a canonical α can in fact be chosen. We then use Theorem 3 and minimality of x to show that any of the minimal-support α which generate x as above is in fact also minimal in C. We arrive at $x \in Z$. To conclude that also $x \in \min(Z)$, we use that any $x' \in Z$ with smaller support than x would also be in $\mathrm{TF}(\mathcal{P}_1 \mid_{\mathrm{p}} \mathcal{P}_2)$ (Lemma 1), hence contradicting minimality of x in $\mathcal{P}_1 \mid_{\mathrm{p}} \mathcal{P}_2$.

Lemma 3 (Soundness part 2). *Let $\mathcal{P}_1$, $\mathcal{P}_2$, X_1, X_2 and W^{s} be as given in Definition 9. Then* $\mathrm{MTF}^{\mathrm{Par}}(X_1, X_2, W^{\mathrm{s}}) \subseteq \mathrm{MTF}(\mathcal{P}_1 \mid_{\mathrm{p}} \mathcal{P}_2)$

The proof carries on from Lemma 1. To show that the elements of $\min(Z)$ are in fact minimal in $\mathcal{P}_1 \mid_{\mathrm{p}} \mathcal{P}_2$, we use that all minimal-support (although not necessarily canonical) flows are represented in Z by completeness (Lemma 2).

Together the two previous lemmas prove our main T-flow theorem:

Theorem 5 (Soundness and completeness). *Let $\mathcal{P}_1$, $\mathcal{P}_2$, X_1, X_2 and W^{s} be as given in Definition 9. Then* $\mathrm{MTF}^{\mathrm{Par}}(X_1, X_2, W^{\mathrm{s}}) = \mathrm{MTF}(\mathcal{P}_1 \mid_{\mathrm{p}} \mathcal{P}_2)$

The size of matrices X and C may be reduced by removing columns which have all 0-entries in C; these columns are also flows in the composite net and can be included directly.

The flows in Z may not be minimal, which is why the minimisation function must be applied as a last step. This is illustrated by the following example.

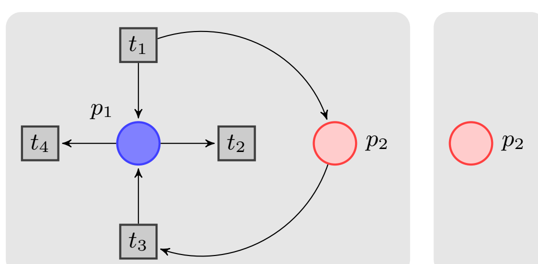


Fig. 3. Two Petri nets illustrating how Definition 9 can give rise to non-minimal flows in Z.

Example 5. Figure 3 shows two Petri nets: the left, $\mathcal{P}_1$, has two places of which one is shared with the right, $\mathcal{P}_2$, consisting of just a single place. The restriction of $\mathcal{P}_1$ to the place p_1 (corresponding to W^-) has four minimal T-flows represented by $x_1 = (t_1, t_2)$, $x_2 = (t_2, t_3)$, $x_3 = (t_3, t_4)$ and $x_4 = (t_1, t_4)$. The "minimal" combinations of these which preserve the flow for the shared place p_2 (corresponding to the minimal flows of C) are $x_1 + x_2 = (t_1, 2 \cdot t_2, t_3)$, $x_1 + x_3 = (t_1, t_2, t_3, t_4)$ and $x_2 + x_4 = (t_1, t_2, t_3, t_4)$. But the latter two flows are not minimal because they strictly contain the support of the first.

Minimisation is however *not* necessary in cases where the minimal flows in X are linearly independent. Then we get unique decomposition in the sense that any flow can be written uniquely as combinations of minimal flows (linear independence fails in the above example, for $x_1 + x_3 = x_2 + x_4$). This can be used in the proof of the following theorem:

Theorem 6. *Let X and Z be as given in Definition 9. If the columns of X are linearly independent, then the elements of Z have minimal support (but still may not be canonical).*

5 Minimal Place Flows

As for T-flows we start by looking at an example of how P-flows in a composite net arise from P-flows in parallel components.

Example 6. In example 2 we listed the three minimal P-flows for each of the two Petri nets in Figure 1. These included $x = (\mathrm{CE}, \mathrm{H_2O}, \mathrm{Sugar})$ from the first net and $y = (\mathrm{H_2O}, \mathrm{Sugar}, \mathrm{CE}')$ from the second net. Neither is a flow in the composite net shown in Figure 2 because of interference from the additional transitions. For example, $0t_1$ consumes tokens from Sugar and produces tokens in CE′, and this violates the first flow.

However, because x and y have identical weights for their shared places (namely $1 \cdot \mathrm{H_2O}$ and $1 \cdot \mathrm{Sugar}$), we can "join" them to obtain a new minimal flow $x \frown y = (\mathrm{CE}, \mathrm{H_2O}, \mathrm{Sugar}, \mathrm{CE}')$ for the composite net.

Here is the formal definition of P-flow joins where again we assume the partitioning of flow matrices given in Section 3.1.

Definition 10 (Flow joins). *Let $\mathcal{P}_1$, $\mathcal{P}_2$ be Petri nets and let $x \in \mathrm{PF}(\mathcal{P}_1)$, $y \in \mathrm{PF}(\mathcal{P}_2)$. Write $x = (x^- x^{\mathrm{s}})$, $y = (y^{\mathrm{s}} y^-)$ where, for $\Delta S = S_{\mathcal{P}_1} \cap S_{\mathcal{P}_2}$, x^- represents places $S_{\mathcal{P}_1} \setminus \Delta S$, x^{s} and y^{s} represent places ΔS, and y^- represents places $S_{\mathcal{P}_2} \setminus \Delta S$. If $x^{\mathrm{s}} = y^{\mathrm{s}}$ we say that x and y are* consistent *and define their* join $x \frown y \stackrel{\Delta}{=} (x^- x^{\mathrm{s}} y^-)$.

The join of consistent flows from two parallel nets is a flow in the composite net:

Lemma 4. *Let $\mathcal{P}_1$ and $\mathcal{P}_2$ be Petri nets and let $x \in \mathrm{PF}(\mathcal{P}_1)$, $y \in \mathrm{PF}(\mathcal{P}_2)$. If x and y are consistent then $x \frown y \in \mathrm{PF}(\mathcal{P}_1 \mid_{\mathrm{p}} \mathcal{P}_2)$.*

Conversely, any P-flow z of a parallel composition $\mathcal{P}_1 \mid_{\mathrm{p}} \mathcal{P}_2$ is the join of a P-flow from $\mathcal{P}_1$ and a P-flow from $\mathcal{P}_2$.

Lemma 5. *Let $\mathcal{P}_1$ and $\mathcal{P}_2$ be Petri nets and let $z \in \mathrm{PF}(\mathcal{P}_1 \mid_{\mathrm{p}} \mathcal{P}_2)$. Then there are $x \in \mathrm{PF}(\mathcal{P}_1)$ and $y \in \mathrm{PF}(\mathcal{P}_2)$ s.t. $z = x \frown y$.*

In contrast to Example 6, it is generally not sufficient to join only *minimal* consistent flows. Rather we must obtain two linear combinations of minimal flows from the respective nets in such a way that they become consistent, and then join them to form a flow of the composite net. As for modular T-flows, the weights used in this linear combination must be minimal in some sense in order for there to be any hope of minimality for the resulting join.

The general modular definition of P-flows is given below. Similarly to the definition for T-flows, $[\mathrm{MPF}(\mathcal{P})]$ is a matrix with rows from $\mathrm{MPF}(\mathcal{P})$ in any order.

Definition 11. *Let $\mathcal{P}_1$ and $\mathcal{P}_2$ be Petri nets and let $X = [\mathrm{MPF}(\mathcal{P}_1)]$ and $Y = [\mathrm{MPF}(\mathcal{P}_2)]$ be given. Let X^{s} and Y^{s} be the sub-matrices of X and Y containing only columns for shared places $s \in S_{\mathcal{P}_1} \cap S_{\mathcal{P}_2}$. Define the following:*

1. $C \triangleq \begin{bmatrix} X^{\mathrm{s}} \\ -Y^{\mathrm{s}} \end{bmatrix}$.
2. $Z \triangleq \{\alpha X \frown \beta Y \mid (\alpha\beta) \in \mathrm{MPF}(C)\}$.

We then define $\mathrm{MPF}^{\mathrm{Par}}(X, Y) \triangleq \min(Z)$.

To elaborate on this definition, let $\Delta S = S_{\mathcal{P}_1} \cap S_{\mathcal{P}_2}$, $m = |\Delta S|$, $n_1 = |\mathrm{MPF}(\mathcal{P}_1)|$, $n_2 = |\mathrm{MPF}(\mathcal{P}_2)|$. Then

1. C is an $(n_1 + n_2) \times m$ matrix with the first n_1 rows representing minimal P-flows of $\mathcal{P}_1$ and the last n_2 rows representing *negated* minimal P-flows from $\mathcal{P}_2$, but restricted to the m shared places only.
2. Z contains the joins of consistent linear combinations of flows from the two nets. The weights for this linear combination are chosen exactly so that the resulting flows have the same weights for shared places. Note that the set Z is well-defined because $\mathrm{MTF}(C)$ is finite and unique by Theorem 1.

As for T-flows we have soundness and completeness results, and soundness is split into two separate lemmas.

Lemma 6 (Soundness part 1). *Let Z be as given in Definition 11. Then*

1. $Z \subsetneq \mathrm{PF}(\mathcal{P}_1 \mid_{\mathrm{p}} \mathcal{P}_2)$.
2. $\min(Z) \subsetneq \mathrm{PF}(\mathcal{P}_1 \mid_{\mathrm{p}} \mathcal{P}_2)$.

The proof uses Lemma 4 and the definition of C.

Lemma 7 (Completeness). *Let $\mathcal{P}_1$,$\mathcal{P}_2$,X and Y be as given in Definition 11. Then* $\mathrm{MPF}(\mathcal{P}_1 \mid_{\mathrm{p}} \mathcal{P}_2) \subseteq \mathrm{MPF}^{\mathrm{Par}}(X, Y)$

The proof first uses Lemma 5 to write any $z \in \mathrm{MPF}(\mathcal{P}_1 \mid_{\mathrm{p}} \mathcal{P}_2)$ as $z = x \frown y$ for some $x \in \mathrm{PF}(\mathcal{P}_1)$ and $y \in \mathrm{PF}(\mathcal{P}_2)$. Then the main challenge is to show that there is some d and $(\alpha\beta) \in \mathrm{MPF}(C)$ s.t. $dx = \alpha X$ and $dy = \beta Y$ (for then we can conclude that $dz \in Z$). First the existence of such $(\alpha\beta) \in \mathrm{PF}(C)$ is shown using Theorem 2, the definition of C and the fact that dx and dy are consistent. Minimality of $(\alpha\beta)$ uses an idea similar to the proof of Lemma 2 (completeness for T-flows).

Lemma 8 (Soundness part 2). *Let* $\mathcal{P}_1$*,*$\mathcal{P}_2$*,*X *and* Y *be as given in Definition 11. Then* $\text{MPF}^{\text{Par}}(X,Y) \subseteq \text{MPF}(\mathcal{P}_1 \mid_{\text{p}} \mathcal{P}_2)$

The proof is similar to that of Lemma 3 (soundness for T-flows). Together the last two lemmas prove our main theorem on modular P-flows:

Theorem 7 (Soundness and completeness). *Let* $\mathcal{P}_1$*,*$\mathcal{P}_2$*,*X *and* Y *be as given in Definition 11. Then* $\text{MPF}^{\text{Par}}(X,Y) = \text{MPF}(\mathcal{P}_1 \mid_{\text{p}} \mathcal{P}_2)$

The matrix C in Definition 11 can be reduced in size by removing rows with all 0 entries. Because these do not involve shared places, they are also flows of the composite net and can be included directly.

As for the modular definition of T-flows, minimisation is not necessary in cases where the minimal flows in the rows of C are linearly independent:

Theorem 8. *Let* C *and* Z *be as given in Definition 11. If the rows of* C *are linearly independent, then the elements of* Z *have minimal support (but still may not be canonical).*

6 Compositional Definitions of Minimal Flows

The modular definitions of flows given in the previous sections are not compositional for two reasons: 1) the flows of parallel components are given explicitly and not defined inductively. This is because there is no inductive structure on Petri nets and flows per se. 2) In the case of T-flows, the definition of MTF^{Par} requires more than just the flows of parallel components to be given. It requires the flows of the components *without shared places* (which are super-sets of the flows of the components) and the flow matrix for shared places.

In response to the first problem, we consider a simple calculus of Petri nets, $\mathcal{CP}$, which is a subset of the Calculus of Biochemical Systems (CBS) [19, 23]. In response to the second problem, we define a compositional T-flow function which returns not T-flows, but *a*) the flow function of the net together with *b*) a *function* mapping shared places to T-flows of the restricted net without these places.

6.1 $\mathcal{CP}$: A Calculus of Petri Nets

In the following, some fixed set of places S and transitions $T \triangleq \{0,1\}^*$ are assumed.

Definition 12. *The language* $\mathcal{CP}$ *is the set of programs generated by the following grammar, where* $n_i, n'_j \in \mathbb{N}$ *and* $s_i, s'_j \in S$*:*

$$P ::= \sum n_i \cdot s_i \rightarrow \sum n'_j \cdot s'_j \mid P_1|P_2$$

Intuitively, the program $\sum n_i \cdot s_i \rightarrow \sum n'_j \cdot s'_j$ represents a single Petri net transition (reaction) with input places (reactants) $\{s_i\}$, output places (products) $\{s'_j\}$ and flow functions (stoichiometries) given by the n_i and n'_j. In the biological setting, programs thus correspond directly to reactions taking place in parallel.

Example 7. Below are two programs representing respectively photosynthesis and respiration. All stoichiometries are 1 and have hence been omitted. Note the resemblance with chemical reactions. Also note that there are no reactants in the first reaction of photosynthesis, and no products in the last reaction of respiration.

$$P_1 \stackrel{\Delta}{=} \rightarrow \mathrm{Photons} \mid \mathrm{Photons} + \mathrm{H_2O} \rightarrow \mathrm{CE} + \mathrm{O_2} \mid \mathrm{CE} + \mathrm{CO_2} \rightarrow \mathrm{Sugar}$$
$$P_2 \stackrel{\Delta}{=} \mathrm{Sugar} \rightarrow \mathrm{CE}' + \mathrm{CO_2} \mid \mathrm{CE}' + \mathrm{O_2} \rightarrow \mathrm{Heat} + \mathrm{H_2O} \mid \mathrm{Heat} \rightarrow$$

The parallel composition $P_1 \mid P_2$ then represents combined photosynthesis and respiration.

The denotational semantics for $\mathcal{CP}$ is given in terms of the set $\mathcal{PN}$ of Petri nets.

Definition 13. *Define* $[\![\cdot]\!] : \mathcal{CP} \rightarrow \mathcal{PN}$ *inductively on programs as follows.*

- ***Basis:*** $[\![\sum n_i \cdot s_i \rightarrow \sum n'_j \cdot s'_j]\!] \stackrel{\Delta}{=} (\{s_i\} \cup \{s'_j\}, \{\epsilon\}, W^{\mathrm{in}}, W^{\mathrm{out}})$
  where $W^{\mathrm{in}}(s_i, \epsilon) \stackrel{\Delta}{=} n_i$ *and* $W^{\mathrm{out}}(s'_j, \epsilon) \stackrel{\Delta}{=} n'_j$.
- ***Step:*** $[\![P_1 | P_2]\!] \stackrel{\Delta}{=} [\![P_1]\!] \mid_{\mathrm{p}} [\![P_2]\!]$

In the base case, ϵ denotes the empty string over the binary alphabet. Note the compositional nature of the denotation function.

Example 8. Let P_1 and P_2 be as defined in Example 7. Then $[\![P_1]\!]$ and $[\![P_2]\!]$ are given by the Petri nets shown in Figure 1 (modulo transition naming), and $[\![P_1 \mid P_2]\!]$ is given by the composite Petri net shown in Figure 2 (modulo transition naming).

6.2 Flows in $\mathcal{CP}$

We are now in a position to give compositional definitions of minimal flows for $\mathcal{CP}$ programs. To do so, we first define $\mathcal{P} \setminus \Delta S$ to be the Petri net $\mathcal{P}$ without the places ΔS, and similarly $P \setminus \Delta S$ is the program P without the places ΔS. The power set of a set X is denoted by 2^X, and the domain of a function f is denoted by $\mathrm{dom}(f)$.

Definition 14. *Let* $\mathcal{W} = S \times T \hookrightarrow_{\mathrm{fin}} \mathbb{N}$ *be the set of (partial and finite) flow functions. Define the parameterised minimal T-flows,* $\zeta : \mathcal{CP} \rightarrow \mathcal{W} \times (2^S \rightarrow 2^{(\mathbb{N}^*)})$*, inductively as follows:*

- ***Basis:*** $\zeta(\sum n_i \cdot s_i \rightarrow \sum n'_j \cdot s'_j) \stackrel{\Delta}{=} (W_{\mathcal{P}}, h)$
  where $\mathcal{P} \stackrel{\Delta}{=} [\![\sum n_i \cdot s_i \rightarrow \sum n'_j \cdot s'_j]\!]$ *and* $h(\Delta S) \stackrel{\Delta}{=} \mathrm{MTF}(\mathcal{P} \setminus \Delta S)$.
- ***Step:*** $\zeta(P_1 | P_2) \stackrel{\Delta}{=} (W, h)$
  where
  - $\zeta(P_1) = (W_1, h_1)$ *and* $\zeta(P_2) = (W_2, h_2)$

- *W is composed from W_1 and W_2 as defined in Section 3.*
- $h(\Delta S) \triangleq \mathrm{MTF}^{\mathrm{Par}}(X_1, X_2, W^{\mathrm{ss}})$.
- $X_1 \triangleq h_1(\Delta S')$, $X_2 \triangleq h_2(\Delta S')$.
- $\Delta S' \triangleq \Delta S \cup \Delta S''$.
- $\Delta S'' \triangleq \{s \in S \mid \exists t_1, t_2 \in T.(s, t_1) \in \mathrm{dom}(W_1) \wedge (s, t_2) \in \mathrm{dom}(W_2)\}$ *(i.e. the places shared between $\mathcal{P}_1$ and $\mathcal{P}_2$).*
- *W^{ss} is the sub-matrix of W containing rows for shared places $\Delta S'' \setminus \Delta S$.*

In the inductive step observe how X_1, X_2 and W^{ss} are obtained purely from the results of recursively invoking ζ. Hence the definition is in fact compositional. But compositionality comes at a high price: the return value of ζ "encapsulates" both the flow matrix of the entire net and the flows arising from any restriction of places – all of this information is needed for the composition.

Definition 15. *Define the compositional minimal P-flows, $\xi : \mathcal{CP} \to 2^{(\mathbb{N}^*)}$, inductively as follows:*

– ***Basis:*** $\xi(\sum n_i \cdot s_i \to \sum n'_j \cdot s'_j) \triangleq \mathrm{MPF}([\![\sum n_i \cdot s_i \to \sum n'_j \cdot s'_j]\!])$.
– ***Step:*** $\xi(P_1|P_2) \triangleq \mathrm{MPF}^{\mathrm{Par}}(\xi(P_1), \xi(P_2))$.

Note how we again obtained a compositional definition, albeit in a somewhat simpler manner than for T-flows. This illustrates how modular T and P-flows are intricately different and non-dual because more information is needed in the compositional definition of T-flows.

The following theorem says that the compositional definitions given above work as expected. The proof is by induction on the structure of programs, using Theorems 5 and 7

Theorem 9. *Let P be an $\mathcal{CP}$ program and ΔS a set of places. Then*

1. $\zeta(P) = (W_{\mathcal{P}}, h)$
   where $\mathcal{P} = [\![P]\!]$ *and* $h(\Delta S) = \mathrm{MTF}(\mathcal{P} \setminus \Delta S)$.
2. $\xi(P) = \mathrm{MPF}([\![P]\!])$.

It follows as a special case of 1) that $h(\emptyset) = \mathrm{MTF}([\![P]\!])$.

7 Related Work and Conclusion

7.1 Related Work

The idea that consistent P-flows from two components can be joined to form a P-flow in the composite net (Lemma 4) is not new. Neither is the converse that any place flow in a composite net is a join of place flows from the parallel component (Lemma 5). These results have been stated previously in some form in [27–31].

In [29] an algorithm is given for directly computing the minimal P-flows of a "well-formed net" resulting from a place fusion operation, based on the minimal

P-flows of the net before fusion. But no proof of correctness is given. In [28] a method similar to Definition 11 is proposed for generative sets of P-flows rather than minimal P-flows. Such a method is also presented for "functional subnets" in [31], which in addition considers how to obtain the modules in the first place. However, in neither case is it clear to us how completeness follows from the proofs given, i.e. that the method in fact results in generative families of P-flows. In contrast, we give a full proof of *minimality* of the resulting P-flows (which is stronger than generativity).

Modular definitions of T-flows have received somewhat less attention than P-flows in the literature. To our knowledge, the only existing explicit work on modular T-flows is [29] (for well-formed nets), but this only shows an *example* of how new T-flows can arise after a place fusion. No general definition is given. In [30], a characterisation of *P-flows* arising from a composition of modules is given based on *both* place sharing *and* transition sharing. The duality elucidated in Theorem 4 suggests that a dual characterisation can be given for *T-flows* under place and transition sharing. Nevertheless, the characterisation does not result in methods for finding minimal or generative sets of flows and hence is of little practical use. It also considers flows in $\mathbb{Z}$ rather than in $\mathbb{N}$ as is more common (and harder).

7.2 Conclusion

As the primary contribution, this paper has presented algebraic definitions for obtaining the minimal P and T-flows of parallel Petri nets given the minimal P and T-flows of its components (with some additional information in the case of T-flows). These definitions have then been proven correct. Although the idea used for minimal P-flows is not new, no complete proof has to our knowledge been given before.

We have also shown modular dualities between T/P-flows under place sharing and T/P-flows under transition sharing. This allows our results for place sharing to be easily adapted to transition sharing. On the other hand, we have seen that T and P-flows are *not* dual in the modular sense under place sharing alone, and hence the existing work on modular P-flows under place sharing does not carry over to T-flows.

As an application we have shown how our modular definitions of T and P-flows can be used to define T and P-flows in a compositional manner for a subset of CBS. This has turned out to be harder for T-flows than for P-flows, thus further illustrating the intricate difference between the two when considering place sharing alone.

Future work may consider the computational complexity of calculating minimal flows using our compositional definitions and investigate if improvements can be made over existing algorithms as in e.g. [28]. The inherent compositionality can also be exploited by distributed computation. On the more theoretical side, a potential next step is to extend the results to higher-level coloured Petri nets. These allow species modifications and complexes to be represented compactly and form a semantical foundation of the full CBS.

Acknowledgements

The author would like to thank Gordon Plotkin and Monika Heiner for useful discussions. This work was supported by Microsoft Research through its European PhD Scholarship Programme.

References

1. Murata, T.: Petri nets: properties, analysis and applications. Proc. IEEE **77**(4) (1989) 541–580
2. Goss, P.J.E., Peccoud, J.: Quantitative modeling of stochastic systems in molecular biology by using stochastic Petri nets. PNAS **95**(12) (1998) 6750–6755
3. Peleg, M., et al.: Using Petri net tools to study properties and dynamics of biological systems. Journal of the American Medical Informatics Association **12**(2) (2005) 181–199
4. Hardy, S., Robillard, P.N.: Modeling and simulation of molecular biology systems using Petri nets: Modeling goals of various approaches. J. Bioinformatics and Computational Biology **2**(4) (2004) 619–638
5. Reddy, V.N., et al.: Petri net representation in metabolic pathways. In: Proc. Int. Conf. Intell. Syst. Mol. Biol. (1993) 328–336
6. Zevedei-Oancea, Schuster, S.: Topological analysis of metabolic networks based on Petri net theory. In Silico Biol **3** (2003) 323–345
7. Heiner, M., et al.: Analysis and simulation of steady states in metabolic pathways with Petri nets. In Jensen, K., ed.: Workshop and Tutorial on Practical Use of Coloured Petri Nets and the CPN Tools. (2001) 15–34
8. Genrich, H., et al.: Executable Petri net models for the analysis of metabolic pathways. J STTT **3**(4) (2001) 394–404
9. Voss, K., et al.: Steady state analysis of metabolic pathways using Petri nets. In Silico Biol **3** (2003)
10. Heiner, M., Koch, I.: Petri net based model validation in systems biology. In: Applications and Theory of Petri Nets 2004. Volume 3099 of LNCS., Springer (2004) 216–237
11. Sackmann, A., et al.: Application of Petri net based analysis techniques to signal transduction pathways. BMC Bioinformatics **7**(482) (2006)
12. Lee, D.Y., et al.: Colored Petri net modeling and simulation of signal transduction pathways. Metab Eng **8**(2) (2005) 112–22
13. Heiner, M., et al.: Petri nets for systems and synthetic biology. In Bernardo, M., Degano, P., Zavattaro, G., eds.: SFM 2008. Volume 5016 of LNCS. (2008) 215–264
14. Taubner, C., et al.: Modelling and simulation of the TLR4 pathway with coloured Petri nets. In: Proc. Annual International Conference of the IEEE Engineering in Medicine and Biology Society, Engineering in Medicine and Biology Society (2006) 2009–2012
15. Matsuno, H., et al.: Hybrid Petri net representation of gene regulatory network. Pacific Symposium on Biocomputing **5** (2000) 341–52
16. Steggles, L.J., et al.: Qualitatively modelling and analysing genetic regulatory networks: a Petri net approach. Bioinformatics **23**(3) (2007) 336–343
17. Gilbert, D., et al.: A case study in model-driven synthetic biology. In: Biologically-inspired cooperative computing. Volume 268 of IFIP International Federation for Information Processing., Springer (2008) 163–175

18. Jensen, K.: Coloured Petri Nets: Basic Concepts, Analysis Methods and Practical Use. Volume 1. Springer (1992)
19. Pedersen, M., Plotkin, G.: A language for biochemical systems. In Heiner, M., Uhrmacher, A.M., eds.: Proc. CMSB. LNCS, Springer (2008)
20. Kofahl, B., Klipp, E.: Modelling the dynamics of the yeast pheromone pathway. Yeast **21**(10) (2004) 831–850
21. Krückeberg, F., Jaxy, M.: Mathematical methods for calculating invariants in Petri nets. In: Advances in Petri Nets 1987, covers the 7th European Workshop on Applications and Theory of Petri Nets, London, UK, Springer (1987) 104–131
22. Schuster, S., et al.: A general definition of metabolic pathways useful for systematic organization and analysis of complex metabolic networks. Nature Biotechnology **18** (2000) 326 – 332
23. Plotkin, G.: A calculus of biochemical systems. In preparation
24. Pedersen, M.: Compositional definitions of minimal flows in Petri nets. Technical report, University of Edinburgh (2008) http://www.inf.ed.ac.uk/publications/report/1269.html.
25. Reisig, W.: Petri nets. EATCS Monograps on Theoretical Computer Science. Springer (1982)
26. Memmi, G., Roucairol, G.: Linear algebra in net theory. In: Proc. Advanced Course on General Net Theory of Processes and Systems, Springer (1980) 213–223
27. Jensen, K.: Coloured Petri Pets: Basic Concepts, Analysis Methods and Practical Use. Volume 2. Springer (1995)
28. Bourjij, A., et al.: A decentralized approach for computing invariants in large scale and interconnected Petri nets. In: Proc. IEEE International Conference on Systems, Man, and Cybernetics. Volume 2. (1997) 1741–1746
29. M., I.C.R.: Compositional construction and analysis of Petri net systems. PhD thesis, School of Informatics, University of Edinburgh (1998)
30. Christensen, S., Petrucci., L.: Modular analysis of Petri nets. The Computer Journal **43**(3) (2000) 224–242
31. Zaitsev, D.A.: Decomposition-based calculation of Petri net invariants. In Cortadella, Yakovlev, eds.: Proc. Workshop on Token based Computing (ToBaCo), Satellite Event of the 25-th International conference on application and theory of Petri nets. (2004) 79–83

A Selected Proofs

A.1 Modular T-flows

Proof (Lemma 2). Take any $x \in \mathrm{MTF}(\mathcal{P}_1 \mid_{\mathrm{p}} \mathcal{P}_2)$. Then $Wx = 0$, so also $W^{\mathrm{s}}x = 0$ and $W^{-}x = 0$. Hence $x \in \mathrm{TF}(W^{\mathrm{s}})$ and $x \in \mathrm{TF}(W^{-})$. Observe that X consists exactly of the minimal T-flows of W^{-}. Therefore, by Theorem 2 there are $\alpha \in \mathbb{N}^{|col(X)|^{\mathbf{T}}}$ and $a \in \mathbb{N}$ s.t. $x = \frac{1}{a}X\alpha$, i.e. $xa = X\alpha$. There may generally be multiple such α, so pick one which is canonical and has *minimal decomposition-support* in the sense that no other choices have smaller support. Such a canonical choice *is* indeed possible because it is always the case that $\gcd(\alpha)$ divides a. To see this, let $c = \gcd(\alpha)$; then there is a canonical α' s.t. $ax = Xc\alpha' = cX\alpha'$. Also $\frac{a}{d}x = \frac{c}{d}X\alpha'$ where $d = \gcd(a, c)$. Since x has natural number entries, $\frac{a}{d}$ divides all entries in $\frac{c}{d}X\alpha'$. It follows from Euclid's lemma and $\gcd(\frac{a}{d}, \frac{c}{d}) = 1$

that $\frac{a}{d}$ divides all entries in $X\alpha'$. Canonicity of x then forces $c = d$, and hence $d = \gcd(\alpha)$ divides a as claimed.

We now show that α is a T-flow of C, i.e. that $C\alpha = 0$. The following steps rely on the fact that matrix multiplication is associative:

$$C\alpha = (W^{\mathrm{s}}X)\alpha = W^{\mathrm{s}}(X\alpha) = W^{\mathrm{s}}(xa) = (W^{\mathrm{s}}x)a = 0a = 0$$

Next we show that α is a *minimal* T-flow of C. It is canonical per assumption. To get that α has minimal support, we show that any T-flow α' of C with $\sup(\alpha') \subsetneq \sup(\alpha)$ will also generate x, contrary to our choice of α being the smallest decomposition-support for which this holds. Note here the subtle distinction between minimality of α wrt. decomposition of x and wrt. flows of C; the former holds per assumption, and we will now prove the latter.

So, we have $\sup(\alpha') \subsetneq \sup(\alpha)$ and $C\alpha' = 0$. Then $0 = C\alpha' = (W^{\mathrm{s}}X)\alpha' = W^{\mathrm{s}}(X\alpha')$, so $x' = X\alpha'$ is a T-flow of W^{s}. Any linear combination of T-flows is also a T-flow, so x' is also a T-flow of W^{-}. Together these give $x' \in \mathrm{TF}(W)$. Now since $\sup(\alpha') \subsetneq \sup(\alpha)$ it must also hold that $\sup(x') = \sup(X\alpha') \subseteq \sup(X\alpha) = \sup(x)$. Since x has minimal-support, it must be the case that $\sup(x') = \sup(x)$. By Theorem 3, either $x = nx'$ or $x' = nx$ for some $n \in \mathbb{N}$. But x is canonical, so $x' = nx$ i.e. $x = \frac{1}{n}x' = \frac{1}{n}X\alpha'$. This contradicts our original choice of α to be a minimal-support decomposition of x.

We conclude that $\alpha \in \mathrm{MTF}(C)$ and hence $xa = X\alpha \in Z$. Per assumption x is minimal, so there is no other minimal flow $x'' \in \mathrm{MTF}(\mathcal{P}_1 \mid_{\mathrm{p}} \mathcal{P}_2) \supset Z$ (the inclusion is By Lemma 1) with $\sup(x'') \subsetneq \sup(x)$. Hence $x = \frac{xa}{a} \in \min(Z) = \mathrm{MTF}^{\mathrm{Par}}(X_1, X_2, W^{\mathrm{s}})$.

A.2 Modular P-flows

Proof (Lemma 7). Take any $z \in \mathrm{MPF}(\mathcal{P}_1 \mid_{\mathrm{p}} \mathcal{P}_2)$. By Lemma 5 there are restrictions $x \in \mathrm{PF}(\mathcal{P}_1)$ and $y \in \mathrm{PF}(\mathcal{P}_2)$ of z s.t. $z = x \frown y$. **Claim:** there are $(\alpha\beta) \in \mathrm{MPF}(C)$ and $d \in \mathbb{N}$ such that

$$dx = \alpha X \text{ and } dy = \beta Y$$

Then $dz = dx \frown dy = \alpha X \frown \beta Y \in Z$. Per assumption z is minimal so there is no other flow $z' \in \mathrm{PF}(\mathcal{P}_1 \mid_{\mathrm{p}} \mathcal{P}_2) \supset Z$ (Lemma 6) s.t. $\sup(z') \subsetneq \sup(z) = \sup(dz)$. Hence $z = \frac{dz}{d} \in \min(Z) = \mathrm{MPF}(X_1, X_2, W^{-})$, so we are done.

Proof of claim: By Theorem 2 there are $a, b \in \mathbb{N}$, $\alpha'' \in \mathbb{N}^{|row(X)|}$ and $\beta'' \in \mathbb{N}^{|row(Y)|}$ s.t.

$$\begin{aligned} ax = \alpha'' X \quad &\text{and} \quad by = \beta'' Y \quad \Leftrightarrow \\ abx = \alpha'' bX \quad &\text{and} \quad aby = \beta'' aY \end{aligned}$$

There may generally be many such (α'', β''), so pick one which has *minimal decomposition-support* in the sense that there are no other choices with smaller support satisfying the above equations.

Now let $c = \gcd(a, b)$, $d = \frac{ab}{c}$, $\alpha = \alpha'' \frac{b}{c}$ and $\beta = \beta'' \frac{a}{c}$. Continuing with the equations from above we then get

$$dx = \alpha X \quad \text{and} \quad dy = \beta Y$$

We know that x and y are consistent, i.e. $x^{\mathrm{s}} = y^{\mathrm{s}}$ where x^{s} and y^{s} are the restrictions of x and y to the shared places $S_{\mathcal{P}_1} \cap S_{\mathcal{P}_2}$. Hence also $dx^{\mathrm{s}} = dy^{\mathrm{s}}$. So

$$\begin{aligned} \alpha X^{\mathrm{s}} = dx^{\mathrm{s}} &= dy^{\mathrm{s}} = \beta Y^{\mathrm{s}} \quad \Leftrightarrow \\ \alpha X^{\mathrm{s}} - \beta Y^{\mathrm{s}} &= 0 \quad \Leftrightarrow \\ (\alpha \beta) C &= 0 \end{aligned}$$

It follows that $(\alpha\beta) \in \mathrm{PF}(C)$. We may assume that $(\alpha\beta)$ is canonical, for if it is not, it is always possible to divide through by $\gcd(\alpha\beta)$ since this always divides d. To se why this is the case, let $c = \gcd(\alpha\beta)$. Then there are α' and β' s.t. $dx = c\alpha' X$ and $dy = c\beta' Y$. Now let $e = \gcd(c, d)$ and write $\frac{d}{e} x = \frac{c}{e} \alpha' X$ and $\frac{d}{e} y = \frac{c}{e} \beta' Y$. Since x and y have entries in $\mathbb{N}$, $\frac{d}{e}$ divides all entries in both $\frac{c}{e} \alpha' X$ and $\frac{c}{e} \beta' Y$. From $e = \gcd(c, d)$ and a standard result from number theory we get that $\frac{d}{e}$ divides all entries in $\alpha' X$ and $\beta' Y$. Therefore $\frac{c}{e}$ divides all entries in both x and y, and hence also in $x \frown y = z$. Canonicity of z then forces $c = e$, so c divides d as claimed.

To see that $(\alpha\beta)$ has minimal support in C, suppose towards a contradiction that there is $(\alpha'\beta') \in \mathrm{PF}(C)$ with $\sup(\alpha'\beta') \subsetneq \sup(\alpha\beta) = \sup(\alpha''\beta'')$. From the definition of C it follows that $x' = \alpha' X$ and $y' = \beta' Y$ are consistent, i.e. $x'^{s} = \alpha' X^{\mathrm{s}} = \beta' Y^{\mathrm{s}} = y'^{s}$. They are also place flows of $\mathcal{P}_1$ and $\mathcal{P}_2$ respectively. Lemma 4 then gives that $z' = x' \frown y' \in \mathrm{PF}(\mathcal{P}_1 \mid_{\mathrm{p}} \mathcal{P}_2)$. We know that $\sup(z') \subseteq \sup(z)$, but we cannot have $\sup(z') \subsetneq \sup(c)$ since z is minimal. Hence $\sup(z') = \sup(z)$. By Theorem 3, there is some $n \in \mathbb{N}$ s.t.

$$nz = z' = x' \frown y' = \alpha' X \frown \beta' Y$$

But we also know that $nz = n(x \frown y) = nx \frown ny$. Hence

$$nx = \alpha' X \text{ and } ny = \beta' Y$$

Per assumption either $\sup(\alpha') \subsetneq \sup(\alpha'')$ or $\sup(\beta') \subsetneq \sup(\beta'')$. This contradicts our original choice of α'' or β'' to have minimal decomposition-support.