Electronic Communications of the EASST
Volume X (2008)

Proceedings of the
Seventh International Workshop on
Graph Transformation and Visual Modeling Techniques
(GT-VMT 2008)

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25 pages

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ECEASST Home Page: http://www.easst.org/eceasst/ ISSN 1863-2122

Controlling resource access in Directed Bigraphs

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Abstract: We study *directed bigraph with negative ports*, a bigraphical framework for representing models for distributed, concurrent and ubiquitous computing. With respect to previous versions, we add the possibility that components may *govern* the access to resources, like (web) servers control requests from clients. This framework encompasses many common computational aspects, such as name or channel creation, references, client/server connections, localities, etc, still allowing to derive systematically labelled transition systems whose bisimilarities are congruences.

In order to illustrate the expressivity of this framework, we give the encodings of client/server communications through firewalls, of (compositional) Petri nets and of chemical reactions.

Keywords: Bigraphs, reactive systems, Petri nets, graph-based approaches to service-oriented applications.

1 Introduction

Bigraphical reactive systems (BRSs) are an emerging graphical framework proposed by Milner and others [Mil01, Mil06] as a unifying theory of process models for distributed, concurrent and ubiquitous computing. A bigraphical reactive system consists of a category of *bigraphs* (usually generated over a given *signature of controls*) and a set of *reaction rules*. Bigraphs can be seen as representations of the possible configurations of the system, and the reaction rules specify how these configuration can evolve, i.e., the reaction relation between bigraphs. Often, bigraphs represent terms up-to structural congruence and reaction rules represent term rewrite rules.

Many process calculi have successfully represented as bigraphical reactive systems: λ-calculus [Mil07], CCS [Mil06], π-calculus [BS06, JM04], Mobile Ambients [Jen08], Homer [BH06], Fusion [GM07c], Petri nets [LM06], and context-aware systems [BDE$^+$06]. The advantage of using bigraphical reactive systems is that they provide powerful general results for deriving a labelled transition system *automatically* from the reaction rules, via the so-called *IPO construction*. Notably, the bisimulation on this transition system is always a congruence; thus, bigraphical reactive systems provide general tools for compositional reasoning about concurrent, distributed systems.

Bigraphs are the key structures supporting these results. A bigraph is a set of nodes (the *controls*), endowed with two independent graph structures, the *place graph* and the *link graph* (Figure 1). The place graph is a tree over the nodes, representing the spatial arrangement (i.e., nesting) of the various components of the system. The link graph represents the communication connections between the components, possibly traversing the place structure. A bigraph may be "not ground", in the sense that it may have one or more "holes", or *sites* (the gray boxes) to

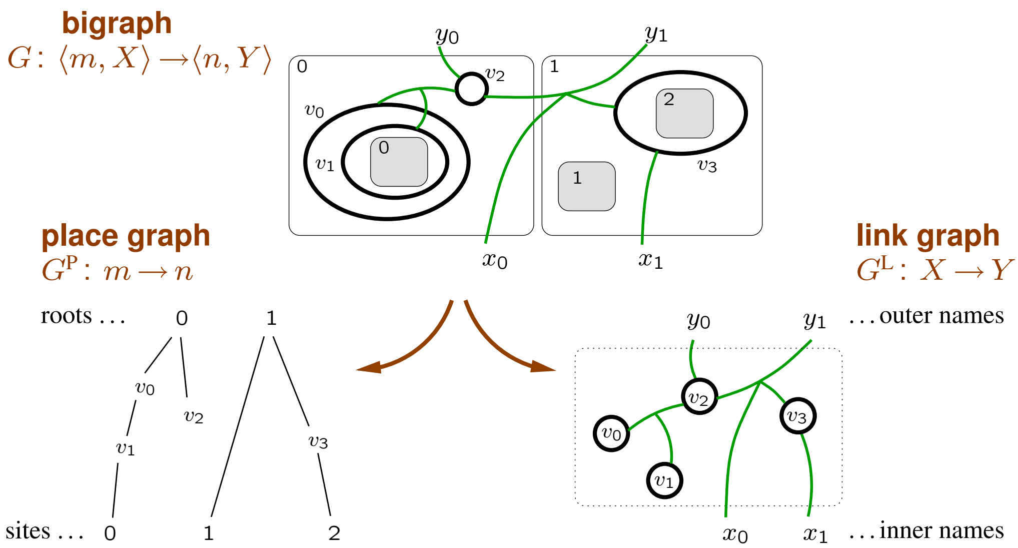


Figure 1: Example of pure bigraph (from [Mil06]).

be instantiated; these holes are specific leaves of the place graph, where other bigraphs can be grafted, respecting the connection links. This operation gives rise to a notion of composition between bigraphs, and hence to a categorical structure.

In Milner's "pure bigraphs" [Mil06], connections are represented by hyper-arcs between nodes (Figure 1). This model has been successfully used to represent many calculi, such as CCS, and (with a small variant) λ-calculus, π-calculus. Nevertheless, other calculi, such as Fusion [PV98], seem to escape this framework. Aiming to a more expressive framework, in previous work [GM07b, GM07c], we have introduced *directed bigraphs*. Pure and directed bigraphs differ only on the link structure: in the directed variant, we distinguish "edges" from "connections". Intuitively, edges represent *(delocalized) resources*, or *knowledge tokens*, which can be *accessed* by controls. Arcs are arrows from ports of controls to edges (possibly through names on the interfaces of bigraphs); moreover, in the version considered in the present paper, we allow arcs to point to other control's ports (Figure 2). Outward ports on a control represent the capability of the control to access to (external) resources; insted, inward ports represent the capability of the control to "stop" or "govern" other node's requests. The presence of both kinds of capabilities is common in distributed scenarios, such as client/server communications, firewalls, web services etc; for instance a system may ask to access to some data, but this attempt may be blocked, checked and possibly redirected by a guarding mechanism. Moreover, controls with inward ports can represent *localized* resources, that is, resources with a position within the place hierarchy; this cannot be represented easily by edges, which do not appear in the place graph.

Notably, these extended have RPO and IPO constructions, there is a notion of normal form, and a sound a complete axiomatization can be given. Therefore, these bigraphs can be conveniently used for building wide reaction systems from which we can synthesize labelled transition systems via the IPO construction, and whose bisimilarity is still a congruence.

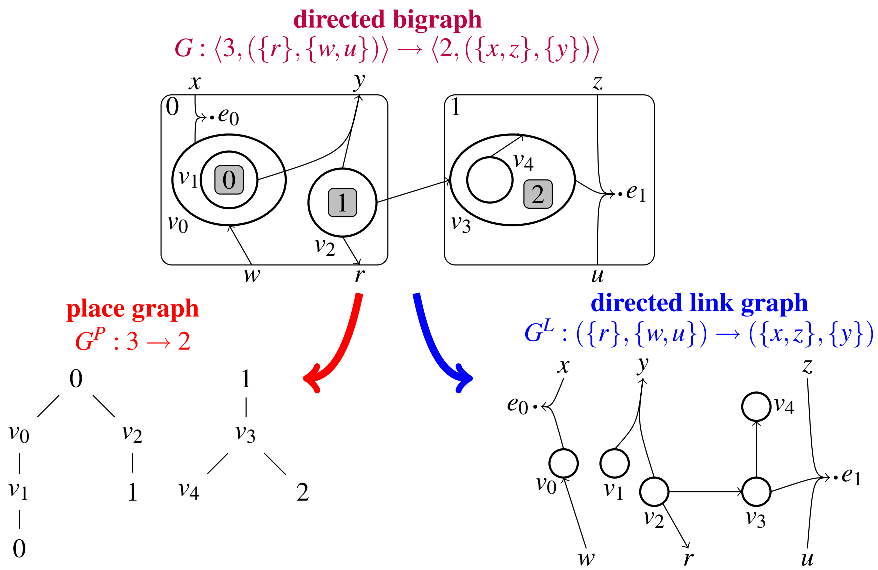


Figure 2: An example of directed bigraph, with negative ports.

Due to lack of space, in this paper we can only skim over these theoretical results; we prefer to focus on some important applications of this framework. In Section 2 we give the basic definitions about directed bigraphs; constructions of RPOs and IPOs are in Appendix A. In Sections 3 we present the elementary bigraphs, which are enough to generate all possible bigraphs; a notion of normal form and a complete axiomatization are in Appendix B. Section 4 is devoted to example applications, highlighting the expressive power of this framework: we show how distributed services and protocols can be represented, by describing a three-tier architecture with a firewall; we will present an encoding of Petri nets, and finally we apply this framework to the representation of chemical reactions. Conclusions and direction for future work are in Section 6.

2 Directed bigraphs over polarized signatures

In this section we introduce directed bigraphs, with inward ("negative") ports on controls, extending [GM07b]. Following previous developments about pure and directed bigraphs, we work in *supported monoidal precategories*; we refer to [JM04, §3] for an introduction.

A *polarized signature* is a signature of controls, which may have two kind of ports: *negative* and *positive*. Let $\mathscr{K}$ be a polarized signature; we denote with $ar^n, ar^p : \mathscr{K} \to \mathbb{N}$ the arity functions of the negative and positive ports, respectively. Thus, for $k \in \mathscr{K}$, the arity function is $ar(k) \triangleq (ar^n(k), ar^p(k))$. A control k is *positive* if it has only positive ports (i.e., $ar^n(k) = 0$); it is *negative* if it has only negative ports (i.e., $ar^p(k) = 0$).

Definition 1 A *polarized interface* X is a pair of sets of names $X = (X^-, X^+)$; the two components are called *downward* and *upward* interfaces, respectively.

A *directed link graph* $A : X \to Y$ is $A = (V, E, ctrl, link)$ where X, Y are the *inner* and *outer* interfaces, V is the set of *nodes*, E is the set of *edges*, $ctrl : V \to \mathscr{K}$ is the *control map*, and $link : \mathsf{Pnt}(A) \to \mathsf{Lnk}(A)$ is the *link map*, where *ports*, *points* and *links* of A are defined as follows:

$$\mathsf{Prt}^n(A) \triangleq \sum_{v \in V} ar^n(ctrl(v)) \qquad \mathsf{Prt}^p(A) \triangleq \sum_{v \in V} ar^p(ctrl(v)) \qquad \mathsf{Prt}(A) \triangleq \mathsf{Prt}^n(A) \cup \mathsf{Prt}^p(A)$$

$$\mathsf{Pnt}(A) \triangleq X^+ \uplus Y^- \uplus \mathsf{Prt}^p(A) \qquad\qquad \mathsf{Lnk}(A) \triangleq X^- \uplus Y^+ \uplus \mathsf{Prt}^n(A) \uplus E$$

The link map cannot connect downward and upward names of the same interface, i.e., the following condition must hold: $(link(X^+) \cap X^-) \cup (link(Y^-) \cap Y^+) = \emptyset$; moreover the link map cannot connect positive and negative ports of the same node.

Directed link graphs are graphically depicted much like ordinary link graphs, with the difference that edges are explicit objects, and not hyper-arcs connecting points and names; points and names are associated to links (that is edges or negative ports) or other names by (simple, non hyper) directed arcs. An example are given in Figure 2. This notation aims to make explicit the "resource request flow": positive ports and names in the interfaces can be associated either to internal or to external resources. In the first case, positive ports and names are connected to an edge or a negative port; these names are "inward" because they offer to the context the access to an internal resource. In the second case, the positive ports and names are connected to an "outward" name, which is waiting to be plugged by the context into a resource.

In the following, by "signature", "interface" and "link graphs" we will intend "polarized signature", "polarized interface" and "directed link graphs" respectively, unless otherwise noted.

Definition 2 The precategory of *directed link graphs* has polarized interfaces as objects, and directed link graphs as morphisms.

Given two directed link graphs $A_i = (V_i, E_i, ctrl_i, link_i) : X_i \to X_{i+1}$ $(i = 0, 1)$, the composition $A_1 \circ A_0 : X_0 \to X_2$ is defined when the two link graphs have disjoint nodes and edges. In this case, $A_1 \circ A_0 \triangleq (V, E, ctrl, link)$, where $V \triangleq V_0 \uplus V_1$, $ctrl \triangleq ctrl_0 \uplus ctrl_1$, $E \triangleq E_0 \uplus E_1$ and

$$link : X_0^+ \uplus X_2^- \uplus \mathsf{Prt}^p(A_0) \uplus \mathsf{Prt}^p(A_1) \to X_0^- \uplus X_2^+ \uplus E \uplus \mathsf{Prt}^n(A_0) \uplus \mathsf{Prt}^n(A_1)$$

is defined as follows:

$$link(p) \triangleq \begin{cases} link_0(p) & \text{if } p \in X_0^+ \uplus \mathsf{Prt}^p(A_0) \text{ and } link_0(p) \in X_0^- \uplus E_0 \uplus \mathsf{Prt}^n(A_0) \\ link_1(x) & \text{if } p \in X_0^+ \uplus \mathsf{Prt}^p(A_0) \text{ and } link_0(p) = x \in X_1^+ \\ link_1(p) & \text{if } p \in X_2^- \uplus \mathsf{Prt}^p(A_1) \text{ and } link_1(p) \in X_2^+ \uplus E_1 \uplus \mathsf{Prt}^n(A_1) \\ link_0(x) & \text{if } p \in X_2^- \uplus \mathsf{Prt}^p(A_1) \text{ and } link_1(p) = x \in X_1^-. \end{cases}$$

The identity link graph of X is $id_X \triangleq (\emptyset, \emptyset, \emptyset_{\mathscr{K}}, id_{X^-} \cup id_{X^+}) : X \to X$.

It is easy to check that composition is associative, and that given a link graph $A : X \to Y$, the compositions $A \circ id_X$ and $id_Y \circ A$ are defined and equal to A.

Definition 1 forbids connections between names of the same interface in order to avoid undefined link maps after compositions. Similarly, links between ports on the same node are forbidden, because these graphs cannot be obtained by composing an "unlinked" node and a context.

It is easy to see that the precategory ′DLG is self-dual, that is ′DLG $\cong$ ′DLG^{op}.

The notions of openness, closeness, leanness, etc. defined in [GM07b] can be easily extended to the new framework, considering negative ports as a new kind of resources. Moreover, the definition of tensor product can be derived extending to negative ports the one given in [GM07b],

Finally, we can define the *(extended) directed bigraphs* as the composition of standard place graphs (see [JM04, §7] for definitions) and directed link graphs.

Definition 3 A *directed bigraph* with signature $\mathscr{K}$ is $G = (V, E, ctrl, prnt, link) : I \to J$, where $I = \langle m, X \rangle$ and $J = \langle n, Y \rangle$ are its inner and outer interfaces respectively. An interface is composed by a *width* (a finite ordinal) and by a pair of finite sets of names. V and E are the sets of nodes and edges respectively, and *prnt*, *ctrl* and *link* are the parent, control and link maps, such that $G^P \triangleq (V, ctrl, prnt) : m \to n$ is a place graph and $G^L \triangleq (V, E, ctrl, link) : X \to Y$ is a directed link graph.

We denote G as combination of G^P and G^L by $G = \langle G^P, G^L \rangle$. In this notation, a place graph and a (directed) link graph can be put together iff they have the same sets of nodes.

Definition 4 The precategory ′DBIG of directed bigraph with signature $\mathscr{K}$ has interfaces $I = \langle m, X \rangle$ as objects and directed bigraphs $G = \langle G^P, G^L \rangle : I \to J$ as morphisms. If $H : J \to K$ is another directed bigraph with sets of nodes and edges disjoint from the respectively ones of G, then their composition is defined by composing their components, i.e.:

$$H \circ G \triangleq \langle H^P \circ G^P, H^L \circ G^L \rangle : I \to K.$$

The identity directed bigraph of $I = \langle m, X \rangle$ is $\langle id_m, id_X \rangle : I \to I$.

Analogously, the tensor product of two bigraphs can be defined tensoring their components.

It is easy to check that for every signature $\mathscr{K}$, the precategory ′DBIG is wide monoidal; the origin is $\varepsilon = \langle 0, (\emptyset, \emptyset) \rangle$ and the interface $\langle n, X \rangle$ has width n. Hence, ′DBIG can be used for applying the theory of *wide reaction systems* and *wide transition systems* as developed by Jensen and Milner; [JM04, §4, §5]. To this end, we need to show that ′DBIG has RPOs and IPOs. Since place graphs are as usual, it suffices to show that directed link graphs have RPOs and IPOs.

Theorem 1 *If a pair $\vec{A}$ of link graphs has a bound $\vec{D}$, there exists an RPO $(\vec{B}, B)$ for $\vec{A}$ to $\vec{D}$.*

As a consequence, ′DLG has IPOs too. See Appendix A for the direct constructions for RPOs and IPOs in directed bigraphs with negative ports, extending the construction given in [GM07b].

Actually, often we do not want to distinguish bigraphs differing only on the identity of nodes and edges. To this end, we introduce the category DBIG of *abstract directed bigraphs*, which is constructed from ′DBIG forgetting the identity of nodes and edges and any idle edge. More precisely, abstract bigraphs are bigraphs taken up-to an equivalence $\approx$ (see [JM04] for details).

Definition 5 Two concrete directed bigraphs G and H are *lean-support equivalent*, written $G \approx H$, if there exists an iso between their nodes and edges sets after removing any idle edges.

The category DBIG of abstract directed bigraphs has the same objects as ′DBIG, and its arrows are lean-support equivalence classes of directed bigraphs.

3 Algebra and Axiomatization

As for directed bigraphs, also in the case of polarized signature it is possible to give a sound and complete axiomatization. In this section, due to lack of space, we describe only the main classes of bigraphs and the elementary bigraphs which can generate all bigraphs according to a well-defined normal form. See Appendix B for the definition of normal form and the normalization theorem. We refer the reader to [GM07a] for an accurate presentation of the notation used here.

First, we introduce two distinct and complementary subclasses of bigraphs: *wirings* and *discrete bigraphs*. that are strongly used in defining the normal form and the axiomatization.

Definition 6 A *wiring* is a bigraph whose interfaces have zero width (and hence has no nodes). The wirings ω are generated by the composition or tensor product of three elements: substitutions $\sigma : (\emptyset, X^+) \to (\emptyset, Y^+)$, fusions $\delta : (Y^-, \emptyset) \to (X^-, \emptyset)$, and closures $\rceil^x_y : (\emptyset, y) \to (x, \emptyset)$.

Definition 7 An interface is *prime* if its width is 1. Often we abbreviate a prime interface $\langle 1, (X^-, X^+)\rangle$ with $\langle (X^-, X^+)\rangle$, in particular $1 = \langle (\emptyset, \emptyset)\rangle$. A prime bigraph $P : \langle m, (Y^-, Y^+)\rangle \to \langle (X^-, X^+)\rangle$ has a prime outer interface and the names in Y^+, X^- are linked to negative ports of P.

An important prime bigraph is $merge_m : m \to 1$, it has no nodes and maps m sites to one root.

Definition 8 A bigraph is *discrete* if it has no edges and every open link has exactly one point.

The discreteness is well-behaved, and preserved by composition and tensor. It is easy to see that discrete bigraphs form a monoidal sub-precategory of ′DBIG.

Definition 9 Let K be any non atomic control with arity (k^-, k^+), let $\vec{x}^-, \vec{x}^+$ be two sequences of distinct names, and let $\vec{Y}^+, \vec{Y}^-$ be two sequences of (possibly empty) sets of distinct names, such that: $|\vec{x}^-| + |\vec{x}^+| = k^+$ and $|\vec{Y}^-| = |\vec{Y}^+| = k^-$. For a K-node v, we define the discrete *ion*

$$K(v,l) : \langle (\vec{x}^-, \vec{Y}^+)\rangle \to \langle (\vec{Y}^-, \vec{x}^+)\rangle$$

as the bigraph with exactly a node v and l is a pair of maps: an iso map $l^p : \vec{x}^- \cup \vec{x}^+ \to \mathsf{Prt}^p(v)$ describing the linking among positive ports and names in $\vec{x}^-$ or $\vec{x}^+$, and another iso map $l^n : \vec{Y}^- \cup \vec{Y}^+ \to \mathsf{Prt}^n(v)$ describing the linking among negative ports and sets of upward inner names (in $\vec{Y}^+$) and sets of downward outer names (in $\vec{Y}^-$). We omit v when it can be understood.

For a prime discrete bigraph P with outer names in (Z^-, Z^+), we define a discrete *molecule* as:

$$(K(l) \otimes id_{(Z^- \setminus \vec{x}^-, Z^+ \setminus \vec{Y}^+)}) \circ P.$$

If K is atomic, we define the discrete *atom*, as an ion without sites:

$$K(l) : (\vec{x}^-, \vec{Y}^+) \to \langle (\vec{Y}^-, \vec{x}^+)\rangle.$$

An arbitrary (non-discrete) ion, molecule or atom is formed by the composition of $\omega \otimes id_1$ with a discrete one. Often we omit $\ldots \otimes id_I$ in the compositions, when there is no ambiguity.

Figure 3 shows the *algebraic signature*, that is a set of elementary bigraphs able to define any other bigraph using composition and tensor product. In Appendix C we list the definition of the *sharing products* that are the intuitive generalization of the ones defined in [GM07a].

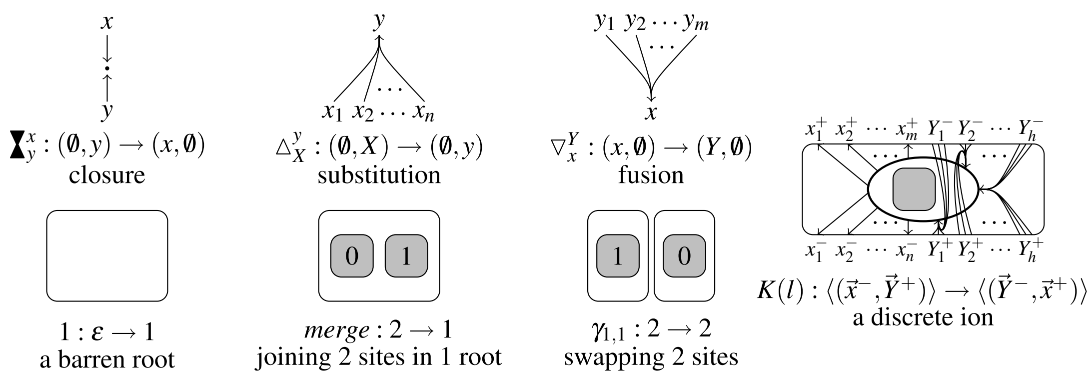


Figure 3: Elementary Bigraphs over polarized signatures.

4 Applications

4.1 Three-tier interaction with access control

As mentioned before, directed bigraphs over polarized signatures allow to represent resource access control, by means of negative ports. This is particularly useful for representing access policies between systems, possibly in different locations; the edges can represent access tokens (or keys), which are global (although known possibly to only some controls). An example and quite common scenario is a client-server connection, where the access to the server is subject to authentication; after the request has been accepted, the server can route it to a back-end service (e.g., a DBMS); see Figure 4. The security policy is implemented by the firewall control, which allows a query to reach the server only if the client knows the correct key (rule AUTH). The server routes the query to the correct back-end service using rules like ROUTE; finally the back-end service provides the data (rule GET). An example computation is shown in Figure 5.

4.2 Compositional Petri Nets

In this section we recall briefly what a Petri net is and we give an encoding of these nets as directed bigraphs; to this end it is preferable to work with sorted links, as in [LM06]. Notice that this encoding yields naturally a notion of composition between Petri nets.

Definition 10 A *place transition net* (*P/T net*) is a 5-tuple (P,T,F,M_i) $(P \cap T = \emptyset)$, where:

- P is the set of *places;* T is the set of *transitions;*
- F is the multiset of *arcs,* linking places to transitions and vice versa: $F \triangleq \langle (P \times T) \cup (T \times P), f : (P \times T) \cup (T \times P) \to \mathbb{N} \rangle$, with the constrain $\forall t \in T.\ \exists p,q \in P.\ (p,t) \in F \land (t,q) \in F$;
- $M : P \to \mathbb{N}$ is a *marking,* giving to each place a number of tokens, a place p is *marked* by M if $M(p) > 0$ and *unmarked* if $M(p) = 0$; M_i is the *initial marking.*

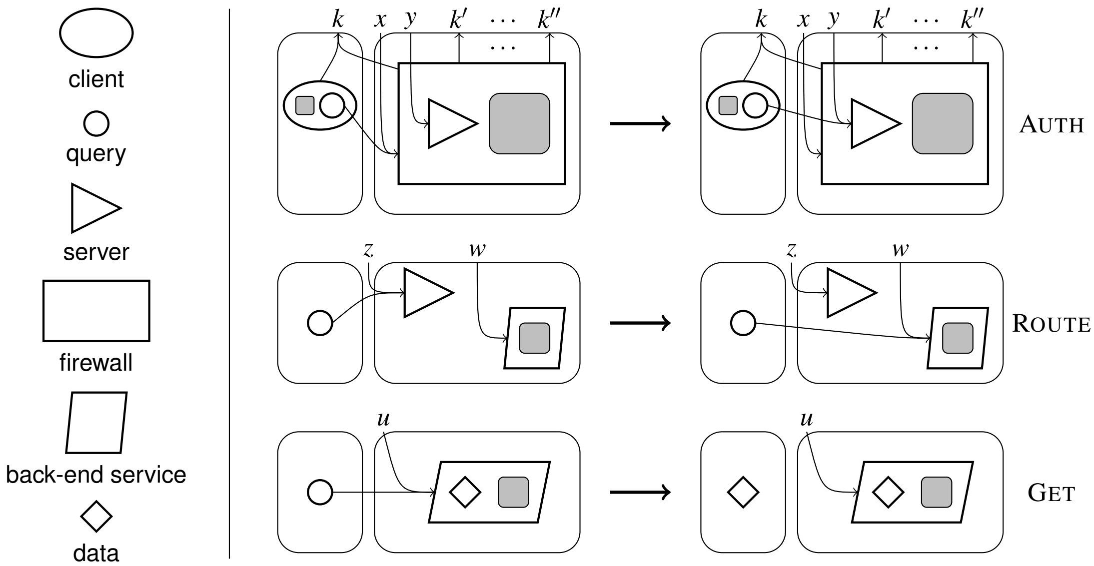


Figure 4: Signatures and rules for three-tier architecture services through a firewall.

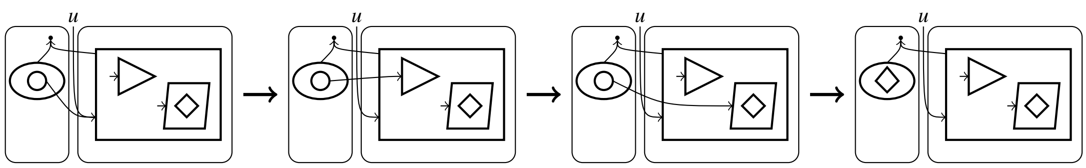


Figure 5: An example of client-server interaction through a firewall.

We define ${}^\bullet t \triangleq \{p \mid (p,t) \in F\}$ to be the *pre-multiset* of the transition t, and $t^\bullet \triangleq \{p \mid (t,p) \in F\}$ the *post-multiset* of the transition t.

A transition t is *enabled* by a marking M if M marks every place in ${}^\bullet t$; a transition *fires* from a marking M to a marking M', written $M \xrightarrow{t} M'$, iff for all $p \in P : M'(p) = M(p) - \sharp({}^\bullet p) + \sharp(p^\bullet)$, where $\sharp({}^\bullet p)$ and $\sharp(p^\bullet)$ are the number of occurrences of p in ${}^\bullet t$, $t^\bullet$, respectively.

Notice that we allow multiple connections between a place and a transition, that is analogous to assign a weight to an arc representing the token that have to be consumed to fire the reaction.

Definition 11 Let $N = (P,T,F,M)$ and $N' = (P',T',F',M')$ be two P/T nets, we say that N and N' are *isomorphic*, if there exist two bijections $\alpha : P \to P'$ and $\beta : T \to T'$, such that:

- $(p,t) \in F$ iff $(\alpha(p),\beta(t)) \in F'$;
- $(t,p) \in F$ iff $(\beta(t),\alpha(p)) \in F'$;
- $M = M' \circ \alpha$.

We recall, as defined in [LM06], the definition of link sorting.

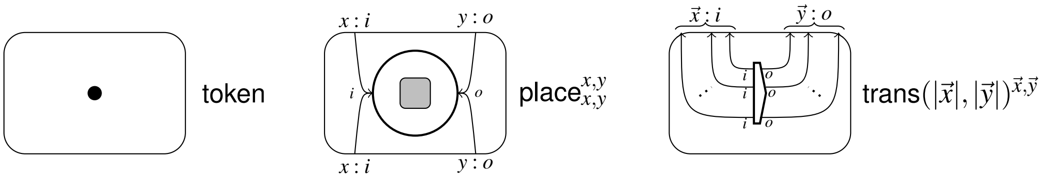


Figure 6: Signature for the encoding of compositional Petri nets.

Definition 12 A *link sorting* is a triple $\Sigma = (\Theta, \mathscr{K}, \Phi)$, where Φ is a set of sorts, and $\mathscr{K}$ is a sorted signature (that is, a signature enriched with a sort to ports of each control). Furthermore, each name in the interface (X^-, X^+) is given a sort, so the interfaces take the form $(\{x_1^- : \theta_1^-, \dots, x_n^- : \theta_n^-\}, \{x_1^+ : \theta_1^+, \dots, x_m^+ : \theta_m^+\})$. Finally, Φ is a rule on such enriched bigraphs, that is preserved by identities, composition and tensor product.

We denote the precategory and category of, respectively, concrete and abstract Σ-sorted directed bigraphs with $'\mathrm{DBIG}(\Sigma)$ and $\mathrm{DBIG}(\Sigma)$.

Definition 13 A *positive-negative sorting* $\Sigma = (\Theta, \mathscr{K}, \Phi)$ has sorts: $\Theta = \{\theta_1, \dots, \theta_n\}$. The signature $\mathscr{K}$ assigns sorts to ports arbitrarily. The unique Φ rule is: a point and a link (except of edges) can be connected if they are equally sorted.

In order to define an encoding for compositional Petri nets, we introduce a positive-negative sorting Σ_{petri}, having sort $\Theta_{petri} \triangleq \{i, o\}$ and sorted signature:

$$\mathscr{K}_{petri} \triangleq \{\mathsf{token} : (0,0),\ \mathsf{place} : (\{1:i, 1:o\}, 0),\ \mathsf{trans}(h,k) : (0, \{h:i, k:o\})\} \qquad \text{where } h,k > 0$$

where the controls token and trans are both atomic, while the control place is passive. Finally, the Φ rule ensures that the linking is allowed only among ports having the same sort. An example of use of this sorted signature is shown in Figure 6. The encoding function $[\![\cdot]\!]$ is defined as follows:

$$[\![(P,T,F,M)]\!] = merge_{(|P|+|T|)} \circ \left(id_{|P|} \curlyvee id_{(P\times\{i,o\},\emptyset)} \curlyvee \left(\curlyvee_{t\in T} trans(|^\bullet t|,\ |t^\bullet|)_{(^\bullet t\times\{i\},\ t^\bullet\times\{o\})} \right) \right) \circ$$
$$\left(\sum_{p\in P} place^{(p,i),\ (p,o)}_{(p,i),\ (p,o)} \circ (merge_{(|M(p)|+1)} \circ (\vartriangle^{\{(p,i),\ (p,o)\}} \otimes (\sum_{i=0}^{M(p)} token) \otimes 1)) \right).$$

where, with an abuse of notation, $trans(|^\bullet t|,\ |t^\bullet|)_{(^\bullet t\times\{i\},\ t^\bullet\times\{o\})}$ means that if in the multisets there are some repetitions of places then the ports of *trans* are linked to the same downward inner name (i.e., (p,i) or (p,o)), an alternative definition is to link every port of *trans* to a different downward inner name and then (eventually) "equate" these names using fusions.

Proposition 1 *Let N, N' be two P/T nets, N is isomorphic to N' iff $[\![N]\!] = [\![N']\!]$ up to iso.*

We have a different reaction rule for any pair (h,k) associated to the control trans, in Figure 7 we show the reaction rule for the pair $(3,2)$, that is a transition having 3 inputs and 2 outputs. Moreover, we allow multiple connections between places and transitions, as in Figure 8, and we can have transitions using some places as inputs and outputs, see Figure 9.

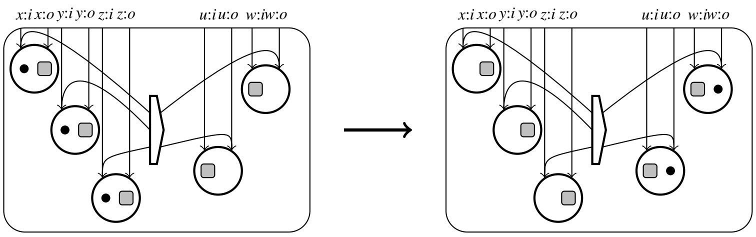


Figure 7: Example of reaction rule in the case of 3 input and 2 output places.

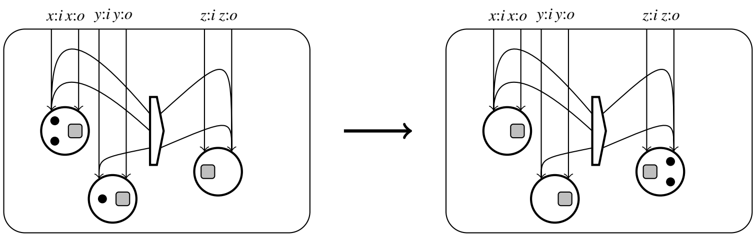


Figure 8: Example of reaction rule in the case of 2 input and 1 output places (with multiple arcs).

Now we can show that the given translation is adequate.

Theorem 2 *Let* (P,T,F,M_i) *be a P/T net,* $M \xrightarrow{t} M'$ *iff* $[\![(P,T,F,M)]\!] \longrightarrow [\![(P,T,F,M')]\!]$.

Proof. (⇒) Suppose $M \xrightarrow{t} M'$, so M enable the transition t, then there exists a trans-node in $[\![(P,T,F,M)]\!]$ encoding the transition t, and the corresponding place-node of ${}^{\bullet}t$ contain the necessary tokens to fire the transition (by translation of M), then we can apply the appropriate rule to perform the reaction reaching the configuration $[\![(P,T,F,M')]\!]$.

(⇐) If $[\![(P,T,F,M)]\!] \longrightarrow [\![(P,T,F,M')]\!]$, there exists a matching of a rule with a sub-bigraph of $[\![(P,T,F,M)]\!]$, in particular the matched nodes have a counter part into the P/T net (P,T,F,M), so the marking M enables a transition t (corresponding to the trans-node), and then $M \xrightarrow{t} M'$. □

An interesting future work is to study the bisimulation induced by the IPO LTS over these compositional Petri nets. We remark however, that this notion of composition is different from that in Open Petri nets, since in the latter the interfaces express also behavioural properties, while in the bigraphical encoding the interfaces express resource requests and offerings.

5 Chemical Reactions

A chemical reactions is a process describing the conversions of a chemical compositions. Always, the chemical changes caused by a reaction involve the motion of electrons in the forming or breaking of *chemical bonds*. For example, the *octet rule* says that atoms tend to gain, lose or share electrons so as to have eight electrons in their outer electron shell.

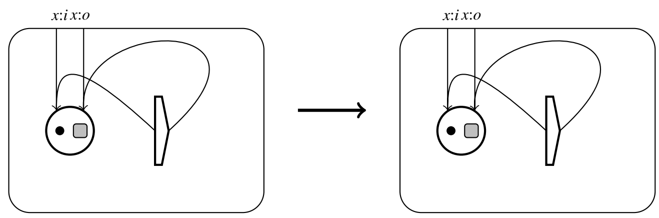


Figure 9: Example of reaction rule in the case of 1 place used as input and output.

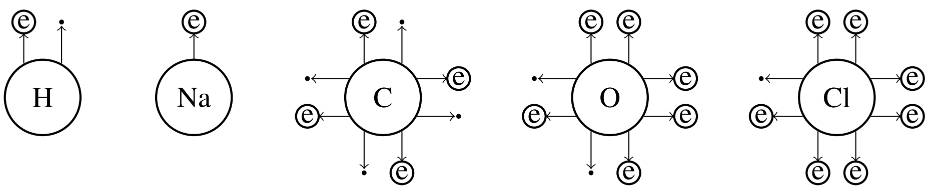


Figure 10: Example of atom encodings in directed link graphs.

In this section, we give an encoding of atoms into directed link graphs, as shown in Figure 10, inspired by the well-known *Lewis structures*. We describe the atoms as nodes, and those nodes have a number of positive ports equal to the number of valence electrons. Each of these ports are linked to an electron, represented as a node having a negative port (accepting incoming connections; for sake of simplicity we identify the node representing the electron with its port, that is, we do not force all incoming connections to be linked to a precise point of the node). Moreover, some nodes can have extra ports, that are initially linked to edges, hydrogen and oxygen can be two examples, the idea is that such a configuration describes the aim of the atom to "capture" electrons to complete its external shell; e.g. an oxygen atom has two missing electrons, so it tries to share these two electrons with a pair of hydrogen atoms forming the water molecule.

We apply this model describing the forming and breaking of bonds among atoms, here we deal with *strong bonds*, that is *covalent* and *ionic bonds*.

Some examples of covalent bonds are shown in Figure 11, the first shows how to hydrogen atoms can share their electron. The second one is well-know and describes the generation of a water molecule from two hydrogen atoms and an oxygen one: the oxygen shares two electrons: one with each hydrogen, in this way it gets the two missing electrons in its external orbit, conversely each hydrogen atom completes its orbit sharing an electron with the oxygen. The latter describes a more complicate situation, where the two carbon atoms (each needing four electron to complete its orbit) share two electron with the other carbon atom, and the remaining two missing electrons are provided by a pair of hydrogen.

In Figure 12, we show an example of ionic bond: given an atom of sodium and a chlorine one, it may happen (by octet rule) that the external electron of sodium is lost by the atom and "captured" by the chlorine, forming a sodium (positive) ion and a chlorine (negative) ion. These two ions attract each other by the electrostatic force caused by the electron exchange. Finally the

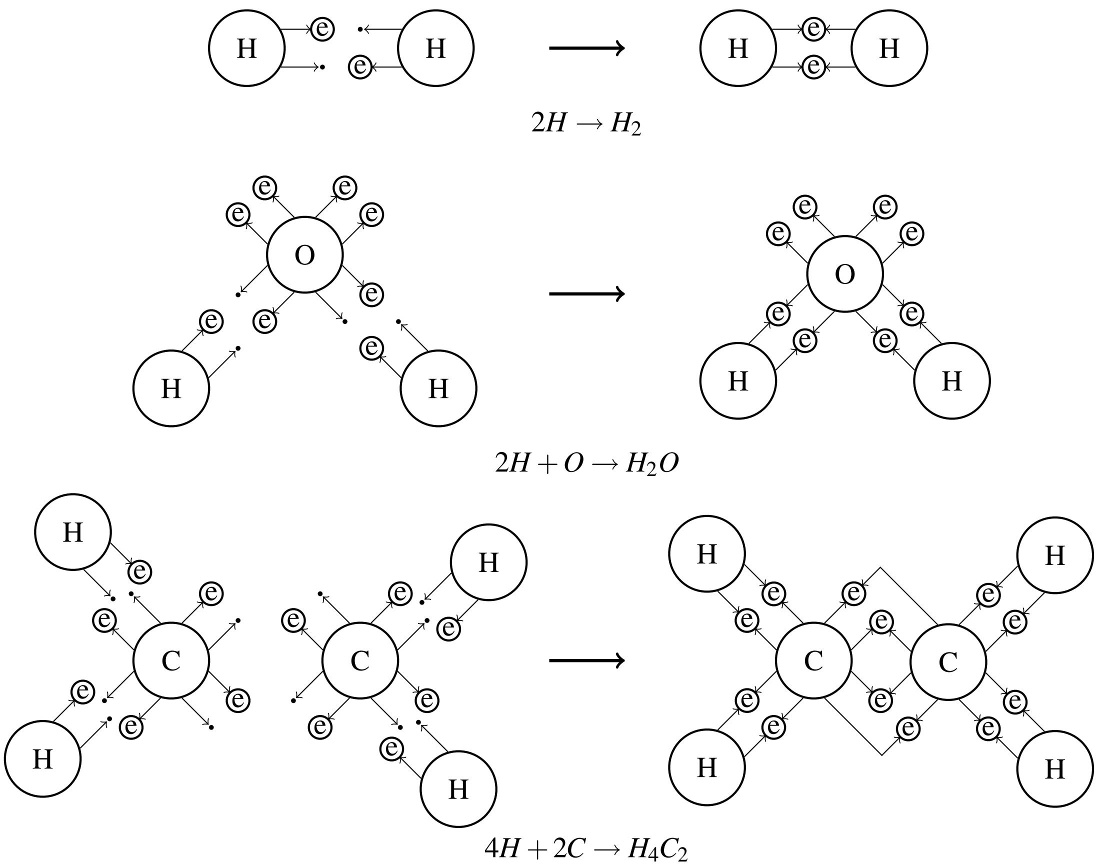


Figure 11: Example of covalent bonds among atoms.

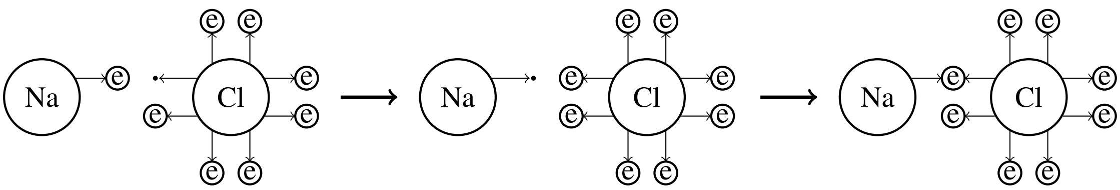
ions can be composed to form sodium-chloride molecule, that is the common salt.

An interesting future work concern to represent the *weak bonds*, i.e. *hydrogen bonds* and *van der Waals bonds*, using the same representation as much as possible.

6 Conclusions

In this paper, we have considered directed bigraphs over *polarized signatures*, a bigraphical model for concurrent, distributed system with resources and controls. The main difference with previous versions of bigraphs is the capability of nodes (i.e., systems) to ask for resource access (via the "positive ports") and to control other's requests, providing access to own resources (via the negative ports). These bigraphs have RPO and IPO constructions, thus allowing to derive systematically labelled transition systems from reactive systems, as in [JM03, GM07c]; notably the bisimilarities induced by these labelled transition systems are always congruences. These directed bigraphs admit also a notion of normal form, and a complete axiomatization.

We have exhibited the expressive power of this framework, by applying it some interesting cases: a three-tier interaction between client, server and back-end service through a firewall, the



$$Na + Cl \to Na^+ + Cl^- \to NaCl$$

Figure 12: Examples of ion bonds among atoms.

Petri nets, and chemical reactions. All these cases are faithfully encoded as directed bigraphs with polarized signatures (possibly with sorting).

An interesting future work is to develop properly the treatment of web service interactions, extending the ideas shown in Section 4.1. In particular, we would like to give a bigraphical semantics of some formal calculus for web services, such as SCC or CC-Pi [BBC+06, BM07].

Another future development is to use this kind of bigraphs as a general framework for systems biology. Some preliminary experiment about the representation of biochemical reactions, not shown in this paper due to lack of space, are promising: ions, electrons, chemical links can be represented as controls and arcs, and the place structure can be fruitfully used to represent nesting of chemical compounds. It would be interesting to encode in directed bigraphs some important formalism for systems biology, such as the κ-calculus [DL04]. Along this line, also the possibility of adding quantitative aspects (i.e., reaction rates) sounds very promising.

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A RPO and IPO constructions

A.1 Construction of relative pushouts and pullbacks

We first give an idea of how the construction works. Suppose $D_0 : X_0 \to Z$, $D_1 : X_1 \to Z$ is a bound for a span $A_0 : W \to X_0, A_1 : W \to X_1$ and we wish to construct the RPO $(B_0 : X_0 \to \hat{X}, B_1 : X_1 \to \hat{X}, B : \hat{X} \to Z)$. In the following we will denote a pair (A_0, A_1) by $\vec{A}$ and the link map of A simply by A. To form the pair $\vec{B}$ we truncate $\vec{D}$ by removing all the edges, nodes and ports not present in $\vec{A}$. Then in the outer interface of $\vec{B}$, we create an outer name for each point unlinked by the truncation: the downward names connected to the same link (name, edge or negative port) must be "bound together", i.e. we must consider all the possible ways to associate a downward name of A_0 with one of A_1 and vice versa; further we must equate an upward name of A_0 with one of A_1 if they are both connected to a point shared between A_0 and A_1. Formally:

Construction 14 A relative pushout $(\vec{B} : \vec{X} \to \hat{X}, B : \hat{X} \to Z)$, for a pair $\vec{A} : W \to \vec{X}$ of link graphs relative to a bound $\vec{D} : \vec{X} \to Z$, will be built in three stages. Since RPOs are preserved by isomorphisms, we can assume the components of X_0 and X_1 disjoint.

nodes and edges If V_i are the nodes of A_i $(i = 0,1)$, then the nodes of D_i are $V_{D_i} = (V_{\bar{i}} \setminus V_i) \uplus V_2$ for some V_2. Define the nodes of B_i and B to be $V_{B_i} \triangleq V_{\bar{i}} \setminus V_i$ $(i = 0,1)$ and $V_B \triangleq V_2$. Edges E_i and ports P_i^p, P_i^n of A_i are treated analogously.

interface Construct the shared codomain $\hat{X} = (\hat{X}^-, \hat{X}^+)$ of $\vec{B}$ as follows: first we define the names in each $X_i = (X_i^-, X_i^+)$, for $i = 0,1$, that must be mapped into $\hat{X} = (\hat{X}^-, \hat{X}^+)$:

$$X_i'^- \triangleq \{x \in X_i^- \mid \exists y \in X_{\bar{i}}^- \text{ s.t. } A_i(x) = A_{\bar{i}}(y) \text{ or } A_i(x) \in (E_i \setminus E_{\bar{i}}) \uplus (P_i^n \setminus P_{\bar{i}}^n)\}$$
$$X_i'^+ \triangleq \{x \in X_i^+ \mid D_i(x) \in (E_2 \uplus P_2^n \uplus Z^+)\}.$$

Let $\mathsf{Res} \triangleq W^- \uplus (E_0 \cap E_1) \uplus (P_0^n \cap P_1^n)$. We define for each $l \in \mathsf{Res}$ the set of names in $X_i'^-$ linked to l:

$$X_i'^-(l) \triangleq \{x \in X_i'^- \mid A_i(x) = l\} \quad (i = 0,1).$$

Now we must "bind together" names connected to the same link, so we create all the possible pairs between a name in $X_0'^-$ and a name in $X_1'^-$. Further we must add to $\hat{X}^-$ all the names in $X_i'^-$ "not associable" to any name of $X_{\bar{i}}'^-$. Then the set of downward names of $\vec{B}$ is:

$$\hat{X}^- \triangleq \bigcup_{l \in \mathsf{Res}} X_0'^-(l) \times X_1'^-(l) \cup \sum_{i \in \{0,1\}} \bigcup_{e \in (E_i \setminus E_{\bar{i}}) \uplus (P_i^n \setminus P_{\bar{i}}^n)} X_i'^-(e).$$

Next, on the disjoint sum $X_0'^+ + X_1'^+$, define $\cong$ to be the smallest equivalence for which $(0, x_0) \cong (1, x_1)$ iff there exists $p \in W^+ \uplus (P_0^p \cap P_1^p)$ such that $A_0(p) = x_0$ and $A_1(p) = x_1$. Then define:

$$\hat{X}^+ \triangleq (X_0'^+ + X_1'^+)/_{\cong}.$$

For each $x \in X_i'^+$ we denote the equivalence class of (i, x) by $\widehat{i,x}$.

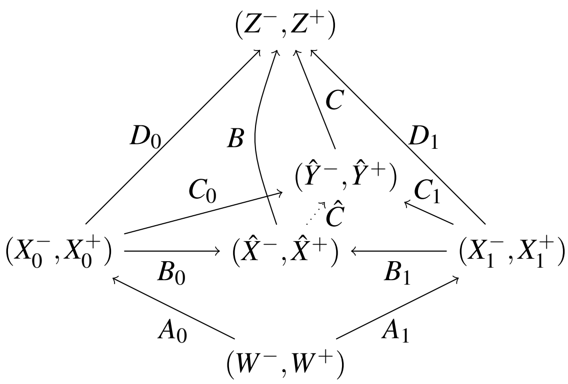

Figure 13: Construction of the unique arrow form the RPO to any other candidate.

links Define the link maps of B_i as follows:

$$\text{for } x \in X_i^+ : \qquad B_i(x) \triangleq \begin{cases} D_i(x) & \text{if } x \in (X_i^+ \setminus X_i'^+) \\ \widehat{i,x} & \text{if } x \in X_i'^+; \end{cases}$$

$$\text{for } p \in P_{\bar{i}}^p \setminus P_i^p : \qquad B_i(p) \triangleq \begin{cases} D_i(p) & \text{if } A_{\bar{i}}(p) \notin X_{\bar{i}}^+ \\ \widehat{\bar{i},x} & \text{if } A_{\bar{i}}(p) = x \in X_{\bar{i}}^+; \end{cases}$$

$$\text{for } \hat{x} \in \hat{X}^- : \qquad B_i(\hat{x}) \triangleq \begin{cases} x & \text{if } \hat{x} = (x,y) \text{ and } i = 0 \\ y & \text{if } \hat{x} = (x,y) \text{ and } i = 1 \\ \hat{x} & \text{if } \hat{x} \in (\hat{X}^- \cap X_i^-) \\ A_{\bar{i}}(\hat{x}) & \text{if } \hat{x} \in (\hat{X}^- \cap X_{\bar{i}}^-). \end{cases}$$

Finally we define the link map of B:

$$\text{for } \hat{x} \in \hat{X}^+ : \qquad B(\hat{x}) \triangleq D_i(x) \text{ where } \hat{x} = \widehat{i,x} \text{ and } x \in X_i^+;$$

$$\text{for } p \in P_2^p \uplus Z^- : \qquad B(p) \triangleq \begin{cases} D_i(p) & \text{if } D_i(p) \in (E_2 \uplus P_2^n \uplus Z^+) \\ D_{\bar{i}}(p) & \text{if } D_i(p) \in (E_{\bar{i}} \setminus E_i) \uplus (P_{\bar{i}}^n \setminus P_i^n) \\ D_i(p) & \text{if } D_{\bar{i}}(p) \in (E_i \setminus E_{\bar{i}}) \uplus (P_i^n \setminus P_{\bar{i}}^n) \\ (x,y) & \text{if } D_0(p) = x \in X_0^- \text{ and } D_1(p) = y \in X_1^-. \end{cases}$$

Theorem 3 *In* 'DLG, *whenever a pair $\vec{A}$ of link graphs has a bound $\vec{D}$, there exists an RPO $(\vec{B}, B)$ for $\vec{A}$ to $\vec{D}$, and Construction 14 yields such an RPO.*

Proof. The proof is in two parts. First we have to check that $(\vec{B}, B)$ is an RPO candidate; this is done by long and tedious calculations. Next, for any other candidate $(\vec{C}, C)$, we have to construct the unique arrow $\hat{C}$ such that the diagram (in Figure 13) commutes. This link graph $\hat{C}$ can be constructed as follows: let be V_C the nodes of C, for $i = 0,1$ the set of nodes of C_i is $V_{C_i} \triangleq (V_{\bar{i}} \setminus V_i) \uplus V_3$, where V_3 is such that $V_2 = V_3 \uplus V_C$; edges E_{C_i} and ports P_{C_i} of C_i are defined analogously. Then $\hat{C}$ has V_3, E_3 and P_3 as sets of nodes, edges and ports respectively. Its link map is defined as follows:

$$\text{for } \widehat{j,x} \in \hat{X}^+ : \qquad \hat{C}(\widehat{j,x}) \triangleq C_j(x);$$

$$\text{for } p \in P_3^p \uplus \hat{Y}^- : \qquad \hat{C}(p) \triangleq \begin{cases} C_i(p) & \text{if } C_i(p) \in (E_3 \uplus P_3^n \uplus \hat{Y}^+) \\ C_0(p) & \text{if } C_0(p) \in (\hat{X}^- \cap X_0^-) \\ C_1(p) & \text{if } C_1(p) \in (\hat{X}^- \cap X_1^-) \\ (x,y) & \text{if } C_0(p) = x \in X_0^- \text{ and } C_1(p) = x \in X_1^- \end{cases}$$

□

As an immediate consequence, we can calculate RPBs as well.

Corollary 1 *In* $'$DLG, *whenever a pair* $\vec{D} : \vec{X} \to W$ *of link graphs has a co-bound* $\vec{A} : Z \to \vec{X}$*, there exists an RPB* $(\vec{B} : \hat{X} \to \vec{X}, B : Z \to \hat{X})$ *for* $\vec{A}$ *to* $\vec{D}$*, and Construction 14 can be used for calculating such an RPB.*

Proof. Consider the pair $\overline{\vec{D}} : \overline{W} \to \overline{\vec{X}}$, which is in $'$DLG since $'$DLG is self-dual; this pair has the bound $\overline{\vec{A}} : \overline{\vec{X}} \to \overline{Z}$, and hence, for Theorem 3, Construction 14 yields an RPO $(\vec{C} : \overline{\vec{X}} \to \overline{\hat{X}}, C : \overline{\hat{X}} \to \overline{Z})$. Then, take $\vec{B} \triangleq \overline{\vec{C}}$ and $B \triangleq \overline{C}$. □

A.2 Construction of idem-relative pushouts

We now proceed to characterise all the IPOs for a given pair $\vec{A} : W \to \vec{X}$ of link graphs. The first step is to establish consistency conditions.

Definition 15 We define four *consistency conditions* on a pair $\vec{A} : W \to \vec{X}$ of link graphs.

CDL0 $ctrl_0(v) = ctrl_1(v)$ if $v \in V_0 \cap V_1$;

CDL1 if $p \in P_0^p \cap P_1^p$ and $A_i(p) \in W^- \uplus (E_0 \cap E_1) \uplus (P_0^n \cap P_1^n)$, then $A_{\bar{i}}(p) = A_i(p)$;

CDL2 if $p_2 \in P_0^p \cap P_1^p$ and $A_i(p_2) \in (E_i \setminus E_{\bar{i}}) \uplus (P_i^n \setminus P_{\bar{i}}^n)$, then $A_{\bar{i}}(p_2) = x_{\bar{i}}$ for some $x_{\bar{i}} \in X_{\bar{i}}^+$, and further if $A_{\bar{i}}(p) = A_{\bar{i}}(p_2)$ then $p \in W^+ \uplus (P_0^p \cap P_1^p)$ and $A_i(p) = A_i(p_2)$, or $p \in (P_{\bar{i}}^p \setminus P_i^p)$ and exists $x_i \in X_i^-$ such that $A_i(x_i) = A_i(p_2)$;

CDL3 for each $p \in P_i^p \setminus P_{\bar{i}}^p$ such that $A_i(p) \in W^- \uplus (E_0 \cap E_1) \uplus (P_0^n \cap P_1^n)$, then exists $x_{\bar{i}} \in X_{\bar{i}}^-$ such that $A_{\bar{i}}(x_{\bar{i}}) = A_i(p)$.

Informally, CDL1 says that if a shared point p in A_i is linked to a shared link l, then in $A_{\bar{i}}$ the shared point p must be linked to the same l. CDL2 says that if the link of a shared point p_2 in A_i is closed and unshared, then its link in $A_{\bar{i}}$ must be an outer upward name, further any peer p of p_2 in $A_{\bar{i}}$ must also be its peer in A_i, or if p is not shared, then in A_i there exists an outer downward name linked to the unshared edge of p_2. Finally, CDL3 says that if an unshared point in A_i is linked to a shared link, then in $A_{\bar{i}}$ there is an outer downward name linked to the shared link.

Proposition 2 *If a pair of link graphs $\vec{A}$ has a bound, then the consistency conditions hold.*

Now, assuming the consistency conditions of Definition 15, we shall construct a non-empty family of IPOs for $\vec{A}$ denoted by $IPO(\vec{A})$.

Construction 16 Assume the consistency conditions for the pair $\vec{A} : W \to \vec{X}$ of link graphs. We define $\vec{C} : \vec{X} \to Y$ an IPO for $\vec{A}$ as follows:

nodes and edges Define the nodes of C_i to be $V_{C_i} \triangleq V_{\bar{i}} \setminus V_i$. Edges and ports of C_i are defined analogously.

interface For $i = 0,1$ choose any subset L_i^+ of idle names in X_i^+. Define

$$\tilde{P}_i^p \triangleq \{p \in P_i^p \setminus P_{\bar{i}}^p \mid A_i(p) \in X_i^+ \text{ and } \nexists p' \in W^+ \uplus (P_i^p \cap P_{\bar{i}}^p) \text{ s.t. } A_i(p) = A_i(p')\}$$

and choose $Q_i^+ \subseteq A_i(\tilde{P}_i^p)$. Let be $K_i^+ = X_i^+ \setminus (L_i^+ \cup Q_i^+)$, define $K_i'^+ \subseteq K_i^+$, the names to be mapped to the codomain Y^+. Then we define (for $i = 0,1$):

$$X_i'^- \triangleq \{x \in X_i^- \mid \exists y \in X_{\bar{i}}^- \text{ s.t. } A_i(x) = A_{\bar{i}}(y) \text{ or } A_i(x) \in (E_i \setminus E_{\bar{i}}) \uplus (P_i^n \setminus P_{\bar{i}}^n)\}$$
$$K_i'^+ \triangleq \{x \in K_i^+ \mid \forall p \in W^+ \uplus (P_0^p \cap P_1^p).A_i(p) = x \in X_i^+ \Rightarrow A_{\bar{i}}(p) \in X_{\bar{i}}^+\}.$$

As in Construction 14, let $\mathsf{Res} \triangleq W^- \uplus (E_0 \cap E_1) \uplus (P_0^n \cap P_1^n)$ we define for each $l \in \mathsf{Res}$ the set $X_i'^-(l)$ of names linked to l, and define:

$$Y^- \triangleq \bigcup_{l \in \mathsf{Res}} X_0'^-(l) \times X_1'^-(l) \cup \sum_{i \in \{0,1\}} \bigcup_{e \in (E_i \setminus E_{\bar{i}}) \uplus (P_i^n \setminus P_{\bar{i}}^n)} X_i'^-(e).$$

Next, on the disjoint sum $K_0'^+ + K_1'^+$, define $\simeq$ to be the smallest equivalence for which $(0,x_0) \simeq (1,x_1)$ iff there exists $p \in W^+ \uplus (P_0^p \cap P_1^p)$ such that $A_0(p) = x_0$ and $A_1(p) = x_1$. Then define:

$$Y^+ \triangleq (K_0'^+ + K_1'^+)/_{\simeq}.$$

For each $x \in K_i'^+$ we denote the equivalence class of (i,x) by $\widehat{i,x}$.

links For $i = 0,1$, choose two arbitrary functions:

$$\eta_i : L_i^+ \to (E_{\bar{i}} \setminus E_i) \uplus (P_{\bar{i}}^n \setminus P_i^n);$$
$$\xi_i : Q_i^+ \to \{l \in (E_{\bar{i}} \setminus E_i) \uplus (P_{\bar{i}}^n \setminus P_i^n) \mid \exists x \in X_{\bar{i}}^- \text{ s.t. } A_{\bar{i}}(x) = l\};$$

and for each $l \in \mathsf{Res}$ for which there exists $x_i \in X_i^-$ and $p \in P_{\bar{i}}^p \setminus P_i^p$ such that $A_i(x_i) = l$ and $A_{\bar{i}}(p) = l$, choose an arbitrary function:

$$\theta_i^l : \{p \in P_{\bar{i}}^p \setminus P_i^p \mid A_{\bar{i}}(p) = l\} \to X_i'^-(l).$$

Then define the link maps $C_i : X_i \to Y$ as follows:

$$\text{for } x \in X_i^+ : \qquad C_i(x) \triangleq \begin{cases} A_{\bar{i}}(p) & \text{if } x \in K_i^+ \setminus K_i'^+, \text{ then} \\ & \exists p \in W^+ \uplus (P_0^p \cap P_1^p) \text{ s.t. } A_i(p) = x \\ \widehat{i,x} & \text{if } x \in K_i'^+ \\ \eta_i(x) & \text{if } x \in L_i^+ \\ \xi_i(x) & \text{if } x \in Q_i^+; \end{cases}$$

$$\text{for } p \in P_{\bar{i}}^p \setminus P_i^p : \qquad C_i(p) \triangleq \begin{cases} A_{\bar{i}}(p) & \text{if } A_{\bar{i}}(p) \in (E_{\bar{i}} \setminus E_i) \uplus (P_{\bar{i}}^n \setminus P_i^n) \\ \widehat{\bar{i},x} & \text{if } A_{\bar{i}}(p) = x \in X_{\bar{i}}^+ \setminus Q_{\bar{i}}^+ \\ \theta_i^l(p) & \text{if } A_{\bar{i}}(p) = l \in \mathsf{Res} \\ \theta_i^e(p) & \text{if } p \in \tilde{P}_{\bar{i}}^p \text{ and } e = \xi_{\bar{i}}(A_{\bar{i}}(p)); \end{cases}$$

$$\text{for } y \in Y^- : \qquad C_i(y) \triangleq \begin{cases} x & \text{if } \hat{x} = (x,y) \text{ and } i = 0 \\ y & \text{if } \hat{x} = (x,y) \text{ and } i = 1 \\ y & \text{if } y \in Y^- \cap X_i^- \\ A_{\bar{i}}(y) & \text{if } y \in Y^- \cap X_{\bar{i}}^-. \end{cases}$$

The maps η_i are called *elision*; because the idle names L_i^+ in A_i are not exported in the IPO interface Y, but instead mapped into C_i.

The maps ξ_i are called *inversion*; this refers to the fact that in the bound $C_{\bar{i}}$ of $A_{\bar{i}}$ we can invert the direction of some link from upward to downward. In this way we can connect a port p of $P_i \setminus P_{\bar{i}}$ to an edge e in $E_{\bar{i}} \setminus E_i$ also when there is no shared port, connected to the same name of p, which is linked to e in $A_{\bar{i}}$.

The maps θ_i^l are called *random link*; this refers to the fact that if a link has more then one name linked to it, then in the bound it is indifferent to which name a point is linked to, because the effect of composition is the same.

There is a distinct IPO for each choice of L_i^+, Q_i^+, η_i, ξ_i and θ_i^l.

Theorem 4 *A pair $\vec{C} : \vec{X} \to Y$ is an IPO for $\vec{A} : W \to \vec{X}$ iff it is generated (up to isomorphism) by Construction 16.*

Proof. ($\Rightarrow$) $\vec{B}$ is an IPO for $\vec{A}$ iff it is the legs of an RPO w.r.t. some bound $\vec{D}$. So we can assume w.l.o.g. that $\vec{B}$ is generated by Construction 14. Now apply Construction 16 to create $\vec{C}$ by choosing $\vec{L}^+$, $\vec{Q}^+$, $\vec{\eta}$, $\vec{\xi}$ and $\vec{\theta}^l$ as in $\vec{D}$. Then $\vec{C}$ coincides with $\vec{B}$.

($\Leftarrow$) Consider any $\vec{C}$ generated by Construction 16. Now apply the Construction 14 to yield an RPO $(\vec{B}, B)$ for $\vec{A}$ to $\vec{C}$. Then $\vec{B}$ coincides with $\vec{C}$. □

B Algebra

Here, we show how derive all bigraphs from the elementary ones by composition and tensor product. Before giving a formal result, we provide an intuitive explanation of the meaning of these elementary bigraphs.

- The first three bigraphs build up all wirings, i.e. all link graphs having no nodes. All substitutions (fusions, resp.) can be obtained tensoring elementary substitutions $\triangle^y_X$ (fusions $\triangledown^Y_x$, resp.); the tensor products of singleton substitutions $\triangle^y_x$ or singleton fusions $\triangledown^x_y$ give all renamings. Composition and tensor product of substitutions, fusions and closures give all wirings.
- The next three bigraphs define all placings, i.e. all place graphs having no nodes; for example $merge_m : m \to 1$, merging m sites in a unique root, are defined as:

  $$merge_0 \triangleq 1 \qquad merge_{m+1} \triangleq merge \circ (id_1 \otimes merge_m).$$

  Notice that $merge_1 = id$ and $merge_2 = merge$, and that all permutations π are constructed by composition and tensor product from the place symmetry $\gamma_{1,1}$.
- Finally, for expressing any direct bigraph we need to introduce only the discrete ions $K(l) : \langle(\vec{x}^-,\vec{Y}^+)\rangle \to \langle(\vec{Y}^-,\vec{x}^+)\rangle$. In particular, we can express any discrete atoms as $K(l) \circ 1$.

The following proposition shows that every bigraph can be expressed in a normal form, called *discrete diagonal normal form* (DDNF). We will use D, Q and N to denote discrete, prime and discrete bigraphs, and discrete molecules respectively.

Theorem 5 *1. A bigraph G on signature $\mathscr{K}$ can be expressed uniquely (up to iso) as:*

$$G = (\omega \otimes id_n) \circ D \circ (\omega' \otimes id_m) \tag{1}$$

where D is a discrete bigraph and ω, ω' are two wirings satisfying the following conditions:

i. in ω, if two outer downward names are peer, then their target is an edge;

ii. in ω' there are no edges, and no two inner upward names are peer.

2. Every discrete bigraph $D : \langle n, Z\rangle \to \langle m, W\rangle$, may be factored uniquely (up to iso) on the width m in the following form:

$$D = \alpha \otimes \left(\begin{pmatrix} (Q_0 \otimes \chi^{out}_{1,0} \otimes \chi^{out}_{2,0} \otimes \dots & & &)\circ \\ (\chi^{in}_{0,1} \otimes Q_1 \otimes \chi^{out}_{2,1} \otimes \dots & & &)\circ \\ (\chi^{in}_{0,2} \otimes \chi^{in}_{1,2} \otimes Q_2 \otimes \dots & & &)\circ \\ & \ddots & & \\ (& \dots \otimes Q_{m-3} & \otimes \chi^{out}_{m-2,m-3} \otimes \chi^{out}_{m-1,m-3} &)\circ \\ (& \dots \otimes \chi^{in}_{m-3,m-2} \otimes Q_{m-2} & \otimes \chi^{out}_{m-1,m-2} &)\circ \\ (& \dots \otimes \chi^{in}_{m-3,m-1} \otimes \chi^{in}_{m-2,m-1} \otimes & Q_{m-1} &) \end{pmatrix} \circ (\pi \otimes id_{dom(\vec{Q})}) \right)$$

shortly:

$$D = \alpha \otimes (\chi(Q_0, \dots, Q_{m-1}) \circ (\pi \otimes id_{dom(\vec{Q})})) \tag{2}$$

- *where α is a renaming;*
- *π is a permutation;*

- *each* $Q_i : \langle h_i, (X_i^-, X_i^+)\rangle \to \langle (Y_i^-, Y_i^+)\rangle$ *(for* $i \in \{0,\dots,m-1\}$*) is prime and discrete;*
- $\chi_{i,l}^{out}$ *(*$\chi_{i,l}^{in}$ *resp.) are the identities on the outer (inner resp.) names of* Q_i *at level* $l \in \{0,\dots,m-1\}$*, which are not used by* $Q_l,\dots,Q_{i-1}$ *(*$Q_{i+1},\dots,Q_l$ *resp.). Formally:*

$$\chi_{i,l}^{out} \triangleq id_{\langle (Y_i^- \setminus (\biguplus_{j=l}^{i-1} X_j^-), Y_i^+ \setminus (\biguplus_{j=l}^{i-1} X_j^+))\rangle} \qquad \text{for } i > l$$

$$\chi_{i,l}^{in} \triangleq id_{\langle h_i, (X_i^- \setminus (\biguplus_{j=i+1}^{l} Y_j^-), X_i^+ \setminus (\biguplus_{j=i+1}^{l} Y_j^+))\rangle} \qquad \text{for } i < l.$$

3. *Every prime and discrete* Q*, may be factored uniquely (up to iso) in the following form:*

$$Q = (merge_{n+p} \otimes id_{codom(\vec{N})}) \circ (id_n \otimes \chi(N_0,\dots,N_{p-1})) \circ (\pi \otimes id_{dom(\vec{N})}) \tag{3}$$

where χ *is defined as in 2.*

4. *Every discrete molecule* N*, may be factored uniquely (up to iso) in the following form:*

$$N = (K(l) \otimes id_{(codom(Q)\setminus(\vec{x}^-,\vec{Y}^+))}) \circ Q. \tag{4}$$

Furthermore, the expression is unique up to iso on the parts and reordering of N*s in* Q*.*

These equations can be used for normalizing any bigraph G as follows; first, we apply equations (1), (2) to G once, obtaining an expression containing prime discrete bigraphs $Q_0,\dots,Q_{m-1}$. These are decomposed further using equations (3), (4) repeatedly: each Q_i is decomposed into an expression containing molecules $N_{i,0},\dots,N_{i,p_i-1}$, each of which is decomposed in turn into an ion containing another prime discrete $Q'_{i,j}$. The last two steps are repeated recursively until the ions are atoms or have only holes as children. Note that 1 is a special case of Q when $n = p = 0$.

Notice that if the signature has only positive controls, then all the "Q_i layers" can be collapsed in a unique one, obtaining a normal form that is very similar to the Milner's DNF (see [Mil06]).

Furthermore, a renaming is discrete but not prime (since it has zero width); this is why the factorization has such a factor. The uniqueness of that factorization depends on the fact that prime bigraphs have upward inner names and downward outer names linked to negative ports.

In Table 1 we give a set of axioms which we prove to be sound and complete.

Each of these equations holds only when both sides are defined; in particular, recall that the tensor product of two bigraphs is defined only if the name sets are disjoint. It is important to notice that for ions only the renaming axiom is needed (because names are treated positionally).

Theorem 6 *Let* E_0, E_1 *be two expressions constructed from the elementary bigraphs by composition and tensor product. Then,* E_0 *and* E_1 *denote the same bigraph in* DBIG *if and only if the equation* $E_0 = E_1$ *can be proved by the axioms in Table 1.*

Proof. The proof is similar to that of [JM04, Theorem 10.2]. The "if" direction is simple to prove, since it requires to check that each axiom is valid. The "only if" direction is in two steps. First, we prove by induction on the structure of expressions, that the equality between an expression and its DDNF is derivable from the axioms. Next, since DDNFs are taken up to iso, we prove that the equality between isomorphic DDNFs is provable from the axioms. This is proved by showing that the axioms can prove the isomorphisms of the components of a DDNF, which are ions, prime and discrete bigraphs, and discrete bigraphs. □

Categorical Axioms

$A \circ id = A = id \circ A \qquad A \circ (B \circ C) = (A \circ B) \circ C$

$A \otimes id_\varepsilon = A = id_\varepsilon \otimes A \qquad A \otimes (B \otimes C) = (A \otimes B) \otimes C$

$\gamma_{I,\varepsilon} = id_I \qquad \gamma_{J,I} \circ \gamma_{I,J} = id_{I \otimes J} \qquad \gamma_{I \otimes J,K} = (\gamma_{I,K} \otimes id_J) \circ (id_I \otimes \gamma_{J,K})$

$(A_1 \otimes B_1) \circ (A_0 \otimes B_0) = (A_1 \circ A_0) \otimes (B_1 \circ B_0)$

$\gamma_{I,K} \circ (A \otimes B) = (B \otimes A) \circ \gamma_{H,J} \qquad$ (where $A : H \to I, B : J \to K$)

Link Axioms

$\triangle^x_x = id_{(\emptyset,x)} \quad \nabla^x_x = id_{(x,\emptyset)} \quad \bowtie^x_y \circ \triangle^y_z = \bowtie^x_z \quad \nabla^z_x \circ \bowtie^x_y = \bowtie^z_y \quad \nabla_x \circ \bowtie^x_y \circ \triangle^y = id_\varepsilon$

$\triangle^z_{(Y \uplus y)} \circ (id_{(\emptyset,Y)} \otimes \triangle^y_X) = \triangle^z_{(Y \uplus X)} \qquad (id_{(Y,\emptyset)} \otimes \nabla^X_y) \circ \nabla^{(Y \uplus y)}_z = \nabla^{(X \uplus Y)}_z$

Place Axioms

$merge \circ (1 \otimes id_1) = id_1 \qquad merge \circ \gamma_{1,1} = merge$

$merge \circ (merge \otimes id_1) = merge \circ (id_1 \otimes merge)$

Node Axioms

Let $K(l) : \langle(\vec{x}^-, \vec{Y}^+)\rangle \to \langle(\vec{Y}^-, \vec{x}^+)\rangle$

$(id_1 \otimes \alpha^+ \otimes \zeta^-) \circ K(l) = K(l')$ with $l' = ((id_{\vec{x}^-} \cup \alpha^+) \circ l^p, ((\zeta^-)^{op} \cup id_{\vec{Y}^+}) \circ l^n)$

$K(l) \circ (id_1 \otimes \alpha^- \otimes \zeta^+) = K(l'')$ with $l'' = ((\alpha^- \cup id_{\vec{x}^+}) \circ l^p, (id_{\vec{Y}^-} \cup (\zeta^+)^{op}) \circ l^n)$

where $\alpha^+ : \vec{x}^+ \to \vec{z}^+, \alpha^- : \vec{x}^- \to \vec{z}^-$ are renamings and

$\zeta^- : \vec{Z}^- \to \vec{Y}^-, \zeta^+ : \vec{Z}^+ \to \vec{Y}^+$ are surjective fusions.

Table 1: Axiomatization for the abstract directed bigraphs.

C Sharing products

Here we remark some variants of the tensor product (presented in [GM07a]), whose allow the sharing of names. Process calculi often have a parallel product $P \mid Q$, that allows the processes P and Q to share names. In directed bigraphs, this sharing can involve inner downward names and/or outer upward names, as described by the following definitions.

Definition 17 The *outer sharing product* ($\curlywedge$), *inner sharing product* ($\curlyvee$) and *sharing product* ($\|$) of two objects $X = (X^-, X^+), Y = (Y^-, Y^+)$ and of two link graphs $A_i : X_i \to Y_i$ $(i = 0, 1)$ are defined as follows:

$$(X^-, X^+) \curlywedge (Y^-, Y^+) \triangleq (X^- \uplus Y^-, X^+ \cup Y^+)$$
$$(X^-, X^+) \curlyvee (Y^-, Y^+) \triangleq (X^- \cup Y^-, X^+ \uplus Y^+)$$

$$A_0 \curlywedge A_1 \triangleq (V_0 \uplus V_1, E_0 \uplus E_1, ctrl_0 \uplus ctrl_1, link_0 \uplus link_1) : X_0 \otimes X_1 \to Y_0 \curlywedge Y_1$$
$$A_0 \curlyvee A_1 \triangleq (V_0 \uplus V_1, E_0 \uplus E_1, ctrl_0 \uplus ctrl_1, link_0 \uplus link_1) : X_0 \curlyvee X_1 \to Y_0 \otimes Y_1$$
$$A_0 \parallel A_1 \triangleq (V_0 \uplus V_1, E_0 \uplus E_1, ctrl_0 \uplus ctrl_1, link_0 \uplus link_1) : X_0 \curlyvee X_1 \to Y_0 \curlywedge Y_1$$

defined when interfaces are defined and A_i have disjoint node and edge sets.

The *outer sharing product*, *inner sharing product* and *sharing product* of two objects $I = \langle m,X\rangle, J = \langle n,Y\rangle$ and of two bigraphs $G_i : I_i \to J_i$ $(i = 0,1)$ are defined by extending the corresponding products on their link graphs with the tensor product on widths and place graphs:

$$\langle m,X\rangle \curlywedge \langle n,Y\rangle \triangleq \langle n+m, X \curlywedge Y\rangle \qquad \langle m,X\rangle \curlyvee \langle n,Y\rangle \triangleq \langle n+m, X \curlyvee Y\rangle$$
$$G_0 \curlywedge G_1 \triangleq \langle G_0^P \otimes G_1^P, G_0^L \curlywedge G_1^L\rangle : I_0 \otimes I_1 \to J_0 \curlywedge J_1$$
$$G_0 \curlyvee G_1 \triangleq \langle G_0^P \otimes G_1^P, G_0^L \curlyvee G_1^L\rangle : I_0 \curlyvee I_1 \to J_0 \otimes J_1$$
$$G_0 \parallel G_1 \triangleq \langle G_0^P \otimes G_1^P, G_0^L \parallel G_1^L\rangle : I_0 \curlyvee I_1 \to J_0 \curlywedge J_1.$$

defined when interfaces are defined and G_i have disjoint node and edge sets.

It is simple to verify that $\curlywedge$, $\curlyvee$ and $\parallel$ are associative, with unit ε.

Another way of constructing a sharing product of two bigraphs G_0, G_1 is to disjoin the names of G_0 and G_1, then take the tensor product of the two bigraphs and finally merge the name again:

Proposition 3 *Let G_0, G_1 be bigraphs with disjoint node and edge sets. Then*

$$G_0 \curlywedge G_1 = \sigma(G_0 \otimes \tau G_1 \zeta) \qquad G_0 \curlyvee G_1 = (G_0 \otimes \tau G_1 \zeta)\delta \qquad G_0 \parallel G_1 = \sigma(G_0 \otimes \tau G_1 \zeta)\delta$$

where the substitution σ and τ are defined in the following way: if z_i $(i \in n)$ are the upward outer names shared by G_0 and G_1, and w_i are fresh names in bijection with the z_i, then $\tau(z_i) = w_i$ and $\sigma(w_i) = \sigma(z_i) = z_i$ $(i \in n)$. The substitution δ and ζ are defined in a very similar way, but acting on the downward inner names.

Definition 18 The *prime outer sharing product* and *prime sharing product* of two objects $I = \langle m,X\rangle, J = \langle n,Y\rangle$ and of two bigraphs $G_i : I_i \to J_i$ $(i = 0,1)$ are defined as follows:

$$\langle m,X\rangle \bar{\curlywedge} \langle n,Y\rangle \triangleq \langle 1, X \curlywedge Y\rangle$$
$$G_0 \bar{\curlywedge} G_1 \triangleq merge_{(width(J_0)+width(J_1))} \circ (G_0 \curlywedge G_1) : I_0 \otimes I_1 \to J_0 \bar{\curlywedge} J_1$$
$$G_0 \mid G_1 \triangleq merge_{(width(J_0)+width(J_1))} \circ (G_0 \parallel G_1) : I_0 \curlyvee I_1 \to J_0 \bar{\curlywedge} J_1.$$

defined when interfaces are defined and G_i have disjoint node and edge sets.

It is easy to show that $\bar{\curlywedge}$ and $\mid$ are associative, with unit 1 when applied to prime bigraphs. Note that for a wiring ω and a prime bigraph P, we have $\omega \bar{\curlywedge} P = \omega \curlywedge P$ and $\omega \mid P = \omega \parallel P$, because in this case these products have the same meaning.

D Directed Bigraphical Reactive and Transition Systems

In order to define reactive systems over directed bigraphs, we need to define how a parametric rule, a "redex-reactum" pair of bigraphs, can be instantiated. Essentially, in the application of a rule, the "holes" in the reactum must be filled with the parameters appearing in the redex. This relation can be expressed by a function mapping each site of the reactum to a site of the redex.

Definition 19 An *instantiation* ρ from (width) m to (width) n, written $\rho :: m \to n$, is determined by a function $\bar{\rho} : n \to m$. For any pair X, this function defines the map $\rho : Gr\langle m, X\rangle \to Gr\langle n, X\rangle$ as follows. Decompose $g : \langle m, X\rangle$ (using the DDNF) into

$$g = \omega \circ \chi(Q_0, \dots, Q_{m-2}, q_{m-1})$$

where χ is defined as in Theorem 5, and with $\omega : Y \to X$, each Q_i ($i \in m-1$) prime discrete, and q_{m-1} ground prime discrete. Then define:

$$\rho(g) \triangleq \omega \circ (\chi^{\|}(S_0, \dots, S_{n-2}, s_{n-1}) \curlywedge id_{(\emptyset, Y^+)})$$

where $\chi^{\|}$ is defined like χ, but it uses $\|$ operator instead of $\otimes$, and $|S_j| \doteq |Q_{\bar{\rho}(j)}|$ for $j \in n$, changing the interfaces of Ss accordingly to the order of the composition.

If $\bar{\rho}$ is injective, surjective or bijective then ρ is said to be *affine, total* or *linear* respectively.

Suppose ρ is not linear, the reactum is not defined if the removed or duplicated parts of the parameter have connections between nodes in two different locations (i.e., connections between a positive port and a negative one) or have outer accessible local resources (i.e. negative ports). In fact, the resources cannot be anymore accessible, because the parts containing them are removed; or it is unclear which resources of the copies still remain accessible. So, to use not linear ρ, a sufficient (but not necessary) condition is that parameters have no connections crossing boundaries of different locations and have no outer accessible local resources.

If ρ is not affine then it replicates at least one of the factor d_i. Outer sharing product is used because copies will share names. Moreover, the outer upward names of $S_0 \dots S_{n-2}, s_{n-1}$ may be fewer than Y^+, because ρ may be not total, so we add $id_{(\emptyset, Y^+)}$ to $\rho(g)$ to ensure that the composition with ω is defined (here idle names can be generated).

Definition 20 A ground reaction rule is a pair (r, r'), where r and r' are ground with the same outer interface. Given a set of ground rules, the reaction relation $\longrightarrow$ over agents is the least, such that $Dr \longrightarrow Dr'$ for each active context D and each ground rule (r, r').

A parametric reaction rule has a redex R and reactum R', and takes the form:

$$(R : I \to J, R' : I' \to J, \rho)$$

where I and I' have widths m and m' respectively. The third component $\rho :: m \to m'$ is an instantiation. For any X and discrete $d : I \otimes X$, the parametric rule generates the ground rule:

$$((R \otimes id_X) \circ d, (R' \otimes id_X) \circ \rho(d)).$$

Definition 21 A *directed bigraphical reactive system* (DBRS) over the polarized signature $\mathscr{K}$, denoted by $\mathscr{D}(\mathscr{K}, \mathscr{R})$ is the precategory $'\mathrm{DBIG}(\mathscr{K})$ equipped with a set $\mathscr{R}$ of reaction rules.

Now we can prove the following important result:

Proposition 4 *DBRSs are wide reactive systems over a wide monoidal precategory*

This result ensures that DBRSs inherit from the theory of WRSs the definition of transition system based on IPOs [Mil06].

Definition 22 A *transition* for a DBRS $\mathscr{D}(\mathscr{K},\mathscr{R})$ is a quadruple (a, L, λ, a'), written as $a \xrightarrow{L}_{\lambda} a'$, where a and a' are ground bigraphs and there exist a ground reaction rule $(r, r') \in \mathscr{R}$ and an active context D such that $La = Dr$, and $\lambda = width(D)(width(cod(r)))$ and $a' \simeq Dr'$.

A transition is *IPO* if the (L, D) is an IPO for (a, r).

Definition 23 A *directed bigraphical transition system* (DBTS) $\mathscr{L}$ for $\mathscr{D}$ is a pair $(\mathscr{I}, \mathscr{T})$:

- $\mathscr{I}$ is a set of interfaces; the agents of $\mathscr{L}$ are the ground bigraphs with outer interfaces in $\mathscr{I}$;
- $\mathscr{T}$ is a set of transitions whose sources and targets are agents of $\mathscr{L}$.

The *full* (*IPO*, resp.) transition system consists of all interfaces, with all (IPO, resp.) transitions.

From [Mil06, Theorem 4.6] we have that in any DBRS with the IPO transition system, wide bisimilarity is a congruence.