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Computation in the Informatic Jungle

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Abstract

Informatics bridges Turing-computation and interactive behaviour; examples of the latter include ubiquitous/pervasive and biological systems. But how does a model of computation fit within a model of less disciplined informatic behaviour? This paper offers a precise treatment of that relationship, identifying a class of *calculational* bigraphical reactive systems. We show how such a system contains a confluent calculation sub-model, and how calculation only ever enables, never prevents, informatic behaviour of the larger model. We submit these results as a modest but essential beginning of a unified informatic theory.

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1 Introduction

Computing technology and informatic behaviour appear to demand different models. On the one hand is the notion of Turing-complete computation, largely underlying computational artifacts;on the other hand are models describing semi-natural or natural interactive behaviour within complexly structured systems. These latter models are essential for a coherent informatic theory: the ubiquitous and/or pervasive systems of the future (some of which exist already), while promising to add quality to our lives, may not be as well-understood as traditional computing on the one hand, and naturally-occurring physical phenomena on the other.

Informatics bridges between the two. It involves artifacts, and even natural (e.g. biological) systems, that interact within an often undisciplined environment, but also calculate in a disciplined way. But how does a model of Turing-computation sit within a model of less disciplined informatic behaviour? For this, it is essential that the former model can be seen as an instance of the latter. The latter model must be generic, instantiable to many applications (e.g. biological systems or wireless networks), and one such application must be classical computation. This paper offers a candidate for this relationship. We show how computation — represented by general recursive equations — can be regarded as a sub model of a bigraphical reactive system.

Bigraphs [1, 2, 3, 4, 5, 6] model the behaviour of large mobile informatic systems, often termed pervasive or ubiquitous systems. They are inspired by process calculi, especially CCS [7], π-calculus [8, 9] and Mobile Ambients [10], but are generic; they specialise applications as varying as biological phenomena and the built environment. Many well-known process calculi have been represented in bigraphs [1, 3, 11, 4, 12, 13], and their several theories are recovered in varying degrees within bigraph theory. This theory can be found, with bibliography, in a recent text book [1]. For further material see [14, 15].

A *bigraphical reactive system* (BRS) is a collection of bigraphs enriched with reaction rules, allowing complex systems to reconfigure themselves. The large variety of BRSs is achieved by means of sorting [4, 6, 3, 16, 17, 18], a generalisation of the sort structure of many-sorted algebra. BRSs can model both concrete structures (e.g. buildings, wireless networks) as well as abstract ones (e.g. data and control structures). Thus computation may be treated as a sub-BRS of a BRS that models real-world behaviour.

This paper identifies a class of calculational BRSs. In these, calculational behaviour is represented by an *unfolding* reaction, as distinct from the less disciplined *liberal* reaction, which models interactive behaviour such as communication, physical motion or even biological development. We prove that unfolding really is diciplined: it is confluent, and, in a sense to be made precise, it may *enable* but never *disable* liberal reaction. We submit these results as a beginning of a unified informatic theory.

Overview. In Sections 2 and 3, we recall the structure and dynamics of BRSs. Then in Section 4, we give an example of a calculational BRS. In the remainder of the paper, we put this example on a formal foundation. First, in Section 5, we study interplay of reaction relations in an abstract setting. Then, in Section 6, we introduce unfolding BRSs: BRSs disciplined enough that we may think of "reaction" as "calculation". Finally, in Section 7, we define a Calculational BRS as a BRS which has an unfolding sub-BRS, and subject to certain conditions, unfolding never preempts reaction. We proceed to lift these results to sorted BRSs. In Section 8 we recall sorted BRSs, and in Section 9 and 10, we examine the interplay of sorting and calculation, giving a sufficient condition for a sorting to preserve confluence and unfolding never preempting reaction. BRS.

2 Free bigraphs

A *free bigraphical reactive system* is specified by a *signature* $\mathcal{K}$ that defines its static structure, and a *reaction regime* $\mathcal{R}$ that defines its dynamics. In this section, we review the static structure of bigraphs using a running example. We first recall their basic structure, then their composition, and finally their algebra.Limitation of space forces us to omit many details, which can be found in [1, 3].

Basic structure. Consider the diagram in Figure 1. In its centre is a bigraph g, representing part of a built environment consisting of buildings B, rooms R and computers C, among which agents A move and communicate. A bigraph consists of two structures on a single finite node-set: a *placing* (depicted left of g), which is an ordered forest of its nodes that defines their nesting, and a *linking* (depicted right of g) that partitions all the ports of its nodes, defining their

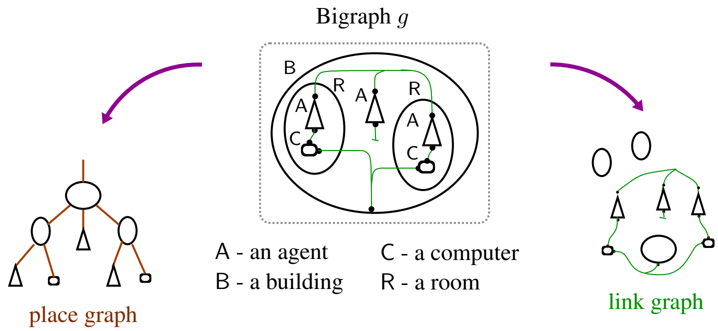


Figure 1: Bigraph g

linkage. We see how placing and linking intertwine. Three agents in different places are linked in a conference call; each agent in a room is logged in to a computer there; and all the computers in a building are linked in its local-area network. In this example, placing models physical nesting of computers and agents in rooms etc., and linking models connections, virtual or physical.

Each *node* in a bigraph has a *control*. In g, controls are A, B, C, R, mnemonics for Agent, Building, Computer, and Room. We have indicated controls both by a letter and by the geometrical shape — agents A are triangles, computers C are small rounded boxes etc. We often omit the letter and rely on shape to indicate control. The control of a node dictates the number of its *ports*, the end-points of linking. In diagrams, ports are indicated by the little dots on the nodes.

Bigraphs are parametrised on the set of available controls and their number of ports (arities). The signature for our example is $\mathcal{K}_{\mathsf{built}} = \{\mathsf{A} : 2,\ \mathsf{B} : 1,\ \mathsf{C} : 2,\ \mathsf{R} : 0\}$.

Definition 1. *A signature $\mathcal{K}$ is a set of* controls *with finite* arities.

Composition. In Figure 2, we show how g arises as the composition of two other bigraphs G and d. Here, g from

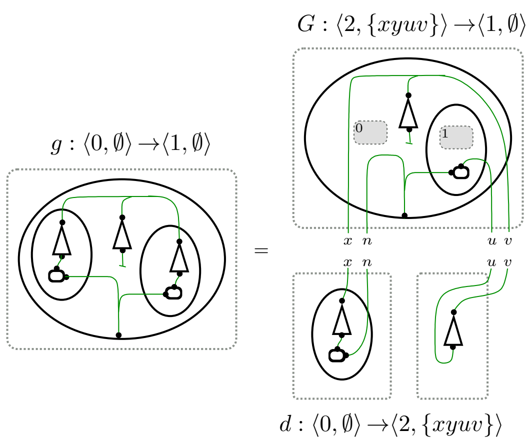


Figure 2: Composition of bigraphs: $g = G \circ d$

Figure 1 is at the left of the equal-sign. At the right are two bigraphs, G and $d.G$ resembles g, except the left-most room of g has been replaced by a *site*, depicted as a grey box with a 0 in it. The agent in the right-most room of g has been similarly replaced with a site 1. The missing room, agents and computer are in d at the bottom. Whereas both g and G have only a single nesting hierarchy each, d has two, indicated by its two dashed boxes, its two *regions*. In the left is the replaced room, agent, and computer; in the right the replaced agent. The linkage of g has been similarly split, with *names* at the bottom of G and at the top of d serving as points of indirection.

Bigraphs are composed separately in the placing and the linking. In the placing, we plug the left-most region of d into site 0 of G, and the right-most region of d into site 1 of G. (Regions are numbered left-to-right: we plug region 0 in site 0 etc.) In the linking, we splice together links along names. Thus, the composition $G \circ d$, yields exactly g. Two bigraphs compose only if they have compatible sets of names and sites/regions; compatible *interfaces*. An interface takes the form $\langle m, X\rangle$ where m is a natural number, the number of sites/regions, and X is a set of names. G and d share the interface $\langle 2, \{xyuv\}\rangle$.

Each bigraph has in fact two interfaces: one downwards, and one upwards. When we say that "G and d are compatible" and speak of their composition $G \circ d$, we mean that the upwards interface of d is equal to the downwards[1] interface of G. Writing out the full interfaces of G, and d, we find $G : \langle 2, \{xyuv\}\rangle \to \langle 1, \emptyset\rangle$, and $d : \langle 0, \emptyset\rangle \to \langle 2, \{xyuv\}\rangle$. Thus, e.g., G has names $\{xyuv\}$ downwards, no names upwards, 2 sites, and 1 region. Note that the upwards interface of d is the same as the downwards interface of G.

A useful intuition for readers acquainted with process algebras or term-rewriting is to think of bigraphs b with interfaces $b : \langle 0, \emptyset\rangle \to \langle n, Y\rangle$ for some n, Y as processes or terms, and other bigraphs $B : \langle m, X\rangle \to \langle n, Y\rangle$ as multi-hole contexts, the number of holes given by m. This intuition is so important that we introduce a term for the former kind: we call them *ground* bigraphs. Ground bigraphs are written in lower-case letters, non-ground in capitals: d is ground, G is non-ground.

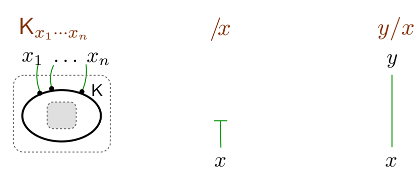
Bigraphs have a partial tensor: If G, H have disjoint upwards and downwards names, then $G \otimes H$ is simply the concatenation of their regions. An example is in Figure 3.

In summary, a bigraph comprises two graph structures over a shared set of nodes: a placing and a linking. Each node has an associated control, controls being given by an ambient signature. A bigraph B has an interface $B : \langle m, X\rangle \to \langle n, Y\rangle$, indicating that it has n regions, m sites, names X downwards and names Y upwards.

Through their interfaces, composition, and tensor, bigraphs over a particular signatureform a symmetric partial monoidal category — an *spm* category [1, 3]:

Definition 2 (free bigraphical system)**.** *The* free bigraphical system $\mathrm{B}{\small G}(\mathcal{K})$ *is the symmetric partial monoidal (spm) whose objects are interfaces and morphisms are bigraphs over the signature* $\mathcal{K}$*.*

Algebra. It is often convenient to represent bigraphs algebraicallyrather than graphically. All bigraphs are in fact generated by composition and monoidal product from a small set of elementary ones [1, 5, 19]. We recall here the parts of this algebra we will need for examples. Of the elementary bigraphs, we will use the *ion* $\mathsf{K}_{x_1 \cdots x_n} : \langle 1, \emptyset\rangle \to \langle 1, x_1 \cdots x_n\rangle$; a single region containing only K, in turn containing a site; *closure* $/x : \langle m, \{x\}\rangle \to \langle m, \emptyset\rangle$, which closes an x-link, and the *substitution* y/x, which re-directs names:



mm We also use the derived operators of Figure 3:

Parallel product $G_1 \parallel G_2$	– like $G_1 \otimes G_2$ but allows names to be shared
Prime product $G_1 \mid G_2$	– like $G_1 \parallel G_2$ but merges regions into one
Nesting $G.F$	– like $G \circ F$ but G has no inner names, and the outer names of F are exported.

We now have enough syntax to write our examples g, D and d algebraically:

$$
\begin{aligned}
g &= /x/n(\mathsf{B}_n.(\mathsf{Room}_{xn} \mid /c\mathsf{A}_{xc} \mid \mathsf{Room}_{xn})) \qquad \textit{where } \mathsf{Room}_{xn} \stackrel{\text{def}}{=} \mathsf{R}./c(\mathsf{A}_{xc} \mid \mathsf{C}_{cn})\\
d &= \mathsf{Room}_{xn} \parallel \mathsf{A}_{vu}\\
G &= /x/n(\mathsf{B}_n.(\boxed{0} \mid /s\mathsf{A}_{xs} \mid \mathsf{R}.(\boxed{1} \mid \mathsf{C}_{un})) \mid x/v)\ .
\end{aligned}
$$

[1] What we here call "upwards" and "downwards" is usually called "outer" and "inner".

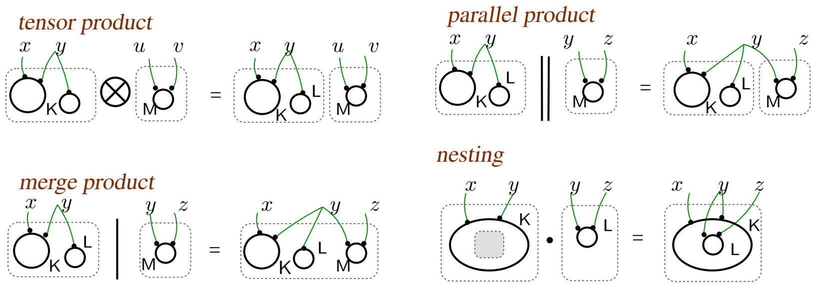


Figure 3: Operator examples

The closure "$/x$" binds x; terms are up to alpha-conversion. Of course, many terms denote the same free bigraph. However, under the axiomatisation [5, 19], two terms are equal iff they denote the same bigraph. This justifies our term "free" bigraph, since $\mathrm{BG}(\mathcal{K})$ is the free interpretation of those axioms. Note that sortings of bigraphs will (typically) not be free in this sense.

We conclude this section by defining three notions we shall need later: "ground" and "discrete" bigraphs, and "guarded" nodes. Ground bigraphs we saw already above.

Definition 3 (ground, guarded, discrete)**.** *A bigraph B is* ground *if it has interface $\langle 0, \emptyset\rangle \to \langle n, Y\rangle$ for some n, y. It is* discrete *if its linking is a bijection of ports and upwards names. A node or site in a bigraph is* guarded *if it occurs inside another node.*

We saw both ground and non-ground bigraphs above, but not discrete ones — they all had links between a port of a computer and a port of an agent. In Figure 4, the two bigraphs under B2 are both discrete. Finally, in d in Figure 2, the agent A linked to u, v is not guarded, whereas the agent A linked to x, n is guarded by a R-node.

3 Dynamics

Bigraphs can be reconfigured by *reaction* or *rewriting* rules. First, we must distinguish between those bigraphical controls which allow dynamic behaviour within them, and those which do not. We call the former "active", the latter "passive".

Definition 4 (activity, dynamic signature)**.** *A signature is* dynamic *if it assigns to each control a* status *of either* active *or* passive*. A bigraph $G : \langle m, X\rangle \to \langle n, Y\rangle$ is* active *if every ancestor of every site $i \in m$ has status* active.

In the built-environment of the preceding section, all controls are active; so all bigraphs are too: reaction can happen anywhere. If, e.g., either the control B (Building, flat oval) or R (Room, tall oval) were passive, then the bigraph G of Figure 2 would be passive. Intuitively, if non-ground bigraphs are contexts, then active ones are evaluation contexts.

For brevity, we treat a number m as a finite ordinal: the set $\{0, 1, \ldots, m-1\}$ of its predecessors. Note the use of the "nesting" operator (dot) of Figure 3.

Definition 5 (reaction rule)**.** *A* reaction rule *in $\mathrm{BG}(\mathcal{K})$ is a triple (R, R', η) of a* redex *$R : \langle m, \emptyset\rangle \to \langle n, Y\rangle$, a* reactum *$R' : \langle m', \emptyset\rangle \to \langle n, Y\rangle$, and a map $\eta : m' \to m$ of finite ordinals. A* parameter *for R is a discrete ground bigraph $d : \langle 0, \emptyset\rangle \to \langle m, X\rangle = d_0 \otimes \cdots \otimes d_{m-1}$; we call the d_i* parameter factors*. Define $d' \stackrel{\text{def}}{=} d_{\eta(0)} \parallel \cdots \parallel d_{\eta(m'-1)}$. For every parameter d the rule generates the* ground *rule $(r, r') = (R.d, R'.d')$. Ground rules yield a* reaction relation *by closing them under active bigraphs H: When $H \circ r$ defined, $H \circ r \longrightarrow H \circ r'$.*

In Figure 4 are three reaction rules. While reaction rules are generally on the form (R, R', η), for these particular rules η is the identity, so in Figure 4 we show simply the redex R and reactum R' of each rule. Call this set of rules $\mathcal{R}_{\mathsf{built}}$. Rule B1 allows an agent to abandon a conference call. B2 allows an agent outside a room to enter it. As we shall see, links will follow, and the special case of no links is included. This rule is parametric; the redex's site allows other occupants in the room. Finally, B3 allows an agent to be logged in to a nearby computer

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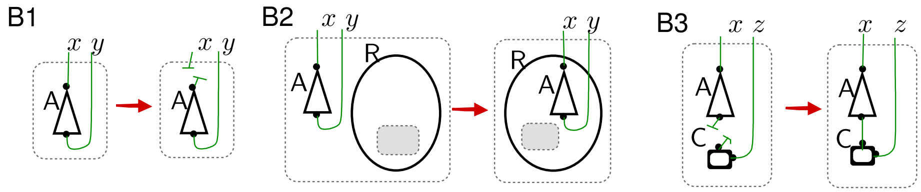
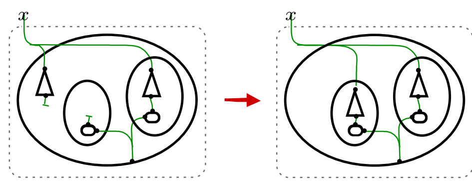


$$\mathsf{B1} : \mathsf{A}_{xy} \longrightarrow x \,|\, /x\mathsf{A}_{xy} \qquad \mathsf{B2} : \mathsf{A}_{xy} \,|\, \mathsf{R}.\square \longrightarrow \mathsf{R}.(\square \,|\, \mathsf{A}_{xy})$$
$$\mathsf{B3} : /y\mathsf{A}_{xy} \,|\, /y\mathsf{C}_{yz} \longrightarrow /y(\mathsf{A}_{xy} \,|\, \mathsf{C}_{yz}) \,.$$

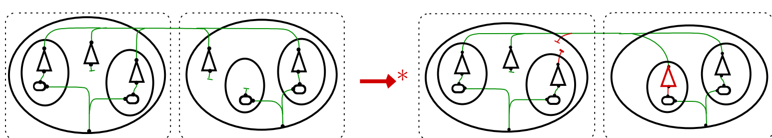
Figure 4: Example reaction rules $\mathcal{R}_{\mathsf{built}} = \{\mathsf{B1}, \mathsf{B2}, \mathsf{B3}\}$.

We apply B2 to a bigraph h, obtaining the reaction $h \longrightarrow h'$:

$h =$  $= h'$

Call the redex and reactum of B2 for R, R': B2 is the rule $(R, R', [1 \mapsto 1])$. This rule generates ground rules $R.d \longrightarrow R'.d$ for any discrete $d : \langle 0, \emptyset\rangle \to \langle 1, X\rangle$ (because η is trivial, $d' = d$; we return to η shortly). The reaction relation is further closed under arbitrary contexts, so to establish the reaction $h \longrightarrow h'$, it is sufficient to factorise h into $h = H \circ R.d$ and similarly $H \circ R'.d = h'$. We do so in Figure 5. Because of the nesting $R.d$ and $R'.d$, the names u, v are forwarded across R and R'. In general, a reaction rule (R, R', η) induces a reaction $f \longrightarrow f'$ when $f = F \circ R.d$ and $f = F \circ R'.d'$, where d' is obtained from d via η as specified in Definition 5, *provided* that F in question is active. In Figure 5, H is active because the building control B (flat oval) is. If it were not, there would not be reaction $h \longrightarrow h'$.

Let us see the result of applying B1, B2, B3 once each in a bigraph with two buildings. They may occur in any order, except that B2 must precede B3.



A realistic model will have many more rules and much non-determinism, i.e. many *critical pairs* of applicable rules, each of which would preempt the other. For example, a rule for an agent to leave a room is likely to form a critical pair with B3.

We now explain the role of the map η and the necessity of parameters being "ground" and "discrete" in the above definition of reaction rules. First, η. The redex R and reactum R' of the rule B2 above both have exactly one site. We have seen that in reaction, a parameter d of R is simply retained as the parameter d of R'. Thus B2 is a linear rule: its parameter is neither duplicated nor discarded. Non-linear reaction rules are also allowed:

$$\mathsf{R}.\square \longrightarrow \mathsf{R} \qquad\qquad \mathsf{R}.\boxed{0} \longrightarrow \mathsf{R}.(\boxed{0} \,|\, \boxed{1})$$

The first one says that a room may spontaneously lose all contents; the second that a room may spontaneously duplicate its contents. Even though the real world certainly would not exhibit this behaviour — rooms do not duplicate people! — a failing sensor network might believe it did. Applying these rules to a bigraph $\mathsf{R}.(\mathsf{C}_{yz})$ we find:

$$\mathsf{R}.(\mathsf{C}_{yz}) \longrightarrow \mathsf{R}.() \qquad\qquad \mathsf{R}.(\mathsf{C}_{yz}) \longrightarrow \mathsf{R}.(\mathsf{C}_{yz} \,|\, \mathsf{C}_{yz})$$

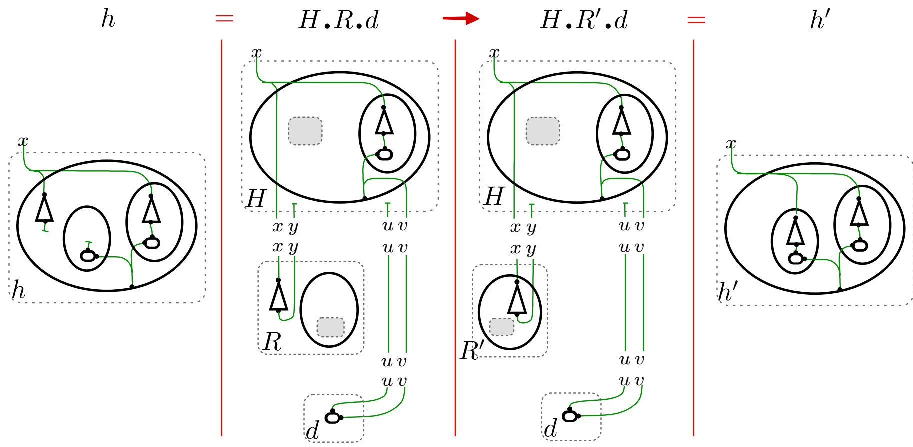


Figure 5: Reaction $h \longrightarrow\!\!\triangleright\ h'$ deconstructed

Both reactions are based on a parameter $d = \mathsf{C}_{yz}$; this parameter is discarded in the first case and duplicated in the second. In general, for a redex $R : \langle m, \emptyset\rangle \to \langle n, Y\rangle$, a parameter consists of m factors. For a reactum $R' : \langle 0, \emptyset\rangle \to \langle n, Y\rangle$, we must know, for each $i < n$ of R', which of the m factors of R should be inserted under i. The map $\eta : m \to n$ tells us that. E.g., the second of the above two rules have redex $\langle 1, \emptyset\rangle \to \langle 1, \emptyset\rangle$ and reactum $\langle 2, \emptyset\rangle \to \langle 1, \emptyset\rangle$; the map $\eta : 2 \to 1$ is in this case $[0 \mapsto 0, 1 \mapsto 0]$.

Finally, why must parameters be ground and discrete? They are ground simply to make reaction apply only to ground bigraphs; reaction of bigraph contexts have yet to be useful. They are discrete because there is no obvious right way to duplicate non-discrete parameters. Similar considerations causes the restriction that redex and reactum have no downwards names. Refer to one of [1, 3, 6, 20] for details. We now define:

Definition 6 (free bigraphical reactive system)**.** *A* free bigraphical reactive system (BRS) $\mathrm{B{\small G}}(\mathcal{K}, \mathcal{R})$ *consists of* $\mathrm{B{\small G}}(\mathcal{K})$ *equipped with a set* $\mathcal{R}$ *of reaction rules. A* free sub-BRS of $\mathrm{B{\small G}}(\mathcal{K}, \mathcal{R})$ *consists of* $\mathrm{B{\small G}}(\mathcal{K}', \mathcal{R}')$*, where* $\mathcal{K}' \subseteq \mathcal{K}$*.*

Using the signature $\mathcal{K}_{\mathsf{built}}$ of the preceding section, and the reaction rules $\mathcal{R}_{\mathsf{built}}$ of Figure 4, we may form a BRS $\mathrm{B{\small G}}(\mathcal{K}_{\mathsf{built}}, \mathcal{R}_{\mathsf{built}})$. A sub-BRS will come later.

The combination of bigraphical structure and dynamics is powerful and flexible enough to capture the both the term-structure and and the reaction semantics of major calculi such as CCS [1, 3], various π-calculi [6], Petri-nets [4], and λ-calculus [13]. Multi-site redexes are crucial to most of these.

4 Calculation example

In this section, we demonstrate by example how we embed calculation into a BRS, and we sketch our main results on the interplay between calculation and reaction. We formalise the notions and sketches introduced here in the subsequent sections.

Consider the reaction rule B2 of Figure 4 for an agent entering a room:

$$\mathsf{B2}: \quad \mathsf{A}_{xy} \,|\, \mathsf{R}.\square \longrightarrow\!\!\triangleright\ \mathsf{R}.(\square \,|\, \mathsf{A}_{xy}) \,.$$

How can we refine this rule, so that an agent is only admitted to a room if she satisfies some condition? Let us imagine that she uses a swipe card. This is easily modelled by increasing the arity of A from 2 to 3, adding a port; in an agent-node A_{xyz}, z is the extra link. The identity of an agent can now be given manifestation a Tag_z node, also linked to this z. We now require that each room contains an Admit-molecule, containing the names of – i.e. tags linked to – all the agents it can admit. In this simple case, we can refine the rule B2 so that only these named agents can enter:

$$\mathsf{B2}': \quad \mathsf{A}_{xyz} \,|\, \mathsf{R}.(\boxed{0} \,|\, \mathsf{Admit}.(\boxed{1} \,|\, \mathsf{Tag}_z)) \longrightarrow\!\!\triangleright\ \mathsf{R}.(\boxed{0} \,|\, \mathsf{A}_{xyz} \,|\, \mathsf{Admit}.(\boxed{1} \,|\, \mathsf{Tag}_z)) \,.$$

No calculation was needed here, because the matching of bigraphs, in particular the detection of a redex occurrence, is powerful enough to enforce the condition.

In contrast, suppose admission depends upon a numerical condition: that each room has a lower age-limit for the agents that may enter it. Now each agent must carry her age, and each room its limit. Admission now involves calculation: before an agent can enter, we must *calculate* whether the agent's age is greater than the room's age-limit.

We add a sub-BRS performing that calculation. Take controls $\mathcal{K}_{\leq} = \{\leq : 0,\ \mathsf{Succ} : 0,\ \mathsf{Zero} : 0,\ \mathsf{True} : 0,\ \mathsf{False} : 0\}$, and reaction rules $\mathcal{R}_{\leq} = \{\mathsf{L1}, \mathsf{L2}, \mathsf{L3}\}$ given by:

$$\mathsf{L1} : \mathsf{Zero} \leq \square \longrightarrow \mathsf{True} \qquad \mathsf{L2} : \mathsf{Succ}(\square) \leq \mathsf{Zero} \longrightarrow \mathsf{False}$$
$$\mathsf{L3} : \mathsf{Succ}(\boxed{0}) \leq \mathsf{Succ}(\boxed{1}) \longrightarrow \boxed{0} \leq \boxed{1}$$

We write the control "$\leq$" infix for readability[2]; we ought to write, e.g., $\leq\ .(\square \otimes \mathsf{Zero})$. We now have a BRS $\mathrm{BG}(\mathcal{K}_{\leq}, \mathcal{R}_{\leq})$, which we shall embed in $\mathrm{BG}(\mathcal{K}_{\mathsf{built}}, \mathcal{R}_{\mathsf{built}})$, in essence embedding calculation in it. We proceed as follows. First, we modify the rules $\mathcal{R}_{\mathsf{built}}$ to use calculation. We factor the rule B2 into two stages. In the first, the following rule initiates the calculation:

$$\begin{aligned}\mathsf{B2.1} : \quad & \mathsf{A}_{xy}.\mathsf{Age}.\boxed{0} \mid \mathsf{R}.(\boxed{1} \mid \mathsf{Agelimit}.\boxed{2}) \longrightarrow \\ & /z\, \mathsf{A}'_{xyz}.\mathsf{Age}.\boxed{0} \mid \mathsf{R}'_{z}.(\boxed{1} \mid \mathsf{Agelimit}.\boxed{2} \mid \mathsf{Pass}.(\boxed{2} \leq \boxed{0}))\ .\end{aligned}$$

With Tag_z replaced by Agelimit, we no longer need the extra port on A introduced above, and so revert to A having arity 2. We do add new controls Agelimit and A', though, so altogether we need to work within a signature $\mathcal{K}'_{\mathsf{built}} = \mathcal{K}_{\mathsf{built}} \cup \{\mathsf{Agelimit} : 0,\ \mathsf{A}' : 3\}$. Observe that A, R have become A', R', committing them to a mutual reaction that depends upon the outcome of the comparison. The transitory pair $(\mathsf{A}', \mathsf{R}')$ is linked at z to avoid confusion with other such pairs that may be simultaneously formed.

In the second stage, the following two rules either permit or deny the entry:

$$\begin{aligned}\mathsf{B2.2} : \quad & /z\, \mathsf{A}'_{xyz}.\boxed{0} \mid \mathsf{R}'_{z}.(\boxed{1} \mid \mathsf{Pass}.\mathsf{True}) \quad \longrightarrow \quad \mathsf{R}.(\boxed{1} \mid \mathsf{A}_{xy}.\boxed{0}) \\ \mathsf{B2.3} : \quad & /z\, \mathsf{A}'_{xyz}.\boxed{0} \mid \mathsf{R}'_{z}.(\boxed{1} \mid \mathsf{Pass}.\mathsf{False}) \quad \longrightarrow \quad \mathsf{A}_{xy}.\boxed{0} \mid \mathsf{R}.\boxed{1}\ .\end{aligned}$$

In the presence of $\mathrm{BG}(\mathcal{K}_{\leq}, \mathcal{R}_{\leq})$, the rules $\mathsf{B2.1}, \mathsf{B2.2}, \mathsf{B2.3}$ in a sense implements a *conditional* rule. Here the condition is simple, but the principle applies for arbitrarily complex conditions. Thus the embedding of calculation adds considerable power.

Formally, this is how we add calculation: Define a set of reaction rules $\mathcal{R}'_{\mathsf{built}} = \{\mathsf{B1}, \mathsf{B2.1},\ \mathsf{B2.2},\ \mathsf{B2.3}, \mathsf{B3}\}$ (with $\mathsf{B1}, \mathsf{B3}$ from Figure 4). Now construct $\mathrm{BG}(\mathcal{K}'_{\mathsf{built}} \cup \mathcal{K}_{\leq}, \mathcal{R}'_{\mathsf{built}} \cup \mathcal{R}_{\leq})$. This BRS embeds $\mathrm{BG}(\mathcal{K}_{\leq}, \mathcal{R}_{\leq})$ as a sub-BRS for calculation; the admission rules B2.i in a sense rely on this sub-BRS to perform numerical calculation.

But how does the calculation sub-BRS interact with our original BRS? For instance, the reaction rule L1 of $\mathrm{BG}(\mathcal{K}_{\leq}, \mathcal{R}_{\leq})$ discards its parameter and thus might destroy a redex of $\mathrm{BG}(\mathcal{K}'_{\mathsf{built}}, \mathcal{R}'_{\mathsf{built}})$. We would like calculation in $\mathrm{BG}(\mathcal{K}_{\leq}, \mathcal{R}_{\leq})$ to never destroy redexes of $\mathrm{BG}(\mathcal{K}'_{\mathsf{built}}, \mathcal{R}'_{\mathsf{built}})$, and only create them for rules such as B2.2 and B2.3.

Let us be precise about this notion of "disciplined interplay". Call reaction in the calculating sub-BRS *unfolding*, and write it $\hookrightarrow$; call reaction in the host BRS *liberal*, and write it the usual way, $\longrightarrow$. For $\mathrm{BG}(\mathcal{K}_{\mathsf{built}} \cup \mathcal{K}_{\leq}, \mathcal{R}'_{\mathsf{built}} \cup \mathcal{R}_{\leq})$, $\mathcal{R}_{\leq}$ gives rise to unfolding $\hookrightarrow$ and $\mathcal{R}'_{\mathsf{built}}$ to liberal reaction $\longrightarrow$.We prove in Theorem 26 that, under suitable conditions: (1) unfolding $\hookrightarrow$ is confluent, and (2) whenever a bigraph a has both a liberal reaction $a \longrightarrow a'$ and an unfolding $a \hookrightarrow^* b$, then there exists a b' s.t. $a' \hookrightarrow^* b'$ and $b \longrightarrow b'$. In this case we say that unfolding respects liberal reaction. Diagrammatically:

$$\begin{array}{ccc} a \longrightarrow a' & & a \longrightarrow a' \\ \big\downarrow{*} & \text{implies for some } b' & \big\downarrow{*} \qquad \big\downarrow{*} \\ b & & b \longrightarrow b' \end{array}$$

That unfolding is confluent ensures that given a choice between different possible unfoldings, it does not matter which is chosen: intuitively, if one such choice enables a liberal reaction, it remains available even if not made right away.

[2]This notation implies an ordering among the children of the "$\leq$"-node. Such an ordering is readily enforced by wrapping children in special "first','"second" etc. controls, indicating which child constitutes which argument. We omit these controls, again for readability.

Unfolding respecting liberal reaction means that it does not destroy liberal reaction: we can find $b \longrightarrow\!\!\!\triangleright\, b'$. Unfolding may of course create a liberal redex.The correct intuition is that calculation is cheap, more or less of it makes little difference. Reaction may create or destroy calculation, because it can duplicate or discard a factor of its parameter – which may already be calculating! This is admitted by the use of $\hookrightarrow^*$ rather than $\hookrightarrow$.We shall formalise this intuition later, proving that if we take unfolding as an equivalence — a structural congruence if you will —, then reaction is in a sense closed under this equivalence.

The idea of introducing calculation by combining BRSs was introduced in [21, 22], where a much cruder notion of sub-BRS was used. The present paper takes this idea much further, on the one hand by allowing much more interplay between the calculational and the ambient BRS, on the other by systematically studying this interplay.

Next, we study the interplay of sets ofreaction rules in an abstract setting. We use that study when we prove unfolding confluent in Section 6; and when we prove that unfolding respects liberal reaction in Section 7.

5 Parametric Reactive Systems

We now leave bigraphs behind for a while, considering instead an abstraction of bigraphs we call Parametric Reactive Systems (PRSs). Studying the interplay of PRSs will help us understand the interplay of liberal and unfolding reaction in bigraphs. A PRS is a particular case of a *reactive system* [23], where reaction is given not by ground rules, but by parametric ones. This extra structure helps us reason about that interplay.

Recall that bigraphs have a partial tensor, and thus form an spm: a symmetric partial monoidal category. Write ϵ for the tensor unit; a morphism is *ground* if its domain is ϵ. We tame the partiality by taking an *object-definite spm*:

Definition 7 (ground, object-definite)**.** *If $\mathcal{C}$ is an spm, then a sub-spm $\mathcal{D}$ of $\mathcal{C}$ is* ground *if every ground morphism of $\mathcal{C}$ is also a morphism of $\mathcal{D}$. An spm is* object-definite *if f, g have $f \otimes g$ defined whenever $\mathsf{cod}(f) \otimes \mathsf{cod}(g)$ and $\mathsf{dom}(f) \otimes \mathsf{dom}(g)$ are.*

Bigraphs are object-definite, as is every standard smc.

Definition 8 (PRS)**.** *A* parametric reactive system *(PRS) comprises an object-definite spm-category $\mathcal{C}$; a ground spm-subcategory $\mathcal{D}$ of active contexts, prefix-closed under decomposition*[3] $(R : x \to y, R' : x' \to y, \rho)$*. Here, the* instantiation map *ρ is a function $\mathcal{C}(\epsilon, x) \to \mathcal{C}(\epsilon, x')$. An* occurrence *of a redex R in a ground morphism a is a pair (C, d) s.t. $a = C \circ R \circ d$ and C is active, that is $C \in \mathcal{D}$. In this case, a has a* reaction*$a \longrightarrow\!\!\!\triangleright\, a' = C \circ R' \circ \rho(d)$. A PRS is* active *if every context is active, i.e., if $\mathcal{D} = \mathcal{C}$.*

Here R, R', d etc. are morphisms of $\mathcal{C}$, and ϵ, x, x' are objects. This definition generalises Definitions 5 and 6 from highly-structured bigraphs to abstract object-definite spm categories. In Definition 5 we exploited the monoidal structure of bigraphs to specify, via a map η, how sites of the reactum would be plugged from sites of the redex, altogether telling us how to form the parameter d' for the reactum from a parameter d for the redex. Here we abstract away from the details of taking d to d', saying simply that a reaction rule comes with a function ρ, which for each possible parameter d for the redex tells you the corresponding parameter $\rho(d)$ for the reactum.

An η of any bigraphical reaction rule uniquely determines an instantiation map $\overline{\eta}$. In fact, a BRS fixes a PRS with the same reaction relation by taking every BRS rule (R, R', η) to PRS-rules $(R \otimes \mathsf{id}_X, R' \otimes \mathsf{id}_X, \overline{\eta})$ for X which has those tensors defined. Here $\overline{\eta}$ re-interprets η as an instantiation map as mentioned above, cf. [1, Def'n 8.3, p.90]).

The notion of active contexts here is standard for reactive systems. Active contexts of bigraphs do form a ground sub-category, and a category of bigraphs is active iff every control is. The "ground" requirement is an inconsequential technical requirement, sufficient to obtain the following lemma:

Lemma 9. *Let $a : \epsilon \to x$ be a ground morphism and $C : x \otimes y \to z$ an active context of a PRS $\mathcal{P}$. Then $C \circ (f \otimes 1_z)$ is an active context of $\mathcal{P}$.*

Intuitively, this lemma says that inserting a ground-term into a one of hole of a multi-hole context gives you a new active context.

[3] $E \circ F = D \in \mathcal{D} \Rightarrow F \in \mathcal{D}$ and if also $H \in \mathcal{D}$ then $E \circ H \in \mathcal{D}$. This relaxes reactive systems enough to include bigraphs; we conjecture it is still strong enough to give the usual bisimulation congruence result.

We shall now work our way to sufficient conditions for a PRS to be confluent, and for one PRS to respect another, as sketched in the previous section. We then apply these conditions to bigraphs in the next two sections. First, confluence.

Definition 10 (confluence)**.** *A relation $\rightarrow$ is* confluent *if, whenever $a \rightarrow^* b$ and $a \rightarrow^* c$, then there exists d such that $b \rightarrow^* d$ and $c \rightarrow^* d$.*

Theorem 11. *Let $\mathcal{P}$ be a PRS, and let $\multimap$ be a binary relation s.t. $\rightarrowtriangle \;\subseteq\; \multimap \;\subseteq\; \rightarrowtriangle^*$. Suppose moreover that when $a \rightarrowtriangle b$ and $a \multimap c$, then there exists d with $c \rightarrowtriangle^* d$ and $b \multimap d$.*

$$
\begin{tikzcd}
a \arrow[r, -{Triangle[open]}] \arrow[d, -o] & b \\
c &
\end{tikzcd}
\qquad \textit{implies for some } d \qquad
\begin{tikzcd}
a \arrow[r, -{Triangle[open]}] \arrow[d, -o] & b \arrow[d, -o] \\
c \arrow[r, -{Triangle[open]}, "*"'] & d
\end{tikzcd}
$$

Then $\mathcal{P}$-reaction $\rightarrowtriangle$ is confluent.

Proof. We first prove that under this assumption, if $a \rightarrowtriangle^* b$ and $a \multimap c$, then $b \multimap d$ and $c \rightarrowtriangle^* d$.

$$
\begin{tikzcd}
a \arrow[r, -{Triangle[open]}, "*"] \arrow[d, -o] & b \\
c &
\end{tikzcd}
\qquad \text{implies for some } d \qquad
\begin{tikzcd}
a \arrow[r, -{Triangle[open]}, "*"] \arrow[d, -o] & b \arrow[d, -o] \\
c \arrow[r, -{Triangle[open]}, "*"'] & d
\end{tikzcd}
\tag{1}
$$

By induction on n in $a \rightarrowtriangle^n b$. For $n = 0$, take $d = c$ and (1) is trivial, so suppose $a \rightarrowtriangle a' \rightarrowtriangle^n b$. We find

$$
\begin{tikzcd}
a \arrow[r, -{Triangle[open]}] \arrow[d, -o] & a' \arrow[r, -{Triangle[open]}, "n"] \arrow[d, -o] & b \arrow[d, -o] \\
c \arrow[r, -{Triangle[open]}, "*"'] & b' \arrow[r, -{Triangle[open]}, "*"'] & d
\end{tikzcd}
$$

where b' and the left-most square follows from the assumption, and d and the right-most square from the induction hypothesis.

We now prove confluence, that is, if $a \rightarrowtriangle^* b$ and $a \rightarrowtriangle^* c$, then there exists some d with $b \rightarrowtriangle^* d$ and $c \rightarrowtriangle^* d$. We proceed by induction on n in $a \rightarrowtriangle^n b$. Again, if $n = 0$ we are done with $c = d$, so suppose $a \rightarrowtriangle a' \rightarrowtriangle^n b$. We find

$$
\begin{tikzcd}
a \arrow[r, -{Triangle[open]}] \arrow[d, -{Triangle[open]}, "*"'] & a' \arrow[r, -{Triangle[open]}, "n"] \arrow[d, -{Triangle[open]}, "*"'] & b \arrow[d, -{Triangle[open]}, "*"] \\
c \arrow[r, -o] & b' \arrow[r, -{Triangle[open]}, "*"'] & d
\end{tikzcd}
$$

where b' and the left-most square follows from (1) using that $a \rightarrowtriangle a'$ implies $a \multimap a'$, and d and the right-most square follows from the induction hypothesis. Because $\multimap$ implies $\rightarrowtriangle^*$, we have $c \rightarrowtriangle^* d$. $\square$

Here is a suitable relation for using this theorem to establish confluence:

Definition 12 (parallel reaction)**.** *Let $\mathcal{P}$ be a PRS, and let a, b be ground bigraphs. We write $a \rightarrowtriangle\!\!\triangleright b$ iff*

$$
a = E \circ \bigotimes_{i \leq n} R_i \circ d_i \qquad \textit{and} \qquad b = E \circ \bigotimes_{i \leq n} R'_i \circ \rho_i(d_i)
$$

s.t. E is active and (R_i, R'_i, ρ_i) are rules of $\mathcal{P}$ for $1 \leq i \leq n$.

Intuitively, $a \longrightarrow\!\!\triangleright\!\!\triangleright b$ means that a contains $n{\geq}0$ separate redexes, and will become b after doing the corresponding n reactions in any order. Observe that $a \longrightarrow\!\!\triangleright b$ implies $a \longrightarrow\!\!\triangleright\!\!\triangleright b$, which in turn implies $a \longrightarrow\!\!\triangleright^* b$.

We move on to consider the interplay of two PRSs, proving that unfolding respects liberal reaction in bigraphs: when $a \longrightarrow\!\!\triangleright a'$ and $a \hookrightarrow^* b$, there must exist some b' with $a' \longrightarrow\!\!\triangleright b'$ and $b \hookrightarrow^* b'$ (see (**??**)). It will be enough if (1) no liberal and unfolding redexes overlap, and (2) liberal instantiation preserves parallel unfolding, in a sense to be made precise, and (3) the unfolding PRS is active.

First, we formalise redexes "not overlapping". There are three ways redexes may not overlap: they are disjoint ("parallel"), one resides in a parameter of the other ("dominated"), or they actually do overlap, but have the same effect in reaction ("equivalent").

Definition 13 ($\|, >, \simeq$)**.** *Let $\mathcal{P}, \mathcal{Q}$ be (possibly identical) PRSson the same spm-category, and let R, S be redexes of $\mathcal{P}$, $\mathcal{Q}$, respectively. Suppose (C, d) and (D, e) are occurences of R and S in the same morphism; that is, $C \circ R \circ d = D \circ S \circ e$. We then say that:*

1. *(C, d) and (D, e) are* parallel*, written $(C, d) \parallel (D, e)$, if there exists E with $C = E \circ (- \otimes S \circ e)$ and $D = E \circ (R \circ d \otimes -)$.*

2. *(C, d)* dominates *(D, e), written $(C, d) > (D, e)$, if there exists D_0 with $D = C \circ R \circ D_0$ and $d = D_0 \circ S \circ e$.*

3. *(C, d) and (D, e) are* equivalent*, written $(C, d) \simeq (D, e)$, if both occurrences yields the same reactions; i.e., for each rule (R', R'', ρ) of $\mathcal{P}$ with $C \circ R' \circ d$ defined, there is a rule (S', S'', ϱ) of $\mathcal{Q}$ s.t. $C \circ R'' \circ \rho(d) = D \circ S'' \circ \varrho(e)$; and symmetrically.*

Next, we formalise instantiation of one PRS preserving parallel reaction of another.

Definition 14 ("instantiation respects")**.** *Let $\mathcal{P}, \mathcal{Q}$ be PRSs on the same spm-category. We say that $\mathcal{P}$-*instantiation respects *$\mathcal{Q}$*-reaction *iff for any $\mathcal{P}$-rule (R, R', ρ) and all d with $\rho(d)$ defined, if $d \longrightarrow\!\!\triangleright\!\!\triangleright_{\mathcal{Q}} d'$, then $\rho(d) \longrightarrow\!\!\triangleright\!\!\triangleright_{\mathcal{Q}} \rho(d')$.*

We can now state the key connection between spm-structure and reaction relations.

Theorem 15 (interplay of PRSs)**.** *Let $\mathcal{P}, \mathcal{Q}$ be PRSs on the same spm-category and suppose $a \longrightarrow\!\!\triangleright_{\mathcal{P}} b$ and $a \longrightarrow\!\!\triangleright_{\mathcal{Q}} a'$, with underlying occurrences γ, δ. Then:*

1. *If $\gamma \parallel \delta$ then there exists b' s.t. $a' \longrightarrow\!\!\triangleright_{\mathcal{P}} b'$ and $b \longrightarrow\!\!\triangleright_{\mathcal{Q}} b'$.*

2. *If $\gamma > \delta$, $\mathcal{P}$-instantiation respects $\mathcal{Q}$-reaction, and $\mathcal{Q}$ is active, then there exists b' with $a' \longrightarrow\!\!\triangleright_{\mathcal{P}} b'$ and $b \longrightarrow\!\!\triangleright\!\!\triangleright_{\mathcal{Q}} b'$.*

In diagrams:

$$\begin{tikzcd} a \arrow[r, "\mathcal{P}"] \arrow[d, "\mathcal{Q}"'] & b \\ a' & \end{tikzcd} \qquad 1.\ \begin{tikzcd} a \arrow[r, "\mathcal{P}"] \arrow[d, "\mathcal{Q}"'] & b \arrow[d, "\mathcal{Q}"] \\ a' \arrow[r, "\mathcal{P}"'] & b' \end{tikzcd} \qquad 2.\ \begin{tikzcd} a \arrow[r, "\mathcal{P}"] \arrow[d, "\mathcal{Q}"'] & b \arrow[d, "\mathcal{Q}"] \\ a' \arrow[r, "\mathcal{P}"'] & b' \end{tikzcd}$$

Proof. We have $C \circ R \circ d = a = D \circ S \circ e$ for rules (R, R', ρ) and (S, S', ϱ) of $\mathcal{P}, \mathcal{Q}$, respectively. Moreover, we have $a \longrightarrow\!\!\triangleright_{\mathcal{P}} b = C \circ R' \circ \rho(d)$ and $a \longrightarrow\!\!\triangleright_{\mathcal{Q}} a' = D \circ S' \circ \varrho(e)$.

Part 1. Suppose $(C, d) \parallel (D, e)$. Then there exists E, E_0, E_1 s.t. $a = E \circ (E_0 \circ R \circ d \otimes E_1 \circ S \circ e)$, $C = E \circ (E_0 \circ - \otimes E_1 \circ S \circ e)$, and $D = E \circ (E_0 \circ R \circ d \otimes E_1 \circ -)$. Then

$$\begin{aligned} b &= C \circ R' \circ \rho(d) \\ &= E \circ (E_0 \circ R' \circ \rho(d) \otimes E_1 \circ S \circ e) \\ &\longrightarrow\!\!\triangleright_{\mathcal{Q}} E \circ (E_0 \circ R' \circ \rho(d) \otimes E_1 \circ S' \circ \rho(e)) \\ &= b' \end{aligned}$$

$$
\begin{aligned}
a' &= D \circ S' \circ \varrho(d) \\
&= E \circ (E_0 \circ R \circ d \otimes E_1 \circ S' \circ \varrho(e)) \\
&\longrightarrow\!\!\triangleright_{\mathcal{P}} E \circ (E_0 \circ R' \circ \rho(d) \otimes E_1 \circ S' \circ \varrho(e)) \\
&= b'
\end{aligned}
$$

Here, reactions are justified by noting that from C, D active it follows that E, E_0, E_1 active, whence $E \circ (E_0 \circ R' \circ \rho(d) \otimes E_1 \circ -)$ and $E \circ (E_0 \circ - \otimes E_1 \circ S' \circ \varrho(e))$ are active using Lemma 9, noting that active-contexts form an spm.

Part 2. Suppose $(C, d) > (D, e)$. Then there exists D_0 with $d = D_0 \circ S \circ e$ and $D = C \circ R \circ D_0$. We compute:

$$
\begin{aligned}
a' &= D \circ S' \circ \varrho(e) \\
&= C \circ R \circ D_0 \circ S' \circ \varrho(e) \\
&\longrightarrow\!\!\triangleright_{\mathcal{P}} C \circ R' \circ \rho(D_0 \circ S' \circ \varrho(e)) \\
&= b'
\end{aligned}
$$

$$
\begin{aligned}
b &= C \circ R' \circ \rho(d) \\
&= C \circ R' \circ \rho(D_0 \circ S \circ e) \\
&\longrightarrow\!\!\triangleright\!\!\triangleright_{\mathcal{Q}} C \circ R' \circ \rho(D_0 \circ S' \circ \varrho(e)) \\
&= b'
\end{aligned}
$$

Where the latter step follows because $\mathcal{P}$-instantiation (here, ρ) respects $\mathcal{Q}$-reaction, $D_0 \circ S \circ e \longrightarrow\!\!\triangleright_{\mathcal{Q}} D_0 \circ S' \circ \varrho(e)$, and every context active for $\mathcal{Q}$ □

Intuition: If a contains two redexes, one from $\mathcal{P}$, one from $\mathcal{Q}$, then these redexes yield reactions $a \longrightarrow\!\!\triangleright_{\mathcal{P}} a'$ and $a \longrightarrow\!\!\triangleright_{\mathcal{Q}} b$. Now, (1) if the redexes are parallel, the reactions commute. (2) If the $\mathcal{P}$-redex has the $\mathcal{Q}$-redex in its parameter, then the $\mathcal{P}$-reaction $a \longrightarrow\!\!\triangleright_{\mathcal{P}} a'$ will at worst discard or duplicate the $\mathcal{Q}$-redex, since $\mathcal{P}$-instantiation preserves (parallel) reaction of $\mathcal{Q}$. So after executing the copies of the $\mathcal{Q}$-redex in parallel $a' \longrightarrow\!\!\triangleright\!\!\triangleright_{\mathcal{Q}} b$, one will find the same thing as if one had first used the original $\mathcal{Q}$-redex $a \longrightarrow\!\!\triangleright_{\mathcal{Q}} b$, and *then* duplicated or discarded its reactum by using the $\mathcal{P}$-redex $b \longrightarrow\!\!\triangleright_{\mathcal{P}} b'$. This insight is key in defining unfolding later.

Notation. When $a = E \circ (\bigotimes_{i \le n} r_i)$, we take $E^k = E \circ [(\bigotimes_{i<k} r_i) \otimes - \otimes (\bigotimes_{k<i} r_i)]$. For object-definite spms, E^k is defined when a is.

Lemma 16. *Let $\mathcal{P}$ be a PRS. Then $\mathcal{P}$-reaction is confluent if P is active, $\mathcal{P}$-instantiation respects $\mathcal{P}$-reaction, and the following holds. Whenever a has reactions $a \longrightarrow\!\!\triangleright b$ and $a \longrightarrow\!\!\triangleright\!\!\triangleright c$, then these reactions have underlying occurrences $a = C \circ R \circ d$ and $a = E \circ (\bigotimes_{i \le n} R_i \circ d_i)$, such that at least* one *of the following three statements is true.*

1. *Either there exists i with*

$$
\begin{aligned}
d_i &= D_i \circ R \circ d \\
C &= E^i \circ R_i \circ D_i
\end{aligned}
$$

2. *Up to equivalence of occurrences there exists $I \subseteq 1, \ldots, n$ and k, E' such that*[4]

$$
\begin{aligned}
d &= D \circ \bigotimes_{i \in I} R_i \circ d_i \\
E &= E' \circ [(R \circ D) \otimes -] \\
C &= E' \circ [- \otimes \bigotimes_{j \in \complement I} R_j \circ d_j)]
\end{aligned}
$$

[4]That is, suppose $(C, d) \simeq (\bar{C}, \bar{d})$ and for some $\bar{E}$, each $(C^i, d_i) \simeq (\bar{E}^i, \bar{d}_i)$, then there exists k, E' satisfying the equations, only substituting $\bar{C}/C$, $\bar{d}/d$ etc.

3. *For some i, the occurrence (C, d) is equivalent to the occurrence (E^i, d_i).*

Proof. We prove that $\mathcal{P}$ in this case satisfies the preconditions of Theorem 11; confluence is then immediate. So suppose for some a we have $a \longrightarrow\!\!\triangleright\, b$ and $a \longrightarrow\!\!\triangleright\!\!\triangleright\, c$. Then $a = C \circ R \circ d$ and $a = E \circ (\bigotimes_{i \leq n}(R_i, d_i))$. By assumption we must have either (1), (2), or (3) above satisfied. The case (3) is trivial; we consider the other two cases separately.
(1). We compute.

$$\begin{aligned}
b &= C \circ R' \circ \rho(d) \\
&= E \circ [(R_1 \circ d_1) \otimes \cdots \otimes (R_i \circ D_i \circ R' \circ \rho(d)) \otimes \cdots \otimes (R_n \circ d_n)] \\
&\longrightarrow\!\!\triangleright\!\!\triangleright\, E \circ [(R_1' \circ \rho_1(d_1)) \otimes \cdots \otimes (R_i' \circ \rho_i(D \circ R' \circ \rho(d))) \otimes \cdots \otimes (R_n' \circ \rho_n(d_n))] \\
&= d
\end{aligned}$$

And, the other way around:

$$\begin{aligned}
c &= E \circ [(R_1' \circ \rho_1(d_1)) \otimes \cdots \otimes (R_i' \circ \rho_i(d_i)) \otimes \cdots \otimes (R_n' \circ \rho_n(d_n))] \\
&= E \circ [(R_1' \circ \rho_1(d_1)) \otimes \cdots \otimes (R_i' \circ \rho_i(D \circ R \circ d)) \otimes \cdots \otimes (R_n' \circ \rho_n(d_n))] \\
&\longrightarrow\!\!\triangleright\!\!\triangleright\, E \circ [(R_1' \circ \rho_1(d_1)) \otimes \cdots \otimes (R_i' \circ \rho_i(D \circ R' \circ \rho(d))) \otimes \cdots \otimes (R_n' \circ \rho_n(d_n))] \\
&= d
\end{aligned}$$

(2). We compute.

$$\begin{aligned}
b &= C \circ R' \circ \rho(d) \\
&= E' \circ [- \otimes \bigotimes_{j \in \complement I} R_j \circ d_j] \circ R' \circ \rho(d) \\
&= E' \circ [(R' \circ \rho(D \circ \bigotimes_{i \in I} R_i \circ d_i)) \otimes (\bigotimes_{j \in \complement I} R_j \circ d_j)] \\
&= E' \circ [(R' \circ \rho(D \circ \bigotimes_{i \in I} R_i \circ d_i)) \otimes (\bigotimes_{j \in \complement I} R_j \circ d_j)] \\
&\longrightarrow\!\!\triangleright\!\!\triangleright\, E' \circ [(R' \circ \rho(D \circ \bigotimes_{i \in I} R_i' \circ \rho_i(d_i))) \otimes (\bigotimes_{j \in \complement I} R_j \circ d_j)] \\
&\longrightarrow\!\!\triangleright\!\!\triangleright\, E' \circ [(R' \circ \rho(D \circ \bigotimes_{i \in I} R_i' \circ \rho_i(d_i))) \otimes (\bigotimes_{j \in \complement I} R_j' \circ \rho_j(d_j))] \\
&= d
\end{aligned}$$

Where the composite reaction $\longrightarrow\!\!\triangleright\!\!\triangleright\!\longrightarrow\!\!\triangleright\!\!\triangleright$ is also parallel because the underlying reactions takes place on either side of a tensor[5] The other way around:

$$\begin{aligned}
c &= E \circ (\bigotimes_{i \leq n}(R_i', \rho(d_i))) \\
&= E' \circ [(R \circ D) \otimes -] \circ \pi \circ (\bigotimes_{i \leq n}(R_i', \rho(d_i))) \\
&= E' \circ [(R \circ D \circ \bigotimes_{i \in I}(R_i' \circ \rho_i(d_i))) \otimes \bigotimes_{j \in \complement I} R_j' \circ \rho_j(d_j)] \\
&\longrightarrow\!\!\triangleright\, E' \circ [(R' \circ \rho(D \circ \bigotimes_{i \in I}(R_i' \circ \rho_i(d_i)))) \otimes \bigotimes_{j \in \complement I} R_j' \circ \rho_j(d_j)] \\
&= d
\end{aligned}$$

$\square$

[5] In general, tensor preserves parallel reaction: if $a \longrightarrow\!\!\triangleright\!\!\triangleright\, b$ and $c \longrightarrow\!\!\triangleright\!\!\triangleright\, d$ then $a \otimes b \longrightarrow\!\!\triangleright\!\!\triangleright\, c \otimes d$.

For certain bigraph redexes, *any* instantiation respects parallel reactions.

Lemma 17. *Let $\mathcal{P}, \mathcal{Q}$ be PRSs induced by BRSs, and suppose every redex of $\mathcal{Q}$ has codomain $\langle 1, X\rangle$. Then $\mathcal{P}$-instantiation respects $\mathcal{Q}$-reaction.*

Bigraphs with domain $\langle 1, X\rangle$ are usually called "prime"; all redexes we have seen in examples so far have been prime. An example of a non-prime bigraph is d in Figure 2. The maps η of bigraphical reaction rules do not necessarily preserve parallel reaction of non-prime redexes. To see this, suppose d was a redex of some rule. If d appears also as a parameter for some other rule, the map η of that rule might discard the left region, but retain the right. But then $d \longrightarrow\!\!\triangleright\, d'$ for some d', but applying the instantiation map $\overline{\eta}$ to obtain $\overline{\eta}(d)$, we lost half the redex, and so have $\overline{\eta}(d) \not\longrightarrow\!\!\triangleright\!\!\triangleright$.

The above lemma is crucial to the present development; indeed, we currently see no easy path to extending the present development to wide unfoldings.

In subsequent section, we shall apply these theorems to BRSs. The relevant structure of BRSs is essentially captured by the following factorisation lemma.

Lemma 18. *Let $\hat{a}$ be an agent of a concrete BRS, and suppose $\hat{C} \circ \hat{r} = \hat{D} \circ \hat{s}$ with $\mathsf{cod}(\hat{r}) \otimes \mathsf{cod}(\hat{s})$ defined.*

1. *If the support of $\hat{r}$ is disjoint from the support of $\hat{s}$, $\hat{r}$ is epi, and $\hat{s}$ is epi; then there exists $\hat{E}$ with*

$$\hat{C} = \hat{E} \circ (- \otimes \hat{s}) \tag{2}$$

$$\hat{D} = \hat{E} \circ (\hat{r} \otimes -) \tag{3}$$

2. *If $r = \hat{R} \circ \hat{d}$ and the support of $\hat{s}$ is contained in the support of $\hat{d}$, and $\hat{s}$ has no edges and is epi; then there exists $\hat{D}_0$ with*

$$\hat{D} = \hat{C} \circ \hat{R} \circ \hat{D}_0 \tag{4}$$

$$\hat{d} = \hat{D}_0 \circ \hat{s} \tag{5}$$

Proof. Part 1. Suppose $\mathsf{cod}(\hat{r}) = (n, X)$ and $\mathsf{cod}(\hat{s}) = (m, Y)$. Note that because $\hat{r} \otimes \hat{s}$ defined, X, Y must be disjoint. We define $\hat{E} : (n + m, X \cup Y) \to \mathsf{cod}(\hat{a})$. The support of $\hat{E}$ is $|\hat{a}| \setminus (|\hat{r}| \cup |\hat{s}|)$. The parent map of $\hat{E}$ is the obvious restriction of the parent map of $\hat{a}$, extended with $\hat{E}(i) = \hat{C}(i)$ for $i < n$ and $\hat{E}(j + n) = \hat{D}(j)$ for $n \leq j < n + m$. Clearly, $\hat{E}(v)$ is defined for all $v \in \hat{E}$ or $\hat{a}$ cannot be ground. The link map of $\hat{E}$ is the obvious restriction of the link map of $\hat{a}$, extended with $\hat{E}(x) = \hat{C}(x)$ for $x \in X$, and $\hat{E}(y) = \hat{D}(y)$ for $y \in Y$. We show that this link map is defined for all points p in $\hat{E}$. Suppose for a contradiction that at p it is not. Clearly $\hat{a}(p)$ is then an edge. If $\hat{a}(p) \in |r|$ then also $p \in |r|$, but that contradicts $p \in |\hat{E}|$; similarly if $\hat{a}(p) \in |s|$. From r epi we get (2), and from s epi we get (3).

Part 2. We similarly find a place graph D_0^P. We construct also a link graph D_0^L. Supposing $\hat{R}$ has names Y in its inner face and $\hat{s}$ names X in its outer face, we have to construct $D_0^L : X \to Y$. Suppose $\hat{s}(p) = y \in Y$. Take $D_0^L(y) = \hat{d}(p)$. To see this well-defined, suppose also $D_0^L(p') = y$; because $\hat{C} \circ \hat{r} = \hat{D} \circ \hat{s}$, necessarily p, p' has the same parent also in $\hat{d}$. Clearly we have found a D_0 satisfying (5). Now (4) follows from $\hat{s}$ epi. □

6 Unfolding

We now step down from the abstract PRSs and return to bigraphs and BRSs. In this section, we define *unfolding* BRSs, which perform calculation. We shall prove that those are confluent, and we shall see that $\mathrm{BG}(\mathcal{K}_{\leq}, \mathcal{R}_{\leq})$ is in fact an unfolding BRS.

We begin with a summary of *atomic* unfolding, as introduced in Section 11.2 of the book [1]; we then generalise it to parametric unfolding. An atomic *unfolding* rule is a reaction rule (r, r', η) in which the redex r consists of just a control, the reactum has no sites, and consequently, η is empty; a rule $(\mathsf{K}_{\vec{x}}, r', [])$. We call the control K a *seed*. The redex $\mathsf{K}_{\vec{x}}$, has n distinct names $\vec{x}$, and the reactum $r' : \langle 0, \emptyset\rangle \to \langle 1, \vec{x}\rangle$ may contain occurrences of K and other seeds.

Unfolding thus can represent recursion, e.g., a CCS user-defined recursion $A(\vec{x}) \stackrel{\text{def}}{=} P_A$, and so extends the bigraphical encoding of finite CCS [3, 1] to infinite CCS, and similarly for CSP [24].

Unfortunately, atomic unfolding is too weak, e.g, it cannot represent $\mathrm{BG}(\mathcal{K}_{\le}, \mathcal{R}_{\le})$. Hence, parametric unfolding, where we allow *parametric* seeds. These unfold differently for different parameter *patterns*. So each parametric seed K has a set of patterns Δ_{K}, each being a discrete bigraph $P : \langle m, \emptyset \rangle \to \langle k, X \rangle$ containing no seeds. Parametric unfolding recalls the standard form of a parametric redex in term-rewriting or pattern-matching rules in a functional languages such as SML, only in bigraphs rather than terms.

Discrete patterns are a technical convenience; requiring so does not seem to adversely affect expressiveness. We conjecture that the results in this paper holds for arbitrary patterns.

In $\mathrm{BG}(\mathcal{K}_{\le}, \mathcal{R}_{\le})$, the control "$\le$" is a parametric seed, with set of patterns[6]

$$\Delta_{\le} = \{\square \parallel \mathsf{Zero},\ \mathsf{Zero} \parallel \mathsf{Succ}(\square),\ \mathsf{Succ}(\boxed{0}) \parallel \mathsf{Succ}(\boxed{1})\}$$

. Note that these patterns are discrete.

Definition 19 (unfolding rule, BRS)**.** *A* (parametric) unfolding rule *is a reaction rule of the form* $(\mathsf{K}_{\vec{x}} \bullet P,\ U,\ \eta)$ *where* K *is a parametric seed and* $P \in \Delta_{\mathsf{K}}$ *is a pattern of* K*. A BRS* $\mathrm{BG}(\mathcal{K}, \mathcal{R})$ *is an* unfolding *BRS if every rule of* $\mathcal{R}$ *is an unfolding rule.*

We will usually drop the "parametric" and speak simply of "unfolding rules". In the sequel, we shall imagine the set of patterns Δ_{K} for a control K fixed by the signature.

$\mathrm{BG}(\mathcal{K}_{\le}, \mathcal{R}_{\le})$ is in fact an unfolding BRS as its reaction rules $\mathcal{R}_{\le}$ are unfolding ones under the patterns $\Delta_{\le}$. Composing the seed "$\boxed{0} \le \boxed{1}$" with the patterns of $\Delta_{\le}$', yields the redexes of rules L1, L2, and L3.

Unfolding BRSs will be our notion of calculation. As presented, they are, however, not confluent. Even with the discipline of distinct seed controls and patterns, nothing prevents patterns from overlapping. But we can require that they do not:

Definition 20 (orthogonal)**.** *A set of patterns* Δ *is* orthogonal *if its patterns are pairwise inconsistent, i.e., if for any two distinct patterns* $P, Q \in \Delta$ *and all parameters* d, e, $P \bullet d \not\simeq Q \bullet e$*. An unfolding BRS is* orthogonal *if all its seeds have orthogonal patterns.*

And this is enough! With redexes not overlapping, Theorems 15 and 11 of the preceding section can be used to establish that orthogonal, unfolding BRSs are confluent.

Definition 21 (free calculus)**.** *A* free calculus *is an orthogonal, unfolding BRS.*

Theorem 22. *In an a free calculus, unfolding is confluent.*

Proof. Let $\mathcal{U}$ be the PRS induced by a free calculus. It is sufficient to show that $\mathcal{U}$ satisfies the preconditions of Lemma 16. Every redex of $\mathcal{U}$ has prime redex, so by Lemma 17, $\mathcal{U}$-instantiation respects $\mathcal{U}$-reaction. Now consider some ground bigraph a and rules (R, R', ρ) and $R_i, R'_i \rho_i$.

$$C \circ R \circ d = a = E \circ (\bigotimes_{i \le n} R_i \circ d_i) \tag{6}$$

First note that we can choose all the constituent variables such that the tensor of any pair among R, R_i is defined. Now observe that the equation (6) holds in the category $\mathcal{U}$ iff each constituent has a pre-image in the concrete pre-category '$\mathcal{U}$ underlying $\mathcal{U}$. Thus, we have

$$\hat{C} \circ \hat{R} \circ \hat{d} = \hat{a} = \hat{E} \circ (\bigotimes_{i \le n} \hat{R}_i \circ \hat{d}_i) \tag{7}$$

in '$\mathcal{U}$. Observe that $R = K \bullet P$ and $R_i = K_i \bullet P_i$ for seeds K, K_i and discrete bigraphs P, P_i with no seed controls. Write v for the unique node of $\hat{R}$ with control K and u_i for each of the unique nodes of $\hat{R}_i$ with control K_i. We proceed by cases on the relative positioning of v and the u_i. There are three cases: either (1) $v = u_i$ for some i; (2)

[6] We again omit details of distinguishing the first and second argument.

some u_i is a proper ancestor of v, (3) no u_i is an ancestor of v, and v is a proper ancestor of u_i for exactly $i \in I$ for some possibly empty subsequence $I \subseteq \{1, \dots n\}$.

Case 1. Assume $v = u_i$. Then, writing B^P for the place component of a bigraph B, we must have $\hat{R}^P \circ \hat{d}^P = \hat{R}^P \circ \hat{e}^P$. Thus, because $\hat{R}, \hat{d}, \hat{S}, \hat{e}$ are all discrete, there exists substitutions[7] σ, τ s.t. $\hat{R}.\hat{d} = \sigma\hat{R}_i.\tau\hat{d}_i$. Thus $\hat{R}.\hat{d} \simeq \hat{R}_i.\hat{\tau}d_i$. But then, because $\mathcal{U}$ is unfolding, we must have $R = R_i$, $R' = R'_i$ and $\eta = \eta_i$, lest orthogonality of patterns be violated. It follows that $\sigma = \mathsf{id}$. Because unfolding redexes are mono, we find from $\hat{R}.\hat{d} = \hat{R}.\tau\hat{e}$ that $d = \tau e$. Using that unfolding ground rules are epi and pushing through the substitution τ, we find from $\hat{C} \circ (\hat{R} \otimes \mathsf{id}_X) \circ \tau\hat{e} = \hat{E}^i \circ (\hat{R}_i \otimes \mathsf{id}_{X_i}) \circ \hat{d}_i$ that $C\tau' = \hat{E}^i$ for $\tau' = \tau \otimes \mathsf{cod}(R) \otimes \mathsf{id}_1$. We compute:

$$\begin{aligned}\hat{C} \circ (\hat{R}' \otimes \mathsf{id}_X) \circ \overline{\eta}(\hat{d}) &= \hat{C} \circ (\hat{R}'_i \otimes \mathsf{id}_X) \circ \overline{\eta}(\tau\hat{d}_i) \\ &= \hat{C} \circ (\hat{R}'_i \otimes \mathsf{id}_X) \circ \tau\overline{\eta}_i(\hat{d}_i) \\ &= \hat{E}^i \circ (\hat{R}'_i \otimes \mathsf{id}_{X_i}) \circ \overline{\eta}_i(\hat{d}_i)\end{aligned}$$

The penultimate step exploits that in the case of BRSs, linking commutes with instantiation; cf. Proposition 8.4 of [1]; the last step pushes through the substitution τ. Thus this pair of occurrences are equivalent.

Case 2. Assume that u_i is an ancestor of v. Because v has seed control, it is not in $\hat{R}_i$; thus, it is in $\hat{d}_i$. Clearly $|(\hat{R} \otimes \mathsf{id}_X) \circ \hat{d}| \subseteq |\hat{d}_i|$. We now get the factorisation (1) of Lemma 16 using Lemma 18, part 2.

Case 3. Assume that v has no u_i as an ancestor, and assume wlog (choose equivalent occurrences of the redexes if necessary) that the descendants of v among u_i are exactly those with $i < k$ for some k. Because redexes of $\mathcal{U}$ contain a unique root seed, clearly $\hat{R}$ and $\hat{R}_i$ for $k < i \leq n$ all have disjoint support, and equally clearly, $|\hat{R}|$ contains the support of $\hat{R}_j, \hat{d}_j$ for $1 \leq j \leq k$. We now have the following.

$$\hat{C} \circ \hat{R} \circ \hat{d} = \hat{E} \circ [(\bigotimes_{i \leq k} R_i \circ d_i) \otimes (\bigotimes_{j > k} R_j \circ d_j)]$$

A little more concisely, hoping that the gentle reader will infer the definitions of $\hat{E}_{i,j}$ and $\hat{r}_i$:

$$\hat{C} \circ \hat{R} \circ \hat{d} = \hat{E}_{1,k} \circ \bigotimes_{i \leq k} \hat{r}_i$$

Observing that $\hat{R} \circ \hat{d}$ is discrete and epi, we apply Lemma 18, part 2, to find $\hat{D}_0$ with

$$\begin{aligned}\hat{E}_{1,k} &= \hat{C} \circ \hat{R} \circ \hat{D}_0 \\ \hat{d} &= \hat{D}_0 \circ \bigotimes_{i \leq k} r_i\end{aligned}$$

But then we have

$$\hat{C} \circ \hat{R} \circ \hat{D}_0 \circ \bigotimes_{i \leq k} r_i = E_{k+1,n} \circ \bigotimes_{j > k} r_j$$

where $\hat{R} \circ \hat{D}_0 \circ \bigotimes_{i \leq k} r_i$ and $\bigotimes_{j > k} r_j$ have disjoint support, and both are discrete and epi, so by Lemma 18, part 1, we find $\hat{E}'$ with

$$\begin{aligned}\hat{C} &= \hat{E}' \circ (- \otimes \bigotimes_{j > k} r_j) \\ \hat{E}_{k+1,n} &= \hat{E}' \circ (R \circ D_0 \circ \bigotimes_{i \leq k} r_i \otimes -)\end{aligned}$$

But then we have $\hat{E} \circ [\bigotimes_{i \leq k} r_i \otimes \bigotimes_{j > k} r_k] = \hat{E}_{k+1,n} \circ \bigotimes_{j > k} r_k = \hat{E}' \circ (R \circ D_0 \circ \bigotimes_{i \leq k} r_i \otimes \bigotimes_{i > k} r_j)$ we find by $\bigotimes_{i \leq k} r_i \otimes \bigotimes_{j > k} r_k$ epi that

$$\hat{E} = \hat{E}' \circ (R \circ D_0 \otimes -),$$

which is what we needed to prove. □

[7] We allow ourselves the notation "σf" where we should write "$(\sigma \otimes \mathsf{id}_{\mathsf{width}(f)}) \circ f$"; and similarly for $f\sigma$.

$\mathrm{B}\textsc{g}(\mathcal{K}_{\le}, \mathcal{R}_{\le})$ is a free calculus. In general, a free calculus has controls besides seeds; they are *constructors*, and those with rank 0 are *constants*. In $\mathrm{B}\textsc{g}(\mathcal{K}_{\le}, \mathcal{R}_{\le})$ we have constructors Zero, True, False of rank 0 and Succ of rank 1.

Notation. In keeping with familiar notation, we write a comma for the monoidal product $\otimes$, and we write a context such as Cons occurring in a parametric seed $\mathsf{K}_{\vec{x}}.P$ as $\mathsf{Cons}(\boxed{i}, \boxed{j})$, where the indices i and j indicate the ordinal positions of these two sites in the inner width of P.

We give a second example: Lists. Constructors are Cons of rank 2 and Nil of rank 0. An arbitrary finite list with members $\{d_i : i \in n\}$ takes the form

$$\mathsf{Cons}.(d_0 \otimes \mathsf{Cons}.(\cdots \mathsf{Cons}.(d_{n-1} \otimes \mathsf{Nil}) \cdots)) \,.$$

Names of the d_i can be shared or closed as necessary. The constructors Cons and Nil happen to have arity 0, but non-zero arities can be useful. One example is the Tag-node introduced in Section 4: by putting Tags inside Cons-nodes, we can form lists of identities and compute with them. A recursive function over lists is represented by a seed and its unfolding. E.g, concatenating two lists is done by the seed Append of with patterns $\Delta_{\mathsf{Append}} = \{\mathsf{Cons}.(\boxed{0} \otimes \boxed{1}) \otimes \boxed{2},\ \mathsf{Nil}\}$ and unfolding rules:

$$\begin{array}{rcl} \mathsf{Append}.(\mathsf{Cons}.(\boxed{0} \otimes \boxed{1}) \otimes \boxed{2}) & \hookrightarrow & \mathsf{Cons}.(\boxed{0} \otimes \mathsf{Append}.(\boxed{1} \otimes \boxed{2})) \\ \mathsf{Append}.(\mathsf{Nil} \otimes \Box) & \hookrightarrow & \Box \,. \end{array}$$

The class of free calculi has the computing power of Turing-machines; this is straightforwardly verified using the standard encoding into orthogonal term-rewriting [25][8]

Theorem 23. *Free calculi with finite signatures and rule-sets are Turing complete.*

Proof. We make the following inconsequential constraints on Turing machines: We consider single-head, single-tape machines; there are no transitions to the initial state q_0 or from the halting state q_h; the machine is never stuck, i.e., the transition $\delta(q, b)$ is defined for every $q \neq q_h$ and every symbol b. The alphabet is $\{0, 1, \mathsf{x}\}$. The initial configuration of a machine is in state q_0 with the input starting immediately to the right of the read/write head.

We give an adaptation of the standard encoding of Turing machines into orthogonal term-rewriting systems [25]. First note that ordered sub-nodes in bigraphs are readily encoded by encapsulating each sub-node in a control indicating its position. So if we have a control f, supposedly taking two arguments or sub-nodes, we encapsulate these in controls first, second; we then encode, e.g., $f(x, y)$ where f is a constructor and x, y variables as $\mathsf{f}.(\mathsf{first}.\boxed{0} \mid \mathsf{second}.\boxed{1})$. (This is to avoid sorting or ranking, but rather stay in a free BRS.) We write $\mathsf{f}(\boxed{0}, \boxed{1})$ as a short-hand for $\mathsf{f}.(\mathsf{first}.\boxed{0} \mid \mathsf{second}.\boxed{1})$.

Using these orderings, we easily encode lists like described above. Rather than writing $\mathsf{Cons}.(\mathsf{first}.\boxed{0} \mid \mathsf{second}.\boxed{1})$, we write simply $\boxed{0} \cdot \boxed{1}$.

We can now encode a Turing machine $M = \langle q_0, q_h, Q, \delta \rangle$ as the unfolding BRS over signature $\Sigma_M = \{q : 0 \mid q \in Q\} \cup \{\mathsf{first}, \mathsf{second}, 0, 1, \mathsf{x}, \bullet\}$ with rules as follows. $\bullet$ is used to simulate to infinite blank tape at either end of the footprint of the machine for a given execution. We represent a state as a control q and two lists: the tape at the left of the read/write-head, and the tape including and to the right of the read-write head.

For each transition	there are reaction rules for each $a \in \{0, 1, \mathsf{x}\}$	
$\delta(q, b) = (q', b', R)$	$q(\boxed{0}, b \cdot \boxed{1}) \hookrightarrow q'(b' \cdot \boxed{0}, \boxed{1})$	(R1)
$\delta(q, b) = (q', b', L)$	$q(a \cdot \boxed{0}, b \cdot \boxed{1}) \hookrightarrow (\boxed{0}, a \cdot (b' \cdot \boxed{1}))$	(R2)
	$q(\bullet, b \cdot \boxed{0}) \hookrightarrow q'(\bullet, \mathsf{x} \cdot (b' \cdot \boxed{0}))$	(R3)
$\delta(q, \mathsf{x}) = (q', b', R)$	$q(\boxed{0}, \bullet) \hookrightarrow q'(b' \cdot \boxed{0}, \bullet)$	(R4)
$\delta(q, \mathsf{x}) = (q', b', L)$	$q(a \cdot \boxed{0}, \bullet) \hookrightarrow b' \cdot (a \cdot \boxed{0})$	(R5)
	$q(\bullet, \bullet) \hookrightarrow q'(\bullet, b' \cdot \bullet)$	(R6)

The rules are split on cases according to whether the machine must read outside its footprint (R1-3) or not (R4-6). The left-moving rules are further split on whether the move takes the machine outside its footprint (R3,6) or not (R4,5).

[8] Thanks to Jakob Grue Simonsen for pointing suggesting this encoding to me. The present formulation is an adaptation of the one used in his [26].

Write $\mathcal{R}_M$ for these rules. We must prove that the $\text{BG}(\Sigma_M, \mathcal{R}_M)$ is unfolding and orthogonal. It is unfolding with seeds Q; each seed $q \in Q$ has, for $a, b \in \{0, 1, \mathsf{x}\}$, patterns a subset of

$$\Delta_q = \left\{ \begin{array}{rl} \boxed{0} \otimes b \cdot \boxed{1}, & \text{(R1)} \\ \boxed{0} \otimes \bullet, & \text{(R4)} \\ \hline a \cdot \boxed{0} \otimes b \cdot \boxed{1}, & \text{(R2)} \\ \bullet \otimes b \cdot \boxed{0}, & \text{(R3)} \\ a \cdot \boxed{0} \otimes \bullet, & \text{(R5)} \\ \bullet \otimes \bullet & \text{(R6)} \end{array} \right\} .$$

The patterns above the lines are induced by transitions $(\,-\,,\,-\,,R)$, the one below the line by transitions $(\,-\,,\,-\,,L)$. Because the original machine M is non-deterministic, the machine cannot move both left and right on the same input. Hence Δ_q can contain either (R4) or (R5),(R6) but not both; and similarly, for a fixed b, it can contain either (R1) or (R2),(R3). It is now straightforward to verify that each Δ_q is orthogonal: For (R1), $b \neq \bullet$ [R4]; it is mutually exclusive with [R2,R3] and again $b \neq \bullet$ [R6]. For (R4), $b \neq \bullet$ [R2,R3] and it's mutually exclusive with [R5,R6]. For (R2), $a \neq \bullet$ [R3], $b \neq \bullet$ [R5,R6]. For (R3), $b \neq \bullet$ [R5,R6]. For (R5), $a \neq \bullet$. □

7 Calculation

Finally, we define formally a calculational BRS, and pin down the interplay of unfolding and liberal reaction. So far, we have sketched calculation as an embedding of a free calculus C in a free BRS A. We will need some restrictions, though, to ensure that unfolding in C does not adversely affect reaction in A, as sketched in Section 4. It will be sufficient to require (1) that redexes of A and C never overlap, and (2) that no redex of A ever occurs in a parameter of C. This way, A may duplicate or discard entire redexes of C, but C can never discard, destroy, or duplicate a redex of A; we can now apply Theorem 15.

For the latter restriction, no A-redexes in C-parameters, we focus on bigraphs where no C-node has A-children. We call such a bigraph *layered*. Every bigraph in Section 4 is layered, as no $\mathcal{K}_{\leq}$-node ever has a $\mathcal{K}_{\mathsf{built}}$-child. Of course, not every bigraph is layered; in a free BRS *all* controls can be freely mixed. For instance, the seemingly non-sensical bigraph $\mathsf{Succ}(\mathsf{A}_{xy})$, which has agent A of $\mathcal{K}_{\mathsf{built}}$ sitting inside a $\mathcal{K}_{\leq}$-node, is nonetheless a bigraph of $\text{BG}(\mathcal{K}_{\mathsf{built}} \cup \mathcal{K}_{\leq}, \mathcal{R}_{\mathsf{built}} \cup \mathcal{R}_{\leq})$. However, we can ensure that layered bigraphs are preserved by reaction. Altogether, we get the following definition.

Definition 24. (calculational BRS) A free BRS $A = \text{BG}(\mathcal{K}_A, \mathcal{R}_A)$ is *calculational* if it has a sub-BRS $C = \text{BG}(\mathcal{K}_C, \mathcal{R}_C)$ which is a free calculus, and such that:

1. No A-redex contains a C-seed.
2. In a liberal rule (R, R', η), if a site i of R' is guarded by a C-node, then so is the site $\eta(i)$ of R.
3. Each region of a liberal redex is guarded by a node of control $\mathcal{K}_A \setminus \mathcal{K}_C$, a *liberal* node.

A free calculus have two reaction relations: ordinary reaction $\longrightarrow\!\!\triangleright$ is the reaction relation of $\text{BG}(\mathcal{K}_A, \mathcal{R}_A \setminus \mathcal{R}_C)$; unfolding $\hookrightarrow$ is the reaction relation of $\text{BG}(\mathsf{active}(\mathcal{K}_A), \mathcal{R}_C)$, where $\mathsf{active}(\mathcal{K}_A)$ is the same signature as $\mathcal{K}_A$ except every control is active.

Notice that the unfolding $\hookrightarrow$ does not respect passive controls of $\mathcal{K}_A$: unfolding may occur anywhere, anytime. Intuitively, we would like to think of, say, "$\mathsf{Zero} \leq \mathsf{Succ}(\mathsf{Zero})$" and "$\mathsf{True}$" as equivalent, and thus also, say, the larger bigraphs $\mathsf{R}(\mathsf{Zero} \leq \mathsf{Succ}(\mathsf{Zero})$ and $\mathsf{R}(\mathsf{True})$ as equivalent. To make sure that liberal reaction behaves *as if* it was closed under this equivalence, we must be able to unfold (convert) the former to the latter, no matter whether $\mathsf{Zero} \leq \mathsf{Succ}(\mathsf{Zero})$ is locked within a passive control or not. We formalize these ideas below.

If the signature $\mathcal{K}_A$ is in fact active, the reaction and unfolding relations $\longrightarrow\!\!\triangleright$ and $\hookrightarrow$ form a partitioning of the standard reaction relation for $\text{BG}(\mathcal{K}_A, \mathcal{R}_A)$.

Because of the first condition above, we never need to convert from, e.g., $\mathsf{R}(\mathsf{True})$ to $\mathsf{R}(\mathsf{Zero} \leq \mathsf{Succ}(\mathsf{Zero}))$. A-redexes cannot contain unfinished computations (seeds, "$\leq$"), only values normal forms (constructors, "$\mathsf{True}, \mathsf{Zero}, \mathsf{Succ}$"). The second and third conditions ensures that A-reaction preserves layering:

Proposition 25. *If g is layered and $g \longrightarrow\!\!\!\!\triangleright\ g'$ or $g \hookrightarrow g'$, then g' is layered.*

We can now state and prove our main result: calculation is confluent, and never preempts liberal reaction. The proof relies on Theorems 22 and 15.

Theorem 26. *In a free calculational BRS, unfolding is (1) confluent, and (2) respects liberal reaction. That is, for layered ground bigraphs a, b, if $a \longrightarrow\!\!\!\!\triangleright\ b$ and $a \hookrightarrow^* a'$, then $a' \longrightarrow\!\!\!\!\triangleright\ b'$ and $b \hookrightarrow^* b'$ for some b'.*

Proof. First observe that whenever $a \hookrightarrow a'$ and $a \longrightarrow\!\!\!\!\triangleright\ b$ we have for some b' that $b \hookrightarrow^* b'$ and $a' \longrightarrow\!\!\!\!\triangleright\ b'$, then it follows by induction that whenever $a \hookrightarrow^* a'$ and $a \longrightarrow\!\!\!\!\triangleright\ b$ also $a' \longrightarrow\!\!\!\!\triangleright\ b'$ and $b \hookrightarrow^* b'$. Thus, using the above proposition and Theorem 15, it is sufficient to show that for every layered a, every two occurrences γ, δ from $\mathrm{BG}(\mathcal{K}_A, \mathcal{R}_A \setminus \mathcal{R}_C)$ respectively $\mathrm{BG}(\mathsf{active}(\mathcal{K}_A), \mathcal{R}_C)$ in a has either $\gamma \parallel \delta$ or $\gamma > \delta$.

So consider an agent a, with such occurrences $(C, d), (D, e)$.

$$C \circ (R \otimes \mathsf{id}_X) \circ d = a = D \circ (S \otimes \mathsf{id}_Y) \circ e \;. \tag{8}$$

As previously, the equation (8) holds in the category of $\mathrm{BG}(\mathcal{K}_A) = \mathrm{BG}(\mathsf{active}(\mathcal{K}_A))$ iff each constituent has a pre-image in the underlying concrete pre-category, and we thus find there that

$$\hat{C} \circ (\hat{R} \otimes \mathsf{id}_X) \circ \hat{d} = \hat{a} = \hat{D} \circ (\hat{S} \otimes \mathsf{id}_Y) \circ \hat{e} \;.$$

Write v for the unique root of $\hat{S}$. We proceed by cases on the relative positioning of the node v and the nodes of $\hat{R}$. There are four cases: (1) either v is itself in $\hat{R}$, (2) v is an ancestor of some w in $\hat{R}$, (3) v is a descendant of some w in $\hat{R}$, or (4) none of (1)-(3). As we shall see, (1) and (2) are impossible.

Case 1. Assume $v \in \hat{S}$. This is impossible because w has seed control and R contains no seeds. Contradiction.

Case 2. Assume v is an ancestor of some node w in $\hat{R}$. But then by assumption w has an ancestor w' in $\hat{R}$ which is a root of $\hat{R}$. Again by assumption, this w' has liberal control, and thus, again by assumption, cannot be a descendant of v, which has non-liberal seed control. Contradiction.

Case 3. Assume that v is a descendant of some node w in $\hat{R}$. Again because v has seed control, it is not in $\hat{R}$, whence $|(\hat{S} \otimes \mathsf{id}_Y) \circ \hat{e}| \subseteq |\hat{d}|$, and we may apply Lemma 18 to find $(C, d) > (D, e)$.

Case 4. Suppose v is not a node of $\hat{R}$, and that is neither an ancestor or a descendant of any node of $\hat{R}$. Clearly $(\hat{R} \otimes \mathsf{id}_X) \circ \hat{d}$ and $\hat{S} \otimes \mathsf{id}_Y) \circ \hat{e}$ have disjoint support. We apply Lemma 18 to find $(C, d) \parallel (D, e)$.

$\square$

We conclude by lifting unfolding to a "structural congruence", and proving that liberal reaction is in a sense closed under this structural congruence.

Corollary 27. *For a free calculational BRS, define structural congruence $\equiv$ as the symmetric, reflexive, and transitive closure of $\hookrightarrow$; and define unfolding reaction $\longrightarrow\!\!\!\!\blacktriangleright\ = \hookrightarrow^* \longrightarrow\!\!\!\!\triangleright$. Then for layered bigraphs a, b, unfolding reaction is closed under structural congruence: if $a \equiv a'$ and $a \longrightarrow\!\!\!\!\blacktriangleright\ b$, then $a' \longrightarrow\!\!\!\!\blacktriangleright\ b'$ and $b \equiv b'$.*

Proof. We first show an auxiliary lemma: if $a \equiv a'$ then for some c, $a \hookrightarrow^* c$ and $a' \hookrightarrow^* c$. By induction on the number on n steps taken by $\equiv$. For $n = 0$, $a = a'$ so take $c = a = a'$ and we are done. For $n > 0$, suppose $a \equiv a'$ in $n + 1$ steps. There are two cases.

$$\begin{tikzcd} a \arrow[r, phantom, "\equiv"] \arrow[dr, hook, "*"'] & a'' \arrow[r, hook] \arrow[d, hook, "*"] & a' \arrow[d, hook, "*"] \\ & c' \arrow[r, hook, "*"] & c \end{tikzcd} \qquad \begin{tikzcd} a \arrow[r, phantom, "\equiv"] \arrow[dr, hook, "*"'] & a'' \arrow[d, hook, "*"] & a' \arrow[l, hook'] \\ & c & \end{tikzcd}$$

In both cases, the triangle follows from the induction hypothesis. In the first case, the square follows from confluence of $\hookrightarrow$. The second case is immediate.

Now suppose $a \equiv a'$ and $a \longrightarrow\!\!\blacktriangleright\, b$. Then $a \hookrightarrow^* a'' \longrightarrow\!\!\triangleright\, b$ for some a''. We erect the following diagram.

$$
\begin{tikzcd}
a \arrow[r, phantom, "\equiv"] \arrow[d, hook, "*"'] & a' \arrow[d, hook, "*"'] \\
a'' \arrow[r, hook, "*"] \arrow[d, -{Triangle[open]}] & c' \arrow[d, -{Triangle[open]}] \\
b \arrow[r, hook, "*"] & c
\end{tikzcd}
$$

Here the top-square follows from $\hookrightarrow$ the preceding auxiliary lemma and Theorem 26 part (1), noting that $a'' \equiv a'$. The bottom square follows from Theorem 26 part (2); noting that because unfolding preserve layering, b and c' are both layered. □

Our next step, in order to understand calculation in practical applications, is to lift our theory of free calculational BRSs to sorted ones.

8 Static Sorting

So far we have dealt only with *free* bigraphical structure, with little constraint on placing and linking in bigraphs over an arbitrary signature. But every application domain requires some such constraint. For example, in our built environment we wish a room to contain only agents and computers, and these in turn to contain no nodes; also an agent's upper port to be linked only to other agents and its lower port only to a computer, in turn linked only to other computers.

Elementary structural constraints on bigraphs may be expressed in terms of a set of *place sorts* and/or a set of *link sorts*. Interfaces are then enriched by the assignment of sorts to their sites and names. Also, in terms of such sorts, controls are subjected to a discipline governing their nesting and linking.

Example 28. *We construct a sorting $\mathcal{S}_{\mathsf{built}}$ for our built environment as follows: Define a set $\mathsf{ps}_{\mathsf{built}} \stackrel{\text{def}}{=} \{\mathsf{a}, \mathsf{b}, \mathsf{c}, \mathsf{r}, \breve{\mathsf{ac}}, \breve{\mathsf{ar}}\}$ of place sorts. The first four are for regions whose outer nodes must be respectively agents, buildings, computers and rooms; $\breve{\mathsf{ac}}$ is for a region whose outer nodes must be agents or computers; similarly $\breve{\mathsf{ar}}$ for agents or rooms. Thus the place component m of $\langle m, X\rangle$ is enriched to any sequence in $(\mathsf{ps}_{\mathsf{built}})^m$, and the bigraphs in any sorted homset are limited to those satisfying the above constraint. Similarly we define a set $\mathsf{ls}_{\mathsf{built}}$ of link sorts, enrich the link component X of an interface by assigning a link sort to each $x \in X$; finally imposing the above link constraints.*

Such constraints suffice [4, 3, 6, 13] for several applications, including the encoding of process calculi, but can only impose limits on places and links independently. We now summarise a richer notion of sorting [16, 17, 18].

We have seen that an interface in a free bigraph can have many different enrichments in a sorted bigraph; in contrast, a sorted homset $\hat{I} \to \hat{J}$ may *exclude* members of the corresponding free homset. Put another way, we can think of the sorting as a functor from any spm category to free bigraphs that may not be bijective either for interfaces or for homsets, but is *faithful* – i.e. injective for each homset. This insight is realised in [16, 17, 18]. Moreover, such sortings can be defined not just for bigraphs but for for any categories. Here, in the spirit of [18], we proceed first to define sortings for spm categories, and later to specialise them to bigraphs.

Definition 29 (sorting)**.** *A* sorting *for an spm category A is a faithful spm functor $\mathcal{S} : \hat{A} \to A$. Call it* onto *if it is surjective on objects. Call it* reflective *if it reflects composition and monoidal product; that is, if $\mathcal{S}(\hat{a}) = a_1 \circ a_2$ then there exist $\hat{a}_1$ in $\hat{a}_2$ such that $\hat{a} = \hat{a}_1 \circ \hat{a}_2$, and similarly for the monoidal product.*

We shall use a hat, as in $\hat{a}$, to denote entities in the domain of a sorting. In previous work [16, 17, 18] the onto condition was required for all sortings, it is convenient here to relax it. This allows us spm sub-categories as sortings, particularly inclusion functors embedding BRS within larger ones. Recall that a sub-category of A is an inclusion functor into A, and the notion of spm sub-category is defined similarly. Whereas inclusion functors are not in general reflective, it is straightforward to verify that those of sub-BRSs are.

We now turn to sortings for a free bigraphical system $\mathrm{B}\textsc{g}(\mathcal{K})$:

Definition 30 (sorted BS)**.** *A* sorted *bigraphical system $\hat{A} = \mathrm{BG}(\mathcal{S})$ over $\mathcal{K}$ is a reflective sorting $\mathcal{S} : \hat{A} \to \mathrm{BG}(\mathcal{K})$. Call it a bigraph sorting.*

The reader may have expected further conditions for a bigraph sorting, since bigraph algebra is richer than spm algebra. But the only operations (apart from nullary ones, i.e. constants) in a free BS are composition and monoidal product; it is just the spm category generated by these constants, subject to certain equations [5, 19]. The constants are of five kinds: 1 and *join* for placing, closure $/x$ and substitution y/X for linking, and $\mathsf{K}_{\vec{x}}$ for node-ions. The axioms are proved to be complete.

In a bigraph sorting $\mathcal{S} : \hat{A} \to \mathrm{BG}(\mathcal{K})$ each such constant c will have zero or more pre-images in $\hat{A}$ – at most one per homset $\hat{I} \to \hat{J}$ because $\mathcal{S}$ is faithful. Each pre-image may therefore be denoted unambiguously as $\mathsf{c} : \hat{I} \to \hat{J}$. So an expression in bigraph algebra, enriched by ascribing a homset to each constant, denotes a unique (if any) morphism in $\hat{A}$. Indeed, one can often omit the homset when it can be understood; for example in a link-sorted BS one may write the substitution x/y without mentioning the sorts of x and y if clear from context. Thus algebraic manipulation in a sorted BS is both possible and easy.

Proposition 31. *Each bigraph axiom $E_1 = E_2$, enriched with homsets for constants, is sound for $\hat{A} = \mathrm{BG}(\mathcal{S})$ in the sense that the axiom holds in* BG*($\mathcal{S}$) whenever E_1 and E_2 are well-defined in $\hat{a}$.*

This result adds insight into bigraphical sortings, but we pursue it no further here.

Example 32. *As a simple example of a sorting $\mathcal{S} : \hat{A} \to A$ for a free BS $A = \mathrm{BG}(\mathcal{K}_{\mathsf{ccs}})$, consider the encoding of CCS into bigraphs [1, 3]. It has controls* Get *and* Send *for sending and receiving messages, and* Alt *for forming an alternation (a sum of alternative actions). It has two place-sorts:* p *for processes and* a *for alternations. With the above treatment of sortings the interfaces of $\hat{A}$ will take the form $\langle s, X\rangle$, with $s \in \{\mathsf{p}, \mathsf{a}\}^*$. The sorting discipline requires that the sorts of places should alternate (no pun intended): the children of every* p *node should have sort* a*, and vice versa. Sorts are assigned to all places in an interface, to ensure that the discipline is preserved under composition.*

A situation relevant to the present paper is when one BS 'sits inside' another. Suppose that $C = \mathrm{BG}(\mathcal{K}_C)$ and $A = \mathrm{BG}(\mathsf{K}_{\mathsf{lib}} \uplus \mathcal{K}_C)$ are free BSs. The two disjoint signatures play a symmetrical role within A; the bigraphs may mix $\mathsf{K}_{\mathsf{lib}}$-nodes freely with $\mathcal{K}_C$-nodes. We may wish to destroy this symmetry by declaring that the children of a $\mathcal{K}_C$-node must also be $\mathcal{K}_C$-nodes. The idea is that – when dynamic rules are added – the behaviour dictated by $\mathcal{K}_C$-rules for a $\mathcal{K}_C$ node and its descendants within A will be exactly as if C were in isolation. This discipline would embody *layering* of p. 19.

Layering can be represented by a sorting. Introduce two place sorts, lib and c; then define $A_C = \mathrm{BG}(\mathsf{K}_{\mathsf{lib}}, C)$ to have interfaces $\langle s, X\rangle$ where $s \in \{\mathsf{lib}, \mathsf{c}\}^*$, and to include all bigraphs in which the children of a lib-place may have either sort, but those of a c-place must have sort c. Thus we have a layered sorting $\mathcal{S}_C : A_C \to A$. We shall use this sorting later, when dynamics are introduced and C is a calculus.

9 Sorted dynamics

Let $A = \mathrm{BG}(\mathcal{K}, \mathcal{R})$ be a free BRS, and let $\mathcal{S} : \hat{A} \to \mathrm{BG}(\mathcal{K})$ be a sorting. The question now arises: how do we lift the reaction rules $\mathcal{R}$, to form rules $\hat{\mathcal{R}}$ for a sorted bigraphical reactive system $\hat{A} = \mathrm{BG}(\mathcal{S}, \hat{\mathcal{R}})$, in such a way that the induced reaction relation for $\hat{A}$ is related nicely to that for A? This question was treated previously in [17, 16]; presently, we give a stronger answer.

We shall continue to write sorted entities with a hat, e.g. a sorted BS $\hat{A}$ and all entities (objects, arrows, rule-sets or rules) pertaining to it.

Definition 33 (sorted BRS)**.** *Let $\mathcal{S} : \hat{A} \to A = \mathrm{BG}(\mathcal{K})$ be a bigraph sorting, and let A be equipped with rules $\mathcal{R}$, forming a free BRS $A = \mathrm{BG}(\mathcal{S}, \mathcal{R})$. A* sorted *BRS $\hat{A} = \mathrm{BG}(\mathcal{S}, \hat{\mathcal{R}})$ is the result of equipping $\hat{A}$ with a sorted rule-set $\hat{\mathcal{R}}$. These rules take the form*

$$(\hat{R} : \hat{I} \to \hat{J},\ \hat{R}' : \hat{I}' \to \hat{J},\ \eta)$$

where $\mathcal{S}(\hat{I}, \hat{I}') = (m, m')$ and $\eta : m' \to m$. As in Definition 5, for every parameter $\hat{d} : \hat{I} \otimes \hat{X} = \hat{d}_0 \otimes \cdots \otimes \hat{d}_{m-1}$, with $\mathcal{S}(\hat{d})$ discrete, the rule generates a ground rule $(\hat{r}, \hat{r}') = (\hat{R}\centerdot\hat{d}, \hat{R}'\centerdot\hat{d}')$, where $\hat{d}' = \hat{d}_{\eta(0)} \parallel \cdots \parallel \hat{d}_{\eta(m'-1)} \parallel \hat{X}$.

We will discuss how to transfer reaction from the original the sorted category. The following is the basic notion under investigation:

Definition 34 (preserve & create rules)**.** *We say that $\mathcal{S}$* preserves *rules if, whenever $(\hat{R}, \hat{R}', \eta) \in \hat{\mathcal{R}}$, then $(\mathcal{S}(\hat{R}), \mathcal{S}(\hat{R}'), \eta) \in \mathcal{R}$. We say that $\mathcal{S}$* creates *rules if, whenever $(\mathcal{S}(\hat{R}), R', \eta) \in \mathcal{R}$, then $(\hat{R}, \hat{R}', \eta) \in \hat{\mathcal{R}}$ for some $\hat{R}'$ such that $\mathcal{S}(\hat{R}') = R'$.*

We now explain how to ensure that $\mathcal{S} : \hat{A} \to A$ preserves and create rules. If we define sorted rules $\hat{\mathcal{R}}$ to mirror the free rules in $\mathcal{R}$, the following will be sufficient. The critical point is that, given a free rule (R, R', η), there may exist a $\mathcal{S}$-preimage $\hat{R}$ of R but no appropriate $\mathcal{S}$-preimage of R'. The following definition simply assumes away that situation.

Definition 35 ("sorting respects")**.** *A bigraph sorting $\mathcal{S} : \hat{A} \to A$* respects *rules $\mathcal{R}$ for A if whenever there is a rule $(\mathcal{S}(\hat{R}), R', \eta)$ of $\mathcal{R}$, there exists a pre-image $\hat{R}'$ of R' s.t. $(\hat{R}, \hat{R}', \eta)$ is a valid sorted reaction rule for $\hat{A}$.*

Here is the lifting itself.

Lemma 36. *Let $\mathcal{S} : \hat{A} \to A$ be a bigraph sorting, and let A be equipped with rules $\mathcal{R}$, forming a free BRS $A = \mathrm{BG}(\mathcal{S}, \mathcal{R})$. Define $\hat{\mathcal{R}}$ as follows: For every rule $(R : m \to J,\ R' : m' \to J,\ \eta)$, whenever $\hat{I},\ \hat{I}', \hat{R}, \hat{R}'$ are $\mathcal{S}$-sorted preimages of $m,\ m',\ R$ and R', we include a rule $(\hat{R}, \hat{R}', \eta)$ in $\hat{\mathcal{R}}$. This assignment form a sorted BRS $\mathrm{BG}(\mathcal{S}, \hat{\mathcal{R}})$. Then, if $\mathcal{S} : \hat{A} \to A$ respects $\mathcal{R}$, it preserves and creates rules.*

We now extend preserving and creating to ground rules and reaction relations:

Definition 37 (preserve & create ground rules)**.** *Let $\mathcal{S} : \hat{A} \to A$ be a sorting, where A and $\hat{A}$ are equipped with ground rule-sets $\mathcal{R}$ and $\hat{\mathcal{R}}$ respectively. Then:*

1. *$\mathcal{S}$ preserves ground rules if, whenever $(\hat{r}, \hat{r}') \in \hat{\mathcal{R}}_{\mathrm{g}}$, then $(\mathcal{S}(\hat{r}), \mathcal{S}(\hat{r}')) \in \mathcal{R}_g$.*
2. *$\mathcal{S}$ preserves reaction if $\hat{g} \longrightarrow \hat{g}'$ implies that $\mathcal{S}(\hat{g}) \longrightarrow \mathcal{S}(\hat{g}')$.*
3. *$\mathcal{S}$ creates ground rules if, when $(\mathcal{S}(\hat{r}), r') \in \mathcal{R}_{\mathrm{g}}$, then $(\hat{r}, \hat{r}') \in \hat{\mathcal{R}}_{\mathrm{g}}$ for some pre-image $\hat{r}'$ of r'.*
4. *$\mathcal{S}$ creates reaction, if when $\mathcal{S}(\hat{g}) \longrightarrow g'$ then $\hat{g} \longrightarrow \hat{g}'$ for some pre-image $\hat{g}'$ of g'.*

The following lemma helps move reactions across sortings.

Lemma 38. *Let $\mathcal{S} : \hat{A} \to A$ be a BRS sorting. Then*

1. *If $\mathcal{S}$ preserves rules then it preserves ground rules.*
2. *If $\mathcal{S}$ preserves ground rules then it preserves reaction.*
3. *If $\mathcal{S}$ creates rules then it creates ground rules.*
4. *If $\mathcal{S}$ creates ground rules then it creates reaction.*

Proof. 1. Assume $\mathcal{S}$ preserves rules, and suppose $(\hat{r}, \hat{r}')$ is a ground rule in $\hat{A}$. Then there is a rule $(\hat{R}, \hat{R}', \eta)$ with $(\hat{r}, \hat{r}') = (\hat{R}.\hat{d}, \hat{R}'.\hat{d}')$, where $\hat{d} = \hat{d}_0 \otimes \cdots \otimes \hat{d}_{m-1}$ with $\mathcal{S}(\hat{d})$ discrete and $\hat{d}' = d_{\eta(0)} \otimes \cdots \otimes d_{\eta(m'-1)}$. We have to prove that $(r, r') \stackrel{\text{def}}{=} (\mathcal{S}(\hat{r}), \mathcal{S}(\hat{r}'))$ is a ground rule in A.

By assumption there is a rule (R, R', η) in A, where $\mathcal{S}(\hat{R}) = R$, $\mathcal{S}(\hat{R}') = R'$. Therefore, setting $d_i \stackrel{\text{def}}{=} \mathcal{S}(\hat{d}_i)$ for $i \in m$, we have $d = d_0 \otimes \cdots \otimes d_{m-1} = \mathcal{S}(\hat{d})$ is discrete. Therefore, setting $d' \stackrel{\text{def}}{=} d_{\eta(0)} \parallel \cdots \parallel d_{\eta(m'-1)}$ there is a ground rule $(R.d, R'.d')$ in A. This is exactly the required ground rule (r, r').

2. Assume $\mathcal{S}$ preserves ground rules, and suppose $\hat{g} \longrightarrow \hat{g}'$ in $\hat{A}$. Then there is a ground rule $(\hat{r}, \hat{r}')$ and context $\hat{H}$ such that $\hat{g} = \hat{H} \circ \hat{r}$ and $\hat{g}' = \hat{H} \circ \hat{r}'$. But by assumption there is a ground rule $(\mathcal{S}(\hat{r}), \mathcal{S}(\hat{r}'))$ in A, and we readily find that $\mathcal{S}(\hat{g}) \longrightarrow \mathcal{S}(\hat{g}')$ as required.

3. Assume $\mathcal{S}$ creates rules, and suppose (r, r') is a ground rule in A with $r = \mathcal{S}(\hat{r})$. We have to find $\hat{r}'$ in $\hat{A}$ such that $r' = \mathcal{S}(\hat{r}')$ and $\hat{r} \longrightarrow \hat{r}'$.

Now $(r, r') = (R.d, R'.d')$ with discrete $d = d_0 \otimes \cdots \otimes d_{m-1}$ and $d' = d_{\eta(0)} \parallel \cdots \parallel d_{\eta(m'-1)}$, where (R, R', η) is a rule in A. Since $\mathcal{S}$ reflects nesting, there exist $\hat{R}$ and $\hat{d}$ such that $\hat{r} = \hat{R}.\hat{d}$, $\mathcal{S}(\hat{R}) = R$ and $\mathcal{S}(\hat{d}) = d$. Because $\mathcal{S}$ creates rules, we find $\hat{R}'$ with $\mathcal{S}(\hat{R}') = R'$ and $(\hat{R}, \hat{R}', \eta)$ a rule of $\mathcal{S}$. By reflection of $\otimes$ we have $\hat{d} = \hat{d}_0 \otimes \cdots \otimes \hat{d}_{m-1}$ where $\mathcal{S}(\hat{d}_i) = d_1$ for $i \in m$. So, defining $\hat{d}' \stackrel{\text{def}}{=} \hat{d}_{\eta(0)} \parallel \cdots \parallel \hat{d}_{\eta(m'-1)}$, there is a ground rule $(\hat{R}.\hat{d}, \hat{R}'.\hat{d}')$ in $\hat{A}$, easily seen to be the one required.

4. Assume $\mathcal{S}$ creates ground rules, and suppose $g \longrightarrow g'$ in A, where $g = \mathcal{S}(\hat{g})$. We have to prove that there exists $\hat{g}'$ such that $\hat{g} \longrightarrow \hat{g}'$ in $\hat{A}$, with $\mathcal{S}(\hat{g}') = g'$.

By supposition, there is a ground rule (r, r') in A with $g = H \circ r$ and $g' = H \circ r'$. By reflection of composition, there exist $\hat{H}$ and $\hat{r}$ in $\hat{A}$, with $\mathcal{S}(\hat{H}) = H$, $\mathcal{S}(\hat{r}) = r$ and $\hat{g} = H \circ r$. By assumption there exists $\hat{r}'$ with $\mathcal{S}(\hat{r}') = r'$, such that $(\hat{r}, \hat{r}')$ is a ground rule in $\hat{A}$. But then $\hat{H} \circ \hat{r} \longrightarrow \hat{H} \circ \hat{r}'$ in $\hat{A}$, and we are done by taking $\hat{g}' = \hat{H} \circ \hat{r}'$. ☐

Using Lemmas 36, 38 and, crucially, that sortings are faithful, we can prove that if we impose a sorting on a free BS equipped with rules, we can equip the sorted BS with rules, such that the sorted reaction relation mirrors the free one.

Theorem 39. *Let A be a free BS equipped with rules $\mathcal{R}$ to make a free BRS $A = \text{BG}(\mathcal{K}, \mathcal{R})$, and let $\mathcal{S} : \hat{A} \to A$ be a bigraph sorting respecting $\mathcal{R}$. Then we can equip $\hat{A}$ with rules, yielding a sorted BRS $\hat{A} = \text{BG}(\mathcal{S}, \hat{\mathcal{R}})$ such that:*

- *$\mathcal{S}$ preserves and creates reaction.*
- *Reaction is confluent for $\mathcal{S}(g)$ in A iff it is confluent in $\hat{A}$.*

Proof. The first part follows directly from the three lemmas. For the second part, let us just prove the forward implication, Let $g = \mathcal{S}(\hat{g})$, and assume that $\hat{g} \longrightarrow^* \hat{g}_0$ and $\hat{g} \longrightarrow^* \hat{g}_1$ in $\hat{A}$. Then, by iterating the preservation of reaction, we find $g \longrightarrow^* g_0$ and $g \longrightarrow^* g_1$ in A, where $g_i = \mathcal{S}(\hat{g}_1)$ $(i = 0, 1)$. By confluence in A we deduce that $g_0 \longrightarrow^* g'$ and $g_1 \longrightarrow^* g'$ for some g.

Now, by iterating the creation of reaction, we find that $\hat{g}_0 \longrightarrow^* \hat{g}'_0$ and $\hat{g}_1 \longrightarrow^* \hat{g}'_1$ in A, where $\mathcal{S}(g'_0) = \mathcal{S}(g'_1) = g'$. But in a reaction the homset remains constant, so by faithfulness of $\mathcal{S}$ we deduce that $\hat{g}'_0 = \hat{g}'_1$. This completes the proof of confluence for $\hat{g}$. ☐

Notice that the proof of confluence relies crucially on the functor being faithful.

10 Sorted calculation

Let us revert to our principal aim: to understand the role of calculation in a BRS, by means of sorting structure. In Definition 24, given a calculus C we defined the notion of a free calculational BRS over C. This leads naturally to the following:

Definition 40 (calculational BRS). *Let $C = \text{BG}(\mathcal{K}_C, \mathcal{R}_C)$ be a free calculus, and $A = \text{BG}(\mathsf{K}_{\mathsf{lib}}, \mathcal{R}_{\mathsf{lib}}, \mathcal{K}_C, \mathcal{R}_C)$ be a free calculational BRS over C. Let $\mathcal{S} : \hat{A} \to A$ be a bigraph sorting that preserves and creates rules, and let $\hat{\mathcal{R}}_{\mathsf{lib}}$ and $\hat{\mathcal{R}}_C$ be the rules created from $\mathcal{R}_{\mathsf{lib}}$ and $\mathcal{R}_C$. Then $\hat{A}$, denoted by $\text{BG}(\mathcal{S}, \hat{\mathcal{R}}_{\mathsf{lib}}, \hat{\mathcal{R}}_C)$, is a* calculational *BRS.*

Now all that was done in Section 9 can be applied independently to the two reaction relations in $\hat{A}$: liberal reaction $\longrightarrow$ due to $\mathcal{R}_{\mathsf{lib}}$ and unfolding $\hookrightarrow$ due to $\mathcal{R}_C$.

Theorem 41. *Let A be a free calculational BRS over C, with liberal rules $\mathcal{R}_{\mathsf{lib}}$ and unfolding rules $\mathcal{R}_C$. Let $\mathcal{S} : \hat{A} \to A$ be a bigraph sorting that creates and preserves rules, so that $\hat{A} = \text{BG}(\mathcal{S}, \hat{\mathcal{R}}_{\mathsf{lib}}, \hat{\mathcal{R}}_C)$ is a calculational BRS. If the $\mathcal{S}$-image of $\hat{A}$ contains only layered bigraphs, then, in $\hat{A}$:*

1. *Unfolding $\hookrightarrow$ is confluent.*
2. *Unfolding respects liberal reaction; that is, if $\hat{f} \longrightarrow \hat{f}'$ and $\hat{f} \hookrightarrow^* \hat{g}$, then $\hat{g} \longrightarrow \hat{g}'$ and $\hat{f}' \hookrightarrow^* \hat{g}'$ for some $\hat{g}'$.*

Proof. Part (1). By Theorem 22 unfolding in A is confluent. Then from Theorem 39 we get unfolding confluent in $\hat{A}$. For (2), observe that Theorem 39 also gives us that $\mathcal{S}$ preserves and creates reaction. Now suppose $\hat{f} \longrightarrow\!\!\triangleright \hat{f}'$ and $\hat{f} \hookrightarrow^* \hat{g}$. Then because $\mathcal{S}$ preserves reaction, also $f \longrightarrow\!\!\triangleright f'$ and $f \hookrightarrow^* g$, and because $\mathcal{S}$ has image all layered bigraphs, by Theorem 26, we find $g \longrightarrow\!\!\triangleright g'$ and $f' \hookrightarrow^* g'$ for some g'. Using that $\mathcal{S}$ creates reaction, we find $\hat{g}', \hat{g}''$, both with image g', s.t. $\hat{g} \longrightarrow\!\!\triangleright \hat{g}'$ and $\hat{f}' \hookrightarrow^* \hat{g}''$. But reaction preserves homsets, so by $\mathcal{S}$ faithful, we find $\hat{g}' = \hat{g}''$. □

Recall from Theorem 26 that respect for a *free* calculational BRS A only holds for layered bigraphs. But our condition that the $\mathcal{S}$-image of $\hat{A}$ consists only of layered bigraphs ensures respect in $\hat{A}$; we may say that such a sorting *creates* layering.

11 Conclusion

We have embedded calculation in a model of interactive or liberal behaviour, by defining a calculational BRS as a free BRS which embeds an unfolding sub-BRS performing calculation. We have proved that such unfolding is confluent, and that it respects liberal behaviour: unfolding may enable liberal behaviour, never prevents it. To prove so, we have generalised reactive systems to parametric reactive ones, and given conditions sufficient for confluence and the above "respect". Finally, we have generalized these results to encompass also sorted BRSs.

With an eye to applications, we have lifted these results across bigraph sortings, in the process giving theorems which help move reaction behaviour across sortings, as well as clarifying the interplay between bigraph axioms and reflective bigraph sortings. We leave open several questions. We have commented on bigraph sortings in a sense reserving equational structure of bigraphs, but those comments are hardly the last say on that matter. Also, we have presently seen how bigraph sortings may preserve and create reaction, but have neither investigated the abstract case of parametric systems, nor treated transitions, neither in parametric or bigraphical reactive systems.

On the broader question of the relationship of informatic behaviour and calculation, we have taken but a tiny first step. A next step could be to see which existing calculi with calculating components, e.g., spi-calculus [28] or CCP [29], are calculational in the present sense. Understanding the ubiquitous and/or pervasive systems of the future seems to necessitate a better understanding of that relationship. We have a good understanding of calculation in itself; we need to understand it also in the context of informatic behaviour!

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