Completeness for Identity-free Kleene Lattices

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Abstract

We provide a finite set of axioms for identity-free Kleene lattices, which we prove sound and complete for the equational theory of their relational models. Our proof builds on the completeness theorem for Kleene algebra, and on a novel automata construction that makes it possible to extract axiomatic proofs using a Kleene-like algorithm.

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1 Introduction

Relation algebra is an efficient tool to reason about imperative programs. In this approach, the bigstep semantics of a program P is a binary relation $[P]$ between memory states [20, 22, 6, 16, 1]. This relation is built from the elementary relations corresponding to the atomic instructions of P, which are combined using standard operations on relations, for instance composition and transitive closure, that respectively encode sequential composition of programs, and iteration (while loops). Abstracting over the concrete behaviour of atomic instructions, one can compare two programs P, Q by checking whether the expressions $[P]$ and $[Q]$ are equivalent in the model of binary relations, which we write as $\mathcal{R}el \models [P] = [Q]$.

To enable such an approach, one should obtain two properties: decidability of the predicate $\mathcal{R}el \models e = f$, given two expressions e and f as input, and axiomatisability of this relation. Decidability makes it possible to automate the verification process, thus alleviating the burden for the end-user [17, 14, 9, 25, 28]. Axiomatisation offers a better way of understanding the equational theory of relations and provides a certificate for programs verification. Indeed, an axiomatic proof of $e = f$ can be seen as a certificate, which can be exchanged, proofread, and combined in a modular way. Axiomatisations also make it possible to solve hard instances manually, when the existing decision procedures have high complexity and/or when considered instances are large [24, 17, 7].

Depending on the class of programs under consideration, several sets of operations on relations can be considered. In this paper we focus on the following set of operations: composition ($\cdot$), transitive closure ($\_^+$), union ($+$), intersection ($\cap$) and the empty relation (0).

* Full version of the extented abstract in Proc. CONCUR 2018 [13].

The expressions generated by this signature are called KL^--expressions. An example of an inequality in the corresponding theory is $\mathcal{R}el \models (a \cap c) \cdot (b \cap d) \leq (a \cdot b)^+ \cap (c \cdot d)$: when a, b, c, d are interpreted as arbitrary binary relations, we have $(a \cap c) \cdot (b \cap d) \subseteq (a \cdot b)^+ \cap (c \cdot d)$. The operations of composition, union and transitive closure arise naturally when defining the bigstep semantics of sequential programs. In contrast, intersection, which is the operation of interest in the present paper, is not a standard operation on programs. This operation is however useful when it comes to specifications: it allows one to express local conjunctions of specifications. For instance, a specification of the shape $(a \cap b)^+$ expresses the fact that execution traces must consist of sequences of smaller traces satisfying both a and b.

The operations of KL^- contain those of identity-free regular expressions, whose equational theory inherits the good properties of *Kleene algebra* (KA).We summarise them below.

First recall that each regular expression e can be associated with a set of words $\mathcal{L}(e)$ called its language. Valid inequations between regular expressions inequalities can be characterised by language inclusions [29]:

$$\mathcal{R}el \models e \leq f \quad \text{iff} \quad \mathcal{L}(e) \subseteq \mathcal{L}(f) \tag{1}$$

Second, we have the celebrated equivalence between regular expressions and non-deterministic finite automata (NFA) via a *Kleene theorem*: for every regular expression e, there is an NFA such that $\mathcal{L}(e)$ is the language of A, and conversely. Decidability follows (in fact, PSPACE-completeness). Lastly, although every purely equational axiomatisation of this theory must be infinite [30], Kozen has proved that Conway's finite quasi-equational axiomatisation [12] is sound and complete [19]. (There is also an independent proof of this result by Boffa [8], based on the extensive work of Krob [26].)

Those three results nicely restrict to identity-free Kleene algebra (KA^-), which form a proper fragment of Kleene algebra [21]. It suffices to consider languages of non-empty words: Equation (1) remains, Kleene's theorem still holds, and we have the following characterisation, where we write $\mathsf{KA}^- \vdash e \leq f$ when $e \leq f$ is derivable from the axioms of KA^-:

$$\mathcal{L}(e) \subseteq \mathcal{L}(f) \quad \text{iff} \quad \mathsf{KA}^- \vdash e \leq f \tag{2}$$

There are counterparts to the first two points for KL^--expressions. Each KL^--expression e can be associated with a set of graphs $\mathcal{G}(e)$ called its graph language, and valid inequations of KL^--expressions can be characterised through these languages of graphs. A subtlety here is that we have to consider graphs modulo homomorphisms; writing ${}^{\triangleleft}\mathcal{G}$ for the closure of a set of graphs $\mathcal{G}$ under graph homomorphisms, we have [10]:

$$\mathcal{R}el \models e \leq f \quad \text{iff} \quad {}^{\triangleleft}\mathcal{G}(e) \subseteq {}^{\triangleleft}\mathcal{G}(f) \tag{3}$$

KL^--expressions are equivalent to a model of automata over graphs called Petri automata [10]. As for KA^--expressions, a Kleene-like theorem holds [11]: for every KL^--expression e, there is a Petri automaton whose language is $\mathcal{G}(e)$, and conversely. Decidability (in fact, EXPSPACE-completeness) of the equational theory follows [10, 11].

What is missing to this picture is an axiomatisation of the corresponding equational theory. In the present paper, we provide such an axiomatisation, which we call KL^-, and which comprises the axioms for identity-free Kleene algebra (KA^-) and the axioms of *distributive lattices* for $\{+, \cap\}$. Completeness of this axiomatisation is the difficult result we prove here:

$${}^{\triangleleft}\mathcal{G}\,(e) \subseteq {}^{\triangleleft}\mathcal{G}\,(f) \quad \text{entails} \quad \mathsf{KL}^- \vdash e \leq f \tag{4}$$

We proceed in two main steps. First we show that $\mathcal{G}\,(e) \subseteq \mathcal{G}\,(f)$ entails $\mathsf{KL}^- \vdash e \leq f$, using a technique inspired from [23], this is what we call *completeness for strict language* *inclusion.*The second step is much more involved. There we exploit the Kleene theorem for Petri automata [11]: starting from expressions e, f such that ${}^{\triangleleft}\mathcal{G}(e) \subseteq {}^{\triangleleft}\mathcal{G}(f)$, we build two Petri automata $\mathscr{A}, \mathscr{B}$ respectively recognising $\mathcal{G}(e)$ and $\mathcal{G}(f)$. Then we design a product construction to synchronise $\mathscr{A}$ and $\mathscr{B}$, and a Kleene-like algorithm to extract from this construction two expressions e', f' such that $\mathcal{G}(e) = \mathcal{G}(e')$, $\mathsf{KL}^- \vdash e' \leq f'$, and $\mathcal{G}(f') \subseteq \mathcal{G}(f)$. This *synchronised Kleene theorem* suffices to conclude using the first step.

To our knowledge, this is the first completeness result for a theory involving Kleene iteration and intersection. Identity-free Kleene lattices were studied in depth by Andréka, Mikulás and Németi [3]; they have in particular shown that over this syntax, the equational theories generated by binary relations and formal languages coincide. But axiomatisability remained opened. The restriction to the identity-free fragment is important for several reasons. First of all, it makes it possible to rely on the technique used in [10] to compare Petri automata, which does not scale in the presence of identity. Second, this is the fragment for which the Kleene theorem for Petri automata is proved the most naturally [11]. Third, 'strange' laws appear in the presence of 1 [2], *e.g.*, $1 \cap (b \cdot a) \leq a \cdot (1 \cap (b \cdot a)) \cdot b$, and axiomatisability is still open even in the finitary case where Kleene iteration is absent—see the erratum about [2].

Proofs of completeness for other extensions of Kleene algebra include Kleene algebra with tests (KAT) [20], nominal Kleene algebra [23], and Concurrent Kleene algebra [27, 18]. The latter extension is the closest to our work since the parallel operator of concurrent Kleene algebra shares some properties of the intersection operation considered in the present work (*e.g.*, it is commutative and it satisfies a weak interchange law with sequential composition).

The paper is organised as follows. In Sect. 2, we recall KL^--expressions, their graph language and the corresponding model of Petri automata. In Sect. 3 we give our axiomatisation and state the completeness result. Then we show it following the proof scheme presented earlier: in Sect. 4 we show completeness for strict language inclusions, we recall in Sect. 5 the Kleene theorem of KL^- expressions, on which we build to show our synchronised Kleene theorem in Sect. 6.

2 Expressions, graph languages and Petri automata

2.1 Expressions and their relational semantics

We let $a, b \ldots$ range over the letters of a fixed alphabet X. We consider the following syntax of KL^--*expressions*, which we simply call expressions if there is no ambiguity:

$$e, f ::= e \cdot f \;\mid\; e + f \;\mid\; e \cap f \;\mid\; e^+ \;\mid\; 0 \;\mid\; a \qquad (a \in X)$$

We denote their set by Exp_X and we often write ef for $e \cdot f$. When we remove intersection $(\cap)$ from the syntax of KL^--expressions we get KA^--*expressions*, which are the identity-free regular expressions.

If $\sigma : X \to \mathcal{P}(S \times S)$ is an interpretation of the letters into some space of relations, we write $\widehat{\sigma}$ for the unique homomorphism extending σ into a function from Exp_X to $\mathcal{P}(S \times S)$. An inequation between two expressions e and f is *valid*, written $\mathcal{R}el \models e \leq f$, if for every such interpretation σ we have $\widehat{\sigma}(e) \subseteq \widehat{\sigma}(f)$.

2.2 Terms, graphs, and homomorphisms

We let $u, v \ldots$ range over expressions built using only letters, $\cap$ and $\cdot$, which we call *terms*. (Terms thus form a subset of expressions: they are those expressions not using 0, + and $\_^+$.)

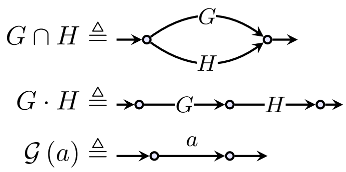


Figure 1 Operations on graphs.

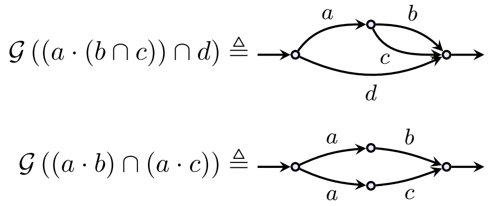


Figure 2 Graphs associated with some terms.

We will use 2-pointed labelled directed graphs, simply called *graphs* in the sequel. Those are tuples $\langle V, E, s, t, l, \iota, o\rangle$ with V (resp. E) a finite set of vertices (resp. edges), $s, t : E \to V$ the *source* and *target* functions, $l : E \to X$ the *labelling* function, and $\iota, o \in V$ two distinguished vertices, respectively called *input* and *output*.

As depicted in Fig. 1, graphs can be composed in series or in parallel, and a letter can be seen as a graph with a single edge labelled by that letter. One can thus recursively associate to every term u a graph $\mathcal{G}(u)$ called the *graph of* u. Two examples are given in Fig. 2; graphs of terms are *series-parallel* [31].

▶ **Definition 1** (Graph homomorphism)**.** A *homomorphism* from $G = \langle V, E, s, t, l, \iota, o\rangle$ to $G' = \langle V', E', s', t', l', \iota', o'\rangle$ is a pair $h = \langle f, g\rangle$ of functions $f : V \to V'$ and $g : E \to E'$ that respect the various components: $s' \circ g = f \circ s$, $t' \circ g = f \circ t$, $l = l' \circ g$, $\iota' = f(\iota)$, and $o' = f(o)$.

We write $G' \lhd G$ if there exists a graph homomorphism from G to G'.

Such a homomorphism is depicted in Fig. 3. A pleasant way to think about graph homomorphisms is the following: we have $G \lhd H$ if G is obtained from H by merging (or identifying) some nodes, and by adding some extra nodes and edges. For instance, the graph G in Fig. 3 is obtained from H by merging the nodes $1, 2$ and by adding an edge between the input and the output labelled by d.

The starting point of the present work is the following characterisation:

▶ **Theorem 2** ([5, Thm. 1], [15, p. 208])**.** *For all terms u, v, $\mathcal{R}el \models u \leq v$ iff $\mathcal{G}(u) \lhd \mathcal{G}(v)$.*

2.3 Graph language of an expression

To generalise the previous characterisation to KL^--expressions, one interprets expressions by sets (languages) of graphs: graphs play the role of words for KA-expressions.

▶ **Definition 3** (Term and graph languages of expressions)**.** The *term language* of an expression e, written $[\![e]\!]$, is the set of terms defined recursively as follows:

$$[\![e \cdot f]\!] \triangleq \{u \cdot v \mid u \in [\![e]\!] \text{ and } v \in [\![f]\!]\} \qquad [\![0]\!] \triangleq \emptyset$$
$$[\![e \cap f]\!] \triangleq \{u \cap v \mid u \in [\![e]\!] \text{ and } v \in [\![f]\!]\} \qquad [\![a]\!] \triangleq \{a\}$$
$$[\![e + f]\!] \triangleq [\![e]\!] \cup [\![f]\!] \qquad [\![e^+]\!] \triangleq \bigcup_{n>0} \{u_1 \cdot \dots \cdot u_n \mid \forall i, u_i \in [\![e]\!]\}$$

The *graph language* of e is the set of graphs $\mathcal{G}(e) \triangleq \{\mathcal{G}(u) \mid u \in [\![e]\!]\}$.

Note that for every term u, $[\![u]\!] = \{u\}$, so that the graph language of u thus contains just the graph of u. This justifies the overloaded notation $\mathcal{G}(u)$. Given a set S of graphs, we write ${}^{\lhd}S$ for its downward closure w.r.t. $\lhd$: ${}^{\lhd}S \triangleq \{G \mid G \lhd G', G' \in S\}$. We obtain:

▶ **Theorem 4** ([10, Thm. 6])**.** *For all expressions e, f, $\mathcal{R}el \models e \leq f$ iff ${}^{\lhd}\mathcal{G}(e) \subseteq {}^{\lhd}\mathcal{G}(f)$.*

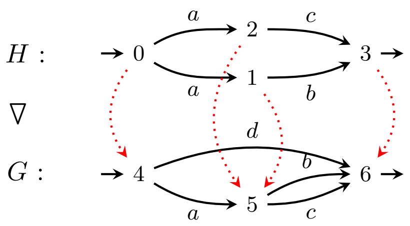


Figure 3 A graph homomorphism.

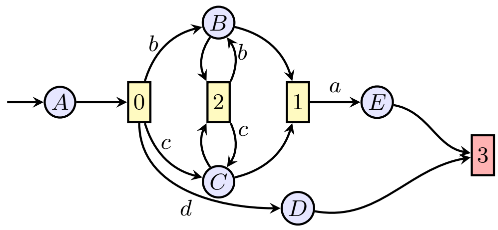


Figure 4 A Petri automaton.

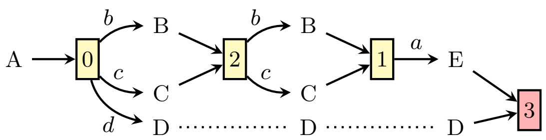


Figure 5 Run of a Petri automaton.

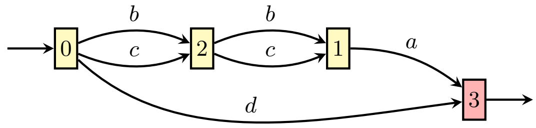


Figure 6 Graph of a run.

2.4 Petri automata

We recall the notion of Petri automata [10, 11], an automata model that recognises precisely the graph languages of our expressions.

▶ **Definition 5** (Petri Automaton). A *Petri automaton (PA)* over the alphabet X is a tuple $\mathscr{A} = \langle P, \mathcal{T}, \iota \rangle$ where:

- P is a finite set of *places*,
- $\mathcal{T} \subseteq \mathcal{P}(P) \times \mathcal{P}(X \times P)$ is a set of *transitions*,
- $\iota \in P$ is the *initial place* of the automaton.

For each transition $t = \langle {}^{\triangleleft}t, t^{\triangleright} \rangle \in \mathcal{T}$, ${}^{\triangleleft}t$ is assumed to be non-empty; ${}^{\triangleleft}t \subseteq P$ is the *input of* t; and $t^{\triangleright} \subseteq X \times P$ is the *output of* t. We write $\pi_2(t^{\triangleright}) \triangleq \{p \mid \exists a, \langle a, p \rangle \in t^{\triangleright}\}$ for the set of the output places of t. Transitions with empty outputs are called *final*.

A PA is depicted in Fig. 4: places are represented by circles and transitions by squares.

Let us now recall the operational semantics of PA. Fix a PA $\mathscr{A} = \langle P, \mathcal{T}, \iota \rangle$ for the remainder of this section. A *state* of this automaton is a set of places. In a given state $S \subseteq P$, a transition $t = \langle {}^{\triangleleft}t, t^{\triangleright} \rangle$ is *enabled* if ${}^{\triangleleft}t \subseteq S$. In that case, we may fire t, leading to a new state $S' = (S \setminus {}^{\triangleleft}t) \cup \pi_2(t^{\triangleright})$. We write $S \xrightarrow{t}_{\mathscr{A}} S'$ in this case.

▶ **Definition 6** (Run of a PA). A *run* is a sequence $\langle S_1, t_1, S_2, \ldots, t_{n-1}, S_n \rangle$, where S_i are states, t_i are transitions such that $S_i \xrightarrow{t_i}_{\mathscr{A}} S_{i+1}$ for every $i \in [1, n-1]$, $S_1 = \{\iota\}$ and $S_n = \emptyset$.

A run of the PA from Fig. 4 is depicted in Fig. 5; this run gives rise to a graph, depicted in Fig. 6; see [11, Def. 3] for a formal definition in the general case.

▶ **Definition 7** (Graph language of a PA). The *graph language of a PA* $\mathscr{A}$, written $\mathcal{G}(\mathscr{A})$, consists of the graphs of its runs.

PA are assumed to be *safe* (in standard Petri net terminology, places contain at most one *token* at any time—whence the definition of states as sets rather than multisets) and to accept only series-parallel graphs. These two conditions are decidable [11]. Here we moreover assume that all PA have the same set of places P.

PA and KL^{-}-expressions denote the same class of graph languages:

$$e \cap (f \cap g) = (e \cap f) \cap g \qquad e \cap f = f \cap e \qquad e \cap e = e$$

$$e \cap (f + g) = (e \cap f) + (e \cap g) \qquad e \cap (e + f) = e \qquad e + (e \cap f) = e$$

$$e + (f + g) = (e + f) + g \qquad e + f = f + e \qquad e + e = e$$

$$e{\cdot}(f{\cdot}g) = (e{\cdot}f){\cdot}g \quad e{\cdot}(f{+}g) = e{\cdot}f{+}e{\cdot}g \quad (e{+}f){\cdot}g = e{\cdot}g{+}f{\cdot}g \quad e{+}0 = e \quad e{\cdot}0 = 0 = 0{\cdot}e$$

$$e + e{\cdot}e^+ = e^+ = e + e^+{\cdot}e \qquad e{\cdot}f + f = f \;\Rightarrow\; e^+{\cdot}f + f = f \qquad f{\cdot}e + f = f \;\Rightarrow\; f{\cdot}e^+ + f = f$$

Figure 7 KL^-: the first three lines correspond to distributive lattices, the last three to KA^-.

▶ **Theorem 8** (Kleene theorem [11, Thm. 18]).
(i) *For every expression e, there is a Petri automaton $\mathscr{A}$ such that $\mathcal{G}(e) = \mathcal{G}(\mathscr{A})$.*
(ii) *Conversely, for every Petri automaton $\mathscr{A}$, there is an expression e such that $\mathcal{G}(e) = \mathcal{G}(\mathscr{A})$.*

3 Axiomatisation and structure of completeness proof

Let us introduce now our axiomatisation.

▶ **Definition 9.** The axioms of KL^- are the union of
- the axioms of identity-free Kleene algebra (KA^-) [21], and
- the axioms of a distributive lattice for $\{+, \cap\}$.

It is easy to check that those axioms are valid for binary relations, whence soundness of KL^-:

▶ **Theorem 10** (Soundness). *If $\mathsf{KL}^- \vdash e \leq f$ then $\mathcal{R}el \models e \leq f$.*

The rest the paper is devoted the converse implication, which thanks to Thm. 4 amounts to:

▶ **Theorem 11** (Completeness). *If ${}^{\triangleleft}\mathcal{G}(e) \subseteq {}^{\triangleleft}\mathcal{G}(f)$ then $\mathsf{KL}^- \vdash e \leq f$.*

The following very weak form of Thm. 11 is easy to obtain from the results in the literature:

▶ **Proposition 1.** *For all terms u, v, $\mathcal{G}(u) \triangleleft \mathcal{G}(v)$ entails $\mathsf{KL}^- \vdash u \leq v$.*

Proof. Follows from Thm. 4, completeness of semilattice-ordered semigroups [4] for relational models, and the fact the the axioms of KL^- entail those of semilattice-ordered semigroups. ◀

As explained in the introduction, our first step consists in proving KL^- completeness w.r.t. strict graph language inclusions, *i.e.*, not modulo homomorphisms:

▶ **Theorem 12** (Completeness for strict language inclusions). *If $\mathcal{G}(e) \subseteq \mathcal{G}(f)$ then $\mathsf{KL}^- \vdash e \leq f$.*

The proof is given in Sect. 4. Our second step is to get the following theorem (Sect. 6):

▶ **Theorem 13** (Synchronised Kleene Theorem). *If $\mathscr{A}, \mathscr{B}$ are PA such that ${}^{\triangleleft}\mathcal{G}(\mathscr{A}) \subseteq {}^{\triangleleft}\mathcal{G}(\mathscr{B})$, then there are expressions e, f such that:*

$$\mathcal{G}(\mathscr{A}) = \mathcal{G}(e), \quad \mathsf{KL}^- \vdash e \leq f, \quad \text{and} \quad \mathcal{G}(f) \subseteq \mathcal{G}(\mathscr{B}).$$

The key observation for the proof is that the state-removal procedure used to transform a PA into a KL^- expression is highly non-deterministic. When considering two PA at a time, one can use this flexibility in order to synchronise the computation of the two expressions, so that they become easier to compare axiomatically. The concrete proof is quite technical and requires us to first recall many concepts from the proof [11] of Thm. 8(ii) (Sect. 5); it heavily relies on both Thm. 12 and Prop. 1.

Completeness of KL^- follows using Thm. 8(i) and Thm. 12 as explained in the introduction.

4 Completeness for strict language inclusion

Recall that the graph language of an expression e, $\mathcal{G}(e)$, is defined as the set of graphs of the term language of e, $[\![e]\!]$. We first prove that KL^- is complete for term language inclusions:

▶ **Proposition 2.** *If* $[\![e]\!] \subseteq [\![f]\!]$ *then* $\mathsf{KL}^- \vdash e \leq f$.

Proof. We follow a technique similar to the one recently used in [23]. We consider the maximal KA^--subexpressions, and we compute the atoms of the Boolean algebra of word languages generated by those expressions. By KA^- completeness [19, 21], we get KA^- (and thus KL^-) proofs that those are equal to appropriate sums of atoms. We distribute the surrounding intersections over those sums and replace the resulting intersections of atoms by fresh letters. This allows us to proceed recursively (on the intersection-depth of the terms), using substitutivity to recover a KL^- proof of the starting inequality. ◀

The difference between the term language and the graph language is that intersection is interpreted as an associative and commutative operation in the latter. We bury this difference by defining a 'saturation' function s on KL^--expressions such that for all e,

$$(\dagger)\quad \mathsf{KL}^- \vdash s(e) = e, \qquad \text{and} \qquad (\ddagger)\quad [\![s(e)]\!] = \{u \mid \mathcal{G}(u) \in \mathcal{G}(e)\}\ .$$

Intuitively, this function uses distributivity and idempotency of sum to replace all intersections appearing in the expression by the sum of all their equivalent presentations modulo associativity and commutativity. For instance, $s(a\cap(b\cap c))$ is a sum of twelve terms (six choices for the ordering times two choices for the parenthesing). Technically, one should be careful to expand the expression first by maximally distributing sums, in order to make all potential n-ary intersections apparent. For instance, $((a\cap b)+d)\cap c$ expands to $((a\cap b)\cap c)+(d\cap c)$ so that its saturation is a sum of twelve plus two terms. For the same reason, all iterations should be unfolded once: we unfold and expand $(a\cap b)^+\cap c$ into $((a\cap b)\cap c)+((a\cap b)\cdot(a\cap b)^+\cap c)$ before saturating it. We finally obtain Thm. 12 using (‡), Prop. 2, and (†):

$$\mathcal{G}(e)\subseteq\mathcal{G}(f) \quad\Rightarrow\quad [\![s(e)]\!]\subseteq[\![s(f)]\!] \quad\Rightarrow\quad \mathsf{KL}^-\vdash s(e)\leq s(f) \quad\Rightarrow\quad \mathsf{KL}^-\vdash e\leq f$$

5 Kleene theorem for Petri automata

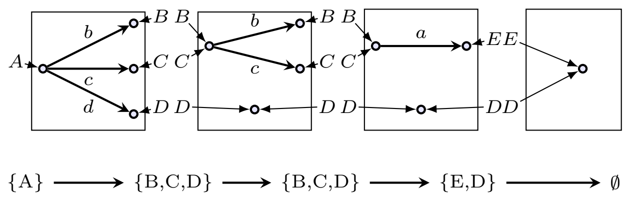
To prove the synchronised Kleene theorem (Thm. 13), we cannot use the Kleene theorem for PA (Thm. 8) as a black box: we use in a fine way the algorithm underlying the proof of the second item. We thus explain how it works [11] in details.

Recall that to transform an NFA $\mathscr{A}$ to a regular expression e, one rewrites it using the rules of Fig. 8 until one reaches an automaton where there is a unique transition from the initial state to the final one, labelled by an expression e. While doing so, one goes through generalised NFA, whose transitions are labelled by regular expressions instead of letters.

Figure 8 Rewriting rules for state-removal procedure.

We use the same technique for PA: we start by converting the PA into a NFA over a richer alphabet, which we call a *Template Automaton (TA)*, then we reduce this automaton using the rules of Fig. 8 until we get a single transition labelled by the desired expression.

To get some intuitions about the way we convert a PA into an NFA, consider the run in Fig. 5 and its graph in Fig. 6. One can decompose the run and the graph as follows:



The graph can thus be seen as a word over an alphabet of 'boxes', and the run as a path in an NFA whose states are sets of places of the PA. The letters of the alphabet, the above boxes, can be seen as 'slices of graphs'; they arise naturally from the transitions of the starting PA (Fig. 4 in this example).

5.1 Template automata

In order to make everything work, we need to refine both this notion of states and this notion of boxes to define template automata:

- states (sets of places) are refined into *types*. We let σ, τ range over types. A type is a tree whose leaves are labelled by places. When we forget the tree structure of a type τ, we get a a state $\overline{\tau}$. See [11, Def. 10] for a formal definition of types, which is not needed here. We call *singleton types* those types whose associated state is a singleton.
- letters will be *templates*: finite sets of boxes like depicted above but with edges labelled with arbitrary KL^--expressions; we define those formally below.

Given a directed acyclic graph (DAG) G, we write $\min G$ (resp. $\max G$) for the set of its sources (resp. sinks). A DAG is non-trivial when it contains at least one edge.

► **Definition 14** (Boxes). Let σ, τ be types. A *box* from σ to τ is a triple $\langle \overrightarrow{\mathfrak{p}}, G, \overleftarrow{\mathfrak{p}} \rangle$ where G is a non-trivial DAG with edges labelled in Exp_X, $\overrightarrow{\mathfrak{p}}$ is a map from $\overline{\sigma}$, the *input ports*, to the vertices of G, and $\overleftarrow{\mathfrak{p}}$ is a bijective map from $\overline{\tau}$, the *output ports*, to $\max G$, and where an additional condition relative to types holds [11, Def. 11]. (This condition can be kept abstract here.) A *basic* box is a box labelled with letters rather than arbitrary expressions. A *1-1* box is a box between singleton types.

We let α, β range over boxes and we write $\beta : \sigma \to \tau$ when β is a box from σ to τ.

We represent boxes graphically as in Fig. 15. Inside the rectangle is the DAG, with the input ports on the left-hand side and the output ports on the right-hand side. The maps $\overrightarrow{\mathfrak{p}}$ and $\overleftarrow{\mathfrak{p}}$ are represented by the arrows going from the ports to vertices inside the rectangle.

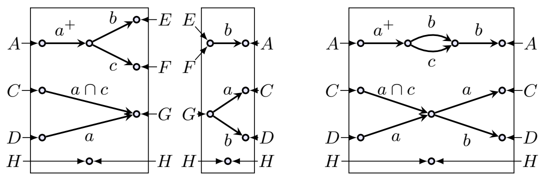


Figure 9 Two boxes and their composition.

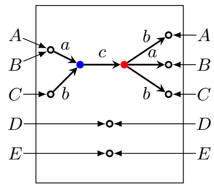


Figure 10 An atomic box.

Note that unlike $\overleftarrow{\mathfrak{p}}$, the map $\overrightarrow{\mathfrak{p}}$ may reach inner nodes of the DAG. 1-1 boxes are those with exactly one input port and one output port.

Boxes compose like in a category: if $\alpha : \sigma \to \tau$ and $\beta : \tau \to \rho$ then we get a box $\alpha \cdot \beta : \sigma \to \rho$ by putting the graph of α to the left of the graph of β, and for every port $p \in \overline{\tau}$, we identify the node $\overleftarrow{\mathfrak{p}_1}(p)$ with the node $\overrightarrow{\mathfrak{p}_2}(p)$. For instance the third box in Fig. 15 is obtained by composing the first two.

The key property enforced by the condition on types (kept abstract here) is the following:

▶ **Lemma 15.** *A 1-1 box is just a series-parallel 2-pointed graph labelled in Exp_X.*

Accordingly, one can extract a KL^--expression from any 1-1 box β, which we write $e(\beta)$ and call its *expression*.

▶ **Definition 16** (Templates)**.** A *template* $\Gamma : \sigma \to \tau$ is a finite set of boxes from σ to τ. A *1-1 template* is a template of 1-1 boxes. The *expression* of a 1-1 template, written $e(\Gamma)$, is the sum of the expressions of its boxes.

Templates can be composed like boxes, by computing all pairwise box compositions.

▶ **Definition 17** (Box language of a template)**.** A basic box is *generated* by a box β if it can be obtained by replacing each edge $x \xrightarrow{e} y$ of its DAG by a graph $G' \in \mathcal{G}(e)$ with input vertex x and output vertex y. The *box language* of a template Γ, written $\mathcal{B}(\Gamma)$, is the set of basic boxes generated by its boxes.

As expected, the box language of a template $\Gamma : \sigma \to \tau$ only contains boxes from σ to τ. Thanks to Lem. 15, when Γ is a 1-1 template, its box language can actually be seen as a set of graphs, and we have:

▶ **Proposition 3.** *For every 1-1 template Γ, we have $\mathcal{B}(\Gamma) = \mathcal{G}(e(\Gamma))$.*

We can finally define template automata:

▶ **Definition 18** (Template automaton (TA))**.** A *template automaton* is an NFA whose states are types, whose alphabet is the set of templates, whose transitions are of the form $\langle \sigma, \Gamma, \tau \rangle$ where $\Gamma : \sigma \to \tau$, and with a single initial state and a single accepting state which are singleton types. A *basic TA* is a TA whose all transitions are labelled by basic boxes.

By definition, a word accepted by a TA is a sequence of templates that can be composed into a single 1-1 template Γ, and thus gives rise to a set of graphs $\mathcal{B}(\Gamma)$. The *graph language of a TA $\mathscr{E}$*, written $\mathcal{G}(\mathscr{E})$, is the union of all those sets of graphs.

An important result of [11] is that we can translate every PA into a TA:

▶ **Proposition 4.** *For every PA $\mathscr{A}$, there exists a basic TA $\mathscr{E}$ such that $\mathcal{G}(\mathscr{A}) = \mathcal{G}(\mathscr{E})$.*

TA were defined so that they can be reduced using the state-removal procedure from Fig. 8. Templates can be composed sequentially and are closed under unions, so that now we only miss an operation $\_^*$ on templates to implement the first rule. Since we work in an identity-free (and thus star-free) setting, it suffices to define a strict iteration operation $\_^+$; and to rely on the following shorthands $\Delta \cdot \Gamma^* = \Delta \cup \Delta \cdot \Gamma^+$ and $\Gamma^* \cdot \Delta = \Delta \cup \Gamma^+ \cdot \Delta$.

Such an operation is provided in [11]:

▶ **Proposition 5.** *There exists a function $\_^+$ on templates such that if the TA obtained from a PA $\mathscr{A}$ through Prop. 4 reduces to a TA $\mathscr{E}$ by the rules in Fig. 8, then $\mathcal{G}(\mathscr{A}) = \mathcal{G}(\mathscr{E})$.* [1]

One finally obtains the Kleene theorem for PA by reducing the TA until it consists of a single transition labelled by a 1-1 template Γ: at this point, $e(\Gamma)$ is the desired KL^--expression.

5.2 Computing the iteration of a template

We need to know how the above template iteration can be defined to obtain our synchronised Kleene theorem, so that we explain it in this section. This section is required only to understand how we define a synchronised iteration operation in Sect. 6.

First notice that templates on which we need to compute $\_^+$ are of type $\sigma \to \sigma$. We first define this operation for a restricted class of templates, which we call *atomic*.

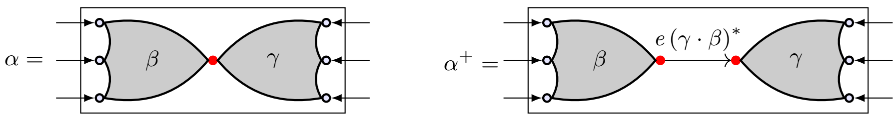
▶ **Definition 19** (Atomic boxes and templates, Support)**.** A box $\beta = \left\langle \overrightarrow{\mathfrak{p}}, G, \overleftarrow{\mathfrak{p}} \right\rangle : \sigma \to \sigma$ is *atomic* if its graph has a single non-trivial connected component C, and if for every vertex v outside C, there is a unique port $p \in \overline{\sigma}$ such that $\overrightarrow{\mathfrak{p}}(p) = \overleftarrow{\mathfrak{p}}(p) = v$. An *atomic template* is a template composed of atomic boxes.

The *support* of a box $\beta : \sigma \to \sigma$ is the set $supp(\beta) \triangleq \left\{p \mid \overrightarrow{\mathfrak{p}}(p) \neq \overleftarrow{\mathfrak{p}}(p)\right\}$. The support of a template is the union of the supports of its boxes.

The following property of atomic boxes, makes it possible to compute their iteration:

▶ **Lemma 20** ([11, Lem. 7.18])**.** *The non-trivial connected component of an atomic box $\beta : \sigma \to \sigma$ always contains a vertex c, s.t. for every port p mapped inside that component, all paths from $\overrightarrow{\mathfrak{p}}(p)$ to a maximal vertex visit c. We call such a vertex a* bowtie *for β.*

Notice that the bowtie of a box is not unique. For instance, the atomic box in Fig. 10 contains two bowties: the blue and the red nodes.
We compute the iteration of an atomic box as follows. First choose a bowtie for this box, then split it at the level of this node into the product $\alpha = \beta \cdot \gamma$. The box $\gamma \cdot \beta$ is 1-1, we can thus extract from it a term $e(\gamma \cdot \beta)$. We set α^+ to be the template consisting of α and the box obtained from α by replacing the bowtie by an edge labelled $e(\gamma \cdot \beta)^+$. For the sake of conciseness, we denote this two-box template as on the right below, with an edge labelled with a starred expression.



[1] This statement is not simpler because, unfortunately, there is no function $\_^+$ on templates such that $\mathcal{B}(\Gamma^+) = \mathcal{B}(\Gamma)^+$).

Data: Atomic template Γ
Result: A template Γ^+ s.t. $\mathcal{B}(\Gamma^+) = \mathcal{B}(\Gamma)^+$
if $\Gamma = \emptyset$ **then**
  Return $\emptyset$
else
  Write $\Gamma = \Delta \cup \{\alpha\} \cup \Sigma$ such that $\mathit{supp}\,(\Delta) \subseteq \mathit{supp}\,(\alpha)$ and $\mathit{supp}\,(\Sigma) \cap \mathit{supp}\,(\alpha) = \emptyset$;
  Choose a bowtie for α;
  Split α into $\beta \cdot \gamma$ at the level of this bowtie;
  Return $(\Delta^+ \cdot \Sigma^*) \cup (\Delta^* \cdot \Sigma^+) \cup (\Delta^* \cdot \delta \cdot \Delta^* \cdot \Sigma^*)$, where δ is the two-box template depicted on the right.
end

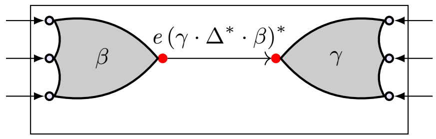


Figure 11 Iteration of an atomic template.

It is not difficult to see that $\mathcal{B}(\alpha^+) = \mathcal{B}(\alpha)^+$. Depending on the bowtie we have chosen, the box α^+ will be different. This is why we will write $\alpha^+_{\bowtie}$ to say that the bowtie $\bowtie$ has been selected for the computation of the iteration.

Now we need to generalise this construction to compute the iteration of an atomic template. For this, we need the following property, saying that the supports of atomic boxes of the same type are either disjoint or comparable:

▶ **Lemma 21.** *For all atomic boxes $\beta, \gamma : \sigma \to \sigma$, we have either 1) $\mathit{supp}\,(\beta) \subseteq \mathit{supp}\,(\gamma)$, or 2) $\mathit{supp}\,(\gamma) \subseteq \mathit{supp}\,(\beta)$, or 3) $\mathit{supp}\,(\beta) \cap \mathit{supp}\,(\gamma) = \emptyset$.*

We can compute the iteration of an atomic template by the algorithm in Fig. 11; intuitively, atomic boxes with disjoint support can be iterated in any order: they cannot interfere; in contrast, atomic boxes with small support must be computed before atomic boxes with strictly larger support: the iteration of the latter depends on that of the former. (Also note that since $\mathit{supp}\,(\Delta) \subseteq \mathit{supp}\,(\alpha)$ we have also $\mathit{supp}\,(\Delta^+) \subseteq \mathit{supp}\,(\alpha)$ thus the template $\gamma \cdot \Delta^* \cdot \beta$ is 1-1 and it gives rise to an expression $e\,(\gamma \cdot \Delta^* \cdot \beta)$.)

We finally compute the iteration of an arbitrary template $\Gamma : \sigma \to \sigma$ as follows: from each connected component of the graph of each box in Γ stems an atomic box; let $\mathit{At}(\Gamma)$ be the set of all these atomic boxes; we set $\Gamma^+ = \mathit{At}(\Gamma)^+$.

The overall algorithm contains two sources of non-determinism. First, one can partially choose in which order to process the atomic boxes. This is reflected by the choice of the box α, which we will call the *pivot*. For instance if $\Gamma = \{\alpha_1, \alpha_2, \beta\}$ such that $\mathit{supp}\,(\alpha_1) = \mathit{supp}\,(\alpha_2)$ and $\mathit{supp}\,(\beta) \cap \mathit{supp}\,(\alpha_1) = \emptyset$, then we can choose either α_1 or α_2 as the pivot, and the computation will respectively start with the computation of α_2^+ or that of α_1^+, yielding two distinct expressions. (In contrast, choices about boxes with disjoint support do not change the final result.) Second, every box of the template is eventually processed, and one must thus choose a bowtie for all of them. We write $\Gamma^+_{\bowtie,\leq}$ to make explicit the choice of the bowties and the computation order.

6 Synchronised Kleene theorem for PA

We can now prove Thm. 13. To synchronise the computation of two expressions e, f for two PA $\mathscr{A}, \mathscr{B}$ respectively, we construct a *synchronised product automaton* $\mathscr{E} \times \mathscr{F}$ between a TA $\mathscr{E}$ for $\mathscr{A}$ and a TA $\mathscr{F}$ for $\mathscr{B}$.

The states of this automaton are triples $\langle \sigma, \eta, \tau \rangle$ where σ and τ are types, *i.e.*, states from the TA $\mathscr{E}$ and $\mathscr{F}$, and $\eta : \overline{\tau} \to \overline{\sigma}$ is a function used to enforce coherence conditions. Its transitions have the form $\langle \langle \sigma, \eta, \tau \rangle, \langle \Gamma, \Delta \rangle, \langle \sigma', \eta', \tau' \rangle \rangle$ where $\langle \sigma, \Gamma, \sigma' \rangle$ is a transition of $\mathscr{E}$, $\langle \tau, \Delta, \tau' \rangle$ is a transition of $\mathscr{F}$, and Γ and Δ satisfy a certain condition which we call *refinement*, written $\Gamma \leq \Delta$.

The overall strategy is as follows. We reduce $\mathscr{E} \times \mathscr{F}$ using the rules of Fig. 8, where the operations $\cdot$ and $\cup$ are computed pairwise. The operation $\_^*$ is also computed pairwise, but in a careful way, exploiting the non-determinism of this operation to ensure that we maintain the refinement relation. We eventually get a single transition labelled by a pair of 1-1 templates Γ and Δ such that $\mathcal{B}(\Gamma) = \mathcal{G}(\mathscr{A})$, $\mathcal{B}(\Delta) = \mathcal{G}(\mathscr{B})$, and $\Gamma \leq \Delta$. To conclude, it suffices to deduce $\mathsf{KL}^- \vdash e(\Gamma) \leq e(\Delta)$ from the latter property. To sum-up, what we need to do now is:

- **Refinement**: define the refinement relation $\leq$ on templates;
- **Initialisation**: define $\mathscr{E} \times \mathscr{F}$ so that refinement holds;
- **Stability**: show that the refinement relation is maintained during the rewriting process;
- **Finalisation**: show that refinement between 1-1 templates entails KL^- provability.

6.1 Refinement relation

We first generalise graph homomorphisms to templates; this involves dealing with multiple ports, with finite sets, and with edge labels which are now arbitrary KL^--expressions. For the latter, we do not require strict equality but KL^--derivable inequalities.

▶ **Definition 22** (Box and template homomorphisms)**.** Let $\sigma, \tau, \sigma', \tau'$ be four types with two functions $\eta : \overline{\sigma} \to \overline{\tau}$ and $\eta' : \overline{\sigma'} \to \overline{\tau'}$. Let $\beta = \left\langle \overrightarrow{\mathfrak{p}}_\beta, \langle V_\beta, E_\beta, s_\beta, t_\beta, l_\beta \rangle, \overleftarrow{\mathfrak{p}}_\beta \right\rangle$ be a box of type $\tau \to \tau'$ and let $\alpha = \left\langle \overrightarrow{\mathfrak{p}}_\alpha, \langle V_\alpha, E_\alpha, s_\alpha, t_\alpha, l_\alpha \rangle, \overleftarrow{\mathfrak{p}}_\alpha \right\rangle$ be a box of type $\sigma \to \sigma'$. A homomorphism from α to β is a pair $\langle f, g \rangle$ of functions $f : V_\alpha \to V_\beta$ and $g : E_\alpha \to E_\beta$ s.t.:

- $s_\beta \circ g = f \circ s_\alpha$, $t_\beta \circ g = f \circ t_\alpha$,
- $\forall e \in E_\alpha, \quad \mathsf{KL}^- \vdash l_\beta \circ g(e) \leq l_\alpha(e)$,
- If $\{v\} \subseteq V_\alpha$ is a trivial connected component, so is $f(v)$.
- $\overrightarrow{\mathfrak{p}}_\beta \circ \eta = f \circ \overrightarrow{\mathfrak{p}}_\alpha$ and $\overleftarrow{\mathfrak{p}}_\beta \circ \eta' = f \circ \overleftarrow{\mathfrak{p}}_\alpha$. (We call this condition (η, η')-*compatibility.*)

We write $\beta \lhd_{\eta,\eta'} \alpha$ when there exists such a homomorphism. For two templates $\Gamma : \tau \to \tau'$ and $\Delta : \sigma \to \sigma'$, we write $\Gamma \lhd_{\eta,\eta'} \Delta$ if for all $\beta \in \Gamma$, there exists $\alpha \in \Delta$ such that $\beta \lhd_{\eta,\eta'} \alpha$.

We abbreviate $\Gamma \lhd_{\eta,\eta'} \Delta$ as $\Gamma \lhd \Delta$ when Γ, Δ are 1-1 templates, or when $\sigma = \tau$, $\sigma' = \tau'$ and η, η' are the identity function id. A box homomorphism is depicted in Fig. 12.

The above relation on templates is not enough for our needs; we have to extend it so that it is preserved during the rewriting process. We first write $\Gamma \sqsubseteq \Delta$ when $\mathcal{B}(\Gamma) \subseteq \mathcal{B}(\Delta)$, for two templates Γ, Δ of the same type. Refinement is defined as follows:

▶ **Definition 23** (Refinement)**.** We call *refinement* the relation on templates defined by $\leq_{\eta,\eta'} \triangleq \lhd_{\eta,\eta'} \cdot (\lhd_{\mathrm{id},\mathrm{id}} \cup \sqsubseteq)^*$, where $\_^*$ is reflexive transitive closure.

The following proposition shows that refinement implies provability of the expressions extracted from 1-1 templates. This gives us the finalisation step.

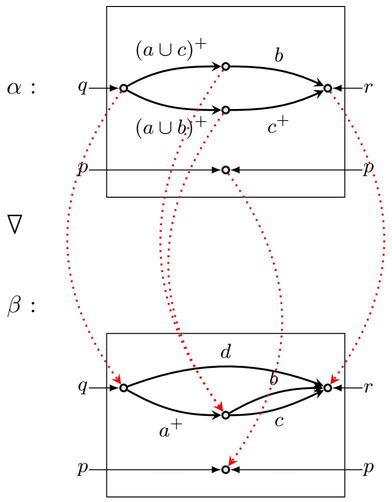


Figure 12 A box homomorphism.

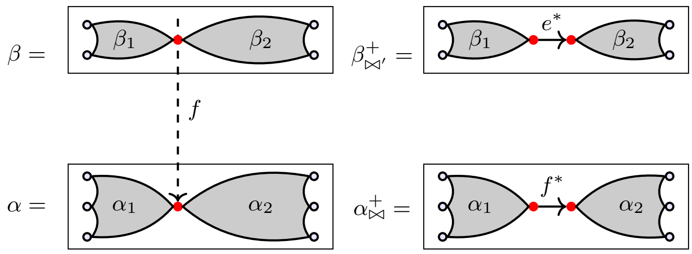


Figure 13 Bowtie compatible boxes.

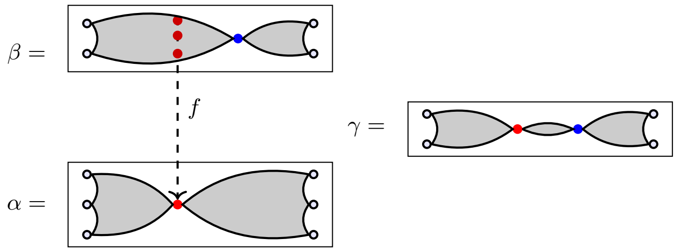


Figure 14 Case of bowtie incompatible boxes.

▶ **Proposition 6.** *If Δ, Γ are 1-1 templates such that $\Delta \leq \Gamma$, then* $\mathsf{KL}^- \vdash e(\Delta) \leq e(\Gamma)$.

Proof. When $\Delta \subseteq \Gamma$, it follows from Prop. 3 and Thm. 12; when $\Delta \lhd \Gamma$, it follows from Prop. 1. We conclude by transitivity. ◀

6.2 Synchronised product automaton (initialisation)

▶ **Definition 24** (2-Template automata (2-TA))**.** A *2-template automaton* is an NFA whose states are tuples of the form $\langle \tau, \eta, \sigma \rangle$ where τ, σ are types and $\eta : \overline{\sigma} \to \overline{\tau}$, whose alphabet is the set of pairs of templates, whose transitions are of the form $\langle \langle \sigma, \eta, \tau \rangle, \langle \Gamma, \Delta \rangle, \langle \sigma', \eta', \tau' \rangle \rangle$ where $\Gamma : \sigma \to \sigma'$, $\Delta : \tau \to \tau'$, and $\Gamma \leq_{\eta, \eta'} \Delta$, and with a single initial state and a single accepting state which consist of singleton types.

If $\mathcal{T}$ is a 2-TA, we denote by $\pi_1(\mathcal{T})$ (resp. $\pi_2(\mathcal{T})$) the automaton obtained by projecting the alphabet, the states and the transitions of $\mathcal{T}$ on the first (resp. last) component. Note that $\pi_1(\mathcal{T})$ and $\pi_2(\mathcal{T})$ are TA.

▶ **Definition 25** (Synchronised product of TA)**.** Let $\mathscr{E}, \mathscr{F}$ be two TA. The *synchronised product* of $\mathscr{E}$ and $\mathscr{F}$, written $\mathscr{E} \times \mathscr{F}$ is the 2-TA where $\langle \langle \tau, \eta, \sigma \rangle, \langle \Gamma, \Delta \rangle, \langle \tau', \eta', \sigma' \rangle \rangle$ is a transition of $\mathscr{E} \times \mathscr{F}$ iff $\langle \tau, \Gamma, \tau' \rangle$ is a transition of $\mathscr{E}$, $\langle \sigma, \Delta, \sigma' \rangle$ is a transition of $\mathscr{F}$ and $\Gamma \leq_{\eta, \eta'} \Delta$. (And with initial and accepting states defined from those of of $\mathscr{E}$ and $\mathscr{F}$.)

Note that we enforce refinement in the definition of this product, so that $\pi_1(\mathscr{E} \times \mathscr{F})$ is a sub-automaton of $\mathscr{E}$ and $\pi_2(\mathscr{E} \times \mathscr{F})$ is a sub-automaton of $\mathscr{F}$. Thus $\mathcal{G}(\pi_1(\mathscr{E} \times \mathscr{F})) \subseteq \mathcal{G}(\mathscr{E})$ and $\mathcal{G}(\pi_2(\mathscr{E} \times \mathscr{F})) \subseteq \mathcal{G}(\mathscr{F})$. When $\mathscr{E}, \mathscr{F}$ are TA coming from PA $\mathscr{A}, \mathscr{B}$ such that ${}^{\lhd}\mathcal{G}(\mathscr{A}) \subseteq {}^{\lhd}\mathcal{G}(\mathscr{B})$, we can use the results from [11] about simulations to strengthen the first inclusion into an equality:

▶ **Theorem 26.** *Let $\mathscr{A}, \mathscr{B}$ be two PA, $\mathscr{E}, \mathscr{F}$ be basic TA such that $\mathcal{G}(\mathscr{A}) = \mathcal{L}(\mathscr{E})$ and $\mathcal{G}(\mathscr{B}) = \mathcal{L}(\mathscr{F})$ (given by Prop. 4). If ${}^{\lhd}\mathcal{G}(\mathscr{A}_1) \subseteq {}^{\lhd}\mathcal{G}(\mathscr{A}_2)$ then:*

- $\mathcal{G}(\pi_1(\mathscr{E} \times \mathscr{F})) = \mathcal{G}(\mathscr{A})$;
- $\mathcal{G}(\pi_2(\mathscr{E} \times \mathscr{F})) \subseteq \mathcal{G}(\mathscr{B})$.

Proof. The second point follows from the observation above. The first one comes from the simulation result ([11, Prop. 9.10]) for PA. Indeed, if ${}^{\lhd}\mathcal{G}(\mathscr{A}) \subseteq {}^{\lhd}\mathcal{G}(\mathscr{B})$, then there is a simulation ([11, Def. 9.2]) between $\mathscr{A}$ and $\mathscr{B}$. This implies that for every run $\langle \tau_1, \Gamma_1, \tau_2, \ldots, \Gamma_{n-1}, \tau_n \rangle$ of $\mathscr{E}$, there is a run $\langle \sigma_1, \Delta_1, \sigma_2, \ldots, \Delta_{n-1}, \sigma_n \rangle$ of $\mathscr{F}$ and a set of mapping $\eta_i : \overline{\sigma_i} \to \overline{\tau_i}$, $i \in [1, n]$ such that $\Gamma_i \lhd_{\eta_i, \eta_{i+1}} \Delta_i$ for every $i \in [1, n-1]$. ◀

6.3 Maintaining refinement during reductions

Let us finally show that refinement is stable by composition, union, and iteration.

▶ **Theorem 27** (Stability of refinement by $\cdot$ and $\cup$).
- *If* $\Gamma_1 \leq_{\eta,\eta'} \Gamma_2$ *and* $\Delta_1 \leq_{\eta',\eta''} \Delta_2$ *then* $\Gamma_1 \cdot \Delta_1 \leq_{\eta,\eta''} \Gamma_2 \cdot \Delta_2$.
- *If* $\Gamma_1 \leq_{\eta,\eta'} \Gamma_2$ *and* $\Delta_1 \leq_{\eta,\eta'} \Delta_2$ *then* $\Gamma_1 \cup \Delta_1 \leq_{\eta,\eta'} \Gamma_2 \cup \Delta_2$.

Proof. To show the first property it suffices to show the following results:

$$\text{If} \quad \Gamma_1 \lhd_{\eta,\eta'} \Gamma_2 \quad \text{and} \quad \Delta_1 \lhd_{\eta',\eta''} \Gamma_2 \quad \text{then} \quad \Gamma_1 \cdot \Delta_1 \lhd_{\eta',\eta''} \Gamma_2 \cdot \Delta_2. \qquad (L_1)$$

$$\text{If} \quad \Gamma_1 \sqsubseteq \Gamma_2 \quad \text{and} \quad \Delta_1 \sqsubseteq \Delta_2 \quad \text{then} \quad \Gamma_1 \cdot \Delta_1 \sqsubseteq \Gamma_2 \cdot \Delta_2. \qquad (L_2)$$

$$\text{If} \quad \Gamma_1 \lhd \Gamma_2 \quad \text{and} \quad \Delta_1 \sqsubseteq \Delta_2 \quad \text{then} \quad \Gamma_1 \cdot \Delta_1 \ (\lhd \cdot \sqsubseteq)^* \ \Gamma_2 \cup \Delta_2. \qquad (L_3)$$

To show (L_1), consider a box $\alpha_1 \in \Gamma_1$ and $\beta_1 \in \Delta_1$. By hypothesis, there is a box $\alpha_2 \in \Gamma_2$ and an (η, η')-compatible homomorphism $h = \langle f, g \rangle$ from α_2 to α_1 and a box $\beta_2 \in \Delta_2$ and an (η', η'')-compatible homomorphism $h' = \langle f', g' \rangle$ from β_2 to β_1. Let $h'' = \langle f'', g'' \rangle$, where f'' equals f in $\mathrm{dom}(f)$ and f' in $\mathrm{dom}(f')$, and g" equals g in $\mathrm{dom}(g)$ and g' in $\mathrm{dom}(g')$. Using (η, η')-compatibility of h and (η', η'')-compatibility of h', it is easy to show that h'' is an (η, η'')-compatible homomorphism from $\alpha_2 \cdot \beta_2$ to $\alpha_1 \cdot \beta_1$, which concludes the proof of (L_1). (L_2) follows easily from the definition of $\sqsubseteq$. For (L_3), note that $\Delta_1 \lhd \Delta_1$ (we choose the identity homomorphism), thus by (L_1), we have that $\Gamma_1 \cdot \Delta_1 \lhd \Gamma_2 \cdot \Delta_1$. By (L_2), we have that $\Gamma_2 \cdot \Delta_1 \sqsubseteq \Gamma_2 \cdot \Delta_2$, which concludes the proof.

To show the first property, we proceed by induction on the length of the sequences justifying that $\Gamma_1 \leq_{\eta,\eta'} \Gamma_2$ and $\Delta_1 \leq_{\eta',\eta"} \Delta_2$, using $(L_1), (L_2)$ and (L_3) for the base cases.

To show the second property, we follow the same proof schema, showing results similar to $(L_1) - (L_3)$ where $\cdot$ is replaced by $\cup$. ◀

▶ Remark. Thm. 27 justifies our definition of $\leq_{\eta,\eta'}$. Indeed, a more permissive definition would seem natural, but the first property of Thm 27 would fail. For instance, if $\Gamma_1 \sqsubseteq \Gamma_2$ and $\Delta_1 \lhd_{\eta,\eta'} \Delta_2$, we do not have in general that $\Gamma_1 \cdot \Delta_1 \leq_{\eta,\eta'} \Gamma_2 \cdot \Delta_2$.

The main theorem of this section is Thm 28, stating that the refinement relation is stable under iteration.

▶ **Theorem 28** (Stability of refinement by $\_^+$). *If* $\Gamma \leq_{\eta,\eta} \Delta$ *then there are bowtie choices* $\bowtie, \bowtie'$ *and computation orders* $\preceq, \preceq'$*, for* Γ *and* Δ *respectively, such that:* $\Gamma^+_{\bowtie,\preceq} \leq_{\eta,\eta} \Delta^+_{\bowtie',\preceq'}$.

Proof. To prove Thm. 28, it is enough to show the following properties.
- If $\Gamma \sqsubseteq \Delta$ then, for every bowtie choices $\bowtie, \bowtie'$, and every computation orders $\preceq, \preceq'$ for Γ and Δ respectively, we have that $\Gamma^+_{\bowtie,\preceq} \sqsubseteq \Delta^+_{\bowtie',\preceq'}$.
- If $\Gamma \lhd_{\eta,\eta} \Delta$ then there are two bowtie choices $\bowtie, \bowtie'$ and two computation orders $\preceq, \preceq'$, for Γ and Δ respectively, such that $\Gamma^+_{\bowtie,\preceq} \leq_{\eta,\eta} \Delta^+_{\bowtie',\preceq'}$.

The first property follows from $\mathcal{B}(\Gamma^+_{\bowtie,\preceq}) = \mathcal{B}(\Gamma)^+$ for every bowtie choice $\bowtie$ and order $\preceq$.

For the sake of clarity, we give here the proof of the second proposition in the case where Γ and Δ are singletons of atomic boxes $\{\alpha\}$ and $\{\beta\}$ respectively. The general case is treated in App. B. Let $\bowtie, \bowtie'$ be bowtie choices for α and β respectively, and let $h = \langle f, g\rangle$ be a homomorphism from β to α.

Let us first treat the case where $f^{-1}(\bowtie) = \{\bowtie'\}$ (we say that α, β are bowtie compatible). This is illustrated by the boxes α, β of Fig. 13, where the bowties are the red nodes. If we decompose α and β at the level of their bowties, we get $\alpha = \alpha_1 \cdot \alpha_2$ and $\beta = \beta_1 \cdot \beta_2$, where $\alpha_2 \cdot \alpha_1$ and $\beta_2 \cdot \beta_1$ are 1-1 boxes. We write $e = e\,(\alpha_2 \cdot \alpha_1)$ and $f = e\,(\beta_2 \cdot \beta_1)$. The boxes $\alpha^+_{\bowtie}$ and $\beta^+_{\bowtie'}$ are depicted in Fig. 13. Let us show that there is a homomorphism from $\beta^+_{\bowtie'}$ to $\alpha^+_{\bowtie}$. The homomorphism h induces a homomorphism h_1 from β_1 to α_1 and a homomorphism h_2 from β_2 to α_2 (Lem. 42 in App. B). Combining h_1 and h_1, we get almost a homomorphism from $\beta^+_{\bowtie'}$ to $\alpha^+_{\bowtie}$ (See Fig. 13), we need only to show that $\mathsf{KL}^- \vdash e \leq f$. But this follows from Prop. 6: indeed, we can combine h_1 and h_2 to get a homomorphism from $\beta_2 \cdot \beta_1$ to $\alpha_2 \cdot \alpha_1$. We have thus that $\alpha^+_{\bowtie} \lhd_{\eta,\eta} \beta^+_{\bowtie'}$ ((η,η)-compatibility is easy).

Let us now treat the case where $N := f^{-1}(\bowtie)$ is not necessarily $\{\bowtie'\}$ (N is illustrated by the red node of β in Fig. 14). Let γ be the box obtained from β by merging the nodes N (see Fig. 14). There are two bowtie choices for γ: a bowtie $\bowtie_b$ inherited from β (blue in Fig. 14) and a bowtie $\bowtie_r$ coming from the nodes of N (red in Fig. 14).

Let h' be the homomorphism from β to γ that maps each node (and each edge) to itself, except for the nodes of N which are mapped to $\bowtie_r$. If we consider the bowtie $\bowtie_b$ for γ, then β and γ are bowtie compatible w.r.t. to h', thus $\gamma^+_{\bowtie_b} \lhd \beta^+_{\bowtie'}$ using the previous case.

Let h'' be the homomorphism from γ to α, which is exactly h except that it maps the node $\bowtie_r$ to the bowtie $\bowtie$ of α. If we consider the bowtie $\bowtie_r$ for γ, then γ and α are bowtie compatible w.r.t. h'', thus $\alpha^+_{\bowtie} \lhd_{\eta,\eta} \gamma^+_{\bowtie_r}$ using the previous case again.

Notice finally that $\gamma^+_{\bowtie_r} \sqsubseteq \gamma^+_{\bowtie_b}$. To sum up, we have: $\alpha^+_{\bowtie} \lhd_{\eta,\eta} \gamma^+_{\bowtie_r} \sqsubseteq \gamma^+_{\bowtie_b} \lhd \beta^+_{\bowtie'}$. ◀

The last case in this proof explains the need to work with refinement ($\leq$) rather than just homomorphisms ($\lhd$): when starting from templates that are related by homomorphism and iterating them, the templates we obtain are not necessarily related by a single homomorphism, only by a sequence of homomorphisms and inclusions.

7 Future work

We have proven that KL^- axioms are sound and complete w.r.t. the relational models of identity-free Kleene lattices, and thus also w.r.t. their language theoretic models, by the results from [3].

Whether one can obtain a finite axiomatisation in presence of identity remains open. This question is important since handling the identity relation is the very first step towards handling *tests*, which are crucial in order to model the control flow of sequential programs precisely (*e.g.*, as in Kleene algebra with tests [20]).

An intermediate problem, which is still open to the best of our knowledge, consists in finding an axiomatisation for the fragment with composition, intersection and identity (not including transitive closure) [2, see errata available online].

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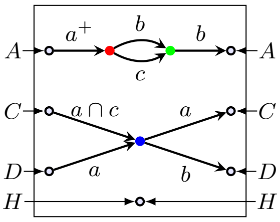


Figure 15 Example of a box.

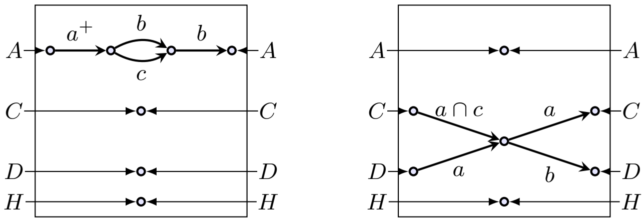


Figure 16 Atomic boxes stemming from the box of Fig. 15.

A Iteration of a template

In this section, we address in detail the definitions relative to the construction of the iteration of a template.

We have seen that there are two sources of non-determinism when computing the iteration of a template (Algorithm 11). The first is the bowtie choice and the second is the computation order. Let us introduce them more precisely.

A.1 Bowtie choice for a template

We have seen in Sec. 5.2 that the non-trivial connected component of an atomic box can be associated with a specific node called its bowtie (Lem.20). We do the same for non atomic boxes.

▶ **Definition 29** (Connected component of a box). If $\beta = \langle \overrightarrow{\mathfrak{p}}, G, \overleftarrow{\mathfrak{p}} \rangle$ is a box, we denote by $\mathcal{C}(\beta)$ the set of non-trivial connected components of G, which we call simply connected component of β.

▶ **Lemma 30** (Bowtie lemma [11, Lem. 7.1]). *Let $B = \langle \overrightarrow{\mathfrak{p}}, G, \overleftarrow{\mathfrak{p}} \rangle$ be a box of type $\tau \to \tau$. For every $C \in \mathcal{C}(\beta)$ there is a vertex c such that for every port p where $\overrightarrow{\mathfrak{p}}(p) \in C$, all paths from $\overrightarrow{\mathfrak{p}}(p)$ to a maximal vertex of C visit c. We call such a vertex a bowtie for C.*

▶ **Definition 31** (Bowtie choice for a template). A *bowtie choice* for a box is a function mapping a bowtie to every connected component.

A *bowtie choice* for a template is a function mapping a bowtie to every connected component of every box.

▶ Remark. When β is atomic, it has only one connected component, so we may identify the bowtie choice that maps this component to a node, with the node itself.

▶ **Example 32.** Consider the box of Figure 15. It has two connected components. The first has two bowtie choices: the red and the green node. The second has only one bowtie choice, the blue node.

▶ **Notation 1.** *If α is an atomic box and $\bowtie$ is a bowtie choice for α, then we can decompose α at the level of this bowtie to get two boxes such that $\alpha = \alpha_1 \cdot \alpha_2$. We write $\alpha \overset{\bowtie}{=} \alpha_1 \cdot \alpha_2$ for this decomposition. In Fig. 17, the box α can be decomposed at the level of its bowtie (the blue node) into α_1 and α_2.*

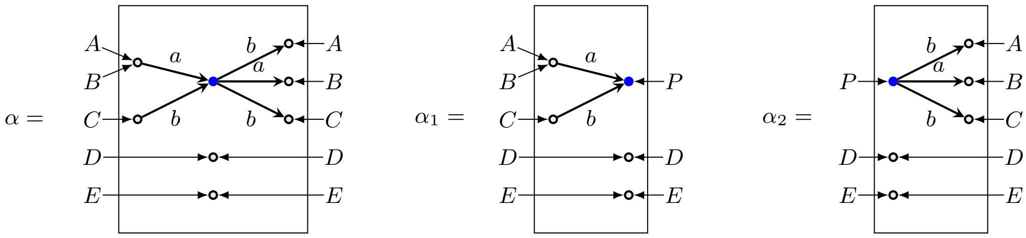


Figure 17 Decomposition of an atomic box.

A.2 Computation order

Let us analyse computation order of algorithm 11 in the simple case where $\Gamma = \{\alpha, \beta\}$. If $supp\,(\alpha) \subsetneq \beta$ then the algorithm starts necessarily by processing α. If $supp\,(\alpha) \cap supp\,(\beta) = \emptyset$, then the order in which the computation proceeds does not matter, and we will get the same result no matter if we start with processing α or β. The only case where we have a freedom to choose the computation order, and in which this order may affect the result is when $supp\,(\alpha) = supp\,(\beta)$. In general, to specify the computation order, it is enough to order the elements of Γ having the same support.

▶ **Definition 33** (Computation order)**.** A *computation order* for an atomic template Γ is a partial order $\preceq$ on its elements such that if $\alpha \preceq \beta$ then $supp\,(\alpha) = supp\,(\beta)$.

A.3 Atomic template of a template

To compute the iteration of a template, we start by decomposing its boxes into atomic ones.

▶ **Definition 34** ($At(\Gamma)$)**.** Let $\beta : \sigma \to \sigma$ be a box. From each $C \in \mathcal{C}(\beta)$ stems an atomic box of the same type having C as a connected component. We set $At(\beta)$ to be the set of atomic boxes stemming from its connected components.

If $\Gamma : \sigma \to \sigma$ is a template we write $At(\Gamma)$ for the set of boxes stemming from the connected components of the boxes of Γ.

For instance, the boxes of Figure 16 are the boxes stemming from the connected components of the box of Figure 15.

▶ Remark. Note that every bowtie choice for Γ induces a bowtie choice for $At(\Gamma)$.

▶ **Definition 35.** A computation order for a template Γ is a computation order for $At(\Gamma)$.

A.4 The iteration algorithm

Fig. 18 shows the algorithm computing the iteration of an atomic template, parameterised by a bowtie choice and a computation order.

If $\bowtie$ is a bowtie choice and $\preceq$ is a computation order for Γ, we set $\Gamma^+_{\bowtie,\preceq} := At(\Gamma)^+_{\bowtie,\preceq}$.

B Stability of $\leq$ under iteration

In the whole section, we will work under the following proviso:

▶ **Proviso 1.** *We suppose that all templates are of type $\tau \to \tau$ and that all the box and template homomorphisms are (η, η)-compatible, where τ is a fixed type and $\eta : \overline{\tau} \to \overline{\tau}$ a fixed mapping. We will not write explicitly $\lhd_{\eta,\eta}$ for (η, η)-compatible homomorphisms but simply*

Data: Atomic template Γ, a bowtie choice $\bowtie$ and a computation order $\preceq$ for Γ
Result: A template $\Gamma^+_{\bowtie,\preceq}$ such that $\mathcal{B}(\Gamma^+_{\bowtie,\preceq}) = \mathcal{B}(\Gamma)^+$
if $\Gamma = \emptyset$ **then**
  Return $\emptyset$
else
  Write $\Gamma = \Delta \cup \{\alpha\} \cup \Sigma$ such that $\mathit{supp}\,(\Delta) \subseteq \mathit{supp}\,(\alpha)$, $\forall \alpha' \in \Delta$ if $\mathit{supp}\,(\alpha)' = \mathit{supp}\,(\alpha)$ then $\alpha' \preceq \alpha$, and $\mathit{supp}\,(\Sigma) \cap \mathit{supp}\,(\alpha) = \emptyset$;
  Set $\bowtie' := \bowtie (C)$, where $\mathcal{C}(\alpha) = \{C\}$.
  Split α into $\alpha \overset{\bowtie'}{=} \beta \cdot \gamma$;
  Return $(\Delta^+ \cdot \Sigma^*) \cup (\Delta^* \cdot \Sigma^+) \cup (\Delta^* \cdot \delta \cdot \Delta^* \cdot \Sigma^*)$, where δ is the two-box template depicted on the right.
end

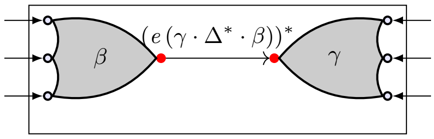


Figure 18 Algorithm computing the iteration of an atomic template

$\lhd$. *All the theorems, propositions, lemmas of this section hold under this proviso, which will not be mentioned explicitly in their statements.*

In this section, we will show the following theorem:

▶ **Theorem 36.** *If $\Delta \lhd \Gamma$ then there are two bowtie choices $\bowtie, \bowtie'$ for Δ and Γ respectively, and two computation orders $\preceq, \preceq'$ for Δ and Γ respectively such that: $\Delta^+_{\bowtie,\preceq} \leq \Gamma^+_{\bowtie',\preceq'}$.*

To prove theorem 36, we will show that template homomorphisms can be decomposed into simpler template homomorphisms $\lhd_1$ and $\lhd_2$ (Def. 37, Def. 39, Prop. 7). It is thus enough to show Thm. 36 in the case where $\Delta \lhd_1 \Gamma$ and $\Delta \lhd_2 \Gamma$, these results are precisely Prop. 8 and Prop. 9.

B.1 Decomposing $\lhd$ into $\lhd_1$ and $\lhd_2$

Let us first define the template homomorphisms $\lhd_1$ and $\lhd_2$.

▶ **Definition 37** ($\lhd_1$)**.** Let α, β be two boxes. We set $\alpha \lhd_1 \beta$ if there are bowtie choices $\bowtie, \bowtie'$ for α and β respectively, and a box homomorphism h from β to α such that:

- If $C \in \mathcal{C}(\beta)$ then $h(C) \in \mathcal{C}(\alpha)$.
- If $C, D \in \mathcal{C}(\beta)$ and $C \neq D$ then $h(C) \neq h(D)$.
- If $C \in \mathcal{C}(\beta)$ then $h(\bowtie' (C)) = \bowtie (h(C))$.

If Γ, Δ are templates, we set $\Gamma \lhd_1 \Delta$ if for every $\alpha \in \Gamma$, there is $\beta \in \Delta$ such that $\alpha \lhd_1 \beta$.

Figure 19 shows two boxes α, β such that $\alpha \lhd_1 \beta$. Indeed, the blue connected component of β and its bowtie are mapped to the blue connected component of α and its bowtie. The same holds for the red connected component.

To define the homomorphism $\lhd_2$, we need to define formally the operation of "merging" (or "identifying") nodes in a graph.

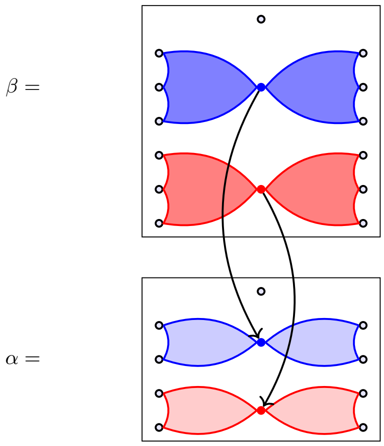


Figure 19 Boxes α, β such that $\alpha \lhd_1 \beta$.

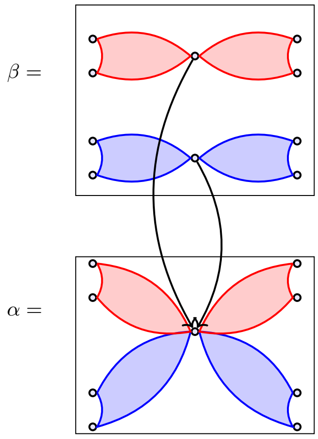


Figure 20 Boxes α, β such that $\alpha \lhd_2 \beta$.

▶ **Definition 38** (Identification of nodes in a graph)**.** Let $G = \langle V, E\rangle$ be a graph and $N_1, \dots, N_k \subseteq V$ be pairwise disjoint sets of nodes. Let $\equiv$ be the smallest equivalence relation on V containing all the pairs $\langle n, m\rangle$, such that $\exists i \in [1, k], n, m \in N_i$. We write $G|_{\equiv\{N_1,\dots,N_k\}}$ for the graph $\langle \{[n] \mid n \in V\}, E'\rangle$ where $[n] = \{m \mid m \equiv n\}$ and $\langle [n], x, [m]\rangle \in E'$ if and only if $\langle n, x, m\rangle \in E$.

Let $\beta = \left\langle \overrightarrow{\mathfrak{p}}, G, \overleftarrow{\mathfrak{p}} \right\rangle$ is a box, and $N_1, \dots, N_k$ be pairwise disjoint sets of the nodes of G. We write $\beta|_{\equiv\{N_1,\dots,N_k\}}$ for the box $\left\langle \overrightarrow{\mathfrak{p}}', G|_{\equiv\{N_1,\dots,N_k\}}, \overleftarrow{\mathfrak{p}}' \right\rangle$ where $\overrightarrow{\mathfrak{p}}'$ and $\overleftarrow{\mathfrak{p}}'$ are defined by: $\overrightarrow{\mathfrak{p}}'(x) = [n]$ if $\overrightarrow{\mathfrak{p}}(x) = n$ and $\overleftarrow{\mathfrak{p}}'(x) = [n]$ if $\overleftarrow{\mathfrak{p}}(x) = n$.

▶ **Definition 39** ($\lhd_2$)**.** Let α, β be two boxes. We set $\alpha \lhd_2 \beta$ if there is a bowtie choice $\bowtie$ for β and $C, D \in \mathcal{C}(\beta)$ such that when we set $N = \{\bowtie(C), \bowtie(D)\}$ we have $\alpha = \beta|_{\equiv\{N\}}$. If Γ, Δ are templates, we set $\Gamma \lhd_2 \Delta$ if $\Gamma = \Sigma \cup \{\alpha\}$ and $\Delta = \Sigma \cup \{\beta\}$ such that $\alpha \lhd_2 \beta$.

In other words, $\alpha \lhd_2 \beta$ if α is obtained by "merging" the bowties of two connected components of β. Figure 20 show two boxes α, β such that $\alpha \lhd_2 \beta$.

To show that $\lhd$ can be decomposed into $\lhd_1$ and $\lhd_2$ (Prop. 7), we need the following lemma, which says that the converse image of a connected component by a homomorphism is a collection of connected components.

▶ **Lemma 40.** *Let α, β be two boxes and h be a box homomorphism from β to α. For every $C \in \mathcal{C}(\alpha)$, there is a set $\{C_1, \dots, C_n\} \subseteq \mathcal{C}(\beta)$ such that $h^{-1}(C) = C_1 \cup \dots \cup C_n$.*

Proof. Let $C \in \mathcal{C}(\alpha)$. By contradiction suppose that there is a connected component $C' \in \mathcal{C}(\beta)$ and two nodes $x, y \in C'$ such that $\langle x, a, y\rangle$ is a vertex of the graph of α, $h(x) \in C$ and $h(y) \notin C$. Since h is a homomorphism, we have that there is a vertex in the graph of β between $h(x)$ and $h(y)$, thus $h(y) \in C$. This gives us a contradiction. ◀

Let us show now that we can indeed decompose $\lhd$ into $\lhd_1$ and $\lhd_2$.

▶ **Proposition 7.** *We have that $\lhd \subseteq (\lhd_1 \cup \lhd_2)^+$, where the operation $\_^+$ is the transitive closure on relations.*

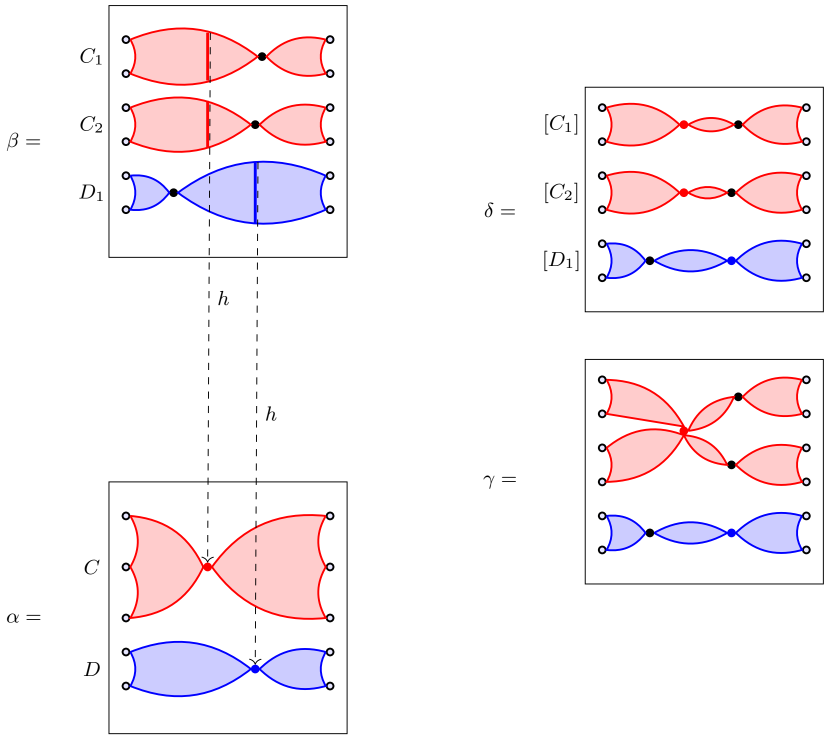


Figure 21 Decomposing $\alpha \lhd \beta$ into $\alpha \lhd_1 \gamma$, $\gamma \lhd_2^+ \delta$ and $\delta \lhd_1 \beta$.

Proof. Let us show that if $\Gamma \lhd \Delta$ then there is $\Sigma_1, \dots, \Sigma_n$ such that $\Sigma_1 = \Gamma$, $\Sigma_n = \Delta$ and for every $i \in [1, n-1]$ either $\Sigma_i \lhd_1 \Sigma_{i+1}$ or $\Sigma_i \lhd_2 \Sigma_{i+1}$. For that, we proceed by induction on the size of Γ.

Let $\alpha \in \Gamma$ and set $\Sigma = \Gamma \setminus \{\alpha\}$. Since $\Gamma \lhd \Delta$, there is a box $\beta \in \Delta$ such that $\alpha \lhd \beta$. Let h be a homomorphism from β to α and let $\bowtie, \bowtie'$ be two bowtie choices for α and β respectively.

Let us show first that there are two boxes γ and δ such that $\alpha \lhd_1 \gamma$, $\gamma \lhd_2^+ \delta$ and $\delta \lhd_1 \beta$. We will illustrate the construction of γ and δ by Figure 21. In this figure, α has two connected components C and D, and β has three connected components C_1, C_2 and D_1 such that $h(C_1 \cup C_2) = C$ and $h(D_1) = D$. The bowtie choices for α and β are illustrated by the nodes in the middle of each connected component.

Let us construct δ. By Lem. 40, we know that for every connected component C of α, $h^{-1}(C) = C_1 \cup \dots \cup C_n$ where $C_i \in \mathcal{C}(\beta)$. We set $C^{-1} = \{C_1, \dots, C_n\}$. For every $C' \in C^{-1}$ we set:

$$b(C, C') = h^{-1}(\bowtie(C)) \cap C'$$

Let $\delta = \beta|_{\equiv\{b(C,C') \mid C \in \mathcal{C}(\alpha), C' \in C^{-1}\}}$. As illustrated by Figure 21, δ is obtained from β by merging in every connected component the nodes that are mapped to a bowtie of α by h.

The box δ has two possible bowtie choices: one inherited from the bowtie $\bowtie'$ of β (the black bowties of δ in Figure 21) and another coming from the nodes $b(C, C')$ that have being merged (the red and the blue bowties for δ in Figure 21). We call the former $\bowtie_1$ and the later $\bowtie_2$.

If we take $\bowtie_1$ as a bowtie choice for δ, then we have easily that $\delta \lhd_1 \beta$.

Let us construct γ now. We set $\bowtie^{-1}(C) = h^{-1}(\bowtie(C))$. Note that we have $\bowtie^{-1}(C) = \bigcup_{C' \in C^{-1}} b(C, C')$. We let

$$\gamma = \beta|_{\equiv\{\bowtie^{-1}(C) \mid C \in \mathcal{C}(\alpha)\}}$$

In other words, if we denote by $[C]$ the connected component of δ coming from the connected component C of β, then γ is obtained by identifying every two nodes $\bowtie_2([C_1])$ and $\bowtie_2([C_2])$, where $C_1, C_2 \in C^{-1}$ and $C \in \mathcal{C}(\alpha)$. If we call $\gamma_1, \ldots, \gamma_k$ these intermediate boxes where we merged only two nodes, we have that $\gamma \lhd_2 \delta_1 \lhd_2 \ldots \lhd_2 \delta_k \lhd_2 \delta$. Figure 21 illustrates the construction of γ.

If we consider the bowtie choice $\bowtie$ of α and the bowtie choice $\bowtie_3$ of γ induced by merging the nodes $\bowtie^{-1}(C)$ of β (The red node of γ in Figure 21), it is easy to see that $\alpha \lhd_1 \gamma$.

Let us make a final observation before showing the general result. Notice that if B, B' are two boxes, and Θ is a template, then $B \lhd_1 B'$ entails $B \cup \Theta \lhd_1 B' \cup \Theta$ and $B \lhd_2 B'$ entails $B \cup \Theta \lhd_2 B' \cup \Theta$. Thus if $B(\lhd_1 \cup \lhd_2)^+ B'$ then $(B \cup \Theta)(\lhd_1 \cup \lhd_2)^+(B' \cup \Theta)$.

Let us go back to the proof of our result. Recall that $\Gamma = \Sigma \uplus \{\alpha\}$, that $\beta \in \Delta$, and that $\alpha(\lhd_1 \cup \lhd_2)^+\beta$. By the remark above, we have that $\Gamma(\lhd_1 \cup \lhd_2)^+(\{\beta\} \cup \Sigma)$. Since $\Gamma \lhd \Delta$ we have also that $\Sigma \lhd \Delta$, thus by induction hypothesis we have $\Sigma(\lhd_1 \cup \lhd_2)^+\Delta$, and again by the remark above, we have that $(\Sigma \cup \{\beta\})(\lhd_1 \cup \lhd_2)^+\Delta$, which concludes the proof. ◀

B.2 $\lhd_1$ is stable under iteration

Let us show now that $\lhd_1$ is stable under iteration:

▶ **Proposition 8.** *If $\Gamma \lhd_1 \Delta$ then there are two bowtie choices $\bowtie, \bowtie'$ and two template orders $\preceq, \preceq'$ for Γ and Δ respectively such that: $\Gamma^+_{\bowtie,\preceq} \leq \Delta^+_{\bowtie',\preceq'}$.*

To show Prop. 8, we need the following lemma.

▶ **Lemma 41.** *If $\alpha_1, \beta_1, \alpha_2, \beta_2$ are atomic boxes such that $\alpha_1 \lhd \beta_1$ and $\alpha_2 \lhd \beta_2$ then:*

- *$supp(\alpha_1) \subseteq supp(\alpha_2) \Rightarrow supp(\beta_1) \subseteq supp(\beta_2)$.*
- *$supp(\alpha_1) \cap supp(\alpha_2) = \emptyset \Rightarrow supp(\beta_1) \cap supp(\beta_2) = \emptyset$.*

Proof. To show this result, let us make first the following observation. If α, β are atomic boxes such that $\alpha \lhd \beta$ then:

$$p \in supp(\beta) \text{ if and only if } \eta(p) \in supp(\alpha).$$

Let us see why this observation holds. We set $\alpha = \langle \overrightarrow{\mathfrak{p}}_\alpha, G, \overleftarrow{\mathfrak{p}}_\alpha \rangle$ and $\beta = \langle \overrightarrow{\mathfrak{p}}_\beta, H, \overleftarrow{\mathfrak{p}}_\beta \rangle$, and let h be a homomorphism from β to α.

Suppose by contradiction that there is $p \in supp(\beta)$ such that $\eta(p) \notin supp(\alpha)$. We set $v = \overrightarrow{\mathfrak{p}}_\beta(p)$ and $w = \overrightarrow{\mathfrak{p}}_\alpha(\eta(p))$. By (η, η)-compatibility, we have $h(v) = w$. Since $p \in supp(\beta)$, $\overrightarrow{\mathfrak{p}}_\beta(p)$ is a node of a non-trivial component of G, thus there is an edge $\langle v, a, u\rangle$ in G. Since h is a homomorphism from β to α we should have an edge $\langle w, b, h(u)\rangle$ in H. But since $\eta(p) \notin supp(\alpha)$, we have that w is an isolated node of H, this gives us a contradiction.

Conversely, if $p \notin supp(\beta)$ then $v := \overrightarrow{\mathfrak{p}}_\alpha(p)$ is an isolated node of β, thus $h(v)$ is an isolated node by definition of a box homomorphism. By $(\eta - \eta)$-compatibility, we have that $\overrightarrow{\mathfrak{p}}_\alpha(\eta(p)) = h(v)$, thus $\eta(p) \notin supp(\alpha)$.

Let us go back to the proof of our lemma. Suppose that $supp(\alpha_1) \subseteq supp(\alpha_2)$ and let $p \in supp(\beta_1)$. By the observation above, we have that $\eta(p) \in supp(\alpha_1)$ thus $\eta(p) \in supp(\alpha_2)$. By the above observation again, we have $\eta(p) \in supp(\alpha_2)$.

Suppose that $p \in supp\,(\beta_1) \cap supp\,(\beta_2)$. By the above observation, we have that $\eta(p) \in supp\,(\alpha_1) \cap supp\,(\alpha_2)$. ◀

▶ **Lemma 42.** *Let α, β be two atomic boxes and h be a homomorphism from β to α. Let $\bowtie, \bowtie'$ be bowtie choices for α, β, and let $\alpha \overset{\bowtie}{=} \alpha_1 \cdot \alpha_2$ and $\beta \overset{\bowtie'}{=} \beta_1 \cdot \beta_2$. If $h(\bowtie') = \bowtie$ then $\alpha_1 \lhd \beta_1$ and $\alpha_2 \lhd \beta_2$.*

Proof. We show that the homomorphism h induces a homomorphism from β_i to α_i, for $i = 1, 2$. For that we only need to show that h maps the graph of β_1 to the graph of α_1 and maps the graph of β_2 to the graph of α_2. In other words, for $i = 1, 2$:

$$n \text{ is a node of } \beta_i \text{ if and only if } h(n) \text{ is a node of } \alpha_i$$

Suppose (by symmetry) that there is a node n of β_1 such that $h(n) \in \alpha_2$. There is a path from n to $\bowtie$ in the graph of β. This path can be mapped by h to a path from $h(n)$ to $\bowtie'$ in the graph of α. This is not possible by well-typedness of the α. ◀

Let us show now Prop. 8.

Proof of Prop. 8. It is not difficult to see that if $\Gamma \lhd_1 \Delta$ then $At(\Gamma) \lhd_1 At(\Delta)$, thus we suppose *w.l.o.g.* that Γ and Δ are atomic.

Let $\bowtie, \bowtie'$ be the bowtie choices for Γ and Δ respectively, witnessing that $\Gamma \lhd_1 \Delta$. We set $\Gamma = \{\alpha_1, \ldots, \alpha_n\}$. Since $\Gamma \lhd \Delta$, we have that for every $i \in [1, n]$, there is $\beta_i \in \Delta$ such that $\alpha_i \lhd_1 \beta_i$. We set $\Sigma = \{\beta_1, \ldots, \beta_n\}$. Since $\Sigma \subseteq \Delta$, it is enough to show that there are $\preceq, \preceq'$ such that $\Gamma^+_{\bowtie,\preceq} \leq \Sigma^+_{\bowtie',\preceq'}$.

Let $\preceq$ be a template order for Γ. Let us define a template order $\preceq'$ for Σ. Note that if $supp\,(\beta_i) = supp\,(\beta_j)$, by Lem. 41 we cannot have $supp\,(\alpha_i) \cap supp\,(\alpha_j) = \emptyset$, thus by Lem. 21, either $supp\,(\alpha_i) \subseteq supp\,(\alpha_j)$ or $supp\,(\alpha_j) \subseteq supp\,(\alpha_i)$. We set define $\preceq'$ as follows:

$$\beta_i \preceq' \beta_j \quad \text{iff} \quad supp\,(\alpha_i) \subsetneq supp\,(\alpha_j) \qquad \text{or} \qquad supp\,(\alpha_i) = supp\,(\alpha_j) \quad \text{and} \quad \alpha_i \preceq \alpha_j$$

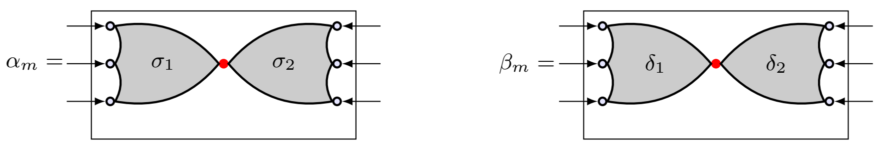
Let us show now, by induction on Γ, that $\Gamma^+_{\bowtie,\preceq} \leq \Sigma^+_{\bowtie',\preceq'}$. We decompose Γ into $\Gamma_1 \cup \{\alpha_m\} \cup \Gamma_2$ such that:

1. $\forall \alpha \in \Gamma_1$, $supp\,(\alpha) \subseteq supp\,(\alpha_i)$.
2. If $\alpha \preceq \alpha_m$ then $\alpha \in \Gamma_1$.
3. $\forall \alpha \in \Gamma_2$, $supp\,(\alpha) \cap supp\,(\alpha_m) = \emptyset$.

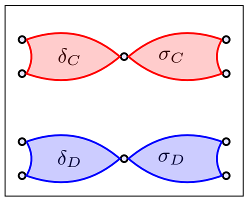
We set $\Gamma_1 = \{\alpha_k\}_{k \in I}$, $\Gamma_2 = \{\alpha_k\}_{k \in J}$ and $\Sigma_1 = \{\beta_k\}_{k \in I}$, $\Sigma_2 = \{\beta_k\}_{k \in J}$. We have that $\Sigma = \Sigma_1 \cup \{\beta_m\} \cup \Sigma_2$. Let us show that this decomposition of Σ is relevant for the computation of its iteration, in particular that β_m can be chosen as a pivot.

- $\forall \beta \in \Sigma_1$, $supp\,(\beta) \subseteq supp\,(\beta_m)$. (By item 1 above and Prop. 41)
- If $\beta \preceq' \beta_m$ then $\beta \in \Sigma_1$. (Indeed, by definition of $\preceq'$, if $\beta_j \preceq' \beta_m$ then $supp\,(\alpha_j) \subseteq supp\,(\alpha_m)$ thus $\alpha_j \in \Gamma_1$ and then $\beta_j \in \Sigma_1$.)
- $\forall \beta \in \Sigma_2$, $supp\,(\beta) \cap supp\,(\beta_i) = \emptyset$. (By item 3 above and Prop. 41).

To compute the iteration of Γ and Σ, we decompose the pivots α_m and β_m at the level of their bowtie choices: $\alpha_m \overset{\bowtie}{=} \sigma_1 \cdot \sigma_2$ and $\beta_m \overset{\bowtie'}{=} \delta_1 \cdot \delta_2$.



$\beta =$



$\alpha =$

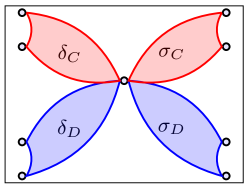
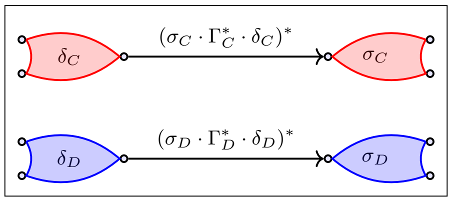


Figure 22 Boxes α, β in the proof of Prop. 9

$\beta_C^+ \cdot \beta_D^+ =$



$\alpha_{C \cdot D}^+ =$

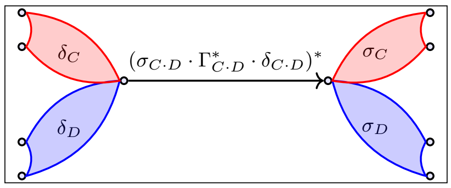


Figure 23 Boxes $\alpha_{C \cdot D}^+$ and $\beta_C^+ \cdot \beta_D^+$ of the proof of Prop. 9

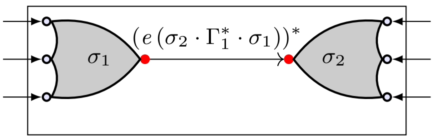
If we set $\Gamma_i^+ = (\Gamma_i)^+_{\bowtie, \preceq}$ and $\Sigma_i^+ = (\Sigma_i)^+_{\bowtie', \preceq'}$, for $i = 1, 2$ then we have:

$$\Gamma^+_{\bowtie, \preceq} = (\Gamma_1^+ \cdot \Gamma_2^*) \cup (\Gamma_1^* \cdot \Gamma_2^+) \cup (\Gamma_1^* \cdot {\alpha_m}^+ \cdot \Gamma_1^* \cdot \Gamma_2^*)$$

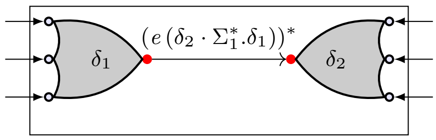
$$\Sigma^+_{\bowtie', \preceq} = (\Sigma_1^+ \cdot \Sigma_2^*) \cup (\Sigma_1^* \cdot \Sigma_2^+) \cup (\Sigma_1^* \cdot {\beta_m}^+ \cdot \Sigma_1^* \cdot \Sigma_2^*)$$

Where ${\alpha_m}^+$ are and ${\beta_m}^+$ are the following boxes.

$\alpha_m^+ =$



$\beta_m^+ =$



By induction hypothesis, we have that $\Gamma_1^+ \leq \Sigma_1^+$ and $\Gamma_2^+ \leq \Sigma_2^+$. Since $\leq$ is stable by set union and composition, it is enough to show that $\alpha_m^+ \leq \beta_m^+$ to conclude. More precisely, we will show that $\alpha_m^+ \lhd \beta_m^+$.

Since $\alpha_m \lhd_1 \beta_m$, we know by Lem. 42 that $\sigma_1 \lhd \delta_1$ and $\sigma_2 \lhd \delta_2$. To show that $\alpha_m^+ \lhd \beta_m^+$, it is enough to show that $\mathsf{KL}^- \vdash (e\,(\sigma_2 \cdot \Gamma_1^* \cdot \sigma_2))^+ \leq (e\,(\delta_2 \cdot \Sigma_1^* \cdot \delta_1))^+$ or simply that $\mathsf{KL}^- \vdash e\,(\sigma_2 \cdot \Gamma_1^* \cdot \sigma_1) \leq e\,(\delta_2 \cdot \Sigma_1^* \cdot \delta_1)$. For that observe that $\sigma_2 \cdot \Gamma_1^* \cdot \sigma_1 \leq \delta_2 . \Sigma_1^* \cdot \delta_1$ (because $\sigma_2 \lhd \delta_2$, $\Gamma_1^* \leq \Sigma_1^*$ and $\sigma_1 \lhd \delta_1$). We can thus conclude by Prop. 6. ◀

B.3 $\lhd_2$ is stable under iteration

▶ **Proposition 9.** *If $\Gamma \lhd_2 \Delta$ then there are two bowtie choices $\bowtie, \bowtie'$ and two computation orders $\preceq, \preceq'$ for Γ and Δ respectively such that: $\Gamma^+_{\bowtie, \preceq} \leq \Delta^+_{\bowtie', \preceq'}$.*

Proof. Since $\Gamma \lhd_2 \Delta$, we can write $\Gamma = \Sigma \cup \{\alpha\}$ and $\Delta = \Sigma \cup \{\beta\}$ such that $\alpha \lhd_2 \beta$. This means that there is a bowtie choice $\bowtie'$ for β, and two connected components C and D of the graph of β, such that α is obtained by merging $\bowtie(C)$ and $\bowtie(D)$. We denote by $C \cdot D$ the connected component of α obtained by merging C and D at the level of $\bowtie(C)$ and $\bowtie(D)$. (see Figure 22)

Let us define a bowtie choice $\bowtie$ for α. For the connected component $C \cdot D$, we set $\bowtie(C \cdot D)$ to be the node resulting from the merge of $\bowtie'(C)$ and $\bowtie'(D)$. For the other connected components, $\bowtie$ and $\bowtie'$ coincide. We extend $\bowtie$ and $\bowtie'$ to bowtie choices for Γ and Δ.

Let β_C, β_D and $\alpha_{C \cdot D}$ be the atomic boxes stemming respectively from the connected component C, D and $C \cdot D$. Observe that we can write $At(\Gamma)$ and $At(\Delta)$ as $At(\Gamma) = \Theta \cup \{\alpha_{C \cdot D}\}$ and $At(\Delta) = \Theta \cup \{\beta_C, \beta_D\}$.

Let $\preceq$ be a template order on $At(\Gamma)$ for which $\alpha_{C \cdot D}$ is minimal. Let $\preceq'$ be a template order on $At(\Delta)$ for which β_C and β_D are maximal elements.

We set $\Gamma_C = \{\delta \mid \delta \in \Theta, supp\,(\delta) \subseteq supp\,(\alpha_C)\}$ and $\Gamma_D = \{\delta \mid \delta \in \Theta, supp\,(\delta) \subseteq supp\,(\alpha_D)\}$. The computation of $At(\Gamma)^+_{\bowtie,\preceq}$ starts with the computation of $(\Gamma_C \cup \Gamma_D \cup \{\alpha_{C \cdot D}\})^+_{\bowtie,\preceq}$ and that of $At(\Delta)^+_{\bowtie',\preceq'}$ starts with the computation of $(\Gamma_C \cup \Gamma_D \cup \{\beta_C, \beta_D\})^+_{\bowtie',\preceq'}$. Both carry on in exactly the same way, using respectively $(\Gamma_C \cup \Gamma_D \cup \{\alpha_{C \cdot D}\})^+_{\bowtie,\preceq}$ and $(\Gamma_C \cup \Gamma_D \cup \{\beta_C, \beta_D\})^+_{\bowtie',\preceq'}$ as black-boxes. It is thus enough to show that:

$$(\Gamma_C \cup \Gamma_D \cup \{\alpha_{C \cdot D}\})^+_{\bowtie,\preceq} \leq (\Gamma_C \cup \Gamma_D \cup \{\beta_C, \beta_D\})^+_{\bowtie',\preceq'}$$

We decompose β_C, β_D and $\alpha_{C \cdot D}$ as follows (See Figure 22):

$$\begin{array}{lcl} \beta_C & \overset{\bowtie'}{=} & \delta_C \cdot \sigma_C \\ \beta_D & \overset{\bowtie'}{=} & \delta_D \cdot \sigma_D \\ \alpha_{C \cdot D} & \overset{\bowtie}{=} & \delta_{C \cdot D} \cdot \sigma_{C \cdot D} \end{array}$$

Since $\preceq$ and $\preceq'$ (resp. $\bowtie$ and $\bowtie'$) coincide on the elements of Θ, we will write Γ_C^+ (resp. Γ_D^+) for the iteration of Γ_C (resp. Γ_D) under the bowtie choice $\bowtie$ and the template order $\preceq$ or under the bowtie choice $\bowtie'$ and the template order $\preceq'$.

Since $supp\,(\Gamma_C) \cap supp\,(\Gamma_D) = \emptyset$, we have that $\Gamma_C^+ \cdot \Gamma_D^+ = \Gamma_D^+ \cdot \Gamma_C^+$, we denote this product simply by $\Gamma_{C \cdot D}^+$. We have also that:

$$\begin{array}{lcl} (\Gamma_C \cup \Gamma_D \cup \{\alpha_{C \cdot D}\})^+_{\bowtie,\preceq} & = & \Gamma_{C \cdot D}^+ \ \cup \ (\Gamma_{C \cdot D}^* \cdot \alpha_{C \cdot D}^+ \cdot \Gamma_{C \cdot D}^*) \\ (\Gamma_C \cup \Gamma_D \cup \{\beta_C, \beta_D\})^+_{\bowtie,\preceq} & \supseteq & \Gamma_{C \cdot D}^+ \ \cup \ (\Gamma_{C \cdot D}^* \cdot \beta_C^+ \cdot \beta_D^+ \cdot \Gamma_{C \cdot D}^*) \end{array}$$

Where $\alpha_{C \cdot D}^+$ and $\beta_C^+ \cdot \beta_D^+$ are the boxes depicted in Figure 23. It is not difficult to see that $\alpha_{C \cdot D}^+ \lhd \beta_C^+ \cdot \beta_D^+$, whence the result. ◀