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Strategic portgraph rewriting: an interactive modelling and analysis framework*

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We present strategic portgraph rewriting as a basis for the implementation of visual modelling and analysis tools. The goal is to facilitate the specification, analysis and simulation of complex systems, using portgraphs. A system is represented by an initial graph and a collection of graph rewriting rules, together with a user-defined strategy to control the application of rules. The strategy language includes constructs to deal with graph traversal and management of rewriting positions in the graph. We give a small-step operational semantics for the language, and describe its implementation: the graph transformation and visualisation tool PORGY.

Keywords: portgraph, graph rewriting, strategies, simulation, analysis, visual environment

1 Introduction

In this paper we present strategic portgraph rewriting as a basis for the design of PORGY – a visual, interactive environment for the specification, debugging, simulation and analysis of complex systems. PORGY has a graphical interface [23] and an executable specification language (see Fig. 1), where a system is modelled as a portgraph together with portgraph rewriting rules defining its dynamics (see Sect. 2).

Reduction strategies define which (sub)expression(s) should be selected for evaluation and which rule(s) should be applied (see [9,19] for general definitions). They are present in programming languages such as Clean [24], Curry [17], and Haskell [18] and can be explicitly defined to rewrite terms in languages such as ELAN [8], Stratego [31], Maude [21] or Tom [5]. They are also present in graph transformation tools such as PROGRES [29], AGG [12], Fujaba [22], GROOVE [28], GrGen [14] and GP [27]. PORGY's strategy language draws inspiration from these previous works, but a distinctive feature of PORGY's language is that it allows users to define strategies using not only operators to combine graph rewriting rules but also operators to define the location in the target graph where rules should, or should not, apply.

The main contribution of this paper is the definition of a strategic graph program (see Sect. 3): it consists of an initial *located graph* (that is, a portgraph with two distinguished subgraphs P and Q

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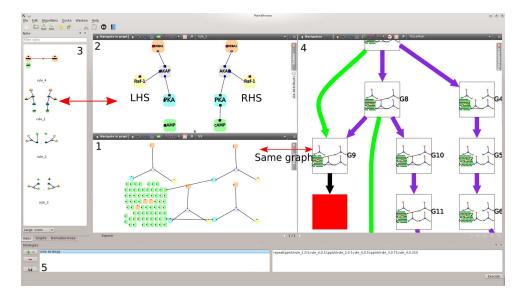


Figure 1: Overview of PORGY: (1) editing one state of the graph being rewritten; (2) editing a rule; (3) all available rewriting rules; (4) portion of the derivation tree, a complete trace of the computing history; (5) the strategy editor.

specifying the position where rewriting should take place, and the subgraph where rewriting is banned, respectively), and a set of rewrite rules describing its dynamic behaviour, controlled by a strategy. We formalise the concept of strategic graph program, showing how located graphs generalise the notion of a term with a rewrite position, and provide a small-step operational semantics for strategic graph programs (Sect. 4).

Strategies are used to control PORGY's rewrite engine: users can create graph rewriting derivations and specify graph traversals using the language primitives to select rewriting rules and the position where the rules apply. A rewriting position is a subgraph, which can be interactively selected (in a visual way), or can be specified using a *focusing* expression. Alternatively, rewrite positions could be encoded in the rewrite rules using markers or conditions, as done in other languages based on graph rewriting which do not have focusing primitives [27].

PORGY and its strategy language were first presented in [2, 13]. Unlike those papers, the notion of portgraph considered in this paper includes attributes for nodes, ports and also edges, which are taken into account in the definition of portgraph morphism. In addition, the strategy language includes a sublanguage to deal with properties of graphs, which facilitates the specification of rewrite positions and banned subgraphs (to be protected during rewriting). The operational semantics of the language, including the non-deterministic sublanguage, is formally defined using a transition system.

2 Port Graph Rewriting

Several definitions of graph rewriting are available, using different kinds of graphs and rewriting rules (see, for instance, [6, 7, 11, 15, 20, 26]). In this paper we consider *port graphs* with *attributes* associated to nodes, ports and edges, generalising the notion of port graph introduced in [3].

Intuitively, a port graph is a graph where nodes have explicit connection points called *ports*; edges are attached to ports. Nodes, ports and edges are labelled and may have attributes. For instance, a port

may be associated to a state (e.g., active/inactive or principal/auxiliary) and a node may have properties such as colour, shape, label, etc. Attributes may be used to define the behaviour of the modelled system and for visualisation purposes (as illustrated in examples later).

Port graph with attributes A *labelled port graph with attributes* is a tuple $G = (V_G, lv_G, E_G, le_G)$ where:

- V_G is a finite set of nodes.
- lv_G is a function that returns, for each $n \in V_G$, a node label N (the node's name), a set $\{p_1, \ldots, p_n\}$ of port labels (each with its own set of attribute labels and assigned value labels), and a set of attribute labels (each with a value label). We write $Interface(N) = \{p_1, \ldots, p_n\}$.
 - We consider the function lv_G as a family of functions: lv_Gname , lv_Gports , $lv_Gattributes$, $lv_GattributeValue$, $lv_GportAttributeS$, $lv_GportAttributeValue$, which, when applied to a node, return its name, ports, attributes, values, port attributes and port attribute values, respectively.
- E_G is a finite set of edges; each edge has two attachment ports $(v_1, p_1), (v_2, p_2)$, where $v_i \in V_G, p_i \in Interface(lv_Gname(v_i))$. Edges are undirected, so $\langle (v_1, p_1), (v_2, p_2) \rangle$ is an unordered pair, and two nodes may be connected by more than one edge on the same ports.
- le_G is a labelling function for edges, which returns for each $e \in E_G$ an edge label, its attachment ports $(v_1, p_1), (v_2, p_2)$ and its set of attribute labels, each with an associated value.
 - le_G can also be seen as a family of functions le_G name, le_G ports, le_G attributes, le_G attributeValue.

Let G and H be two port graphs. A *port graph morphism* $f:G\to H$ maps nodes, ports, edges, node attributes and their values, port attributes and their values, and edge attributes and their values, from G to H, such that all labels are preserved, the attachment of edges is preserved and the set of pairs of attributes and values for nodes, ports and edges are also preserved. If G contains variable labels, the morphism must instantiate the variables. Intuitively, the morphism identifies a subgraph of H that is equal to G except at positions where G has variables (at those positions H could have any value). Due to space constraints we omit the formal definition.

Port graphs are transformed by applying port graph rewriting rules. A port graph rewrite rule $L \Rightarrow R$ can itself be seen as a port graph, consisting of two port graphs L and R called the *left-* and *right-hand side* respectively, and one special node \Rightarrow , called *arrow node*. The left-hand side of the rule, also called pattern, is used to identify subgraphs in a given graph, which should be replaced by the right-hand side of the rule. Intuitively, the arrow node describes the way the new subgraph should be linked to the remaining part of the graph, to avoid dangling edges [11,15] during rewriting.

Given a finite set \mathscr{R} of rules, a port graph G rewrites to G', denoted by $G \to_{\mathscr{R}} G'$, if there is a rule r in \mathscr{R} and a morphism g such that $G \to_{r}^{g} G'$. This induces a reflexive and transitive relation on port graphs, called *the rewriting relation*, denoted by $\to_{\mathscr{R}}^{*}$. Each *rule application* is a rewriting step and a *derivation*, or computation, is a sequence of rewriting steps.

Given a port graph G and a set of port graph rewrite rules \mathscr{R} , the *derivation tree* of G, written $DT(G,\mathscr{R})$, is a labelled tree such that the root is labelled by the initial port graph G, and its children are all the derivation trees $DT(G_i,\mathscr{R})$ such that $G \to_{\mathscr{R}} G_i$. The edges of the derivation tree are labelled with the rewrite rule and the morphism used in the corresponding rewrite step. We will use *strategies* to specify the rewrite derivations of interest.

3 Strategic graph programs

Located graph A *located graph* G_P^Q consists of a port graph G and two distinguished subgraphs P and Q of G, called respectively the *position subgraph*, or simply *position*, and the *banned subgraph*.

In a located graph G_P^Q , P represents the subgraph of G where rewriting steps may take place (i.e., P is the focus of the rewriting) and Q represents the subgraph of G where rewriting steps are forbidden. We give a precise definition below; the intuition is that subgraphs of G that overlap with P may be rewritten, if they are outside Q. The subgraph P generalises the notion of rewrite position in a term: if G is the tree representation of a term t then we recover the usual notion of rewrite position P in T0 be the node at position T2 in the tree T3, and T4 to be the part of the tree above T5 (to force the rewriting step to apply from T4 downwards).

When applying a port graph rewrite rule, not only the underlying graph G but also the position and banned subgraphs may change. A *located rewrite rule*, defined below, specifies two disjoint subgraphs M and N of the right-hand side R that are used to update the position and banned subgraphs, respectively. If M (resp. N) is not specified, R (resp. the empty graph \emptyset) is used as default. Below, we use the operators \cup, \cap, \setminus to denote union, intersection and complement of portgraphs. These operators are defined in the natural way on port graphs considered as sets of nodes, ports and edges.

Located rewrite rule A *located rewrite rule* is given by a port graph rewrite rule $L \Rightarrow R$, and optionally a subgraph W of L and two disjoint subgraphs M and N of R. It is denoted $L_W \Rightarrow R_M^N$. We write $G_P^Q \to_{L_W \Rightarrow R_M^N}^R G_{P'}^{Q'}$ and say that the located graph G_P^Q rewrites to $G_{P'}^{Q'}$ using $L_W \Rightarrow R_M^N$ at position P avoiding Q, if $G \to_{L \Rightarrow R} G'$ with a morphism g such that $g(L) \cap P = g(W)$ or simply $g(L) \cap P \neq \emptyset$ if W is not provided, and $g(L) \cap Q = \emptyset$. The new position subgraph P' and banned subgraph Q' in G' are defined as $P' = (P \setminus g(L)) \cup g(M)$, $Q' = Q \cup g(N)$; if M (resp. N) are not provided then we assume M = R (resp. $N = \emptyset$).

In general, for a given located rule $L_W \Rightarrow R_M^N$ and located graph G_P^Q , more than one morphism g, such that $g(L) \cap P = g(W)$ and $g(L) \cap Q$ is empty, might exist (i.e., several rewriting steps at P avoiding Q might be possible). Thus, the application of the rule at P avoiding Q produces a *set of located graphs*.

To control the application of the rules, we introduce a strategy language whose syntax is shown in Table 1. *Strategy expressions* are generated by the grammar rules from the non-terminal *S*. A strategy expression combines *applications* of located rewrite rules, generated by the non-terminal *A*, and *position updates*, using *focusing expressions* generated by *F*. The application constructs and some of the strategy constructs are strongly inspired from term rewriting languages such as ELAN [8], Stratego [31] and Tom [5]. Focusing operators are not present in term rewriting languages (where the implicit assumption is that the rewrite position is defined by traversing the term from the root downwards).

The syntax presented here extends the one in [13] by including a language to define subgraphs of a given graph by selecting nodes that satisfy some simple properties (see Table 2).

The focusing constructs are a distinctive feature of our language. They are used to define positions for rewriting in a graph, or to define positions where rewriting is not allowed. They denote functions used in strategy expressions to change the positions P and Q in the current located graph (e.g., to specify graph traversals). We describe them briefly below.

- CrtGraph, CrtPos and CrtBan, applied to a located graph G_P^Q , return respectively the whole graph G, P and Q.
- AllNgb, OneNgb and NextNgb denote functions that apply to pairs consisting of a located graph G_P^Q and a subgraph G' of G. If Pos is an expression denoting a subgraph G' of the current graph G,

```
Let L,R be port graphs, M,N positions, \rho a property, m,n integers, p_{i=1...n} \in [0,1]

(Strategies) S ::= A \mid U \mid S; S \mid \text{repeat}(S) \mid \text{while}(S) \text{do}(S)

\mid (S) \text{orelse}(S) \mid \text{if}(S) \text{then}(S) \text{else}(S)

\mid \text{ppick}(S_1, p_1, \dots, S_n, p_n)

(Applications) A ::= \text{Id} \mid \text{Fail} \mid \text{all}(T) \mid \text{one}(T)

(Transformations) T ::= L_W \Rightarrow R_M^N

(Position Update) U ::= \text{setPos}(F) \mid \text{setBan}(F) \mid \text{isEmpty}(F)

(Focusing) F ::= \text{CrtGraph} \mid \text{CrtPos} \mid \text{CrtBan} \mid \text{AllNgb}(F)

\mid \text{OneNgb}(F) \mid \text{NextNgb}(F) \mid \text{Property}(\rho, F)

\mid F \cup F \mid F \cap F \mid F \setminus F \mid \emptyset
```

Table 1: Syntax of the Strategy Language.

```
Let n \in \nabla_{\mathcal{N}} \cup \nabla_{\mathcal{E}} \cup \nabla_{\mathcal{A}} \cup \nabla_{\mathcal{D}} and value \in \nabla_{\mathcal{V}} \cup \mathcal{X}_{\mathcal{V}}.

(Properties) \rho := (Elem, Expr)
Elem := Node \mid Edge \mid Port \mid Function
Expr := Name = n \mid Name \neq n \mid function\text{-}name
\mid attribute \ Relop \ value
Relop := = |!=|>|<|\leq|\geq
```

Table 2: Syntax of the Property Language.

then by writing AllNgb(Pos) we obtain the subgraph of G consisting of all immediate successors of the nodes in G', where an immediate successor of a node v is a node that has a port connected to a port of v. OneNgb(Pos) returns a subgraph of G consisting of one immediate successor of a node in G', chosen non-deterministically. NextNgb(Pos) computes successors of nodes in G' using for each node only the subset of its ports that have the attribute "next"(so NextNgb(Pos) returns a subset of the nodes returned by AllNgb(Pos)).

- Property(ρ , F) is used to select a subgraph of a given graph, satisfying a certain property, specified by ρ . It can be seen as a filtering construct: If the expression F generates a subgraph G' then Property(ρ , F) returns a subgraph containing only the nodes and edges from G' that satisfy the decidable property ρ .
 - Property ((Node, Name = Add),F) returns all the nodes of the subgraph defined by the expression F that are labelled "Add".
 - Property((Port, Active != True),F) returns all the nodes of the subgraph defined by the expression *F* that have a port with an attribute labelled *Active* that is not set to the value *True*.

• \cup , \cap and \setminus are union, intersection and complement of portgraphs which may be used to combine multiple Property operators. We give other examples in Section 5.

Strategic graph program A *strategic graph program* consists of a finite set of located rewrite rules \mathcal{R} , a strategy expression S (built from \mathcal{R} using the grammar in Table 1) and a located graph G_P^Q . We denote it $\left[S_{\mathcal{R}}, G_P^Q\right]$, or simply $\left[S, G_P^Q\right]$ when \mathcal{R} is clear from the context.

4 Semantics of strategic graph programs

Intuitively, a strategic program consists of an initial port graph, together with a set of rules that will be used to reduce it, following the given strategy. Formally, the semantics of a strategic graph program $\left[S,G_P^Q\right]$ is specified using a transition system (that is, a set of configurations with a binary relation on configurations), defining a *small step* operational semantics in the style of [25].

Definition A configuration is a multiset $\{O_1, \ldots, O_n\}$ where each O_i is a strategic graph program.

Given a strategic graph program $\left[S_{\mathscr{R}},G_{P}^{\mathcal{Q}}\right]$, we will define sequences of transitions according to the strategy S, starting from the *initial configuration* $\left\{\left[S,G_{P}^{\mathcal{Q}}\right]\right\}$. A configuration is *terminal* if no transitions can be performed.

We will prove that all terminal configurations in our transition system consist of *program values* (or simply values, if there is no ambiguity) of the form $[Id, G_P^Q]$ or $[Fail, G_P^Q]$. In other words, there are no blocked programs: the transition system ensures that, for any configuration, either there are transitions to perform, or we have reached values.

Below we provide the transition rules for the core sublanguage, that is, the sublanguage that does not include the non-deterministic operators one(), OneNgb(), () orelse(), ppick() (the non-deterministic sublanguage is presented in Sect. A in the Appendix).

Transitions The transition relation \longrightarrow is a binary relation on configurations defined as follows:

$$\{O_1,\ldots,O_k\}\longrightarrow \{O'_{11},\ldots,O'_{1m_1},\ldots,O'_{km_k}\}$$

if $O_i \to \{O'_{i1}, \dots, O'_{im_i}\}$, for $1 \le i \le k$, where $k \ge 1$ and some of the O'_{ij} might be values. The auxiliary relation \to is defined below (see Definition 4) using axioms and rules.

A configuration $\{O_1, \ldots, O_k\}$ is a multiset of graph programs representing nodes in the derivation tree generated by the initial graph program; the transition relation performs reductions in parallel at all the positions in the derivation tree where there is a reducible graph program. We can see a configuration $\{O_1, \ldots, O_k\}$ as a parallel set of processes, but, unlike the standard definitions in process calculi, the objects inside a configuration do not communicate.

Definition The transition relation \rightarrow on individual strategic graph programs is defined by induction.

There are no axioms/rules defining transitions for a program where the strategy is ld or Fail (these are terminal).

Axioms for the operator all:

$$\frac{}{[\mathtt{all}(L_W \Rightarrow R_M^N), G_P^Q] \to \{[\mathsf{Id}, G_1{}_{P_1}^{Q_1}], \dots, [\mathsf{Id}, G_k{}_{P_k}^{Q_k}]\}} \ LS_{L_W \Rightarrow R_M^N}(G_P^Q) = \{G_1{}_{P_1}^{Q_1}, \dots, G_k{}_{P_k}^{Q_k}\}$$

$$\frac{}{[\mathtt{all}(L_W \Rightarrow R_M^N), G_P^{\mathcal{Q}}] \to \{[\mathsf{Fail}, G_P^{\mathcal{Q}}]\}} \, LS_{L_W \Rightarrow R_M^N}(G_P^{\mathcal{Q}}) = \emptyset$$

where $LS_{L_W\Rightarrow R_M^N}(G_P^Q)$, the set of legal reducts of G_P^Q for $L_W\Rightarrow R_M^N$, or legal set for short, contains all the located graphs $G_{iP_i}^{Q_i}$ $(1\leq i\leq k)$ such that $G_P^Q\to_{L_W\Rightarrow R_M^N}^{g_i}G_{iP_i}^{Q_i}$ and g_1,\ldots,g_k are pairwise different.

As the name of the operator indicates, all possible applications of the rule are considered. The strategy fails if the rule is not applicable.

Position Update and Focusing: Next we give the semantics of the commands that are used to specify and update positions via focusing constructs. The focusing expressions generated by the grammar for the non terminal F in Tab. 1 have a functional semantics (see below). In other words, an expression F denotes a function that applies to the current located graph, and computes a subgraph of G. Since there is no ambiguity, the function denoted by the expression F will also be called F.

$$\begin{split} \frac{1}{[\mathtt{setPos}(F),G_P^Q] \to \{[\mathsf{Id},G_{P'}^Q]\}} \, F(G_P^Q) &= P' \text{ (resp. } Q' \text{ for setBan())} \\ \frac{1}{[\mathtt{isEmpty}(F),G_P^Q] \to \{[\mathsf{Id},G_P^Q]\}} \, F(G_P^Q) &= \emptyset \\ \\ \frac{1}{[\mathtt{isEmpty}(F),G_P^Q] \to \{[\mathsf{Fail},G_P^Q]\}} \, F(G_P^Q) &\neq \emptyset \end{split}$$

$$\begin{array}{lll} \operatorname{CrtGraph}(G_P^Q) & = & G & \operatorname{CrtPos}(G_P^Q) & = & P & \operatorname{CrtBan}(G_P^Q) & = & Q \\ \operatorname{AllNgb}(F)(G_P^Q) & = & G' & \text{where G' consists of all immediate successors of nodes in $F(G_P^Q)$} \\ \operatorname{NextNgb}(F)(G_P^Q) & = & G' & \text{where G' consists of the immediate successors, } \\ & & & via \text{ ports labelled "next", of nodes in $F(G_P^Q)$} \\ \operatorname{Property}(\rho,F)(G_P^Q) & = & G' & \text{where G' consists of all nodes in $F(G_P^Q)$ satisfying ρ} \\ (F_1 \circ p F_2)(G_P^Q) & = & F_1(G_P^Q) \circ p F_2(G_P^Q) & \text{where op is \cup,\cap,\setminus} \\ \end{array}$$

Note that with the semantics given above for setPos() and setBan(), it is possible for P and Q to have a non-empty intersection. A rewrite rule can still apply if the redex overlaps P but not Q.

Sequence: The semantics of sequential application, written S_1 ; S_2 , is defined by two axioms and a rule:

$$\begin{split} \overline{[\mathsf{Id};S,G_P^Q] \to \{[S,G_P^Q]\}} & \overline{[\mathsf{Fail};S,G_P^Q] \to \{[\mathsf{Fail},G_P^Q]\}} \\ \overline{[S_1,G_P^Q] \to \{[S_1^1,G_{1P_1}^{Q_1}],\dots,[S_1^k,G_{kP_k}^{Q_k}]\}} \\ \overline{[S_1;S_2,G_P^Q] \to \{[S_1^1;S_2,G_{1P_1}^{Q_1}],\dots,[S_1^k;S_2,G_{kP_k}^{Q_k}]\}} \end{split}$$

The rule for sequences ensures that S_1 is applied first.

Conditional: The behaviour of the strategy $if(S_1)then(S_2)else(S_3)$ depends on the result of the strategy S_1 . If S_1 succeeds on (a copy of) the current located graph, then S_2 is applied to the current graph, otherwise S_3 is applied.

$$\frac{\exists G', M \text{ s.t. } \{[S_1, G_P^Q]\} \longrightarrow^* \{[\mathsf{Id}, G'], M\}}{[\mathsf{if}(S_1) \mathsf{then}(S_2) \mathsf{else}(S_3), G_P^Q] \to \{[S_2, G_P^Q]\}}$$

$$\frac{\not\exists G', M \ s.t. \ \{[S_1, G_P^Q]\} \longrightarrow^* \{[\mathsf{Id}, G'], M\}}{[\mathsf{if}(S_1) \mathsf{then}(S_2) \mathsf{else}(S_3), G_P^Q] \to \{[S_3, G_P^Q]\}}$$

Note that S_1 may produce some success but also some failure results. To ensure a unique result, the strategy S_1 should terminate and be deterministic; the class Cond of strategies generated by the following grammar satisfies these conditions:

$$Cond ::= Cond; Cond \mid all(T) \mid isEmpty(F)$$

where

$$F ::= \mathtt{AllNgb}(F) \mid \mathtt{NextNgb}(F) \mid \mathtt{Property}(\rho, F) \mid \cup \mid \cap \mid \setminus \mid \emptyset$$

Semantics of while loops: Iteration is defined using a conditional as follows:

$$\overline{[\texttt{while}(S_1)\texttt{do}(S_2),G_P^Q] \to \{[\texttt{if}(S_1)\texttt{then}(S_2;\texttt{while}(S_1)\texttt{do}(S_2))\texttt{else}(\mathsf{Id}),G_P^Q]\}}$$

5 Examples

Using focusing (specifically the Property construct), we can create concise strategies that perform traversals¹. In this way, we can for instance switch between *outermost and innermost term rewriting* (on trees). This is standard in term-based languages such as ELAN [8] or Stratego [31] [10]; here we can also define traversals in graphs that are not trees. More examples can be found in [2,23].

Graph analysis The following strategy allows us to check if a graph is connected. using a standard connectivity test. Assuming that all nodes of the initial graph have the Boolean attribute *state* set to false, we just need one rewriting rule, which simply sets *state* to *true* on a node. We start with the strategy *pick-one-node* to randomly select a node *n* as a starting point. Then, the rule is applied to all neighbours of *n*. When the rule cannot be applied anymore, the position subgraph is set to all neighbours of the previously used nodes which still have *state* to *false* (visit-neighbours-at-any-distance). The strategy continues until the position subgraph is empty. If the rule can still be applied somewhere in the graph, there is a failure (check-all-nodes-visited).

```
pick-one-node: \mathtt{setPos}(\mathtt{CrtGraph}); \\ one(R); \\ \mathtt{setPos}(\mathtt{Property}((Node, state == true, \mathtt{CrtGraph})); \\ visit-neighbours-at-any-distance: \mathtt{setPos}(\mathtt{AllNgb}(\mathtt{CrtPos})); \\ \mathtt{while}(\mathtt{not}(\mathtt{isEmpty}(\mathtt{CrtPos})))\mathtt{do}(\\ \mathtt{if}(R)\mathtt{then}(R)\mathtt{else}(\\ \mathtt{setPos}(\mathtt{AllNgb}(\mathtt{CrtPos}) \setminus \\ \mathtt{Property}((Node, state == true), CrtGraph)))); \\ check-all-nodes-visited: \mathtt{setPos}(\mathtt{CrtGraph}); \\ \mathtt{if}(R)\mathtt{then}(\mathtt{Fail})\mathtt{else}(\mathtt{Id})
```

¹Working examples can be downloaded from http://tulip.labri.fr/TulipDrupal/?q=porgy.

Biochemical Network Biochemical networks contain different types of molecules interacting over time, maintaining necessary regulation mechanisms. The challenge for biologists is building models that explain how/when specific molecules reach given concentrations and whether these quantities can be used to track the system, reliably predict its evolution and simulate for instance a regulation mechanism. Knowledge gained from wet lab experiments suggests that a regulation mechanism relates to the evolution pattern of the concentration of a particular molecule type. Hypothesis were made that these concentrations should evolve stepwise, following a staircase pattern. Moreover, biologists assumed that a non-deterministic combination of only four biochemical reactions (rules r1, r2, r3 and r4) is complex and powerful enough to fully explain the studied phenomenon. We use the ppick() operator to reproduce this behaviour. Several iterations were necessary with our domain experts, reasoning about the system and testing several different combinations of rules, to design adequate rule sets and strategy. The final strategy is:

```
repeat(
ppick(r1,0.5,r4,0.5);
ppick(r2,0.5,r4,0.5);
ppick(r3,0.75,r4,0.25))
```

More details on the biological background of this case study are available in [1,2]; for more details of this example in Porgy see [23].

6 Properties

A strategic graph program $\left[S,G_P^Q\right]$ is *strongly terminating* (or just terminating) if there is no infinite transition sequence out of the initial configuration $\left\{\left[S,G_P^Q\right]\right\}$, otherwise it is non-terminating. It is *weakly terminating* if we can reach a configuration having at least one value.

For the core part of the language (that is, excluding the constructs ppick, orelse, repeat, one and OneNgb), strategic graph programs have at most one terminal configuration (none if the program is non-terminating).

Result set Given a strategic graph program $\left[S,G_P^Q\right]$, we can associate a set of results to each sequence of transitions out of the initial configuration $\left\{\left[S,G_P^Q\right]\right\}$: the *result set* associated to a sequence of transitions is the set of values in the configurations in the sequence. If the sequence of transitions out of the the initial configuration $\left\{\left[S,G_P^Q\right]\right\}$ ends in a terminal configuration then the result set of the sequence is a *program result*. If a strategic graph program does not reach a terminal configuration (in case of non-termination) then the program result is undefined (\bot) .

Note that there may be more than one derivation out of the initial configuration $\{S, G_P^Q\}$ ending in a terminal configuration. However, if we exclude the non-deterministic constructs, we can prove that each strategic graph program has at most one program result, which is a set of program values (Prop. 6.0.3).

Graph programs are not terminating in general, however we can identify a terminating sublanguage (i.e. a sublanguage for which the transition relation is terminating) and we can characterise the strategic graph programs that yield terminal configurations. In the proof of termination, we need a lemma.

Lemma 6.1 If $[S_1, G_P^Q]$ is strongly terminating and S_2 is such that $[S_2, G_P']$ is strongly terminating for any G_P' , then $[S_1; S_2, G_P^Q]$ is strongly terminating.

Property 6.0.1 (Termination) The sublanguage that excludes the while and repeat constructs is strongly terminating.

Property 6.0.2 (Progress: Characterisation of Terminal Configurations) For every strategic graph program $[S, G_P^Q]$ that is not a value (i.e., $S \neq Id$ and $S \neq Fail$), there exists a configuration C such that $\{[S, G_P^Q]\} \rightarrow C$.

Proof By induction on S. According to Definition 4 and its probabilistic extension, for every strategic graph program $[S, G_P^Q]$ different from $[\mathsf{Id}, G_P^Q]$ or $[\mathsf{Fail}, G_P^Q]$ there is an axiom or rule that applies (it suffices to check all the cases in the grammar for S).

The language contains non-deterministic operators in each of its syntactic categories: OneNgb for Position Update, one for Applications and ppick, orelse and repeat for Strategies. For the sublanguage that excludes them, we have the property:

Property 6.0.3 (Result Set) Each strategic graph program in the sublanguage that excludes OneNgb, one, ppick, orelse and repeat has at most one program result.

Proof If we exclude those constructs, the transition system is deterministic, so there is at most one derivation out of any given graph program. Hence there is at most one program result.

With respect to the computation power of the language, it is easy to state the Turing completeness property. The proof is similar to that in [16].

Property 6.0.4 (Completeness) The set of all strategic graph programs $\left[S_{\mathcal{R}}, G_P^Q\right]$ is Turing complete, i.e. can simulate any Turing machine.

7 Implementation

Porgy is implemented on top of the visualisation framework Tulip [4] as a set of Tulip plugins. The strategy language is one of these plugins. A version of Tulip bundled with Porgy can be downloaded from http://tulip.labri.fr/TulipDrupal/?q=porgy.

Our first challenge was to implement portgraphs, because Tulip only supports nodes and edges from a graph theory point of view. We had to develop an abstract layer on top of the Tulip graph library to be able to easily work with portgraph.

When applying a rule $L \Rightarrow R$ on a graph G, the first operation is to match the left-hand side L inside G. This problem, known as the graph-subgraph isomorphism, still receives a great attention from the community. We have implemented the original Ullman's algorithm [30] because its implementation is straightforward and it is used as a reference in many papers.

The derivation tree is implemented thanks to the metanode (a node which represents a graph) and quotient graph functionnalities of Tulip (a graph of metanodes). Each node of the derivation tree (except the red ones) represents a state of G. Inside each node, the user sees an interactive drawing of the graph (see panel 4 of Fig. 1). See [23] for more details about the interactive features of Porgy and how we implemented them.

The strategy plugin is developed with the Spirit C++ library from Boost². This plugin works as a compiler: its inputs are a strategy defined as a text string and the Tulip graph datastructure, the output are low-level Tulip graph operations. Boost (precisely its Random library) is also used to generate the random numbers needed for the probabilistic operators. For instance, we use a non-uniform generator for ppick() to be able to choose a strategy following the given probabilities.

²see http://www.boost.org/libs/spirit for more details

8 Conclusion

The strategy language defined in this paper is part of PORGY [2], an environment for visual modelling and analysis of complex systems through port graphs and port graph rewrite rules. It offers also a visual representation of rewriting traces as a derivation tree. The strategy language is used in particular to guide the construction of this derivation tree. The implementation uses the small-step operational semantics of the language. Some of these steps require a copy of the strategic graph program; this is done efficiently in PORGY thanks to the cloning functionalities of the underlying TULIP system [4]. Verification and debugging tools for avoiding conflicting rules or non-termination are planned for future work.

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A Appendix – Probabilistic extension

To define the semantics of the non-deterministic and probabilistic constructs in the language we will generalise the transition relation.

We denote by \rightarrow_p a transition step with probability p. The relation \rightarrow defined in the previous section can be seen as a particular case where p = 1, that is, \rightarrow corresponds to \rightarrow_1 .

The relation \longrightarrow also becomes probabilistic:

$$\{O_1,\ldots,O_k,V_1,\ldots,V_j\}\longrightarrow_p \{O'_{11},\ldots,O'_{1m_1},\ldots,O'_{km_k},V_1,\ldots,V_j\}$$

if $O_i \to_{p_i} \{O'_{i1}, \dots, O'_{im_i}\}$, for $1 \le i \le k$ (where $k \ge 1$ and some of the O'_{ij} might be values) and $p = p_1 \times \dots \times p_k$.

We write $M \longrightarrow_p^* M'$ if there is a sequence of transitions \longrightarrow_{p_i} from configuration M to M', such that the product of probabilities is p.

We are now ready to define the semantics of the remaining constructs in the strategy language. *Probabilistic Choice of Strategy:*

$$\overline{\left[\operatorname{ppick}(S_1,p_1,\ldots,S_n,p_n),G_P^Q\right]\to_{p_i}\left\{\left[S_j,G_P^Q\right]\right\}}$$

Non-deterministic Choice of Reduct: The non-deterministic one operator takes as argument a rule or several rules in parallel (in the latter case, we create a new rule, as explained above). It selects only one amongst the set of legal reducts $LS_{L_W \Rightarrow R_M^N}(G_P^Q)$, non-deterministically. Since all of them have the same probability of being selected, in the axiom below $p = 1/|LS_{L_W \Rightarrow R_M^N}(G_P^Q)|$.

$$\frac{1}{[\operatorname{one}(L_W \Rightarrow R_M^N), G_P^Q] \to_p \{[\operatorname{Id}, G_{P'}'^{\underline{Q'}}]\}} \; G'^{\underline{Q'}}_{P'} \in LS_{L_W \Rightarrow R_M^N}(G_P^Q)$$

$$\frac{}{[\mathsf{one}(L_W \Rightarrow R_M^N), G_P^Q] \to_1 \{[\mathsf{Fail}, G_P^Q]\}} \ LS_{L_W \Rightarrow R_M^N}(G_P^Q) = \emptyset$$

Priority choice:

$$\frac{[S_1,G_P^Q]\longrightarrow_p^*\{[\mathsf{Id},G'],M\}}{[(S_1)\mathsf{orelse}(S_2),G_P^Q]\to_{p/n}\{[\mathsf{Id},G']\}} \quad \frac{[S_1,G_P^Q]\longrightarrow_p^*\{[\mathsf{Fail},G_1'],M\}}{[(S_1)\mathsf{orelse}(S_2),G_P^Q]\to_p\{[S_2,G_P^Q]\}}$$

Here, S_1 is applied to G_P^Q and if with probability p we reach a configuration with $n \ge 1$ successful leaves $[\operatorname{Id}, G_i]$, then with probability p/n there is a transition to one of the successful configurations $[\operatorname{Id}, G']$. However, if with probability p we reach a fail, then S_2 is applied to the initial graph with probability p. We assume that the implementation will take the shortest path $[S_1, G_P^Q] \longrightarrow_p^* \{[\operatorname{Id}, G'], M\}$ that generates a success.

We chose to define (S_1) orelse (S_2) as a primitive operator instead of encoding it as $if(S_1)$ then (S_1) else (S_2) since the language has non-deterministic operators: evaluating S_1 in the condition and afterwards in the "then" branch of the if-then-else could yield different values. The semantics given above ensures that if S_1 can succeed then it can be successfully applied.

Iteration of a given strategy:

The construction repeat(S) iterates the strategy S.

$$\frac{[S,G_P^Q] \longrightarrow_p^* \{[\mathsf{Id},G'],M\}}{[\mathsf{repeat}(S),G_P^Q] \to_{p/n} \{[\mathsf{repeat}(S),G']\}} \quad \frac{[S,G_P^Q] \longrightarrow_p^* \{[\mathsf{Fail},G_1'],M\}}{[\mathsf{repeat}(S),G_P^Q] \to_p \{[Id,G_P^Q]\}}$$

where again we assume that $n \ge 1$ is the number of successful leaves in the configuration $\{[\mathsf{Id}, G'], M\}$ *Non-deterministic position update and focusing:*

The commands setPos(F), setBan(F) and isEmpty(F) are non-deterministic if the expression F is non-deterministic. The operator OneNgb(F) introduces non-determinism. The axioms are similar to the ones we gave in the previous section, but now the transitions are indexed by a probability.