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THE MANUAL FOR COLORED PETRI NETS IN SNOOPY – QPN^c/SPN^c/CPN^c/GHPN^c

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The Manual for Colored Petri Nets in Snoopy – $\label{eq:colored} QPN^C/SPN^C/CPN^C/GHPN^C$

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The Manual for Colored Petri Nets in Snoopy $-\mathcal{QPN}^{\mathcal{C}}/\mathcal{SPN}^{\mathcal{C}}/\mathcal{CPN}^{\mathcal{C}}/\mathcal{GHPN}^{\mathcal{C}}$

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Abstract

Colored Petri nets are an excellent formalism for modeling and analyzing complex systems. In Snoopy, we have implemented functionalities for editing, and animating/simulating colored qualitative Petri nets $(\mathcal{QPN^C})$, colored stochastic Petri nets $(\mathcal{SPN^C})$, colored continuous Petri nets $(\mathcal{CPN^C})$, and colored generalized hybrid Petri nets $(\mathcal{GHPN^C})$. In this manual, we demonstrate how to construct colored Petri nets step by step using a simple example and describe some key modeling problems, e.g. automatic coloring Petri nets, specifying initial markings, or specifying rate functions. We also give our annotation language and describe how to use this language to declare or define inscriptions of colored Petri nets, e.g. color sets, are expressions or guards. In addition, we describe the animation, simulation, and analysis of colored Petri nets and show possible import/export relationships among different net classes. Finally, we give some examples to demonstrate the application of colored Petri nets. In summary, this manual contains a number of relevant materials for understanding, constructing, simulating and analyzing colored Petri nets so that the user will have no difficulties in using colored Petri nets.

^{*}Please sent all questions, comments and suggestions how to improve this material to this address.

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1 Introduction

Petri nets provide a formal and clear representation of systems based on their firm mathematical foundation for the analysis of system properties. However, standard Petri nets do not easily scale. So attempts to simulate systems by standard Petri nets have been mainly restricted so far to relatively small models. They tend to grow quickly for modeling complex systems, which makes it more difficult to manage and understand the nets, thus increasing the risk of modeling errors. Two known modeling concepts improving the situation are hierarchy and color. Hierarchical structuring has been discussed a lot, while the color has gained little attention so far. Thus, we investigate how to apply colored Petri nets to modeling and analyzing biological systems. To do so, we not only provide compact and readable representations of complex systems, but also do not lose the analysis capabilities of standard Petri nets, which can still be supported by automatic unfolding. Moreover, another attractive advantage of colored Petri nets for a modeler is that they provide the possibility to easily increase the size of a model consisting of many similar subnets just by adding colors.

In Snoopy, we have implemented prototypes for editing, and animating/simulating colored qualitative Petri nets $(\mathcal{QPN}^{\mathcal{C}})$, colored stochastic Petri nets $(\mathcal{SPN}^{\mathcal{C}})$, colored continuous Petri nets $(\mathcal{CPN}^{\mathcal{C}})$, and colored generalized hybrid Petri nets $(\mathcal{CHPN}^{\mathcal{C}})$. In this manual, we will give relevant materials for understanding, constructing, simulating and analyzing colored qualitative/stochastic/continuous/hybrid Petri nets, so that the user will have no difficulties in using colored Petri nets. In this manual, we concentrate on color-specific features; see [HRR+08], [RMH10], and [MRH12] for a general introduction into Snoopy, and [Liu12] for more background information re the use of colored Petri nets in systems biology.

1.1 Colored Petri nets

Colored Petri nets [GL79], [GL81], [Jen81], combine Petri nets with capabilities of programming languages to describe data types and operations, thus providing a flexible way to create compact and parameterizable models. In colored Petri nets, tokens are distinguished by the "color" rather than having only the "black" one. Additionally, are expressions, an extended version of arc weights, specify which tokens can flow over the arcs, and guards that are in fact Boolean expressions define additional constraints on the enabling of transitions [JKW07].

By way of introduction let us consider Figure 1 which gives a colored Petri net modeling the well-known textbook example of dinning philosophers. Philosophers sit around a round table. Between each pair of philosophers there is one fork on the table. The philosophers either think or eat. In order to eat, they have to take the following steps: (1) take the left fork, (2) take the right fork and then start eating, (3) put the right fork back, and (4) put the left fork back. In the colored Petri net model, changing the number of philosophers means changing the number of colors in the net.

In our implementation, QPN^{C} is a colored extension of qualitative Place/Transition nets (extended by different kinds of arcs, e.g. inhibitor arc, read arc, reset arc and equal

arc [HRR+08]), $\mathcal{SPN}^{\mathcal{C}}$ is a colored extension of biochemically interpreted stochastic Petri nets introduced in [GHL07] and extended in [HLG+09], $\mathcal{CPN}^{\mathcal{C}}$ is a colored extension of continuous Petri nets introduced in [GHL07], and $\mathcal{GHPN}^{\mathcal{C}}$ is a colored extension of generalized hybrid Petri nets introduced in [HH11].

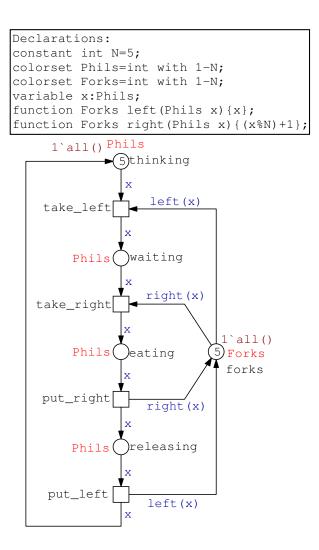


Figure 1: A colored Petri net modeling dinning philosophers. All declarations are given on top (see Section 3 for how to read them). all() is a marking function to specify that all the colors in one color set are set to the same coefficient (here it is 1). See B.2 for a textual notation of this Petri net.

1.2 Some notes

In Snoopy, we provide a similar editing environment for $\mathcal{QPN}^{\mathcal{C}}$, $\mathcal{SPN}^{\mathcal{C}}$, $\mathcal{CPN}^{\mathcal{C}}$ and $\mathcal{GHPN}^{\mathcal{C}}$; therefore the following descriptions will equally apply to $\mathcal{QPN}^{\mathcal{C}}$, $\mathcal{SPN}^{\mathcal{C}}$, $\mathcal{CPN}^{\mathcal{C}}$ and $\mathcal{GHPN}^{\mathcal{C}}$, except those concerning animation, simulation and analysis, but all these differences will be noted clearly.

1.3 Features - overview

Before exploring all features in detail in the following sections, we give a brief overview for the expected features here.

1.3.1 Features for modeling

- Drawing of the Petri net graph as usual.
- Rich data types for color set definition, see Section 3.1.1.
 - Simple types: dot, int, string, bool, enum, index,
 - Compound types: product, union.
- Flexible user-defined functions.
- Concise specification of initial marking for larger color sets, see Section 2.4.1.
- Rate function definition for each transition instance (for $SPN^{C}/CPN^{C}/GHPN^{C}$), see Section 2.4.3.
- Several extended arc types, such as inhibitor arc, read arc (often also called test arcs), equal arc, reset arc, and modifier arc, which are popular add-ons enhancing modeling comfort [HRR+08], see Section 2.4.4.
- Several special transitions. Snoopy supports stochastic transitions with freestyle rate functions as well as three deterministically timed transition types: immediate firing, deterministic firing delay, and scheduled firing, see [HLG+09] for details.
- Automatically convert the type of a node or edge to another type.
- Compute and show bindings (instances) for each transition.
- Compute and show token colors and numbers for each place.
- Random Generation of initial marking (only for SPN^{C}), see Section 2.4.2.
- Define auxiliary variables (observers) based on colored places, see Section 2.4.5.
- Automatically colorize some special subnets:
 - Colorize any selected subnet,

- Colorize twin nets,
- Colorize T-invariants/master nets.

1.3.2 Features for animation (for QPN^{C}/SPN^{C})

- Running animation automatically or controlling the animation manually.
 - Automatic animation,
 - Single-step animation by manually choosing a binding.

1.3.3 Features for simulation (for $SPN^{\mathcal{C}}/\mathcal{CPN}^{\mathcal{C}}/\mathcal{GHPN}^{\mathcal{C}}$)

- Simulation is done on an automatically unfolded Petri net.
- Show or export simulation results for colored or uncolored places/transitions separately or together.
- Several simulation algorithms to simulate $SPN^{\mathcal{C}}$, including the Gillespie stochastic simulation algorithm (SSA) [Gil77].
- Several simulation algorithms to simulate $\mathcal{CPN}^{\mathcal{C}}$, including the Euler algorithm, Runge-Kutta algorithm, etc. [HH11].

1.3.4 Other features

- Highlighting places of the same color set by specifying a true color.
- Highlighting different inscriptions (color sets, marking, arc expressions or guards) with different colors.
- All colored net classes are exported to different net formalisms within Snoopy (see Figure 2), see Section 5 for details.
- Export $QPN^{\mathcal{C}}$ and $SPN^{\mathcal{C}}$ to APNN.
- Export/import beyond Snoopy, e.g. export to CPN tools, see Section 5 for details.

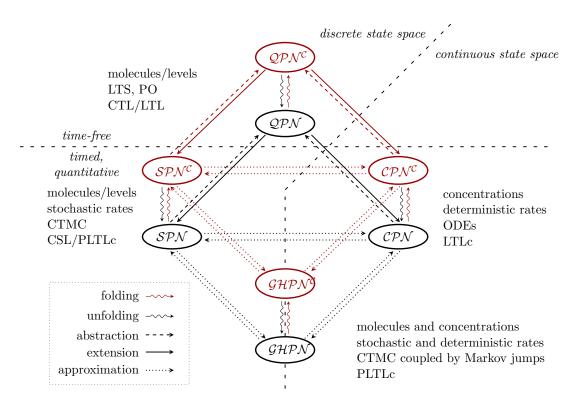


Figure 2: Export relationships among different net formalisms.

2 Modeling

In this section, we will first demonstrate how to construct a colored Petri net and consider several key modeling problems afterwards.

2.1 General modeling procedure - an introductory example

This section will present a general step-by-step procedure of how to construct a colored Petri net $(\mathcal{QPN^C}/\mathcal{SPN^C}/\mathcal{CPN^C}/\mathcal{GHPN^C})$ on the basis of a standard Petri net. A simple example will be used for the illustration of the procedure.

2.1.1 Transform a standard Petri net into a colored Petri net

One possibility to construct a colored Petri net is the transformation of an existing standard Petri net into a $\mathcal{QPN}^{\mathcal{C}}/\mathcal{SPN}^{\mathcal{C}}/\mathcal{CPN}^{\mathcal{C}}/\mathcal{GHPN}^{\mathcal{C}}$. The following sections will concentrate on $\mathcal{SPN}^{\mathcal{C}}$, but all steps can be equally applied to $\mathcal{QPN}^{\mathcal{C}}$, $\mathcal{CPN}^{\mathcal{C}}$ and $\mathcal{GHPN}^{\mathcal{C}}$. We start with the following steps:

- Open a standard SPN (in our example "Copynet.spstochpn", see Figure 3) that should be transformed into a colored SPN^{C} .
- Go to the menu bar, select File/Export and choose "Export to colored stochastic Petri net" (see Figure 4). Define the path where you want to save the transformed Petri net. All Petri net elements (places, transitions, arcs) and their properties (markings, rate functions, arc weights) will be used for the construction of the corresponding colored Petri net.

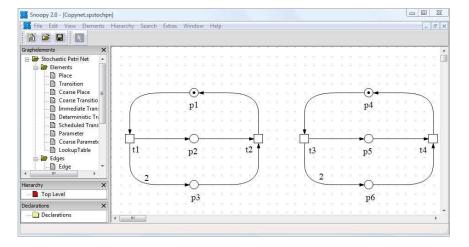


Figure 3: Open a stochastic Petri net.

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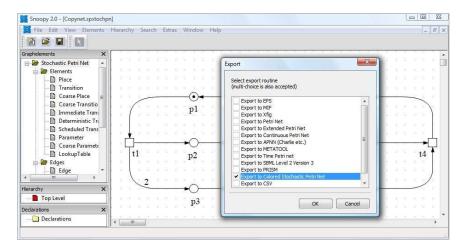


Figure 4: Export to colored stochastic Petri net.

2.1.2 Define similar subnets in the Petri net

We now need to subdivide the Petri net and fold it. We proceed as follows:

- Open the transformed Petri net (shown in Figure 5). Please note that the transformed Petri net is now opened in the $\mathcal{SPN}^{\mathcal{C}}$ environment. The transformation of the Petri net can be recognized by the assigned default color set Dot to all places of the original Petri net.
- Define similar subnets contained in the Petri nets. The Petri net shown in Figure 5 can obviously be divided into two subnets. Therefore, the color set that we will assign to the Petri net consists of two colors. For example: colorset Copy = int with 1-2. See Section 3.1.1 for how to define color sets.

2.1.3 Define declarations

We have to declare or define the color sets, variables, constants and functions that we want to apply to our $SPN^{\mathcal{C}}$ model. In the first step we define the color set according to the following procedure:

- Click on the tab "Colorsets" in declarations menu (left sidebar) and the color set definition dialogue will appear (shown in Figure 6).
- Define name, type (choose one in the drop down list) and colors of your color set.
- Check the syntax to proof your expressions.

For our running examples we will define the color set named "Copy" of the type integer (shortly int) with the colors 1 and 2 (see Figure 6)

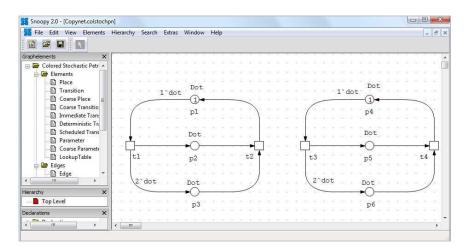


Figure 5: The transformed colored Petri net.

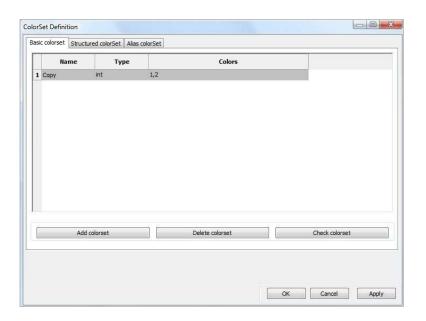


Figure 6: Define color sets.

In the next step we define the variables (shown in Figure 7) that we want to use. The procedure is analogous to the definition of the color set. In our running examples we define the variable "x", whose color set is "Copy" that can be chosen in the drop down list.

Following the same procedure to declare constants and functions.

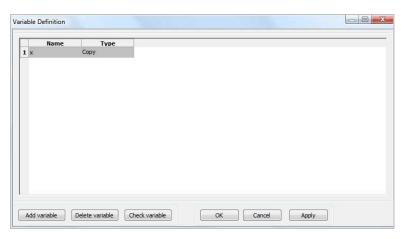


Figure 7: Declare variables.

2.1.4 Assign color sets to places and define initial markings

Now we need do apply the defined color set to the places of the colored Petri net.

- Open the "Edit Properties dialog" of a certain place.
- In the General tab, specify the name of a place.
- In the Marking tab, specify the color set in the "Colorset" box and edit the initial marking in the "MarkingList" (see Figure 8). You can always check the defined color sets with a click open the button "Colorset". If you want to apply the same marking for every color of this place use the function "all()", which means that all the colors in this color set are set to the same coefficient (here it is 1). (See Section 2.4.1 for more details on how to define initial markings.)

It is also possible to edit a group of places and set their color set and marking at once. Just selected the places you want to edit and proceed like above.

- Select a group of places.
- Click *Edit—Edit selected elements*, and then a dialogue to specify the properties appear, e.g. see Figure 9.
- In the Marking tab, specify the color set in the "Colorset" box and edit the initial marking in the "MarkingList".

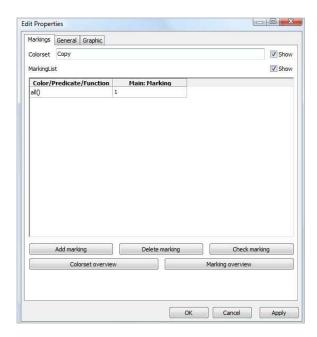


Figure 8: Specify initial marking.

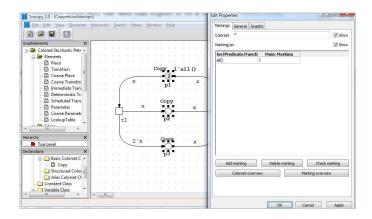


Figure 9: Specify inital markings for a group of places.

2.1.5 Define arc expressions

In the next step, we define the expression for each arc. (See Section 3.2.2 for how to write arc expressions.)

- Open the "Edit Properties dialog" of a certain arc.
- In the Expression tab, write the expression, which can be aided by the expression assistant (Figure 10). Please note that this field should not be empty.



Figure 10: Write arc expressions.

In our example, we use the arc weight separated with "`" from the variable x. You can also edit multiple arcs by selecting a group of arcs and edit them like above.

2.1.6 Define guards for transitions

The guard of a transition can be edited as follows, if they are needed (see also section Section 3.2.3).

- Open the "Edit Properties dialog" of a transition.
- Write the guard expression in the "Guard" tab (see Figure 11). You have also the possibility to use the guard assistant to define the guard.

Again, you can edit multiple transitions by selecting a group of transitions.



Figure 11: Write guards.

2.1.7 Define rate functions for transitions (for $SPN^{C}/CPN^{C}/GHPN^{C}$)

You can also edit the rate functions for transitions if they are needed by applying the following procedure. You have also the possibility to use the rate function assistant to define the rate functions.

- Open the "Edit Properties dialog" of a transition.
- Write the rate function expression in the "Function" tab (see Figure 12).

See Section 2.4.3 for how to write rate functions. Rate functions are only available for SPN^{C} , CPN^{C} and $GHPN^{C}$.

For every mentioned step above there exists a check of the syntax. With the help of the check function you can find and avoid mistakes. You can find this function in each dialogue mentioned above.

After applying all the steps to our running example, we obtain the following colored Petri net model (see Figure 13). We don't need the right subnetwork anymore, because we established this copy by assigning a color set consisting of two colors to the left one. This Petri net is equivalent to the original Petri net of Figure 3. With the help of colored Petri nets we can easily increase the number of copies by changing the declaration of the color set instead of creating multiple graphical copies of the same subnet.

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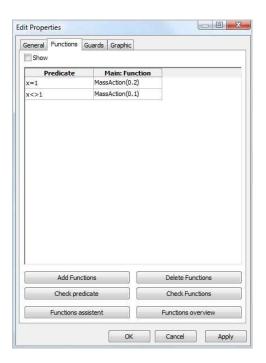


Figure 12: Write rate functions.

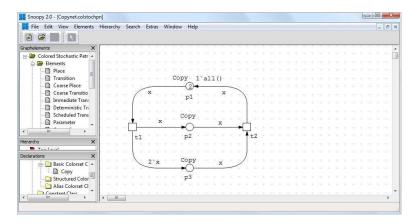


Figure 13: The colored Petri net model.

2.2 Constructing colored Petri nets

Colored Petri nets allow a more compact and parametric representation of a system by folding similar subnets. So it is possible to represent very concisely systems that would have required a huge uncolored net. In this section, we will demonstrate how to construct basic colored Petri net components, so that we can build the whole model based on these components.

2.2.1 Basic colored Petri net components

The key step in the design of a colored Petri net is to construct basic colored Petri net units, through which we can obtain the whole colored Petri net model step by step. This process is also called folding. In the following we will introduce some folding ways to construct basic colored Petri net components, which are illustrated in Figure 14.

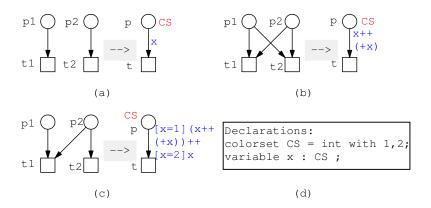


Figure 14: Basic colored Petri net components. For all these three cases, we define the color set as "CS" with two integer colors: 1 and 2. We use color "1" to represent the subnet containing p1 and t1, and color "2" to represent the subnet containing p2 and t2.

Figure 14 (a) shows the folding of two isolated subnets with the same structure. For this simple case, we only need to assign the color set "CS" to the place. We write the arc expression as x, where x is a variable of the type "CS". Thus, we get a basic colored Petri net component, illustrated on the right hand of Figure 14 (a).

In **Figure 14** (b), the net to be folded is extended by two extra arcs from p2 (p1) to t1 (t2), respectively. To fold it, we use the same color set, and just modify the arc expression to x + + (+x), where the "+" in the (+x) is the successor operator, which returns the successor of x in an ordered finite color set. If x is the last color, then it returns the first color. The "++" is the multiset addition operator.

In **Figure 14** (c), the net to be folded gets one extra arc from p2 to t1. To fold it, we use the same color set, and just modify the arc expression to [x = 1](x + (+x)) + +[x = 1](x + (+x)) + + (-x + (+x)) + (-x + (+x)) + + (-x + (+x)) + (-x +

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2]x, meaning: if x = 1, then there are two arcs connecting p with t, while if x = 2, then there is only one arc connecting p with t.

In summary, the following rules apply when folding two similar nets to a colored Petri net. If the two subnets share the same structure, we just have to define a color set and set arc expressions without predicates. If the subnets are similar, but do not have the same structure, we may need to use guards or arc expressions with predicates. However, in either case, if we want to continue to add other similar nets, what we should do is usually to add new colors, and slightly change arc expressions or guards. Using these basic colored Petri net components, we can construct the whole colored Petri net model step by step.

2.2.2 Modeling branch and conflict reactions

In this section, we demonstrate how to construct colored models for two special situations: a branching reaction (One reaction produces several products from reactants.) and conflicting reactions (Several reactions use the same reactants and produce their products independently or concurrently.) Figure 15 and Figure 16 illustrate how to model these two situations, respectively.

Figure 15 shows how to fold a branching reaction into a colored component. For this case, we define two color sets: Dot with one color dot, and CS with two colors b and c. We then assign the color set "Dot" to the place A, and CS to the place P. We define the expression dot for the arc from A to r and b++c for the arc from r to P, which means that when r fires two tokens with colors b and c will be added to P. Please note that the "++" is the multiset addition operator.

Figure 16 shows how to fold conflicting reactions into a colored component. For this case, we use the same color sets. We assign the color set "Dot" to the place A, and CS to the place P. We define the expression dot for the arc from A to r and x for the arc from r to P, where x is a variable of the type "CS".

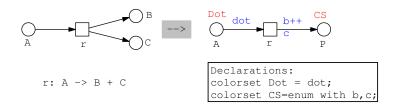


Figure 15: Petri net representation (on the left hand) and colored Petri net representation (on the right hand) of a branching reaction with reactant A and products B and C.

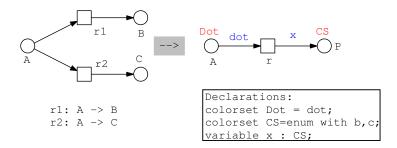


Figure 16: Petri net representation (on the left hand) and colored Petri net representation (on the right hand) of two conflicting reactions with reactant A producing B or C.

2.2.3 Modeling nets with logical nodes

In this section we will discuss how to deal with nets with logical nodes, illustrated in Figure 17 to Figure 21.

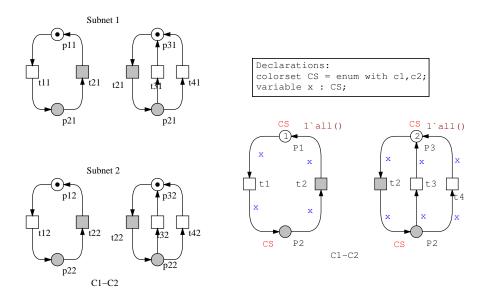


Figure 17: Case 1. In this case, we fold Subnet1 and Subnet2 (on the left hand) to a colored component (on the right hand). Each logical node has a unique copy in each subset.

2.3 Automatic colorizing

Now, three ways are supported to automatically colorize selected subnets.

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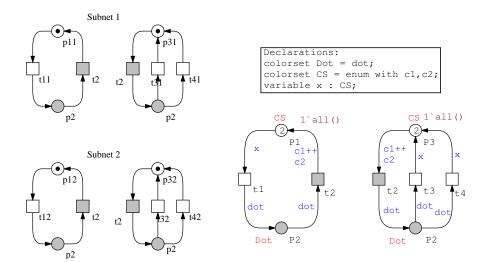


Figure 18: Case 2. In this case, either the transition t2 or place p2 only have one unique copy in both subnets.

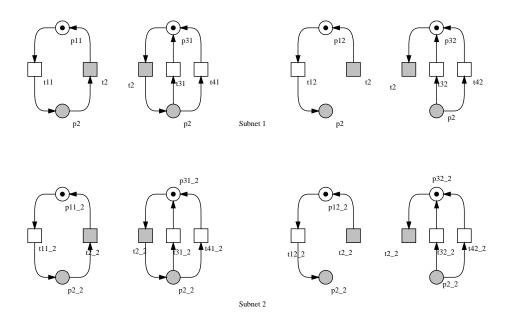


Figure 19: Case 3. Each logical node has a unique copy in each subset.

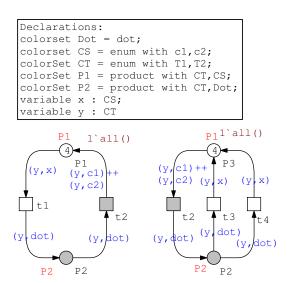


Figure 20: Colored Petri net model for Figure 19. Each logical node has a unique copy in each subset. Each subnet has the same structure and uses the same color set CS.

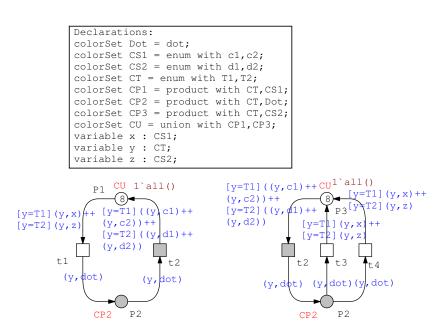


Figure 21: Colored Petri net model for Figure 19. Each logical node has a unique copy in each subset. Each subnet allows a different structure and uses a different color set. Here Subnet 1 uses the color set CS1, and Subnet 2 uses the color set CS2.

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2.3.1 Colorizing any subset

Go to the menu bar, select Extras/Folding/Colorize and then the user can colorize a selected subnet. During this process, the user can set a new color set (for places) and variable name (for edges). After this is done, all places have the same color set and all edges the same expression.

2.3.2 Colorizing twin nets

Go to the menu bar, select Extras/Folding/Generate twin nets and then the user can create twin nets for a given net.

2.3.3 Colorizing T-invariants

Go to the menu bar, select Extras/Folding/Generate master nets and then the user can create a color Petri net model for the given T-invariant file. The user then can demonstrate T-invariants on this colored net.

2.4 Some other key modeling problems

2.4.1 Specifying initial markings

We provide several ways for specifying initial markings:

- Specifying colors and their corresponding tokens as usual,
- Specifying a set of colors with the same number of tokens,
- Using a predicate to choose a set of colors and then specifying the same number of tokens,
- Using the all() function to specify for all colors a specified number of tokens.

Table 1 gives some examples for specifying initial marking.

Table 1: Specification of initial markings. $Colorset\ CS = int\ with\ 1-100.$

Color/Predicate/Function	marking
1	1
4,5,7	2
x > 10	3
all()	4

2.4.2 Random generation of initial marking (for SPN^{C})

For $SPN^{\mathcal{C}}$, we support random generation of an initial marking by applying the following steps (see Figure 22):

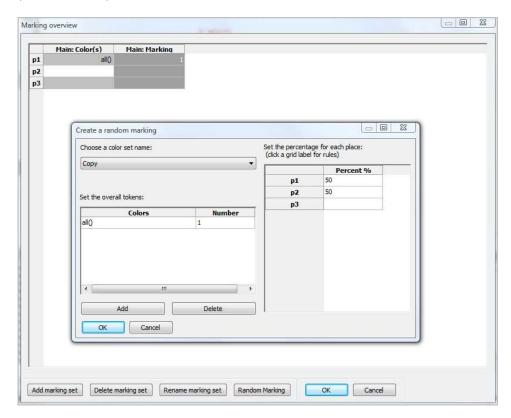


Figure 22: Random generation of initial marking.

- 1. Enter the marking overview dialogue,
- 2. Select a marking set that will hold the generated initial marking, e.g. the main set in Figure 22, and then click the "Random Marking" button. The random marking definition dialogue will appear.
- 3. In this dialogue, you need to do the following things:
 - Choose a color set, e.g. "Copy" in Figure 22, based on which we define random marking.
 - Set the total tokens, e.g. all() is used in Figure Figure 22, based on which we do the random assignment.
 - Set the percentage of each place, which decides how many tokens will be assigned to each place.

The rules for the setting of the percentage are as follows:

- If the percentage domain is an integer, then this will be considered as the percentage.
- If the percentage domain is set to 0, then the marking for this place is set to 0.
- If the percentage domain keeps empty, then this place will keep the old marking unchanged.

2.4.3 Specifying rate functions

As there are four kinds of transitions (stochastic, immediate, deterministic and scheduled), we have to choose a suitable kind. Then we have to define the rate functions for the stochastic transitions, the weights for the immediate transition, the delays for the deterministic transitions, and the periodic values for the scheduled transitions. But their specifications have a similar procedure.

We start with the specification of predicates of rate functions. When writing predicates, there are some notes you should notice:

- For a same binding, only one predicate is allowed to be evaluated to true in the situation of more than one predicates. For example, in Table 2, we have two predicates, x = 1 and x = 2. For each binding, only one of these is evaluated to true. However, we are not allowed to write the predicates like this, x = 1 and x > 1, as these two predicates are evaluated to true for the binding x = 1.
- If the predicates of a transition do not cover all the instances of this transition, then the rate functions of these instances that are not covered are set to 0. For example, if we only use a predicate x = 1, this predicate will not cover the transition instance when x equals 2.

There are three ways for the specification of rate functions: at the colored level or at the instance level (Here we call each unfolded transition corresponding to a colored transition a transition instance of this colored transition.) or a combination of both of them. For any way, we should first use predicates to choose a or a set of transition instances and then specify rate functions.

(1) Specifying rate functions at the colored level

We can specify rate functions by referencing names of colored places, just like specifying rate functions for stochastic Petri nets. For instance, in Figure 23 we can do it at the colored level like shown in the #1 and #2 of Table 2.

(2) Specifying rate functions at the instance level

We can also specify rate functions at the instance level. To do this, in a rate function, we reference a colored place, followed by [color/variable], which denotes the place instance by the specified "color" or "variable". For instance, in Figure 23 we can do it at the instance level as shown in the #3 of Table 2.

#	Predicate	Rate function
1	true	P2 * P3
2	x = 1	P2 * P3
	x = 2	5 * P2 * P3
3	true	P1[1] * P1[2]
4	true	P1[1] * P1[2] * P2 * P3
5	x = 1	P1[1] * P1[2] * P2 * P3
	x = 2	5 * P1[1] * P1[2] * P2 * P3

Table 2: Specifying rate functions.

In addition, we can also combine the above ways to specify rate functions, like shown in the #4 and #5 of Table 2.

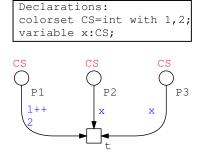


Figure 23: An example to demonstrate how to specify rate functions. The operator ++ in the arc expression 1++2 is the multiset addition operator.

2.4.4 Extended arc types

We support the following extended arc types, which are popular add-ons enhancing modeling comfort (see Figure 24 for graphical representation in Snoopy):

- inhibitor arc,
- read arc,
- equal arc,
- reset arc, and
- modifier arc.

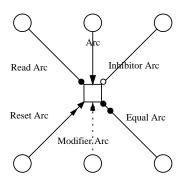


Figure 24: Special arcs in Snoopy.

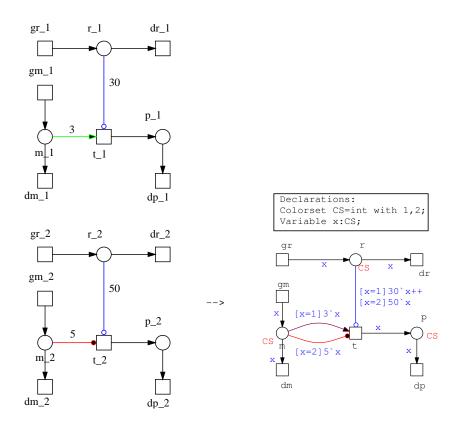


Figure 25: An example for demonstrating the folding involving extended arcs.

Figure 25 gives an example for demonstrating the folding involving extended arcs, which contains two cases: 1) two special arcs are the same kind, and 2) two arcs are different kinds.

2.4.5 Definition of auxiliary variables (observers)

We can also define auxiliary variables (observers), which are extra performance measures, e.g. the sum of some places. This definition follows the following procedure:

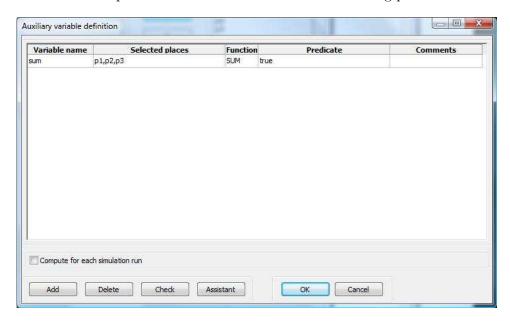


Figure 26: Definition of auxiliary variables.

- 1. Enter the simulation dialogue,
- 2. Enter the plot editing dialogue,
- 3. In this dialogue, click the auxiliary variable definition button, and then enter the auxiliary variable definition dialogue (see Figure 26). In this dialogue, we will do the following things for defining a new auxiliary variable:
 - Define the name for a new auxiliary variable.
 - Select a set of colored places.
 - \bullet Choose an operation. So far, we only support the SUM operation.
 - Define a predicate, which is used to select the instances of colored places, based on which we will compute the values of the auxiliary variable.

Please note that there is a checkbox on the bottom for enabling the computation of auxiliary variables for each simulation run.

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2.4.6 Consistency checks

In the rate function of a transition, only preplaces of this transition are allowed. However sometimes we may omit some preplaces in writing rate functions for different reasons. Therefore, we support to automatically check unused preplaces in rate functions, so that we can reexamine the rate functions. Consistency check is a part of syntax check. The principles we consider are as follows:

- If a rate function is constant, then we only check unused preplaces connected by modifier arcs,
- If a rate function contains places, then we check all unused preplaces.

The following is a consistency check result, which is taken from the Halo model.

- \bullet 11:08:35: Warning: The rate function for r3_1 has unused modifier pre-places: SRI_510
- 11:08:35: Warning: The rate function for r3_2 has unused modifier pre-places: SRI_510
- 11:08:35: Warning: The rate function for r3_6 has unused pre-places: CheB
- 11:08:35: Warning: The rate function for r3_7 has unused pre-places: CheB

3 Annotation Language

In this section, we will describe the annotation language developed for Snoopy's colored Petri nets.

3.1 Declarations

3.1.1 Color sets

We provide two groups of data types to define color sets of colored Petri nets. The simple types can be directly used, but the compound ones must be based on defined color sets. The BNF form for the data type definition is given in Appendix A.2.

- Simple types: dot, int, string, bool, enum, index,
- Compound types: product, union.

Compared with CPN tools [CPN11], we do not support the list and record data types. The reason for not providing the record type is that the record type can be replaced by the product type. For the list type, the reason is that we only want to support finite color sets so as to get an unfolding Petri net from any color Petri net. In the following, we will describe each data type in detail.

(1) dot

We define a dot data type to declare a color set "Dot" with only one default black color "dot".

(2) int

Integers are numerals without a decimal point. Here only non-negative integers are supported.

• Declaration Syntax:

Integers seperated by "," or "-". Here are some legal definitions:

- 1,2,3
- 1-3
- 1,3,5-7
- 1-n

For example, "1,3,5-7" defines the color set that has the following colors: "1,3,5,6,7". We can also support a constant in the integer color set definition, for example, in the "1-n", n is an integer constant (See Section 3.1.4 for constant declarations.).

• Operations:

- $-i_1+i_2$ addition
- $-i_1-i_2$ subtraction
- $-i_1 * i_2$ multiplication
- $-i_1/i_2$ division, quotient
- $-i_1 \% i_2$ modulus, remainder

(3) string

Strings are specified by sequences of printable ASCII characters surrounded with double quotes.

• Declaration Syntax:

Strings separated by "," or "-". We also support very weak regular expressions to define strings, but they will be separated by "[]". Here are some legal definitions:

- *a, b, c*
- a-c
- *a*, *c*, *e*-*g*
- [a][e, f, g]

For example, a, c, e-g defines the color set that has the following colors: a, c, e, f, g. [a][e, f, g] defines the colors: ae, af, ag.

- Operations:
 - -s1+s2 concatenate the strings s1 and s2.

(4) bool

The boolean values are true and false.

• Declaration Syntax:

false, true.

- Operations:
 - -!b negation of the boolean value b,
 - -b1 & b2 boolean conjunction, and,
 - $-b1 \mid b2$ boolean disjunction, inclusive or.

(5) enum

Enumerated values are explicitly named as identifiers in the declaration.

• Declaration Syntax:

Strings separated by "," or "-". We also support very weak regular expressions to define enumeration values, but they will be separated by "[]". Here are some legal definitions:

- \bullet a, b, c
- a-c
- \bullet a, c, e-g
- [a][e, f, g]

For example, a, c, e-g defines the color set that has the following colors: a, c, e, f, g. [a][e, f, g] defines the colors: ae, af, ag.

The color set definition for enum is like that of string. The difference is that an enum color should be an identifier.

• Operations:

There are no standard operations.

(6) index

Indexed values are sequences of values composed of an identifier and an indexspecifier.

• Declaration Syntax:

index id with [intexp1 - intexp2]. For example, we can define an index color set as: colorset Philosopher with index phil[1-5].

• Operations:

There are no standard operations.

(7) product

A product color set is a tuple of previously declared color sets.

• Declaration Syntax:

Defined color sets separated by ",". For example, we can define a product color set as: $colorset\ Philosopher\ with\ product\ H2O \times Level$, where H2O and Level are two previously defined color sets.

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• Operations:

There are no standard operations.

(8) union

A union color set is a disjoint union of previously declared color sets.

• Declaration Syntax:

Defined color sets separated by ",". For example, we can define a union color set as: colorset Salad with union Fruit, Dish, where Fruit and Dish are two previously defined color sets.

• Operations:

There are no standard operations.

3.1.2 Subsets of color sets

We can also define subsets for a defined color set in the following two ways:

- Enumerate the colors that will appear in a subset, separated by ','.
- Using a logic expression (predicate) to select a group of colors, see Section 3.2.3 for how to define a predicate.

For example, suppose $Colorset\ CS = int\ with\ 1 - 10$, $Variable\ x: CS$ and then we can define a subset CS_sub for the color set CS using the logic expression x <> 10, which selects the colors, 1-9, for the subset CS_sub .

3.1.3 Variables

A variable is an identifier whose value can be changed during the execution of the model. They have the following characteristics:

- They are declared with a previously declared color set.
- They are bound to the variety of different values from their color set by the simulator as it attempts to determine if a transition is enabled.
- There can be multiple bindings simultaneously active on different transitions. These bindings can exist simultaneously because they have different scopes.
- They allow are expressions with the ability to reference different values.

Variables can be used in the following situations (Suppose Colorset $CS = int \ with \ 1-10; \ Variable \ x : CS$):

- arc expressions, e.g., x+1,
- guard, e.g., x < 5,
- marking predicate definition, e.g., x < 6,
- rate function predicate definition, e.g., x < 7.

3.1.4 Constants

A constant has a value and corresponding data type or color set. For example, we can define a constant as follows: $constant \ N = int \ with \ 5$. We can also define a constant of the integer type based on an existing constant, e.g $constant \ M = int \ with \ N+5$. Constants can be used in the arc expressions, guards, predicates and integer color set definition.

Constants can be used in the following cases (Suppose $Colorset\ CS = int\ with\ 1-10;$ $Variable\ x:CS;\ Constant\ N:CS\ with\ 5$):

- arc expressions, e.g., x + N,
- guard, e.g., x < N,
- integer colorset definition, e.g., x < N,
- marking predicate definition, e.g., x < N,
- marking definition, e.g., we can set a color having a number of N,
- rate function predicate definition, e.g., x < N.

3.1.5 Functions

We can also define functions that are used in the whole net. A user-defined function contains the following components:

- Function name, which is an identifier,
- Parameter list, separated by ",",
- Function body, which is an expression, and
- Return type, which is the type of the return value.

When we write a function body, we can use all the defined constants and all the operators in Table 3. A function body should comply with the BNF forms in Appendix A.3. However, please be careful when using the operator ++ and make sure that this will return only one single value or empty as we at present do not support that the user-defined function returns more than one values (colors).

Specifically speaking, a user-defined function can be used in the following situations:

- expressions on arcs,
- guards on transitions,
- predicates in rate functions of transitions, and
- predicates in marking definitions of places.

In Figure 1, we use two user-defined functions. For example,

Forks
$$Left(Phils x) \{ x \}.$$

In this function, Forks is the type of the return value, which is an integer color set. Left is the function name. Phils x defines the parameter of this function. x is the function body, which returns the left folk.

Forks Right(Phils x) {
$$(x\%N) + 1$$
 }.

This function returns the right fork. % is the modulus operator.

In Figure 37, we also use user-defined functions (See Table 5 for details.). For example, the function Fun1 is defined as follows:

$$P Fun1(HbO2 x, Level y) \{ [y = L]1`(x + 1, y) + +[y = H]1`(x, y) \}.$$

In this function, P is the type of the return value, which is a product color set. Fun1 is the function name. HbO2 x, Level y define two parameters of this function, where x is of the type HbO2 and y of Level. [y=L]1`(x+1,y)++[y=H]1`(x,y) is the function body, which means when y equals L it returns one token with the color (x+1,y) and when y equals H it returns one token with the color (x,y). See Section 3.2.2 for more details about how to read function bodies.

3.2 Expressions

3.2.1 Operators and built-in functions

We support the operators summarized in Table 3 and some built-in functions, which are illustrated in Table 4.

3.2.2 Arc expressions

Arc expressions can be defined according to the BNF forms illustrated in Appendix A.3. Arc expressions can use all the constants, variables and user-defined functions and all the operators in Table 3.

For example, in Figure 35 (see Table 5 for its declarations), we use three different expressions: dot, e.g. on the arc from transition t1 to place O2, x, e.g. from t1 to HbO2L and x + 1, e.g. from HbO2L to t1. Among these, dot is a default constant color, x is a variable and x + 1 is an addition expression.

Table 3: Operators in the annotation language.

Priority	Operator	Executed operation	
	Operator	Successor, which returns the successor of the current	
10 +			
		color in an ordered finite color set. If the current color	
		is the last color, then it returns the first color.	
Predecessor, whi		Predecessor, which returns the predecessor of the current	
	_	color in an ordered finite color set. If the current color	
		is the first color, then it returns the last color.	
	@ Index extracting, which returns the index of an index		
	:	Extracting a component from a product color.	
	!	Logical not.	
9	*,/,%,^	Arithmetic multiplicity, division, modulus, power.	
8	+	Arithmetic addition, or string concatenation.	
	_	Arithmetic subtraction.	
7	<,<=	Less than, less than or equal to.	
	>,>=	Greater than, greater than or equal to.	
6	=,<>	Equal, unequal.	
5	&	Logical and.	
4		Logical or.	
3	,	Used in a tuple expression.	
2	`	Separating the coefficients and the color.	
1	++	Multiset addition, connecting two multiset expressions.	

Table 4: Built-in functions in the annotation language.

Function	Executed operation		
all()	Return all colors of a color set, only used in the arc expressions.		
abs()	Return the absolute value.		

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In Figure 36, we can see more complex expressions. For example, [y = L]dot on the arc from place O2 to transition t1 means that if y equals L it returns a token with the color dot, otherwise an empty value. In fact, y = L is a predicate of this expression.

3.2.3 Predicates/guards

Predicates/guards are in fact boolean expressions, which should be evaluated to boolean values. Guards are used for transitions, which decide which transition instances exist, while predicates are used in other situations. Predicates/guards can contain user-defined functions. Specifically speaking, we use the predicates in the following situations:

- Subset definition of color sets, where a predicate is used to select a group of colors to form a subset.
- Initial marking specification, where a predicate is used to select a group of colors.
- Rate function specification, where a predicate is used to select a group of transition instances.
- Arc expression specification, where a predicate is used to decide if the current arc
 is used or not.

For example, in Figure 35 (see Table 5 for its declarations), in the expression [y = L]dot, y = L is a predicate of this expression, where when y = L is evaluated to true, this expression returns one token dot, otherwise it returns empty. In addition, there is a guard x <> 4 e.g. on transitions t1, which means when this guard is evaluated to true, there exists a transition instance of t1.

4 Animation, Simulation and Analysis

In this section, we will demonstrate how to animate/simulate/analyze $\mathcal{QPN}^{\mathcal{C}}$, $\mathcal{SPN}^{\mathcal{C}}$, $\mathcal{CPN}^{\mathcal{C}}$, and $\mathcal{GHPN}^{\mathcal{C}}$.

4.1 Animation (for QPN^{C}/SPN^{C})

When a Petri net model is opened, then the user can click the *View—Start Anim-Mode* to prepare animation. Before opening the animation dialogue, the syntax will be checked automatically for this model. The user can choose automatic animation or a manual one, in which case the user can select a binding. In the following, we will in detail describe it. Figure 27 shows the animation interface.

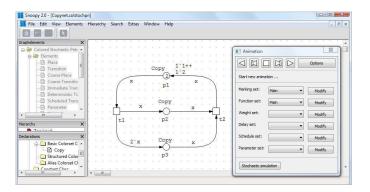


Figure 27: Animation interface.

4.1.1 Automatic animation

When the user clicks the *Play forward/Pause* button, the automatic animation will begin/pause. Figure 28 shows one animation snapshot.

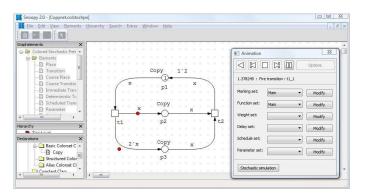


Figure 28: One animation snapshot.

4.1.2 Manual animation

When the user just clicks the transition to fire, then the binding selection dialogue will appear if this transition is enabled. For example, when we click the transition t1, we will get Figure 29. Then the user can select manual binding.

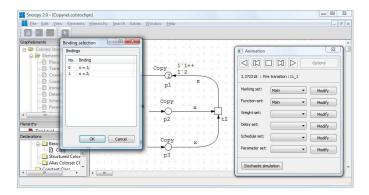


Figure 29: Manual animation snapshot.

4.2 Simulation (for $SPN^{c}/CPN^{c}/GHPN^{c}$)

When the user clicks the *View—Start Simulation-Mode*, the simulation dialogue will appear. During this process, an implicit unfolding is done, which unfolds a colored Petri net to a standard Petri net.

4.2.1 Run simulation

In the simulation dialogue (Figure 30), the user can first set simulation parameters, and then click the *Start simulation* button to start simulation. The settings include:

- Setting a marking set,
- Setting a rate function/weight/delay/schedule set,
- Setting a parameter set,
- Setting a simulation run interval, output step count, and simulation run number, and
- Choosing a simulation algorithm.

4.2.2 Show simulation results

The user can choose to show simulation results as a table or plot. Further, in a table or plot, the user can choose which information to be shown: colored, unfolded or both. For example, Figure 31 gives the plot of colored places.

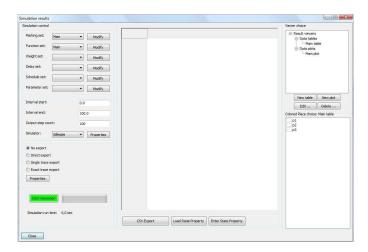


Figure 30: Simulation interface.

Plus, the user can edit the table or plot to change what information to be shown (Figure 32).

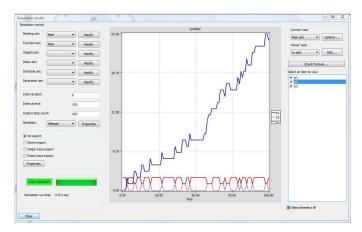


Figure 31: Plot for simulation results.

4.2.3 Export simulation results

The user can choose which information to be exported to a file: colored, unfolded or both.

4.3 Analysis

4.3.1 Analysis using Charlie

We can export a colored Petri net to an uncolored Petri net, and then use Charlie [Cha11], [Fra09] to analyze its properties, e.g. P-invariants and T-invariants, or generate

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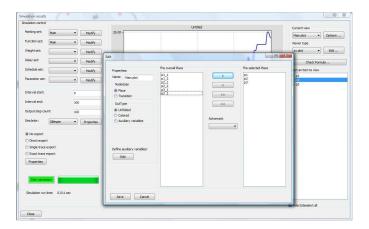


Figure 32: Edit plot.

its reachability graph.

4.3.2 Analysis using Marcie

We can also export a colored stochastic Petri net to a stochastic Petri net, and then use Marcie [Mar11], [SH09] to model check it.

4.3.3 Analysis using the MC2 tool

The MC2 tool [MC210] is used to analyze simulation traces of a stochastic model, so we can use MC2 to directly analyze simulation traces of a colored stochastic/continuous Petri net.

4.3.4 Analysis using CPN tools

We can export a colored Petri net produced by Snoopy to another colored Petri net readable by the CPN tools [CPN11]. So we can make use of the analysis tool of CPN tools [CPN11], [ASAP11] to analyze colored Petri nets at the colored level.

5 Export/Import

5.1 Common export/import

5.1.1 Export to APNN

A colored Petri net can be exported to an APNN file which then can be read by Charlie or Marcie for further analysis.

5.1.2 Export to CANDL

A colored Petri net can be exported to an CANDL file which then can be read by Marcie for further analysis. See Appendix B.1 for the CANDL grammar.

5.1.3 Import CANDL

The user can import a CANDL file of a colored Petri net. See Appendix B.1 for the CANDL grammar.

5.1.4 Export declarations to a CSV file

We can export declarations of a colored Petri net to a csv file, which then can be used for publication purposes or imported by other nets, i.e., when we create a new colored net, we can import declarations from a CSV file for this new net.

5.1.5 Import declarations from a CSV file

Before defining a new colored Petri net, we can import declarations from a CSV file to reuse the declaration information which has been defined before.

5.2 QPN^{C} export/import

5.2.1 Export to colored extended Petri nets

An extended Petri net can be exported to a colored extended Petri net (QPN^{C}) by defining a color set Dot. After this transformation, the new net has the following features:

- All the places are set to the same color set *Dot*.
- All the arcs are set to the same expression dot.

5.2.2 Export to extended Petri nets

A colored extended Petri net can be unfold to an extended Petri net just by exporting it to an extended Petri net. During this process, all isolated nodes (places or transitions) are removed.

5.2.3 Export to colored stochastic Petri nets

A colored extended Petri net $(\mathcal{QPN}^{\mathcal{C}})$ can be transformed into a colored stochastic Petri net. All information is kept during this process, and all rate functions for the transformed $\mathcal{SPN}^{\mathcal{C}}$ are set to MassAction(1).

5.2.4 Export the structure to extended Petri nets

The structure of a colored extended Petri net $(\mathcal{QPN}^{\mathcal{C}})$ can be exported to an extended Petri net. In this specific case, there is no unfolding involved.

5.2.5 Export to CPN tools

A colored extended Petri net $(\mathcal{QPN}^{\mathcal{C}})$ can be transformed to a file read by CPN tools [CPN11]. After this transformation, sometimes we have to modify the arc or guard expressions to let them comply with the syntax of CPN tools. In summary, the following points should be noted:

- Modify user-defined functions in the declaration part,
- Change the syntax of predicates to the if-then-else syntax supported by CPN tools,
- Replace the operators of successor, predecessor etc. with user-defined functions,
- Modify arc expressions that belong to the union type.

5.3 SPN^{C} export/import

5.3.1 Export to colored stochastic Petri nets

A stochastic Petri net can be exported to a colored stochastic Petri net by defining a color set *Dot*. After this transformation, the new net has the following features:

- All the places are set to the same color set *Dot*.
- All the arcs are set to the same expression dot.

5.3.2 Export to stochastic Petri nets

A colored stochastic Petri net can be unfolded to a stochastic Petri net just by exporting it to a stochastic Petri net. During this process, all isolated nodes (places or transitions) are removed.

5.3.3 Export to colored extended Petri nets

A colored stochastic Petri net can be transformed to a colored extended Petri net. After this transformation, all information about rate functions is lost.

5.3.4 Export to colored continuous/hybrid Petri nets

A colored stochastic Petri net can be transformed to a colored continuous/hybrid Petri net.

5.3.5 Export the structure to stochastic Petri nets

The structure of a colored stochastic Petri net (SPN^{C}) can be exported to a stochastic Petri net. In this specific case, there is no unfolding involved.

5.3.6 Export to CPN tools

A colored stochastic Petri net (SPN^C) can be transformed to a file read by CPN tools [CPN11]. After this transformation, sometimes we have to modify the arc or guard expressions to let them comply with the syntax of CPN tools.

5.4 $\mathcal{CPN}^{\mathcal{C}}$ export/import

5.4.1 Export to colored continuous Petri nets

A continuous Petri net can be exported to a colored continuous Petri net by defining a color set *Dot*. After this transformation, the new net has the following features:

- All the places are set to the same color set *Dot*.
- All the arcs are set to the same expression dot.

5.4.2 Export to continuous Petri nets

A colored continuous Petri net can be unfolded to a continuous Petri net just by exporting it to a continuous Petri net. During this process, all isolated nodes (places or transitions) are removed.

5.4.3 Export to colored stochastic/hybrid Petri nets

A colored continuous Petri net can be transformed to a colored stochastic/hybrid Petri net.

5.4.4 Export the structure to continuous Petri nets

The structure of a colored continuous Petri net $(\mathcal{CPN}^{\mathcal{C}})$ can be exported to a continuous Petri net. In this specific case, there is no unfolding involved.

5.5 $\mathcal{GHPN}^{\mathcal{C}}$ export/import

5.5.1 Export to colored hybrid Petri nets

A hybrid Petri net can be exported to a colored hybrid Petri net by defining a color set *Dot*. After this transformation, the new net has the following features:

- All the places are set to the same color set *Dot*.
- All the arcs are set to the same expression dot.

5.5.2 Export to hybrid Petri nets

A colored hybrid Petri net can be unfolded to a hybrid Petri net just by exporting it to a continuous Petri net. During this process, all isolated nodes (places or transitions) are removed.

5.5.3 Export to colored stochastic/continuous Petri nets

A colored hybrid Petri net can be transformed to a colored stochastic/continuous Petri net.

5.5.4 Export the structure to hybrid Petri nets

The structure of a colored hybrid Petri net $(\mathcal{GHPN}^{\mathcal{C}})$ can be exported to a hybrid Petri net. In this specific case, there is no unfolding involved.

6 Examples

6.1 Cooperative ligand binding

We consider an example of the binding of oxygen to the four subunits of a hemoglobin heterotetramer. The hemoglobin heterotetramer in the high and low affinity state binds to none, one, two, three or four oxygen molecules. Each of the ten states is represented by a place and oxygen feeds into the transitions that sequentially connect the respective places. The qualitative Petri net model is illustrated in Figure 33 (taken from [MWW10]).

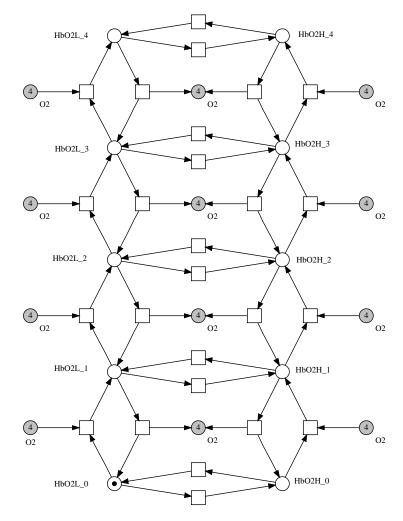


Figure 33: Cooperative binding of oxygen to hemoglobin represented as a Petri net model [MWW10]. For clarity, oxygen is represented in the form of multiple copies (logical places) of one place.

Now we begin to construct a colored Petri net model for Figure 33. For this, we first

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partition Figure 33 into five subnets, each of which is embraced by a rectangle and is defined as a color. So we can use five integers, 0-5, to represent these five subnets. We then group similar places, which are marked with an identical color. The places in each group (with a specific color) are considered as a colored place. The net after partitioning and grouping is shown in Figure 34.

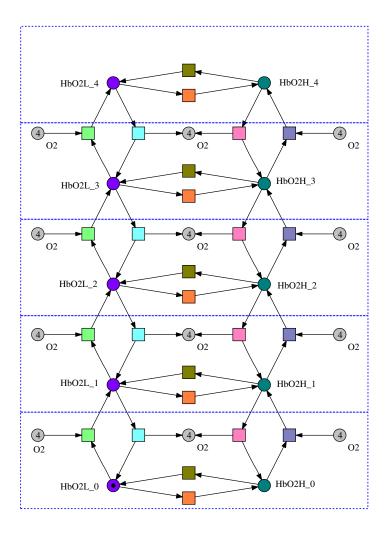


Figure 34: Cooperative binding of oxygen to hemoglobin represented as a Petri net model, which has been partitioned into subnets.

Now we obtain for Figure 33 a $\mathcal{QPN}^{\mathcal{C}}$ model, illustrated in Figure 35, and further a more compact $\mathcal{QPN}^{\mathcal{C}}$ model (Figure 36) by continuing folding the left and right parts. From Figure 35, we can see that the colored Petri net model reduces the size of the corresponding standard Petri net model. Moreover, comparing Figure 35 with Figure 36, we can also see that we can build colored Petri net model with different level of structural details, which is especially helpful for modeling complex biological

systems. After automatic unfolding, these two colored models yield exactly the same Petri net model as given in Figure 33, i.e., the colored models and the uncolored model are equivalent. The declarations for these two $\mathcal{QPN}^{\mathcal{C}}$ models of the cooperative ligand binding are given in Table 5.

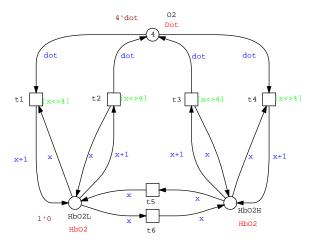


Figure 35: $QPN^{\mathcal{C}}$ model for the cooperative binding of oxygen to hemoglobin, given as a standard Petri net in Figure 33. For declarations of color sets and variables, see 5.

Table 5: Declarations for the $QPN^{\mathcal{C}}$ models of the cooperative ligand binding.

```
Declarations

colorset Dot = dot;

colorset HbO2 = int with 0-4;

colorset Level = enum with H,L;

colorset P = product with HbO2 × Level;

variable x: HbO2;

variable y: Level;

Function P Fun1(HbO2 x, Level y) {[y=L]1`(x+1,y)++[y=H]1`(x,y)};

Function P Fun2(HbO2 x, Level y) {[y=H]1`(x+1,y)++[y=L]1`(x,y)};
```

Besides, we give another colored model (see Figure 37), which uses user-defined functions and is equivalent to Figure 36. In this model, we define two functions Fun1 and Fun2 to replace lengthy expressions. See Table 5 for details about these two functions. From these colored nets, we can also see that the folding operation does reduce the

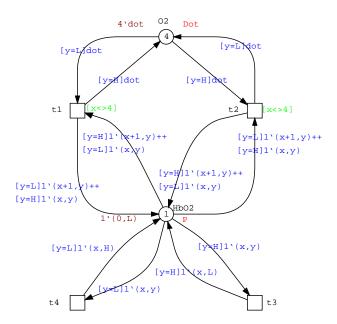


Figure 36: $QPN^{\mathcal{C}}$ model for the cooperative binding of oxygen to hemoglobin, given as a standard Petri net in Figure 33. For declarations of color sets and variables, see Table 5.

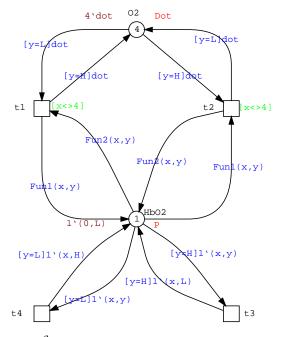


Figure 37: Another $\mathcal{QPN}^{\mathcal{C}}$ model for the cooperative binding of oxygen to hemoglobin, which uses user-defined functions and is equivalent to Figure 36. For declarations of color sets and variables, see Table 5.

size of the net description for the prize of more complicated inscriptions. The graphic complexity is reduced, but the annotations of nodes and edges creates a new challenge. This is not unexpected since a more concise write-up must rely on more complex components. Therefore, it is necessary to build a colored Petri net model at a suitable level of structural details.

6.2 Repressilator

In this section, we will demonstrate the SPN^{C} using an example of a synthetic circuit - the repressilator, which is an engineered synthetic system encoded on a plasmid, and designed to exhibit oscillations [EL00]. The repressilator system is a regulatory cycle of three genes, for example, denoted by g_a, g_b and g_c, where each gene represses its successor, namely, g_a inhibits g_b, g_b inhibits g_c, and g_c inhibits g_a. This negative regulation is realized by the repressors, p_a, p_b and p_c, generated by the genes g_a, g_b and g_c respectively [LB07].

As our purpose is to demonstrate the $SPN^{\mathcal{C}}$, we only consider a relatively simple model of the repressilator, which was built as a stochastic π -machine in [BCP08]. Based on that model, we build a stochastic Petri net model (Figure 38), and further a $SPN^{\mathcal{C}}$ model for the repressilator (shown on the left hand of Figure 39). This colored model when unfolded yields the same uncolored Petri net model in Figure 38.

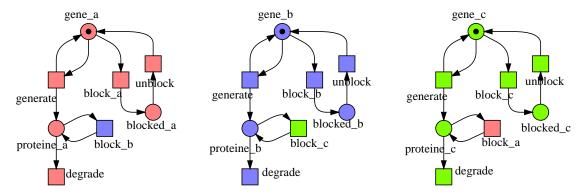


Figure 38: Stochastic Petri net model for the repressilator. The highlighted transitions are logical transitions.

For the $SPN^{\mathcal{C}}$ model in Figure 39, there are three colors, a, b, and c to distinguish three similar components in Figure 38. The predecessor operator "-" in the arc expression -x returns the predecessor of x in an ordered finite color set. If x is the first color, then it returns the last color.

As described above, the $\mathcal{SPN}^{\mathcal{C}}$ will be automatically unfolded to a stochastic Petri net, and can be simulated with different simulation algorithms. On the right hand of Figure 39 a snapshot of a simulation run result is given. The rate functions are given in Table 6 (coming from [PC07]). The $\mathcal{SPN}^{\mathcal{C}}$ model exhibits the same behavior compared with that in [PC07].

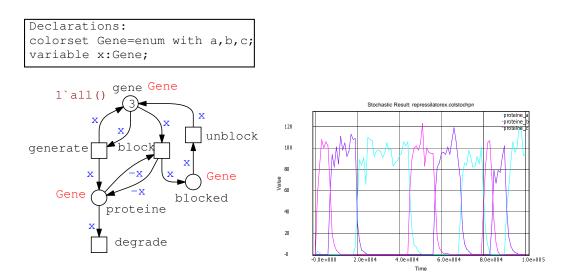


Figure 39: SPN^{C} model of the standard Petri net given in Figure 38, and one simulation run plot for the repressilator. For rate functions, see Table 6.

Table 6: Rate functions for the $\mathcal{SPN}^{\mathcal{C}}$ model of the repressilator.

Transition	Rate function
generate	0.1*gene
block	1.0*proteine
unblock	0.0001*blocked
degrade	0.001*proteine

From Figure 39, we can see that the $SPN^{\mathcal{C}}$ model reduces the size of the original stochastic Petri net model to one third. More importantly, when other similar subnets have to be added, the model structure does not need to be modified and what has to be done is only to add extra colors.

For example, we consider the generalized repressilator with an arbitrary number n of genes in the loop that is presented in [MHE+06]. To build its $\mathcal{SPN}^{\mathcal{C}}$ model, we just need to modify the color set as n colors, and do not need to modify anything else. For example, Figure 40 gives the conceptual graph of the generalized repressilator with n=9 (on the left hand), and one simulation plot (on the right hand), whose rate functions are the same as in Table 6. Please note, the $\mathcal{SPN}^{\mathcal{C}}$ model for the generalized repressilator is the same as the one for the three-gene repressilator, and the only difference is that we define the color set as n colors rather than 3 colors. This demonstrates a big advantage

of color Petri nets, that is, to increase the colors means to increase the size of the net.

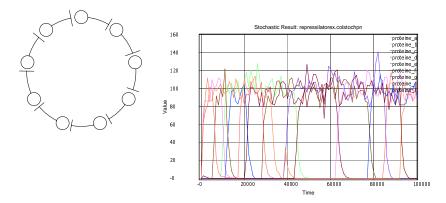


Figure 40: Conceptual graph and one simulation run plot for the repressilator with 9 genes.

6.3 Where to find more examples

In [GLG+11], [GLT+11], colored (both stochastic and continuous) Petri nets have been used to describe the phenomenon of Planar Cell Polarity (PCP) signaling in Drosophila wing. Two colored models (abstract and refined) has been developed, which model a group of cells on a two-dimensional grid, corresponding to a fragment of the wing tissue. Moreover each cell is partitioned into seven virtual compartments, so these two models has a two-level hierarchy. In addition, these models involve product color sets, subsets of color sets, user-defined functions and etc.

More case studies can be found in [GH11], [Liu12], e.g.

- Gradient,
- Dictyostelium colony formation,
- Phase variation in bacterial colony growth,
- C. Elegans vulval development,
- Coupled Ca^{2+} channels,
- Membrane systems.

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References

- [ASAP11] ASAP: http://www.daimi.au.dk/~ascoveco/asap.html (2011)
- [BCP08] R. Blossey, L. Cardelli, A. Phillips: Compositionality, Stochasticity and Cooperativity in Dynamic Models of Gene Regulation. HFSP Journal. 2(1), 17-28 (2008)
- [BNF11] BNF: http://en.wikipedia.org/wiki/Backus_Naur_Form (2011)
- [Cha11] Charlie a Software Tool to Analyze Place/Transition Nets: http://www-dssz.informatik.tu-cottbus.de/DSSZ/Software/Charlie (2011)
- [CPN11] CPN tools: http://cpntools.org/ (2011)
- [EL00] M.B. Elowitz, S. Leibler: A Synthetic Oscillatory Network of Transcriptional Regulators. Nature. 403, 335-338 (2000)
- [Fra09] A. Franzke: Charlie 2.0 a Multi-Threaded Petri Net Analyzer. Diploma Thesis, Brandenburg University of Technology Cottbus. (2009)
- [GH11] D. Gilbert, M. Heiner: Petri nets for multiscale Systems Biology: http://multiscalepn.brunel.ac.uk (2011)
- [GHL07] D. Gilbert, M. Heiner, S. Lehrack: A Unifying Framework for Modelling and Analysing Biochemical Pathways Using Petri Nets. Proc. International Conference on Computational Methods in Systems Biology. LNCS/LNBI, 4695, 200-216 (2007)
- [Gil77] D.T. Gillespie: Exact Stochastic Simulation of Coupled Chemical Reactions. Journal of Physical Chemistry. 81(25), 2340-2361 (1977)
- [GL79] H.J. Genrich, K. Lautenbach: The Analysis of Distributed Systems by Means of Predicate/Transition-Nets. Semantics of Concurrent Computation. LNCS, 70, 123-146 (1979)
- [GL81] H.J. Genrich, K. Lautenbach: System Modelling with High-Level Petri Nets. Theoretical Computer Science. 13(1), 109-135 (1981)
- [GLG+11] Q. Gao, F. Liu, D. Gilbert, M. Heiner, D. Tree: A Multiscale Approach to Modelling Planar Cell Polarity in Drosophila Wing using Hierarchically Coloured Petri Nets. Proc. 9th International Conference on Computational Methods in Systems Biology (CMSB 2011). ACM digital library (2011)
- [GLT+11] Q. Gao, F. Liu, D. Tree, D. Gilbert: Multi-cell Modeling Using Coloured Petri Nets Applied to Plannar Cell Polarity. Proc. 2th International Workshop on Biological Processes & Petri nets. CEUR Workshop Proceedings, 724, 135-150 (2011)
- [HH11] M. Herajy, M. Heiner: Hybrid Representation and Simulation of Stiff Biochemical Networks through Generalised Hybrid Petri Nets. Technical Report, Brandenburg University of Technology Cottbus, Department of Computer Science (2011)

- [HLG+09] M. Heiner, S. Lehrack, D. Gilbert, W. Marwan: Extended Stochastic Petri Nets for Model-based Design of Wetlab Experiments. Transaction on Computational Systems Biology XI. LNCS/LNBI, 5750, 138-163 (2009)
- [HRR+08] M. Heiner, R. Richter, C. Rohr, M. Schwarick: Snoopy A Tool to Design and Execute Graph-Based Formalisms. [Extended Version]. Petri Net Newsletter. 74, 8-22 (2008)
- [Jen81] K. Jensen: Coloured Petri Nets and the Invariant-Method. Theoretical Computer Science. 14(3), 317-336 (1981)
- [JKW07] K. Jensen, L.M. Kristensen, L.M. Wells: Coloured Petri Nets and CPN Tools for Modelling and Validation of Concurrent Systems. International Journal on Software Tools for Technology Transfer. 9(3/4), 213-254 (2007)
- [LB07] A. Loinger, O. Biham: Stochastic Simulations of the Repressilator Circuit. Physical Review. 76(5), 051917(9) (2007)
- [Liu12] F. Liu: Colored Petri Nets for Systems Biology, Ph.D. Thesis, BTU Cottbus, Dep. of CS, (2012)
- [Mar11] Marcie a Tool for Qualitative and Quantitative Analysis of Generalized Stochastic Petri Nets. http://www-dssz.informatik.tu-cottbus.de/DSSZ/Software/Marcie (2011)
- [MC210] MC2 website: MC2 A PLTL Model Checker. University of Glasgow, http://www.brc.dcs.gla.ac.uk/~drg/courses/sysbiomres/software/mc2 (2010)
- [MHE+06] S. Muller, J. Hofbauer, L. Endler, C. Flamm, S. Widder, P. Schuster: A Generalized Model of the Repressilator. Journal of Mathematical Biology. 53, 905-937 (2006)
- [MWW10] W. Marwan, A. Wagler, R. Weismantel: Petri Nets as a Framework for the Reconstruction and Analysis of Signal Transduction Pathways and Regulatory Networks. Natural Computing. 10(2), 639-654 (2010)
- [MRH12] W. Marwan, C. Rohr, M. Heiner: Petri nets in Snoopy: A unifying framework for the graphical display, computational modelling, and simulation of bacterial regulatory networks, in Jv Helden and A Toussaint and D Thieffry (Eds.), Methods in Molecular Biology Bacterial Molecular Networks, chapter 21, Humana Press, series Methods in Molecular Biology, Vol. 804, pp. 409–437 (2012)
- [PC07] A. Phillips, L. Cardelli: Efficient, Correct Simulation of Biological Processes in the Stochastic Pi-Calculus. Proc. Computational Methods in Systems Biology. LNCS, 4695, 184-199 (2007)
- [RMH10] C. Rohr, W. Marwan, M. Heiner: Snoopy a Unifying Petri Net Framework to Investigate Biomolecular Networks: Bioinformatics. 26(7), 974-975 (2010)

[SH09] M. Schwarick, M. Heiner: CSL Model Checking of Biochemical Networks with Interval Decision Diagrams. Proc. 7th International Conference on Computational Methods in Systems Biology (CMSB 2009), LNBI 5688, 296-312 (2009)

A Annotation Language

A.1 Introduction to BNF

A Backus-Naur Form (BNF) specification is a set of derivation rules [BNF11], written as

$$\langle \text{symbol} \rangle ::= expression$$

$$| \text{"terminal"}$$

where:

- 1. (symbol) is a nonterminal; expression consists of one or more sequences of symbols; more sequences are separated by the vertical bar, |, indicating a choice, the whole being a possible substitution for the symbol on the left.
- 2. Symbols that never appear on a left side are terminals, which are notated by using the double quotation marks "".
- 3. Symbols that appear on a left side are non-terminals.
- 4. ::= means "is defined as".
- 5. \perp means "empty" or "null".

A.2 BNF for the data type definition

```
\langle \text{Type} \rangle ::=
                                        \langle \text{SimpleType} \rangle \mid \langle \text{CompoundType} \rangle
                                         ⟨TypeIdentifier⟩ | ⟨StructuredType⟩
      \langle SimpleType \rangle ::=
   (TypeIdentifier)
                                ::=
                                         ⟨UnsignedInteger⟩ | ⟨Boolean⟩ | ⟨String⟩
(UnsignedInteger)
                                         "int"
                                ::=
             (Boolean)
                                         "bool"
                                ::=
                (String)
                                         "string"
                                ::=
\langle StructuredType \rangle
                                ::= \langle \text{Enumeration} \rangle \mid \langle \text{Index} \rangle
     (Enumeration)
                                ::=
                                         (IdentifierList)
     \langle IdentifierList \rangle
                                ::= \langle Identifier \rangle | \langle Identifier List \rangle "," \langle Identifier \rangle
                                         ⟨Identifier⟩"["⟨IndexSpecifier⟩"]"
                 \langle \mathrm{Index} \rangle
                                ::=
                                          "int"
   (IndexSpecifier)
                                ::=
(CompoundType)
                                ::= \langle Product \rangle \mid \langle Union \rangle
             (Product)
                                ::= \langle \text{Type} \rangle \text{"} \times \text{"} \langle \text{Type} \rangle \mid \langle \text{Product} \rangle \text{"} \times \text{"} \langle \text{Type} \rangle
                \langle Union \rangle ::= \langle Type \rangle \mid \langle Union \rangle", "\langle Type \rangle
```

A.3 BNF for the annotation language

```
\langle \text{ColorExpr} \rangle
                                          (MultiSetExpr)
                                 ::=
    (MultiSetExpr)
                                          \langle Predicate \rangle \mid \langle MultiSetExpr \rangle \langle MSAdditionOp \rangle \langle Predicate \rangle
                                 ::=
                                         "++"
  (MSAdditionOp)
                                 ::=
           (Predicate)
                                         ⟨SeparatorExpr⟩ | "["⟨OrExpr⟩"]"⟨SeparatorExpr⟩
                                 ::=
                                          \langle \text{TupleExpr} \rangle \mid \langle \text{SeparatorExpr} \rangle \langle \text{SeparatorOp} \rangle \langle \text{TupleExpr} \rangle
   (SeparatorExpr)
                                 ::=
      (SeparatorOp)
                                 ::=
          (TupleExpr)
                                         (OrExpr) | "("(CommaExpr)")"
                                 ::=
                                         \langle \text{TupleExpr} \rangle \mid \langle \text{CommaExpr} \rangle \langle \text{CommaOp} \rangle \langle \text{TupleExpr} \rangle
      (CommaExpr)
                                 ::=
                                         ","
         (CommaOp)
                                 ::=
               \langle OrExpr \rangle
                                 ::= \langle AndExpr \rangle \mid \langle OrExpr \rangle \langle OrOp \rangle \langle AndExpr \rangle
                 \langle OrOp \rangle
                                 ::=
            \langle AndExpr \rangle
                                 ::=
                                        \langle \text{EqualExpr} \rangle \mid \langle \text{AndExpr} \rangle \langle \text{AndOp} \rangle \langle \text{EqualExpr} \rangle
                                         "&"
               \langle AndOp \rangle
                                 ::=
         (EqualExpr)
                                 ::=
                                         \langle \text{RelationExpr} \rangle \mid \langle \text{EqualExpr} \rangle \langle \text{EqualOp} \rangle \langle \text{RelationExpr} \rangle
                                         "=" | "<>"
            (EqualOp)
                                 ::=
     (RelationExpr)
                                 ::= \langle AddExpr \rangle \mid \langle RelationExpr \rangle \langle RelationOp \rangle \langle AddExpr \rangle
                                         "<" | "<=" | ">=" | ">"
        (RelationOp)
                                 ::=
            \langle AddExpr \rangle
                                         \langle MultiplicityExpr \rangle \mid \langle AddExpr \rangle \langle AddOp \rangle \langle MultiplicityExpr \rangle
                                 ::=
                                          "+" | "-"
               \langle AddOp \rangle
                                 ::=
                                         \langle \text{UnaryExpr} \rangle \mid \langle \text{MultiplicityExpr} \rangle \langle \text{MultiplicityOp} \rangle \langle \text{UnaryExpr} \rangle
(MultiplicityExpr)
                                 ::=
                                         "*" | "/" | "%" | "^"
   ⟨MultiplicityOp⟩
                                 ::=
         (UnaryExpr)
                                         \langle PostfixExpr \rangle \mid \langle UnaryOp \rangle \langle PostfixExpr \rangle
                                 ::=
                                         "+" | "-" | "@" | "!"
            (UnaryOp)
                                 ::=
        (PostfixExpr)
                                 ::= \langle AtomExpr \rangle \mid \langle PostfixExpr \rangle"["\langle AtomExpr \rangle"]"
                                          \langle PostfixExpr \rangle ":" \langle AtomExpr \rangle
                                   ::= \langle Constant \rangle \mid \langle Variable \rangle \mid \langle Function \rangle \mid "("\langle ColorExpr \rangle")"
          \langle AtomExpr \rangle
            \langle Constant \rangle
                                 ::= \langle Integer \rangle \mid \langle String \rangle
             (Variable)
                                 ::= \langle Identifier \rangle
                                        ⟨Identifier⟩ "("⟨ArgumentList⟩")" "{"⟨FunctionBody⟩"}"
            (Function)
                                 ::=
                                         \langle OrExpr \rangle \mid \langle ArgumentList \rangle \langle CommaOp \rangle \langle OrExpr \rangle
    (ArgumentList)
                                 ::=
    ⟨FunctionBody⟩
                                         (MultiSetExpr)
                                 ::=
                                 ::= \langle \text{Digit} \rangle \mid \langle \text{Integer} \rangle \langle \text{Digit} \rangle
               (Integer)
                                 ::= \langle LetterOrDigit \rangle \langle String \rangle \langle LetterOrDigit \rangle
                 (String)
            (Identifier)
                                 ::= \langle Letter \rangle \mid \langle Identifier \rangle \langle LetterOrDigit \rangle
```

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```
\begin{split} \langle \text{LetterOrDigit} \rangle & ::= & \langle \text{Letter} \rangle \mid \langle \text{Digit} \rangle \\ \langle \text{Digit} \rangle & ::= & \text{``0-9''} \\ \langle \text{Letter} \rangle & ::= & \text{``a-zA-Z_-''} \end{split}
```

B Colored Abstract Net Definition Language (CANDL)

B.1 BNF

```
\langle \text{NetType} \rangle "[" \langle \text{Identifier} \rangle "]" "{" \langle \text{Net} \rangle "}"
              \langle Start \rangle ::=
                                 "colpn" | "colxpn" | "colcpn" | "colhpn"
         (NetType)
                          ::=
                                  "colspn" | "colgspn" | "colxspn"
                \langle \text{Net} \rangle ::= \langle \text{Constants} \rangle
                                 (SimpleColorsets)
                                  (CompoundColorsets)
                                 (Variables)
                                  (Functions)
                                  (Places)
                                  (Observers)
                                  (Transitions)
        (Constants)
                                 "constants:" (ConstList)
                                 \perp \mid \langle ConstDef \rangle \mid \langle ConstDef \rangle \langle ConstList \rangle
        (ConstList)
                          ::=
        \langle ConstDef \rangle
                          ::= \langle ConstType \rangle \langle Identifier \rangle \langle ConstInit \rangle ";"
                                "int" | "double" | "bool" | "string"
      \langle ConstType \rangle
                          ::=
                                 \perp | "=" \langle ConstExpr \rangle
        \langle ConstInit \rangle
                          ::=
(SimpleColorsets)
                          ::=
                                  "simplecolorsets:" (SimpleCsList)
   \langle SimpleCsList \rangle
                                 \langle SimpleCsDef \rangle \mid \langle SimpleCsDef \rangle \langle SimpleCsList \rangle
                          ::=
                                 ⟨SimpleCsType⟩⟨Identifier⟩⟨SimpleCsInit⟩";"
    \langle SimpleCsDef \rangle
                          ::=
  (SimpleCsType)
                          ::=
                                 "dot" | "int" | "bool" | "string" | "enum" | "index"
                                 ⟨SimpleColorset⟩
                            (SimpleCsInit)
                                 (DotCsInit) | (IntCsInit) | (BoolCsInit) | (StringCsInit)
                          ::=
                            ⟨EnumCsInit⟩ | ⟨IndexCsInit⟩ | ⟨Predicate⟩
                                 "dot"
        (DotCsInit)
                          ::=
         (IntCsInit)
                                 \langle IntCsDef \rangle \mid \langle IntCsDef \rangle \langle IntCsDelim \rangle \langle IntCsInit \rangle
                          ::=
         \langle IntCsDef \rangle
                                 \langle Integer \rangle \mid \langle Constant \rangle
                          ::=
                                 "," | "-"
      (IntCsDelim)
                          ::=
                                 "true" "," "false"
      (BoolCsInit)
                          ::=
     (StringCsInit)
                                 (String) | (String)"," (StringCsInit)
                          ::=
     (EnumCsInit)
                                 ⟨Identifier⟩ | ⟨Identifier⟩","⟨EnumCsInit⟩
                          ::=
```

```
⟨Identifier⟩"["⟨Integer⟩","⟨Integer⟩"]"
          \langle IndexCsInit \rangle ::=
                                    "compoundcolorsets:" (CompoundCsList)
(CompoundColorsets)
                             ::=
   (CompoundCsList)
                                    \perp \mid \langle CompoundCsDef \rangle \mid \langle CompoundCsDef \rangle \langle CompoundCsList \rangle
                             ::=
                                    ⟨CompoundCsType⟩⟨Identifier⟩⟨CompoundCsInit⟩";"
   \langle CompoundCsDef \rangle
                             ::=
 (CompoundCsType)
                                    "product" | "union" | (CompoundColorset)
                             ::=
   (CompoundCsInit)
                                    (CsComponents) | (Predicate)
                             ::=
                                    \langle Colorset \rangle \mid \langle Colorset \rangle"," \langle CsComponents \rangle
      (CsComponents)
                             ::=
                                    "variables:" (VariableList)
             (Variables)
                             ::=
          (VariableList)
                                    \perp \mid \langle VariableDef \rangle \mid \langle VariableDef \rangle \langle VariableList \rangle
                                    \langle Colorset \rangle \langle Identifier \rangle";"
          ⟨VariableDef⟩
                             ::=
            (Functions)
                                    "functions:" (FunctionList)
                             ::=
                                    \perp \mid \langle FunctionDef \rangle \mid \langle FunctionDef \rangle \langle FunctionsList \rangle
         (FunctionList)
                             ::=
         ⟨FunctionDef⟩
                             ::=
                                   ⟨FunctionType⟩⟨Identifier⟩ "("⟨FunctionParams⟩")" ⟨FunctionBody⟩ ";"
       ⟨FunctionType⟩
                                    \langle SimpleCsType \rangle \mid \langle CompoundCsType \rangle
                             ::=
     (FunctionParams)
                                    ⊥ | ⟨FunctionParam⟩ | ⟨FunctionParam⟩","⟨FunctionParams⟩
                             ::=
      (FunctionParam)
                                    \langle FunctionType \rangle \langle Identifier \rangle
                             ::=
                                    "{" (ColorExpr)"}"
       (FunctionBody)
                             ::=
                                    "places:" (PlaceList)
                 (Places)
                             ::=
             \langle PlaceList \rangle
                                   \langle PlaceDef \rangle \mid \langle PlaceDef \rangle \langle PlaceList \rangle
                             ::=
                                  ⟨PlaceType⟩⟨Colorset⟩⟨Identifier⟩⟨PlaceInit⟩";"
             (PlaceDef)
                             ::=
                                   \perp | "discrete:" | "continuous:"
           \langle PlaceType \rangle
                             ::=
                                    "=" "{" (Assignments) "}"
             (PlaceInit)
                             ::=
                                   ⟨Assignment⟩ | ⟨Assignment⟩","⟨Assignments⟩
         (Assignments)
                             ::=
                                    "{"\langle ConstExpr\rangle"" \langle ColorExpr\rangle"}"
          (Assignment)
                             ::=
                                    "observers:" (ObserverList)
            (Observers)
                             ::=
         (ObserverList)
                                   \perp \mid \langle ObserverDef \rangle \mid \langle ObserverDef \rangle \langle ObserverList \rangle
                             ::=
                                   ⟨Identifier⟩"="⟨ObserverInit⟩";"
         ⟨ObserverDef⟩
                             ::=
                                    "{" (Predicate)"," (ObserverFunc)"}"
         ⟨ObserverInit⟩
                             ::=
                                    ⟨ObserverOp⟩ "("⟨CsComponents⟩")"
        (ObserverFunc)
                             ::=
                                    "+"
          (ObserverOp)
                             ::=
```

```
(Transitions)
                                 "transitions:" (TransList)
                          ::=
                          ::= \langle TransDef \rangle \mid \langle TransDef \rangle \langle TransList \rangle
          \langle TransList \rangle
          \langle TransDef \rangle
                          ::= \langle TransType \rangle \langle Identifier \rangle \langle Guard \rangle
                                 ":" (ConditionList)
                                 ":" (UpdateList)
                                 ⟨RateFunctionList⟩";"
                                 "stochastic:" | "immediate:" |
                                                                          "deterministic:"
        \langle TransType \rangle
                          ::=
                                 "scheduled:" | "continuous:"
                                \perp | "["\langlePredicate\rangle"]"
             (Guard)
                          ::=
                          := \bot \mid \langle ConditionDef \rangle \mid \langle ConditionDef \rangle "&" \langle ConditionList \rangle
    (ConditionList)
    \langle ConditionDef \rangle
                          ::= "[""{"\ColorExpr\"}""<="\Place\"<""{"\ColorExpr\"}""]"
                                 "[""{"\ColorExpr\"}""<="\Place\"]"
                                 "[""{"\ColorExpr\"}""="\Place\"]"
                                 "[" "{" (ColorExpr) "}" ">" (Place) "]"
                                 "["\langle Place \rangle"<" "{"\langle ColorExpr \rangle"}""]"
                                 "["\langle \mathrm{Place}\rangle"=""\{"\langle \mathrm{ColorExpr}\rangle"\}""]"
                                 "["\langle Place \rangle">=""{"\langle ColorExpr \rangle"}""
                                 "[" (Place) "]"
                                 \perp \mid \langle UpdateDef \rangle \mid \langle UpdateDef \rangle "&" \langle UpdateList \rangle
       (UpdateList)
                          ::=
        ⟨UpdateDef⟩
                          ::=
                                 "["\langle Place\rangle \langle UpdateOp\"\{"\langle ColorExpr\rangle "\}" "]"
                                 "+" | "-" | "="
        \langle UpdateOp \rangle
                          ::=
⟨RateFunctionList⟩
                                 \perp | ":" "{" (RateFunctions) "}"
                          ::=
                                 ⟨RateFunction⟩ | ⟨RateFunction⟩","⟨RateFunctions⟩
   (RateFunctions)
                          ::=
                                 "{" (Predicate) ":" (RateFunctionDef) "}"
    ⟨RateFunction⟩
                          ::=
                                 \langle ColorPattern \rangle \mid \langle Pattern \rangle \mid \langle ArithmeticFunction \rangle
(RateFunctionDef)
                          ::=
                                "[" (ColorExpr)"]" | "#""(" (Identifier)")"
     ⟨ColorPattern⟩
                          ::=
            (Pattern)
                          ::=
                                 ⟨Func1Param⟩ "("⟨ArithmeticFunction⟩")"
                                 ⟨Func2Param⟩ "("⟨ArithmeticFunction⟩","⟨ArithmeticFunction⟩")"
                                 ⟨Func2Param⟩ "("⟨ArithmeticFunction⟩","⟨ArithmeticFunction⟩")"
                                 (ArithmeticFunction)"," (ArithmeticFunction)"," (ArithmeticFunction)
     ⟨Func1Param⟩
                                 "MassAction"
                          ::=
     ⟨Func2Param⟩
                                 "LevelInterpretation"
                          ::=
                                 "MichaelisMenten"
                                 "Inhibit"
```

```
"Read"
                                     "Equal"
                                     \langle \text{Term} \rangle \mid \langle \text{Term} \rangle \langle \text{AddOp} \rangle \langle \text{ArithmeticFunction} \rangle
(ArithmeticFunction)
                              ::=
                                     "+" | "-"
                \langle AddOp \rangle
                              ::=
                   \langle \text{Term} \rangle
                                     \langle Factor \rangle \mid \langle Factor \rangle \langle MultOp \rangle \langle Term \rangle
                              ::=
                                     "*" | "/" | "^"
               \langle MultOp \rangle
                              ::=
                 \langle Factor \rangle
                                    \langle Atom \rangle | "-" \langle Factor \rangle
                              ::=
                  \langle Atom \rangle
                              ::=
                                     \langle Integer \rangle
                                     (Float)
                                     (Constant)
                                     (Place)
                                     "("(ArithmeticFunction)")"
                                     ⟨UnOp⟩ "("⟨ArithmeticFunction⟩")"
                                     ⟨BinOp⟩ "("⟨ArithmeticFunction⟩ "," ⟨ArithmeticFunction⟩ ")"
                 \langle UnOp \rangle ::=
                                    "abs" | "exp" | "sqr" | "sqrt" | "floor"
                                     "ceil" | "sin" | "asin" | "cos" | "acos"
                                     "tan" | "atan" | "log10" | "log"
                                     "pow" | "min" | "max"
                 \langle BinOp \rangle
                              ::=
                                     (Identifier) //name of a defined constant
              (Constant)
                              ::=
      (SimpleColorset)
                                     (Identifier) //name of a defined simple color set
                              ::=
⟨CompoundColorset⟩
                                     (Identifier) //name of a defined compound color set
                              ::=
               \langle Colorset \rangle
                                     ⟨SimpleColorset⟩ | ⟨CompoundColorset⟩
                              ::=
               \langle Variable \rangle
                                     (Identifier) //name of a defined variable
                              ::=
                                     (Identifier) //name of a defined place
                   ⟨Place⟩
                              ::=
```

B.2 Example

For illustration we give the introductory dinning philosophers example, see Figure 1, in CANDL notation which has been generated by Snoopy's export feature.

```
colpn [phil]
constants:
    int N = 5;
simplecolorsets:
    dot Dot = dot;
    int Phils = 1-N;
    int Forks = 1-N;
compound color sets:
variables:
    Phils x;
functions:
    Forks left (Phils x)
        \{x\};
    Forks right (Phils x)
        \{ (x\%N)+1 \} ;
places:
    Phils thinking = \{ \{1`all()\} \};
    Phils waiting = \{(0) \text{ all } ()\};
    Phils eating = { {0`all()} };
    Phils releasing = \{ \{0`all()\} \};
    Forks forks = \{ \{1`all()\} \};
observers:
```