Formalising Knowledge-intensive Nuclear Fuel Process Models Using Pattern Theory

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Abstract. In this paper we present a formalisation for a previously elaborated model-based approach for representing knowledge intensive processes in the domain of nuclear knowledge management. It is shown how a Nuclear Fuel Cycle Process Model can be formalised and represented visually by using the concepts of pattern theory. The formalisation is then applied to the configuration of acquisition paths and the analysis of the evolution of the models. Thereby a basis for the application of formal queries and advanced visual analyses can be established.

Keywords: Nuclear knowledge management, Modelling, Pattern Theory, Formalisation

1 Introduction

In [1] a framework for the knowledge-based process modelling for nuclear inspections was introduced. The goal of this approach was to provide a method for externalizing the implicit knowledge of nuclear workers and nuclear inspectors in order to facilitate nuclear knowledge management. Thereby, it is aimed for the preservation of the knowledge about nuclear processes as well as for the increase in efficiency and effectiveness of inspection management.

In the following we will regard the application domain of nuclear verification and in particular the Nuclear Fuel Cycle Process Model (NFCM) - see figure 1 for an example. The intention of this paper is to process these models in order to check for their consistency or automate the generation of safeguards objectives inferred from the model. This is one example of processing that can be achieved based on rules such as "if x nuclear activity takes place then activity y can follow". The task of automatically generating objectives from existing models does not in itself represent a complex job, however the formalisation of rules is demanding and requires domain knowledge. This example of formalisation is meant to serve as basis for applying more complex algorithms, e.g. stochastic approaches. For this purpose it is necessary to formalise the elements and relationships of the NFCM model type. To do so we will revert to pattern theory [5]. In section 2 we will briefly outline the fundamentals of pattern theory and apply them for illustrating the formalisation of the NFCM model type in section 3. Based on the formalisation we will then discuss two possible application scenarios in section 4. Section 5 discusses related work and section 6 concludes the paper with an outlook to future steps.

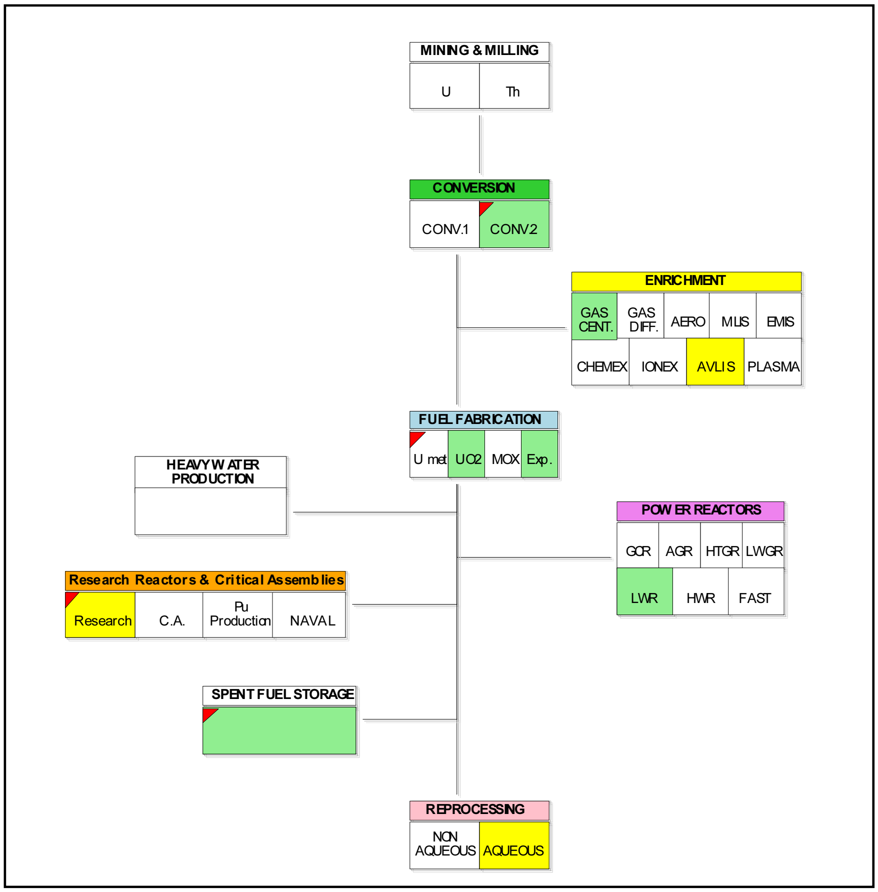

Fig. 1. Nuclear Fuel Cycle Model represented with a modelling language implemented in ADOxx and based on the notation for describing States Physical Model [11]

2 Fundamentals of Pattern Theory

Pattern theory stems from the field of applied mathematics and offers a graphical and mathematical formalism, which may bring us a step forward in closing the gap between a machine processable languages and easy to use domain/specific modelling languages. Through the use of so called generators that represent atomic elements, in our case diagrammatic modelling language primitives, principles of regularity can be formalised. Generators can be positive pixel values in an image, states in a Markov Chain, geometric objects such as vectors and surface elements, or rewriting rules in language theory. Rules of transformation are the generators (formal grammars). Transformations allowed by the rules are constrained by using the bonds between the generating rules [5].

2.1 Elements of Pattern Theory

Pattern theory was first introduced by Grenander in [3]. In the following a canonical introduction will be provided presenting the algebraic constructs that can describe the structure of the *generators* as well as their admissible combination into configurations. Properties of a generator are defined with in-bonds, out-bonds and attributes. To a given generator corresponds the arity $\omega(g)$. The arity tells us the maximum number of connections to the generator and represents the sum of in-arity and the out-arity. Generators can appear more than once in a configuration. To keep them separate, identifying marks as parts of attributes are used. The direction of the bonds may be in-wards or out-wards. Properties of the generator can therefore be described as follows:

$$\begin{aligned}\omega_{in}(g) =& 2, \omega_{out}(g) = 2\\ \omega(g) =& \omega_{in}(g) + \omega_{out}(g) = 4\\ B_v =& \{\beta_0, \beta_1, \beta_2, \beta_3\}\\ B_s =& \{0, 1, 2, 3\}\end{aligned} \tag{1}$$

To each bond corresponds a bond value β from bond value space B. $B(g)$ shall be denoted by the combination of bond structure B_s and bond values B_v. For any $g \in G$, the notation $B_s(g)$ will mean the set $\{b_j; j = 1, 2, \ldots \omega(g)\}$ and $B_v(g)$ will mean the set $\{b_j; j = 1, 2, \ldots \omega(g)\}$ where b_j means bond coordinate. Configurations that satisfy a certain given constraint are known as regular. A generator with its bonds represents a structure that can be combined with other generators to form regular or partially regular configurations. A good analogy is the one that resembles the behavior of molecules which can be made of more atoms which are held together with their chemical bonds [4]. For each two generators the pair of bond values is either regular (true) or irregular (false). With this the local regularity is established that can be formalised with the structure formula in equation 2.

$$\bigwedge_{\langle k,k' \rangle} \rho\left[\beta_j(g_i), \beta_{j'}(g_{i'})\right] = TRUE \tag{2}$$

The algebraic component will express the rules of regularity whereas the optionally probabilistic one the variability. Pattern theory attempts to combine these two opposing themes [4]. The aim of the next section will be to express the rules of the nuclear fuel cycle modelling language, i.e. the process structures.

3 Formalising the Nuclear Fuel Cycle Model (NFCM)

We will use configurations or sub-configurations to represent existing or potential weapons material acquisition paths modelled with NFCM. Local regularity of connected generators (modelling primitives) will be formalised in order for us to be able to check the consistency of modeled acquisition paths or infer inspection objectives. Both serve as examples of intended processing however many other analysis tasks would also be possible.

To represent a nuclear fuel cycle process each of the major nuclear activities can be represented with a generator. This generator is then connectable to other generators based on their structure (bonds) and bond value – which in our case represents the nuclear material going in and out of these activities. The relation between different generators is based on the matching in and out-bond values. Each generator contains a structure and based on regularity rules, possible combinations of nuclear activities in the fuel cycle can be represented as a regular configuration. These rules of regularity for this example application were extracted from the *Physical Model (PM)*. PM is a document that defines each of the activities in the nuclear fuel cycle and the associated indicators [6–10].

When dealing with a model such as NFCM that represents the nuclear fuel cycle and can therefore be used to model an acquisition path, there are two levels of granularity that can be considered for the formalisation. The first is to take each activity of the nuclear fuel cycle as a generator and the second is to use the specific nuclear activity technologies as the atomic elements of this modelling language represented with generators. Technologies and materials used are represented with the modelling elements of the NFCM, where an activity is represented as a large square. The technologies associated with the activity are shown as sub entities and are represented with smaller sized squares. An example of such a model and its elements was already shown in figure 1.

For the purpose of applying algorithms such as analyzing potential acquisition paths, the second granularity level was determined to be the appropriate one. The value assigned to the bond relating any two generators is based on the material that is produced by one nuclear activity and fed into the other. Based on the experiment made by applying the lower level of granularity – i.e. generators as activities – difficulties were encountered to formalise the NFCM models. These mainly stem from one or more of the following issues:

1. Technologies that represent an activity can mean semantically different things: In some cases they represent distinct technologies and in others they are generalised. For example, the conversion activity is often ambiguous and it is impossible to express semantic correctness as to which conversion phase the MLIS (Molecular laser isotope separation) enrichment is related to.
2. In regard to the direction of the link between two activities, the aspect of bi-directional relation cannot be formalised with the approach shown. For

instance, in the case of the activities, conversion and enrichment material going to enrichment returns for conversion into fuel elements or similar. It is not possible to distinguish based on the bond value the direction modelled or in other cases the two directional relation.

To address these issues we will apply a higher level of formalism where modelling activities are actually classes of generators, whereas generators represent technologies each activity is characterised with. In other words, the technology associated to the nuclear activity is the atom of the modelling language. Technologies in the example model in figure 1 are shown as smaller boxes within each nuclear activity modelling element. Generators as elements of the generator class are identified with the name of the technology and are sequentially indexed from 0 to 30 (i.e. g_3, g_{23}). As shown below, all generators g_i are presented including the generator classes G^i they belong to. There are in total 31 generators. Classes of generators represent nuclear fuel cycle phases shown to contain generators representing the associated technology. Each class corresponds to a modelling element from the NFCM, whereas the generators are the specific technology activities:

$$G^0 = \{\text{Mining and Milling}\} \tag{3}$$

$$G^1 = \{\text{Conv1}, \text{Conv2}\} \tag{4}$$

$$G^2 = \{\text{Gas cent}, \text{Gas diff}, \text{AERO}, \text{MLIS}, \text{EMIS}, \text{CHEMEX}, \text{IONEX}, \text{AVLIS}, \\ \text{PLASMA}\} \tag{5}$$

$$G^3 = \{\text{Umet}, \text{UO2}, \text{MOX}, \text{EXP}\} \tag{6}$$

$$G^4 = \{\text{GCR}, \text{AGR}, \text{HTGR}, \text{LWGR}, \text{LWR}, \text{HWR}, \text{FAST}\} \tag{7}$$

$$G^5 = \{\text{Research Reactor}, \text{C.A.}, \text{Pu Production}, \text{NAVAL}\} \tag{8}$$

$$G^6 = \{\text{Spent Fuel Storage}\} \tag{9}$$

$$G^7 = \{\text{Non-aqueous}, \text{aqueous}\} \tag{10}$$

$$G^8 = \{\text{Heavy Water}\} \tag{11}$$

The nuclear fuel cycle generator space G consists of the union of all generator spaces $G = \bigcup_{\alpha \in A}, G^{\alpha}, G = \bigcup_{i=0}^{8} G^{i}$. Where α is called generator index. Generators can also have attributes, which together with its structure (i.e. bonds), represent the properties of a generator [3]. Being able to also formalise attributes of generators has an important impact in addressing problems such as the second issue discovered above in the specific case of formalizing NFCM. All generators have common attributes in NFCM, therefore $a \forall g \in G$ is the scale of the known or expected development. This can be "production" or "research", represented with the notation colours "yellow" and "green" on the model level. An example of an attribute formalisation could thus be: $a(g_i) =$ "Research".

The relation between the generators will be represented with the binary function ρ where the bonds that fit together are formalised. Matching bond values that are represented with β is the basis for defining the relations between the generators. Nuclear material going in and out of a nuclear activity is represented with β values of generators connected through bond coordinates: (i, j); j is called bond coordinates for g_i. Next, a selected set of generators of the nuclear fuel cycle phases for the NFCM modelling language will be formalised with the level of detail proposed. This is meant to demonstrate the application of pattern theory and offer a mathematical framework based on this theory so that the models can be processed through algorithms and mechanisms.

In the following we will illustrate the details of the formalisation by using the examples of g_1 - Conversion 1 (pre-Conversion), g_2 - Conversion 2 (post-Conversion), and g_3 - Gas centrifuges.

3.1 g_1 – Conversion 1 (pre-Conversion)

Conversion 1, which is also called pre-conversion, includes all activities related to chemical transformations of natural nuclear material in order to provide feed material for isotope separation or reactor fuel fabrication [6]. The generator g_1 is characterized in the following, whereby bond values assigned based on the nuclear material as shown in equation 16. Each of the nuclear materials and the matching technologies are represented by bond values and the structure of generators.

$$B_s = \{0, 1, 2, 3, 4, 5, 6, 7, 8, 9\} \tag{12}$$

$$B_v = \{\beta_0, \beta_1, \beta_2, \beta_3, \beta_4, \beta_5, \beta_6, \beta_7, \beta_8, \beta_9\} \tag{13}$$

$$\omega_{in}(g_1) = 2 \tag{14}$$

$$\omega_{out}(g_1) = 8 \tag{15}$$

$$\beta_0 = UOC, \beta_1 = ThConc, \beta_2 = UF_6, \beta_3 = UCl_4, \beta_4 = ThO_2, \beta_5 = Thmet,$$
$$\beta_6 = UF_4, \beta_7 = UO_3, \beta_8 = Umet, \beta_9 = UO_4 \tag{16}$$

3.2 g_2 – Conversion 2 (post-Conversion)

Next, the bond relation between a conversion 1 generator and the enrichment activities is formalised. Conversion 2, also known as "re-conversion" or "post-conversion", includes all chemical transformations subsequent to enrichment or reprocessing for the purpose of manufacturing reactor fuel elements [7]. Input and output nuclear material is represented with in-bond and out-bond values that are shown in equation 21.

$$B_s = \{0, 1, 2, 3, 4, 5, 6, 7, 8\} \tag{17}$$

$$B_v = \{\beta_0, \beta_1, \beta_2, \beta_3, \beta_4, \beta_5, \beta_6, \beta_7, \beta_8\} \tag{18}$$

$$\omega_{in}(g_2) = 5 \tag{19}$$

$$\omega_{out}(g_2) = 4 \tag{20}$$

$$\beta_0 = Pumet, \beta_1 = PuNO_3, \beta_2 = UF_6e, \beta_3 = UCl_4e, \beta_4 = Umet_{in}$$
$$\beta_5 = UO_2, \beta_6 = PuO_2, \beta_7 = Pumet, \beta_8 = Umet_{out} \quad (21)$$

β_4 and β_8 both show bond values with Umet (Enrichment of Uranium Metal) nuclear material. This example shows them as two separate β indicating that Umet can be both input and output. Figure 2 shows the graphical representation of this generator.

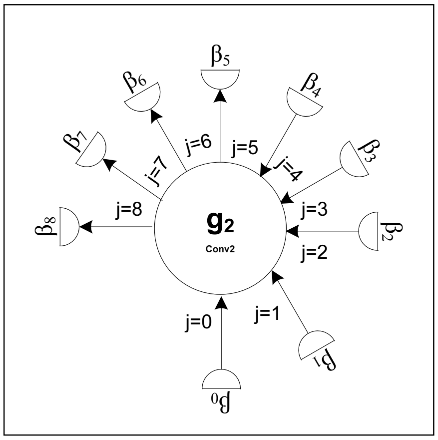

Fig. 2. Generator representing Conversion 2 activity

3.3 g_3 – Gas centrifuges

Gas centrifuges use the principle of centrifugal fields for the separation of gases of different molecular weight. UF_6 gas is fed into mounted rotating cylinders [10]. Gas centrifuges are represented with the generator g_3. Its two bonds are characterised by two β values shown in equation 25. β_0 represents the bond to the conversion 1 generator where UF_6 is used as feed material. Moreover, β_1 represents the product of the gas centrifuge enrichment which is subsequently processed in conversion 2. Use of gas centrifuges is represented with the generator g_3. Use of gas centrifuges requires UF_6 feed material which is generated during conversion 1. The issue documented above as 1 can be resolved at this level of formalism since both directions of the material and therefore the bond between the two generators can be explicitly represented. This issue actually is non existent here since conversion 1 and conversion 2 represent two different generators.

$$B_s = \{0, 1\} \tag{22}$$
$$B_v = \{\beta_0, \beta_1\} \tag{23}$$
$$\omega_{in}(g_3) = 1, \omega_{out}(g_3) = 1 \tag{24}$$
$$\beta_0 = UF_6, \beta_1 = UF_6(enriched) \tag{25}$$

The expression in equation 26 restricts the configuration of generators by local constraints. Therefore, a pair of bond values (β', β'') is regular if $\rho(\beta', \beta'') = TRUE$ or irregular if $\rho(\beta', \beta'') = FALSE$. The product space $B \times B$ of the bond value space B crossed with itself given a truth valued function represented with ρ, where for the bond pair g_3 and g_1 a local constraint is shown in equation 27.

$$\rho : B \times B \rightarrow \{TRUE, FALSE\} \tag{26}$$
$$\rho\,[\beta_j(g_1), \beta_{j'}(g_3)] = TRUE \tag{27}$$
$$\begin{aligned} \rho\,[\beta_2(conv.1), \beta_0(gasscent)] &= TRUE \\ \rho\,[\beta_1(gasscent), \beta_2(conv.2)] &= TRUE \end{aligned} \tag{28}$$

The expression in equation 28 shows the bond between the conversion activity where UF_6 is sent for enrichment and the same is returned for post-conversion or reconversion represented with the generator g_2. The directionality is not an issues since for both feed materials and enrichment UF_6 are formalised with separate bonds.

4 Application of the Formalism: Acquisition Path Configuration and Analysis of Evolution

The generators creating the generator space G can be glued together and the bonds determine which combination can hold. This resembles the behaviour of atoms – which here would be generators – that are connected into molecules or in this case configurations. The next step is to form a configuration of generators that can bond. In the example here with the nuclear fuel cycle model, the generators representing nuclear activities are the atoms that need to be combined in a configuration. Thus, acquisition paths can be represented as a combination of bonding nuclear activities into potential routes of acquiring a nuclear weapon by using the generators formalised in the previous section.

As shown in figure 3, internal bonds make up the configuration of the physical model for the fictitious state *Ruritania*. The panel on the right shows the generators used to represent the activities shown with the NFCM model. The state enriches uranium (U) and fabricates UO_2 fuel which is used for an LWR (Light Water Reactor). Furthermore, the state has research activities for U metal enrichment using AVLIS (Atomic Vapour Laser Isotope Separation). The enriched U metal is used for fabricating fuel elements that are irradiated in a research

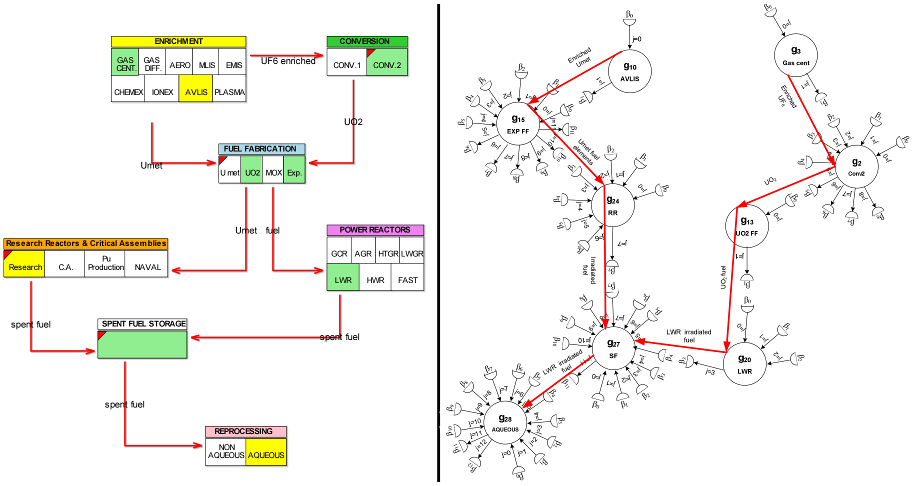

Fig. 3. Representation of the NFCM model shown above with the pattern theory formalism on the right

reactor. In the presence of a Spent Fuel Storage at a research scale some of the irradiated fuel is reprocessed using the aqueous method.

Bonds denoted by $b_1, b_2, \ldots b_\omega$ represent generator coordinates which build the configuration architecture of the model. By σ a connector is denoted that represents a graph of sites that are connected with their bonds. An example configuration for Ruritania can be expressed as in equation 29. The configuration codifying the instance of the NFCM on the left panel consists of nine generators differently connected to each other through their internal bonds. Generators g_{20} and g_{24} both bond to the generator g_{27}. The same can also be diagrammatically expressed by having two identical copies of the generator g_{27} which can then be kept separately by using identifying marks as parts of the attributes. The same is true should there be a need to use more than one copy of a generator. It should however be clear from the context that this is intended [3].

$$\begin{aligned} c =& \sigma(g_1, g_2, \ldots, g_n) \\ c' =& \sigma(g_2, g_3, g_10, , g_13, g_20, g_15, g_24, g_27, g_28) \end{aligned} \tag{29}$$

The configuration is based on the values function ρ which defines the pair of bond values that can be related. It shows all two generators that can bond, making up a configuration consisting of two bonds locally regular for any couple of bonds $(i, j) - (i', j')$. For a configuration to be regular in addition to local regularity it needs to be globally regular. For this the connection type is used. Connection type can be linear for linear chain graphs or tree for tree shaped graphs. This represents the last piece to also define regularity. A configuration is defined to be globally regular if $\sigma \in \Sigma$; where Σ represents the physical arrangement of generators, which in the case of a modelling language is linear. A configuration is called regular if it is both locally and globally regular therefore for a configuration space $C(R)$ where $R = \langle G, S, \rho, \Sigma \rangle$ is referred to as regularity; where S represents similarity group and G represents the generator space.

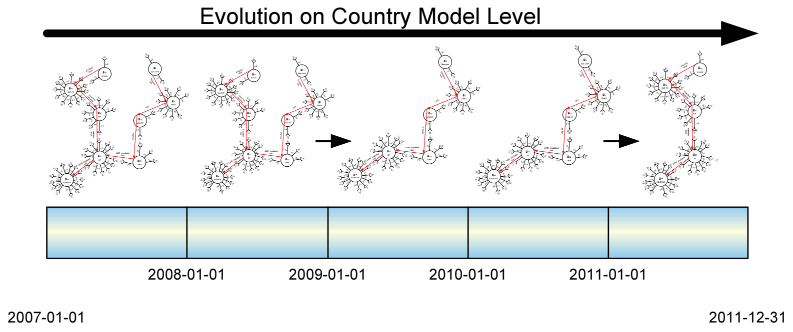

Fig. 4. Application of the Formalisms for Analysing the Evolution over Time

Further to the codification of the NFCM models where pattern theory can be used as an intermediate language for transformation or analysis of inspection process structures, NFCM model-level evolution can be analysed over a timeline for a country or group of countries (see figure 4). In addition, process structures can be seen as configurations representing NFCM models created by experts which are comparable to other models. Such acquisition path configurations represent information structures that need to be stored and retrieved. This introduces the need to find storage mechanisms for configurations created which can then be queried to answer expert questions. Similar to the archetypes introduced with the electronic health records, configurations can represent information structures that can then be queried with a predefined query language similar to SQL.

5 Related Work

There are various formalization approaches that could be also used to achieve the any of the evaluated use cases. Their application depends on the problem at hand. Pattern theory contains a graphical formalism similar to using graphs with the important distinction that generators compared to nodes representing elements of a model would be typed (Activity, Parallelity, etc.) and can carry other attributes that can add semantics to the formal representation. Using graph theory in this context is regarded as semantically inferior to pattern theory. A property of a generator is its structure admitting for the definition of so-called bonds, which define connections to and from a generator. In a model, a generator can be a primitive that represents a pixel of the modelled elements (image) or conceptually the element itself. In our case, generators represent modelling elements which in the example chosen are the activities that can lead to the acquisition of a weapons grade nuclear material.

Pattern theory as introduced originally had a purpose of identifying patterns rather than what is commonly known as pattern recognition. Taking this as a starting position it is important to note that in the context of representing models created by domain experts this formalism serves the transformation of models into patterns that can be analysed by various algorithms and mechanisms. Formalised in a precise language that will allow us to transform user-friendly models to mathematically concise elements.

It can be observed that generators of the pattern theory are also nodes of a graph. However, they also contain a structure as a property. In other words, the generators are the grammars. They represent grammars placed on a graph. In this way we can represent the logical sentence structure but can also formalise all possible connections to neighbouring generators. This formalism is not apparent with graph grammar where rules or operations would have to be explicitly represented in a non-graphical way to support the graph. Furthermore, another important property of a generator is that it can carry attributes. This is very useful for typing generators according to the visual elements to which they map to. The graphical formalism of pattern theory allows for an easy transformation from concrete syntax to abstract syntax due to the visual similarity of the modelling elements and the generators. Graphs offer also a level of visualization, however they lack the connection rules available for generators and their bonds.

When comparing pattern theory to Chomsky's formal grammar, generators of pattern theory are the rules of transformation. They are the formal grammar. Transformations allowed by the rules are constrained by the consistency placed with bonds [5]. Generators are grammatical rules whereas the bond-values are subsets of the terminals and non-terminals.

Petri nets are another abstract formal model that can be used to represent visual languages. Some research was performed in this area where Petri nets are linked to graph grammars to formalise animations of a visual modelling environment. The use of grammars as an intermediary formalism to represent visual elements indicates that Petri nets may not be best at representing visual models [2].

6 Conclusion

As mentioned at the beginning pattern theory is more about identifying patterns or generating patterns that represent realistic structures. These in our case are constrained by the modelling language. What is unique about the formalised acquisition paths is that the generated patterns resemble also the visual model created by a domain expert. They represent signatures that are regular and can be treated also for variability. Configurations represent also probabilistic structures, which allow for expressing variation.

Pattern theory represents a formalism that is graphically very descriptive for representing process structures while allowing for definition of regularity in addition to variability. Between purely graph representations and graph grammars which are rule intensive and formalisms such as Petri nets that are unique in studying behavioural properties, pattern theory finds its place as a mixture that strikes the optimal balance of both properties. It serves as an intermediary language between domain specific languages and formal languages.

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