WATSON-CRICK PETRI NET AND PLACE-LABELLED PETRI NET CONTROLLED GRAMMAR USING FORMAL LANGUAGE THEORY

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لِ لِللَّهِ ٱلرَّحْمَدِ ٱلرَّحِي بْسُ

In the Name of Allah, the Most Gracious, the Most Merciful

To my beloved husband, son, parents and families.

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ABSTRACT

Formal language theory is a branch of applied discrete mathematics and theoretical computer science. A Watson-Crick automaton is an automaton that works on tapes which are double-stranded sequences of symbols related by Watson-Crick complementarity that are similar to the DNA molecules. A Petri net is a model of information flow in systems that provides a useful mathematical formalism for modelling concurrent systems. In this thesis, the relation between Watson-Crick automata and Petri nets is investigated to consider the massive parallelism in Watson-Crick automata. Thus, a new concept called Watson-Crick Petri net is introduced. Besides that, the structural properties of Watson-Crick Petri net are found, namely a single start place, a run place and the stop transition. Also, the generative power of Watson-Crick Petri net is determined. Besides using Watson-Crick complementarity in Petri nets, a context-free grammar is also considered in this research. A Petri net controlled grammar is a type of a context-free grammar equipped with Petri nets, where the successful derivation of the grammar can be simulated by the sequence of occurrences of the net. The production rules of a grammar, for all variants of Petri net controlled grammars that have been introduced, are associated only with transitions of a Petri net. Therefore, a place-labelled Petri net controlled grammar is introduced in this research. The place labelling enables the parallel application of production rules in Petri net controlled grammars to be considered. The effects of labelling strategies and the set of final markings, along with lower and upper bounds are chosen in order to increase the generative power of place-labelled Petri net controlled grammar. Besides that, the structural properties and structural subclass of place-labelled Petri net controlled grammar are also found in this thesis.

ABSTRAK

Teori bahasa formal adalah satu cabang matematik diskret gunaan dan sains komputer teori. Sebuah automaton Watson-Crick ialah automaton yang bertindak pada pita yang merupakan simbol jujukan dwibebenang yang berkaitan dengan pemelengkap Watson-Crick yang serupa dengan molekul DNA. Jaring Petri adalah sebuah model aliran maklumat dalam sistem yang menyediakan formalisme matematik yang berguna untuk pemodelan sistem-sistem serentak. Dalam tesis ini, hubungan antara automata Watson-Crick dan jaring Petri telah dikaji untuk mempertimbangkan keselarian besar-besaran dalam automata Watson-Crick. Dengan itu, suatu konsep baharu yang dipanggil sebagai jaring Petri Watson-Crick telah diperkenalkan. Selain itu, sifat-sifat struktur jaring Petri Watson-Crick telah diperoleh, iaitu sebuah tempat permulaan tunggal, sebuah tempat larian dan peralihan berhenti. Tambahan lagi, kuasa generatif jaring Petri Watson-Crick telah ditentukan. Selain menggunakan pemelengkap Watson-Crick dalam jaring Petri, sebuah tatabahasa konteks-bebas juga dipertimbangkan dalam penyelidikan ini. Sebuah tatabahasa dikawal jaring Petri adalah satu jenis tatabahasa konteks-bebas yang dilengkapi jaring Petri, di mana terbitan kejayaan tatabahasanya boleh disimulasikan oleh jujukan terjadinya jaring itu. Peraturan pengeluaran sebuah tatabahasa, untuk kesemua jenis tatabahasa dikawal jaring Petri yang telah diperkenalkan, dikaitkan hanya dengan peralihan daripada sebuah jaring Petri. Oleh itu, sebuah tatabahasa dikawal jaring Petri pelabelan-tempat diperkenalkan dalam penyelidikan ini. Pelabelan tempat itu membolehkan penggunaan selari peraturan pengeluaran dalam tatabahasa dikawal jaring Petri dipertimbangkan. Kesan strategi pelabelan dan set penandaan akhir, bersama dengan batasan bawah dan atas telah ditentukan supaya dapat meningkatkan kuasa generatif tatabahasa dikawal jaring Petri pelabelan-tempat. Selain itu, sifat-sifat struktur dan subkelas struktur tatabahasa dikawal jaring Petri pelabelan-tempat juga telah diperoleh dalam tesis ini.

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LIST OF SYMBOLS/NOTATIONS

Additive operation +-Adenine А -Σ Alphabet _ Cardinality of a set X|X|-Concurrent composition Δ -С Cytosine -Element of \in _ Φ Empty set -Empty string λ -Equal =-Greater than >-Greater than or equal to \geq -Guanine G _ \subseteq Inclusion _ \cap Intersection -Less than <-Less than or equal to \leq -Multiplicative operation Х -Natural numbers \mathbb{N} -∉ Not element of -Not equal \neq -Strict Inclusion \subset _

- - Subtraction operation
- ρ Symmetric relation
- - Token
- T Thymine
- \cup Union

LIST OF ABBREVIATIONS

CF	-	Context-free
CS	-	Context-sensitive
DNA	-	Deoxyribonucleic acid
MAT	-	Matrix
$p\mathbf{BN}$	-	Place-labelled bounded Petri net controlled grammar
pk BN	-	k-place-labelled bounded Petri net controlled grammar
PN	-	Petri net
$p\mathbf{ON}$	-	Place-labelled ordinary net controlled grammar
$p\mathbf{PN}$	-	Place-labelled Petri net controlled grammar
$p\mathbf{SM}$	-	State machine of place-labelled Petri net controlled grammar
RE	-	Recursively enumerable language
REG	-	Regular language
RWCPn	-	Reverse Watson-Crick Petri net
SM	-	State machine
WCPn	-	Watson-Crick Petri net

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CHAPTER 1

INTRODUCTION

1.1 Introduction

Many real world problems are solved by a combination of mathematical and computational techniques. Mathematics and computer science are also used in the field of biomolecular sciences. For example in deoxyribonucleic acid (DNA) computing, a mathematical model which is an abstraction of the biological properties called a Watson-Crick automaton, is introduced for computational purposes. Watson-Crick automata were inspired by the Watson-Crick complementarity of nucleotides in the double-stranded DNA molecules. Thus, these automata work on tapes which are double-stranded sequences of symbols related by Watson-Crick complementarity that are similar to the DNA molecules. Besides that, Watson-Crick automata are also counterpart of a system known as sticker system, is involved the recombination behavior of DNA molecules by the sticking activities between the dominoes of DNA molecules and the initial dominoes (axioms) of sticker system. [1]. The sticker system is an abstraction of the way of using the Watson-Crick complementarity as in Adleman's DNA computing experiment [2].

DNA computing uses two main features of DNA molecules, namely Watson-Crick complementarity and massive parallelism. DNA molecules consist four bases which are adenine (A), thymine (T), guanine (G), and cytosine (C). The adenine and guanine bases are double-ring molecules called purines, whereas the cytosine and thymine bases are single-ring molecules called pyrimidines. Thermodynamically stable hydrogen bonding occurs between thymine and adenine, and between cytosine and guanine [3]. These base pairing are also called as Watson-Crick complementarity. Massive parallelism allows the development of many copies of DNA strands which carry out operations on the encoded information simultaneously.

However, Watson-Crick automata exploit the Watson-Crick complementarity feature of DNA molecules only. Hence, some additional controls have been considered in order to create a mathematical model that efficiently exploit main features of DNA molecules. In this research, the relation of Watson-Crick complementarity and Petri nets is determined.

Besides that, this research also studies Petri nets with context-free grammars. A Petri net controlled grammar is a context-free grammar equipped with a Petri net where the successful derivations of the grammar is controlled by the occurrence sequences of the net. In Petri net controlled grammars, the production rules of a grammar are associated with transitions of a Petri net. In this research, a new model known as place-labelled Petri net controlled grammar is developed in order to introduce the concurrency mechanism in grammars. This model still uses Petri nets with contextfree grammars, however the production rules of a grammar are associated with places of a Petri net called as place labelling strategies.

1.2 Research Background

In the late 1950s, the idea of performing massively parallel computations in nanotechnology was first stated by Feynman [4]. Consequently in 1994, Adleman was the first who demonstrated a DNA experiment that massive biomolecular computations are feasible [2]. Adleman's experiment succeeded to compute a Hamiltonian

path in a graph by using DNA. Sticker systems introduced by Kari et al., is a computability model which is an abstraction of the computation using the Watson-Crick complementarity [1]. In this computation model, the language generating devices are based on the sticker operation of DNA molecules such as the ligation and annealing operations.

A Watson-Crick automaton is another mathematical model which abstracts DNA properties for computational purposes. Watson-Crick automaton was inspired by the Watson-Crick complementarity of nucleotides in the double-stranded DNA molecules. These automata have two reading heads which work on double-stranded sequences. One of the main characteristics of Watson-Crick automata is that, the characters on corresponding positions from the two strands of the input are similar with the Watson-Crick complementarity of DNA nucleotides.

In 1962, Petri introduced a Petri net as a new model for information flow in discrete event systems [5]. This model provided an elegant and useful mathematical formalism for modelling concurrent systems and their behaviors. Since Petri nets successfully describe and analyse the flow of information and the control of action in such systems, they can also be suitable tools for studying the properties of formal languages. Petri nets are initially used as language generating/accepting tools in previous studies [6], and they have been widely applied as regulation mechanisms for grammar systems [7], automata [8,9] and grammars [10–12].

A Petri net controlled grammar is, in general, a context-free grammar equipped with a Petri net where transitions are labelled with productions of the grammar. Then, the language consists of all terminal strings that can be obtained by applying sequence of productions which is the image of an occurrence sequence of the Petri net under the labelling function. Several variants of Petri net controlled grammars have been introduced and investigated from previous researches. For instance, a generalization of regularly controlled grammars is investigated in [11, 13], where the concept of control of derivations in context-free grammars by arbitrary Petri nets is introduced.

Besides that, *k*-Petri net controlled grammars and their generative power, closure properties and infinite hierarchies have been discussed in [14, 15]. In addition, the grammars controlled by the structural subclasses of Petri nets, namely state machines, marked graphs, causal nets, free-choice nets, asymmetric choice nets and ordinary nets are explored in [10, 16]. The research on Petri net controlled grammars is continued by investigating Petri nets with place capacities. A Petri net with place capacity regulates the defining grammar by permitting only those derivations where the number of each nonterminal in each sentential form is bounded by its capacity [12, 17].

1.3 Problem Statements

In DNA computing, Watson-Crick complementarity and massive parallelism are main two features of DNA molecules. Watson-Crick complementarity occurs in DNA molecules, enables far-reaching conclusions on the information encoded on the DNA strands. According to the Watson-Crick complementarity principle, the information on the strand can be decoded by checking only the information Besides that, massive parallelism of DNA strands encoded on other strand. allows construction of many copies of DNA strands and operations on the encoded information simultaneously and parallelly in a test tube. A model introduced earlier, namely Watson-Crick automata is developed to investigate the Watson-Crick complementarity of DNA molecules. This model did not fulfill main features of DNA molecules. Thus, a new model is introduced in this research, namely Watson-Crick Petri net to investigate the Watson-Crick complementarity and massive parallelism of DNA molecules. This model relates Watson-Crick complementarity with a model of concurrent, asynchronous and parallel systems namely Petri net.

A Petri net controlled grammar is a Petri net with respect to a context-free

grammar. The successful derivations of the grammar can be simulated using the occurrence sequences of the net and transitions of the net are labelled with productions of the grammar. In this research, a new variant of Petri net controlled grammar is introduced by considering the place labelling strategies in Petri net controlled grammar. The place labelling strategies enable us to consider parallel applications of production rules in Petri net controlled grammars, which allows the development of formal language based models for parallel discrete event systems.

In this research, the following questions will be answered. First, how can Watson-Crick complementarity be related to Petri net in a new mathematical model? Next, what are the computational properties of Petri net controlled grammars when the place labelling strategies are considered? Lastly, what is the generative power of the languages generated by Watson-Crick Petri nets and place-labelled Petri net controlled grammars?

1.4 Research Objectives

The objectives of this research are:

- 1. to relate Watson-Crick complementarity and context-free grammars with Petri nets,
- 2. to examine Petri net controlled grammars by adding the place labelling strategies,
- 3. to introduce Watson-Crick Petri nets and place-labelled Petri net controlled grammars,
- 4. to determine the structural properties of Watson-Crick Petri nets and placelabelled Petri net controlled grammars,
- 5. to analyse the generative power of Watson-Crick Petri nets and placelabelled Petri net controlled grammars.

1.5 Scope of the Study

The scope of this research involves the study of computational model of deoxyribonucleic acid, formal languages and Petri nets. From previous research, Watson-Crick automata is developed to investigate the Watson-Crick complementarity of DNA molecules. In creating a model that fulfills DNA molecules main features, namely Watson-Crick complementarity and massive parallelism, Watson-Crick complementarity is related to a model based on the concept of parallelism namely Petri nets. Besides that, context-free grammar in formal language theory is also used to relate with Petri nets in order to increase the generative power of a Petri net.

1.6 Research Methodology

This research is divided into two parts. The first part is to study of deoxyribonucleic acid, Watson-Crick automata and Petri nets. A Watson-Crick automaton is a model of automaton that uses the Watson-Crick complementarity feature of DNA molecules. In Chapter 3, Watson-Crick Petri net is introduced in developing a model that fulfills main features of DNA molecules namely Watson-Crick complementarity and massive parallelism. Watson-Crick Petri net is a model that relates Watson-Crick complementarity to Petri nets. Moreover, some examples are presented to illustrate this model. Some structural properties of Watson-Crick Petri nets such as reverse Watson-Crick Petri nets and *k*-Watson-Crick Petri nets are investigated. The languages of Watson-Crick Petri nets are analysed.

Next, the existing model of Petri net controlled grammar is modified by replacing transition labelling strategies with the place labelling strategies. Hence, a new model, namely place-labelled Petri net controlled grammar is developed. The languages of place-labelled Petri net controlled grammar are investigated by using labelling strategies. The generative power of place-labelled Petri net controlled grammar are also presented by the investigation of their lower and upper bound. Moreover, the structural properties of place-labelled Petri net controlled grammar such as a single start place, reduction to ordinary nets, removal of dead places and place-labelled bounded Petri net controlled grammars are presented in this research. Lastly, a structural subclass of place-labelled Petri net controlled grammar, namely state machine is also determined. The research framework is given in Figure 1.1.



Figure 1.1 Research framework

1.7 Significance of Findings

Nowadays, the development of DNA computing in the field of computer science has rises. Thus, variants of new computational models are developed to investigate the bio-molecular computing advantages. Therefore, the result of this research will enhance contribution from mathematicians in the field of molecular biology and computer science by linking Watson-Crick complementarity with Petri net. This relation enables both features of DNA molecules, namely Watson-Crick complementarity and massive parallelism to be fulfilled. Moreover, this relation also enables the properties of Watson-Crick automata to be investigated by using Petri nets. Besides that, the use of place labelling strategies in Petri net controlled grammars increases the generative power of Petri net controlled grammars. Moreover, the place labelling strategies enables parallel application of production rules in Petri net controlled grammars, which leads to the development of formal language based models for parallel discrete event systems.

1.8 Research Gap

In DNA computing, there are two features of DNA molecules namely Watson-Crick complementarity and massive parallelism. Watson-Crick complementarity naturally occurs in DNA molecules based on DNA strand and is always constructed in pairs of A-T and C-G. On the other hand, massive parallelism allows developing many copies of DNA strands and carrying out of operations on the encoded information simultaneously.

From previous research, one computational model namely Watson-Crick automata is built to investigate the first feature of DNA molecules. However, Watson-Crick automata do not fulfill both features of the DNA molecules since Watson-Crick automata do not fulfill the massive parallelism. Hence, it is interesting to relate WatsonCrick automata with a model of concurrent, asynchronous and parallel systems namely Petri net, in order to increase the generative power of DNA-based devices. Also, the relation enables the possibility for the development of DNA computing in the field of Petri net.

Furthermore, in the study of Petri net with other fields, it is interesting to investigate the properties of the Petri net equipped with context-free grammar in formal language theory. Thus, it is also interesting to add label of production rules at the places of the Petri net known as the place labelling strategies. The research gap is given in Figure 1.2.



Figure 1.2 Research gap

1.9 Thesis Organisation

This thesis contains seven chapters. The first chapter serves as an introduction to the whole thesis. This chapter introduces the relation of Watson-Crick complementarity with Petri nets to fulfill the main features of DNA molecules, namely Watson-Crick complementarity and massive parallelism. Besides, the idea of replacing transition labelling strategies with the place labelling strategies in Petri net controlled grammars is also introduced in order to increase the generative power of Petri net controlled grammars. In addition, Chapter 1 also includes the research background, problem statement, research objectives, scope of the study, research methodology, significance of findings and research gap.

Next, in Chapter 2, the literature review of this research is presented. This includes some concepts of DNA molecules, formal language theory, automata and Petri net. Moreover, some preliminaries used in this research are also provided in this chapter.

Chapter 3 presents the relation Watson-Crick complementarity in Petri net. In this chapter, a new model of Watson-Crick Petri net is introduced. Some examples of Watson-Crick Petri net are illustrated to show how this model works. Besides that, some structural properties of this model, namely a single start place, a run place and the stop transition are provided. Also, some new variants of Watson-Crick Petri net which are reverse Watson-Crick Petri net and *k*-Watson-Crick Petri net are also introduced.

The languages of Watson-Crick Petri net are discussed in Chapter 4. Here, the Watson-Crick Petri net languages determined by the labelling strategies and the set of final markings are introduced. Also, some examples which illustrate the Watson-Crick Petri net languages are presented to demonstrate the model. Furthermore, some closure properties of Watson-Crick Petri net languages are shown using some examples and theorems.

In Chapter 5, place-labelled Petri net controlled grammar is introduced, and some examples of place-labelled Petri net controlled grammar are illustrated. Moreover, the languages of place-labelled Petri net controlled grammar determined by labelling strategies are presented in some theorems. Next, the lower and upper bound of place-labelled Petri net controlled grammar are given.

The structural properties of place-labelled Petri net controlled grammar namely a single start place, reduction to ordinary nets, removal of dead places and placelabelled bounded Petri net controlled grammars are illustrated by some examples in Chapter 6. Some theorems related to these structural properties have also been presented. Moreover, the languages of place-labelled Petri net controlled grammar determined by the set of final markings are presented in some theorems. The generative power of place-labelled Petri net controlled grammar is also shown using the structural subclass of place-labelled Petri net controlled grammar namely the state machine.

Lastly, Chapter 7 presents the summary of this research. Some suggestions for future research are also given in this chapter. The content of this thesis is illustrated in Figure 1.3.

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