UNIVERSITI PUTRA MALAYSIA

MODELING OF STATIC AND DYNAMIC COMPONENTS OF BIO-NANOROBOTIC SYSTEMS

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MODELING OF STATIC AND DYNAMIC COMPONENTS OF BIO-NANOROBOTIC SYSTEMS

By

HAMIDREZA KHATAEE GAVGANI

Thesis Submitted to the School of Graduate Studies, Universiti Putra Malaysia in Fulfilment of the Requirements for the Degree of Master of Science

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DEDICATION

To

My parents, Jamshid and Rouhiyeh, for their love, support, and understanding.

Abstract of thesis presented to the Senate of Universiti Putra Malaysia
in fulfilment of the requirement for the degree of Master of Science

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Chair: Teh Noranis Mohd Aris, PhD

Faculty: Computer Science and Information Technology

Computational modeling techniques can facilitate to achieve in applications of biological nanocomponents for the development of potential bio-nanorobotic systems through representing the properties of these components. This work focuses on the current library of components for the development of bio-nanorobots and considers the recently reported static (e.g. C_{60} and C_{70} fullerenes) and dynamic (e.g. kinesin and muscle myosin nanomotors) components for modeling. This thesis proposes two new computational techniques to model these static and dynamic components.

The first modeling technique applies graph algorithms to compute a new set of optimal weighted structural properties of C_{60} and C_{70} fullerenes. C_{60} and C_{70} fullerene nanoparticles are composed of 60 and 70 equivalent carbon atoms, respectively, arranged as hollow cages. In this technique, the graph-based structural models of the fullerenes are proposed using their real structural information. Then, these graph-based structural models of the fullerenes and graph algorithms based on dynamic programming are applied to compute a new set of optimal weighted

physical properties of the components including Wiener, hyper-Wiener, Harary and reciprocal Wiener indices as well as Hosoya and hyper-Hosoya polynomials. In addition, a graph algorithm based on greedy methods is employed to compute a new set of optimal weighted electronic properties of the fullerenes via computing their Minimum Weight Spanning Trees (MWSTs). The computed optimal weighted physical and electronic properties of the fullerenes showed a good agreement with the mathematics of the properties as well as the principles of the employed graph algorithms.

The second modeling technique applies agent technology to propose comprehensive structural and behavioral models of kinesin and muscle myosin protein nanomotors that can introduce the nanomotors as autonomous and intelligent nanosystems. In this technique, kinesin and muscle myosin nanomotors are introduced as physical intelligent agents. Agent-based structural models of the nanomotors are proposed using composite diagram of Unified Modeling Language (UML) to introduce the sensors and actuators of the nanomotors. Moreover, agent-based behavioral models of the nanomotors are developed using state machine diagrams of UML to illustrate the internal autonomous and intelligent decision-making processes of the nanomotors. The agent-based behavioral state machine models of the nanomotors are validated with comparing their mathematical definitions, developed as Deterministic Finite Automatons (DFAs) and their respective grammars, to the natural behaviors of the nanomotors. Finally, the behavioral DFA models of the nanomotors are implemented as their software agent models. Accordingly, the outputs of the software agent models were in good agreement with the natural behaviors of the nanomotors.

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia
sebagai memenuhi keperluan untuk ijazah Master Sains

PEMODELAN KOMPONEN STATIK DAN DINAMIK SISTEM BIO-NANOROBOTIK

Oleh

HAMIDREZA KHATAEE GAVGANI

Julai 2012

Pengerusi: Teh Noranis Mohd Aris, PhD

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Teknik pemodelan pengkomputeran boleh membantu aplikasi biologikal nanokomponen untuk pembangunan bagi meningkatkan potensi sistem bio-nanorobotik melalui sifat komponen ini. Tumpuan kerja diberikan kepada komponen perpustakaan semasa dalam pembangunan bio-nanorobotik dan mengambilkira laporan statik terkini (seperti *fullerenes* C_{60} dan C_{70}) dan komponen dinamik (seperti *kinesin* dan otot *myosin nanomotors*) di dalam pemodelan komponen ini. Tesis ini mencadangkan dua teknik pengkomputeran baru untuk memodelkan komponen statik dan dinamik.

Teknik pemodelan pertama mengaplikasikan algorithma grafik untuk mengira satu set baru wajaran optimum struktur sifat *fullerenes* C_{60} dan C_{70}. *Fullerene nanoparticles* C_{60} dan C_{70} terdiri daripada 60 dan 70 *atom* karbon yang masing-masing setara dan disusun sebagai sangkar berongga. Di dalam teknik ini, struktur model *fullerenes* berasaskan graf menggunakan maklumat struktur sebenar mereka dicadangkan. Kemudian, struktur model *fullerenes* berasaskan graf dan algoritma graf berdasarkan pengaturcaraan dinamik digunakan untuk mengira satu set baru

wajaran optimum sifat fizikal komponen termasuklah *Wiener*, *hyper-Wiener*, *Harary* dan salingan indeks *Wiener* serta *Hosoya* dan polinomial *hyper-Hosoya*. Di samping itu, algoritma graf yang berasaskan kaedah tamak digunakan untuk mengira satu set baru wajaran optimum sifat elektronik *fullerenes* melalui pengiraan *Minimum Weight Spanning Tress (MWSTs)*. Pengiraan wajaran optimum sifat fizikal dan elektronik *fullerenes* menunjukkan satu keserasian yang baik dengan sifat-sifat matematik serta prinsip algoritma graf yang digunakan.

Teknik pemodelan kedua menggunakan teknologi ejen bagi mencadangkan struktur dan tingkah laku model *kinesin* dan otot *myosin nanomotors protein* yang komprehensif yang mana dapat memperkenalkan *nanomotors* sebagai autonomi dan nanosistem yang cerdik. Di dalam teknik ini, *kinesin* dan otot *myosin nanomotors* diperkenalkan sebagai ejen fizikal pintar. Struktur model *nanomotors* berasaskan ejen dicadangkan menggunakan rajah komposit *Unified Modeling Language (UML)* untuk memperkenalkan penderia dan penggerak *nanomotors*. Selain itu, model tingkah laku *nanomotors* berasaskan ejen dibangunkan menggunakan rajah *UML state machine* bagi menggambarkan autonomi dalaman dan proses pembuatan keputusan cerdik *nanomotors*. Model *nanomotors* berasaskan ejen tingkah laku *state machine* telah disahkan dengan membandingkan definisi matematik mereka, dibangunkan sebagai *Deterministic Finite Automatons (DFAs)* menggunakan tatabahasa tertentu, kepada tingkah laku semulajadi *nanomotors*. Akhir sekali, tingkah laku model *DFA nanomotors* dilaksanakan sebagai model ejen perisian. Sehubungan dengan itu, output bagi model ejen perisian dibuktikan sangat serasi dengan tingkah laku semulajadi *nanomotors*.

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I certify that a Thesis Examination Committee has met on 25 July 2012 to conduct the final examination of Hamidreza Khataee Gavgani on his thesis entitled "**Modelling of Static and Dynamic Components of Bio-Nanorobotic Systems**" in accordance with the Universities and University Colleges Act 1971 and the Constitution of the Universiti Putra Malaysia [P.U.(A) 106] 15 March 1998. The Committee recommends that the student be awarded the Master of Science.

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This thesis was submitted to the Senate of University Putra Malaysia and has been accepted as fulfilment of the requirement for the degree of Master of Science. The members of the Supervisory Committee were as follows:

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DECLARATION

I declare that the thesis is my original work except for quotations and citations which have been duly acknowledged. I also declare that it has not been previously, and is not currently, submitted for any other degree at University Putra Malaysia or at any other institution.

HAMIDREZA KHATAEE GAVGANI

Date: 25 July 2012

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