



MOBILE AD HOC MOLECULAR NANONETWORKS

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# ABSTRACT

## MOBILE AD HOC MOLECULAR NANONETWORKS

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Recent developments in nanotechnology have enabled the fabrication of nanomachines with very limited sensing, computation, communication, and action capabilities. The network of communicating nanomachines is envisaged as nanonetworks that are designed to accomplish complex tasks such as drug delivery and health monitoring. For the realization of future nanonetworks, it is essential to develop novel and efficient communication and networking paradigms. In this thesis, the first step towards designing a mobile ad hoc molecular nanonetwork (MAMNET) with electrochemical communication is taken. MAMNET consists of mobile nanomachines and infostations that share nanoscale information using electrochemical communication whenever they have a physical contact with each other. In MAMNET, the intermittent connectivity introduced by the mobility of nanomachines and infostations is a critical issue to be addressed. In this thesis, an analytical framework that incorporates the effect of mobility into the performance of electrochemical communication among nanomachines is presented. Using the analytical model, numerical analysis for the performance evaluation of MAMNET is obtained. Results reveal that MAMNET

achieves adequately high throughput performance to enable frontier nanonetwork applications with sufficiently low communication delay.

Keywords: Nanomachines, molecular neuro-spike communication, mobile ad hoc molecular nanonetworks, epidemic modeling, delay performance, throughput performance.

# ÖZ

## HAREKETLİ TASARSIZ MOLEKÜLER NANOĞLAR

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Nanoteknolojideki son gelişmeler sınırlı algılama, hesaplama, iletişim ve aksiyon kabiliyeti olan nanomakinelerin üretimini mümkün kılmaktadır. Birbiriyle haberleşen nanomakinelerin oluşturduğu nanoğlar, vücuda alınan ilaçların istenilen yerlere iletilmesi ve vücut içi sağlık kontrolü gibi karmaşık görevlerin üstesinden gelebilmek amacıyla tasarlanmıştır. Nanoğ fikrinin gerçeğe dönüştürülmesi için yeni ve verimli haberleşme ve ağ modelleri gerekmektedir. Bu tezde, elektrokimyasal haberleşmeyi kullanan hareketli tasarsız moleküler nanoğ (MAMNET) tasarlamak için ilk adım atıldı. MAMNET, birbirleriyle fiziksel bağlantı kurduklarında elektrokimyasal haberleşme ile bilgi paylaşımı yapan hareketli nanomakine ve bilgi istasyonlarından oluşmaktadır. MAMNET için nanomakinelerin ve bilgi istasyonlarının hareketli olmasından kaynaklanan aralıklı bağlantı, üzerinde düşünülmesi gereken önemli bir konudur. Bu tezde, hareketliliğin yol açtığı sonuçlar ve elektrokimyasal haberleşmenin performansı analitik bir çerçevede birleştirilerek sunulmuştur. Bu analitik model kullanılarak MAMNET'in performansı üzerine sayısal analizler yapılmıştır. Elde edilen sonuçlara göre MAMNET gelecekteki öncü nanoğ uygulamaları için yeterli

derecede yüksek çıktıyı, yeterli miktarda gecikme ile sağlayabilecek niteliktedir.

Anahtar Kelimeler: Nanomakine, moleküler sinirsel haberleşme, hareketli tasarsız moleküler nanoağ, salgın modellemesi, gecikme performansı, çıktı performansı



*To Demet*

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# CHAPTER 1

## INTRODUCTION

Nanotechnology is a new interdisciplinary field that grows attention in the early 2000s. Although the concept of nanotechnology is half century old, the advancements accelerated in the early years of the last decade [1]. Nanotechnology can be defined as the processing, separation, consolidation and deformation of materials on atomic or molecular scale [2]. At this scale, new behaviors and properties, that cannot be seen at macroscopic level, are observed for nanomaterials or nanoparticles. These new behaviors and properties are exploited to create nanodevices [14].

Nanotechnology utilizes the knowledge of the fields of natural sciences such as physics, chemistry and molecular biology as well as engineering and computer science. The cooperation of scientists from different fields enables the creation of novel materials and devices on the order of nanometers. Nanotechnology promises many new applications in almost every field of life.

### 1.1 Nanomachines

Rapid growth in nanotechnology provides favorable development in miniaturization and fabrication of nanomachines with simple sensing, computation, communication, and action capabilities. Nanomachines are molecular scale devices, that consist of an arranged set of molecules. The development of nanomachines is under extensive research.

In literature, three different ways are proposed for the development of nanomachines,

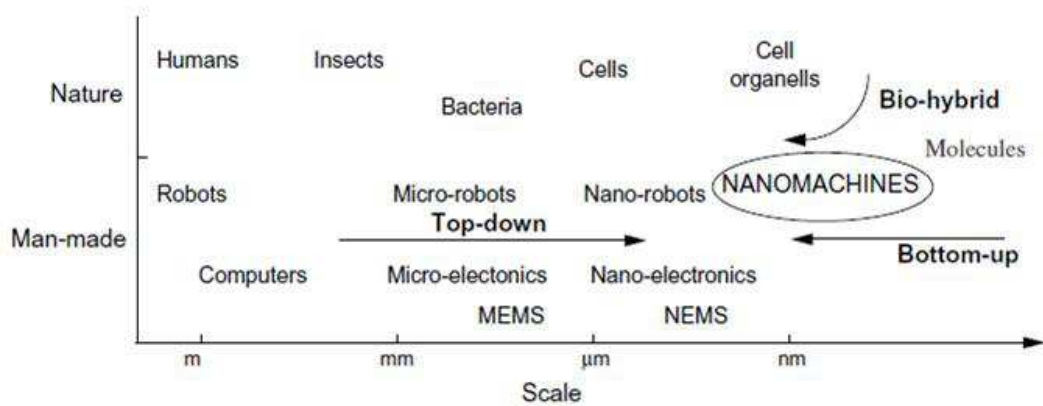


Figure 1.1: Approaches for the development of nanomachines [1].

namely, bottom-up, top-down and bio-hybrid approaches [1]. In bottom-up approach, the molecules or atoms are assembled to form nanomachines. In-top down approach, the design of nanomachines is realized by downsizing current microelectronic technologies. The third approach in developing nanomachines is the bio-hybrid approach. In this approach, biological entities can either be modified to develop nanomachines or used as the building blocks of nanomachines.

In nature, there are already many molecular-scale phenomena that are able to perform very simple tasks. For example, a chloroplast in a plant cell stands as a nanomachine including arrays of molecules that act as tuned optical antennas for absorption and transformation of solar energy. Mitochondrion can be envisioned as a nanomachine used for controlled combustion of organic molecules to generate Adenosine triphosphate (ATP) for fulfilling energy needs of cellular activities. A flagellar motor attached on the membrane of many bacterial cells is a highly structured combination of proteins for providing cellular movement [3]. Nature-made nanomachines can be exploited to learn and understand the principles governing the operation of nanomachines and their interactions [3].

## 1.2 Nanonetworks

A single nanomachine has very limited capabilities. The interconnection of nanomachines, however, enables to accomplish complex tasks by collaboration of nanoma-

chines. The networks of communicating nanomachines, i.e., *nanonetworks*, are expected to enable very large set of new applications in genetic engineering, health monitoring, military surveillance systems, as well as industrial and environmental applications [1]. The potential applications can be briefed as follows.

- **Health care applications.** The tiny size of nanomachines allows them to be deployed in human body. Therefore, nanonetworks promise many new applications for health care. For example, nanomachines can be used in the immune system support. They can be used to detect and eliminate foreign agents [6, 7]. Moreover, they can also be used as bio-hybrid implants to support or replace lost tissues [9]. The in body deployment of nano sensor networks can enable early diagnosis by controlling certain parameters such as cholesterol level and hormonal activities [9]. One thing to keep in mind for health care applications is that, the nanomachines should be bio-compatible.
- **Military applications.** The applications of nanonetworks on military field are countless. These applications range from smart military equipments [10] to chemical or biologic agent detection and elimination [11].
- **Industrial applications.** Nanonetworks can be used in developing functionalized materials and products [1]. For example, nanonetworks can be used in developing clothes that regulates the body temperature [10]. On the other hand, nano sensor networks can be used in food and water quality control to detect small agents and toxic components that cannot be detected by current detecting technologies [1].
- **Environmental applications.** Nanonetworks can also be used in biodegradation, air pollution control, animals and biodiversity control [1]

The nature-made nanomachines also form nanonetworks to accomplish the vital functions of the organism. Therefore, in designing nanonetworks, it is reasonable to inspire by existing biological nanonetworks. In living organisms, cells communicate in various ways. For example, lymphocytes called B-cells and T-cells constitute immune network to defend the organism against infection. B-cells and T-cells can be considered as nanomachines having the capabilities of recognizing, learning and

destroying the antigens. When an antigen is recognized by some B-cells that are genetically matching the antigens, these B-cells communicate with other B-cells by emitting antibody molecules to their surrounding environment. This way, the B-cells that genetically match with the antigen are quickly produced in the bone marrow to completely eliminate the antigens [4]. Existing communication paradigms between cells may be adopted for the realization of nanonetworks [16].

### **1.3 Communication Among Nanomachines**

Communication of nanomachines is one of the most important challenges in realizing a nanonetwork. Classical communication and network paradigms cannot be directly used in nanonetworks. This is because of the new challenges and requirements introduced by the limited capabilities of nanomachines. These challenges and requirements can be briefed as follows:

- Scale of the nanomachines is on the order of micro meter, therefore, traditional transceiver circuitries cannot be mounted into nanomachines.
- Current encoding and decoding techniques are not feasible due to very limited processing capability of nanomachines.
- For in vivo application scenarios, nanomachines need to be biocompatible in order not to be rejected by the organism.
- Mobility of nanomachines is governed by the physical rules in this regime [5].
- Nanomachines are extremely susceptible to any change in the communication environment such as rapid concentration change or quaking.
- Communication or noise signal characteristics cannot be easily anticipated due to severely unreliable nature of the communication medium.

In literature, different communication techniques, namely, acoustic, electromagnetic, molecular and nanomechanical, are proposed for the communication of nanomachines [7]. Traditional electromagnetic communication technologies cannot be di-

rectly used in the communication between nanomachines because of the size restrictions. In [12], a single carbon nanotube (CNT) is shown to be designed as radio circuitry. Although the size of the CNT radio is promising, it has major drawbacks to be used in the communication nanomachines. For example, it needs a power supply of 200 Volts to operate. At nano level, acoustic communication is also not feasible due to the size of current ultrasonic transducers. On the other hand, the main drawback of nanomechanical communication is that it requires a physical contact between nanomachines. Molecular communication which is already used by biological entities is a promising approach for the communication of nanomachines.

#### **1.4 Molecular Communication**

Molecular communication is a new paradigm, that enables the communication of nanomachines through the use of molecules as communication carriers [16]. Molecular communication is inspired by the natural inter-cellular communication paradigm in which cells communicate using molecules. It is an interdisciplinary approach spanning bio, nano and communication technologies.

The superiority of molecular communication over previously proposed communication techniques is the size of transceivers. In nature, there already exist many molecular transceivers. Therefore, the integration of molecular transceivers to nanomachines is more feasible [1]. Furthermore, molecular communication is purely biocompatible in its nature which makes it suitable for in-vivo applications. On the other hand, molecular communication has also drawbacks such as low signal propagation speed and high susceptibility to environmental conditions. The significant differences between molecular communication and traditional communication paradigms are summarized in Table 1.1.

Despite the significant differences between molecular and traditional communication paradigms, the steps followed in both communication paradigms are identical. The communication process based on molecular signaling involves the following steps:

1. *Encoding*: In molecular communication, the signals are encoded onto the information molecules. The information can be encoded on some molecular features

Table 1.1: Traditional vs. molecular communication [16].

	<i><b>Molecular Communication</b></i>	<i><b>Traditional Communication</b></i>
<i>Communication carrier</i>	Molecules	Electromagnetic Waves
<i>Signal type</i>	Chemical	Electromagnetic
<i>Signal speed</i>	Extremely slow	Light speed
<i>Noise</i>	Particles and molecules in medium	Electromagnetic fields and signals
<i>Encoded information</i>	Phenomena, chemical states or processes	Voice, text and video
<i>Energy consumption</i>	Low	High

like polarity, magnetization and structures [16].

2. *Transmission*: Actually, this process is the release of encoded information molecules to the medium.
3. *Signal Propagation*: The released information molecules propagate through the channel between transmitter and receiver. In the propagation process, either information molecules diffuse freely or some carriers like molecular motors [18] are used to carry them.
4. *Reception*: The information molecules released into the channel finally reach to the receiver.
5. *Decoding*: The information is then decoded to useful information such as reaction, data storing, actuation commands [1].

In order to enable molecular communication, the steps followed in molecular signaling should be well defined and investigated.

## 1.5 Related Work

For the realization of frontier nanonetworks, it is imperative to develop new and efficient communication and network techniques. The aim of these techniques is to

overcome unique challenges and fulfill requirements of nanonetworks. By virtue of the great potential in nature-made nanomachines and nanonetworks, researchers have been recently inspired by natural nanoscale communication techniques.

In literature, there exist several research efforts about the communication of nanomachines. The majority of these efforts are inspired from natural molecular-scale communication phenomena. Molecular communication is one of the most promising technique that enables communication among nanomachines using molecules as communication carriers [16]. The first attempt for the design of a molecular communication system is made in [21]. A molecular communication paradigm using artificial cells is discussed in [23]. In [19], a design of a molecular communication system based on intercellular calcium signaling is introduced. Molecular communication systems using biological molecular motors [18], and vesicles [22] as communication carriers are introduced as well. In [17] a molecular communication channel is modeled as a binary symmetric channel and mutual information and capacity expressions are derived for that channel.

In literature, there also exist several research efforts for realizing nanonetworks. In [13], nanotechnology enabled wireless sensor networks are discussed from a device perspective. In [5], the concept of carbon nanotube-based nanoscale ad hoc networks is introduced. A survey on electromagnetic wireless nanosensor networks is presented in [14].

## **1.6 Motivation and Overview of This Work**

The existing studies in the literature consider the nanomachines as immobile network nodes. However, mobile nanomachines may be indispensable for many nanonetwork applications. Clearly, these applications necessitate the realization of MAMNET. A possible example that necessitates the mobility of nanomachines is a nanonetwork designed for coordinated cancer cell detection by identifying unique properties of cancer cells. Artificial mobile nodes can be specifically designed for detecting cancer cells and informing a central control that the human has cancer cells. In MAMNET, nanomachines sense the environment to gather some environmental information about

a chemical state, or the existence of certain antibodies. In MAMNET, the main aim is to deliver the information collected by mobile nanomachines to mobile *infostations*, that are central control units that make decisions according to the collected information, or gateways that connect MAMNET to a micro-device.

However, the mobility of nanomachines also incurs a new set of crucial challenges that must be addressed for the realization of MAMNET. One of the main challenges introduced by the mobility of nanomachines is the intermittent connectivity, i.e., nanomachines can communicate only when they are in physical contact. Therefore, this intermittent connectivity clearly imposes a high level of latency on nanoscale communication in MAMNET. To the best of our knowledge, the feasibility and performance of an ad hoc nanonetwork, composed of mobile nanomachines communicating through electrochemical means, have not yet been investigated.

The aim of this work is to introduce and investigate the feasibility of MAMNET and provide an analytical framework for its evaluation. The communication of mobile nanomachines is inspired by the cellular communication paradigm in immune system. In adaptive immune system, the immune response starts by the recognition of antigens by T-cells. However, T-cells cannot directly recognize antigens. First, antigen presenting cells (APCs) recognize the antigen entering the body. Then, APCs and T-cells collide and adhere to each other by surface molecules. The adhesion of these cells forms an immunological synapse. T-cells are activated by the interaction of major histocompatibility complex molecules on the surface of APCs with T-cell receptors [8]. With the transfer of antigen information to T-cells, the immune response starts.

In MAMNET, the communication of nanomachines is inspired by the natural cellular communication in adaptive immune system and established through three main phases, namely, collision, adhesion and transmission. In collision phase, nanomachines randomly collide with each other. In adhesion phase, nanomachines stuck to each other. Finally, the information is transmitted in the transmission phase. For the transmission of information, in this work, we propose a new communication paradigm, namely, *molecular neuro-spike communication*, that is based on the neural communication which is the fastest and most reliable communication between



cells. This molecular neuro-spike communication scheme can be used in the communication of adjacent nanomachines and classified as a molecular short range communication paradigm. Analytical framework is obtained by integrating the models for collision, adhesion and transmission. Using the analytical model developed, it is shown that, MAMNET is feasible with sufficiently low communication delay and high throughput.

The remainder of this thesis is organized as follows. In Chapter 2, we give an overview of the architecture of MAMNET, and underline the design issues and assumptions made. Then, we model the collision and adhesion of nanomachines in Chapter 3. In Chapter 4, using the principles of neural communication, we model the neuro-spike transmission between two adherent nanomachines. Based on this model, we derive an analytical expression for the capacity of molecular neuro-spike channel to evaluate the suitability of the model to MAMNET. Moreover, in Chapter 5, we develop an analytical framework and derive expressions for the distribution of communication delay in the network and average throughput. We present the numerical results about the performance of the MAMNET in Chapter 6 and conclude the thesis in Chapter 7.

## CHAPTER 2

### MOBILE AD HOC MOLECULAR NANONETWORK COMMUNICATION MODEL

MAMNET is composed of two kinds of mobile nanonodes, namely, nanomachines and infostations. Nanonode refers to both nanomachine and infostation. As shown in Fig. 2.1, both nanomachines and infostation roam in an aqueous environment. Nanomachines and infostations are assumed as modified cells with additional capabilities. The environment should have the appropriate conditions for functioning of cells in terms of temperature, pH and medium viscosity to enable the operation of nanomachines [1]. We assume that nanomachines sense the environment using nanosensors and gather some environmental information. Infostations can be thought as central controls that make decisions according to the collected information, or they can be thought as gateways that connect MAMNET to a micro-device.

We assume that nanomachines are pre-programmed to sense the environment and collect simple information in response to the observed phenomena. This information should be transmitted to an infostation. However, nanomachines and infostations do not always have a direct communication interface because of mobility. In order for a nanomachine to transmit the generated information, the nanomachine and the infostation should first collide, then adhere to each other. We assume that the volume containing MAMNET is much larger than the size of a single nanonode. Therefore, the meeting probability of a nanomachine and an infostation is very low. Thus, it is inefficient for a nanomachine to directly transmit information to an infostation. Instead, intermediary nanomachines can be used as relay nodes.

In order to understand the information flow in MAMNET, consider the nanonetwork

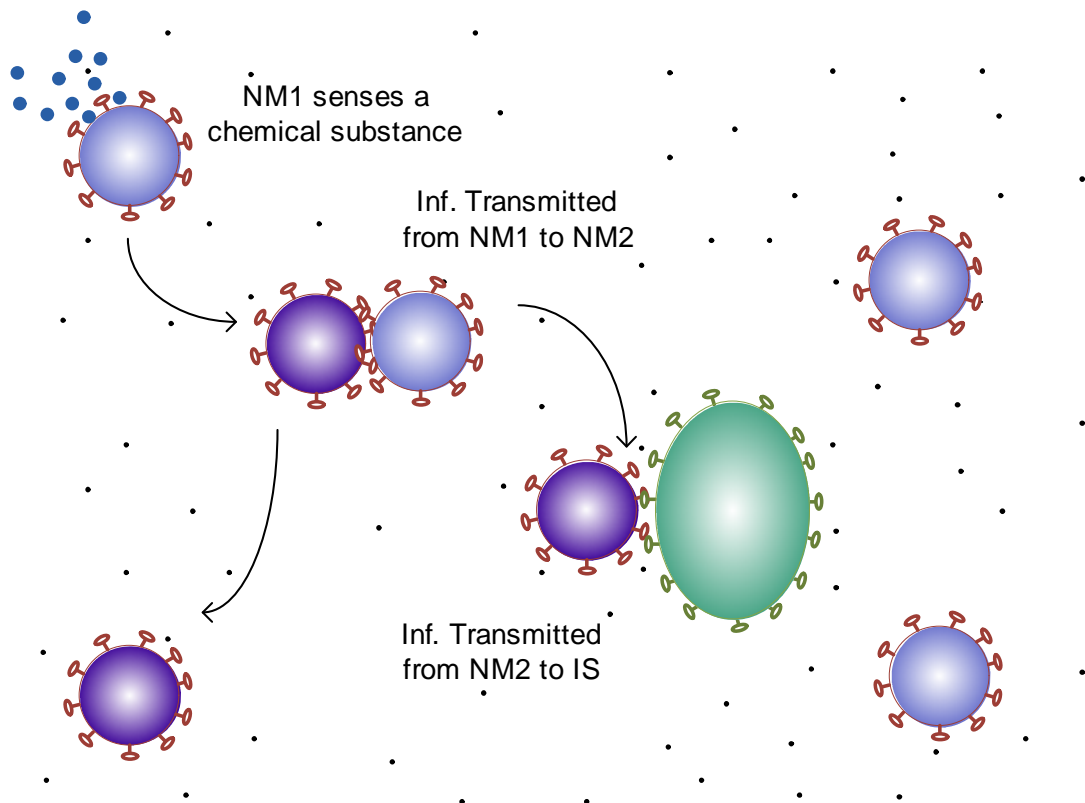


Figure 2.1: Information flow in MAMNET.

in Fig. 2.1. Nanomachine 1 is assumed to be the source of the information that is to be communicated to the infostation. Nanomachine 1 tries to transmit the information to every nanomachine it meets. The nanomachines that newly acquire the information behave the same and this clearly increases the probability of information delivery. Before the transmission of information, nanonodes should first collide and adhere to each other. In other words, before the transmission of information there are two preliminary phases:

1. *Collision phase:* In this phase, mobile nanonodes randomly collide with each other. Here, we assume that nanomachines and infostations do not have any additional capability for mobility or collision. The movement of nanonodes is only due to the external factors and modeled in Chapter 3.
2. *Adhesion phase:* In this phase, collided nanonodes adhere to each other via the surface mounting molecules called, ligands and receptors. They adhere by means of the ligand-receptor binding process. According to the ligand-receptor

binding process, ligand molecules on the surface of one nanonode bind to the receptors of an other nanonode. A certain number of bonds should be established between the nanonodes in order for successful adhesion.

The performance of MAMNET directly depends on the interaction of nanomachines and infostations. The interactions are triggered by collision and adhesion of nanomachines and infostation. Therefore, it is important to know the collision rate, i.e., the number of collisions occur per unit time in the network, and the adhesion probability of collided nanomachines and infostations. In Chapter 3, the complete analysis of collision and adhesion is given. Moreover, collision rate and adhesion probability are derived in order to be used in the performance evaluation of MAMNET.

After collision and adhesion, nanomachines are ready to transmit the information. The information transmission between nanonodes is the key issue to be addressed. In this thesis, *molecular neuro-spike communication* is proposed for the communication of mobile nanomachines and infostations. The details of molecular neuro-spike communication are presented in Chapter 4.

In MAMNET, the information spreads over the network by the three phases defined above. In Chapter 5, the flow of information in MAMNET is modeled using the collision, adhesion and transmission models. In order to evaluate the performance of MAMNET we define three performance metrics, i.e., average throughput, system throughput and communication delay. Average throughput is defined as the average amount of information reached to an infostation per unit time. Furthermore, the system throughput is defined as the average amount of information transmitted in the network. Communication delay is defined as the time past from the generation of an information by a nanomachine until its arriving to any infostation. In Chapter 5, an analytical framework is derived to obtain average throughput, system throughput and average communication delay. Using the analytical models, the performance of MAMNET is evaluated.

## CHAPTER 3

### COLLISION AND ADHESION OF NANOMACHINES

In nature, the behaviors of cells are significantly affected by contacts with other cells [26]. In their environment, mobile biological cells collide with each other and cellular adhesion occurs between the collided cells. One of the main processes that adhesion is involved is the communication between cells. The cell adhesion is accomplished by the ligand-receptor binding process. When the cells collide, ligand molecules on the surface of one cell are captured by the receptors of other cell. Adhesion is also involved in shaping the structure of multicellular organisms [28]. Recent studies show that adhesion also has a critical role in intracellular and intercellular signaling [29]. For example, the cell adhesion molecules called integrins play both direct and indirect roles in signaling. Integrins can directly activate intracellular signaling processes by activating the signal transduction pathways especially that are leading to activation of mitogen-activated protein (MAP) kinases. The integrins also involve in the modulation of MAP kinase cascades and G protein-coupled receptor cascades by interaction of integrin with other membrane receptors, which describes their indirect role [29]. Another example can be neural cell adhesion molecules (N-CAMs), which belong to a family of  $Ca^{2+}$  dependent cell adhesion molecules and have a function in neural cells [30].

In this thesis, we adopt the natural cellular signaling paradigm for the communication among nanomachines. Nanomachines should be in physical contact with each other in order to communicate. The physical contact is established through the collision and adhesion of nanonodes. Therefore, we need to model the collision and adhesion of nanonodes.

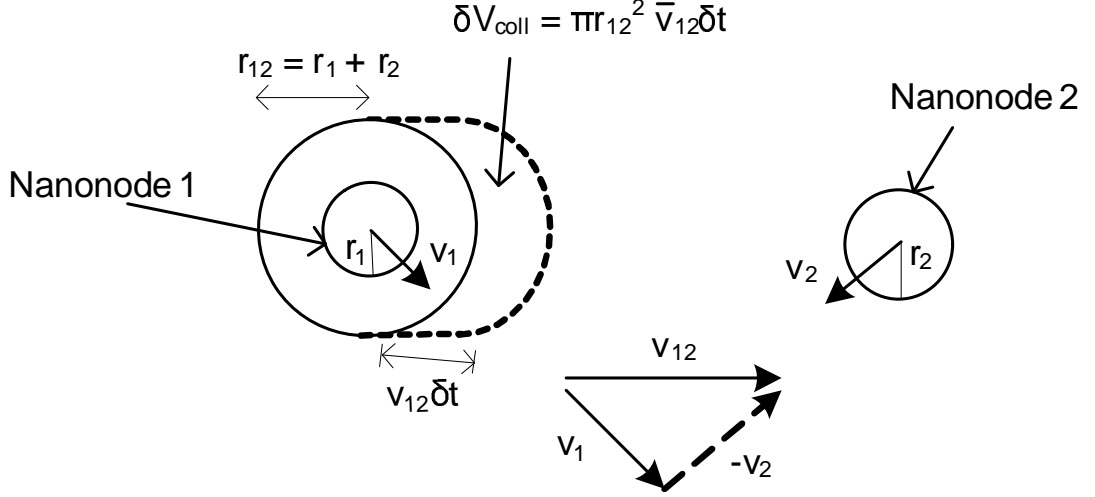


Figure 3.1: Collision of two nanomachines. Nanomachine 1 and nanomachine 2 collide in the time interval  $\delta t$  if nanomachine 2 is in the collision volume  $\delta V_{coll}$  in  $\delta t$ .

### 3.1 Collision of Nanomachines

In MAMNET, information is transmitted from a nanomachine to another or to an infostation. The information can be transmitted only if the nanonodes are in direct contact. In order to be in direct contact, the nanonodes first collide, and then adhere. Therefore, the number of collisions per unit time directly affects the performance of MAMNET. A higher collision rate means more interactions between nanonodes which leads to a lower communication delay and a higher throughput. In this section, we model the collision of nanonodes and derive the collision rates.

The collision of nanomachines in MAMNET can be resembled to the meeting of nodes in the traditional mobile ad hoc networks. In traditional mobile ad hoc networks, the nodes are assumed to be moving according to a certain mobility model, such as random direction, random waypoint and random walker mobility models, and node meeting rates are derived for these mobility models. A similar approach can be followed in deriving the collision rate of nanomachines. In order to model the collision rate, firstly, the movement of nanomachines in an aqueous environment should be investigated.

Since nanomachines are very tiny components with limited capabilities, it is assumed that nanomachines do not have a capability of controlling their movement. Thus, the

movement of nanomachines is only due to the external factors. In fact, the movement of nanomachines can be described as Brownian motion. Brownian motion explains the movement of particles in a fluid as due to the total movement of small molecules composing the fluid [24]. Nanomachines can be thought as the particles moving in a fluid, and, hence, their motion can be described as Brownian motion.

Nanomachines are assumed to be contained in a volume  $V$  and moving according to Brownian motion. We also assume that the nanomachine radius  $r$  is small compared to the volume  $V$ . We first obtain the probability that the nanomachines collide within the next infinitesimal time interval  $\delta t$ , given that the first nanomachine's center is located at the position  $(x_1, y_1, z_1)$ . Two nanomachines collide in the next  $\delta t$ , only if the second nanomachine is in the volume that is covered by the first nanomachine with respect to the second nanomachine. This collision volume  $\delta V_{coll}$  is shown in Fig. 3.1 and expressed as

$$\delta V_{coll} = \pi r_{12}^2 v_{12} \delta t \quad (3.1)$$

where  $r_{12} = r_1 + r_2$  and  $v_{12}$  is the relative velocity of the first nanomachine with respect to the second nanomachine. By using the relative velocity, the second nanomachine is considered as stationary and only the first nanomachine is considered moving with velocity  $v_{12}$  rather than  $v_1$ . Thus, the probability that the second nanomachine is located in volume  $\delta V_{coll}$  is expressed by

$$p_{x_1, y_1, z_1} = \iiint_{\delta V_{coll}} f(x, y, z) dx dy dz \quad (3.2)$$

where  $f(x, y, z)$  is the probability density function(pdf) of spatial node distribution in a volume  $V$  in which the nanomachines are moving according to the Brownian motion. For small values of  $r$ , the points  $f(x, y, z)$  in  $V$  can be approximated by  $f(x_1, y_1, z_1)$ . This gives the probability of a collision within the next infinitesimally small time interval, given that the first node's starting position is  $(x_1, y_1, z_1)$ , i.e.,

$$p_{x_1, y_1, z_1} \approx \pi r_{12}^2 v_{12} \delta t f(x_1, y_1, z_1) \quad (3.3)$$

Then, by unconditioning this probability on the position of the first node, i.e., integrating over all starting positions of the first node, the probability of collision within

the next infinitesimally small time interval  $\delta t$  can be obtained as

$$\begin{aligned} p &= \iiint_V p_{x_1, y_1, z_1} f(x_1, y_1, z_1) dx_1 dy_1 dz_1 \\ &\approx \pi r_{12}^2 v_{12} \delta t \iiint_V f^2(x_1, y_1, z_1) dx_1 dy_1 dz_1 \end{aligned} \quad (3.4)$$

(3.4) is specific for the relative speed  $v_{12}$  of the first node according to the second node. Averaging it over the velocity distributions of the nanonodes, the collision rate for nanodes can be approximated as

$$R_c \approx \pi r_{12}^2 E[v_{mn}] \iiint_V f^2(x_1, y_1, z_1) dx_1 dy_1 dz_1 \quad (3.5)$$

where  $E[v_{mn}]$  is the average relative speed of the nanomachines. In order to evaluate the collision rate, the spatial node distribution  $f(x, y, z)$ , and average relative speed  $E[v_{mn}]$  for the nanomachines moving according to Brownian motion are required. The effect of average relative speed on performance is discussed in Chapter 6. The spatial node distribution for Brownian motion is uniform, i.e.,  $f(x, y, z) = 1/V$ . Thus,  $R_c$  can be approximated as

$$R_c \approx \pi r_{12}^2 E[v_{mn}] \iiint_V 1/V^2 dx_1 dy_1 dz_1 \approx \frac{\pi r_{12}^2 E[v_{mn}]}{V} \quad (3.6)$$

Since the size of nanomachines are identical, for nanomachine-nanomachine collision,  $r_{12} = 2r$ , where  $r$  is the radius of a nanomachine. Then, from (3.6), the collision rate for nanomachines can be expressed as

$$R_c \approx \frac{4\pi r^2 E[v_{mn}]}{V} \quad (3.7)$$

The collision rate of an infostation and a nanomachine follows a similar argument except that infostations could have a different radius compared to nanomachines. For nanomachine-infostation collision  $r_{12} = r + r_i$ , where  $r_i$  is the radius of an infostation. Then, similar to the collision rate of nanomachines, the collision rate of an infostation and a nanomachine can be written as

$$R_{ic} \approx \frac{\pi(r + r_i)^2 E[v_{ni}]}{V} \quad (3.8)$$

where  $E[v_{ni}]$  is the average relative speed of the nanomachine and infostation.



The collision rates  $R_c$  and  $R_{ic}$  are essential to understand the interaction rate of nanomachines and infostations. However, the collision rates are not the ultimate parameters that affect the MAMNET performance since the collided nanomachines should also adhere with each other to enable molecular neuro-spike communication.

Next, the adhesion of nanomachines is modeled.

### 3.2 Adhesion of nanomachines

After the collision between nanomachines, the collided nanomachines adhere with each other via the binding of the surface molecules called ligands and receptors, as shown in Fig. 3.2. In MAMNET, nanomachines need to adhere successfully in order to enable information transmission. Therefore, the adhesion probability of nanomachines is also a critical issue when evaluating the performance of MAMNET. In this section, we model the adhesion of nanomachines and analytically derive the adhesion probability.

In nature, the binding process of two cells, i.e., cell adhesion, is an important issue. Cell adhesion is involved in a variety of processes such as migration, invasion, embryogenesis, wound healing and cell-to-cell communication. One of the most important processes that adhesion involved, is intercellular communication [29]. With the adhesion of cells, there exists a natural communication interface between cells.

In this work, the natural cellular adhesion paradigm is adopted to enable the adhesion of nanomachines. In literature, there exist several research efforts on modeling the adhesion between cells [20], [26]. Here, the adhesion model developed in [20] is adapted. Accordingly, nanomachines are assumed to have ligands and receptors which mediate adhesion. The adhesion process is heavily affected by the density of ligands and receptors and the contact area of the collided nanomachines.

Adhesion is considered as a random event and the state of the system is considered as a probability vector  $[p_0, p_1, \dots, p_n, \dots, p_{A_c m_{min}}]$  where  $m_{min}$  is the minimum of surface densities of receptors and ligands and  $A_c$  is the area of contact [20]. In other words, adhesion could be mediated by any number of bonds ranging from 0 to  $A_c m_{min}$ .

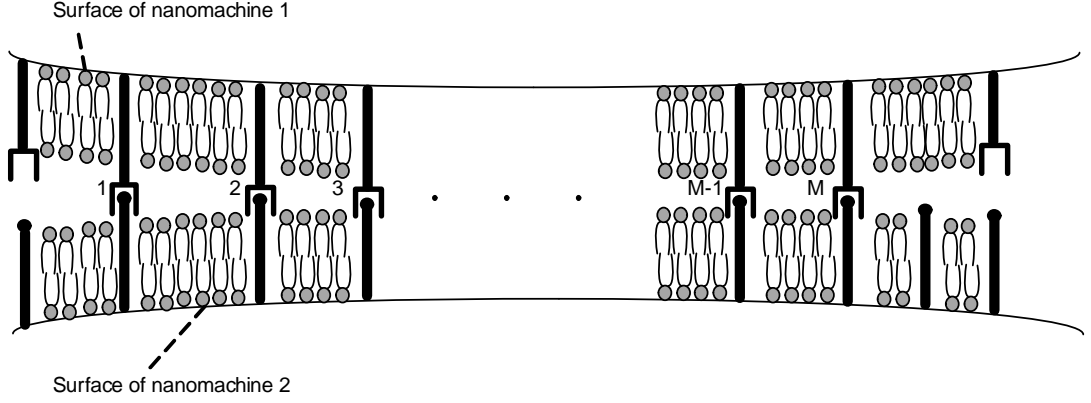


Figure 3.2: Nanomachine Adhesion. Nanomachine 1 and Nanomachine 2 are attached to each other by  $M$  ligand receptor pairs.

For forming any number of bonds, there is a defined likelihood given by  $p_n$ . Here, nanomachines are assumed to adhere when at least  $c$  bonds are formed between them. Hence, our aim is to derive the probability that nanomachines adhere via at least  $c$  bonds, and the closed-form expression of  $p_n$  is needed in deriving this. In [20], a closed-form expression is found for  $p_n$  under a set of certain assumptions for two cells, such as either ligands or receptors outnumbers the other one. When two nanomachines are just brought together ( $t = 0$ ), there is no bond, hence,

$$p_n(0) = \begin{cases} 1 & , n = 0 \\ 0 & , n \neq 0 \end{cases} \quad (3.9)$$

With the contact of nanomachines, bonds start to form according to a single step reversible reaction. The chemical reaction of  $v_r$  receptors (designated  $M_r$ ) binding to  $v_l$  ligands (designated  $M_l$ ) to form  $v_b$  bonds (designated  $M_b$ ) can be expressed as



where  $k_f^0$  and  $k_r^0$  are the forward and reverse rate constants, respectively.

In the stochastic model of chemical kinetics, the state of the system, described by the single step reversible chemical reaction (3.10), is represented by the probability vector  $[p_0, p_1, \dots, p_n, \dots, p_{A_c, m_{min}}]$ . In [25], a stochastic model of chemical kinetics is discussed and master equations are derived in order to describe the state of the system. Actually, these master equations can be used to describe the rate of change in

probability  $p_n(t)$ . However, it is not possible to obtain closed-form solutions for the master equations. Rather, in the current literature, two simplified versions of master equations are discussed in order to obtain closed-form expressions. In [20], a simplified version of the master equations is discussed under the condition that either ligands or receptors excessively outnumber the other one. Under that condition and with  $v_r = v_l = v_b = 1$ , i.e., a bond is formed by the binding of a ligand to a receptor, the master equations can be simplified as [20]

$$\begin{aligned} \frac{dp_n}{dt} = & \left[ A_c m_{min} - (n-1) \right] m_{max} k_f^0 p_{n-1} - \\ & - \left[ (A_c m_{min} - n) m_{max} k_f^0 + n k_r^0 \right] p_n + (n+1) k_r^0 p_{n+1} \end{aligned} \quad (3.11)$$

Assuming either ligands or receptors excessively outnumber the other one,  $p_n(t)$  is found to be in the form of binomial distribution and can be given as [20]

$$p_n(t) = \binom{A_c m_{min}}{n} [p(t)]^n [1 - p(t)]^{A_c m_{min} - n} \quad (3.12)$$

where  $p(t)$  is the probability of forming one bond given by

$$p(t) = \frac{1 - e^{-kt}}{1 + (m_{max} K_a^0)^{-1}} \quad (3.13)$$

where  $K_a^0 = k_f^0/k_r^0$  is the equilibrium association constant and  $k = m_{max} k_f^0 + k_r^0$  is the overall rate of reaction.

After the collision event between two nanomachines, they are assumed to stay in contact with each other during an average contact duration  $\tau_c$ .  $\tau_c$  is affected by the physical properties of the environment, relative velocities and physical surface properties of the nanomachines. The effect of  $\tau_c$  on performance is discussed in Chapter 6. We also assume that the collided nanomachines adhere to each other if at least  $c$  bonds are formed during a contact duration  $\tau_c$ . Hence, the probability that the collided nanomachines adhere to each other, i.e.,  $R_a$ , can be given as

$$R_a = 1 - \sum_{i=0}^{c-1} p_i(\tau_c) \quad (3.14)$$

Note that we do not present a different adhesion probability for the nanomachine-infostation interaction. This is because the physical properties used in the derivation

of adhesion rates are the same for both nanomachines and infostations. The adhesion probability derived in this section is very important to understand the interaction of nanomachines. The communication between nanomachines can only be possible after successful adhesion.

## CHAPTER 4

### MOLECULAR NEURO-SPIKE COMMUNICATION

In this chapter, molecular neuro-spike communication is explained in detail. First, the basics of molecular neuro-spike communication are described. Then, the performance of the proposed scheme is evaluated using the channel error probability and channel capacity. Lastly, successful information transmission probability is derived to be used in the performance evaluation of MAMNET.

#### 4.1 Basics of Molecular Neuro-Spike Communication

When nanomachines collide and successfully adhere, the nanomachine that has an information wants to transmit its information to the other one. The nanomachine that transmits the information is called the transmitter nanomachine (TN) and the nanomachine that receives the information is called the receiver nanomachine (RN). After the adhesion of nanomachines, there exists a small gap, synapse, between the TN and RN. This synapse is the communication media for nanomachines. Since TN and RN cannot remain adhered for a long time, a fast and reliable communication paradigm is needed to enable the information transmission between nanomachines. Among the existing inter-cellular communication paradigms, the communication between neuron cells is the fastest one. Therefore, in our model, we adopt the principles of neural communication to enable the information transmission among nanomachines.

In human body, there already exist at least two types of natural synapses between cells, namely, the neuronal synapse and the immunological synapse. These specialized contacts directly transfer highly controlled secretory signals between the adja-

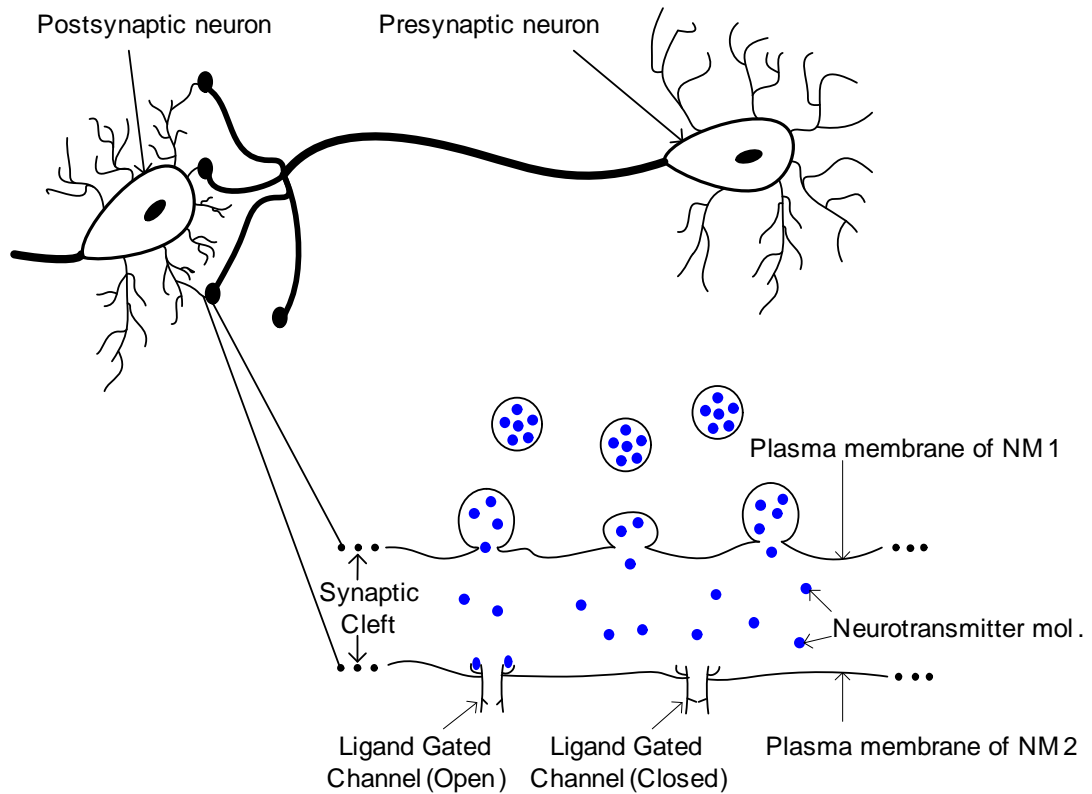


Figure 4.1: Neuro-spike transmission between nanomachines. Neurotransmitters emitted from the transmitter nanomachine (TN), diffuse through the gap between the nanomachines and reach the receiver nanomachine (RN).

cent cells [27]. The neuronal synapse is formed between the neurons and it retains the connectivity of the neuron cells throughout the life, whereas the immunological synapse is formed by the instant contacts of immune cells. Although nervous system and immune system have totally different roles in human life, in both systems cells need to communicate, and this is accomplished in the synapse. Therefore, synapses play a critical role in the cell-to-cell communication.

In nervous system, neural signals propagate in the form of electrochemical waves. These electrochemical waves are basically action potentials that propagate along axons and transmitted to other neurons. Action potential is basically an electrical pulse which has approximately 80 mV amplitude. At synapse, action potentials or *spikes* are transmitted from one neuron to another by electrochemical means. The signal is transmitted by means of chemical messengers called neurotransmitters. Neurotransmitters are contained in vesicles. The coming pulse or action potential, releases the neurotransmitters on the pre-synaptic neuron, and then, the neurotransmitters bind to

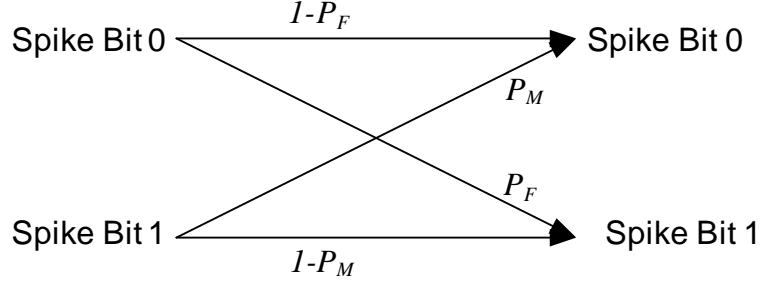


Figure 4.2: Channel model of synaptic transmission. Transmission probabilities are shown for the binary channel.

the receptors on the post-synaptic neuron. Binding of a neurotransmitter to a receptor opens a channel which lies between inside and outside of the post-synaptic neuron. These channels let the flow of ions to the neuron or out of the neuron. The net movement of ions causes the membrane potential of the post-synaptic neuron to change rapidly. In this way, spikes or action potentials are transmitted to the next neuron.

In this work, we adopt the principles of neural communication to our model. The communication between nanomachines is realized with spike transmission as shown in Fig. 4.1. The communication process based on molecular neuro-spike communication involves the following steps:

1. *Encoding*: Similar to the traditional digital communication, we define 2 bit levels, i.e., spike bit 0 and spike bit 1 corresponding to logic 0 and 1. The information is encoded on the concentration of the released neurotransmitter molecules. The transmission of consecutive spike bits are separated by a certain time interval. For spike bit 1, neurotransmitters are released to the channel, whereas for spike bit 0 no releasing occurs in the specified time interval.
2. *Transmission*: Actually, this process is the signaling initiation. Whenever a TN wants to send a spike bit 1, it simply activates the release of vesicles that contain neurotransmitters.
3. *Signal Propagation*: The released neurotransmitters propagate in the synaptic channel formed between the adherent nanomachines. The aim of the neurotransmitters is to bind to the receptors on the RN.
4. *Reception*: The neurotransmitters released into the synaptic channel reach the

RN and bind to the receptors on the RN plasma membrane as in Fig. 4.1. The binding of neurotransmitters to receptors opens ligand gated channels that let the flow of ions into or out of the RN. The flow of ions changes the membrane voltage.

5. *Decoding*: RN nanomachine monitors the plasma membrane voltage for the certain time interval specified in encoding stage. If RN observes a rapid change in the membrane voltage at this time interval it decides the received bit as spike bit 1, otherwise the decision is spike bit 0.

In an ideal channel, the spike bit sent by a transmitter nanomachine should be perfectly received by the receiver nanomachine. However, in practice there exist two kinds of errors as shown in Fig. 4.2, namely, false alarm and miss errors. Probabilities for these errors can be defined as

$$\begin{aligned}
 P_F &= Prob[Y = 1|X = 0] \\
 P_M &= Prob[Y = 0|X = 1]
 \end{aligned}
 \tag{4.1}$$

where  $X$  and  $Y$  are the input and output symbols, respectively. In order to derive these probabilities, a close look at neuronal synapse would be helpful. In [31], a cortical synapse is modeled as a binary channel and the information-theoretical capacity is derived for two different coding paradigms, i.e., signal estimation and signal detection. Although this synaptic transmission model ignores certain aspects like paired-pulse facilitation, vesicle depletion and calcium buffering, it represents a simplified and compact picture of synaptic transmission. Therefore, we adopt the synaptic transmission model in [31] and accordingly derive the channel capacity expression.

In Fig. 4.3, the block diagram of the channel model of synaptic transmission is shown [31]. The input to the channel,  $X(t)$ , is a spike bit. If the input is spike bit 1, vesicles containing neurotransmitters are released by the TN to the synaptic cleft. For spike bit 0, no vesicles are released.

Neurotransmitters binding to the receptors on the RN membrane open channels that let the flow of ions. The flow of ions create an Excitatory Postsynaptic Potential (EPSP) on the RN. In Fig. 4.3, EPSP profile or shape of RN is modeled by a filter with impulse response  $h(t)$  [31]. In Fig. 4.3, the random variable  $q$ , which has



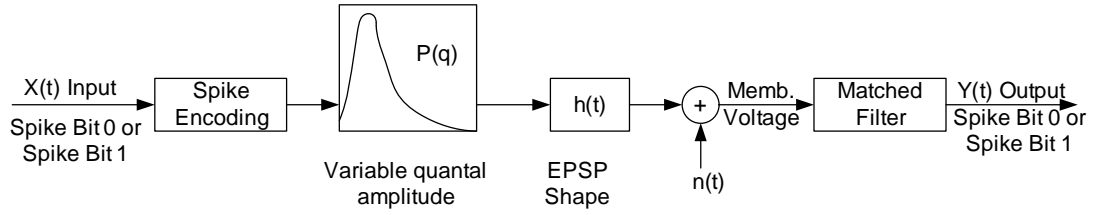


Figure 4.3: Block diagram of the channel model of synaptic transmission [31]. Spikes sent from the transmitter nanomachines pass through a filtering process and an additive gaussian noise is corrupted at the post-synaptic membrane. The decision by the receiver nanomachine is based on the matched filter.

probability density  $P(q)$ , models the variability in the size of EPSP. The number of neurotransmitter molecules released by the TN, the number of available postsynaptic receptors on the RN and several other factors are responsible for this variability. In Fig. 4.3, there exists also an additive noise,  $n(t)$ , coupled to the response of RN. The noise  $n(t)$  accounts for the other noise sources in the membrane of the RN such as thermal noise and channel noise [32].

## 4.2 Information Theoretical Capacity of Molecular Neuro-Spike Communication

For molecular neuro-spike channel, it is essential to investigate the channel properties and performance to enable communication with high capacity. Here, firstly, single spike bit error probability expression is derived. Secondly, channel capacity is discussed. Although, single spike bit error probability and channel capacity expressions are not be directly used in the analytical model of MAMNET, they give insight on the performance of molecular neuro-spike communication. Lastly, the probability of successful information transmission is derived to be used in the analytical model of MAMNET.

In molecular neuro-spike communication, at the receiver side, the aim is to optimally detect the presence or absence of a single spike through the knowledge of membrane voltage  $V_m(t)$  of RN. In [31], it is shown that the optimal decision rule is to compare the correlation  $r$  between  $V_m(t)$  and  $h(t)$  to a threshold  $\theta$ . Thus, the decision rule can

be written as

$$\begin{aligned} r \geq \theta &\Rightarrow Y = 1, \\ r < \theta &\Rightarrow Y = 0 \end{aligned} \quad (4.2)$$

With this decision rule, the false alarm and miss probabilities are written as

$$\begin{aligned} P_F &= \text{Prob}[r \geq \theta | X = 0] \\ P_M &= \text{Prob}[r < \theta | X = 1] \end{aligned} \quad (4.3)$$

In [31], the probabilities of miss and false alarm are derived for both stochastic and deterministic vesicle release processes. In our model, we use the probabilities derived for deterministic vesicle release, i.e.,

$$P_F = \frac{1}{2}[1 - \text{Erf}(\theta)] \quad (4.4)$$

$$P_M = \frac{1}{2} \left[ 1 + \int_0^\infty \text{Erf}(\theta - q\sqrt{SNR})P(q) dq \right] \quad (4.5)$$

where  $\text{Erf}(x)$  is the error function,  $\theta$  is the threshold used to decide whether spike is received or not, and  $SNR$  is the signal-to-noise ratio on the post-synaptic potential.

Based on the false alarm and miss probabilities, the molecular neuro-spike channel can now be modeled as a binary symmetric channel. TN emits spike bit 1 with probability  $p_1$  and spike bit 0 with probability  $(1 - p_1)$ . Then, the probability of error for one spike bit can be written as

$$P_E = p_1 P_M + (1 - p_1) P_F \quad (4.6)$$

The value of  $P_E$  depends both on the threshold  $\theta$  and  $SNR$ . For small values of  $\theta$ ,  $P_M$  is low whereas  $P_F$  is high. On the other hand, for large values of  $\theta$ ,  $P_F$  is low whereas  $P_M$  is high. Therefore,  $P_E$  should be evaluated with varying  $\theta$  in order to find an optimum value for  $\theta$ . In Fig. 4.4, the dependencies of  $P_E$ ,  $P_M$  and  $P_F$  on  $\theta$  are shown for a fixed value of  $SNR = 10$  assuming an equally-likely prior probability ( $p_1 = 0.5$ ).

The dependence of  $P_E$  on  $SNR$  is more obvious. With decreasing  $SNR$ , the probability of error increases. Furthermore,  $SNR$  also has an impact on the optimum value of

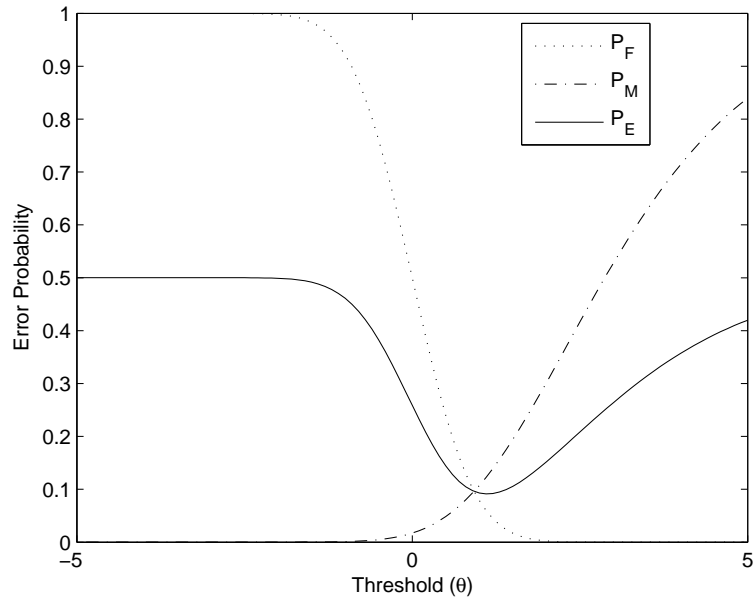


Figure 4.4: Plot of the false alarm, miss and channel error probabilities in molecular neuro-spike channel for a fixed value of  $SNR = 10$  with varying  $\theta$ . A prior probability of  $p_1 = 0.5$  is assumed.

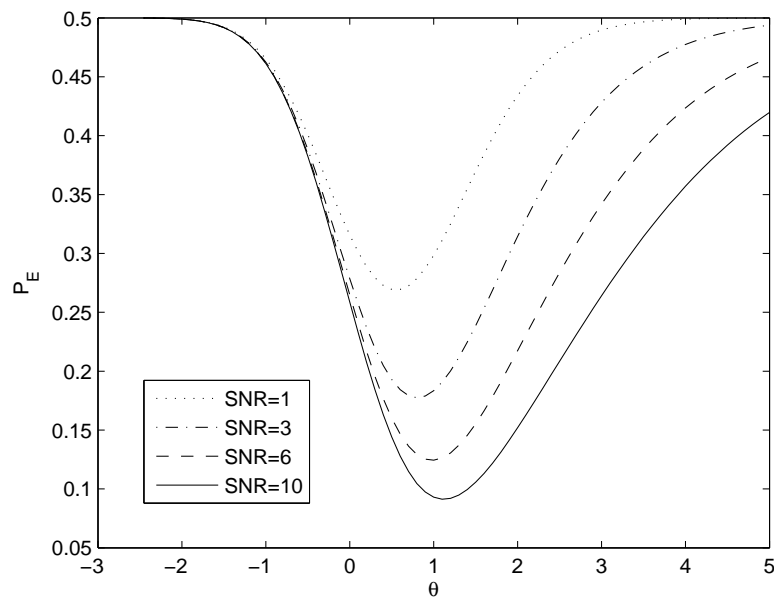


Figure 4.5: Plot of the channel error probability in molecular neuro-spike channel with varying  $\theta$  for different values of  $SNR$ . A prior probability of  $p_1 = 0.5$  is assumed.

threshold. As can be seen in Fig. 4.5, the optimum value of  $\theta$  becomes closer to 0 as the value of  $SNR$  decreases.

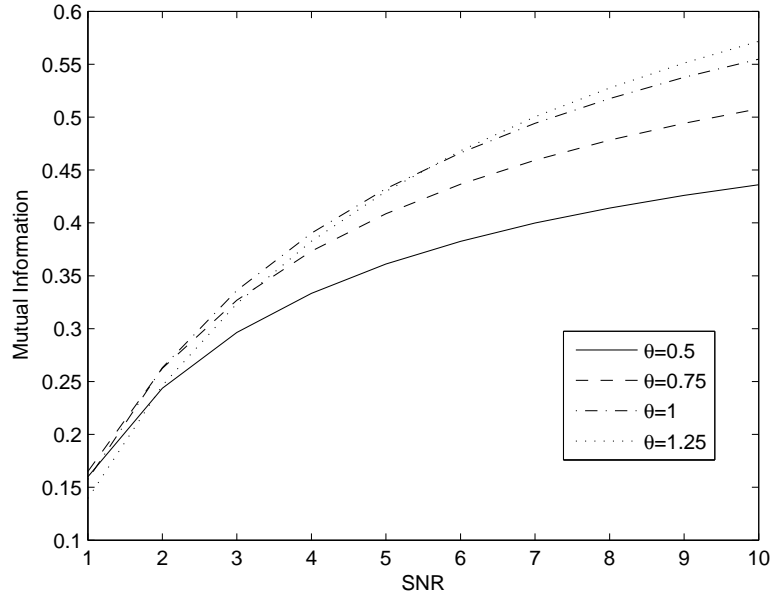


Figure 4.6: Plot of mutual information with varying  $SNR$  for different values of  $\theta$ . A prior probability of  $p_1 = 0.5$  is assumed.

The performance of the molecular neuro-spike communication can be further quantified by the mutual information. The transition matrix of the molecular neuro-spike channel can be written as follows

$$P(Y|X) = \begin{pmatrix} p_1(1 - P_M) & (1 - p_1)P_F \\ p_1P_M & (1 - p_1)(1 - P_F) \end{pmatrix} \quad (4.7)$$

Using the transition matrix in (4.7), the mutual information  $I(X; Y)$  between  $X$  and  $Y$  can be derived as follows

$$\begin{aligned} I(X; Y) &= H(Y) - H(Y|X) \\ &= H(p_1P_M + (1 - p_1)(1 - P_F)) - (p_1H(P_M) + (1 - p_1)H(P_F)) \end{aligned} \quad (4.8)$$

where  $H(z)$  denotes the binary entropy function  $H(z) = -z \log_2(z) - (1 - z) \log_2(1 - z)$ . Mutual information corresponds to how much one can guess about the input with the knowledge of the output.  $\theta$  and  $SNR$  have a direct effect on the value of mutual information. For low  $SNR$  values, mutual information can be very low. However, as  $SNR$  increases the mutual information increases as well, as shown in Fig. 4.6. The optimum value of  $\theta$  changes with  $SNR$ .

In a synaptic channel, spikes can be transmitted by 3 ms differences which is com-

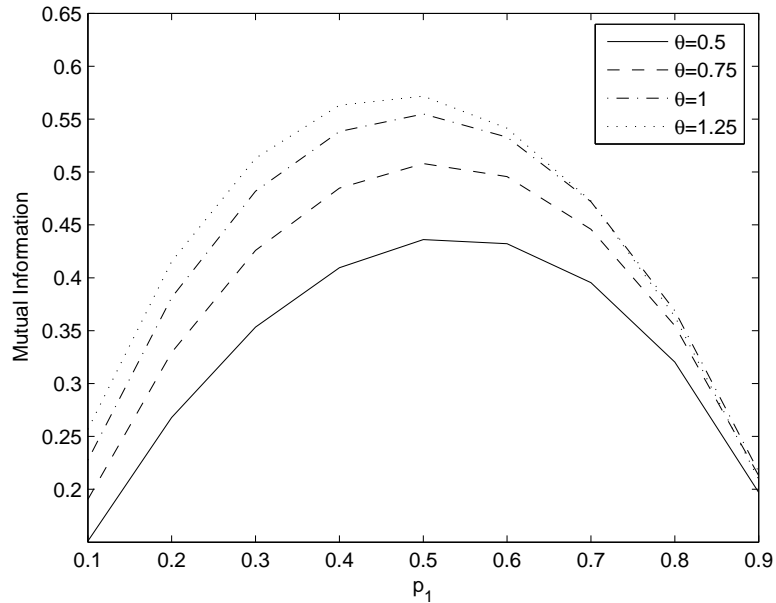


Figure 4.7: Plot of mutual information with varying  $p_1$  for different values of  $\theta$ . A high  $SNR$  value is assumed ( $SNR = 10$ ).

posed of a 0.5 ms action potential pulse and 2.5 ms of recovery time. Thus, a theoretical bandwidth of 333 bps can be reached. This corresponds to an ideal synaptic channel with  $I(X; Y) = 1$ , i.e., every bit transmitted contains exactly 1 bit of information. However, in practice there exist channel errors and this rate cannot be achieved.

The capacity of the molecular-neuro spike channel can be obtained by maximizing the mutual information over all input distributions, i.e.,

$$C = \max_{p_X}(I(X; Y)) \quad (4.9)$$

As can be seen in Fig. 4.7, the mutual information can be at most 0.57 for the channel under consideration. This corresponds to a bandwidth of approximately  $333 \times 0.57 \approx 190$  bps. Even if it is slightly larger than half of the ideal bandwidth of an ideal synaptic channel, it is a considerably high bandwidth.

By analyzing single spike bit error probability and channel capacity expressions, it is shown that molecular neuro-spike channel promises a reliable and fast communication. Therefore, molecular neuro-spike communication stands as a promising solution for the communication of adherent nanomachines in MAMNET. In evaluat-

ing the performance of MAMNET, information transmission probability is needed. Information transmission probability can be described as the successful transmission of all the information from TN to RN.

The information stored in the TN is encoded to spikes and sent to the RN. The probability of successful information transmission is analogous to the successful transmission of all spike bits in the message. Hence, successful information transmission probability is

$$R_t = (1 - P_E)^n \quad (4.10)$$

where  $n$  is the number of spike bits contained in the message. The probability in (4.10) represents the successful transmission probability of an information between adherent nanonodes and used in the analytical model of MAMNET.

## CHAPTER 5

### ANALYTICAL FRAMEWORK FOR MOBILE AD HOC MOLECULAR NANONETWORK

In this chapter, a closed form expression for the distribution of the delay in MAM-NET is derived. Furthermore, average throughput and system throughput expressions are obtained. The propagation of a single message is modeled using the principles of epidemic disease spreading. Because of the intermittent connectivity between nanomachines and infostations, intermediary nanomachines need to be used. For this purpose, a store-carry-forward scheme is proposed. When a nanomachine having an information encounters with another nanomachine that does not have a copy of the information, it forwards the information to the other nanomachine. This is analogous to epidemic disease spreading.

In mobile ad hoc networks, epidemic disease spreading techniques are already applied to the performance analysis of network architectures with intermittent connectivity [33], [34], [35]. By epidemic analogy, nanomachines can be in 3 different states, i.e., *infected*, *suspicious* and *recovered*. The message which should be transmitted to an infostation, is analogous to the agent of a disease. An infected nanomachine is the one that has a copy of the message. A nanomachine is said to be suspicious when it does not have a copy of the message, but could potentially acquire a copy of the message from the infected ones. A nanomachine is recovered after it has offloaded the message to the infostation.

Our model is developed upon the Markov model for the basic epidemic disease spreading [36]. In Fig. 5.1,  $S(t)$ ,  $I(t)$  and  $R(t)$  describes the numbers of susceptible, infected and recovered nanomachines, respectively. The model is based on three

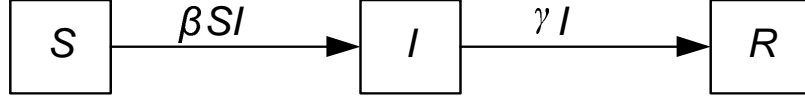


Figure 5.1: S-I-R Model. Markov chain model of an epidemic disease spreading. S, I, R represents the susceptible, infected and the recovered states respectively.

assumptions, which can be adopted for our model as follows.

- i. An infected nanomachine makes contacts, that are ended with the successful transmission of message, with  $\beta(N - 1)$  others per unit time where  $N$  represents the total number of nanomachines in MAMNET. Since  $S/(N - 1)$  proportion of these contacts are with the suspicious ones, the number of infections per unit time can be derived as  $(\beta(N - 1))(S/(N - 1))I = \beta SI$ .
- ii. A proportion  $\gamma$  of infected individuals leave the infected class per unit time.
- iii. The total number of individuals in the system is constant.

In MAMNET, by its definition, the parameter  $\beta$  contains collision ( $R_c$ ), adhesion ( $R_a$ ) and transmission rates ( $R_t$ ) for nanomachines. Therefore,  $\beta = R_c \times R_a \times R_t$ . On the other hand,  $\gamma$  represents the contact rate, that ends with successful transmission, between a nanomachine and an infostation. Therefore,  $\gamma = R_{ic} \times R_a \times R_t$ . If there are more than one infostation, the parameter  $\gamma$  should be multiplied by the number of infostations. This is because, the delivery of message to any infostation means recovery.

The first aim is to analytically obtain the cumulative distribution of the message delay in the network. The message delivery delay  $T_d$  is defined as the time elapsed from a packet is first generated by a nanomachine to the time when this packet is first offloaded to an infostation. The initial conditions for the system can be defined as follows. At time  $t = 0$ , only one nanomachine is infected, i.e.,  $I(0) = 1, S(0) = N - 1$ . Until offloading, the entire number of nanomachines  $N$  will be contained in either  $I$  state or  $S$  state, i.e.,  $S + I = N, R(t) = 0$  for  $t < T_d$ . At the time of offloading,  $R(T_d) = 1$ .

In order to find message delay distribution, we need the model until a copy of the



message is offloaded to any infostation, i.e., the transient solution of the Markov Chain in Fig. 5.1. The transient solution is the solution for the following differential equation:

$$\frac{dI}{dt} = \beta S I = \beta N I - \beta I^2 \quad (5.1)$$

With the initial condition of  $I(0) = 1$ , the solution of (5.1) is

$$I(t) = \frac{N}{1 + (N - 1)e^{-\beta N t}} \quad (5.2)$$

Using (5.1), the cumulative distribution function (CDF) of the message delay can be found. The CDF describes the probability that the message is transmitted to an infostation by time  $t$  and denoted by  $F(t) = Pr(T_d < t)$ . In [33], a similar discussion is followed about the delay distribution and  $F(t)$  is derived. Here, the argument in [33] is adopted. The aim is to find a differential equation for  $F(t)$  and solving it by the initial condition specified by the system.

The differential equation for  $F(t)$  can be written as

$$\frac{dF}{dt} = \lim_{\epsilon \rightarrow 0} \frac{F(t + \epsilon) - F(t)}{\epsilon} \quad (5.3)$$

where  $\epsilon$  is an arbitrary positive small number close to 0. Note that,  $F(t) = 1 - Pr(T_d > t)$  and  $F(t + \epsilon) = 1 - Pr(T_d > t + \epsilon)$ . In order to find  $F(t)$  using (5.3),  $Pr(T_d \geq t + \epsilon)$  is needed. Assuming  $Pr(\text{event in } [0, t])$  is independent of  $Pr(\text{event in } [t, t + \epsilon])$ ,

$$\begin{aligned} & Pr(T_d > t + \epsilon) | T_d > t \\ &= 1 - Pr(t < T_d < t + \epsilon | T_d > t) \\ &= 1 - \epsilon \gamma I(t) \end{aligned} \quad (5.4)$$

where  $\gamma I(t)$  is the offload rate. From (5.4),  $Pr(T_d > t + \epsilon)$  can be calculated as

$$\begin{aligned} Pr(T_d > t + \epsilon) &= Pr(T_d > t) Pr(T_d > t + \epsilon | T_d > t) \\ &= Pr(T_d > t) (1 - \epsilon \gamma I(t)) \end{aligned} \quad (5.5)$$

This can be used to derive the differential equation for  $F(t)$ , i.e.,

$$\begin{aligned} \frac{dF}{dt} &= \lim_{\epsilon \rightarrow 0} \frac{[1 - Pr(T_d > t + \epsilon)] - [1 - Pr(T_d > t)]}{\epsilon} \\ &= \lim_{\epsilon \rightarrow 0} \frac{-1}{\epsilon} Pr(T_d > t) (1 - \epsilon \gamma I(t) - 1) \\ &= \gamma I(t) Pr(T_d > t) \\ &= \gamma \frac{N}{1 + e^{-\beta N t} (N - 1)} [1 - F(t)] \end{aligned} \quad (5.6)$$

For the solution of (5.6), an initial condition is required. Note that,  $F(0)$  represents the probability that the nanomachine which generates the message is adherent with infostation such that it can directly transmit the message to the infostation. Therefore,  $F(0)$  can be given by

$$F(0) = \frac{4\pi(r_i^3 - r^3)}{3V} \quad (5.7)$$

Using the initial conditions specified,  $F(t)$  can be derived as

$$F(t) = 1 - K \left( \frac{N-1}{N-1 + e^{\beta N t}} \right)^{\frac{\gamma}{\beta}} \quad (5.8)$$

where  $K = \left[ \frac{N-1}{N} \right]^{\frac{\gamma}{\beta}} [1 - F(0)]$ . With this expression in hand, the probability that a message is transmitted to an infostation for a given time can be obtained. Inversely thinking, the average time needed to transmit the information to an infostation can also be calculated. Average delivery delay can be found using CDF of message delivery delay, i.e.,

$$\begin{aligned} E[T_d] &= \int_0^{\infty} 1 - F(t) dt \\ &= \int_0^{\infty} K \left( \frac{N-1}{N-1 + e^{\beta N t}} \right)^{\frac{\gamma}{\beta}} dt \end{aligned} \quad (5.9)$$

Assuming  $\gamma/\beta \in N^+$ ,  $E[T_d]$  can be analytically expressed as

$$E[T_d] = \begin{cases} \frac{F(0) \ln N}{\gamma(N-1)} & , \gamma/\beta = 1 \\ \frac{F(0)(1-N)}{\beta N^2} \left[ \sum_{k=2}^{\gamma/\beta} \frac{\beta}{\beta + \gamma - k\beta} \left( \frac{N}{N-1} \right)^k - \left( \frac{N}{N-1} \right)^{1+\gamma/\beta} \log N \right] & , \gamma/\beta \geq 2 \end{cases} \quad (5.10)$$

Note that, the analytical result in (5.10) are only valid for  $\gamma/\beta \in N^+$ . On the other hand, by numerically evaluating the integral in (5.9),  $E[T_d]$  can be calculated for any  $\gamma$  and  $\beta$ . The numerical results for average delivery delay are presented in Chapter 6.

Using the average delivery delay, average throughput of MAMNET can also be calculated. Considering from an infostation point of view,  $n$  spike bits are transmitted from a nanomachine source to an infostation in an average time of  $E[T_d]$ . Hence, the average throughput of MAMNET can be described as

$$T_{avg} = \frac{n}{E[T_d]} \quad (5.11)$$

On the other hand, considering the whole system, an average number of  $I(E[T_d])$  nanomachines get infected, i.e., apart from source, an average number of  $I(E[T_d]) - 1$  copies of the message exist in the network. This means that, an average of  $(I(E[T_d]) - 1) \times n$  spike bits are transmitted between nanomachines until the message arrives into an infostation. Also accounting for the  $n$  spike bits transmitted to infostation, the system throughput can be written as

$$T_{sys} = \frac{I(E[T_d])n}{E[T_d]} \quad (5.12)$$

Note that, results obtained integrate the models of collision, adhesion and molecular neuro-spike communication into a single framework. All aspects of MAMNET are covered by this model. The expressions derived for  $E[T_d]$ ,  $T_{avg}$  and  $T_{sys}$  clearly describe the performance of MAMNET. These expressions can be used to investigate the feasibility and evaluate performance of MAMNET. Using the model derived here, next, the performance of MAMNET is evaluated.

## CHAPTER 6

### PERFORMANCE ANALYSIS OF MOBILE AD HOC MOLECULAR NANONETWORK

In this chapter, we evaluate the performance of MAMNET by using average message delay and system throughput expressions derived in previous chapter. The variations of these performance metrics are observed with respect to communication and networking parameters in MAMNET. We use MATLAB to obtain analytical results. The aim is to investigate delay and throughput performance and gain insight on the feasibility of MAMNET. There are many parameters affecting the performance of MAMNET. The parameters used in the analysis are given in Table 1. In the following sections, the effects of these parameters are investigated.

#### 6.1 Effect of Relative Speed and Size of Nanomachines

We first observe the effect of relative speed and size of nanomachines on average delay and system throughput. Nanomachines and infostation are contained in a volume of  $10^6 \mu m^3$ . Nanomachine size is on the order of typical mammalian cells, i.e. having a diameter of 5-10  $\mu m$ . Since infostations have more complex roles than nanomachines, they are assumed to have larger dimensions than nanomachines, e.g., around 10-20  $\mu m$ .

In Fig. 6.1, Fig. 6.2 and Fig. 6.3, average message delay, average throughput and system throughput are shown for different  $r$  with varying  $E[v_m]$ , respectively. For  $r = 7.5 \mu m$ , average message delivery delay ranges from a few hundreds to a thousand seconds. Although these can be considered as huge message delays for traditional net-

Table 6.1: Simulation Parameters

<i>Radius of a nanomachine (<math>r</math>)</i>	7.5 ( $\mu\text{m}$ )
<i>Radius of an infostation (<math>r_i</math>)</i>	15 ( $\mu\text{m}$ )
<i>Average relative speed of nanomachines (<math>E[v_{nm}]</math>)</i>	1 ( $\mu\text{m}/\text{sec}$ )
<i>Average relative speed of nanomachines and infostation (<math>E[v_{ni}]</math>)</i>	1 ( $\mu\text{m}/\text{sec}$ )
<i>Volume (<math>V</math>)</i>	1000000 ( $\mu\text{m}^3$ )
<i>Area of contact (<math>A_c</math>)</i>	3 ( $\mu\text{m}^2$ )
<i>Surface density of receptors (<math>m_r</math>)</i>	100 ( $1/\mu\text{m}^2$ )
<i>Surface density of ligands (<math>m_l</math>)</i>	75 ( $1/\mu\text{m}^2$ )
<i>Forward binding rate (<math>k_f^0</math>)</i>	$1.32 \times 10^{-7}$ ( $\mu\text{m}^2/\text{sec}$ )
<i>Reverse binding rate (<math>k_r^0</math>)</i>	0.36 ( $1/\text{sec}$ )
<i>Contact time <math>\tau_c</math></i>	1 ( $\text{sec}$ )
<i>Minimum number of required bonds for proper adhesion (<math>c</math>)</i>	40
<i>Prior probability of sending spike bit 1 (<math>p_1</math>)</i>	0.5
<i>Threshold for decision of spike bit (<math>\theta</math>)</i>	1.1
<i>Signal to noise ration on RN (SNR)</i>	10
<i>Length of message (<math>n</math>)</i>	8 (bits)
<i>Number of nanomachines (<math>N</math>)</i>	20

works, these values are very reasonable for MAMNET. The volume in nanomachines contained is 565 times larger than a nanomachine volume. Furthermore, the average relative speed of nanomachines is very low. Hence, the collision rate in MAMNET is low, e.g., with the values specified in Table 6.1, on average, only 14 collisions occur between nanomachines in 1000 seconds. Therefore, it is reasonable to end up with message delays on the order of a few thousand seconds. The system throughput follows a similar argument. Considering the effect of low collision rate and the information message is encoded by 8 spike bits, it is also reasonable to encounter with a system throughput on the order of few spike bits per 10 seconds.

In Fig. 6.1, average message delivery delay decreases with increasing relative speed of nanomachines. On the other hand, in Fig. 6.2 and Fig. 6.3, average throughput and system throughput increase with  $E[v_{nm}]$ . This is because, by increasing the relative speed of nanomachines the collision rate is amplified and this causes more nanomachines to get infected. Therefore, the number of information transfers in MAMNET increases, which yields a higher throughput. Moreover, the message is delivered to an infostation more quickly.

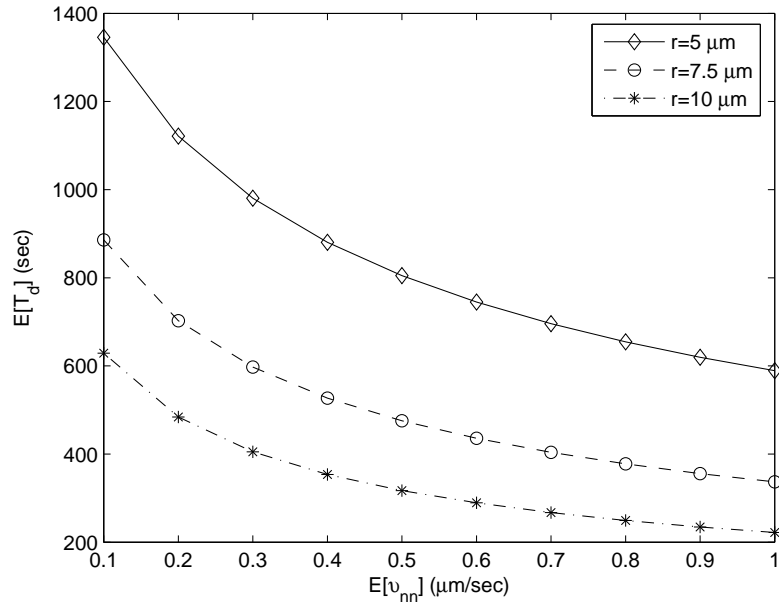


Figure 6.1: Average message delay with varying average relative speed of nanomachines for different values of nanomachine radius.

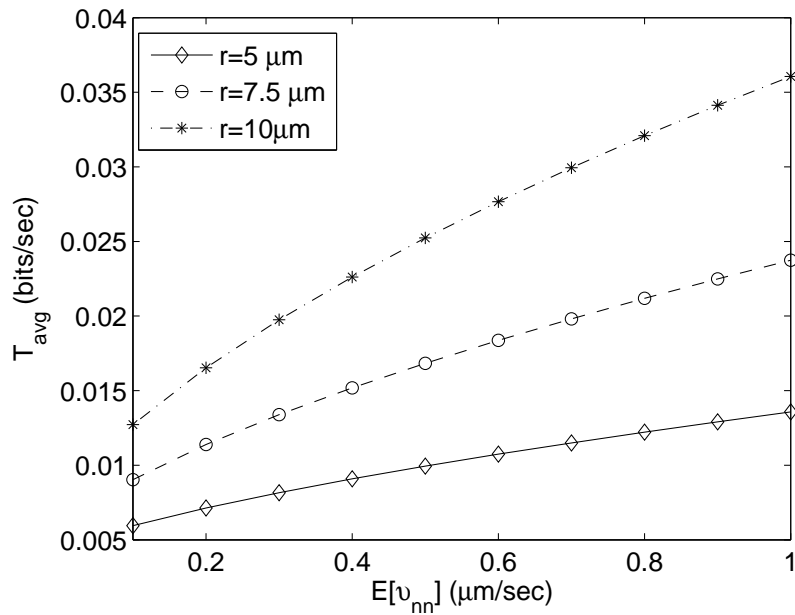


Figure 6.2: Average throughput with varying average relative speed of nanomachines for different values of nanomachine radius.

Fig. 6.1, Fig. 6.2 and Fig. 6.3 also show the effect of  $r$  on  $E[T_d]$  and  $T_{sys}$ , respectively. The increase in  $r$  also causes collision rate to increase and this yields a higher throughput and lower message delivery delay. Actually,  $r$  is analogous to the trans-

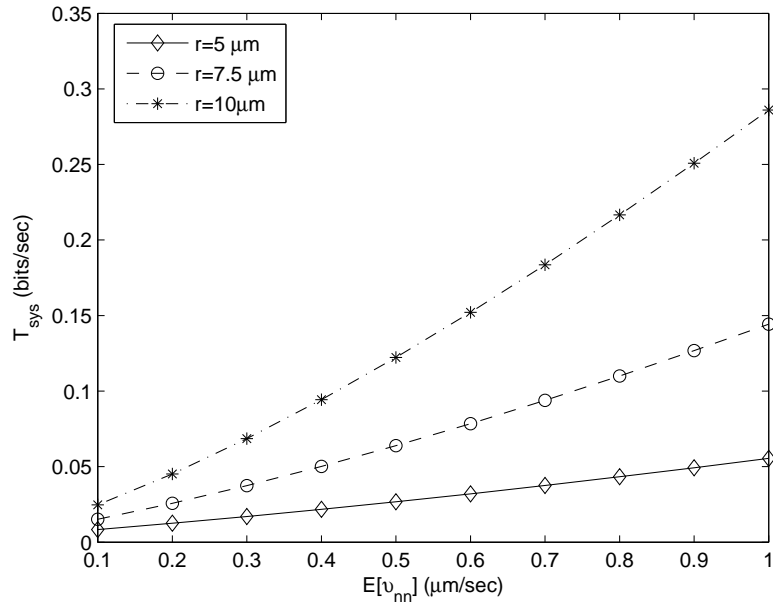


Figure 6.3: System throughput with varying average relative speed of nanomachines for different values of nanomachine radius.

mission range of mobile nodes in traditional mobile ad hoc networks. The larger the transmission range, the higher the probability of meeting of nodes. However, the transmission range is limited in traditional mobile ad hoc networks because of limited power. Similarly, it seems reasonable to make larger nanomachines to increase the performance, however, one has to consider that these nanomachines can be used in applications where the dimensions of the nanomachines is a critical issue.

## 6.2 Effect of Relative Speed and Size of Infostations

Here, the effects of relative speed and the size of infostations on performance are discussed.  $E[T_d]$ ,  $T_{avg}$  and  $T_{sys}$  are shown for different infostation radius values with varying relative speed in Fig. 6.4, Fig. 6.5 and Fig. 6.6, respectively. Increasing  $r_i$  and  $E[v_{ni}]$  increases the collision rate  $R_{ic}$  of nanomachines and infostation. Therefore, the interactions between nanomachines and infostation increase which further yield a better delay performance and higher system throughput.

However, the system throughput performance does not have such a direct relation.

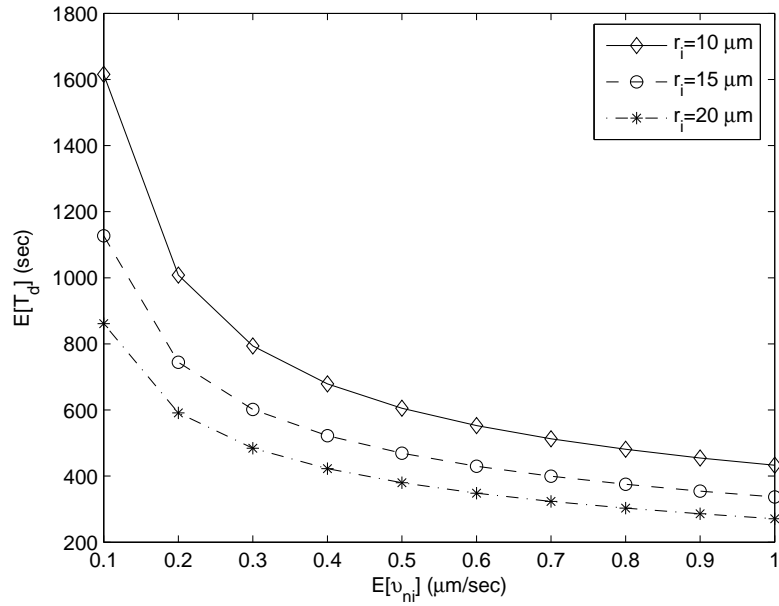


Figure 6.4: Average message delay with varying average relative speed of nanomachine and infostation for different values of infostation radius.

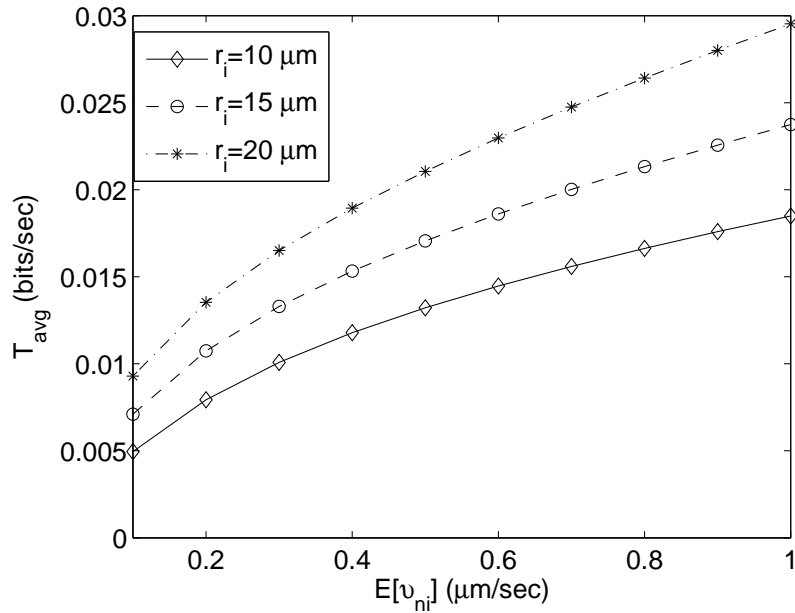


Figure 6.5: Average throughput with varying average relative speed of nanomachine and infostation for different values of infostation radius.

This is because, system throughput is defined as the average number of spike bits transmitted in the *system* until the offloading of a message. For  $E[v_{ni}] = 0.1$ , the collision rate of nanomachines and infostations are extremely low, creating a high



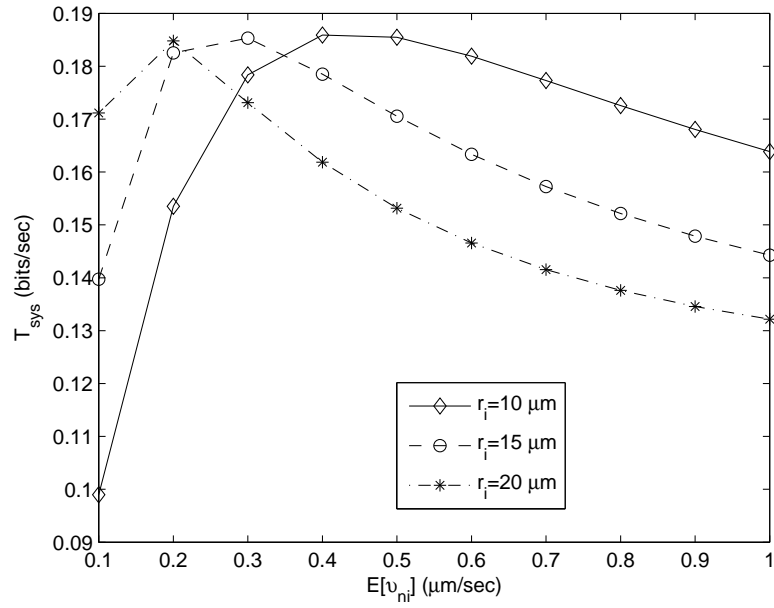


Figure 6.6: System throughput with varying average relative speed of nanomachine and infostation for different values of infostation radius.

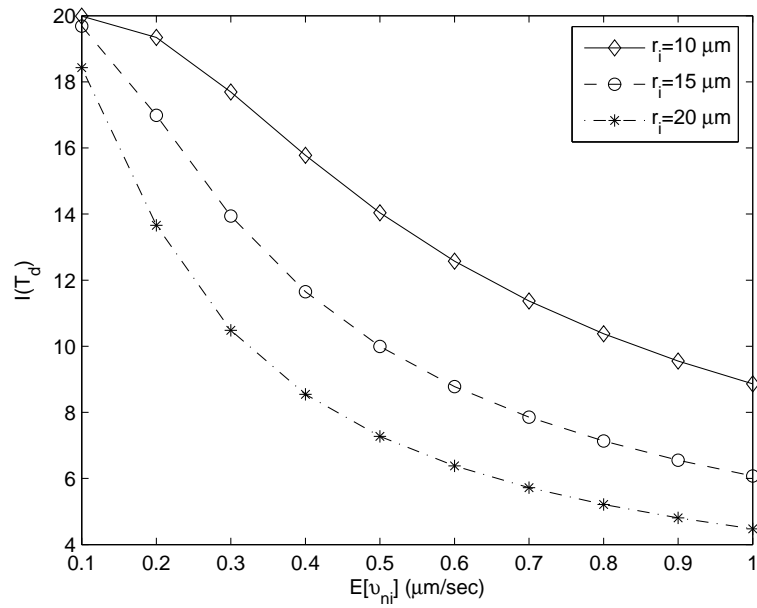


Figure 6.7: Average number of infected nanomachines at the instant of message delivery with varying average relative speed of nanomachine and infostation for different values of infostation radius.

message delivery delay. Until the delivery of the message almost all of the nanomachines get infected. Doubling  $E[v_{ni}]$  causes the message delivery delay to decrease

significantly. However, the number of infected nanomachines does not change at the same pace. Thus, the throughput increases significantly because of the significant decrease in average message delivery delay. Further increasing of  $E[v_{ni}]$  causes message delivery delay to decrease, and also the number of infected nanomachines decreases as well. Therefore, the system throughput performance decreases.

### 6.3 Effect of Contact Time

In Fig. 6.8, average message delay and system throughput are shown with varying contact time. A long contact time yields a high adhesion probability. Therefore,  $E[T_d]$  decreases and  $T_{sys}$  increases with increasing  $\tau_c$ . In Fig. 6.8, after a certain value of  $\tau_c$ , the performance of MAMNET does not change. The reason for that can be observed more clearly in Fig. 6.9. The contact time of nanonodes has only an effect on the adhesion probability. Actually, at  $\tau_c = 1.1$  second, the adhesion probability becomes 1, and after that point, the adhesion rate does not change. For  $\tau_c = 0.75$  second, adhesion probability ( $R_a$ ) is 0.3, i.e., approximately one third of the collisions are resulted in successful adhesion. On the other hand, for  $\tau_c = 1.1$ ,  $R_a = 1$ , i.e., all the collisions are resulted in successful adhesion. Thus,  $E[T_d]$  and  $T_{sys}$  become constant after  $\tau_c = 1.1$  second.

### 6.4 Effect of Number of Bonds Required for Successful Adhesion

Another critical parameter defined in Chapter 3 is the number of bonds required for successful adhesion. The effect of number of bonds required for successful adhesion on MAMNET performance is analyzed in Fig. 6.10. With the increase in the number of bonds required for successful adhesion, the adhesion of nanomachines becomes more difficult. Therefore, the adhesion probability decreases, which implies a decrease in the interaction of nanomachines. Hence, average message delivery delay increases and system throughput decreases with increasing number of bonds required for successful adhesion.

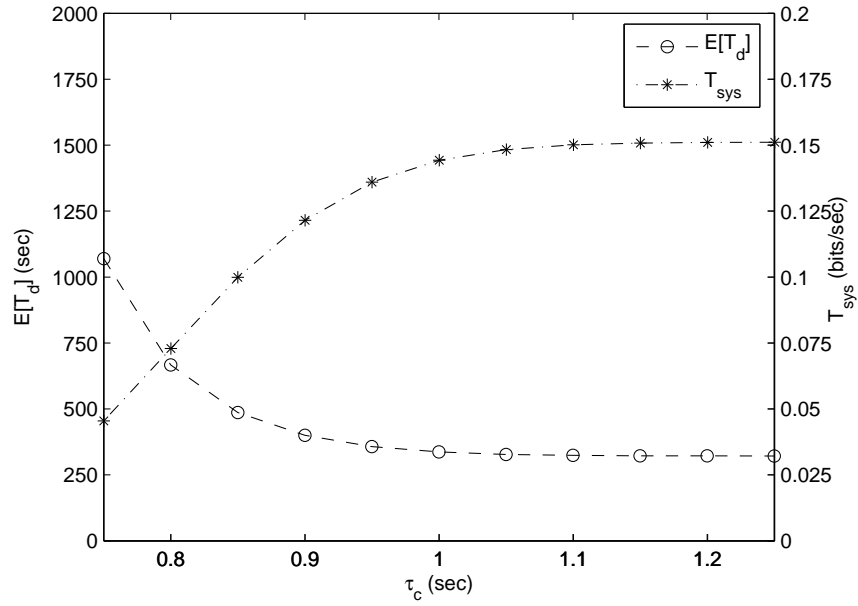


Figure 6.8: Average message delay and system throughput with varying contact time.

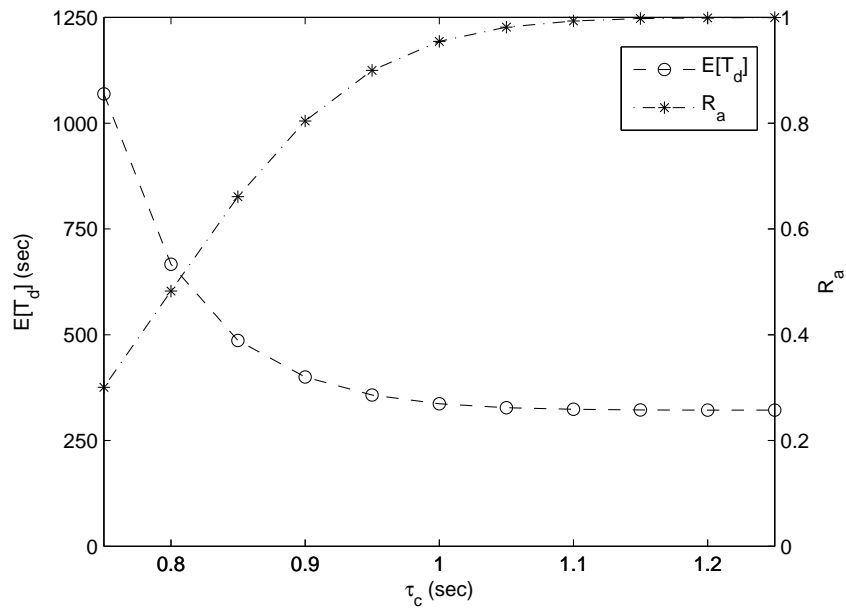


Figure 6.9: Adhesion probability and average message delay with varying contact time.

### 6.5 Effect of Molecular Neuro-Spike Communication Parameters

Here, the effects of molecular neuro-spike communication parameters on MAMNET performance are explored. Synaptic variability, threshold used for spike detection and

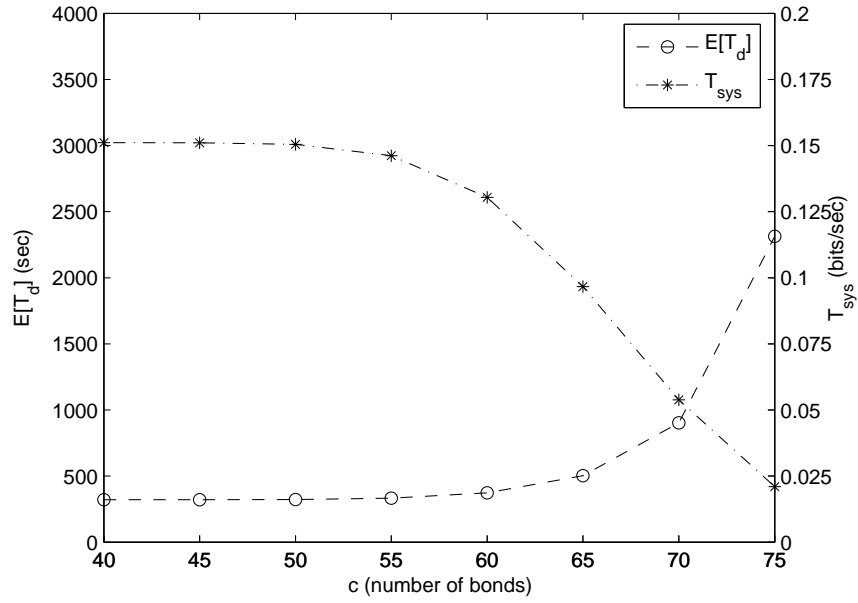


Figure 6.10: Average message delay and system throughput with varying number of bonds required for proper adhesion.

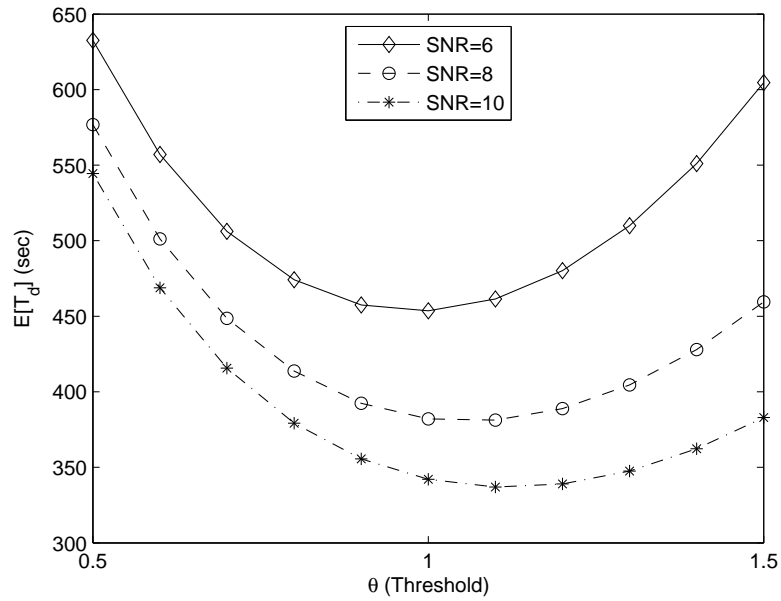


Figure 6.11: Average message delay with varying threshold value for different values of SNR.

signal-to-noise ratio on post-synaptic potential affect molecular neuro-spike communication and thus, MAMNET performance.

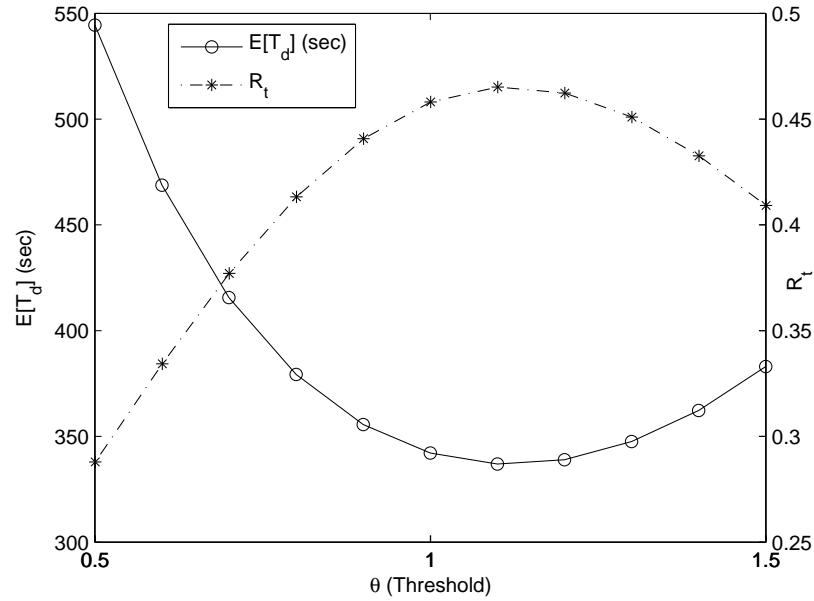


Figure 6.12: Average message delay and transmission probability with varying threshold value.

In Fig. 6.11, average message delivery delay is shown with varying  $\theta$  for different  $SNR$ . The effect of  $SNR$  on delay performance is obvious. With decreasing  $SNR$ , the transmission probability of information decreases and this yields higher delays. The effect of the threshold used for spike detection is more complicated. In Chapter 4, it is pointed out that the choice of the threshold for detection of spikes is very important for molecular neuro-spike communication. There exists a critical value for  $\theta$  to achieve a high channel performance. In Fig. 6.11, the average message delivery delay decreases until a certain value of  $\theta$ . After that point,  $E[T_d]$  start to increase. This is because of the effect of  $\theta$  on transmission probability. In Fig. 6.12, the effects of the threshold used for spike detection on transmission probability and average message delivery delay are shown. It can be seen that, there exists a different critical value of  $\theta$  which makes the transmission probability maximum.

Similar arguments follow for the average throughput and system throughput. The threshold value that makes the transmission probability maximum also maximizes the throughput. In Fig. 6.13 and 6.14, a reverse hook shape exists for the average throughput and system throughput with varying threshold. From Fig. 6.11, Fig. 6.13 and Fig. 6.14, we deduce that the critical value of threshold slightly changes with

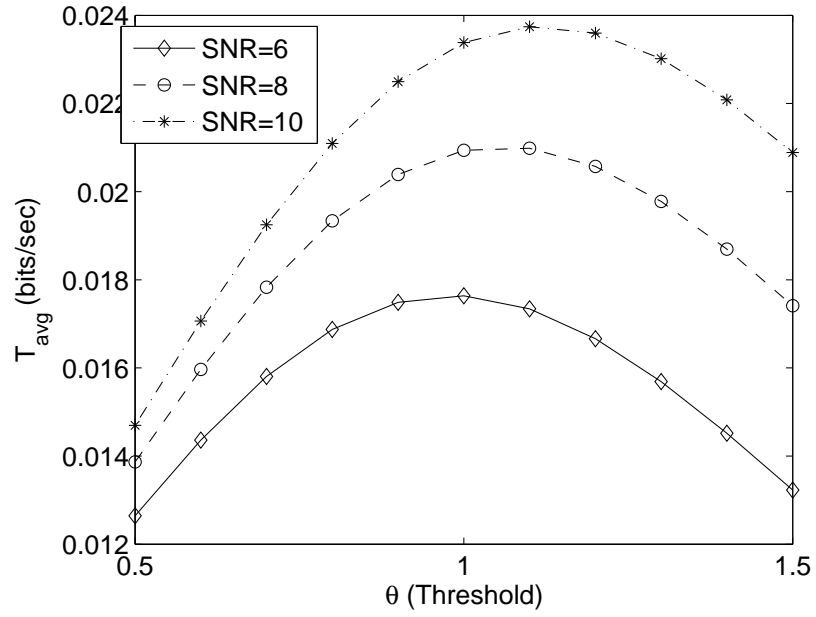


Figure 6.13: Average throughput with varying threshold value for different values of SNR.

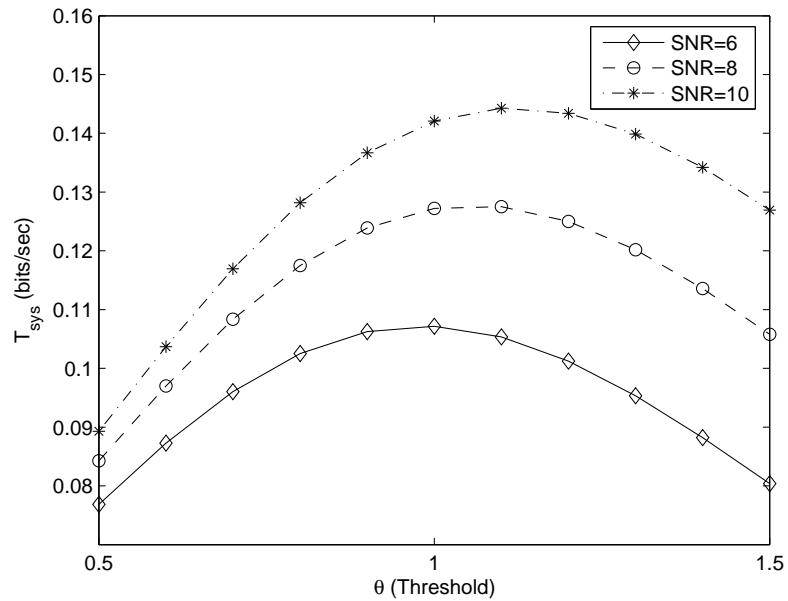


Figure 6.14: System throughput with varying threshold value for different values of SNR.

different *SNR* values. Therefore, a threshold that goes well with all *SNR* values should be chosen to achieve low message delivery delay and high system throughput.

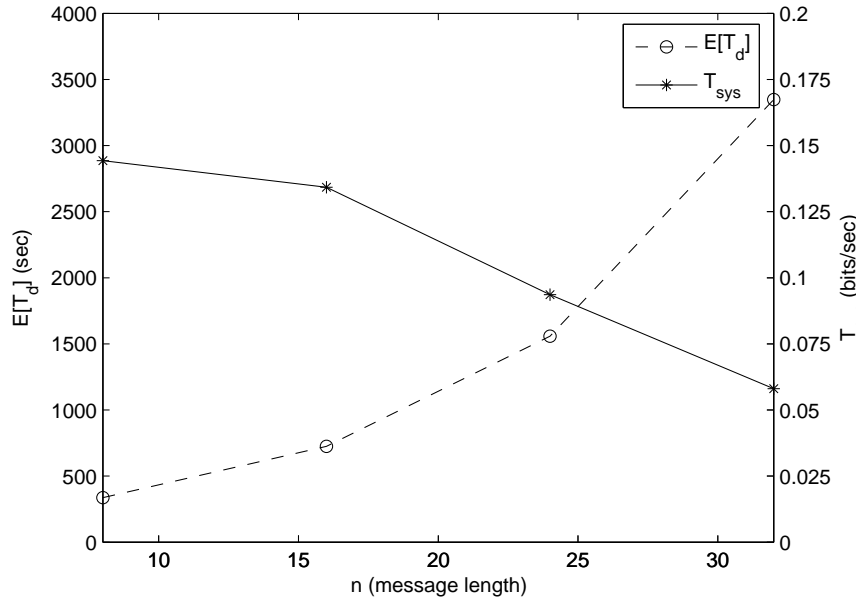


Figure 6.15: Average message delay and system throughput with varying number of spike bits contained in the message.

## 6.6 Effect of Number of Spike Bits Contained in a Message

The number of spike bits used to encode a message is a critical parameter. Because of the limited capabilities of nanomachines, we do not expect them to generate a large amount of information. Nanomachines sensing the environment generate information about the observed phenomena. The information generated by nanomachines is on the order of a few dozen of spike bits. The predefined message strings, and their length are determined before the deployment, and hence, nanomachines are accordingly programmed. The length of the messages depends on the diversity of the phenomena that is desired to be observed in the deployment environment, e.g., with 8 bits 256 different phenomena can be represented.

In Fig. 6.15, the performance of MAMNET is shown for varying  $n$ . With increasing  $n$ , the performance of MAMNET decreases. This is due to the decreased transmission probability of a message. Note that, the successful transmission probability of a message given in (4.10) exponentially decreases with increasing message length. This causes fewer nanomachines to get infected, and eventually, a higher message delivery delay. On the other hand, having more number of spike bits transmitted in a single

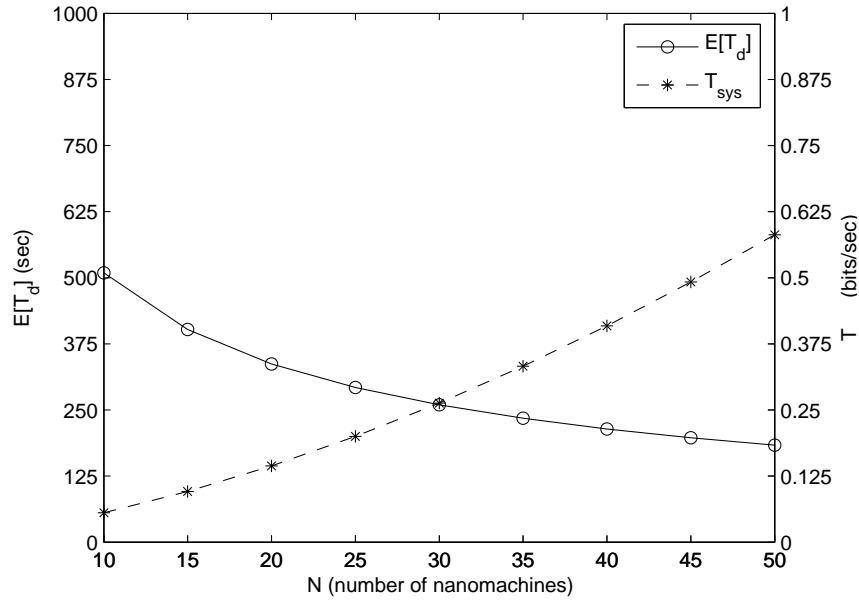


Figure 6.16: Average message delay and system throughput with varying number of nanomachines.

message, one can expect a higher system throughput. However, the decrease in the successful message transmission probability overcomes the increase in the number of spike bits contained in a message. Therefore, system throughput decreases with increasing number of spike bits contained in a message.

## 6.7 Effect of Number of Nanomachines

The number of nanomachines in MAMNET is also a critical parameter for the performance MAMNET. In Fig. 6.16, average message delay and system throughput are shown for varying number of nanomachines. The increasing number of nanomachines increases the connectivity in MAMNET. Therefore, the message can be delivered to an infostation in a lower time. Furthermore, the system throughput increases with increasing number of nanomachines.



## CHAPTER 7

### CONCLUSIONS AND FUTURE WORK

The network of mobile nanomachines is an unexplored area and promising many applications. Since the traditional communication and networking paradigms are not suitable for nanomachines, new communication and networking paradigms should be proposed for the realization of nanonetworks.

In this work, using the stochastic models for collision and adhesion of nanomachines we first derive the rates for the interaction of nanomachines. Then, using the principles of neural communication we provide a new communication paradigm for the realization of mobile ad hoc molecular nanonetworks. We also investigate the performance of molecular neuro-spike channel model by examining single bit error probability and mutual information. Then we model the flow of a single message in MAMNET by using the principles of infectious disease spreading.

We evaluate the performance of MAMNET based on average message delivery delay and system throughput expressions. Our models and numerical analysis clearly show that a mobile ad hoc nanonetwork can be realized with sufficiently low message delivery delay and sufficiently high system throughput. Numerical results also reveal that it is imperative to efficiently and effectively regulate the parameters to achieve better performance. Therefore, the most efficient parameters should be investigated for the application under consideration. The design scheme should select the parameters according to the environmental factors and application dependent requirements.

The main challenge in realizing nanonetworks is the development of nanomachines. Currently, there is a significant research going on the development of hardware components of nanomachines, namely, nanosensors, nanoactuators, nanobatteries and

nanoprocessors. However, for the time being there is no nanomachine that integrates all the hardware components [14].

The bio-hybrid approach for developing nanomachines requires extensive synergy of the knowledge of biology and nanotechnology. First of all, models of biological systems should be developed in detail. Once the models are developed and the operation of biological systems are fully understood, it is essential to develop biological and electronics interfaces. Then, the integration of the biological and electronics components would be possible, which enables the development of new and unlimited applications.

The information and communication technologies have a key role in realizing nanonetworks. Once the nanomachines are built, the information and communication technologies should be ready to enable reliable communication between nanomachines. Molecular neuro-spike communication is a promising solution. However, there are some open issues as well. For example, in encoding stage clearly a method to transform the information stored in a nanomachine to a molecular signal is needed. Similarly, in decoding stage a method for transforming the action potential to the information to be stored in nanomachine is needed.

The small dimensions of nanomachines can enable many new applications that imposes size restrictions. For example, nanomachines deployed to human blood stream can be used in health care applications by monitoring certain parameters in blood. However, the small size of nanomachines also makes them susceptible to external forces, which can be seen as a drawback. Therefore, in designing nanonetworks the susceptibility of nanomachines to environmental factors should be considered.

The introduction of simulation tools for networks was a cutting edge for network design. Similarly, for nanonetworks, the development of simulation tools is very essential to evaluate the performance of nanonetwork models. The existing biological simulation models and network simulation tools should be wrapped to develop simulation tools for nanonetworks. With this simulation tools, researches can able to model nanomachines, molecular communication processes, network traffic, noise sources, etc. [15].

Mobile ad hoc molecular nanonetworks can enable many applications. For example, mobile nanomachines can be used in the immune system support. They can be programmed to detect certain agents and inform a central control about the agents. This enables early diagnosis and increases the chance of treatment of the disease. MAMNET can also be used in the food and water quality control. With the rapid contamination of our globe, it is becoming more and more important to control the quality of foods and water. Nanomachines can also be used to detect chemical or biological agents in foods and water.

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