

# Fundamentals of Diffusion-Based Molecular Communication in Nanonetworks

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## Abstract

Molecular communication (MC) is a promising bio-inspired paradigm for the interconnection of autonomous nanotechnology-enabled devices, or nanomachines, into nanonetworks. MC realizes the exchange of information through the transmission, propagation, and reception of molecules, and it is proposed as a feasible solution for nanonetworks. This idea is motivated by the observation of nature, where MC is successfully adopted by cells for intracellular and intercellular communication. MC-based nanonetworks have the potential to be the enabling technology for a wide range of applications, mostly in the biomedical, but also in the industrial and surveillance fields. The focus of this article is on the most fundamental type of MC, i.e., diffusion-based MC, where the propagation of information-bearing molecules between a transmitter and a receiver is realized through free diffusion in a fluid. The objectives of the research presented in this article are to analyze an MC link from the point of view of communication engineering and information theory, and to provide solutions to the modeling and design of MC-based nanonetworks. First, a deterministic model is realized to study each component, as well as the overall diffusion-based-MC link, in terms of gain and delay. Second, the noise sources affecting a diffusion-based-MC link are identified and statistically modeled. Third, upper/lower bounds to the capacity are derived to evaluate the information-theoretic performance of diffusion-based MC. Fourth, an analysis of the interference produced by multiple diffusion-based MC links in a nanonetwork is provided. This research provides fundamental results that establish a basis for the modeling, design, and realization of future MC-based nanonetworks, as novel technologies and tools are being developed.

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# 1

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## Introduction

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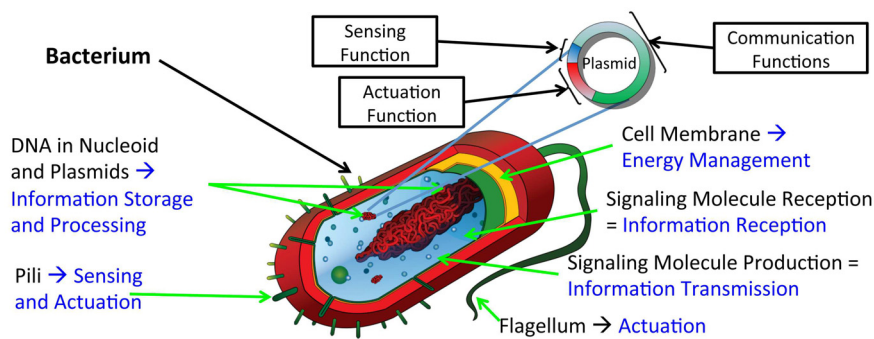
Molecular communication (MC) [2] is a bio-inspired paradigm where the exchange of information is realized through the transmission, propagation, and reception of molecules. This paradigm was first studied in biology, since it is successfully adopted in nature by cells for intracellular and intercellular communication [73]. MC is considered a promising option for communications in nanonetworks [5], which are defined as the interconnections of intelligent autonomous nanometer-scale devices, or nanomachines. Thanks to the feasibility of MC in biological environments, MC-based nanonetworks have the potential to be the enabling technology for a wide range of applications [5], mostly in the biomedical, but also in the industrial and surveillance fields. The objectives of the research presented in this article are to analyze the MC paradigm from the point of view of communication engineering and information theory, and to provide solutions to the modeling and design of MC-based nanonetworks.

## 1.1 Biological Nanomachines and Nanonetworks

Among the more promising research fields of today, nanotechnology is enabling the manipulation of matter at an atomic and molecular scale, from one to a hundred nanometers. One of the goals of nanotechnology is to engineer functional systems based on the unique phenomena and properties of matter at the nanoscale [32]. Currently, a great research effort is spent in the attempt to realize nanoscale machines, also called molecular machines or nanomachines, defined by E. Drexler as “mechanical devices that perform useful functions using components of nanometer-scale and defined molecular structure” [33]. More specifically, nanomachines [5, 3, 4] are expected to have the ability to sense, compute, actuate, manage their energy, and interconnect into networks, termed nanonetworks, to overcome their individual limitations and benefit from collaborative efforts.

Two main types of nanomachines can be identified within the aforementioned definition, namely, synthetic and biological. On the one hand, the synthetic nanomachines are realized either by downscaling from the current micro-scale technologies, such as microelectronics or micro-electro mechanics, or through the use of chemically synthesized nanomaterials [3]. On the other hand, the biological nanomachines are realized either by reusing biological components (e.g., DNA-based memories [52], flagellum-based actuators [18]), or by programming the behavior of biological cells from nature, such as through the genetic engineering of bacteria [41], as illustrated in 1.1.

While the engineering of fully synthetic nanomachines is still in its infancy, the research on the genetic engineering of biological cells is currently in rapid progress, thanks to the advancements made by biotechnology [16]. Several key techniques developed under the umbrella of synthetic biology have made possible today the realization of simple biological nanomachines [87]. As illustrated in Figure 1.1, through the insertion of engineered genetic code in the form of a circular DNA strand (i.e., plasmid) in a bacterium, it will be soon possible to program complete functions, including sensing, actuation, and communication, and have access to the main functionalities of the cell, such as the storage and the processing of information through DNA code, the



**Figure 1.1:** The expected functions of a biological nanomachine realized through the genetic engineering of a bacterium.

sensing and actuation through the use of the *pili* (hairlike appendages), the management of the cell energy through the cell membrane, and the transmission and reception of information through the production and the reception of signaling molecules.

The exchange of information between nanomachines, and their interconnection into nanonetworks, is key to overcome their individual limitations in size, energy and computational capabilities, and benefit from collaborative efforts. In nanonetworks, the applicability of classical communication technologies is limited by several constraints. In particular, the very restricted size of the nanomachines and the peculiarities of the environments in which they are envisioned to operate (e.g., biological scenarios) demand for novel solutions from the perspective of both the choice of the communication medium and the study of suitable communication techniques. While a possible solution to the problem of communication between synthetic nanomachines is suggested by recent studies [3] on nano-structures and on the properties of carbon nano-electronics, the imminent availability of biological nanomachines encourages to study and adopt the communication techniques naturally adopted by biological cells. In this direction, the **Molecular Communication (MC) paradigm**, inspired by the natural cell communication in biology, where message-carrying molecules are synthesized, emitted, collected, and converted to cellular responses through biochemical processes, is expected to be especially attractive

because of its inherent feasibility in a biocompatible environment [2, 5].

## 1.2 Potential Applications of Nanonetworks Enabled by Molecular Communication

Given the tight integration of MC within the biological environment and its feasibility at the cellular scale (nm -  $\mu\text{m}$ ), MC is studied not only as a candidate for nanonetwork communication, but also as a possible tool for the future nanonetworks to interact with the living organisms and their biological processes. As a consequence, the number of potential applications of MC-enabled nanonetworks is very large. Amongst others, the following three main areas deserve a special attention.

**Biomedical applications**, such as disease control and infectious agent detection [93], smart drug delivery systems [43], and intelligent intrabody systems for monitoring glucose, sodium, and cholesterol [34, 60]. These applications are expected to greatly benefit from the use of nanomachines deployed over the body (e.g., through tattoo-like patches) or inside the body (e.g., through pills or intramuscular injection). Since MC is naturally adopted by cells, nanonetworks enabled by this paradigm are envisioned to better integrate with the intra-body biological processes and to show higher biocompatibility when compared to other possible solutions.

**Industrial applications**, such as the monitoring and control of microbial formations. As an example, applications based on bacterial biofilms [27], which are used to clean residual waters coming from different manufacturing processes or to treat organic waste [56], could be greatly enhanced by MC-enabled nanonetworks, since microbial organisms naturally produce and respond to molecular stimuli.

**Surveillance applications** will make use of biological and chemical nanosensors that have an unprecedented sensing accuracy [85, 95]. Nanonetworks composed by several MC-enabled nanosensors could serve for surveillance against biological and chemical attacks [95] by detecting toxic or infectious agents diffusing in the environment.

### 1.3 Research Objectives and Solutions

The focus of this article is on diffusion-based MC, where the propagation of information-bearing molecules between a transmitter and a receiver is realized through free diffusion in a fluid. This choice is motivated by a preliminary analysis, detailed in Chapter 2, which identifies the diffusion-based as the most fundamental type of MC among different options suggested in the literature. As a consequence of the differences between the diffusion-based MC paradigm and classical electromagnetic communication paradigms, the classical communication engineering models and techniques are not directly applicable for the study and the design of diffusion-based MC-enabled nanonetworks. These differences include, but are not limited to, the following:

- The process of diffusion-based molecule propagation is based on radically different phenomena with respect to the electromagnetic wave propagation in classical communication systems. While electromagnetic waves operate the propagation of energy at the speed of light, the molecule diffusion process is caused by the random walk of the molecule Brownian motion in a fluid [76, 29]. As a consequence, while an electromagnetic wave propagates in a defined direction, and with negligible delay for most of the terrestrial communication systems, molecules subject to Brownian motion propagate with a random direction and with a high delay for almost all the transmission ranges of interest.
- The biologically-inspired physical processes that can be adopted to transmit and receive information in a diffusion-based MC-enabled nanonetworks are based on different mechanisms with respect to the modulation and reception of electromagnetic radiations in classical communication systems. While in classical systems antennas transmit and receive electromagnetic radiations through moving charges in metallic conductors, in biological cell bio-signaling [73] information is transmitted through the chemical synthesis of signaling molecules, and received through chemical reactions between incoming signaling molecules and chemical receptors.

As a consequence, there is a need of to build a complete understanding of the diffusion-based MC paradigm from the ground up. The research objectives addressed in this article, and the proposed solutions, have been identified to specifically target this need, and they are summarized as follows. The first research objective is to develop of a deterministic model of diffusion-based MC link, which provides a mathematical characterization of the main physical processes involved in the transmission, propagation, and reception of molecules for the exchange of information between a transmitter and a receiver. The second research objective is to identify and stochastically model the noise sources that affect a diffusion-based MC link. The third research objective is to provide an estimate of the achievable performance of a diffusion-based MC link in terms of information capacity. The fourth research objective is to analyze the interference produced by multiple diffusion-based MC links when present at the same time in a nanonetwork.

#### 1.4 Article Outline

The rest of this article is organized as follows. A preliminary analysis of different MC options from the literature is contained in Chapter 2, which also includes a survey of the results from previous works pertinent to the study of diffusion-based MC. The results obtained through the design and end-to-end modeling of a basic diffusion-based-MC link are presented in Chapter 3, where the contributions of each component of the system are analyzed in terms of gain and delay. In Chapter 4, the most relevant noise sources affecting a diffusion-based MC link are studied through the mathematical expression of their underlying physical processes, and modeled through the use of statistical parameters. Analytical expressions of upper and lower bounds to the information capacity of a diffusion-based MC link are derived in Chapter 5, first by using tools from thermodynamics, and then through a pure information-theoretic approach. In Chapter 6, an analysis of the interference produced by multiple diffusion-based MC links in a nanonetwork is detailed. Finally, a conclusion with the possible future avenues for this research field is provided in Chapter 7.

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