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Exploring the Physical Channel of Diffusion-based Molecular Communication by Simulation

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***Abstract*—Diffusion-based molecular communication is a promising bio-inspired paradigm to implement nanonetworks, i.e., the interconnection of nanomachines. The peculiarities of the physical channel in diffusion-based molecular communication require the development of novel models, architectures and protocols for this new scenario, which need to be validated by simulation. With this purpose, we present *N3Sim*, a simulation framework for diffusion-based molecular communication. *N3Sim* allows to simulate scenarios where transmitters encode the information by releasing molecules into the medium, thus varying their local concentration. *N3Sim* models the movement of these molecules according to Brownian dynamics, and it also takes into account their inertia and the interactions among them. Receivers decode the information by sensing the particle concentration in their neighborhood. The benefits of *N3Sim* are multiple: the validation of channel models for molecular communication and the evaluation of novel modulation schemes are just a few examples.**

I. Introduction

Nanotechnology, the study of nanometer-scale systems, is a multidisciplinary research area with potential applications in the biomedical [1], environmental [2] and industrial fields [3]. A nanomachine is the most basic functional unit able to perform very simple tasks at the nanoscale, including computing, data storage, sensing, actuation and communication.

Nanonetworks, the interconnection of nanomachines, has emerged as a novel research field which has attracted the interest of researchers from the domains of information and communication technology, nanotechnology and biology. One of the main envisaged applications of nanonetworks is in the field of Wireless NanoSensor Networks (WNSN) [4]. A proof of the thriving research activity in this area is the recent appearance of dedicated journals [5] and the organization of specialized workshops and conferences [6].

Nanonetworks will provide means for cooperation and information sharing among nanomachines, allowing them to fulfill more complex tasks. Current communication techniques, such as electromagnetic, mechanical or acoustic communication, cannot be applied at the nanoscale [7]. In consequence, several alternative methods have been proposed to interconnect nanomachines, leading to two novel paradigms to implement communications at the nanoscale: molecular communication [7] and graphene-based electromagnetic communication [8].

In molecular communication, different methods are applied depending on the distance between emitters and receivers. These methods can be classified in three alternatives: short-range (nm to μm), medium-range (μm to mm) and long-range (mm to m). For the *short range*, two methods have been proposed [7]. The first one is molecular signaling, consisting in encoding the information into molecules which are emitted into the medium. The second is based on molecular motors, i.e., protein complexes that are able to transport molecules through microtubules. Two mechanisms have as well been proposed for *medium-range* molecular communication: flagellated bacteria [9] and catalytic nanomotors [10]. Both methods are based on encoding the information in DNA sequences (a DNA packet), which are carried it from transmitter to receiver by using bacteria or nanomotors, respectively. Finally, several techniques have been proposed for the *long range*, such as pheromones, pollen and spores [11].

Among the previous techniques, one of the most widely studied is molecular signaling [12]–[14]. In molecular signaling, transmitters suspended in a fluid medium emit molecules according to a release pattern which encodes the transmitted information. The emitted molecules move following an erratic trajectory, due to the collisions between them and the molecules of the fluid. As a consequence of this movement and of interactions among the emitted molecules (such as collisions and electrostatic forces), the emitted molecules diffuse throughout the medium. This diffusion causes the concentration of molecules to propagate and spread throughout the space. Finally, receivers measure the local concentration of molecules at their neighborhood and decode the transmitted information.

The remainder of this paper is organized as follows. In Section II, we briefly describe diffusion-based molecular communication. Next, Section III describes the related work. In

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Section IV, we outline the architecture of the simulation framework *N3Sim* and in Section V, we present some sample results in order to illustrate its functionalities. Finally, Section VI concludes the paper.

II. Diffusion-based Molecular Communication

Diffusion-based Molecular Communication (DMC) aims to model the previously-described scenario of molecular signaling. In DMC, the evolution of the molecular concentration throughout space and time is modeled as a diffusion process. Depending on the scenario, different diffusion models may be used, which can be grouped into two categories: normal diffusion and anomalous diffusion [15].

On the one hand, *normal diffusion* refers to the case when the movement of the emitted molecules can be modeled by Brownian motion [16], which is valid when viscous forces dominate the motion of the emitted molecules and the interactions among them can be neglected. In this case, the movement of each of the molecules is uncorrelated and the diffusion process can therefore be macroscopically modeled with Fick's laws of diffusion [17].

On the other hand, *anomalous diffusion* appears when interactions among the emitted molecules affect their diffusion process. For instance, in a particular case of molecular signaling known as calcium signaling [18], based on the use of positive-charged calcium ions (Ca^{2+}), the electrostatic forces among these ions impact their diffusion process. Another example of anomalous diffusion includes the case when the concentration of emitted particles is very high and the collisions among them affect their movement, a scenario known as *collective diffusion* [19]. In these cases, the diffusion process can no longer be modeled by Fick's laws of diffusion and it needs to be analyzed with other methods, such as correlated random walk [20].

III. Related Work

Several authors have developed analytical models of the physical channel of DMC [21], [22]. However, to the best of our knowledge, a validation of these models is missing. In order to validate these theoretical models, either an experimental study or simulations are needed. Despite recent advances in synthetic biology, an experimental setup of molecular communication is still very challenging to build; consequently, simulation currently seems the most feasible choice. A simulator would allow to recreate an environment of DMC and measure the relevant metrics to evaluate its performance, such as channel attenuation, delay and throughput. The simulator outputs could be then compared with the results from the analytical models in order to assess their validity and to create novel, more accurate models.

Some authors have previously obtained simulation results of DMC, but restricted to very simple scenarios where the transmitter releases a single particle [23]. Other simulators are based on Fick's laws of diffusion [24] and therefore do not allow the simulation of anomalous diffusion or other effects, such as the noise due to the diffusion itself [25]. *N3Sim* (available at www.n3cat.upc.edu/n3sim) is the first simulation framework for DMC which includes both the cases of normal and anomalous diffusion. In our previous work [26], we provide a high-level overview of *N3Sim*. *N3Sim* has recently allowed to identify several peculiarities of DMC [27], to evaluate an impulse-based modulation for DMC and to validate a characterization of the physical channel of DMC [28].

IV. Simulator Architecture

We designed *N3Sim* in order to simulate a set of nanomachines which communicate among them through molecular diffusion in a fluid medium [21]. The information to be sent by the transmitter nanomachines modulates the rate at which they release molecules, modeled as particles (see Section IV-B), to the medium. For instance, the transmission of a logical bit '1' may be represented by the emission of a set of particles, and the transmission of a bit '0' by the absence of emission. These emissions create variations in the local concentration of particles, which propagate throughout the medium due to the Brownian motion and to interactions among themselves. The receivers are able to estimate the concentration of particles in their neighborhood by counting the number of particles in a volume around their location. From this measurement, they can decode the transmitted information.

Figure 1 shows a block diagram of the steps needed to run a simulation. First, the user specifies the values of the simulation parameters in a configuration file. These parameters include the number and location of transmitters and receivers, the signal to be transmitted, the size of the emitted particles and the diffusion coefficient of the medium, amongst others. A script file allows the user to run multiple simulations automatically using only one configuration file, which is useful to easily evaluate the influence of a specific parameter (e.g., the number of transmitted particles) in the system output. Next, the diffusion simulator takes the configuration file and the automation scripts as input, and performs the actual simulation of the DMC scenario. The diffusion simulator computes the position and velocity of each particle in every time step of the simulation. When the simulation ends, its outputs are stored in receiver files (one per receiver), which contain the concentration measured by each receiver as a function of time. Last, another set of scripts may be used to organize the results from several receivers and graphically represent them into a single plot.

A. Transmitter and Receiver Models

The transmitter is defined by its location in the simulation space and its size, which determines its influence space (i.e., the region where it may release particles). Every transmitter modulates the information to be sent into an associated waveform, which defines its particle release pattern. This waveform may be chosen among a number of predefined waveforms, such as a square pulse, a Gaussian pulse or a pulse train. A custom waveform may be defined by the user as well.

The receiver can be modeled as a sphere or cube able to measure the instantaneous number of particles within its

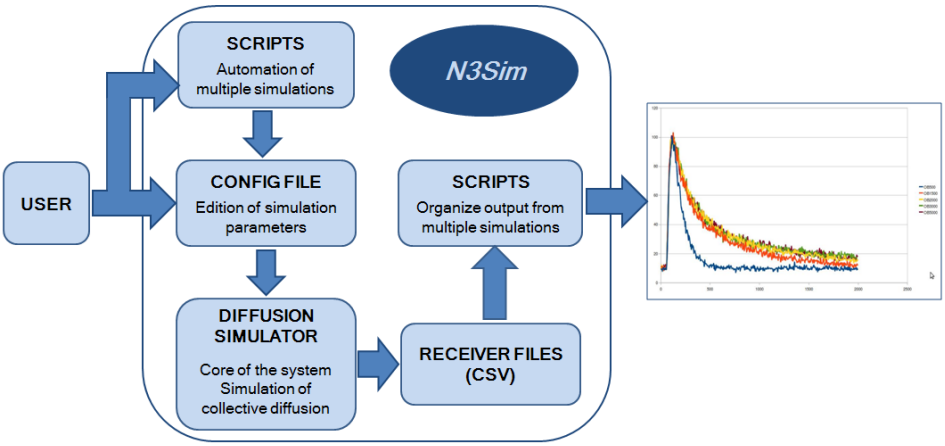

Fig. 1. Block diagram of *N3Sim*

detection range, from which the local concentration can be estimated. This model is an idealization of the ligand-receptor binding mechanism found in nature [29]. Many receiver parameters are customizable; for instance, after the receiver has detected a group of particles, it can either absorb them or be completely transparent to the particles.

N3Sim also allows the user to place multiple transmitters and receivers in the simulation field, thereby simulating a multipoint-to-multipoint communication. The user just needs to define the characteristics of each transmitter and receiver, namely, its position, shape and size, which can be different for each of them. This allows the study of several communication aspects, such as the feasibility of broadcast molecular communication, or the nature of interferences when more than one transmitter emits at the same time.

B. Particle Model

The emitted particles are modeled as indivisible spheres. The main reason for this choice is the simplicity of the collision detection algorithm for this shape. Collisions between the emitted particles and the fluid molecules cause them to diffuse throughout the medium. It would be computationally infeasible to model each of these collisions individually, since the number of collisions between each particle and the fluid molecules is in the order of 10^{20} per second [30]. Fortunately, the seemingly random movement of the suspended particles caused by collisions between the particles and the smaller fluid molecules can be mathematically modeled as Brownian motion. Assuming that the particles have no inertia, Brownian motion allows to statistically calculate their movement, which can be modeled as a Gaussian random variable with zero mean and whose root mean square displacement in each dimension after a time t is $\sqrt{2Dt}$, where D is the diffusion coefficient of the medium [31].

The high-level effect of the particles moving with a Brownian pattern is their diffusion throughout the medium, according to Fick's laws of diffusion [17]. However, Fick's laws do not take into account the influence of interactions among the particles themselves (such as collisions and electrostatic forces), and thus they are only valid when the particle concentration is very low and these interactions are neglected.

In order to simulate environments with anomalous diffusion, which cannot be modeled by Fick's laws of diffusion, *N3Sim* is able to account for the inertia of the emitted particles and the interactions among them. The most relevant interactions which affect the particle diffusion process are collisions and electrostatic forces. For simplicity, collisions among particles are considered elastic (i.e., the total kinetic energy is conserved). Electrostatic forces appear when the emitted particles are ions, which have a non-zero electric charge.

C. Simulation Space

N3Sim can be configured to simulate either a 2-dimensional or a 3-dimensional space. One of the parameters of the simulation space is the initial particle concentration in the medium. If it is zero, both a bounded and an unbounded space can be simulated. However, if the initial particle concentration is greater than zero, the simulation space needs to be bounded, in order to avoid having an infinite number of particles.

When a bounded space is simulated, a cuboidal simulation space is assumed where particles rebound on the space limits. We consider this model to be the most realistic for prospective applications of molecular communication. For instance, in a set of communicating nanomachines located in a blood vessel, whenever a particle collides with the vessel wall (known as *tunica intima*), it will rebound. In order to avoid that the particles released by the transmitters cause the background concentration to increase over time, *N3Sim* includes an optional mechanism which lets some particles disappear when they reach the limits of the simulation space, according to the laws of diffusion.

Moreover, objects can also be set within the scenario in order to simulate obstacles between the transmitters and the receivers. This allows recreating, for example, a scenario where a group of bacteria is crossing the medium and it obstructs the way between transmitters and receivers.

TABLE I
PARAMETERS USED IN THE SIMULATIONS

Parameter	Value
Time step	2 ms
Simulation time	5 s
Transmission distance	50 μm
Transmitter radius	5 μm
Receiver radius	5 μm
Particle radius	0.2 nm
Number of particles released	10^5
Diffusion constant	1 nm^2/ns

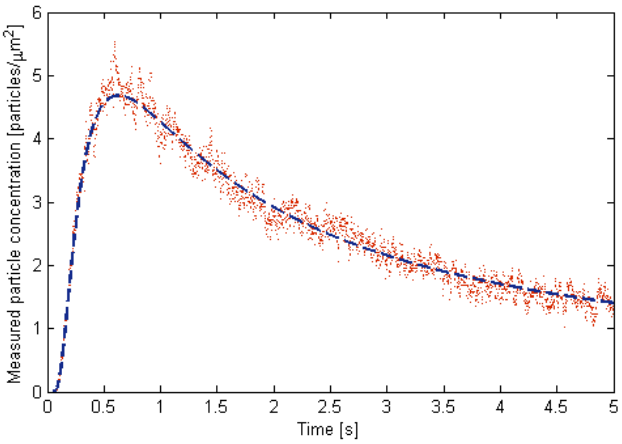

Fig. 2. Received signal when a molecular pulse is transmitted in a scenario of normal diffusion. The red dots show the particle concentration at the receiver as measured by *N3Sim*, and the blue dashed line shows the analytical results of Fick's laws of diffusion.

V. Simulation Results

In order to illustrate the capabilities of the simulator, we show the results of several simple simulations of a point-to-point diffusion-based molecular communication in a 2-dimensional space. Both the transmitter and the receiver have circular shapes. Table I contains the values of the parameters used, which have been selected to mimic a real scenario of molecular signaling among living cells.

A modulation for DMC based on the transmission of molecular pulses, consisting in the release of a number of molecules at the same time instant, has recently been proposed [28]. We perform a simulation in which *N3Sim* computes the particle concentration measured by the receiver when a pulse of 10^5 particles is transmitted, with the purpose of comparing the cases of normal diffusion and anomalous diffusion.

Fig. 2 shows a scenario of normal diffusion, where interactions among the emitted particles are neglected. We observe that when the transmitted signal reaches the receiver location, it is distorted and has a long tail due to the effects of diffusion. As expected in a scenario of normal diffusion, the particle concentration measured by the receiver (red dots), matches the analytical result of Fick's laws of diffusion (blue dashed line).

Fig. 3 shows the results of a simulation with the same parameters, but in an environment of anomalous diffusion. In this case, *N3Sim* simulates the collisions among the emitted particles and their inertia. As we observe in the figure, the measured particle concentration (red dots) no longer matches the results of Fick's laws of diffusion (blue dashed line). In consequence, we conclude that the collisions among the emitted particles and their inertia yield a scenario of superdiffusion, i.e., the particles diffuse faster than predicted by Fick's laws.

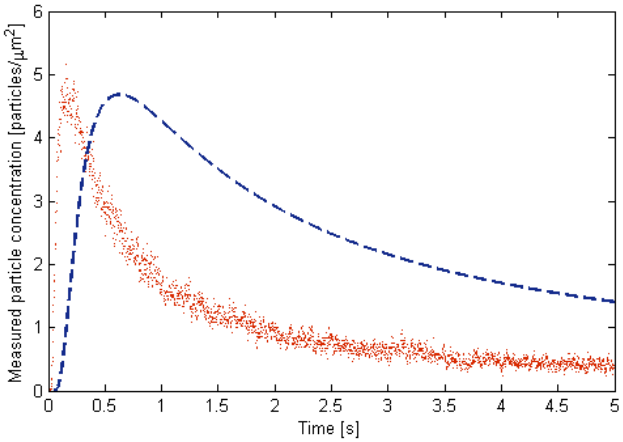

Fig. 3. Received signal when a molecular pulse is transmitted in a scenario of anomalous diffusion. The red dots show the particle concentration at the receiver as measured by *N3Sim*, and the blue dashed line shows the analytical results of Fick's laws of diffusion.

Using the previously-described pulse-based modulation scheme, a stream of information may be sent by transmitting a train of molecular pulses (e.g., different molecule types may be used to encode bits '0' and '1'). Fig. 4 shows the received signal when a train of pulses is transmitted, with the same parameters than in the previous simulation and in a scenario of normal diffusion. Again, the particle concentration measured by the receiver is plotted as a function of time. Since the diffusion-based molecular channel is linear and time-invariant [27], the received signal corresponds to a train of pulses such as that shown in Fig. 2. The minimum time among pulses is determined by the pulse width, which in its turn solely depends on the medium diffusion coefficient and the transmission distance [28]. Therefore, the medium characteristics and the distance between transmitter and receiver nanomachines will ultimately determine the maximum achievable bandwidth with this modulation scheme.

VI. Conclusions

In this work, we have analyzed diffusion-based molecular communication, a promising bio-inspired paradigm to implement nanonetworks, i.e., the interconnection of nanomachines. The physical channel of diffusion-based molecular communication is fundamentally different from that of classical electromagnetic communication; as a consequence, nanonetworks require novel physical channel models, network architectures and communication protocols, which need to be validated by simulation.

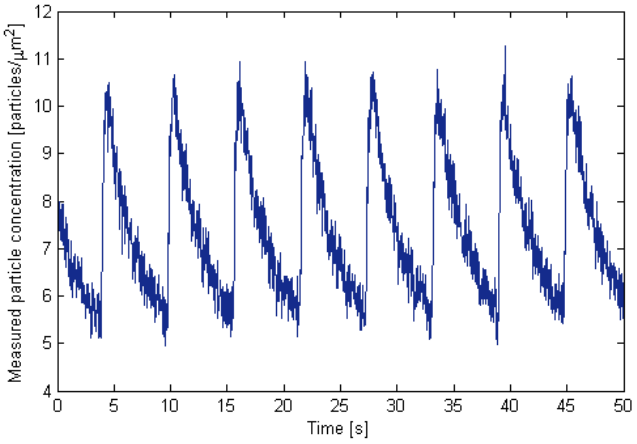

Fig. 4. Received signal when a train of molecular pulses is transmitted, in a scenario of normal diffusion.

With this purpose, we have presented *N3Sim*, a simulation framework for diffusion-based molecular communication, which we consider an essential tool to design and evaluate physical-layer protocols, modulations, resource management schemes and nanomachine components, amongst others. *N3Sim* allows to simulate scenarios where transmitters encode the information by releasing particles into the medium, thus causing a variation in their local concentration. *N3Sim* models the movement of these particles as Brownian motion, and it also takes into account their inertia and the interactions among them. Receivers decode the information by sensing the particle concentration in their neighborhood.

We expect that *N3Sim* will play an important role to evaluate current models, modulations and protocols for diffusion-based molecular communication, and that it will give crucial insights which may help to design novel techniques and schemes.

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