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N3Sim: Simulation framework for diffusion-based molecular communication nanonetworks

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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. *N3Sim* is a simulation framework for nanonetworks with transmitter, receiver, and harvester nodes using Diffusion-based Molecular Communication (DMC). In DMC, 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. Harvesters collect molecules from the environment to reuse them for later transmissions. Receivers decode the information by sensing the particle concentration in their neighborhood. The benefits of *N3Sim* are multiple: the validation of channel models for DMC and the evaluation of novel modulation schemes are just a few examples.

1. Introduction

Nanotechnology, first envisioned by the Nobel laureate physicist Richard Feynman in his famous speech entitled “There’s plenty of room at the bottom” in 1959, is giving rise to devices in a scale ranging from one to a few hundred nanometers. During the last few decades, emerging research areas such as nanoelectronics, nanomechanics and nanophotonics are allowing the development of novel nanomaterials, nanocrystals, nanotubes and nanomachines that promise to revolutionize many fields of science and engineering.

Molecular nanotechnology, popularized by Drexler [1], is a particularly advanced form of nanotechnology based on the ability to build molecular machines by means of mechanosynthesis. Since biology clearly demonstrates that molecular machines are possible (living cells themselves are an example), the manufacture of bio-inspired molecular machines using biomimetic techniques is envisaged in the near future.

Nanotechnology is a multidisciplinary field with almost uncountable potential applications. A few examples are presented next. First, in the biomedical domain, nanoparticles such as dendrimers, carbon fullerenes (buckyballs) and nanoshells are currently used to target specific tissues and organs [2]. Another area where nanotechnology plays an important

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role is environmental science, where molecular and genomic tools are used to uncover the complexity of the induced defense signaling networks of plants [3]. Finally, in the industrial field, molecular-scale filters and pores with well-defined sizes, shapes, and surface properties allow to engineer better functionality in molecular sieving [4].

The envisaged *nanomachines* are the most basic functional units able to perform very simple tasks at the nanoscale, including computing, data storage, sensing, actuation and communication. Cells are a clear example of living nanomachines. Therefore, even though a complete nanomachine has not been manufactured to date, artificial simple nanomachine are expected to become a reality in the near future.

Because of their tiny size, the operation range of nanomachines is limited to their close nano-environment. In consequence, a huge number of them will be required in order to perform meaningful tasks in a real scenario. These nanomachines will also need to control and coordinate their functions, leading to several research challenges in communication at the nanoscale.

Nanonetworks, the interconnection of nanomachines, have emerged as a novel research field which has attracted the interest of researchers from the domains of information and communication technology, nanotechnology and biology. Nanonetworks will provide means for cooperation and information sharing among nanomachines, allowing them to fulfill more complex tasks. As a consequence, nanonetworks are envisage to greatly expand the range of applications of nanotechnology. Sample applications of nanonetworks include Wireless NanoSensor Networks [5] and Graphene-enabled Wireless Networks-on-Chip [6].

Current communication techniques, such as electromagnetic, mechanical or acoustic communication, cannot be directly applied at the nanoscale [7]. Instead, 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 2, we briefly describe diffusion-based molecular communication. Next, Section 3 describes the related work. In Section 4, we outline the architecture of the simulation framework *N3Sim* and Section 5 describes the collision detection implemented in *N3Sim*. In Section 6, we present some sample results in order to illustrate its functionalities. Finally, Section 7 concludes the paper and points to future work directions in this area.

2. Diffusion-based molecular communication

Diffusion is the process by which particles suspended in a fluid experience a random endless movement. The basic diffusion process is based on Brownian motion, which is due to interactions among the fluid particles and the suspended particles. The microscopic dynamics of this process are extremely complex. It was Einstein in 1905 who first suggested equations to describe this process from a macroscopic point of view. Einstein showed that the concentration of Brownian particles $c(x,t)$ satisfies the diffusion equation:

$$\frac{\partial c(x,t)}{\partial t} = D\frac{\partial^2 c(x,t)}{\partial x^2} \tag{1}$$

where $D = K_bT/6\pi Rv$ is the diffusion coefficient, which depends on the Boltzmann constant K_b, the temperature T, the particle radius R and the fluid viscosity v. Assuming that Q particles start from the origin at the initial time $t = 0$, the 3-dimensional diffusion equation has the following solution:

$$c(x,t) = \frac{Q}{(4\pi Dt)^{3/2}} e^{-x^2/4Dt} \tag{2}$$

The first moment of the particle movement is zero, meaning that the Brownian particle is equally likely to move to the left as it is to move to the right. The second moment, which expresses the mean squared displacement of the Brownian particles, is given by