Towards Mastering Complex Particle Movement and Tracking in Molecular Communication Simulation

Fabian Bronner
Paderborn University, Germany
fabian.bronner@ccs-labs.org

Falko Dressler
Paderborn University, Germany
dressler@ccs-labs.org

ABSTRACT

Simulation of molecular communication requires rather application-specific channel models for the physical layer, i.e., the movement of molecules in a target environment. There is already a number of simulators available that apply different concepts for this task. We compare them in terms of geometry of the environment, molecular movement and tracking, as well as visual representation. We identified particle movement and tracking as one of the most challenging research questions in this domain. As a possible solution, we suggest the use of vector fields, which are also used in fluid mechanics, to simulate more complex molecular communication channels.

CCS CONCEPTS

• **Networks** → **Network simulations**; • **Computing methodologies** → *Model development and analysis.*

KEYWORDS

Molecular communication, particle movement, simulation tools

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1 INTRODUCTION

Using molecules as carriers of information to transmit data among nodes is a promising upcoming interest of research often referred to as *molecular communications* (MolCom) [6]. It is mostly interesting for applications where traditional wireless communication is almost impossible or dangerous to use [4]. Application domains include medial environments, e.g., communication within the human body, or industrial facilities, e.g., complex pipes in chemical industry.

Simulation is a key methodology to evaluate communication networks in general. There are established models for simulating radio channels but as a molecular channel is quite different, it requires rethinking about adequate strategies.

Within a molecular channel, molecules carry information in fluid environments (like air or water). So, the movement of these molecules needs to be modeled and, for modeling sender and receiver processes, they need to be tracked very precisely. Here, physical and even chemicals interactions between the molecules and the environment need to be accounted for. A very important task is to find a good trade-off between accuracy and scalability of describing a molecular channel model.

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2 MOLCOM SIMULATORS

There have already been multiple approaches to build simulation tools for molecular communication [1, 2, 5, 7]. We concentrate on how they model a molecular channel. To allow comparisons, we put all simulators listed in Table 1 into operation, experimented with their parameters, and studied their source code.

The characteristics of a molecular channel strongly depend on the geometry of the environment between transmitter and receiver, where carrier molecules propagate the information. nanoNS3 [5] is a simulator based on NS-3. It comes with a list of pre-defined geometries that the user can choose to configure specific variants. BiNS2 [1] has been written in Java and offers similar functionality. It provides a list of scenarios each consisting of a simple geometric environment (e.g., cubic, cylinder). More flexibility is provided by the AcCoRD simulator [7]. The environment is defined by the user who can glue different geometries together to form more complex scenarios. Finally, BloodVoyagerS is a module for NS-3 that provides a model of the human cardiovascular system [2].

Molecules are able to move within the defined environment. There are mainly two forces that cause molecular movement: (i) diffusion due to Brownian motion and (ii) flow of the fluid itself. Additionally, collisions among carriers and the environment influence their trajectory. Diffusion is well covered by BiNS2 and AcCoRD and depends on characteristics of the fluid. In addition, AcCoRD lets the user define a uniform flow. Per time step, a constant vector is added to each molecule's position. In BloodVoyagerS the amount of such a displacement also depends on the type of vessel. This allows for a higher velocity in vessels with lower diameter and vice-versa. BiNS2 supports a more complex method by computing a Poiseuille flow profile in its blood vessel scenario. In contrast, nanoNS3 uses an analytical approach to compute delay and attenuation of transmitted bursts. Therefore, characteristics of flow (in form of pressure drop) and a diffusion coefficient are required.

Due to the analytical approach, nanoNS3 does not offer tracking, but computes delay and attenuation caused by the channel directly. All other simulators track each molecule individually and define a molecule position per simulation time step. Thus, exact molecule coordinates can be computed at arbitrary time steps; this strategy is known as *microscopic*. When molecule positions are bound to a specific subvolume, such as in AcCoRD, it is a *mesoscopic* approach. Here, the environment is subdivided with molecules only being

Table 1: Comparison of molecular simulators in terms of channel characteristics

Simulator	Environment geometry	Molecular movement	Molecular tracking	Visual representation
nanoNS3 [5]	Simple configurable geometries	Diffusion, flow	None (analytical channel description)	None
BiNS2 [1]	Pre-defined scenarios (simple geometries)	Diffusion, Poiseuille flow	Microscopic (per-molecule)	Live 3D rendering
AcCoRD [7]	Combination of multiple configurable geometries	Diffusion, uniform (constant) flow	Microscopic (per-molecule), mesoscopic (subvolumes), hyprid	Textual trace and post-processing in Matlab
BloodVoyagerS [2]	One given scenario (human cardiovascular system)	Different uniform flows (depending on vessel type)	Microscopic (per-molecule)	Textual trace of each molecule

tracked by their respective subvolume. For the sake of completeness, we need to mention NanoNS [3]. It offers a mesoscopic approach by using a lattice structure and molecules bound to the lattice sides.

In order to better understand processes within the molecular channel, most simulators offer visual representation of the environment and the molecules. BloodVoyagerS does not offer a direct visual representation, but the position of each molecule per time step is logged allowing visual analysis in a post-processing step. AcCoRD also logs molecule positions which are later visualized using Matlab scripts to generate 3D plots as well as animations. BiNS2 offers live 3D rendering of the simulation scenario with a freely movable camera. nanoNS3 does not track molecules, thus, it cannot offer a visual representation.

3 INTRODUCING VECTOR FIELDS

Our comparison in Section 2 helped identifying particle movement and tracking as one of the most challenging research questions. First, for practical use cases, even more complex environment geometries need to be modeled such as curved pipe systems. Secondly, and even more important, the investigated simulators support only rather simple movement of particles in a fluid. While this is relatively easy for diffusion, which mainly depends on properties of the environment, it is a lot more difficult for flow. For simulators tracking each molecule individually, we observe that they use simplified flow models and do not allow to simulate more complex fluid mechanics like laminar flow around obstacles or intersections, which can heavily influence molecular movement.

The idea is now to to put more effort into describing the geometry of the environment and implementing more accurate flow handling. We propose to overcome these limitations by using vector fields, which are also used in fluid mechanics. Dedicated software exists for computing such vector fields; this is often referred to as computational fluid dynamics (CFD) software such as *OpenFOAM*. Using such tools, we suggest a workflow that consists of three major steps: (i) Description of the environment within 3D modeling software; (ii) Import of this description in CFD software, which performs flow computations and exports a vector field that allows particle tracing; and (iii) Use of this vector field within a molecular simulator to perform accurate movement of carrier molecules. This results in being able to repeat more accurate simulations without a large increase in computation time as the pre-computed vector field can be re-used. The complexity of the environment then depends on the capabilities of the tool used to generate the field.

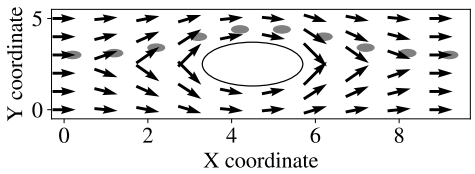

Figure 1: Vector field describing laminar flow around a circular obstacle. Grey dots outline trajectory of a molecule.

Figure 1 outlines an exemplary vector field that also takes an obstacle into account. Basically, through a position of a molecule at time t and position $\vec{p}_{old}$, its position $\vec{p}_{new}$ at $t + \Delta t$ is determined due to the direction and strength of the vector field.

4 CONCLUSION

We compared typical molecular communication simulators and discovered that, while diffusion is well covered, particle movement due to flow is usually oversimplified. Based on these findings, we suggest an approach that builds upon vector fields that can be computed using computational fluid dynamics software. These vector fields support more accurate estimation of the movement of molecules within molecular simulators. We plan to implement this concept and validate simulation results against real world experiments.

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