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Simulating with AcCoRD: Actor-based Communication via Reaction–Diffusion

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ABSTRACT

This paper introduces AcCoRD (Actor-based Communication via Reaction–Diffusion) version 1.0. AcCoRD is a sandbox reaction–diffusion solver designed for the study of molecular communication systems. It uses a hybrid of microscopic and mesoscopic simulation models that enables scalability via user control of local accuracy. AcCoRD is developed in C as an open source command line tool and includes utilities to process simulation output in MATLAB. The latest code and links to user documentation can be found at https://github.com/adamjgnoel/AcCoRD/. This paper provides an overview of AcCoRD's design, including the motivation for developing a specialized reaction–diffusion solver. The corresponding algorithms are presented in detail, including the computational complexity of the microscopic and mesoscopic models. Other novel derivations include the transition rates between adjacent mesoscopic subvolumes of different sizes. Simulation results demonstrate the use of AcCoRD as both an accurate reaction–diffusion solver and one that is catered to the analysis of molecular communication systems. Videos in the supplementary materials demonstrate many of the simulated scenarios. Additional insights from the simulation results include the selection of suitable hybrid model parameters, the impact of reactive surfaces that are in the proximity of a hybrid interface, and the size of a bounded environment that is necessary to assume that it is unbounded. The development of AcCoRD is ongoing, so its future direction is also discussed in order to highlight improvements that will expand its potential areas of application. New features that are being planned at the time of writing include a fluid flow model and more complex actor behavior.

1. Introduction

1.1. Background and motivation

There has been recent interest in designing synthetic wireless communication networks for environments where conventional (i.e., radio frequency) wireless technologies are unsafe, infeasible, or impractical, such as in biological systems. This interest has inspired the idea of adapting natural communication strategies from these biological systems. One such strategy is molecular communication (MC), initially proposed for synthetic networks in [1], where transmitters use physical molecules as information carriers. MC is used for signaling in nature over a wide range of physical scales, from quorum sensing in bacterial communities to communication via pheromones over a kilometer or more, as described in [2] and [3, Ch. 53], respectively. In particular, MC is ubiquitous in communication within and between cells; see [4, Ch. 16].

Natural MC systems are typically designed for the transmission of limited quantities of information, such as a time-varying ON/OFF control signal for some process. However, synthetic MC networks are envisioned for transmitting arbitrarily large amounts of information. These networks could enable new applications in fields including biological engineering, medicine, manufacturing, and environmental modeling; see [5].

Commonly-studied forms of MC include molecular *diffusion*, where molecules passively propagate via collisions with other molecules in a fluid environment. The interest in diffusion for communication engineering, as demonstrated in [6], can be attributed to its speed over very short distances (particularly on the scale of a micron or less), its simplicity (requiring no active propagation mechanism), and the availability of mathematical models to facilitate analysis. In particular, mathematical models

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are needed to determine a channel's impulse response (i.e., the time-varying signal observed at a receiver due to the release of an instantaneous signal by a transmitter). Knowledge of the channel impulse response is essential for meaningful transceiver system design and performance analysis.

There are many seminal texts on the analysis of diffusion, e.g., [7–9]. However, closed-form expressions for the impulse response of a diffusive channel generally require simplifying assumptions and specific system geometries. This reality is an obstacle to the development of MC networks. Most existing research has considered a variation of a common system model. Typically, authors will consider a one- or three-dimensional (i.e., 1D or 3D) unbounded environment, possibly with a uniform fluid flow, with a point source and a receiver that is either an absorbing surface (i.e., molecules are "consumed") or a passive observer.[1]

While the resulting analysis of simplified models is convenient, and uniformity is helpful for comparing transceiver designs, there are a couple of issues with this trend. First, realistic diffusive environments are generally bounded. Approximating an environment as unbounded is only appropriate if it is symmetric and in the absence of other local obstacles, but environments such as cells and cellular tissues are full of obstacles; see [4, Ch. 20]. Second, diffusion is not the only phenomenon that can affect the behavior of a diffusing particle. In addition to fluid flow (which is in general not uniform; see [10]), molecules can undergo chemical reactions (besides absorption at a surface) that convert them into other molecular species or transport them across boundaries. For example, see [11, Ch. 9] for elementary analysis of chemical reactions.

Flow and reactions can significantly modify the channel response, and could even be deliberately introduced to improve communication performance. This was observed by using an electric fan in the macroscale testbench developed in [12], and by adding enzymes to the propagation environment in our own work in [13]. Neither of these strategies could be accurately described using the commonly-studied channel models; the experiments in [12] were fitted to a corrected 1D model in [14], and the enzyme kinetics in [13] were simplified to a first order degradation reaction so that the impulse response could be derived.

The notion that we simplified the analytical model in [13] immediately begs the question of how we verified its accuracy. Furthermore, it was insufficient to determine the *expected* channel behavior; for communications analysis, we are interested in the *probability distribution* of the channel behavior. We addressed both issues in [13] by simulating the detailed model. Unfortunately (and to the best of our knowledge), no existing simulation platform would accommodate the detailed model in [13]. Even though we could have used a *generic reaction–diffusion solver* such as Smoldyn (see [15]) to evaluate the expected channel behavior, it was not suitable for assessing the time-varying channel statistics or for configuring a source to release molecules based on modulating a sequence of random binary data. Our solution in [13] was to internally develop a simulator in MATLAB. However, this simulator was specific to the environment of the model in [13] and not easily portable to other system models. We claim that existing publicly-available MC simulators have similar limitations, e.g. [16–20] (which we will discuss in further detail in Section 2.2).

1.2. The AcCoRD simulator

With these limitations in mind, we have developed the AcCoRD simulator (Actor-based Communication via Reaction–Diffusion). AcCoRD is a generic reaction–diffusion solver that is developed in C and designed for communications analysis. It is an open source project in active development on Github; see [21]. As of the time of writing (November 2016), the latest release is version 1.0. It has the following primary features:

- AcCoRD is a hybrid solver that integrates two simulation models to define 3D environments with flexible local accuracy. Each local region is classified as *microscopic* or *mesoscopic*. Microscopic regions define each molecule individually and evolve over discrete time steps. Mesoscopic regions count the number of molecules in disjoint virtual bins (called *subvolumes*) and evolve over time steps with continuous granularity. We increase the scalability by accommodating the placement of adjacent mesoscopic regions that have subvolumes of different sizes. This feature is based on an extension of the 2D system that we proposed in [22].
- Actors can be distributed throughout the environment as *active* molecule sources (i.e., transmitters) or *passive* observers (i.e., receivers). Transmitters release molecules according to the modulation of a random binary data sequence. The precise number of molecules released and the release times for a given symbol interval can be deterministic or randomized. Receivers can record the number of molecules and (optionally) their positions at any specified interval. Future development will couple these two actor classes to enable transceivers that behave according to their observations.
- Zeroth, first, and second order chemical reactions can be defined locally or globally, i.e., over the entire propagation environment or in a particular set of regions. This general framework can accommodate reactions such as molecule degradation, enzyme kinetics, reversible or irreversible surface binding, ligand–receptor binding, transitions across boundary membranes, and simplified molecular crowding. Surface binding reactions include absorption, i.e., *consumption*, adsorption, i.e., *sticking*, and desorption, i.e., *release* from a surface. Generally, we will refer to adsorption as reversible absorption.
- AcCoRD implements some microscopic behavior in continuous time. Specifically, the release of molecules by active actors, zeroth order reactions, and most first order reactions can occur at any time. Thus, a molecule can undergo multiple reactions in a single microscopic time step, and the accuracy of these phenomena are independent of the chosen time step.
- Independent realizations of a simulation can be repeated an arbitrary number of times (and on different computers) and then aggregated to determine the average behavior and channel statistics.
- The online documentation includes installation and usage instructions for the latest version, descriptions of all configuration options, and many sample configuration files; see [21]. The sample configurations are provided to demonstrate all of AcCoRD's functionality.
- AcCoRD's interface has been designed to be helpful to novice users by providing descriptive output messages. AcCoRD also includes post-processing tools developed in MATLAB. These tools enable the aggregation of simulation output files, plotting receiver observations (either the time-varying behavior or empirical distributions at specified times), and visualizing the physical environment (either as still images or compiled into a video[2]).

[1] A (perhaps surprisingly) large fraction of papers reviewed in [6], including the current authors' own work on MC, can be classified as using such a model.

[2] A series of eight videos are discussed throughout this paper and can be found in the supplementary materials or on YouTube at https://www.youtube.com/watch?v=7QcN6eGrC4w&list=PLZ7uYXG-7XF8UyhFrIuQIiZig1XA89e3i.