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On the asynchronous information embedding for event-driven systems in molecular communications

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ABSTRACT

Molecular communications is emerging as a promising paradigm for nanoscale communications in nanotechnology. Though still at an early stage, research efforts have been devoted and various molecular communication systems have been proposed. However, each proposed system possesses a specific structure to achieve communications in its own way. To our best knowledge, no unified system description exists so far. In this paper, we propose an abstract system structure called an *event-driven system*; a significant group of molecular communication systems can be classified into such an abstract form. We define event-driven systems and further show that, for these systems, there is a signaling scheme called *asynchronous information embedding* which carries additional information while at the same time keeping the original communication mechanisms uninfluenced. Instead of investigating *asynchronous information embedding* in full generality, we consider synchronous type-based systems as a demonstrative example which still captures most of the features. For such type-based systems, we develop an approximation method for obtaining the channel capacity as a general performance measure. Numerical results are provided to show the capacity gain of asynchronous information embedding.

1. Introduction

The term *nanotechnology* was first defined in 1974 [1] as the following: "Nanotechnology mainly consists of the processing of separation, consolidation, and deformation of materials by one atom or by one molecule". Since then, significant progress has been made and the concept of the "nano-machines", which are devices of scale 1–100 nm, has been established. Such nano-machines can be considered as the most basic functional unit, and therefore they can only perform very simple tasks of computation, sensing, etc. One of the core issues of nanotechnology is *how to communicate between two nano-machines*. In the past decades, different communication paradigms have been proposed, among them the most promising one being *molecular communications*, which is defined as the "transmission and reception of information encoded in molecules".

Though still at an early stage, some research efforts have been made in molecular communications. For example, [15] proposes a physical end-to-end model in diffusion-based molecular systems. In [12], a time-slotted system with diffusion-based channels is considered. The work in [6] considers a time-slotted system with information embedded in molecule levels, and [7] considers a similar system with information embedded in molecule types. In [2–4], a series of information-theoretical studies is provided for systems with nano-machines operating on the ligand–receptor binding mechanism. Besides these theoretical studies, laboratory experiments have also been conducted [18,13].

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Although there are several kinds of molecular communication system that have been proposed, each system possesses a specific structure and achieves communications in its own way. There is no systematic classification of these molecular communication systems in the literature so far. In this paper, we define an abstract system structure called an *event-driven system*, and claim that many commonly seen molecular communication systems fall into this category. We also show that these event-driven systems have a great property that one can embed additional information upon the original signaling method without affecting the original messages. We call such a process *asynchronous information embedding* for event-driven systems, and the details are discussed in later sections.

Among recent works, most of the molecular communication systems are assumed to be time-slotted so that the inter-transmission durations are fixed. We call such systems *synchronous* as a counterpart to the terminology "asynchronous". The information of synchronous systems is carried on either the *level* [12,6] or the *type* [7] of molecules. For example, in synchronous level-based systems, the logic "0" or "1" may be represented by transmitting no molecule and one molecule, respectively, at the starting of each time-slot (see Section 3 for rigorous definition of synchronous type-based systems). These synchronous systems are just important examples of event-driven systems. We then study the asynchronous information embedding process under these synchronous systems. We show how to utilize the randomness of inter-transmissions to embed additional information, thus creating a new signaling scheme for molecular communications. Specifically, we develop a full system structure for the *Bernoulli inter-transmissions* and extensively analyze the proposed systems. We will first derive fundamental performance measures, e.g. the error probability. After that, in order to assess the total effect of injecting the random inter-transmissions, we introduce an approximation for the channel capacity and use it as an unified measurement for performance comparison between synchronous and asynchronous systems taking the same average time per channel use.

The rest of this paper is organized as follows. In Section 2, we first define what we mean by an *event-driven system*, and discuss the information embedding method called *asynchronous information embedding* on these systems. In Section 3, we propose a simple system model (synchronous type-based system) that captures the main characteristics of event-driven systems. In Section 4, we analyze the *asynchronous information embedding* process on the systems proposed in Section 3, and also derive the capacity approximation for these systems. In addition, a procedure for system design is discussed at the end of this section. In Section 5, numerical results are presented. Finally, conclusions are made in Section 6.

2. Event-driven systems

Different from time synchronous designs, and inspired by biological systems [11], the *event-driven* concept has been used in computation and system design for a long time [9]. Later, event-driven designs were introduced to communication systems and networks such as sensor networks [17].

2.1. Definition and examples of event-driven systems

Before formally defining an event-driven system, we first introduce some new terminologies for a communication system. For a given communication system, we associate two stochastic processes defined as follows.

Transmission process ($\{T_i\}$, $\{X_i\}$). The transmission process consists of a pair of stochastic processes: the *transmission times* $\{T_i\}$ and the *transmission events* $\{X_i\}$. More precisely, the *transmission times* are the times when the transmitter releases messages (or information), while the *transmission events* represent the transmitted information at the corresponding transmission times.

Decision process ($\{R_i\}$, $\{D_i\}$). The decision process consists of a pair of stochastic processes: the *decision times* $\{R_i\}$ and the *decision events* $\{D_i\}$. More precisely, the *decision times* are the times when the receiver makes decisions. The *decision events* are random variables denoting the outcomes of each decision.

For a communication system, the most general formulation of observation is to model it as a continuous-time stochastic process $C(t)$, where the variable t represents the time index. For instance, the notation $C(t)$ may represent the amplitude of an EM wave, or it may represent the number of received particles. Note that $C(t)$ depends only on the transmission pattern (modulated signal) and the channel effect. The spirit of digital communication is then to design a receiver which, at certain times, utilizes the cumulated observation and prescribed knowledge to make good decisions in relevant hypothesis testing problems.

For example, in classical EM-wave communications, the receiver of a binary phase-shift keying (BPSK) system makes a decision every fixed time duration T by passing the observation results into two matched filters. Fig. 1 illustrates the transmission process and decision process of a BPSK system. As another example, most of the existing molecular communication systems are all supposed to be *synchronized*. That is, the transmitter sends messages periodically with a fixed time duration T, and the receiver makes decisions according to the same period. For *synchronized* systems, the transmission times $\{T_i\}$ and decision times $\{R_i\}$ are all determined numbers (say $T, 2T, 3T, \ldots$), which can also be viewed as a "degenerated" stochastic process.

With the help of the above-defined terminologies, we can now give a formal definition of what we call *event-driven systems*.

Definition. A system is said to be *event driven* if, for every positive integer $i \in \mathbb{N}$, the ith *decision event* is a deterministic function g of the observation at the ith *decision time*. In symbols,

$$D_i = g(C(R_i)), \quad \forall i \in \mathbb{N}. \tag{1}$$

Intuitively speaking, event-driven systems refer to those systems whose decision rules are operating precisely

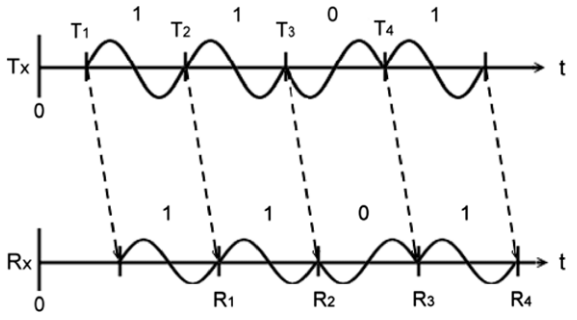

Fig. 1. Receiver of a BPSK system (not event driven).

on the instants of decision times $\{R_i\}$, but do not depend on the long-term behavior of observations. We give some examples, as follows.

- The BPSK system is not event driven, since each decision event D_i depends on the observation within the corresponding time interval $[T_{i-1}, T_i]$, but not only at T_i.
- The molecular system proposed in [2] serves as a classical example of event-driven systems. In [2], the transmitter emits a sequence of chemical substances, and the information is carried on the concentration levels. The receiver makes a decision whenever the concentration of such substance reaches certain levels. The event-driven nature of this system is that the receiver only cares about what levels are reached, and not the transient behaviors of chemical concentrations over time.
- There is another large group of systems in molecular communications that can be classified into event-driven systems. The so-called *particle-based systems* refer to systems whose transmitter conveys information by emitting a sequence of particles. The observation at receiver $C(t)$ in this case is the received particle numbers at time t. Since the particle number is "discrete" in nature, we can model $C(t)$ as a *(compound) counting process*. In such systems, the receiver is often designed to make decisions upon the instant when receiving a particle (or in the terminology of a counting process, upon the arrival times). For these reasons, many particle-based systems fall into the category of event-driven systems. See Fig. 2 for an example.

2.2. Asynchronous information embedding for event-driven systems

In this subsection, we formally discuss the *asynchronous information embedding* process. For each $i \in \mathbb{N}$, we set the following hypothesis testing problem:

$$\begin{cases} H_0 : R_i - R_{i-1} \sim Y_0, \\ H_1 : R_i - R_{i-1} \sim Y_1, \end{cases} \tag{2}$$

where $R_i - R_{i-1}$ is the decision time difference, and Y_0 and Y_1 are two known distributions.[1] We coin the name "asynchronous information embedding" for such process since, as opposed to synchronous systems, the decision times are random and not equally spaced.

We focus on the systems whose decision times are influenced only by the transmission times, but not the transmission events (which is intuitively most cases). We discover that, for event-driven systems, there are conditions guaranteeing that "additional information" is transmitted through the *asynchronous information embedding* process. That is, all the transmission and decision events $\{X_i\}$ and $\{D_i\}$ are kept unchanged, and so are all their derived functionals, e.g. mutual information I, entropy rate H, etc.

Now we give precise conditions for our purpose. Consider a transmission process $(\{T_i\}, \{X_i\})$, its corresponding observation $C(t)$, and decision process $(\{R_i\}, \{D_i\})$. Upon modifying the distributions of transmission times from $\{T_i\}$ to $\{T_i'\}$, we obtain a new observation $C'(t)$ and a new decision process $(\{R_i'\}, \{D_i'\})$. Suppose that the difference of decision times takes on two known distributions:

$$\begin{cases} H_0 : R_i' - R_{i-1}' \sim Y_0 \\ H_1 : R_i' - R_{i-1}' \sim Y_1. \end{cases} \tag{3}$$

Under these hypotheses, we claim that such event-driven system has the following two properties.

(P1) Given the observation value at some decision time, the corresponding decision event is conditionally independent of the decision time. In notation,[2]

$$D_i \perp R_i \mid C(R_i) \tag{4}$$

and

$$D_i' \perp R_i' \mid C'(R_i'). \tag{5}$$

(P2) Suppose further that $C(R_i) = C'(R_i')$ for each i. That is, the observation at each decision time remains unchanged after we modify $\{T_i\}$ into $\{T_i'\}$. Then the outcomes of decision events also remain the same. In notation, $C(R_i) = C'(R_i')$ implies that $D_i = D_i'$.

Proof. The first property is a simple consequence of the definition of event-driven systems, since, given $C(R_i)$ (or $C'(R_i')$), D_i (or D_i') is a deterministic value, and thus independent of T_i (or T_i'). On the other hand, we have again from the definition of event-driven systems that

$$D_i = g(C(R_i)) = g(C'(R_i')) = D_i', \tag{6}$$

since the decision event is a deterministic function of $C(R_i)$ (or $C'(R_i')$) and thus verifies the second property. □

An important interpretation of P1 is that event-driven systems do *not* utilize the timing information to make decisions. In other words, the occurring times R_i do not matter, but only the values of $C(R_i)$. This implication has motivated us to consider additional information embedding utilizing the timing information, thus giving birth to the above asynchronous information embedding process. However, such

[1] The tilde symbol (∼) in Eq. (2) stands for "having the same distribution as".

[2] We use the notation $A \perp B \mid C$ to say that A and B are independent conditioned on C.

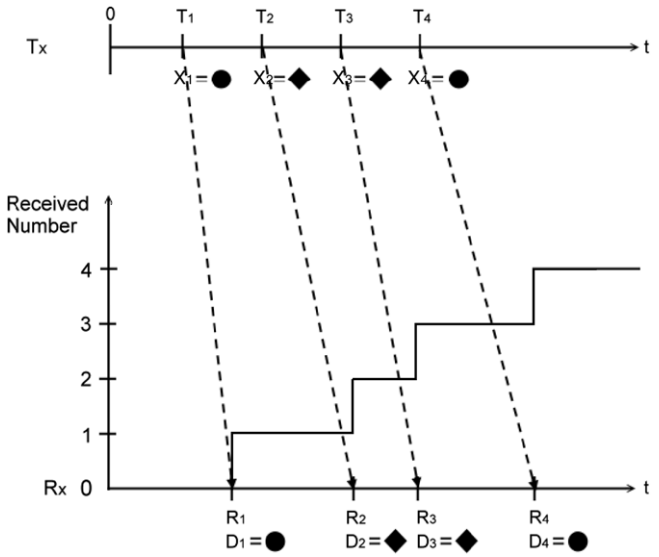

Fig. 2. A type-based molecular communication system (event driven), where the circle represents bit 0, and the diamond represents bit 1.

asynchronous information embedding might possibly influence the performance of the original system in some manner. Nevertheless, P2 eliminates such suspicions by telling us that, for event-driven systems, the decision results are kept unchanged provided that the observations at new decision times remain equal.

Another implication from P2 is that, since $D_i = D'_i$ for each i, the mutual information and entropy rate also remain unchanged:

$$I(X_i; D_i) = I(X_i; D'_i), \tag{7}$$

$$H(D_i) = H(D'_i). \tag{8}$$

It is a classical result that the channel capacity can be expressed in terms of the mutual information I, so Eqs. (7) and (8) imply that the channel capacity is also preserved. In other words, the amount of information transmitted through transmission events $\{X_i\}$ remains the same.

The key point to obtain all these good results is the assumption that "$C(R_i) = C'(R'_i)$" in P2. However, this condition does not always hold, since $C(t)$ might very well be influenced by the modification of transmission times as we embed additional information in time.

For practical applications, we might want to find some weaker conditions which still have acceptable results. The second best we hope is that the observation is "almost unchanged", say $C(R_i) \cong C'(R'_i)$ in some probabilistic sense, which is usually the case in many molecular event-driven systems (see the next subsection for reasons). We now rigorously define what we mean by "$C(R_i) \cong C'(R'_i)$ *in a probabilistic sense*", and then use this condition to prove the following important properties. For event-driven systems, the following hold.

(P3) $C(R_i) \cong C'(R'_i)$ implies that $I(X_i; D_i) \cong I(X_i; D'_i)$.
(P4) $C(R_i) \cong C'(R'_i)$ implies that $H(D_i) \cong H(D'_i)$.

In words, the information amount transmitted through $\{X_i\}$ is "almost" kept provided that the observation at decision times is "almost" the same.

In the following context, $f(\cdot)$ denotes the probability distribution function (p.d.f.) of the corresponding subscripted random variables, and all the integrations are performed in the Lebesgue sense. Given a sequence of transmission events $\{X_i\}$, we say that $C(R_i) \cong C'(R'_i)$ in a probabilistic sense if, for each i, there is a small positive number ϵ such that

$$\int_Z \int_X |f_{X_i, C(R_i)}(x, z) - f_{X_i, C'(R'_i)}(x, z)|\, dx\, dz < \epsilon, \tag{9}$$

where Z and X are the domains of $C(R_i)$ and X_i, respectively. In event-driven systems, since every D_i is a function of $C(R_i)$, we can change condition (9) into the following. For each i, there is a small positive number ϵ such that

$$\int_W \int_X |f_{X_i, D_i}(x, w) - f_{X_i, D'_i}(x, w)|\, dx\, dw < \epsilon, \tag{10}$$

where W is the domain of both D_i and D'_i. Notice that the above formula is similar to the well-known *total-variation distance* between random variables. In other words, we are actually demanding that every pair of (X_i, D_i) is close to (X_i, D'_i) in the sense of total-variation distance.

Now, we can write P3 and P4 into a theorem.

Theorem. *Let the D_i be finitely supported. Suppose that condition (10) holds for some $\epsilon > 0$. Then*

(a) $|H(D) - H(D')| \to 0$ *as* $\epsilon \to 0$,
(b) $|I(X_i; D_i) - I(X_i; D'_i)| \to 0$ *as* $\epsilon \to 0$.

Proof. (a) Suppose that (10) holds true:

$$\int_W \left| f_{D_i}(d) - f_{D'_i}(d) \right| dw$$
$$= \int_W \left| \int_X f_{X_i, D_i}(x, d) - f_{X_i, D'_i}(x, d)\, dx \right| dw$$

$$\leq \int_W \int_X \left| f_{X_i,D_i}(x,d) - f_{X_i,D_i'}(x,d) \right| dx\, dw$$
$$< \epsilon. \tag{11}$$

This shows that $D_i \cong D_i'$ in the sense of total-variation distance. Since the D_i are finitely supported, for every $d \in D$ we have $|f_{D_i}(d) - f_{D_i'}(d)| \leq \epsilon$. Without loss of generality, we can assume the D_i to be binary-valued random variables, so that $H(D_i)$ and $H(D_i)$ take the form

$$H(D_i) = -q \log q - (1-q)\log(1-q), \tag{12}$$

and

$$H(D_i') = -q' \log q' - (1-q')\log(1-q') \tag{13}$$

for some fixed numbers $q, q' \in [0,1]$ with $|q-q'| \leq \epsilon$. The desired result now follows from the fact that all the functions $f_1(q) = q, f_2(q) = 1-q, f_3(q) = \log q, f_4(q) = \log(1-q)$ are continuous, and so are their multiplications and linear combinations.

(b) Using the relation $I(X;Y) = H(X) + H(Y) - H(X,Y)$, we have

$$|I(X_i;D_i) - I(X_i;D_i')|$$
$$= |H(D_i) - H(D_i') + H(X_i,D_i') - H(X_i,D_i')|$$
$$\leq |H(D_i) - H(D_i')| + |H(X_i,D_i') - H(X_i,D_i')|. \tag{14}$$

The first term in (14) tends to 0 by part (a); the second term also tends to 0 by a similar argument as in (a). Therefore, $|I(X_i;D_i) - I(X_i;D_i')|$ tends to 0 as $\epsilon \to 0$. □

This motivates us to propose a communication scheme that embeds information on the *decision times* for event-driven systems. Consider the following scenario: the transmission times are random variables. The decision time difference $T_i - T_{i-1}$ follows

$$\begin{cases} H_0 : T_i - T_{i-1} \sim Y_0, \\ H_1 : T_i - T_{i-1} \sim Y_1, \end{cases}$$

where Y_0 and Y_1 are two known distributions. Then we can form the hypothesis testing problem and solve it simply by computing the likelihood-ratio statistic $\frac{f_{Y_0}(y)}{f_{Y_1}(y)}$ and comparing it to the decision threshold. Suppose further that the observation under H_0 or H_1 is the same; that is, $C(T_i|H_0) = C'(T_i|H_1)$ for all i. Then, by P2, the outcomes of decision events are the same for H_0 and H_1. The above discussion shows that we can transmit information through the transmission times. This tells us that, once the distribution of decision times is controllable, we can embed "additional information" in the sense that, on top of information from the decision events, there are also decodable messages from (between) decision times. Besides, P1 implies that the decision for observation $C(T_i)$ does not involve the decision times, while solving the above hypothesis problems involves *only* the timing information. Therefore, the decision devices for decoding the above hypothesis problems and the observation $C(t)$ can be separated as independent components. In the terminology of the well-studied classical communications, we have utilized the timing information as an *orthogonal signaling* scheme for event-driven systems.

2.3. System realization issues

In this subsection we examine existing molecular systems. We begin by pointing out that most existing molecular systems are *synchronous*, which we define in Section 2.1 as being that the inter-transmission times $T_i - T_{i-1}$ are fixed numbers. For example, the systems in [12,6,7,2–4] are all *synchronous*. Another important observation is that most molecular systems are operating on a *diffusion process*. The diffusion process can be viewed as some partial differential equations that, after the transmitter releases all messages (or after a *transmission process* in our terminology), govern the behavior of observations in time. The solutions of these partial differential equations exhibit exponentially decreasing tails, and therefore are transient at the start and will reach a steady state after some fixed time duration (see [8]). This property is very useful when we require robustness against time interferences caused by diffusion processes. For example, the systems in [12] utilize the Neyman–Pearson lemma to derive the inter-transmission times that ensure very small error probability. The same procedure also applies to systems in [6,7,2–4], which are all operating on diffusion processes.

Recall that the results in Section 2.2 require $C(R_i) \cong C'(R_i')$ in a probabilistic sense. This requirement is easily achieved if we make use of the observations illustrated in the last paragraph. Consider any synchronous molecular system. By properly choosing the inter-transmission times through the Neyman–Pearson lemma as explained above and in [12], we can ensure that

$$D_i \cong D_i' \cong X_i. \tag{15}$$

As a result, all the derivations and results in Section 2.2 apply, so that additional information is guaranteed through asynchronous information embedding.

The above discussions are all based on the ideal assumption that "the distributions of the decision times can be controlled and the decision events do not alter thereafter". The practical situations, however, is not always perfect.

Given an event-driven system, consider its transmission process (S_i, X_i) and decision process (T_i, D_i), where S_i denotes the transmission times, X_i the transmission events, T_i the decision times, and D_i the decision events.

We point out a very important fact about the above mechanism. Although we have proved that the decision rule is invariant when we impose timing information, in the information-theoretic point of view the original system may very well be changed.

In the rest of this paper, we will demonstrate the concept of *asynchronous information embedding* by using a synchronous type-based molecular communication system as an example of an event-driven system. Additional information is embedded by letting the inter-transmission times between two consecutive transmissions be random. Without loss of generality, we choose the simple Bernoulli random variable to demonstrate the whole process. The capacity gain of such a process will also be discussed in the following sections.

3. System model of type-based synchronous systems

We consider a one-dimensional type-based molecular communication system located in a fluid medium. Without loss of generality, suppose that a transmitter is located at the origin and a receiver is at distance x on the positive axis. The transmitter has M types of molecule. Denote the type candidate set by $\mathbb{Q}$. For example, if $\mathbb{Q} = \{A, B\}$, then there are two types of molecule, A and B. After a molecule is released by the transmitter, it diffuses freely in the medium and is assumed to follow *Brownian motion*. We also assume that there are no interactions between transmitted molecules, so each molecule diffuses independently. Once a molecule reaches the receiver, it is captured and discarded. The receiver is assumed to be capable of *recognizing the type* and *computing the time difference between two consecutively received molecules*. Under these assumptions, each molecule experiences a delay which is independent and identical for all molecules. The distribution of the delay d is given by the first hitting time of Brownian motion [10]:

$$f_d(t) = \frac{x}{\sqrt{4\pi D}} \frac{1}{t^{\frac{3}{2}}} \exp\left\{-\frac{(vt - x)^2}{4Dt}\right\}, \tag{16}$$

where D is the diffusion coefficient, x is the distance from the transmitter to the receiver, and v is the drifting velocity. The diffusion coefficient D is given by

$$D = \frac{k_B T}{6\pi nr}, \tag{17}$$

where k_B is the Boltzmann constant, T is the temperature, n is the viscosity of the fluid medium, and r is the radius of the molecule. For simplicity, we assume that the radii for all molecules are the same, so that they have the same diffusion coefficient. These assumptions are usual in molecular communication systems. In the meantime, most existing research also assumes that the inter-transmission durations are fixed, which is a familiar concept rooted in classical *synchronous* communications. We formally define *synchronous type-based systems* [7] as follows.

- The transmitter conveys messages by releasing a sequence of molecules in the type candidate set $\mathbb{Q}$.
- Each molecule in $\mathbb{Q}$ represents a distinct message.
- The inter-transmission duration is a fixed real number T.
- Once the receiver receives a molecule, it recognizes the molecule type and discards the molecule.

The information of systems with above settings is carried on the molecule type. In this paper, we loosen the third restriction to let the inter-transmission times be random and call such systems *asynchronous*. We impose an artificial distribution on the inter-transmission times so that, under suitable decision rules, different realizations of inter-transmission times can be recognized, and therefore information can be transmitted. We coin the term "mixed type–time" for such systems since the information is carried on both the type and time. Formally, we have the following definition of a mixed type–time system.

- The transmitter conveys messages by releasing a sequence of molecules in $\mathbb{Q}$.
- Each molecule in $\mathbb{Q}$ represents a distinct message.
- All inter-transmission times follow a prescribed distribution S. That is, let b_1 and b_2 be the transmission times of any two consecutively transmitted molecules. Then $b_2 - b_1 \sim S$.

For mixed type–time systems, the decision rules at the receiver side are yet to be designed. Although the derivations of decision rules for general S are possible, in this paper we will focus only on the special case of *Bernoulli inter-transmissions*, that is, the case where S is a Bernoulli random variable. This is the simplest version of our asynchronous communication scheme. Despite its simplification, it helps us gain insights into asynchronous systems, and the principles of analysis apply to all finitely supported distributions.

Though from a synchronous type-based system to a mixed type–time system we have only modified one condition, the receiver becomes quite complicated, and we choose to focus on one factor at a time. Instead of directly dealing with a mixed type–time system, we first observe how the random inter-transmissions influence type-based systems. After that, we ignore the information on the molecule type and focus on the timing information. Finally, we combine the above two systems. These steps are formally recorded as studies of following three asynchronous systems.

(i) *Type-based system with i.i.d. random inter-transmissions*
Assume that the inter-transmission times are i.i.d. random variables. We further assume that the information is carried only on the *type* of molecules.

(ii) *Time-based system*
In this system, the transmitted molecules are only for timing purposes and are assumed to carry no information on the type (i.e., the receiver uses only the arrival times for decision). The information is embedded in the inter-transmission times of pairs of consecutively transmitted molecules.

(iii) *Mixed type–time system*
We can embed information in both molecule types and inter-transmission times. The resulting system is a combination of the above two and is just what we have defined as the "mixed type–time system".

Although we do not mention synchronous systems explicitly, we will show in Section 4.1 that synchronous systems are special cases of (i). Therefore, all the results for (i) apply to synchronous systems. Analyses of (i) and (ii) will serve as auxiliaries when we treat (iii).

4. Asynchronous information embedding for type-based synchronous systems

In this section, we discuss in detail the asynchronous information embedding process for the type-based system described in the last section. We will treat all three systems mentioned in Section 3 in the corresponding subsections. In the following, $f(\cdot)$ will denote the p.d.f. and

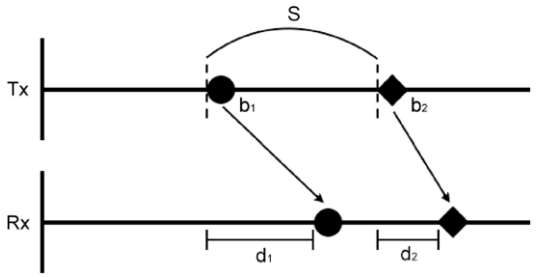

Fig. 3. Asynchronous system.

$F(\cdot)$ the cumulative distribution function (c.d.f.) of relevant distributions.

4.1. Type-based systems with i.i.d. random inter-transmissions

We first derive the crossover error probability that is greatly harmful to system performance in Section 4.1.1, and then use it to compute the capacity approximation in Section 4.1.2.

4.1.1. Crossover error probability

Consider a transmission pair in Fig. 3. Let b_1, b_2 be the transmission times and d_1, d_2 the diffusion times of two molecules, respectively. If the two transmitted molecules are of the same type, then there is no error even if a crossover occurs. However, if they are of different types and if $b_1 + d_1 > b_2 + d_2$, a crossover error occurs. The *error probability* is given by

$$P_e = P(b_1 + d_1 > b_2 + d_2) = \int P(b_2 - b_1 + d_2 < t) f_d(t) dt. \quad (18)$$

Assume that the inter-transmission times are i.i.d. random variables, say $b_2 - b_1 \sim S$. Let $Z \triangleq S + d$. Then

$$P_e = \int P(b_2 - b_1 + d_2 < t) f_d(t) dt = \int P(S + d_2 < t) f_d(t) dt = \int F_Z(t) f_d(t) dt. \quad (19)$$

Note that, for a fixed number $T > 0$, if $S = T$ a.s., then the system reduces to the synchronous case. This suggests that asynchronous systems are more general than synchronous ones.

4.1.2. Capacity approximation

We have derived the crossover probability in Section 4.1.1. In general, to compute the channel capacity we have to consider all levels of crossover. However, in the following we focus on the one-level crossover errors instead of pursuing the general form of all crossovers for the following two reasons.

(i) The general form involves combinatorial terms and is intractable in both computation and analytical form.

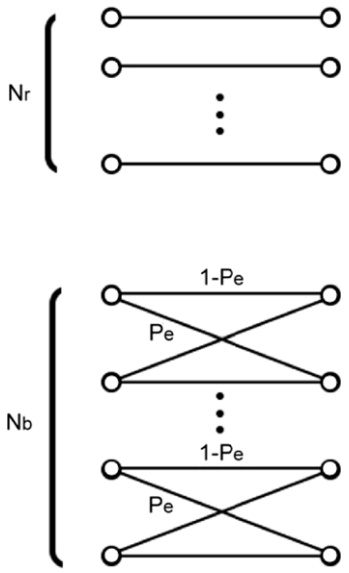

Fig. 4. Channel C.

(ii) We will give a procedure in Section 4.4 to design a system with very small one-level crossover probability. Under such settings, the crossovers of more than two levels can be ignored.

Assume a set of M types of molecule. Suppose that the probability of more than two-level crossover is negligible. We now derive an approximation for the channel capacity by viewing the whole transmission process as independent consecutive transmissions of pairs of molecules. Under this assumption, we can construct an error transition matrix $P_{M^2\times M^2}$ for each pair of molecules. By our analysis above, $P_{M^2\times M^2}$ has the form

$$P = \begin{pmatrix} 1 & 0 & \cdots & \cdots & 0 \\ 0 & 1-P_e & \cdots & P_e & \cdots 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & P_e & \cdots & 1-P_e & \cdots 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & \cdots & \cdots & 1 \end{pmatrix},$$

wherethe rows consisting of a single "1" represent transmission pairs of the same type of molecule and the remaining rows those of different types. This form of matrix has an interpretation in information theory (see Fig. 4).

We can easily see that $N_r = M$ and $N_b = \frac{M^2-M}{2}$. It is well known that the channel capacity of a binary symmetric channel (BSC) is given by $1 - H(P_e)$ [5]. From Fig. 4, we can compute the channel capacity by [5] as

$$2^C = 2^{C_r} + 2^{C_b}, \quad (20)$$

where $C_r = \log N_r = \log M$ and

$$C_b = \log N_b + 1 - H(P_e) = \log\left(\frac{M^2 - M}{2}\right) + 1 - H(P_e).$$

So

$$C = \log(2^{C_r} + 2^{C_b}) = \log\left(M + \frac{M^2 - M}{2} 2^{1-H(P_e)}\right). \quad (21)$$

This derivation shows that the channel capacity C depends only on P_e and the type-number M.

We make some remarks on (21). When considering any transmission pair, all the previously transmitted molecules have impacts on the present transmission pair, so for every transmission pair P_e should be different. However, (21) shows that C_M is a *continuous function* of P_e; thus a small perturbation of P_e causes negligible effect on C_M. Therefore, if we carefully choose the inter-transmission distribution (in Section 4.4), our approximation for channel capacity consequently makes sense.

4.2. Time-based systems

In this section, we analyze systems with information carried only in the inter-transmission times. We derive relevant distributions in Section 4.2.1 and decision rules for various criteria in Section 4.2.2. The results in Section 4.2.2 are the foundations for discussions of system design in Section 4.4.

Consider a consecutive two-molecule transmission with information embedded in the time difference S. The simplest case is that the time difference follows a Bernoulli distribution with parameter π_0. Explicitly, for two fixed numbers $t_0, t_1, t_0 < t_1$,

$$P(S = s) = \begin{cases} \pi_0 & \text{for } s = t_0 \\ 1 - \pi_0 & \text{for } s = t_1. \end{cases}$$

We refer to Fig. 3 again and let b_1, b_2 be the transmission times and d_1, d_2 the diffusion times of two molecules, respectively. We can form the hypothesis testing problem:

$$\begin{cases} H_0 : b_2 - b_1 = t_0, \\ H_1 : b_2 - b_1 = t_1. \end{cases}$$

The *prior* distribution for this system is just $\{\pi_0, 1 - \pi_0\}$ for H_0, H_1, respectively.

4.2.1. Derivations for related distributions

For a fixed hypothesis H_i, put $U = d_1$ and $V = d_2 + t_i$. Then U, V are independent since d_1, d_2 are. Define

$$M = \max\{U, V\} = \max\{d_1, d_2 + t_i\},$$
$$N = \min\{U, V\} = \min\{d_1, d_2 + t_i\}.$$

It is well known from order statistic theory [14] that

$$f_{N,M}(n, m) = f_U(m) f_V(n) + f_U(n) f_V(m) = f_d(n) f_d(m - t_i) + f_d(m) f_d(n - t_i) \quad \text{for } m \geq n. \quad (22)$$

Note that in Section 3 we have only assumed the receiver to be capable of computing the *time differences*, and not the absolute times. Therefore, we *cannot* observe N directly. Instead, our observation is $Q \triangleq M - N = |U - V|$. Denote the realization of Q by q. The distribution of Q can be calculated as follows:

$$\begin{aligned} F_{M-N}(q|H_i) &= P(M - N \leq q|H_i) \\ &= \int_0^\infty \int_0^\infty P(m - n \leq q|H_i) f_{M,N}(m, n|H_i)\, dm\, dn \\ &= \int_0^\infty \int_0^\infty I_{\{m-n\leq q\}} f_{M,N}(m, n|H_i)\, dm\, dn \\ &= \int_0^\infty \int_0^{n+q} f_{M,N}(m, n|H_i)\, dm\, dn, \end{aligned} \quad (23)$$

where $I_{\{\cdot\}}$ is the indicator function. We then differentiate the c.d.f. with respect to q to obtain the p.d.f.:

$$\begin{aligned} f_{M-N}(q|H_i) &= \frac{d}{dq} F_{M-N}(q|H_i) \\ &= \frac{d}{dq} \int_0^\infty \int_0^{n+q} f_{M,N}(m, n|H_i)\, dm\, dn. \end{aligned} \quad (24)$$

Since the integrand of the outer integral is bounded by an integrable function $\int_0^\infty f_{M,N}(m, n) dm$, by Lebesgue's *dominated convergence theorem* (DCT), we can exchange the order of integration and differentiation:

$$\begin{aligned} f_{M-N}(q|H_i) &= \int_0^\infty \frac{d}{dq} \left[\int_0^{n+q} f_{M,N}(m, n|H_i)\, dm\right] dn \\ &= \int_0^\infty f_{M,N}(n + q, n|H_i)\, dn. \end{aligned} \quad (25)$$

4.2.2. Decision rules

Assume first that the *prior* distribution is known and the cost functions are the binary symmetric loss (i.e., we focus on error probability minimization). Consider the *maximum a posteriori probability (MAP)* criterion:

$$\begin{aligned} \operatorname*{argmax}_{i\in\{0,1\}} P(H_i|q) &= \operatorname*{argmax}_{i\in\{0,1\}} \frac{P(H_i, q)}{P(q)} \\ &= \operatorname*{argmax}_{i\in\{0,1\}} P(H_i) P(q|H_i) \\ &= \operatorname*{argmax}_{i\in\{0,1\}} \pi_i f_{M-N}(q|H_i). \end{aligned}$$

It is well known that the *MAP* criterion leads to the likelihood-ratio test [16]:

$$\text{Decide: } \begin{cases} H_0 & \text{if } \Lambda(q) > \dfrac{\pi_1}{\pi_0} \\ \text{randomized} & \text{if } \Lambda(q) = \dfrac{\pi_1}{\pi_0}, \\ H_1 & \text{if } \Lambda(q) < \dfrac{\pi_1}{\pi_0}, \end{cases}$$

where $\Lambda(q)$ is the likelihood-ratio statistic

$$\Lambda(q) \triangleq \frac{f_{M-N}(q|H_0)}{f_{M-N}(q|H_1)} = \frac{\int_0^\infty f_{M,N}(n + q, n|H_0) dn}{\int_0^\infty f_{M,N}(n + q, n|H_1) dn}. \quad (26)$$

Without knowing the *prior* distribution, we consider the minimax criterion. For a fixed decision rule δ, let $P_F(\delta)$

and $P_M(\delta)$ denote the false alarm and missing probability, respectively. The minimax criterion is to consider the following optimization problem:

$$\min_{\delta}\{\max\{P_F(\delta), P_M(\delta)\}\},$$

where the minimization is taken over all decision rules. For the minimax criterion, the resulting decision rule corresponds to the likelihood-ratio test of the least favorable *prior*, which is given by the function

$$V(\pi_0) = \text{the minimum possible}$$
$$\text{Bayes risk for the } \textit{prior}\ \pi_0.$$

Besides Bayes and minimax, we also consider the Neyman–Pearson criterion, which corresponds to the optimization problem

$$\max_{\delta} P_D(\delta) \text{ subject to } P_F(\delta) \le \alpha,$$

where $\alpha < 1$ is a specified level and $P_D(\delta) \triangleq 1 - P_M(\delta)$ is the detection probability. The best way to observe the results of Neyman–Pearson tests is to draw the receiver operating curves (ROCs).

Numerical results of both $V(\cdot)$ and ROCs are given in Section 4.

4.3. Mixed type–time systems

Suppose now that the transmitter embeds information in both the molecule types and inter-transmission times. To assess the performance of the mixed type–time system, we use the capacity approximation derived in previous sections. For ease of illustration, we assume that there are only two types of molecule, say $\mathbb{Q} = \{A, B\}$. The general case for M-type systems can be calculated similarly.

Denote the type-based information bit by A, B and the time-based information bit by H_0, H_1. As in Section 4.1.2, we view the whole transmission process as independent consecutive transmissions of pairs of molecules and separate the two cases.

4.3.1. Same type of molecule

For the decision rule we just derived on time-based systems, let P_F and P_M denote the false alarm probability and missing probability, respectively. If the two transmitted molecules are of the same type, then we have the channel form:

For this channel (see Fig. 5), we have the probability transition matrix

$$P = \begin{pmatrix} 1-P_F & P_F & 0 & 0 \\ P_M & 1-P_M & 0 & 0 \\ 0 & 0 & 1-P_F & P_F \\ 0 & 0 & P_M & 1-P_M \end{pmatrix}.$$

4.3.2. Different types of molecule

Similarly, we have the channel form in Fig. 6.

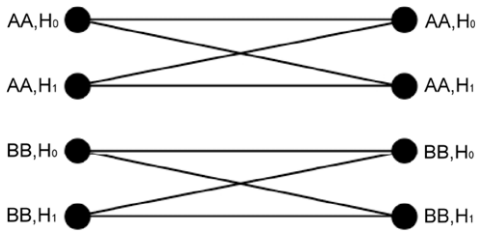

Fig. 5. Channel C_1.

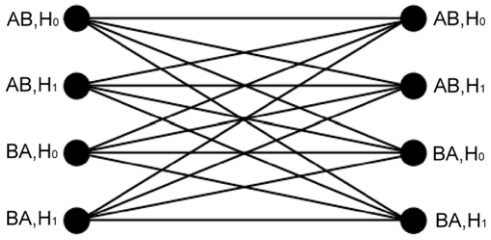

Fig. 6. Channel C_2.

To derive the transition probabilities of this channel, we use the notation in Section 4.2.1, and notice that

$$f_Q(q|H_i, U < V) = \int_0^\infty f(n+q-t_i)f(n)dn, \tag{27}$$

$$f_Q(q|H_i, U \ge V) = \int_0^\infty f(n-t_i)f(n+q)dn. \tag{28}$$

The transition probability of the top link in Fig. 6 can be calculated as

$$P(AB, H_0|AB, H_0) = (1-P_{e0})P_Q(q \in \Gamma_0|H_0, U < V), \tag{29}$$

where Γ_0 is the decision region of H_0 and $P_{e0} = P(U \ge V|AB, H_0)$ is the one-level crossover probability when the transmitting time difference is given by H_0 (see Eq. (19)). Other transition probabilities can be calculated similarly.

The channel capacity for both C_1 and C_2 can be computed by the Blahut–Arimoto algorithm [19], and the total channel capacity is given by

$$C = \log(2^{C_1} + 2^{C_2}). \tag{30}$$

4.4. System design for mixed type–time systems

By system design we mean the assignments of relevant system parameters, namely, t_0, t_1 and the corresponding *prior* distribution π_0. From previous derivations we can see that the performances of both type-based (Section 4.1.2) and time-based (Section 4.2.2) systems are related to the *prior* distribution π_0, so π_0 plays an important role when we incorporate the two systems. The total effect, however, of this *prior* is complicated and intractable in analytical form. In such a situation, the idea is to design t_0 and t_1 so that the controllable performance requirements are satisfied. We therefore propose the following simple and intuitive procedure.

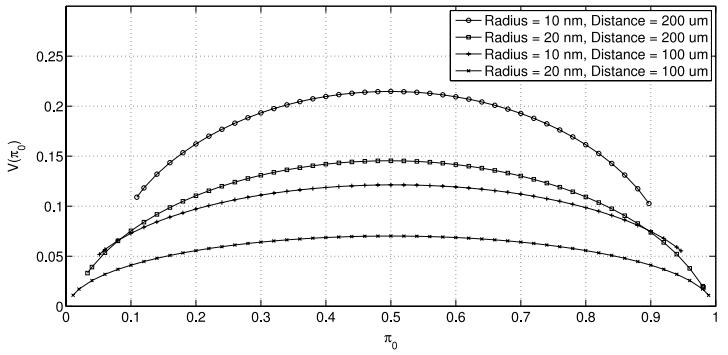

Fig. 7. $V(\pi_0)$ for drift velocity $v = 1\ \mu\text{m/s}$, 300 K water.

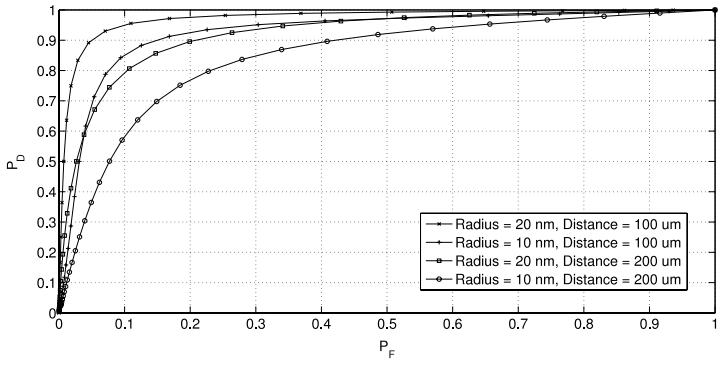

Fig. 8. Receiver operating curves for drift velocity $v = 1\ \mu\text{m/s}$, 300 K water.

(1) Specify two levels, α_1 and α_2, on type-based and time-based systems, respectively.
(2) Choose t_0 so that the level α_1 is satisfied in the type-based system. This can be done by the Neyman–Pearson procedure.
(3) Choose t_1 so that the level α_2 is satisfied in the time-based system. This can be done, again, by the Neyman–Pearson procedure.

Note that when considering time-based systems we adopt the Neyman–Pearson procedure, since the minimax procedure itself does *not* give the resulting performance, the bit error rate (BER). Therefore, if we were to specify a level *beforehand* and ask if the minimax procedure meets our requirement, we have to compute for sets of parameters the resulting BERs and see if any of them is valid. In contrast, the procedure above automatically meets our requirements and provides robustness that is valid for all *prior* distributions and for both type-based and time-based systems, thus guaranteeing a certain level of quality of the overall mixed type–time systems.

5. Numerical results

We present numerical results in this section. In the following, we assume that the fluid medium is 300 K water (so the viscosity is fixed) and the drift velocity $v = 1\ \mu\text{m/s}$. t_0 is set to 100 s and t_1 to 300 s.

Although we do not adopt the minimax procedure, for the sake of completeness we still present the $V(\cdot)$ in Fig. 7. In Fig. 7, all curves are concave, which is in accordance to the theory [16]. We mention that, although the figure looks symmetric, the precise values are not, so we cannot naively set the least favorable *prior* to 0.5. This is just a coincidence for our choices of parameters.

Fig. 8 presents the ROCs. We observe two situations in this figure.

1. For fixed radius (diffusion coefficient), increasing the distance worsens the performance.
2. For fixed distance, increasing the radius (or decreasing the diffusion coefficient) improves the performance.

These facts conform to our intuitions. Informally speaking, the diffusion coefficient represents the "stability" of the molecules. Molecules with large radius tend to be stable in space because of lighter random displacements, and therefore systems with large molecule radii outperform systems with small ones. On the other hand, as the distance increases, the uncertainty of the overall system increases, and thereby the performance degrades.

It is well known that channel capacity is one of the most fundamental performance measures for communication systems. We therefore adopt the channel capacity as the performance measure between synchronous type-based (STB) systems [7] and mixed type–time (MTT) systems.

Table 1
Capacity comparison.

Parameters	STB (100 s)	STB (200 s)	STB (300 s)	MTT
$r = 10\,\text{nm}$, $x = 100\,\mu\text{m}$	1.7620	1.9088	1.9678	2.3479
$r = 10\,\text{nm}$, $x = 200\,\mu\text{m}$	1.6801	1.8290	1.9240	2.0968
$r = 20\,\text{nm}$, $x = 100\,\mu\text{m}$	1.8290	1.9691	1.9955	2.5516
$r = 20\,\text{nm}$, $x = 200\,\mu\text{m}$	1.7336	1.9156	1.9818	2.2826

Table 1 contains the results of capacity approximation derived in Sections 4.1 and 4.3. The inter-transmission durations of synchronous systems are set to be 100 s, 200 s, and 300 s, respectively. As we see in Table 1, the performance of the mixed type–time systems is much better than that of the synchronous counterparts. This fact suggests that carrying additional information in inter-transmission times significantly improves the systems.

6. Conclusions

In this paper, we have defined an abstract system structure called an *event-driven system*, and have shown that, under such a system, we can carry additional information without affecting the original signaling by using a process called *asynchronous information embedding*. We also showed that a great number of commonly seen molecular communication systems fall into this category, including all synchronous systems.

By using a synchronous type-based system as an example, we examined in detail the process of *asynchronous information embedding*. We saw that the channel capacity had been increased after this embedding process. We have also proposed a procedure for designing the system parameters to guarantee a good performance. Numerical results confirmed the feasibility.

The effort in this paper serves as an initial study of a brand new scheme of asynchronous information embedding for molecular communications. Although we focus on Brownian motion channels, the analyses in this paper apply to any diffusion channels as long as the delay distribution is known. Furthermore, we have only analyzed synchronous type-based systems, whereas all procedures in this paper apply to any event-driven system. These problems remain open, and further investigations are needed in the future.

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