Maximum Likelihood Detection for Collaborative Molecular Communication

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Abstract—In this paper, symbol-by-symbol maximum likelihood (ML) detection is proposed for a collaborative diffusion-based molecular communication system. In this system, a fusion center (FC) chooses the transmitter’s symbol that is more likely, given the likelihood of the observations from multiple receivers (RXs). First, two ML detection variants with different levels of computational complexity in perfect reporting are considered. Second, two communication schemes in noisy reporting are considered, namely, 1) decode-and-forward (DF) with multi-molecule-type and ML detection at the FC (MD-ML) and 2) DF with single-molecule-type and ML detection at the FC (SD-ML). Closed-form expressions are derived for the error probabilities of (i) the single-RX system using MD-ML and (ii) the multi-RX system using the lower-complexity ML detection variant. Numerical and simulation results show that ML detection variants and MD-ML achieve a significant error performance improvement over the existing hard fusion rules. For example, the lower-complexity variant achieves a 61-fold improvement and MD-ML achieves a 4-fold improvement for 5 RXs.

I. INTRODUCTION

Molecular communication (MC) has been acknowledged as one of the most promising solutions to implement communication in bio-inspired nanonetworks, due to its unique potential benefits of bio-compatibility and low energy consumption; see [1]. In MC, the information transmission between devices is realized through the exchange of molecules; see [2]. The simplest molecular propagation mechanism is free diffusion, where the information-carrying molecules can propagate from the transmitter (TX) to the receiver (RX) via Brownian motion.

In order to tackle the rapidly decreasing reliability in MC when the TX-RX distance increases, the concept of collaborative MC has been developed in [3, 4] where multiple RXs that share common information are used for collaborative detection. This concept is motivated by practical examples in biological environments, such as when cells or organisms share common information to achieve a specific task, e.g., calcium (Ca$^{2+}$) signaling; see [5].

The majority of existing MC studies have focused on the modeling of a single-RX MC system. Recent studies, e.g., [6–9], have expanded the single-RX MC system to the multi-RX MC system. However, the potential of collaboration among multiple RXs to determine the TX’s intended symbol sequence in a multi-RX MC system has not been established in the literature. Motivated by this, our work in [3, 4] analyzed the error performance of a collaborative diffusion-based MC system where a fusion center (FC) device uses hard fusion rules to combine the local decisions of distributed RXs to improve the detection of the TX’s symbols. Moreover, we considered in [3] a simple soft fusion scheme that achieves lower error probability than the collaborative system with hard fusion rules.

In other fields of communications, e.g., wireless communications, the maximum likelihood (ML) detector is commonly used to achieve the optimal detection performance; see [10, Ch. 5]. In the MC domain, the ML sequence detector has been considered for optimality in several studies, e.g., [11–13]. However, the high complexity of sequence detection is a significant barrier to implement it in the MC domain, even when applying simplified algorithms; see [12, 13]. As such, recent studies have considered symbol-by-symbol ML detection, e.g., [14]. Very recently, [15] considered collaborative ML detection where RXs detect an event and send molecules to a FC over an anomalous diffusion channel.

In this paper, we present symbol-by-symbol ML detection for the collaborative diffusion-based MC system where inter-symbol interference (ISI) is considered. In our proposed system, the FC chooses the TX symbol that was more likely, given the (joint) likelihood of its observations from all of the individual RXs, where the TX sends the same information symbol to all RXs. Thus, the ISI at RXs and the FC is due to the previous symbols transmitted by the TX and RXs, respectively. This work is the first attempt to apply ML detection to the collaborative MC communication system with multiple phases, whereas [14] considered a single RX only and [15] considered a constant event detection probability at each RX, rather than transmission by a TX over a noisy channel. The significance of this paper lies in the fact that our results determine the lower bounds on the error performance that can be achieved in the practical collaborative MC system with hard fusion rules considered in [3, 4].

We consider two different reporting scenarios, namely, perfect reporting and noisy reporting. In perfect reporting, we propose two ML detection variants with different levels of computational complexity. For Variant 1, we measure the likelihood of every individual symbol at each RX, which entails higher computational complexity. For Variant 2, we measure the likelihood of the sum of the symbols at each RX, which entails lower computational complexity and leads to tractable error performance analysis. In noisy reporting, we consider two different communication schemes between the
RXs and the FC, namely, 1) decode and forward (DF) with multi-molecule-type and ML detection at the FC (MD-ML) and 2) DF with single-molecule-type and ML detection at the FC (SD-ML). We note that MD-ML may not be practical in some cases since we need each RX to release a unique type of molecule. However, this assumption gives a lower bound on the error performance of SD-ML. SD-ML is more suitable for environments and devices where the number of types of molecules available is constrained.

Our major contributions are summarized as follows: We derive closed-form analytical expressions for the system error probability for Variant 2 in the perfect reporting scenario and for MD-ML with one RX in the noisy reporting scenario. We are interested in analytically deriving the error performance for MD-ML and SD-ML with multiple RXs in our future work. Using simulation and numerical results, we corroborate the accuracy of our analytical expressions. We demonstrate that symbol-by-symbol ML detection provides a profound error performance gain than hard fusion rules in both perfect and noisy reporting scenarios.

II. SYSTEM MODEL

We consider a collaborative MC system in a three-dimensional space based on [3,4], as illustrated in Fig. 1, which consists of one TX, a “cluster” of K RXs, and one device acting as a FC. We assume that the system has a symmetric topology\(^1\) such that the distances between the TX and the RXs are identical and the distances between the RXs and the FC are also identical. The FC is not included in the set of RXs. For reliable reporting, we generally assume that the FC is close to the cluster of RXs. We also assume that all RXs and the FC are passive spherical observers such that molecules can diffuse through them without reacting. Accordingly, we denote \(V_{RX_k}\) and \(r_{RX_k}\) as the volume and the radius of the \(k\)th RX, \(RX_k\), respectively, where \(k \in \{1,2,\ldots,K\}\). We also denote \(r_{RC}\) as the radius of the FC. For the sake of analysis we assume that all individual observations are independent of each other, although this is relaxed in our simulations. We clarify that we use the terms “sample” and “observation” interchangeably to refer to the number of molecules observed by a RX or the FC at time \(t\).

\(^1\)The assumption of the symmetric topology is adopted for the tractability of error performance analysis. This assumption will be relaxed in future work.

We now present the timing schedules of the system. The transmission interval time from the TX to the RXs is denoted by \(t_{\text{trans}}\) and the report interval time from the RXs to the FC is denoted by \(t_{\text{report}}\). Thus, the symbol interval time from the TX to the FC is given by \(T = t_{\text{trans}}+t_{\text{report}}\). Throughout this paper, we use \(W\) to represent a single information symbol and \(W\) to represent a vector of information symbols. At the beginning of the \(j\)th symbol interval, i.e., \((j-1)T\), the TX transmits \(W_{TX}[j]\). After this, the TX keeps silent until the start of the \((j+1)\)th symbol interval. We denote \(L\) as the length of the symbols transmitted by the TX. We define \(W_{TX} = \{W_{TX}[1], \ldots, W_{TX}[L]\}\) as an \(L\)-length subsequence of the symbols transmitted by the TX, where \(L \leq L\).

In this paper, we address two different reporting scenarios: perfect reporting and noisy reporting. In the perfect reporting scenario, we assume that the FC has perfect knowledge of the observations of all TX – RX links and thus chooses the symbol \(W_{RC}[j]\) based on the observations in the \(j\)th symbol interval. In the noisy reporting scenario, we assume that the FC chooses the symbol \(W_{RC}[j]\) based on its observations of all RX – FC links in the \(j\)th symbol interval. We define \(W_{RC} = \{W_{RC}[1], \ldots, W_{RC}[L]\}\) as an \(L\)-length subsequence of the chosen symbols at the FC. We emphasize that the symbol interval time \(T\) is the same in both reporting scenarios. Next, we describe the transmission of each information symbol and all ML detection approaches in both reporting scenarios.

A. Perfect Reporting

In this scenario, we only consider one-phase transmission of each information symbol from the TX to RXs, since the FC has perfect knowledge of the observations at all RXs. The TX transmits information symbols to the RXs via type \(A_0\) molecules which diffuse independently. In this work we consider that the TX uses ON/OFF keying [16] to convey information, i.e., the TX releases \(S_0\) molecules of type \(A_0\) to convey information symbol “1” with probability \(Pr(W_{TX}[j] = 1) = P_1\), but no molecules to convey information symbol “0”. Each RX\(_k\) observes type \(A_0\) molecules over the TX – RX\(_k\) link and takes \(M_{RX}\) samples in each symbol interval at the same times. The time of the \(m\)th sample for each RX in the \(j\)th symbol interval is given by \(t_{RX}(j,m) = (j-1)T + m\Delta t_{RX}\), where \(\Delta t_{RX}\) is the time step between two successive samples at each RX, \(m \in \{1,2,\ldots,M_{RX}\}\), and \(M_{RX}\Delta t_{RX} < t_{\text{trans}}\). In the perfect reporting scenario, we consider two ML detection variants and simple soft fusion.

**Variant 1:** The FC separately assesses the likelihood of every sample at each RX and chooses the symbol \(W_{RC}[j]\) that is more likely, given the joint likelihood of \(K\) \(M_{RX}\) individual observations at all RXs in the \(j\)th symbol interval.

**Variant 2:** The FC adds each RX’s \(M_{RX}\) observations in the \(j\)th symbol interval, i.e., the FC applies an equal weight to every observation at each RX. The FC then chooses the symbol \(W_{RC}[j]\) that is more likely, given the joint likelihood of \(K\) sums of \(M_{RX}\) observations in the \(j\)th symbol interval.

**Simple soft fusion:** The FC adds all RXs’ \(K\) \(M_{RX}\) observations in the \(j\)th symbol interval, and then makes a decision.
The functional symbol $W_{fc}[j]$ by comparing this sum with a decision threshold $\xi_{fc}$. We emphasize that $\xi_{fc}$ is constant and independent of $W_{tx}^{-1}$. We measured this variant in [3] but did not analyze it.

B. Noisy Reporting

In this scenario, the transmission of each information symbol from the TX to the FC via RXs is completed in two phases. The first phase of the noisy reporting scenario is analogous to the one-phase transmission of perfect reporting. For the second phase, we consider two different communication schemes between the RXs and the FC over a diffusion channel, namely, MD-ML and SD-ML.

**MD-ML**: Each RX detects with an energy detector as described in [12]. The constant detection threshold at RX_k is denoted by $\xi_{ks}$ and is independent of $W_{tx}^{-1}$. We denote $W_{ks}[j]$ as the binary decision on the jth transmitted symbol at RX_k. We define $\hat{W}_{bs}[j] = \{\hat{W}_{bs}[1], \ldots, \hat{W}_{bs}[l]\}$ as an l-length subsequence of the local hard decisions at RX_k.

At the time $(j-1)T + t_{trans}$, each RX_k reports $\hat{W}_{ks}[j]$ via diffusion to the FC. RX_k transmits type $A_k$ molecules, which can be independently detected by the FC. Similar to the TX, each RX uses ON/OFF keying to report its decision to the FC and the RX releases $S_k$ molecules of type $A_k$ to convey information symbol “1”. The FC receives type $A_k$ molecules over the RX_k – FC link and takes $M_{fc}$ samples of each type $A_k$ molecule in every reporting interval. The time of the $m$th sample of the received molecules at the FC in the $j$th symbol interval is given by $t_{fc}(j, m) = (j-1)T + t_{trans} + m\Delta t_{fc}$, where $\Delta t_{fc}$ is the time step between two successive samples over the FC and $m \in \{1, 2, \ldots, M_{fc}\}$. We assume that the $K$ RX_k – FC links are independent. As such, FC has $K$ independent sets of observations from the $K$ RX_k – FC links. The FC adds $M_{fc}$ observations for each RX_k – FC link in the jth symbol interval and the symbol $\hat{W}_{fc}[j]$ is considered in the joint likelihood of the $K$ sums of observations.

**SD-ML**: The behavior of each RX_k in SD-ML is the same as that in MD-ML, except we assume that each RX_k transmits type $A_1$ molecules to report $\hat{W}_{ks}[j]$ to the FC. The number of released type $A_1$ molecules for each RX_k in SD-ML is also denoted by $S_k$. The FC receives type $A_1$ molecules at all $K$ RX_k – FC links and takes $M_{fc}$ samples of type $A_1$ molecules in every reporting interval. The sampling schedule of the FC in SD-ML is the same as that in MD-ML. Thus, the FC has only one set of observations from the $K$ RX_k – FC links. The FC adds $M_{fc}$ observations for all RX_k – FC links in the jth symbol interval and chooses the symbol $\hat{W}_{fc}[j]$ in consideration of the joint likelihood of the sum of observations.

III. ML Detection Design

In this section, we present symbol-by-symbol ML detection design for the collaborative MC system. To this end, for a given TX subsequence $W_{tx}^{-1}$, we formulate the general decision rule of ML detection on the jth symbol transmitted by the TX as

$$\hat{W}_{tx}[j] = \arg\max_{W_{tx}[j]} \mathcal{L}[j],$$

where $\mathcal{L}[j]$ is the joint likelihood of the observations at all RXs or the FC in the jth symbol interval for $W_{tx}^{-1}$. In perfect reporting, $\mathcal{L}[j]$ is the joint likelihood of the observations at the RXs. In noisy reporting, $\mathcal{L}[j]$ is the joint likelihood of the observations at the FC. For the rare case when the likelihoods of $W_{tx}[j] = 1$ and $W_{tx}[j] = 0$ are the same, we assume that the FC chooses the symbol $\hat{W}_{fc}[j] = 1$.

In the remainder of this section, we present $\mathcal{L}[j]$ for Variant 1, Variant 2, MD-ML, and SD-ML. We denote $Q_{fc}[j]$ as the analytical error probability of the collaborative MC system in the jth symbol interval for a given $W_{tx}^{-1}$. We derive $Q_{fc}[j]$ for Variant 2 for perfect reporting and the MD-ML schemes when $K = 1$ for noisy reporting. We also derive $Q_{fc}[j]$ for the simple soft fusion scheme, which we did not present in [3]. By averaging $Q_{fc}[j]$ over all symbol intervals and all possible realizations of $W_{tx}^{-1}$, the analytical average error probability of the collaborative MC system, $\overline{Q}_{fc}$, can be obtained.

A. Perfect Reporting

In this subsection, we first evaluate $\mathcal{L}[j]$ for the two ML detection variants in the perfect reporting scenario. We then analyze the error performance of Variant 2 to provide a lower bound on the achievable error performance of the system in either the perfect or the noisy reporting scenario. We further examine the error performance of simple soft fusion.

1) TX – RX_k Link: We first evaluate the probability of observing a given type $A_0$ molecule, emitted from the TX at $t = 0$, inside $V_{ks}$ at time $t$, $P_{ob_i,0}^{(TX, RX_k)}(t)$. Given independent molecule behavior and assuming that the RXs are sufficiently far from the TX, we use [17, Eq. (6)] to write $P_{ob_i,0}^{(TX, RX_k)}(t)$ as

$$P_{ob_i,0}^{(TX, RX_k)}(t) = \frac{V_{ks}}{(4\pi D_0 t)^{3/2}} \exp\left(-\frac{d_{tx}^2}{4D_0 t}\right),$$

where $D_0$ is the diffusion coefficient of type $A_0$ molecules in $\mu m^2/s$ and $d_{tx}$ is the distance between the TX and RX_k in $\mu m$.

We denote $S_{ob_i,0}^{RX_k}(t)$ as the number of molecules observed within $V_{ks}$ at time $t$ due to the emission of molecules from the current and previous symbol intervals at the TX. As discussed in [12], $S_{ob_i,0}^{RX_k}(t)$ can be accurately approximated by a Poisson random variable (RV) with the mean given by

$$S_{ob_i,0}^{RX_k}(t) = \sum_{i=1}^{\lfloor T/(T-t_{trans})\rfloor} S_0 W_{tx}[i] P_{ob_i,0}^{(TX, RX_k)}(t - (i - 1)T).$$

The sum of $M_{RX}$ samples at RX_k in the jth symbol interval, $S_{ob_i,0}^{RX_k}(j) = \sum_{m=1}^{M_{RX}} S_{ob_i,0}^{RX_k}(t_{RX_k}(j, m))$, is also a Poisson RV whose mean is given by

$$S_{ob_i,0}^{RX_k}(j) = \sum_{i=1}^{j} S_0 W_{tx}[i] \sum_{m=1}^{M_{RX}} P_{ob_i,0}^{(TX, RX_k)}((j-i)T + m\Delta t_{RX_k}).$$

2) ML Detection: Each RX makes $M_{RX}$ observations within each symbol interval. The value of the ith observation at RX_k in the jth symbol interval is labeled $S_{ob_i,0}^{RX_k}$. We consider two ML detection variants in perfect reporting as follows.
Variant 1: The FC chooses the symbol $\hat{W}_{RX}[j]$ that is more likely, given the joint likelihood of $K M_k$ individual observations at all RXs in the $j$th symbol interval. Recall that we assume that all individual observations are independent of each other. Based on this assumption, $L[j]$ is given by

\[
L[j] = \prod_{k=1}^{K} \prod_{m=1}^{M_k} \Pr\left( S_{ob,0}^{RX}(t_{kx}(j, m)) = s_{j,m}^{RX_k} | W_{TX}[j], W_{txj}^{-1} \right).
\]

(5)

Variant 2: The value of the sum for RX$_k$ is labeled $s_{j}^{RX_k}$, where $s_{j}^{RX_k} = \sum_{m=1}^{M_k} s_{j,m}^{RX_k}$. The FC chooses the symbol $\hat{W}_{RX}[j]$ that is more likely, given the joint likelihood of $K$ sums $s_{j}^{RX_k}$ in the $j$th symbol interval. Recall that the $K$ RXs are independent. Thus, $L[j]$ is given by

\[
L[j] = \prod_{k=1}^{K} \Pr\left( S_{ob,0}^{RX_k}(j) = s_{j}^{RX_k} | W_{TX}[j], W_{txj}^{-1} \right).
\]

(6)

It can be shown that (5) and (6) can be evaluated by applying the analysis in Section III-A1 and the probability mass function (PMF) of the Poisson RVs $S_{ob,0}^{RX_k}(t)$ and $S_{ob,0}^{RX_k}(j)$.

3) Error Probability: We now derive $Q_{EC}[j]$ in the perfect reporting scenario for Variant 2. We define the conditional mean of $S_{ob,0}^{RX_k}(j)$ as $\lambda_{k,j} + \lambda_{k,k}[j]$ and $\lambda_{k,k}[j]$ when the $j$th symbol transmitted by the TX is $W_{TX}[j] = 1$ and $W_{TX}[j] = 0$, respectively. We note that $\lambda_{k,k}[j]$ is the expected ISI at RX$_k$ in the $j$th symbol interval due to the previously-transmitted TX symbols $W_{txj}^{-1}$. We consider a collaborative MC system with a symmetric topology, where the RXs have independent and identically distributed observations. Under this assumption, we have $\lambda_{k,[j]} = \lambda_{k}[j]$ and $\lambda_{k,k}[j] = \lambda_{k}[j]$. When not all previous symbols transmitted by the TX are “0”, i.e., $W_{txj}^{-1} \neq 0$, we have $\lambda_{k}[j] > 0$. Under the condition $\lambda_{k}[j] > 0$, we apply the PMF of the Poisson RV $S_{ob,0}^{RX_k}(j)$ and derive the decision rule of Variant 2 as

\[
s_{j}^{RX_k} \geq \xi_{k}[j],
\]

(7)

where $s_{j}^{RX_k} = \sum_{k=1}^{K} s_{j,k}^{RX_k}$, $\xi_{k}[j] = \left[ \frac{\lambda_{k}[j]}{\log(\lambda_{k}[j]/\lambda_{k,0}[j])} \right]$, $\log(\cdot)$ is the natural logarithm, and $\lfloor \cdot \rfloor$ is the nearest integer. Thus, when $W_{txj}^{-1} \neq 0$, we evaluate $Q_{EC}[j]$ for Variant 2 as

\[
Q_{EC}[j] = (1 - P_2) \Pr\left( S_{ob,0}^{RX_k}(j) \geq \xi_{k}[j] | W_{TX}[j] = 0, W_{txj}^{-1} \right) + P_2 \Pr\left( S_{ob,0}^{RX_k}(j) \leq \xi_{k}[j] | W_{TX}[j] = 1, W_{txj}^{-1} \right),
\]

(8)

where $S_{ob,0}^{RX_k}(j) = \sum_{k=1}^{K} S_{ob,0}^{RX_k}(j)$. When all previous symbols transmitted by the TX are “0”, i.e., $W_{txj}^{-1} = 0$, we have $\lambda_{k}[j] = 0$. Under the condition $\lambda_{k}[j] = 0$, we apply the PMF of the Poisson RV $S_{ob,0}^{RX_k}(j)$ and derive the decision rule of Variant 2 as

\[
s_{j}^{RX_k} \geq \xi_{k}[j],
\]

(9)

We note that our evaluation of $L[j]$ mandates the precise knowledge of $W_{txj}^{-1}$ at the FC, which gives a lower bound on the performance error.

Thus, when $W_{txj}^{-1} = 0$, we evaluate $Q_{EC}[j]$ for Variant 2 as

\[
Q_{EC}[j] = (1 - P_2) \Pr\left( S_{ob,0}^{RX_k}(j) > \xi_{k}[j] | W_{TX}[j] = 0, W_{txj}^{-1} \right)
+ P_2 \Pr\left( S_{ob,0}^{RX_k}(j) = \xi_{k}[j] | W_{TX}[j] = 1, W_{txj}^{-1} \right).
\]

(10)

We remark that if the FC instead adds all RXs’ $K M_k$ observations in the $j$th symbol interval to obtain the single sum $s_{j}^{RX_k}$, the error performance of the FC is the same as that of Variant 2. That is, the knowledge of individual $s_{j}^{RX_k}$ for each RX does not improve detection performance over only knowing the sum $s_{j}^{RX_k}$.

We now consider $Q_{EC}[j]$ in the perfect reporting scenario with simple soft fusion. It can be shown that $Q_{EC}[j]$ for simple soft fusion with any realization of $W_{txj}^{-1}$ can be obtained by replacing $\xi_{k}[j]$ with the constant $\xi_{k}$ in (8).

B. Noisy Reporting

In this subsection, we analyze the RX$_k$ – FC link and then evaluate $L[j]$ in the MD-ML and SD-ML schemes. We further derive the error performance for MD-ML when $K = 1$.

1) RX$_k$ – FC Link: We denote $P^{R,EC}_{ob,0}(t)$ as the probability of observing a given $A_k$ molecule, emitted from the center of RX$_k$ at $t = 0$, inside $V_{FC}$ at time $t$. Due to the FC’s intended proximity to each RX$_k$, we find that (2) or [17, Eq. (6)] cannot be used to evaluate $P^{R,EC}_{ob,0}(t)$. Thus, we resort to [18, Eq. (27)] to evaluate $P^{R,EC}_{ob,0}(t)$ as

\[
P^{R,EC}_{ob,0}(t) = \frac{1}{2} \left[ \text{erf} \left( \tau_1 \right) + \text{erf} \left( \tau_2 \right) \right] - \frac{\sqrt{D_{k}}}{d_{res}} \left[ \exp \left( -\frac{\tau_1^2}{\tau_2} \right) - \exp \left( -\frac{\tau_2^2}{\tau_2} \right) \right],
\]

(11)

where $\tau_1 = \frac{\gamma + d_{res}}{2\sqrt{D_{k}}}, \quad \tau_2 = \frac{\gamma - d_{res}}{2\sqrt{D_{k}}}, \quad D_{k}$ is the diffusion coefficient of type $A_k$ molecules in $\frac{m^2}{s}$, and $d_{res}$ is the distance between RX$_k$ and the FC in m.

In MD-ML and SD-ML, we denote $S_{ob,0}^{RX,k}(j)$ as the number of molecules observed within $V_{FC}$ in the $j$th symbol interval, due to the emissions of molecules from the current and the previous emissions by RX$_k$. We emphasize that the TX and RX$_k$ use the same modulation method. The TX – RX$_k$ and RX$_k$ – FC links are both diffusion-based. Therefore, $S_{ob,0}^{RX,k}(j)$ can be accurately approximated by Poisson RVs. We denote $S_{ob,0}^{RX,k}(j)$ as the mean of $S_{ob,0}^{RX,k}(j)$. We obtain $S_{ob,0}^{RX,k}(j)$ by replacing $S_{o}(S_{ob,0}^{RX,k}(j))$, $M_k$, and $\Delta t_{ek}$ in (4) with $S_{o}(S_{ob,0}^{RX,k}(j))$, $M_k$, $\Delta t_{ek}$, respectively. In SD-ML, the sum of $K M_k$ observations at the FC over $K$ RX – FC links in the $j$th symbol interval, $S_{ob,0}^{RX}(j) = \sum_{k=1}^{K} S_{ob,0}^{RX_k}(j)$, is also a Poisson RV whose mean is given by $S_{ob,0}^{RX}(j) = \sum_{k=1}^{K} S_{ob,0}^{RX_k}(j)$.

2) ML Detection: In MD-ML, the FC has $K$ independent sets of observations over the $K$ RX$_k$ – FC links within each symbol interval and the value of the sum of $M_k$ observations at the FC over each RX$_k$ – FC link in the $j$th symbol interval is labeled $s_{j,k}^{RX}$. In SD-ML, the FC has only one set of observations over all $K$ RX$_k$ – FC links within each symbol interval and the value of the sum of $M_k$ observations over $K$ RX$_k$ – FC links in the $j$th symbol interval is labeled $s_{j}^{RX}$. 
**MD-ML:** The FC chooses the symbol $\hat{W}_{tx}[j]$ that is more likely, given the joint likelihood of the $K$ sums $s_{j,k}^{ob}$ in the $j$th interval. Recall that the $K$ RX$_k$–FC links are independent. Based on this assumption, $L[j]$ is given by

$$L[j] = \prod_{k=1}^{K} \left( \Pr \left( \hat{W}_{txk}[j] = 1 | W_{tx}[j], W_{tx}^{-1} \right) \times \Pr \left( S_{ob,k}^{ec,d}[j] = s_{j,k}^{ec} | \hat{W}_{txk}[j] = 1, W_{txk}^{-1} \right) + \Pr \left( \hat{W}_{txk}[j] = 0 | W_{tx}[j], W_{tx}^{-1} \right) \times \Pr \left( S_{ob,k}^{ec,d}[j] = s_{j,k}^{ec} | \hat{W}_{txk}[j] = 0, W_{txk}^{-1} \right) \right),$$

(12)

where we consider an approximate realization of previous symbols $W_{txk}^{-1}$ transmitted by the RX$_k$ when $s_{j,k}$ is observed, i.e., the FC has precise knowledge of $W_{txk}^{-1}$. We note that for MD-ML, it is possible for the FC to obtain the actual $W_{txk}^{-1}$, e.g., the FC could estimate the previous symbols transmitted by each RX$_k$. Here, we assume no error occurs in this estimation to establish a lower bound on error probability.

**SD-ML:** The FC chooses the symbol $\hat{W}_{tx}[j]$ that is more likely, given the likelihood of $s_{j}^{ob}$ in the $j$th interval. To facilitate the evaluation of $L[j]$ for SD-ML, we define $W_{tx}^{RX} = \{ \hat{W}_{txk}[j] \cdots \hat{W}_{txk}[j]\}$ as the set of decisions at all TXs in the $j$th symbol interval. We then define a set $R$ which includes all possible realizations of $W_{tx}^{RX}$ and the cardinality of set $R$ is $2^K$, i.e., $|R| = 2^K$. We further define a subset $R_q$, where $q \in \{0, \cdots, K\}$. $R_q$ includes realizations of $W_{tx}^{RX}$ where the decision at $q$ RXs is “1” and the decision at $K - q$ RXs is “0”. We then derive $L[j]$ as

$$L[j] = \sum_{W_{tx}^{RX} \in R} \Pr \left( W_{tx}^{RX} | W_{tx}[j], W_{tx}^{-1} \right) \times \Pr \left( S_{ob}^{ec,d}[j] = s_{j}^{ec} | W_{tx}^{RX}, W_{txk}^{-1} \right),$$

(13)

where we consider an approximate realization of $W_{txk}^{-1}$, i.e., the FC does not have precise knowledge of $W_{txk}^{-1}$. This consideration is because it is hard for the FC to obtain the actual $W_{txk}^{-1}$ when all RXs transmit the same type of molecule to the FC. The approximated realization of $W_{txk}^{-1}$ is obtained by a biased coin toss method, as discussed in [17]. In (13), we clarify that we need to consider every realization of $W_{tx}^{RX}$ and the corresponding probability to lead to $s_{j}^{ec}$. Since the collaborative MC system has a symmetric topology, the RXs have independent and identically distributed observations. This leads to

$$W_{txk}^{-1} = W_{tx}^{-1} \quad \text{and} \quad \Pr \left( W_{txk}[j] = 1 | W_{tx}[j], W_{tx}^{-1} \right) = \Pr \left( W_{tx}[j] = 1 | W_{tx}[j], W_{tx}^{-1} \right) = \Theta_j. $$

We simplify (13) as

$$L[j] = \sum_{q=0}^{K} \binom{K}{q} \Theta_j^q (1 - \Theta_j)^{K-q} \times \Pr \left( S_{ob}^{ec,d}[j] = s_{j}^{ec} | W_{tx}^{RX} \in R_q, W_{tx}^{-1} \right).$$

(14)

Finally, it is shown that (12) and (14) can be evaluated by applying the analysis in Sections III-A1 and III-B1, the conditional cumulative distribution function (CDF) of the Poisson RV $S_{ob,0}^{ec,d}[j]$, and the conditional PMF of the Poisson RVs $S_{ob,k}^{ec,d}[j]$. We now derive $Q_{ec}[j]$ in the noisy reporting scenario for MD-ML when $K = 1$. We denote the conditional mean of $S_{ob,1}^{ec,d}[j]$ as $\lambda_{1}^{ec}[j] + \lambda_{1}^{ob}[j]$ and $\lambda_{1}^{ob}[j]$ when the $j$th symbol transmitted by RX$_1$ is $\hat{W}_{tx1}[j] = 1$ and $\hat{W}_{tx1}[j] = 0$, respectively. We note that $\lambda_{1}^{ob}[j]$ is the expected ISI at the FC in the $j$th symbol interval due to the previous symbols transmitted by RX$_1$. Applying the PMF of the Poisson RV $S_{ob,1}^{ec,d}[j]$, we obtain the decision rules for MD-ML with $K = 1$. The decision rules are analogous to those of Variant 2 in the perfect reporting scenario in Section III-A3. When $\hat{W}_{tx1}^{-1} = 0$, i.e., $\lambda_{1}^{ob}[j] = 0$, the decision rule can be obtained by replacing $s_{j}^{ob}$ and $\xi_{j}^{ob}$ in (7) with $s_{j}^{ob}$ and $\xi_{j}^{ob}$, respectively, where $\xi_{j}^{ob}$ is given by $\xi_{j}^{ob} = \lambda_{1}^{ob}[j]/(\lambda_{1}^{ob}[j] + \lambda_{1}^{ob}[j]).$ When $\hat{W}_{tx1}^{-1} = 0$, i.e., $\lambda_{1}^{ob}[j] = 0$, the decision rule can be obtained by replacing $s_{j}^{ob}$ with $s_{j}^{ob}$ in (9). Therefore, we evaluate $Q_{ec}[j]$ for MD-ML with $K = 1$ as

$$Q_{ec}[j] = \Pr \left( W_{tx}^{-1} = 0 | W_{tx}^{-1} \right) \left( P_{1} \Pr \left( S_{ob,1}^{ec,d}[j] < S_{ob,0}^{ec,d}[j] \right) + P_{2} \Pr \left( S_{ob,1}^{ec,d}[j] = S_{ob,0}^{ec,d}[j] \right) \right),$$

(15)

IV. NUMERICAL RESULTS AND SIMULATIONS

In this section, we present numerical and simulation results to examine the error performance of ML detection for the collaborative MC system. In this examination we use a particle-based stochastic simulator. We list all the environmental parameters adopted in the examination in Table I and keep them fixed throughout this section. The only parameters that we vary are the detection threshold at RX$_k$, $\xi_{txk}$, the detection threshold at the FC, $\xi_{ec}$, the number of RXs, $K$, the number of samples of the FC, $M_{ec}$, and the time step at the FC, $\Delta t_{ec}$.

| Parameter | Symbol | Units | Fig. 1 | Figs. 2&3 |
|-----------|--------|-------|--------|----------|
| Radius of RXs | $r_{RX}$ | $\mu m$ | 0.225 | 0.225 |
| Radius of FC | $r_{FC}$ | $\mu m$ | - | 0.225 |
| Time step at RX | $\Delta t_{RX}$ | $\mu s$ | 200 | 100 |
| Number of samples by RX | $\lambda_{RX}$ | | 5 | 5 |
| Transmission time interval | $t_{trans}$ | ms | 2 | 1 |
| Report time interval | $t_{report}$ | ms | 0.3 | 0.3 |
| Symbol interval time | $T$ | ms | 2.3 | 1.3 |
| Diffusion coefficient | $D_{L}$ | $m^2/s$ | $10^{-9}$ | $5 \times 10^{-9}$ |
| Length of TX sequence | $L$ | symbols | 10 | 10 |
| Probability of binary | $P_{1}$ | - | 0.5 | 0.5 |
In the following, we assume that the TX releases $S_0 = 5000$ molecules for symbol “1” and the total number of molecules released by all RXs for symbol “1” is fixed at 1000. As such, for MD-ML and SD-ML, each RX releases $S_j = 1000/K$ molecules to report a decision of “1”. We consider a system that consists of at most six RXs. The specific locations of the TX, RXs, and FC are listed in Table II. Furthermore, the simulated error probabilities are averaged over $5 \times 10^4$ independent transmissions of the considered TX symbol sequences.

We compare the error performance of the proposed ML detection for a collaborative MC system with that of three cases, in order to show the performance advantage of the proposed ML detection. The first case is a TX – RX link, referred to as the baseline case in this section, where only one RX exists and there is no FC. The RX implements an energy detector with threshold $\xi_{RX}$ at the RX as in [12]. The second case is the collaborative system with the majority decision rule which we considered in [3] and shows the best error performance among all hard fusion rules. The third case is the collaborative system with the simple soft fusion scheme. In the baseline case, we place the RX at $(2 \mu m, 0.6 \mu m, 0)$, the TX releases 6000 molecules to transmit symbol “1”, and the remaining parameters are as in Table I. For the majority rule and the soft fusion scheme, we consider the same parameters as the ML detection schemes listed in Table I and described above. Thus, we consider that the total number of molecules, the distance away from the TX, the symbol interval time, and all other parameters for the three cases are the same as those for ML detection, ensuring the fairness of the comparison. In the following figures, we clarify that the value of $\xi_{RX}$ is the minimum $\xi_{RX}$ by numerically optimizing $\xi_{RX}$ for MD-ML and SD-ML, $\xi_{RX}$ for the baseline case, $\xi_{FC}$ for the simple soft fusion scheme, and $\xi_{RX}$ and $\xi_{FC}$ for the majority rule. We emphasize that these thresholds are constants that are optimized over all realizations of $W_{RX}^{j-1}$ and all symbol intervals.

In Fig. 2, we consider the perfect reporting scenario. We plot the optimal average global error probability versus the number of collaborative RXs for ML detection Variant 1, Variant 2, the majority rule, and the soft fusion scheme. We first observe that the simulations corroborate the accuracy of the analytical results. Second, we observe that Variants 1 and 2 achieve a significant error performance improvement over the majority rule and the soft fusion scheme. Also, this improvement becomes more remarkable when $K$ increases. For example, when $K = 5$, Variant 1 and Variant 2 bring about 113.5- and 61.2-fold magnitude improvement over the majority rule, respectively. This demonstrates the advantage of ML detection for the collaborative MC system, even though the ML detection is applied on a symbol-by-symbol basis. Third, we observe that the soft fusion scheme slightly outperforms the majority rule. Importantly, we see that the error performance gain from this soft fusion scheme is minimal compared to that achieved from ML detection. This observation is not surprising since the decision rule of Variant 2 is comparing the sum of all RXs’ observations with the adaptive threshold $\xi_{RX}([j])$, while the soft fusion scheme compares this sum with an constant threshold $\xi_{FC}$. Fourth, we observe that Variant 1 outperforms Variant 2. This is due to the fact that the likelihood of every sample at each RX is considered separately in Variant 1, but only the sum of all samples at each RX are considered in Variant 2. Finally, we see that the system error performance improves as $K$ increases, especially for Variants 1 and 2, as expected. In addition, we observe that the rate of error performance improvement almost keep constant when $K$ increases for Variants 1 and 2.

In Fig. 3, we consider a single-RX system in the noisy reporting scenario. We plot the optimal average global error probability versus the number of samples by the FC $M_{FC}$ with $K = 1$ in the noisy reporting scenario.

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**TABLE II**

| Devices | X-axis [µm] | Y-axis [µm] | Z-axis [µm] |
|---------|-------------|-------------|-------------|
| TX      | 0           | 0           | 0           |
| RX1     | 2           | 0.6         | 0           |
| RX2     | 2           | 0.6         | 0           |
| RX3     | 2           | 0           | 0.6         |
| RX4     | 2           | 0           | -0.6        |
| RX5     | 2           | 0.3         | 0.5196      |
| RX6     | 2           | 0.3         | -0.5196     |
| FC      | 2           | 0           | 0           |

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MD-ML. In this figure the report time interval is fixed at $t_{\text{report}} = 0.3\,\text{ms}$ and the time step at the FC for each $M_{\text{fc}}$ is $\Delta_{\text{fc}} = 0.3\,\text{ms}$. We observe that the simulated points accurately match the analytical curves, thereby corroborating the accuracy of our analytical results. We also observe that the system error performance improves as $M_{\text{fc}}$ increases.

In Fig. 4, we plot the optimal average global error probability versus the number of collaborative RXs for MD-ML, SD-ML, and the majority rule in the noisy reporting scenario, Variant 2 in the perfect reporting scenario, and baseline case. In this figure the report time interval is $t_{\text{report}} = 0.3\,\text{ms}$, the number of samples by the FC is $M_{\text{fc}} = 10$, and the time step at the FC is $\Delta_{\text{fc}} = 30\,\mu\text{s}$. Interestingly, we observe that SD-ML outperforms the majority rule when $K = 4$ and $K = 5$, even though all RXs release the same type of molecule in SD-ML. We second observe that MD-ML outperforms the majority rule for all $K$, i.e., MD-ML provides lower error probability than hard fusion rules. Specifically, the error performance of MD-ML and SD-ML achieve 4- and 1.2-fold magnitude improvement over the majority rule, respectively, when $K = 5$. Third, we observe that an accurate match between the simulated point and the analytical curve for Variant 2 and it has a significant improvement over MD-ML, SD-ML, the majority rule, and the baseline case. This observation is consistent with that in perfect reporting in Fig. 2. Fourth, we observe that the MD-ML, SD-ML, Variant 2, and the majority rule of the collaborative MC system outperform the baseline case. Importantly, we further see that the system error performance improves as $K$ increases, as observed in Fig. 2. In addition, we observe that the rate of error performance improvement for MD-ML and SD-ML decreases when $K$ increases. This is because the number of molecules released by each RX decreases for increasing $K$.

V. CONCLUSIONS

In this paper, we presented symbol-by-symbol ML detection for the collaborative diffusion-based MC system. This detection allows us to determine the lower bounds on the error performance that can be achieved in the practical collaborative MC system with hard fusion rules considered in [3, 4]. We considered two variants with different levels of computational complexity in the perfect reporting scenario and MD-ML and SD-ML in the noisy reporting scenario. We derived closed-form analytical expressions for the system error probability for MD-ML with one RX and the perfect reporting variant with lower computational complexity. Simulation results were used to corroborate the accuracy of our expressions. We further showed that symbol-by-symbol ML detection achieves a profound error performance gain than hard fusion rules, although the superiority of SD-ML is not held for all $K$. In our future work, we will investigate other relaying strategies for collaborative MC, such as amplify-and-forward relaying which is suitable for the RXs with limited processing capabilities.

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