Signaling with Identical Tokens: upper bounds with energy constraints

Christopher Rose *Fellow, IEEE* and I. Saira Mian

***Abstract*—As system sizes shrink to the nanoscale, the usual macroscopic methods of communication using electromagnetic and acoustic waves become increasingly difficult and energy-inefficient owing to, essentially, a mismatch between realizable antenna sizes and the propagation characteristics of the medium. Thus, at the scale of microns and below, communication methods which utilize molecular messengers become increasingly attractive, a notion supported by the ubiquity of molecular signaling in biological systems, usually with identical molecules. In a large portion of previous work, time-varying signal molecule/token concentration is used as the observable and various analyses performed. However, from an information-theoretic standpoint, concentration masks the underlying process which consists, fundamentally, of signal token emission, transit through some medium, and reception. We build here on previous work to establish machinery which allows upper bounds to be derived on the identical token timing channel. We then consider the special case of exponential token transit times.**

***Index Terms*—Diffusion channel capacity, molecular signaling, timing channel capacity**

I. Introduction

SCALE-APPROPRIATE signaling methods become important as systems shrink to the nanoscale. [1] For systems with feature sizes of microns and smaller, electromagnetic and acoustic communication become increasingly inefficient since energy coupling from the transmitter to the medium and from the medium to the receiver becomes difficult at usable frequencies. Biological systems, with the benefit of lengthy evolutionary experimentation, seem to have arrived at a ubiquitous solution to this signaling problem at small (and not so small) scales – use of identical molecules ("tokens") which travel through some medium between sender and receiver.

A fair amount of work on nano-scale communications has focused on diffusion of signaling molecules and a large portion of this work has explicitly considered time-varying concentration profiles as the fundamental signal measurement [2]–[8]. While this is an excellent first approach, concentration is a collective property of the process and masks the underlying physics of signal token release by the transmitter and capture by the receiver. This observation begs the question of truly fundamental limits on the capacity of such channels.

In what follows we consider a basic abstraction of molecular signaling wherein identical signaling molecules (tokens) are released from a transmitter according to some transmission schedule and each molecule is perfectly captured at the receiver with some medium-modulated reception schedule [5], [9]. That is, we ignore the reception process since any such *processing* can only decrease channel capacity. Building on previous work [1], [5], [9]–[12], we then provide an upper bound on identical token timing channel capacity, specifically for exponential first passage, but with machinery which should be adaptable to other first passage distributions. Since the molecule release and capture process comprises the underlying physics of concentration-based analyses, in the limit of large numbers of molecules over commensurately large time intervals these results also supply a capacity bound for channels which use time-varying concentration as the information carrier.

II. Paper Organization

We begin with a problem overview and description (almost verbatim from previous work [1]) which (re)introduces the necessary mathematical machinery (sections III and IV). In section V we develop new machinery to derive an upper bound on channel capacity – be begin generally and then specifically present results for exponential first passage in Theorem (5). In section VI we compare the upper bound to previous [1] lower bounds and briefly explore some implications of the results.

III. Problem Description

As previously mentioned, the development of [1], [10]–[12] is repeated here for clarity. Assume that M identical tokens are emitted at times $\{T_m\}$, $m = 1, 2, ..., M$ and each is captured at the receiver at times $\{S_m\}$. The duration of token m's passage between source and destination is a random variable D_m. These D_m are assumed i.i.d. with $f_{D_m}(d) = g(d) = G'(d)$ where $g()$ is some causal probability density with mean $\frac{1}{\mu}$ and CDF (cumulative distribution function) $G()$. We also assume that $g()$ contains no singularities.

Thus, the first portion of the channel is modeled as a sum of random M-vectors

$$\mathbf{S} = \mathbf{T} + \mathbf{D} \tag{1}$$

for which we have

$$f_{\mathbf{S}}(\mathbf{s}) = \int_{\mathbf{0}}^{\mathbf{s}} f_{\mathbf{T}}(\mathbf{t}) \mathbf{g}(\mathbf{s} - \mathbf{t}) d\mathbf{t} \tag{2}$$

where $\mathbf{g}(\mathbf{s} - \mathbf{t}) = \prod_{m=1}^{M} g(s_m - t_m)$ and we impose an emission deadline, $T_m \leq \tau(M)$, $\forall m \in \{1, 2, ..., M\}$.

At this point it is tempting make a direct analogy to *Bits Through Queues* [13]. However, since the tokens are identical we cannot necessarily determine which arrival corresponds to which emission time. Thus, the final output of the channel is a reordering of the $\{S_m\}$ to obtain a set $\{\vec{S}_m\}$ where $\vec{S}_m \leq \vec{S}_{m+1}$, $m = 1, 2, ..., M-1$. We write this relationship as

$$\vec{\mathbf{S}} = P_{\Omega}(\mathbf{S}) \tag{3}$$

where $P_k()$, $k = 1, 2, \cdots, M!$, is a permutation operator and Ω is a permutation index which produces an arrival-time-ordered $\vec{\mathbf{S}}$ from the argument $\mathbf{S}$. That is, $\mathbf{S}$ is sorted by arrival time to produce $\vec{\mathbf{S}}$ The associated emission time ensemble probability density $f_{\mathbf{T}}(\mathbf{t})$ is assumed causal, but otherwise arbitrary. We define the launch and capture of M tokens

[1]We repeat much of the front matter of [1] here for clarity before developing upper bounds in Section V-A

as a "channel use" and if we assume multiple independent channel uses, then the usual coding theorems apply [14] and the channel's figure of merit is the mutual information between $\mathbf{T}$ and $\vec{\mathbf{S}}$, $I(\vec{\mathbf{S}};\mathbf{T})$.

We note that the event $S_i = S_j$ $(i \neq j)$ is of zero measure owing to the no-singularity assumption on $g()$, Thus, for analytic convenience we will assume that $f_{\mathbf{S}}(\mathbf{s}) = 0$ whenever two or more of the s_m are equal. This assumption also assures that the Ω which produces $\vec{\mathbf{S}}$ in equation (3) is unique.

Thus, the density $f_{\vec{\mathbf{S}}}(\vec{\mathbf{s}})$ can be found by "folding" the density $f_{\mathbf{S}}(\mathbf{s})$ about the hyperplanes described by one or more of the s_m equal until the resulting probability density is nonzero only on the region where $s_m < s_{m+1}$, $m = 1, 2, ..., M-1$. Analytically we have

$$f_{\vec{\mathbf{S}}}(\vec{\mathbf{s}}) = \begin{cases} \sum_{n=1}^{M!} f_{\mathbf{S}}(P_n(\vec{\mathbf{s}})) & \vec{s}_1 < \vec{s}_2 < \cdots < \vec{s}_m \\ 0 & \text{otherwise} \end{cases} \tag{4}$$

We can likewise describe $f_{\vec{\mathbf{S}}|\mathbf{T}}(\mathbf{s}|\mathbf{t})$ as

$$f_{\vec{\mathbf{S}}|\mathbf{T}}(\vec{\mathbf{s}}|\mathbf{t}) = \begin{cases} \sum_{n=1}^{M!} f_{\mathbf{S}|\mathbf{T}}(P_n(\mathbf{s})|\mathbf{t}) & \vec{s}_1 < \vec{s}_2 < \cdots < \vec{s}_m \\ 0 & \text{otherwise} \end{cases} \tag{5}$$

which to emphasize the assumed causality of $g()$ we rewrite as

$$f_{\vec{\mathbf{S}}|\mathbf{T}}(\mathbf{s}|\mathbf{t}) = \begin{cases} \sum_{n=1}^{M!} \mathbf{g}(P_n(\mathbf{s}) - \mathbf{t})\mathbf{u}(P_n(\mathbf{s}) - \mathbf{t}) & \text{ordered } s_i \\ 0 & \text{o.w.} \end{cases} \tag{6}$$

where $\mathbf{u}(P_n(\mathbf{s}) - \mathbf{t}) = \prod_{m=1}^{M} u([P_n(\mathbf{s})]_m - t_m)$ and $u()$ is the usual unit step function. (Note that $[P_n(\mathbf{s})]_m$ is the m^{th} component of the vector $P_n(\mathbf{s})$.)

With these preliminaries done, we can now begin to examine the mutual information between $\mathbf{T}$, $\mathbf{S}$ and $\vec{\mathbf{S}}$.

IV. Mutual Information Between $\mathbf{T}$ and $\vec{\mathbf{S}}$

The mutual information between $\mathbf{T}$ and $\mathbf{S}$ is

$$I(\mathbf{S};\mathbf{T}) = h(\mathbf{S}) - h(\mathbf{S}|\mathbf{T}) \tag{7}$$

where $h()$ is differential entropy. Since the S_i given the T_i are mutually independent, $h(\mathbf{S}|\mathbf{T})$ does not depend on $f_{\mathbf{T}}(\mathbf{t})$. Thus, maximization of equation (7) is simply a maximization of the marginal $h(S)$ over the marginal $f_T(t)$, a problem explicitly considered and solved for a mean T_m constraint in [13] and under a deadline constraint with exponential i.i.d. $\{D_m\}$ in [10].

The corresponding expression for the mutual information between $\mathbf{T}$ and $\vec{\mathbf{S}}$ is

$$I(\vec{\mathbf{S}};\mathbf{T}) = h(\vec{\mathbf{S}}) - h(\vec{\mathbf{S}}|\mathbf{T}) \tag{8}$$

Unfortunately, $h(\vec{\mathbf{S}}|\mathbf{T})$ now *does* depend on the input distribution and the optimal form of $h(\vec{\mathbf{S}})$ is non-obvious. So, rather than attempting a brute force optimization of equation (8) by deriving order distributions [5], [9], we invoke simplifying symmetries as in [1], [12]. First, we may assume [1], [12] that

$$f_{\mathbf{T}}(\mathbf{t}) = f_{\mathbf{T}}(P_n(\mathbf{t})) \quad \forall n \tag{9}$$

so that

$$f_{\mathbf{S}}(\mathbf{s}) = f_{\mathbf{S}}(P_n(\mathbf{s})) \quad \forall n \tag{10}$$

That is, $f_{\mathbf{T}}()$ and $f_{\mathbf{S}}()$ are "hypersymmetric". Coupled to the assumption that the first passage density is continuous we have the following theorem, taken from [1], [12]:

Theorem 1:

If $f_{\mathbf{T}}()$ is a hypersymmetric probability density function on emission times $\{T_m\}$, $m = 1, 2, .., M$, and the first passage density is non-singular, then the entropy of the size-ordered outputs $\vec{\mathbf{S}}$ is

$$h(\vec{\mathbf{S}}) = h(\mathbf{S}) - \log M!$$

and the conditional entropy of the size-ordered outputs is

$$h(\vec{\mathbf{S}}|\mathbf{T}) = h(\mathbf{S}|\mathbf{T}) - H(\Omega|\vec{\mathbf{S}},\mathbf{T})$$

where $H(\Omega|\vec{\mathbf{S}},\mathbf{T})$ is the uncertainty about which index Ω produces $P_\Omega(\mathbf{S}) = \vec{\mathbf{S}}$ given both $\mathbf{T}$ and $\vec{\mathbf{S}}$.

We note that $0 \leq H(\Omega|\vec{\mathbf{S}},\mathbf{T}) \leq \log M!$ with equality on the right for any density where all the T_m are equal. Thus, for $f_{\mathbf{T}}()$ hypersymmetric and nonsingular first passage densities we can write the ordered mutual information as (from [1], [12]):

Theorem 2:

$$I(\vec{\mathbf{S}};\mathbf{T}) = I(\mathbf{S};\mathbf{T}) - \left(\log M! - H(\Omega|\vec{\mathbf{S}},\mathbf{T})\right) \tag{11}$$

That is, an information degradation of size $\log M! - H(\Omega|\vec{\mathbf{S}},\mathbf{T}) \geq 0$ is introduced by the sorting operation.

V. Maximizing the Mutual Information

Since $h(\mathbf{S}|\mathbf{T})$ is a constant with respect to $f_{\mathbf{T}}(\mathbf{t})$, maximization of equation (11) requires we maximize $h(\mathbf{S}) + H(\Omega|\vec{\mathbf{S}},\mathbf{T})$. Mutual information is convex in $f_{\mathbf{T}}(\mathbf{t})$ and the space $\mathcal{F}_{\mathbf{T}}$ of feasible hypersymmetric $f_{\mathbf{T}}(\mathbf{t})$ is clearly convex. Thus, we can in principle apply variational [15] techniques to find that hypersymmetric $f_{\mathbf{T}}()$ which attains the unique maximum of equation (8). However in practice, direct application of this method can lead to grossly infeasible $f_{\mathbf{T}}()$, implying that the optimizing $f_{\mathbf{T}}()$ lies along some "edge" or in some "corner" of the convex search space.

So, in what follows, we derive a useful upper bound on $H(\Omega|\vec{\mathbf{S}},\mathbf{T})$ from a previously derived upper bound $H^{\uparrow}(\mathbf{T}) \geq H(\Omega|\vec{\mathbf{S}},\mathbf{T})$. So armed, we then derive an upper bound on $I(\vec{\mathbf{S}};\mathbf{T})$.

A. A Useful Upper Bound On $H(\Omega|\vec{\mathbf{S}},\mathbf{T})$

We state the result as a theorem with proof.

Theorem 3:

Given

$$Q(\cdot) = \bar{G}(|\cdot|) \tag{12}$$

and defining

$$\gamma_T = E_{\mathbf{T}}\left[Q(T_1 - T_2)\right] \tag{13}$$

we have

$$H(\Omega|\vec{\mathbf{S}},\mathbf{T}) \leq E_{\mathbf{T}}\left[H^{\uparrow}(\mathbf{T})\right] \leq M \log\left(1 + \frac{M-1}{2}\gamma_T\right) \tag{14}$$

Proof: Theorem (3) In [12] we derived an upper bound, $H^{\uparrow}(\vec{\mathbf{t}})$, for $H(\Omega|\vec{\mathbf{S}},\vec{\mathbf{t}})$:

$$\sum_{\ell=1}^{M-1}\log(1+\ell)\sum_{m=\ell}^{M-1}\sum_{|\bar{\mathbf{x}}|=\ell}\prod_{j=1}^{m}\bar{G}^{\bar{x}_j}(\vec{t}_{m+1}-\vec{t}_j)G^{1-\bar{x}_j}(\vec{t}_{m+1}-\vec{t}_j) \tag{15}$$

where the $\{\vec{t_j}\}$ are the size-ordered $\{t_i\}$, $G()$and $\bar{G}()$ are, respectively, the CDF and CCDF (complementary cumulative distribution function) of the first passage time. $\bar{\mathbf{x}}$, taken in the context of the summation in m, is a binary (0/1) vector of size m. The bound is satisfied with equality **iff** the first passage density is exponential [12].

We can then define

$$p_{\ell|\vec{\mathbf{t}}}=\frac{1}{M}\sum_{m=\ell}^{M-1}\sum_{|\bar{\mathbf{x}}|=\ell}\prod_{j=1}^{m}\bar{G}^{\bar{x}_j}(\vec{t}_{m+1}-\vec{t}_j)G^{1-\bar{x}_j}(\vec{t}_{m+1}-\vec{t}_j) \tag{16}$$

and use Jensen's inequality to write

$$H^{\uparrow}(\vec{\mathbf{t}})=E_{\ell|\vec{\mathbf{t}}}\left[\log(1+\ell)\right]\le M\log(E[\ell|\vec{\mathbf{t}}]+1) \tag{17}$$

Rewriting $E[\ell|\vec{\mathbf{t}}]$ we have

$$\frac{1}{M}\sum_{m=0}^{M-1}\underbrace{\left[\sum_{\ell=0}^{m}\ell\left(\sum_{|\bar{\mathbf{x}}|=\ell}\prod_{j=1}^{m}\bar{G}^{\bar{x}_j}(\vec{t}_{m+1}-\vec{t}_j)G^{1-\bar{x}_j}(\vec{t}_{m+1}-\vec{t}_j)\right)\right]}_{E[\ell|\vec{\mathbf{t}},m]} \tag{18}$$

and by expanding and regrouping the inner product terms we can show that

$$E[\ell|\vec{\mathbf{t}},m]=\sum_{j=1}^{m}\bar{G}(\vec{t}_{m+1}-\vec{t}_j)$$

which results in

$$H^{\uparrow}(\vec{\mathbf{t}})\le M\log\left(1+\frac{1}{M}\sum_{m=1}^{M-1}\sum_{j=1}^{M}\bar{G}(\vec{t}_{m+1}-\vec{t}_j)\right)$$

(remembering that $E[\ell|\vec{\mathbf{t}},m=0]=0$). Taking the expectation in $\vec{\mathbf{T}}$ yields (via Jensen)

$$H^{\uparrow}(\vec{\mathbf{T}})\le M\log\left(1+\frac{1}{M}\sum_{m=1}^{M-1}\sum_{j=1}^{m}E\left[\bar{G}(\vec{T}_{m+1}-\vec{T}_j)\right]\right) \tag{19}$$

We then note that all ordered differences between the T_i are accounted for in equation (19). For any given $\mathbf{T}$ there are $\frac{M(M-1)}{2}$ ordered terms. Thus, owing to the hypersymmetry of $\vec{\mathbf{T}}$ we have

$$E_{\vec{\mathbf{T}}}\left[H^{\uparrow}(\vec{\mathbf{T}})\right]\le M\log\left(1+\frac{1}{2M}\sum_{i,j,i\neq j}^{M}E\left[\bar{G}(|T_i-T_j|)\right]\right)$$

where the factor of $\frac{1}{2}$ is introduced to account for terms where $T_i<T_j$ which would not appear in the ordered case of equation (19). Finally, hypersymmetry requires that $E\left[\bar{G}(|T_i-T_j|)\right]=\gamma_T$, a constant for $i\neq j$ so that

$$H(\Omega|\vec{\mathbf{S}},\mathbf{T})\le E_{\vec{\mathbf{T}}}\left[H^{\uparrow}(\vec{\mathbf{T}})\right]\le M\log\left(1+\frac{M-1}{2}\gamma_T\right)$$

which matches the result stated in Theorem (3). •

B. Maximizing $h(\mathbf{S})+M\log\left(1+\gamma(M-1)\right)$

The upper bound equation (14) is in terms of $f_{\mathbf{T}}()$ whereas $h(\mathbf{S})$ is a function(al) of $f_{\mathbf{S}}()$. Therefore, we must develop a relationship between $\gamma_T=E\left[Q(T_1-T_2)\right]$ and $\gamma_S=E\left[Q(S_1-S_2)\right]$. This relationship allows us to fix γ_S and maximize $h(\mathbf{S})$ while still maintaining an upper bound on $H(\Omega|\vec{\mathbf{S}},\vec{\mathbf{T}})$. From here onward we assume exponential first passage of tokens.

Theorem 4:

If the first passage density $f_D()$ is exponential then

$$E\left[Q(S_1-S_2)\right]\ge\frac{1}{2}E\left[Q(T_1-T_2)\right]$$

Proof: Theorem (4) Let $\Delta=T_1-T_2$ and $\mathcal{D}=D_2-D_1$. Then $\Delta+\mathcal{D}=S_1-S_2$. For the i.i.d. D_i exponential we have $\bar{G}(d)=e^{-\mu d}$, $d\ge 0$. Thus, $Q(\cdot)=e^{-\mu|\cdot|}$. We then note that $|a+b|\le|a|+|b|$ so that

$$\begin{aligned}E[Q(\Delta+\mathcal{D})] &= E[e^{-\mu|\Delta+\mathcal{D}|}]\\ &\ge E[e^{-\mu|\Delta|-\mu|\mathcal{D}|}]=E[Q(\Delta)]E[Q(\mathcal{D})]\end{aligned}$$

because Δ and $\mathcal{D}$ are independent. Then consider that the density of $\mathcal{D}$ is $f_{\mathcal{D}}(\cdot)=\frac{\mu}{2}e^{-\mu|\cdot|}$ so that $E[Q(\mathcal{D})]=\int_{=\infty}^{\infty}\frac{\mu}{2}e^{-\mu|z|}e^{-\mu|z|}dz=\frac{1}{2}$ which completes the proof. •

Now, suppose we fix $E\left[Q(S_1-S_2)\right]=\gamma_S$. Then, owing to hypersymmetry we have $E\left[Q(S_i-S_j)\right]=\gamma_S\ \forall i,j,i\neq j$. Using standard Euler-Lagrange optimization [15], we can find the density $f_{\mathbf{S}}$ which maximizes $h(\mathbf{S})$ as

$$f^*_{\mathbf{S}}(\mathbf{s})=\frac{1}{A(\beta)}e^{\beta\sum_{\substack{i,j\\ i\neq j}}Q(s_i-s_j)} \tag{20}$$

where

$$A(\beta)=\int e^{\beta\sum_{\substack{i,j\\ i\neq j}}Q(s_i-s_j)}d\mathbf{s} \tag{21}$$

and β is a constant chosen to satisfy $E[Q(S_1-S_2)]=\gamma_S$. The entropy of $\mathbf{S}$ is then

$$h(\mathbf{S})=\log A(\beta)-\beta M(M-1)\gamma_S \tag{22}$$

We note that for $\beta=0$, $f_{\mathbf{S}}()$ is uniform. Increasing β makes $f_{\mathbf{S}}()$ more "peaky" in regions where $s_i\approx s_j$ since $Q(0)=1$ and $Q()$ is monotonically decreasing away from zero. Likewise, decreasing β reduces $f_{\mathbf{S}}()$ in the vicinity of $s_i\approx s_j$. Thus, γ_S increases monotonically with β. The result is that $\gamma'_S()$ is strictly positive.

More formally, we have from the definition of $\gamma_S(\beta)$ that

$$M(M-1)\gamma_S(\beta)=E\left[\sum_{\substack{i,j\\ i\neq j}}Q(s_i-s_j)\right]\equiv\Gamma_S(\beta)$$

Then

$$\Gamma'_S(\beta)=E\left[\left(\sum_{\substack{i,j\\ i\neq j}}Q(s_i-s_j)\right)^2\right]-E^2\left[\sum_{\substack{i,j\\ i\neq j}}Q(s_i-s_j)\right] \tag{23}$$

which is a variance and therefore greater than or equal to zero. Thus, $\gamma'_S(\beta)\ge 0$. And since $0\le\gamma_S(\beta)\le 1$, we must also have $\gamma'_S(\beta)\to 0$ in the limits $\beta\to\pm\infty$.

Now, consider all terms as functions of β as in

$$I(\vec{\mathbf{S}};\mathbf{T}) \begin{array}{ll} \le & \log A(\beta) - \beta M(M-1)\gamma_S(\beta) \\ + & M\log\left(1+\gamma_S(\beta)(M-1)\right) \\ - & h(\mathbf{S}|\mathbf{T}) - \log M! \end{array} \tag{24}$$

We can find extremal points by differentiating equation (24) with respect to β to obtain the first derivative

$$M(M-1)\gamma_S'(\beta)\left(-\beta + \frac{1}{1+\gamma_S(\beta)(M-1)}\right)$$

and the second derivative

$$\begin{array}{c} M(M-1)\gamma_S''(\beta)\left(-\beta + \frac{1}{1+\gamma_S(\beta)(M-1)}\right) \\ + \\ -M(M-1)\gamma_S'(\beta)\left(1+(M-1)\frac{\gamma_S'(\beta)}{(1+\gamma_S(\beta)(M-1))^2}\right) \end{array}$$

which reduces to

$$-M(M-1)\gamma_S'(\beta)\left(1+(M-1)\frac{\gamma_S'(\beta)}{(1+\gamma_S(\beta)(M-1))^2}\right) \le 0$$

when the first derivative is zero – at which point we have

$$\gamma_S^* = \gamma_S(\beta^*) = \frac{1-\beta^*}{(M-1)\beta^*} \tag{25}$$

and note that equation (25) requires $\frac{1}{M} \le \beta^* \le 1$ since $0 \le \gamma_S(\beta) \le 1$. In addition, there is at most one solution to equation (25) since $\frac{1-\beta^*}{(M-1)\beta^*}$ monotonically decreases in β while $\gamma_S(\beta)$ monotonically increases in β. Since the second derivative at the extremal is non-positive, the unique point defined by equation (25) is a maximum.

Unfortunately, solutions to equation (25) have no closed form and numerical solutions for asymptotically large M are impractical. Nonetheless, the constraints on β^* will allow an oblique approach to deriving a bound.

We note again that $\Gamma_S'(\beta)$, is the variance of $\sum_{i\neq j} Q(s_i - s_i)$ and must decrease monotonically in β since as previously discussed, increased β concentrates $f_{\mathbf{S}}()$ around larger values of $\sum_{i\neq j} Q(s_i - s_i)$. Thus,

$$\Gamma_S'(\beta) \le \Gamma_S'(0) \tag{26}$$

$\forall \beta > 0$ which in turn implies

$$\Gamma_S(\beta) \le \beta\Gamma_S'(0) + \Gamma_S(0) \tag{27}$$

$\forall \beta \in (0,1]$.

Assuming exponential first passage, $Q(x) = e^{-\mu|x|}$ and remembering that $\Gamma_S(\beta) = M(M-1)\gamma_S(\beta)$, we can calculate both $\gamma_S(0)$ and $\gamma_S'(0)$ in closed form as

$$\gamma_S(0) \equiv Z(\mu\tau) = \frac{2}{(\mu\tau)^2}\left(\mu\tau + e^{-\mu\tau} - 1\right) \tag{28}$$

and

$$\gamma_S'(0) = \left[\begin{array}{c} (M-2)(M-3)\gamma_S^2(0) + 2Z(2\mu\tau) \\ + \\ 24\frac{M-2}{(\mu\tau)^3}\left(\mu\tau - 2 + e^{-\mu\tau}(2+\mu\tau)\right) \\ - \\ M(M-1)\gamma_S^2(0) \end{array}\right] \tag{29}$$

respectively. Defining $M = \rho\tau$ and taking the limit for large M yields

$$\lim_{M\to\infty} M\gamma_S(0) = \frac{2\rho}{\mu} = \frac{2}{\chi} \tag{30}$$

and

$$\lim_{M\to\infty} (M-1)\gamma_S'(0) = 8\frac{\rho^2}{\mu^2} + 2\frac{\rho}{\mu} = \frac{8}{\chi^2} + \frac{2}{\chi} \tag{31}$$

where

$$\chi \equiv \frac{\mu}{\rho}$$

as in [1]

Again remembering that $\Gamma_S(\beta) = M(M-1)\gamma_S(\beta)$ and utilizing equation (27) we have

$$\gamma_S(0) \le \gamma_S(\beta^*) \le \gamma_S'(0)\beta^* + \gamma_S(0) \tag{32}$$

Thus, the intercept of the monotonically decreasing $\frac{1-\beta}{(M-1)\beta}$ with the right hand side of equation (32) must yield a value larger than $\gamma(\beta^*)$. To solve for this intercept we set

$$\frac{1-\tilde{\beta}}{(M-1)\tilde{\beta}} = \gamma_S'(0)\tilde{\beta} + \gamma_S(0) = \frac{1}{M-1}\tilde{\beta}\left(\frac{8}{\chi^2}+\frac{2}{\chi}\right) + \frac{2}{\chi}\frac{1}{M}$$

so that in the limit of large M we have

$$\tilde{\beta} = \frac{\sqrt{1+\frac{12}{\chi}+\frac{36}{\chi^2}} - (1+\frac{2}{\chi})}{\frac{16}{\chi^2}+\frac{4}{\chi}}$$

which results in

$$(M-1)\gamma(\beta^*) \le \tilde{\beta}\left(\frac{8}{\chi^2}+\frac{2}{\chi}\right) + \frac{2}{\chi} \tag{33}$$

so that for large M we have

$$I(\vec{\mathbf{S}};\mathbf{T}) \begin{array}{ll} \le & \log A(\beta^*) - \beta^* M(M-1)\gamma_S(\beta^*) \\ + & M\log\left(1+\tilde{\beta}\left(\frac{8}{\chi^2}+\frac{2}{\chi}\right)+\frac{2}{\chi}\right) \\ - & h(\mathbf{S}|\mathbf{T}) - \log M! \end{array} \tag{34}$$

To complete the mutual information bound, we could then derive upper bounds on $A(\beta^*) - \beta^* M(M-1)\gamma_S(\beta^*)$. However, in the limit of large $M = \tau/\rho$, the density on $\mathbf{S}$ is effectively constrained to $(\mathbf{0},\boldsymbol{\tau})$ [1] which constrains $h(\mathbf{S}) \le M\log\tau$. Then, since $h(\mathbf{S}|\mathbf{T}) = M(1-\log\mu)$ for exponential first passage, equation (34) produces

$$\frac{I(\vec{\mathbf{S}};\mathbf{T})}{M} \begin{array}{ll} \le & \log\tau - (1-\log\mu) \\ + & \log\left(1+\tilde{\beta}\left(\frac{8}{\chi^2}+\frac{2}{\chi}\right)+\frac{2}{\chi}\right) \\ - & \frac{\log M!}{M} \end{array} \tag{35}$$

Application of Stirling's approximation

$$\lim_{M\to\infty}\frac{\log M!}{M} = \log M - 1$$

in combination with equation (35) produces our main theorem:

Theorem 5:

If the first passage density $f_D()$ is exponential with parameter μ and the average rate at which tokens are released is ρ, then the capacity per token, C_m is upper bounded by

$$C_m \le \log\left(\chi + \tilde{\beta}\left(\frac{8}{\chi}+2\right)+2\right) \tag{36}$$

and the capacity per unit time is upper bounded by

$$C_t \le \rho\log\left(\chi + \tilde{\beta}\left(\frac{8}{\chi}+2\right)+2\right) \tag{37}$$

where $\chi \equiv \frac{\mu}{\rho}$ *and*

$$\tilde{\beta} = \frac{\chi^2\sqrt{1+\frac{12}{\chi}+\frac{36}{\chi^2}} - (\chi^2+2\chi)}{16+4\chi} \tag{38}$$

VI. Discussion & Conclusion

We have derived an upper bound on the mutual information, $I(\vec{\mathbf{S}};\mathbf{T})$ between token launch times $\mathbf{T}$ on a finite interval $(\mathbf{0}, \boldsymbol{\tau}(M))$ and sorted arrival times $\vec{\mathbf{S}}$ in terms of the mean first passage time $1/\mu$ and the number of tokens launched, M. Then, following the channel use discipline described in [1] and deriving bounds for arbitrarily large M, we have produced an upper bound on capacity per token and on capacity per unit time in terms of $\chi = \frac{\mu}{\rho}$, the ratio of token uptake rate μ to token launch rate ρ under the assumption of exponential first passage times.

However, it is important to note that the main part of the development does not require exponential first passage. Any first passage density with finite mean for which a comparable theorem (4) can be derived and for which $\gamma_S(0)$ and $\gamma'(0)$ can be calculated may allow similar bounds to be derived.

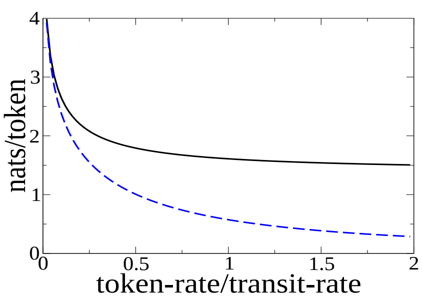

Fig. 1. C_m (nats/token) vs. $1/\chi$ (token-rate per transit-rate). Upper and lower bounds for exponential transit.

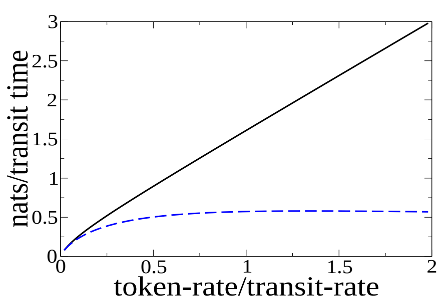

Fig. 2. $C_t = C_m/\chi$ (nats/transit-time) vs. $1/\chi$ (token-rate per transit-rate). Upper and lower bounds for exponential transit.

In FIGURES 1 and 2 we plot the upper bounds of equation (36) and equation (37) along with the lower bounds derived in [1] versus $1/\chi = \rho/\mu$. If token construction is assumed to require some fixed amount of energy [1], then as $\rho/\mu \to 0$, the energy efficiency in nats/joule of the token timing channel increases without bound since the lower bound approaches infinity. However, as might be expected, the corresponding rate of communication also decreases toward zero as $\rho/\mu \to 0$.

This sort of tension between power and rate is typical – consider the well known Gaussian channel where $C = W\log(1+\frac{P}{N_0 W})$. With $P = \frac{\mathcal{E}}{\tau}$ where $\mathcal{E}$ is the energy used per signaling interval, fixed P corresponds to fixed ρ and the capacity of the gaussian channel also approaches zero as $\rho \to 0$. However, the number of bits per joule approaches the finite value $\frac{1}{N_0}$ for the Gaussian channel as $P \to 0$, not ∞. In addition, the Gaussian channel capacity increases as $\log P$. In contrast, if the upper bound derived here is indeed tight, the capacity of the token timing channel increases *linearly* in with power expenditure ρ. For this reason, the gap between the upper and lower bounds of the token timing channel capacity and in particular the tightness of the upper bound described by (5) is a topic of interest currently under investigation.

It is also interesting to note the gap between the nats/token (bits/joule) upper and lower bounds as well. The lower bound decreases monotonically toward zero with a maximum near $\rho/\mu = 1$. In contrast the upper bound approaches $\log 4$ nats/token from above. As stated in previous work, the "sweet spot" near $\rho/\mu = 1$ echoes other previous work [2] which identified an optimal signaling rate with concentration as the observable at the receiver. However, the upper bound derived here, if tight, suggests that the lower bound optimum rate might be an artifact. This too is a topic of significant interest.

Finally, we have not yet exercised these results using values for μ and ρ associated with biological molecular signaling channels, nor have we yet compared our results to the more usual workups which treat token concentration as the observable signal. This is a topic of current work.

References

[1] C. Rose and I.S. Mian. Signaling with identical tokens: Lower bounds with energy constraints. In *Information Theory Proceedings (ISIT), 2013 IEEE International Symposium on*, pages 1839–1843, 2013.

[2] A. Einolghozati, M. Sardari, A. Beirami, and F. Fekri. Capacity of Discrete Molecular Diffusion Channels. In *IEEE International Symposium on Information Theory (ISIT) 2011*, pages 603–607, July 2011. ISBN: 978-1-4577-0594-6.

[3] Josep Miquel Jornet Ian F. Akyildiz and Massimiliano Pierobon. Nanonetworks: A New Frontier in Communications. *Communications of the ACM*, 54(11):84–89, 2011.

[4] M. Pierobon and I.F. Akyildiz. Capacity of a diffusion-based molecular communication system with channel memory and molecular noise. *Information Theory, IEEE Transactions on*, 59(2):942–954, Feb 2013.

[5] T. Nakano, A. W. Eckford, and T. Haraguchi. *Molecular Communication*. Cambridge University Press, 2013.

[6] Arash Einolghozati, Mohsen Sardari, and Faramarz Fekri. Relaying in diffusion-based molecular communication. In *ISIT, 2013*, pages 2959–2963. IEEE, 2013.

[7] A. Einolghozati, M. Sardari, and F. Fekri. Design and analysis of wireless communication systems using diffusion-based molecular communication among bacteria. *Wireless Communications, IEEE Transactions on*, 12(12):6096–6105, 2013.

[8] Arash Einolghozati, Mohsen Sardari, and Faramarz Fekri. Decode and forward relaying in diffusion-based molecular communication between two populations of biological agents. In *Information Conference on Communications, 2014 IEEE ICC*. IEEE, 2014.

[9] A.W. Eckford. Nanoscale communication with Brownian motion. In *CISS'07*, pages 160–165, 2007. Baltimore.

[10] Y-L Tsai, C. Rose, R. Song, and I.S. Mian. An Additive Exponential Noise Channel with a Transmission Deadline. In *IEEE International Symposium on Information Theory (ISIT) 2011*, pages 598–602, July 2011. ISBN: 978-1-4577-0594-6.

[11] R. Song, C. Rose, Y-L Tsai, and I.S. Mian. Wireless Signaling with Identical Quanta. In *IEEE WCNC*, Paris, April 2012.

[12] C. Rose, R. Song, and I.S. Mian. Timing Channels with Multiple Identical Quanta. *IEEE Transactions on Information Theory*, 2014. (to be submitted – draft available: http://arxiv.org/abs/1208.1070).

[13] V. Anantharam and S. Verdu. Bits Through Queues. *IEEE Transactions on Information Theory*, 42(1):4–18, January 1996.

[14] T.M. Cover and J.A. Thomas. *Elements of Information Theory*. Wiley-Interscience, 1991.

[15] F.B. Hildebrand. *Advanced Calculus for Applications*. Prentice Hall, Englewood Cliffs, NJ, 1976.

Acknowledgments

To our extremely helpful and careful anonymous reviewers, we are extremely grateful. This work was supported by NSF-CDI-0835592