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Computation and Communication Cooperation for Molecular Microvascular Networks

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Abstract—Molecular Communication (MC) has attracted significant attention, however, its application is limited due to the lack of computing capacity. Inspired by the concept of Over-the-Air Computation (AirComp), this paper pioneers a computational model for MC within microvascular networks. In this model, the root node acts as the receiver, while other nodes serve as transmitters, employing the microvascular network as a communication medium to directly receive the sum of transmitted information, thereby achieving computational functions in MC. Our model establishes a breakthrough framework, offering guidance for executing computational tasks within MC. Through simulation experiments, we assess our model in terms of computational error rates, thereby demonstrating its feasibility and effectiveness.

Index Terms—Computation and communication cooperation, microvascular network, molecular communication.

I. INTRODUCTION

W ITH the rapid advancement of nanotechnology and information technology, MC has gradually become a research focus in the scientific field [1]. MC has many advantages such as small size [2] and good biocompatibility [3], and is considered to have great potential in realizing nanoscale communication systems.

Specifically, MC utilizing chemical signals for information transmission at the nanoscale, presents an innovative paradigm for applications spanning healthcare, environmental monitoring, and industrial process control [4], [5]. Nonetheless, the unique physical and chemical mechanisms of MC propagation present distinct challenges, such as signal loss, interference, and computational limitations, which significantly affect the performance and dependability of MC systems.

Microvessels, due to its feature of containing rich physiological indicators and distributing throughout the human body, have attracted huge attention recently. They offer the promising means for building a communication channel in the microvascular network and also represent an important

Kezhi Wang is with Department of Computer Science, Brunel University London, Uxbridge, Middlesex, UB8 3PH (email: kezhi.wang@brunel.ac.uk). application domain for MC in the emerging Internet of Bio-Nano Things (IoBNT) context [6].

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Specifically, in [7], the authors proposed a microvascular network of MC system based on a binary tree structure, taking into account the topology of the microvascular network. In [8], the authors considered the human microvascular network composed of three different types of arteries, veins, and capillaries, and considered their different channel characteristics. In [9], the authors developed a mathematical model and particlebased simulator for MC in capillaries and surrounding tissues. This study examined how capillary characteristics, including blood-tissue barrier and blood flow, influenced molecular signal reception, and explored the effects of emission duration, elimination rate, and separation distance.

However, most of the above literature focused on the development of MC models, the challenge of executing computational tasks within MC systems remains unresolved, significantly constraining its potential applications. Also, there are few studies focusing on methods that integrate communication and achieving computing functions.

Against the above background and inspired by the Over-the-Air Computation (AirComp) [10]. In this paper, we propose an innovative framework for MC within microvascular networks where the root node acts as the receiver, while other nodes serve as transmitters, employing the microvasculature network as a communication medium to directly receive the sum of transmitted information, thereby achieving computational functions in MC.

Specially, we allow multiple transmitters to transmit diverse information via different concentrations of chemical molecules, with the receiver directly receives the aggregated information, e.g., the summation, thus, show the potential of realizing computing functions in MC.

Through simulation, we have validated its effectiveness in enhancing both communication and computational efficiency in MC systems. The main contributions of this paper include:

- Inspired by AirComp, we propose an novel computational model for MC systems operating within microvascular networks, effectively combining communication and computing processes.
- We conduct a comprehensive analysis through simulation. The effectiveness and efficiency of the proposed model are thoroughly evaluated.

The successful implementation of this model introduces a novel method of integrated communication and computation into the field of MC. Our research not only shows the potential for addressing the computational limitations that currently

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constrain the applicability of MC but also provides crucial guidance for its evolution.

II. COMPUTATIONAL MODEL FOR MC

In this section, we introduce the developed computational model for MC. Different from traditional MC systems, our proposed system can be construed as an integrated source and channel design that simultaneously facilitates communication and computational functionalities. For traditional MC systems, as shown in Fig. 1(a), the receiver needs to detect the digital modulated data one by one and then perform the computations. However, due to the limitations in molecular computational capabilities, implementing computational functions within body remains quite challenging. Therefore, we propose a MC system with computation function. In this system, multiple transmitters emit molecules that can be aggregated within the channel, utilizing the channel itself as a medium, and we directly demodulate the aggregated data, thereby embedding computational capabilities within the communication process. This removes the need for separate reception and subsequent computation modules, enabling the execution of computational tasks directly within the MC transmission framework.

Fig. 1(b) shows the fundamental principles of the MC computational model, using summation as an example. We assume two transmitters and the receiver share mapping tables. Initially, at the transmitter end, data is mapped onto the quantity of molecules according to a mapping table, with varying quantities representing different pieces of information. Then molecules emitted by two transmitters accumulate in the transmission medium and reach the receiver through advection plus diffusion. Finally, at the receiver, post-mapping the total quantity of received molecules facilitates the implementation of an summation function.



(a) Illustration of the basic principle for traditional model for MC system.



(b) Illustration of the basic principle for computational model for MC system (with an example of summation).

Fig. 1: Two paradigms. (a) Traditional MC system. (b) MC system with computation function.

III. MOLECULAR COMMUNICATION COMPUTATIONAL MODEL IN MICROVASCULAR NETWORKS

In this section, we establish an computational model for the microvascular network within the human body.

A. Microvascular Network Computation Model

Based on the findings in [11], [12], the human body's microvascular network can be conceptualized as a binary tree structure for the purpose of MC modeling. Here, microvessels serve as the edges of the binary tree, and their junctions represent the nodes. A binary tree with M levels can accommodate up to $2^M - 1$ nodes, which are numbered systematically from top to bottom and left to right.

For the generation of our random binary tree, we initially create a complete binary tree. Subsequently, for each node within the tree, we utilize a random number generator that produces only two values, 0 or 1. If the random number generator returns 0 and the node lacks both left and right child node, then that node is removed. This method is employed to generate our random binary tree model. In this model, the position of a node corresponds directly to its identification number, i.e., if there is a node at position 3, then this node is labeled as N_3 .

Based on the findings in [13], the length of each microvessel is approximately 1 mm. Therefore, we set the distance between adjacent nodes at 1 mm.

In this proposed model, transmitters are biologically integrated within the system, specifically designed as cells affixed to the walls of blood vessels. This ensures stable and accurate placement without interference from blood flow. The receiver, conceptualized as advanced nanodevice, is highly mobile and programmable, capable of dynamic interaction within the microvascular network. This receiver is engineered to efficiently manage energy consumption through advanced power management techniques.

Building upon this conceptual framework, Fig. 2 provides a vivid illustration of the MC computational model in the microvascular network. It demonstrates how transmitters, positioned at any node within the binary tree, release signals that traverse the microvascular junctions and converge at the receiver. This effectively captures the essence of computation, i.e., summation in an MC environment, where computation is seamlessly integrated with communications.

Fig. 3 shows an example of the binary tree computation model applied to microvascular networks, highlighting how the receiver N_1 directly aggregates information from transmitters N_4 to N_7 , each transmitting their respective values D_4 to D_7 .

The root node, labeled as N_1 , functions as the receiver in this model, directly assimilating the molecular information from all transmitting nodes in the network. These transmitters



Fig. 2: Illustrative representation of the MC computational model in the microvascular network.

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Fig. 3: An example of binary tree computation model for MC in microvascular networks.

release signals that converge at the root node, where they are immediately processed. Thus, the value at the root node represents the direct summation of the molecular information, expressed as ΣD_m .

B. MC System with Computational Function in Microvascular Networks

This subsection delves into the MC system model in microvascular networks, detailing the processes of molecular transmission and signal reception. We begin by presenting a mathematical model for molecular emission, and then proceed to explore signal detection techniques for configurations with either single or multiple transmitters. The section also includes a derivation of peak detection timing and discusses a multipoint sampling strategy designed specifically for the proposed system.

In the MC system model, the receiver is deployed at the root node, and transmitters are deployed at every other node. The communication process involves transmitters sending symbols, with '0' indicating no molecule emission and positive integers representing the emission of molecules, proportional to the symbol's value times an emission constant E. This process is modeled as below:

$$E(t) = D(t) \cdot E,\tag{1}$$

where E(t) denotes the number of molecules emitted at time t, with D(t) representing the transmitted symbol.

In our model, we assume the emitted molecules are small enough to freely pass through the blood vessel walls, permitting us to employ a free diffusion model. For simplicity, we also assume that these molecules propagate at a constant flow rate.

In traditional single-transmitter single-receiver MC systems, the concentration of molecules detected at any point at time t after a transmitter sends a molecule is given by

$$C(t) = \frac{\beta}{(4\pi Dt)^{\frac{3}{2}}} \exp\left(-\frac{(d-vt)^2}{4Dt}\right),$$
 (2)

where D is diffusion coefficient, v is the flow velocity and d denotes the distance between the transmitter and the center of the spherical receiver. To closely approximate reality, we assume β as the attenuation factor resulting from reactions, degradation, and bifurcation of molecules within the vasculature. In our model, once a channel is established, the value of β is also determined. Thus, after emitting a molecule, the

probability of it reaching the receiver is p = VC(t), where V represents the volume of the receiver.

For passive receivers, peak detection is generally employed. By deriving (2) and setting it to zero, the peak detection time t_d is obtained as

$$t_d = \frac{-3D + \sqrt{9D^2 + d^2v^2}}{v^2},\tag{3}$$

Consequently, at the *i*-th symbol period, detection at the receiver is performed at time t_d , and the total number of molecules received $Y_i(t_d)$ is expressed as

$$Y_{i}(t_{d}) = \sum_{j=0}^{L_{T}} E_{i-j}VC(t_{d}+jT) + n(t_{d})$$
$$= \underbrace{E_{i}VC(t_{d})}_{\text{desired signal}} + \underbrace{\sum_{j=1}^{L_{T}} E_{i-j}VC(t_{d}+jT)}_{\text{ISI}} + \underbrace{n(t_{d})}_{\text{noise}}$$
$$= \lambda_{o} + \lambda_{\text{ISI}} + n(t_{d}), \tag{4}$$

where T is the symbol period, ISI represents the impact of signals from other periods on the current period, $L_T = \min\{i - 1, L\}$, L is the ISI length, and E_i is the number of molecules transmitted in the *i*-th symbol period.

Given that p is small and the number of molecules transmitted by the transmitter is sufficiently large, the number of molecules received can be modeled by a Poisson distribution, with the probability mass function of $Y_i(t_d)$ given by

$$P[Y_i(t_d) = N_{t_d}] = \frac{\Lambda_{t_d}^{N_{t_d}} e^{-\Lambda_{t_d}}}{N_{t_d}!},$$
(5)

where $\Lambda_{t_d} = \lambda_o + \lambda_{\text{ISI}}$ represents the expected noise-free received signal, and N_{t_d} is the number of molecules detected at time t_d .

In our model, which includes M point-source transmitters and a single passive spherical receiver, we process N_s computational data combinations, represented as $[D_1, \ldots, D_{N_s}]$. For computation, the *m*-th transmitter modulates the selected number D_m to E_m , thus designating E_m molecules for transmission.

Since the distance d between different transmitters and the receiver may vary, leading to different peak arrival times for the molecules they emitted, traditional peak detection is no longer applicable for the multi-transmitter model. To address this, we propose multi-point sampling detection. To maintain the receiver's detection complexity comparable to that of traditional systems, we set the number of sampling points to the number of transmitters M, with sampling times corresponding to the peak times of M transmitters. If the sampling times coincide, then we increase the weight of the number of molecules detected at that moment. Let t_{d_m} be the peak detection time for the signal sent by the m-th transmitter. Thus our symbol period or transmission interval $T > \max{t_{d_m}}$. For the *i*-th symbol period, after multi-point sampling detection, the received signal $Y_s(i)$ is given by

$$Y_s(i) = \sum_{j=0}^{L_T} \sum_{m=1}^{M} \sum_{k=1}^{M} E_{i-j,m} V C_m(t_{d_k} + jT) + n(i), \qquad (6)$$

where $E_{i-j,m}$ is the number of molecules transmitted by the *m*-th transmitter in the (i - j)-th symbol period, and $VC_m(t)$ represents the the probability of it reaching the receiver after the *m*-th transmitter emits a molecule. Since the sum of multiple Poisson distributions still follows a Poisson

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distribution, the result of multi-point sampling $Y_s(i)$ follows a Poisson distribution, i.e., $Y(i) \sim P_s(\lambda = \Lambda_i)$, where

$$\Lambda_{i} = \sum_{m=1}^{M} \sum_{k=1}^{M} E_{i,m} V C_{m}(t_{d_{k}}) + \sum_{j=1}^{L_{T}} \sum_{m=1}^{M} \sum_{k=1}^{M} E_{i-j,m} V C_{m}(t_{d_{k}} + jT),$$
(7)

and its probability mass function is given by

$$P(Y_s(i) = N_i) = \frac{\Lambda_i^{N_i} e^{-\Lambda_i}}{N_i!},$$
(8)

where N_i represents the number of molecules detected during the *i*-th symbol period through multi-point sampling detection. The receiver performs MAP demodulation as follows:

$$\hat{\boldsymbol{S}}_{i} = \arg \max_{\boldsymbol{S}_{i} \in \mathcal{Q}} \ln \left(P\left(Y_{s}(i) = N_{i} \mid \boldsymbol{S}_{i}\right) \right)$$

$$= \arg \max_{\boldsymbol{S}_{i} \in \mathcal{Q}} \left(N_{i} \ln \left(\Lambda_{i} \mid \boldsymbol{S}_{i}\right) - \Lambda_{i} \mid \boldsymbol{S}_{i} \right), \qquad (9)$$

where Q is the set of N_s^M computational combinations, and the resulting \hat{S}_i represents the computed result.

IV. NUMERICAL AND SIMULATION RESULTS

In this section, we provides numerical simulation and results for verifying the proposed framework in this paper through MATLAB. The simulation parameters are given in Table I.

Initially, we conduct simulations to compare the computational time of our proposed computational model (CM) against traditional models (TM) (Assuming that the traditional model can achieve the calculation task at this time), Fig. 4. The results clearly demonstrate that our computational model (CM) significantly reduces computational time compared to traditional methods, particularly as the number of transmitters increases. This reduction highlights the efficiency of our proposed model in handling increased computational demands, showcasing its potential for complex communication tasks in scenarios with a high density of transmitters.

Subsequently, we simulated how computational error rates vary with increasing numbers of transmitters within a fivelayer MC model described in Section II-A. We tested transmitter counts from 2 to 9 at a fixed SNR of 50,000, using the maximum a posteriori (MAP) method for detection, and the computational error rate (CER) is calculated by dividing the number of detected errors by the total number of computations Fig. 5(a).

Results indicate that computational error rate (CER) gradually increase with more transmitters. Particularly, the system

 TABLE I: Simulation Parameters

Parameter	Symbol	Value
Signal Period	T	1.5s
Blood Flow Velocity	v	50 µm/s [14]
Receiver Radius	r	1 μm [15]
Distance to Adjacent Node	l	1 mm [13]
ISI Length	L	3
Number of Tree Generations	N1	1000
Number of Computations	N2	10000
Diffusion Coefficient	D	150 μm ² /s
Receiver Computation Time for Two Values	t	0.1s



Fig. 4: The computational efficiency comparison between the molecular communication computing model and the traditional model.



(a) Change in computation error rate (b) Computational error rate variation with an increasing number of trans- with SNR for four transmitters.

Fig. 5: Computational error rates. (a) Variation with an increasing number of transmitters. (b) Variation with SNR for four transmitters.

maintains low error rates for 2 to 5 transmitters. Beyond five transmitters, error rates rise significantly due to denser signal constellations and increased computational combinations (N_s^M) , complicating accurate detection. These challenges necessitate enhancing signal clarity by increasing transmitted molecule counts or employing advanced noise estimation techniques to improve detection accuracy.

In Fig. 5(b), we employ a fixed number of transmitters (four transmitters) to simulate the variation in computational error rate with changes in SNR, within a range of 5,000 to 50,000, in increments of 5,000. As illustrated, there is a discernible downward trend in the computational error rate as the SNR increases. This indicates that the system's ability to resist interference enhances with a higher SNR, leading to improved accuracy in computations. Particularly notable is the significant reduction in error rates beyond a certain SNR threshold, highlighting the system's augmented performance at higher SNR levels.

Following the initial exploration into the impacts of SNR and number of transmitters on computational error rates, we further extend our analysis by conducting a comparative study between MC computational systems and those based on traditional MC system. This study encompasses an SNR spectrum ranging from 50,000 to 500,000 and investigates configurations with 2, 3, and 4 transmitters. The results, as depicted in Fig. 6, elucidate the performance differentials under varying conditions.

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Fig. 6: Comparative analysis of computational error rates across MC computational systems with and traditional technology across a wide SNR range for various transmitter configurations.

In scenarios with two transmitters, MC with computational function system's integration significantly outperforms traditional MC systems across the analyzed SNR range, showcasing its profound impact on computational accuracy.

With the incorporation of three transmitters, the performance landscape becomes progressively intricate. Below an SNR threshold of 400,000, MC with computational function systems demonstrate a marked superiority in computational accuracy over their traditional counterparts. However, upon exceeding this threshold, traditional methodologies exhibit enhanced effectiveness. This transition is attributable to MC with computation system's initial benefit of receiving a greater number of molecules, resulting in higher signal clarity. Nevertheless, as the SNR escalates, traditional approaches also achieve adequate molecular reception, thus showcasing improved operational outcomes.

The addition of a fourth transmitter introduces another layer of complexity to our analysis. In regimes where the SNR is below 200,000, the efficacy of MC with computation systems becomes evident. However, once this SNR threshold is exceeded, traditional model surpass the performance of MC with computation systems. This change is attributed to the exponential rise in computational combinations as the number of transmitters increases, as shown in Fig. 5(a). To mitigate this performance degradation, strategies such as augmenting the quantity of transmitted molecules or employing more accurate noise estimation methods may be required.

Our investigations have revealed that systems characterized by a minimal number of transmitters and lower SNRs benefit from enhanced performance, attributed to fewer computational combinations and increased signal clarity. Nonetheless, the integration of additional transmitters invariably escalates computational error rates. This phenomenon stems from the proliferation of computational combinations, resulting in denser signal constellations that compound the complexity of accurate detection. To overcome this challenge and enhance computational precision in environments with an elevated number of transmitters, it is crucial to increase the quantity of transmitted molecules, refine noise estimation methodologies, or tailor detection algorithms specifically for MC with computation function systems optimization.

V. CONCLUSION

In this letter, we present our computational approach within Molecular Communication (MC), using the microvascular network as a case study. We detail a comprehensive framework and provide a mathematical description of the system. Rigorous simulations confirm the effectiveness and advantages of our proposed system, setting the foundation for addressing computational challenges in MC and furthering molecular computer development. Moving forward, we will focus on enhancing communication performance and developing channel estimation algorithms to mitigate the increased error rates due to a large number of transmitters.

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