IEEE Access
Multidisciplinary | Rapid Review | Open Access Journal

Received October 11, 2018, accepted October 29, 2018, date of publication November 1, 2018, date of current version December 3, 2018.

Digital Object Identifier 10.1109/ACCESS.2018.2879159

Joint Optimization of Molecular Resource Allocation and Relay Positioning in Diffusive Nanonetworks

SATISH K. TIWARI[1], (Student Member, IEEE), TADI RAVI TEJA REDDY[1,2], PRABHAT K. UPADHYAY[1], (Senior Member, IEEE), AND DANIEL BENEVIDES DA COSTA[3], (Senior Member, IEEE)

[1]Discipline of Electrical Engineering, Indian Institute of Technology Indore, Indore 453552, India
[2]Department of Electrical and Computer Engineering, University of California at Los Angeles, Los Angeles, CA 90095, USA
[3]Department of Computer Engineering, Federal University of Ceará, Sobral 62010-560, Brazil

Corresponding author: Satish K. Tiwari (phd1401102014@iiti.ac.in)

This research work was supported by the Council of Scientific and Industrial Research (CSIR), Government of India under Grant Number 22(0763)/18/EMR-II.

ABSTRACT We consider a realistic two-hop diffusion-based molecular communication (DbMC) system with spherical absorbing receivers in the presence of molecular degradation and noises. We address the problem of joint optimization of molecules allocation and relay location for the given detection thresholds in order to minimize the error probability of budget limited DbMC system. Numerical and simulation results reveal the improvement in error performance when molecules distribution and relay placement are in accordance with their joint optimal value. Moreover, it is found that as the relay detection threshold increases, more molecules are needed to be allocated to the source while relay need to be placed closer to the destination in order to satisfy the optimization criteria. Eventually, we demonstrate the effectiveness of our optimization solution through 3D and contour plots illustrating the convergence time.

INDEX TERMS Nanonetworks, molecular communication, diffusion, error performance, molecules allocation, relay positioning, joint optimization.

I. INTRODUCTION

Molecular communication (MC) is a bio-inspired approach for establishing communication in nanonetworks over fluidic environments using chemicals as the information carriers [1]. Owing to its biocompatibility in general, MC finds importance in the cutting-edge *in vivo* biomedical applications [2] such as targeted drug delivery, continuous health monitoring by using Internet of Bio-Nano Things (IoBNT) [3] enabled bio-nanosensors, and so on.

Among the various forms of MC described in [4], the diffusion-based molecular communication (DbMC) has emerged as an effective and energy-efficient method for exchanging information among nanomachines (NMs). In DbMC system, information is encoded in quantity, type or emission frequency of the released molecules. Due to the concentration gradient, these information-bearing molecules traverse across the diffusive medium from the transmitter nanomachine (T_xN) to the receiver nanomachine (R_xN) according to the Brownian motion. On reaching the R_xN, molecular wave interact with the sensors to be decoded and interpreted as the received signal. The performance of DbMC system depends on various design parameters such as molecules allocation, T_xN releasing rate, relay nanomachine (RN) location, detection timing, reception delay, symbol interval, detection threshold, weight values of the detector, path between the NMs, which need to be optimized to achieve the minimum error rate. In [5], optimal number of released molecules for the given detection thresholds was derived in order to minimize the error probability of each hop in a multi-hop DbMC system. A game-theoretic approach has been presented in [6] for the distributed resource allocation in nanoscale MC systems. Salehi *et al.* [7] have derived optimal releasing rate of the T_xN for molecular drug delivery system (DDS) with limited resources. Ntouni *et al.* [8], [9] have specified optimal time for the observation process to minimize the error probability. A symbol interval optimization algorithm has been proposed in [10] and the optimal reception delay to minimize the inter-symbol interference in DbMC system has

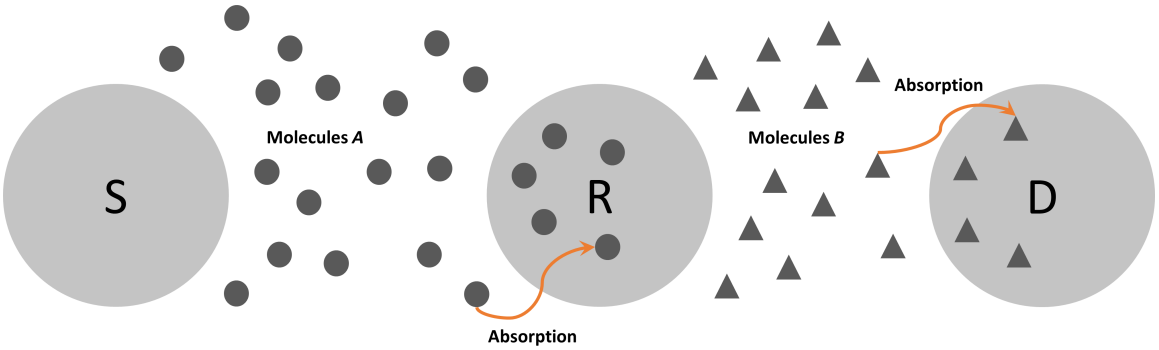


FIGURE 1. Schematic diagram of a two-hop DbMC system with absorbing receivers.

been found recently in [11]. In [12], swarm intelligence algorithm has been implemented in order to evaluate the weight values for the weighted sum detector of a passive receiver in a DbMC system. The ant colony optimization approach has been used in [13] to find the optimal path between the NMs. In [14], an optimization problem for detection threshold has been formulated as quasi-convex and then solved using the bisection method. Whereas, the work in [15] and [16] uses logarithmic barrier, Karush-Kuhn-Tucker conditions and Newton Raphson method sequentially to find the optimal detection threshold. Further, a joint convex optimization problem has been addressed for a cooperative DbMC system to obtain suboptimal detection thresholds using MATLAB-based interior-point algorithm [17]. Tavakkoli *et al.* [18] have proposed a joint RN positioning and R_xN detection threshold optimization problem for the given number of molecules released by the T_xN and the RN, and solved using an iterative algorithm.

However, to the best of our knowledge, the joint optimization of molecules allocation and RN positioning for the given predetermined detection thresholds has not been yet investigated. Note that molecules are limited resource because of the finite availability of molecule synthesizing energy and limited storage capabilities of the reservoir. In fact, such investigation in the context of bio-nanosensor networks [19] is essential for their practical implementation of local DDS [7] where drug molecules may be expensive and their large amount can have ill effects on healthy parts of the body. Above all, the emission of an arbitrary number of molecules would increase multi-source interference for other NMs present in the medium. Therefore, optimal allocation of these molecules and RN placement for the given detection thresholds would reduce the network error without increasing much the complexity of the NMs (i.e., NMs neither need to update their detection thresholds nor require high computational cost involved with the maximum likelihood (ML) detection).

Motivated by above, we investigate the problem of joint optimization of molecules allocation and RN location for a RN-assisted DbMC system that employs spherical absorbing receivers under the influence of molecular degradation and pertinent noises. To this end, we derive an expression for the end-to-end error probability by assuming a decode-and-forward (DF) relaying strategy at the RN. Thereafter, we solve the optimization problem by using an iterative algorithm based on the block coordinate descent algorithm (BCDA). Numerical and simulation results demonstrate that the error performance improves significantly by jointly optimizing the molecular resource allocation and RN location. Moreover, our results highlight the effect of detection thresholds on the joint optimal solution.

II. SYSTEM MODEL

In this paper, we consider a static[1] DbMC system, as illustrated in Fig. 1, wherein communication between a T_xN (node S) and a R_xN (node D) occurs over an unbounded 3-dimensional fluidic environment having uniform temperature and viscosity. The RN (node R) is placed linearly in-between the nodes S and D. We assume node S to be a point source while nodes R and D to be fully absorbing [20] spherical receivers each having radius r. Further, node R is assumed to be a point object (whenever it transmits) and is located at distance $d_{pq} + r$ from end nodes, where d_{pq} is the distance between the center of transmitting node $p \in \{\mathrm{S}, \mathrm{R}\}$ and the nearest point on the surface of receiving node $q \in \{\mathrm{R}, \mathrm{D}\}$. We assume that the transmitting nodes S and R respectively use different types of molecules A and B for information transmission. Nodes R and D have sensors only for the intended molecules A and B respectively. As such, self-interference at node R gets avoided. Moreover, node R employs DF strategy with full-duplex transmission protocol. All nodes are supposed to be synchronized in time, utilizing the strategy mentioned in [21]. We rely on the on-off keying modulation in which N_A and N_B number of molecules are released by the nodes S and R, respectively, for conveying the information bit 1, whereas for bit 0, no molecules are released by them at the beginning of the symbol duration T. These molecules propagate

[1] NMs can be immobilized in the medium in certain scenarios where they get anchored to larger objects or bound to fixed molecules [18].

independently[2] through the molecular channel and may degrade [20] before hitting the receiver nanosensors. As soon as molecules hit the nanosensors, they are removed from the medium and contribute only once to the signal. This activity is described by the first hitting probability function and is derived in [20, eq. (9)] for a spherical absorbing receiver in a 3-dimensional molecular degraded diffusive channel, between nodes p and q, as

$$h_f^{pq}(t) = \frac{r}{d_{pq}+r}\frac{d_{pq}}{\sqrt{4\pi D_f t^3}}\exp\left(-\frac{d_{pq}^2}{4D_f t}\right)\phi(\lambda,t), \quad (1)$$

where D_f is the diffusion coefficient of type, $f \in \{A, B\}$, molecules in the given medium and $\phi(\lambda, t) = \exp(-\lambda t)$ is the survival probability of a molecule, until time t, with degradation rate λ. Hence, the expected fraction of node p transmitted molecules absorbed at node q, at time t, before getting degraded can be calculated by integrating (1) as

$$H_f^{pq}(t) = \int_0^t h_f^{pq}(\acute{t})\quad d\acute{t} = \frac{r}{2(d_{pq}+r)} \times\left[\exp(\psi)\,\mathrm{erfc}\left(\varphi+\sqrt{\lambda t}\right) + \exp(-\psi)\,\mathrm{erfc}\left(\varphi-\sqrt{\lambda t}\right)\right], \quad (2)$$

where $\psi = d_{pq}\sqrt{\lambda/D_f}$ and $\varphi = d_{pq}/\sqrt{4D_f t}$. Consequently, the arrival probability, at node q in the current symbol duration, for a molecule released by node p in the ith previous symbol duration is given by

$$P_{i,f}^{pq} = H_f^{pq}\big((i+1)T\big) - H_f^{pq}\big(iT\big). \quad (3)$$

Besides the residual molecules from prior emissions, molecular signal is also corrupted by the emission from other NMs prevailing in the diffusive medium and the counting error induced at the reception node. As such, the total sensed molecules in the jth symbol duration at node q can be represented as

$$N_f^{pq}[j] = N_{c,f}^{pq}[j] + N_{n_r,f}^{pq}[j] + N_{n_o,f}^{pq}[j] + N_{n_c,f}^{pq}[j], \quad (4)$$

where $N_{c,f}^{pq}[j]$ and $N_{n_r,f}^{pq}[j]$ amount to the respective number of molecules received from the current and prior transmissions. For large N_f, the binomial distributions of $N_{c,f}^{pq}[j]$ and $N_{n_r,f}^{pq}[j]$ can be approximated by the Gaussian distributions $\mathcal{N}\big(a_j^p N_f P_{0,f}^{pq}, a_j^p N_f P_{0,f}^{pq}(1-P_{0,f}^{pq})\big)$ and $\sum_{i=1}^{I}\mathcal{N}\big(a_{j-i}^p N_f P_{i,f}^{pq}, a_{j-i}^p N_f P_{i,f}^{pq}(1-P_{i,f}^{pq})\big)$ respectively [14], [15], where a_j^p and a_{j-i}^p, $\in \{0,1\}$, are the jth current and $(j-i)$th previous transmitted bits respectively by node p, and I symbolizes the number of previous transmissions. Furthermore, $N_{n_o,f}^{pq}[j]$ denotes the sensed number of molecules that were emitted by the other prevailing NMs of the medium and $N_{n_c,f}^{pq}[j]$ signifies the induced counting error at node q, conforming the distributions $\mathcal{N}(\mu_{n_o}^{pq}, \sigma_{n_o}^{2,pq})$ and $\mathcal{N}(0, \sigma_{n_c}^{2,pq})$ respectively [14], [15], where $\sigma_{n_c}^{2,pq}$ depends on the expected number of molecules sensed by node q.

[2]This assumption holds good for sufficiently dilute suspension of the information-carrying molecules.

III. ERROR PROBABILITY ANALYSIS

This section derives the error probability expression for the considered DbMC system. If the detection is erroneous at either of the receiving nodes, error occurs at the destination node. Hence, the jth bit error probability can be evaluated as

$$\begin{aligned}P_e[j] = {} & \Pr(a_j^{\mathrm{S}}=1)\times\big[\Pr(\hat{a}_j^{\mathrm{R}}=0\,|\,a_j^{\mathrm{S}}=1)\times\Pr(\hat{a}_{j+1}^{\mathrm{D}}=0\,|\,a_{j+1}^{\mathrm{R}}=0)\big]\\ & + \Pr(a_j^{\mathrm{S}}=1)\times\big[\Pr(\hat{a}_j^{\mathrm{R}}=1\,|\,a_j^{\mathrm{S}}=1)\times\Pr(\hat{a}_{j+1}^{\mathrm{D}}=0\,|\,a_{j+1}^{\mathrm{R}}=1)\big]\\ & + \Pr(a_j^{\mathrm{S}}=0)\times\big[\Pr(\hat{a}_j^{\mathrm{R}}=1\,|\,a_j^{\mathrm{S}}=0)\times\Pr(\hat{a}_{j+1}^{\mathrm{D}}=1\,|\,a_{j+1}^{\mathrm{R}}=1)\big]\\ & + \Pr(a_j^{\mathrm{S}}=0)\times\big[\Pr(\hat{a}_j^{\mathrm{R}}=0\,|\,a_j^{\mathrm{S}}=0)\times\Pr(\hat{a}_{j+1}^{\mathrm{D}}=1\,|\,a_{j+1}^{\mathrm{R}}=0)\big]\end{aligned} \quad (5)$$

and is given by

$$P_e[j] = \frac{1}{2}\Big(1 + g\big(N_A, d_{SR}\big)\,g\big(N_B, d_{RD}\big)\Big), \quad (6)$$

for the equally likely binary information bits, where $\hat{a}_j^{\mathrm{R}}$ and $\hat{a}_{j+1}^{\mathrm{D}}$ are the detected information bits at nodes R and D respectively in the jth and $(j+1)$th symbol durations, and $\hat{a}_j^{\mathrm{R}} = a_{j+1}^{\mathrm{R}}$. The functions $g(N_A, d_{SR})$ and $g(N_B, d_{RD})$ are calculated as

$$g(N_A, d_{SR}) = Q\left(\frac{\eta_{\mathrm{R}}-\mu_0^{\mathrm{SR}}}{\sqrt{\sigma_0^{2,\mathrm{SR}}}}\right) - Q\left(\frac{\eta_{\mathrm{R}}-\mu_1^{\mathrm{SR}}}{\sqrt{\sigma_1^{2,\mathrm{SR}}}}\right), \quad (7)$$

and

$$g(N_B, d_{RD}) = Q\left(\frac{\eta_{\mathrm{D}}-\mu_1^{\mathrm{RD}}}{\sqrt{\sigma_1^{2,\mathrm{RD}}}}\right) - Q\left(\frac{\eta_{\mathrm{D}}-\mu_0^{\mathrm{RD}}}{\sqrt{\sigma_0^{2,\mathrm{RD}}}}\right), \quad (8)$$

respectively, where $Q(x) = \frac{1}{\sqrt{2\pi}}\int_x^\infty \exp(-\frac{x^2}{2})\mathrm{d}x$. Moreover, the involved statistics are computed as

$$\mu_0^{\mathrm{SR}} = \frac{N_A}{2}\sum_{i=1}^{I} P_{i,\mathrm{A}}^{\mathrm{SR}} + \mu_{n_o}^{\mathrm{SR}}, \quad (9)$$

$$\mu_1^{\mathrm{SR}} = \frac{N_A}{2}\sum_{i=1}^{I} P_{i,\mathrm{A}}^{\mathrm{SR}} + N_A P_{0,\mathrm{A}}^{\mathrm{SR}} + \mu_{n_o}^{\mathrm{SR}}, \quad (10)$$

$$\sigma_0^{2,\mathrm{SR}} = \frac{N_A}{2}\sum_{i=1}^{I} P_{i,\mathrm{A}}^{\mathrm{SR}}(1-P_{i,\mathrm{A}}^{\mathrm{SR}}) + \frac{N_A^2}{4}\sum_{i=1}^{I}(P_{i,\mathrm{A}}^{\mathrm{SR}})^2 + \sigma_{n_o}^{2,\mathrm{SR}} + \sigma_{n_c}^{2,\mathrm{SR}}|_{a_j^{\mathrm{S}}=0}, \quad (11)$$

and

$$\sigma_1^{2,\mathrm{SR}} = N_A P_{0,\mathrm{A}}^{\mathrm{SR}}(1-P_{0,\mathrm{A}}^{\mathrm{SR}}) + \frac{N_A}{2}\sum_{i=1}^{I} P_{i,\mathrm{A}}^{\mathrm{SR}}(1-P_{i,\mathrm{A}}^{\mathrm{SR}}) + \frac{N_A^2}{4}\sum_{i=1}^{I}(P_{i,\mathrm{A}}^{\mathrm{SR}})^2 + \sigma_{n_o}^{2,\mathrm{SR}} + \sigma_{n_c}^{2,\mathrm{SR}}|_{a_j^{\mathrm{S}}=1}, \quad (12)$$

where $\sigma^{2,\mathrm{SR}}_{n_c}|_{a_j^{\mathrm{S}}=0} = \mu_0^{\mathrm{SR}}$ and $\sigma^{2,\mathrm{SR}}_{n_c}|_{a_j^{\mathrm{S}}=1} = \mu_1^{\mathrm{SR}}$. Further, μ_0^{RD}, μ_1^{RD}, $\sigma_0^{2,\mathrm{RD}}$ and $\sigma_1^{2,\mathrm{RD}}$ are calculated likewise. Eventually, η_{R} and η_{D} are the predetermined detection thresholds at nodes R and D respectively.

IV. JOINT OPTIMAL MOLECULES ALLOCATION AND RELAY POSITIONING

As evident from (6), the error probability expression depends on the transmitted number of molecules N_A and N_B, and distances d_{SR} and d_{RD}. Hence, we show interest in the optimal molecules allocation and RN placement that minimizes error probability derived in the previous section. To this end, we formulate a joint optimization problem as

$$\min_{m,n} \; P_e[j], \tag{13}$$

where $m = d_{SR}/(d_{SR}+d_{RD})$ represents relay positioning factor and $n = N_A/(N_A+N_B)$ denotes the fraction of molecular budget allocated to node S. Then, we solve the optimization problem (13) by using BCDA which relies on the concept of fixing all the parameters except one and finding its optimal value that minimizes the objective function. This process is repeated until all the parameters converge [22].

At first, using BCDA, we consider problem (13) for the fixed value of n as

$$\min_{m} \; P_e[j]. \tag{14}$$

Then, we determine convexity of (14) from the numerical results presented in Section V since calculating the second order derivative of $P_e[j]$ with respect to m is cumbersome. $P_e[j]$ follows Jensen's inequality for quasiconvexity [23], i.e., the value of the function on a segment does not exceed the maximum of its values at the endpoints. Alternatively, since $P_e[j]$ is nonincreasing till the minimum point and nondecreasing from thereon, $P_e[j]$ is quasiconvex [23]. Thus, the optimization problem (14) can be solved by using the bisection method provided in Algorithm 1 with convex feasibility problem as

$$\begin{aligned} &\text{Find } m \\ &\text{s.t. } P_e[j] - \theta \leqslant 0. \end{aligned} \tag{15}$$

Algorithm 1 Bisection Method

Choose $\delta \in (0, 1)$ and set $P_e^l = 0$, $P_e^u = 1$;
$P_e^l \leq P_e[\text{optimal } m] \leq P_e^u$
Iterate
1. $\theta = (P_e^l + P_e^u)/2$.
2. Check the convex feasibility problem (15).
3. If enforceable then update $P_e^u = \theta$; else $P_e^l = \theta$.
Until $P_e^u - P_e^l \leq \delta$.

Thereafter, we fix the value of m as the next step of BCDA algorithm and find the optimal n that minimizes the given objective function i.e.,

$$\min_{n} \; P_e[j]. \tag{16}$$

Similar to (14), optimization problem (16) is also quasiconvex that can be solved using Algorithm 1 by replacing m with n and using the new convex feasibility problem as

$$\begin{aligned} &\text{Find } n \\ &\text{s.t. } P_e[j] - \theta \leqslant 0. \end{aligned} \tag{17}$$

Finally, the aforementioned steps are repeated until the values of m and n converge for the optimization problem (13) using the BCDA given in Algorithm 2.

Algorithm 2 BCDA for the Joint Optimization of m and n

Choose $\delta \in (0, 1)$ and set iteration $k = 0$.
Using bisection method in (14), find m^0 for arbitrary n^0.
Iterate
1. For m^{k-1}, find n^k from (16) using bisection method.
2. Invoking n^k, find m^k from (14) using bisection method.
3. Update $k = k + 1$.
Until $\|m^k - m^{k-1}\|$ and $\|n^k - n^{k-1}\| \leq \delta$.

Remark: The addressed problem (13) can be solved by a controller NM [18] having higher computational capability than RN and $\mathrm{R_x N}$. It may use information such as diffusion coefficient and communication distance as the channel state information (CSI) available at the reception nodes. Prior to finding joint optimal molecules allocation and RN location, CSI can be estimated by using training sequence-based channel estimators at the reception nodes. Once the controller node finds the optimal solution, it shares the same with the transmitting nodes each of which are having molecular count limited to $N_A + N_B$ in their reservoirs. This facilitates the release of optimal number of molecules. Moreover, RN may have chemical mechanisms or self-organization capability to move itself towards the optimal position.

V. NUMERICAL AND SIMULATION RESULTS

In this section, we demonstrate the effectiveness of our joint molecules allocation and relay location optimization solution. We further showcase the effect of detection thresholds on the optimal solution which minimizes the error probability of the considered system. We consider a diffusive medium (like blood) with uniform viscosity of 10^{-3} kg $\mathrm{m^{-1}s^{-1}}$ at temperature 310 °K and the information-bearing molecules (as feasible with human insulin hormone like molecules) of compatible radius 2.56 nm [20]. We choose value of several other parameters from [20] as $r = 10$ μm, $D_A = D_B = 79.4$ $\mu\mathrm{m^2 s^{-1}}$, $\lambda = 5.41$ $\mathrm{s^{-1}}$, and $T = 0.2$ s. Furthermore, we select molecular budget $N_A + N_B = 800$, $d_{\mathrm{SR}} + d_{\mathrm{RD}} = 20$ μm, $\mu_{n_o}^{\mathrm{SR}} = \mu_{n_o}^{\mathrm{RD}} = \sigma_{n_o}^{2,\mathrm{SR}} = \sigma_{n_o}^{2,\mathrm{RD}} = 50$, $I = 10$, and $\delta = 10^{-4}$. Results are obtained using Monte Carlo simulation approach (as in [15]) and averaging over 10^4 random realizations of the observations.

Fig. 2 depicts error performance of the considered DbMC system as a function of molecules allocation factor n, for different values of detection thresholds η_{R} and η_{D}, when optimal m is chosen. One can visualize Fig. 2 from 3-dimensional

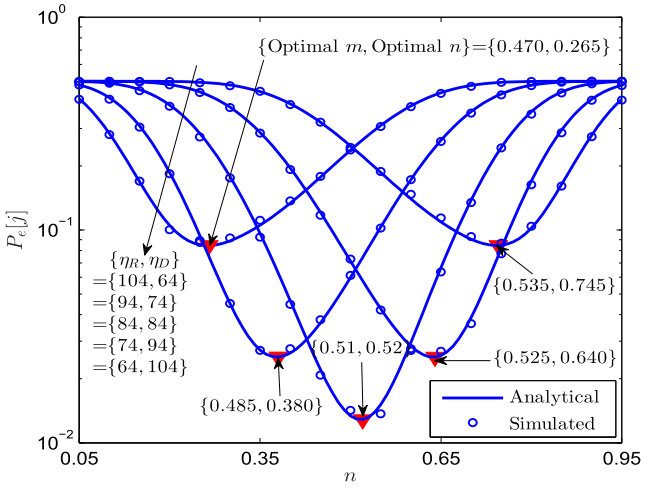


FIGURE 2. $P_e[j]$ as a function of n, with optimal m, for different $\{\eta_R, \eta_D\}$.

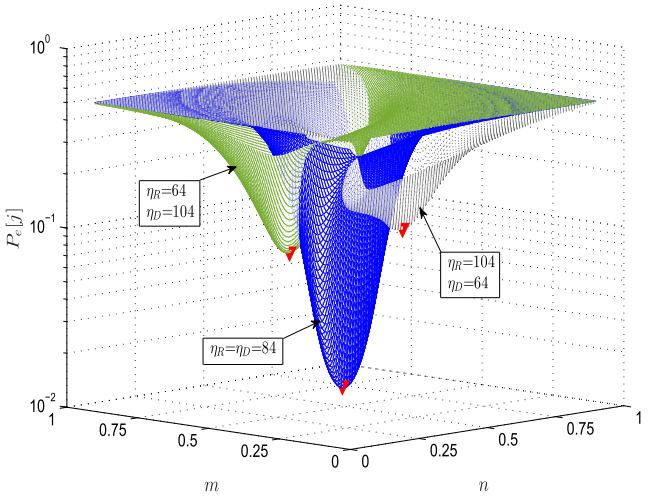


FIGURE 3. $P_e[j]$ as a function of m and n, where ▼ is the optimal $\{m, n\}$.

Fig. 3 by looking along the n axis for the fixed but optimal values of m. Our analytical results, in (6), match well with the simulation points, and the optimal solutions for different $\{\eta_R, \eta_D\}$ coincide with their corresponding minimum error points. Marker '▼' illustrates the joint optimal values of m and n calculated using the BCDA presented in Algorithm 2. Evidently, one can see the increase in optimal n for higher values of detection threshold η_R. This is because T_xN need to release more number of molecules in order to decrease the probability of miss detection. Consequently, optimal m also increases for this increased value of n. On the contrary, T_xN need to release less number of molecules to reduce the probability of false alarm for the lower values of η_R. As a result, optimal m also decreases. Intuitively, for the optimal thresholds of [15], Algorithm 2 provided the joint optimal $\{m, n\}$ as $\{0.51, 0.52\}$ suggesting the placement of RN in the middle, releasing half the molecules at the T_xN, and the other half at the RN. Above all, our analysis helps in achieving the same minimum error performance for the interchanged values of $\{\eta_R, \eta_D\}$, when optimal $\{m, n\}$ are chosen.

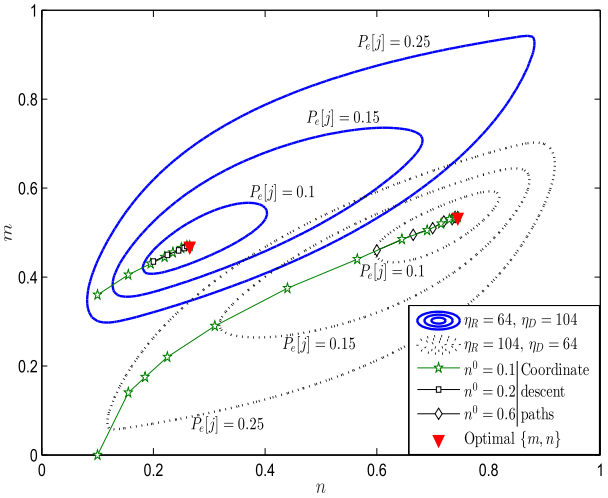


FIGURE 4. Contours or level curves of $P_e[j]$ illustrating coordinate descent paths.

Fig. 4 presents the contours or level curves of $P_e[j]$, for different values of detection thresholds η_R and η_D, along with the coordinate descent paths for different initial values n^0. Fig. 4 can be generated from Fig. 3 by cutting latter along the mn plane at different heights. Apparently, one can observe that $P_e[j]$ is a quasiconvex function of m and n since the lower contour set is convex for any value of $P_e[j]$ [23]. In other words, $P_e[j]$ is quasiconvex since its value for the level curves increases in the outward direction. Further, one can see the coordinate descent paths (or the sequence of solutions corresponding to each BCDA iterations), for different $\{\eta_R, \eta_D\}$ and n^0, leading towards their optimal solutions. Note that a single iteration represents minimization for both the optimization parameters. Algorithm 2 takes 8 and 13 iterations, with $n^0 = 0.1$, to provide the joint optimal solutions for $\{\eta_R = 64, \eta_D = 104\}$ and $\{\eta_R = 104, \eta_D = 64\}$ respectively. Moreover, when n^0 is chosen closer to the optimal n then BCDA takes less iterations for convergence. Specifically, Algorithm 2 requires 6 iterations for $\{\eta_R = 64, \eta_D = 104\}$ with $n^0 = 0.2$ and 7 for $\{\eta_R = 104, \eta_D = 64\}$ with $n^0 = 0.6$. Note that an initial value close to 0.5 will result in faster convergence.

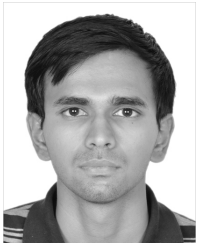
VI. CONCLUSION

We performed the joint optimization of molecules allocation and relay location in order to minimize the end-to-end error probability of a RN-assisted DbMC system. Further, we demonstrated that the error performance minimizes for the joint optimal RN placement and molecular resource allocation. Our results showed that as the relay detection threshold gets increased, more molecules would be required at the source while relay should be shifted towards the destination. The proposed analysis helps in designing a reliable and budget limited DbMC system with minimal computational requirements at the receiving NMs.

REFERENCES

[1] T. Nakano, A. W. Eckford, and T. Haraguchi, *Molecular Communication*. Cambridge, U.K.: Cambridge Univ. Press, 2013.
[2] Q. H. Abbasi *et al.*, "Nano-communication for biomedical applications: A review on the state-of-the-art from physical layers to novel networking concepts," *IEEE Access*, vol. 4, pp. 3920–3935, 2016.
[3] I. F. Akyildiz, M. Pierobon, S. Balasubramaniam, and Y. Koucheryavy, "The Internet of bio-nano things," *IEEE Commun. Mag.*, vol. 53, no. 3, pp. 32–40, Mar. 2015.
[4] N. Farsad, H. B. Yilmaz, A. Eckford, C. B. Chae, and W. Guo, "A comprehensive survey of recent advancements in molecular communication," *IEEE Commun. Surveys Tuts.*, vol. 18, no. 3, pp. 1887–1919, 3rd Quart., 2016.
[5] A. Ahmadzadeh, A. Noel, and R. Schober, "Analysis and design of multi-hop diffusion-based molecular communication networks," *IEEE Trans. Mol. Biol. Multi-Scale Commun.*, vol. 1, no. 2, pp. 144–157, Jun. 2015.
[6] C. Jiang, Y. Chen, and K. J. Ray, "Nanoscale molecular communication networks: A game-theoretic perspective," *EURASIP J. Adv. Signal Process.*, vol. 2015, no. 1, p. 5, Jan. 2015.
[7] S. Salehi *et al.*, "Releasing rate optimization in a single and multiple transmitter local drug delivery system with limited resources," *Nano Commun. Netw.*, vol. 11, pp. 114–122, Mar. 2017.
[8] G. D. Ntouni, V. M. Kapinas, and G. K. Karagiannidis, "On the optimal timing of detection in molecular communication systems," in *Proc. Int. Conf Telecommun. (ICT)*, Limassol, Cyprus, May 2017, pp. 1–5.
[9] G. D. Ntouni, V. M. Kapinas, and G. K. Karagiannidis, "Optimization of the detection process timing in molecular communication systems with flow," in *Proc. Telecommun. Forum (TELFOR)*, Belgrade, Serbia, Nov. 2017, pp. 1–4.
[10] N.-R. Kim, A. W. Eckford, and C.-B. Chae, "Symbol interval optimization for molecular communication with drift," *IEEE Trans. Nanobiosci.*, vol. 13, no. 3, pp. 223–229, Sep. 2014.
[11] B. C. Akdeniz, A. E. Pusane, and T. Tugcu, "Optimal reception delay in diffusion-based molecular communication," *IEEE Commun. Lett.*, vol. 22, no. 1, pp. 57–60, Jan. 2018.
[12] G. D. Ntouni, A. E. Paschos, V. M. Kapinas, G. K. Karagiannidis, and L. J. Hadjileontiadis, "Optimal detector design for molecular communication systems using an improved swarm intelligence algorithm," *IET Micro Nano Lett.*, vol. 13, no. 3, pp. 383–388, Nov. 2017.
[13] I. D. S. Bahri, S. Y. Shin, and S. A. C. Aziz, "Molecular modeling characteristics based on bio-inspired ant colony optimization in long-range nanonetworks," *J. Telecommun., Electron. Comput. Eng.*, vol. 7, no. 2, pp. 27–32, Dec. 2015.
[14] N. Tavakkoli, P. Azmi, and N. Mokari, "Performance evaluation and optimal detection of relay-assisted diffusion-based molecular communication with drift," *IEEE Trans. Nanobiosci.*, vol. 16, no. 1, pp. 34–42, Jan. 2017.
[15] S. K. Tiwari, T. R. T. Reddy, and P. K. Upadhyay, "Error performance optimization using logarithmic barrier function in molecular nanonetworks," *IEEE Commun. Lett.*, vol. 21, no. 11, pp. 2408–2411, Nov. 2017.
[16] S. K. Tiwari and P. K. Upadhyay, "Estimate-and-forward relaying in diffusion-based molecular communication networks: Performance evaluation and threshold optimization," *IEEE Trans. Mol. Biol. Multi-Scale Commun.*, vol. 3, no. 3, pp. 183–193, Sep. 2017.
[17] Y. Fang, A. Noel, N. Yang, A. W. Eckford, and R. A. Kennedy, "Convex optimization of distributed cooperative detection in multi-receiver molecular communication," *IEEE Trans. Mol. Biol. Multi-Scale Commun.*, vol. 3, no. 3, pp. 166–182, Sep. 2017.
[18] N. Tavakkoli, P. Azmi, and N. Mokari, "Optimal positioning of relay node in cooperative molecular communication networks," *IEEE Trans. Commun.*, vol. 65, no. 12, pp. 5293–5304, Dec. 2017.
[19] N. Agoulmine, K. Kim, S. Kim, T. Rim, J.-S. Lee, and M. Meyyappan, "Enabling communication and cooperation in bio-nanosensor networks: Toward innovative healthcare solutions," *IEEE Wireless Commun.*, vol. 19, no. 5, pp. 42–51, Oct. 2012.
[20] A. C. Heren, H. B. Yilmaz, C.-B. Chae, and T. Tugcu, "Effect of degradation in molecular communication: Impairment or enhancement?" *IEEE Trans. Mol. Biol. Multi-Scale Commun.*, vol. 1, no. 2, pp. 217–229, Jun. 2015.
[21] V. Jamali, A. Ahmadzadeh, and R. Schober, "Symbol synchronization for diffusive molecular communication systems," in *Proc. IEEE ICC*, Paris, France, May 2017, pp. 1–7.
[22] P. Tseng, "Convergence of a block coordinate descent method for nondifferentiable minimization," *J. Optim. Theory Appl.*, vol. 109, no. 3, pp. 475–494, 2001.
[23] S. Boyd and L. Vandenberghe, *Convex Optimization*. Cambridge, U.K.: Cambridge Univ. Press, 2004.

SATISH K. TIWARI (S'15) received the B.E. degree in electronics and communication engineering from Rajiv Gandhi Proudyogiki Vishwavidyalaya, Bhopal, India, in 2011, and the M.Tech. degree in communication and networks from the National Institute of Technology, Rourkela, India, in 2014. He is currently pursuing the Ph.D. degree with the Wireless Communications Research Group, Indian Institute of Technology Indore, Indore, India. His research interests include molecular communications, nanonetworking, internet of bio-nano things, detection and estimation theory, and optimization techniques.



TADI RAVI TEJA REDDY received the B.Tech. degree in electrical engineering from the Indian Institute of Technology Indore, Indore, India, in 2018. He is currently pursuing the master's degree in electrical and computer engineering with the University of California at Los Angeles, Los Angeles. His research interests include molecular communications, wireless networks, and optimization techniques. He received the Charpak Research Scholarship by the Government of France in 2017.

PRABHAT K. UPADHYAY (S'09–M'13–SM'16) received the Ph.D. degree in electrical engineering from Indian Institute of Technology Delhi, New Delhi, India, in 2011. He was a Lecturer with the Department of Electronics and Communication Engineering, Birla Institute of Technology, Mesra, Ranchi. He joined as an Assistant Professor in electrical engineering with IIT Indore in 2012, where he has been an Associate Professor since 2017. He has also been leading various research projects in the Wireless Communications Research Group, IIT Indore. He has numerous publications in peer reviewed journals and conferences, and has authored a book and three book chapters. He received the Sir Visvesvaraya Young Faculty Research Fellowship under the Ministry of Electronics and Information Technology, Government of India. He is recently conferred with the IETE-Prof SVC Aiya Memorial Award-2018.

His main research interests include wireless relaying techniques, cooperative communications, MIMO signal processing, hybrid satellite terrestrial systems, cognitive radio, and molecular communications. He is a member of the IEEE Communications Society and the IEEE Vehicular Technology Society, and a Life Member of the Institution of Electronics and Telecommunication Engineers. He was a co-recipient of the best paper awards at the International Conference on Advanced Communication Technologies and Networking, Marrakech, Morocco, in 2018. He is currently serving as an Associate Editor for the IEEE Access and a Guest Editor of the Special Issue on Energy-Harvesting Cognitive Radio Networks in the IEEE Transactions on Cognitive Communications and Networking. He has been involved in Technical Program Committee of several premier conferences.

DANIEL BENEVIDES DA COSTA (S'04–M'08–SM'14) was born in Fortaleza, Ceará, Brazil, in 1981. He received the B.Sc. degree in telecommunications from the Military Institute of Engineering (IME), Rio de Janeiro, Brazil, in 2003, and the M.Sc. and Ph.D. degrees in electrical engineering, Area: Telecommunications, from the University of Campinas, SP, Brazil, in 2006 and 2008, respectively. His Ph.D thesis was awarded the Best Ph.D. Thesis in Electrical Engineering by the Brazilian Ministry of Education (CAPES) at the 2009 CAPES Thesis Contest. From 2008 to 2009, he was a Postdoctoral Research Fellow with INRS-EMT, University of Quebec, Montreal, QC, Canada. Since 2010, he has been with the Federal University of Ceará, where he is currently an Associate Professor.

Prof. da Costa is currently Editor of the IEEE COMMUNICATIONS SURVEYS AND TUTORIALS, the IEEE ACCESS, the IEEE TRANSACTIONS ON COMMUNICATIONS, the IEEE TRANSACTIONS ON VEHICULAR TECHNOLOGY, and the *EURASIP Journal on Wireless Communications and Networking*. He has also served as Associate Technical Editor of the *IEEE Communications Magazine*. From 2012 to 2017, he was Editor of the IEEE COMMUNICATIONS LETTERS. He has served as Area Editor of *KSII Transactions on Internet and Information Systems* and as Guest Editor of several Journal Special Issues. He has been involved on the Organizing Committee of several conferences. He is currently the Latin American Chapters Coordinator of the IEEE Vehicular Technology Society. Also, he acts as a Scientific Consultant of the National Council of Scientific and Technological Development (CNPq), Brazil, and he is a Productivity Research Fellow of CNPq. From 2012 to 2017, he was Member of the Advisory Board of the Ceará. Council of Scientific and Technological Development (FUNCAP), Area: Telecommunications. Currently, he is the Chair of the Special Interest Group on ''Energy-Harvesting Cognitive Radio Networks'' in IEEE Cognitive Networks Technical Committee.

Prof. da Costa is the recipient of four conference paper awards. He received the Exemplary Reviewer Certificate of the IEEE WIRELESS COMMUNICATIONS LETTERS in 2013, the Exemplary Reviewer Certificate of the IEEE COMMUNICATIONS LETTERS in 2016 and 2017, the Certificate of Appreciation of Top Associate Editor for outstanding contributions to the IEEE TRANSACTIONS ON VEHICULAR TECHNOLOGY in 2013, 2015 and 2016, the Exemplary Editor Award of the IEEE COMMUNICATIONS LETTERS in 2016, and the Outstanding Editor Award of the IEEE ACCESS in 2017. He is a Distinguished Lecturer of the IEEE Vehicular Technology Society. He is a Senior Member of IEEE, a Member of the IEEE Communications Society and the IEEE Vehicular Technology Society.