Neural-Inspired Multi-Agent Molecular Communication Networks for Collective Intelligence

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***Abstract*—Molecular Communication (MC) is a pivotal enabler for the Internet of Bio-Nano Things (IoBNT). However, current research often relies on highly capable individual agents with complex transceiver architectures that defy the energy and processing constraints of realistic nanomachines. This paper proposes a paradigm shift towards collective intelligence, inspired by the cortical networks of the biological brain. We introduce a decentralized network architecture where simple nanomachines interact via a diffusive medium using a threshold-based firing mechanism modeled by Greenberg-Hastings (GH) cellular automata. We derive fixed-point equations for steady-state populations via mean-field analysis and validate them against stochastic simulations. We demonstrate that tuning the activation threshold allows the network to exhibit critical transition-like behavior, maximizing susceptibility across the swarm.**

***Index Terms*—Molecular Communication, Internet of Bio-Nano Things, Cellular Automata, Mean-Field Analysis.**

I. Introduction

Molecular Communication (MC) has established itself as a promising paradigm for information exchange in nanonetworks, particularly within the Internet of Bio-Nano Things (IoBNT) domain [1], [3]. While the fundamental limits of point-to-point diffusion channels have been extensively studied, the field is currently shifting towards understanding large-scale, complex collective interactions. Recent works have begun exploring these complex MC topologies using new methodologies, such as analyzing semi-autonomous in vivo computations for nanomachine swarms [6] and investigating the emergence of communication protocols among artificial agents via Graph Neural Networks (GNNs) [2].

Despite these advances, a significant disconnect remains between theoretical models and practical realizability. Existing works frequently investigate structured, deterministic topologies that are unrepresentative of real-life biological environments, where nanomachines are often distributed randomly. Furthermore, current theoretical frameworks frequently rely on idealized assumptions regarding the capabilities of individual agents, such as perfect temporal synchronization, highly complex transceiver designs, and high-precision molecule counting [7]. Current and near-future nanotechnology limits us to the production of simple, resource-constrained agents incapable of such complex individual tasks.

To bridge this gap, we propose a paradigm shift from highly capable individual agents to a network of simple, numerous agents. This approach draws direct inspiration from the cortical networks of the brain, where complex information processing emerges not from a single unit but from collective dynamics. Similar collective intelligence paradigms have recently driven innovations in biological reservoir computing and organoid intelligence [4], [5]. We introduce a decentralized architecture where simple agents operate on a threshold-based firing mechanism: if the concentration of molecules absorbed exceeds a threshold, the agent releases molecules. While continuous-variable neuroscience models possess mean-field theorems, we adopt the discrete Greenberg-Hastings (GH) cellular automaton model, which is computationally advantageous for simulating massive, discrete molecular swarms.

II. System Model

We consider a 3D unbounded medium containing N spherical transceiver agents of radius a_{rx} distributed according to a Poisson point process within a sphere of R. The motion of messenger molecules is governed by free diffusion. We assume an isotropic, homogeneous diffusion coefficient D. Time is slotted into discrete intervals of duration T_s. We employ fully absorbing receivers and assume the agent distribution is sufficiently sparse (i.e., total agent volume is negligible compared to the medium volume) such that no agent significantly obstructs molecule transmission.

The cumulative probability that a molecule emitted by the j-th agent is absorbed by the i-th agent by time t is given by the canonical hitting-time formulation:

$$g_{ij}(t) = \frac{a_{rx}}{d_{ij}} \operatorname{erfc}\left(\frac{d_{ij} - a_{rx}}{\sqrt{4Dt}}\right) \tag{1}$$

where $d_{ij} = |r_i - r_j|$ is the distance between the transceivers. The probability of absorption in the k-th interval is $P_{ij}[k] = g_{ij}(kT_s) - g_{ij}((k-1)T_s)$.

According to the GH model, an agent transitions between three states: quiescent (Q), excited (E), and refractory (R). The state updates are: $Q \to E$ if the received molecules $N^{(R)} > T_{th}$, where T_{th} is the activation threshold; $E \to R$ with probability 1; and $R \to Q$ with probability $\tilde{r}_2$.

Assuming Gaussian arrivals, the number of molecules absorbed by the i-th agent conditioned on the past L states of all agents is $N_i^{(R)}[k] \sim \mathcal{N}(\mu_i[k], {\sigma_i}^2[k])$, with:

$$\mu[k] = N_0 \sum_{l=1}^{L} P[l]x[k-l] \tag{2}$$

$$\sigma^2[k] = N_0 \sum_{l=1}^{L} (P[l] \odot (\mathbf{1} - P[l])) \cdot x[k-l] \tag{3}$$

where N_0 is the emission count, $P[k]$ is the connectivity matrix, $x[k] \in \{0, 1\}$ is the state vector, and $\odot$ denotes element-wise multiplication. By taking the unconditional mean and applying the law of total variance, we derive the steady-state mean-field fixed-point problem:

$$\mathbf{e}^* = \frac{\Gamma(\mathbf{e}^*)}{1 + \Gamma(\mathbf{e}^*)(1 + 1/\tilde{r}_2)} \ , \ \Gamma(\mathbf{e}^*) = 1 - \Phi\left(\frac{T - \boldsymbol{\mu}^*}{\boldsymbol{\sigma}^*}\right) \tag{4}$$

$$\boldsymbol{\mu}^* = N_0 \left(\sum_{\ell=1}^{L} \mathbf{P}[\ell]\right) \cdot \mathbf{e}^* \tag{5}$$

$${\boldsymbol{\sigma}^*}^2 = N_0 \Big(\sum_{\ell=1}^{L} \mathbf{P}[\ell] \odot (\mathbf{1} - \mathbf{P}[\ell])\Big) \cdot \mathbf{e}^* \tag{6}$$

$$+ N_0^2 \Big(\sum_{\ell=1}^{L} \mathbf{P}^2[\ell]\Big) \cdot \mathbf{e}^* \cdot (1 - \mathbf{e}^*) \tag{7}$$

III. Results

We simulate the stochastic dynamics in MATLAB. Agents initialized as 10% excited and the rest quiescent. We calculate the mean and standard deviation of activity across various thresholds.

TABLE I
Simulation Parameters

Parameter	Value	Parameter	Value
Agents (N)	100	Radius (a_{rx})	$4\mu m$
Medium Radius (R)	$20\mu m$	Diff. Coeff (D)	$79.4\mu m^2/s$
Emission (N_0)	100	Memory (L)	5
Time Step (T_s)	1 s	$\tilde{r}_2$	0.5

As shown in Fig. 1, increasing the threshold decreases mean activity. The standard deviation of activity, which measures network susceptibility, peaks during this rapid drop, indicating a phase transition-like behavior. This categorizes the network into a sub-critical saturated phase, a super-critical silent phase, and a critical transitional regime that maximizes the dynamic range of the swarm and should be the ideal operating point.

To validate the mean-field analysis, we compare theoretical excitation probabilities to simulation runs. For this specific validation in Fig. 2, we set $\tilde{r}_2 = 1$ to isolate the excitation dynamics by removing the prolonged refractory period and we use fixed point iteration method to solve Eq. 4.

As seen in Fig. 2, the theoretical estimate strongly aligns with the simulation. The minor divergence at the exact transition point confirms that the mean-field assumption of node independence naturally weakens when the system exhibits high correlation during the critical transition.

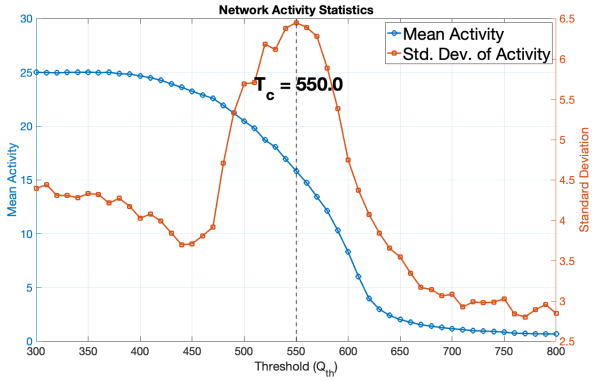

Fig. 1. Mean and standard deviation of activity across varying thresholds.

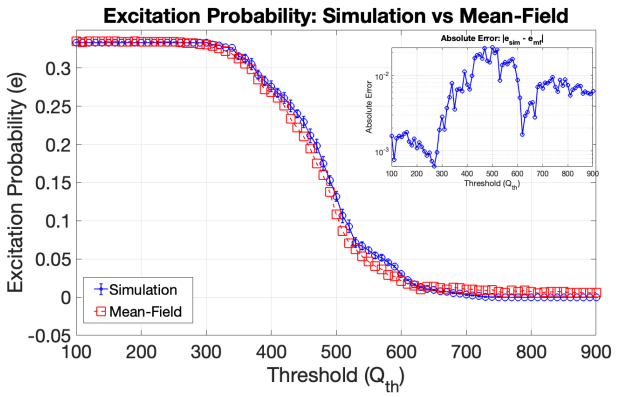

Fig. 2. Theoretical and simulated excitation probabilities (e)

IV. Conclusion

This paper demonstrates that modeling decentralized nanomachines through GH models allows a molecular network to achieve stable, collective operation. By tuning activation thresholds, the network reaches a transitional regime that optimizes signal propagation without requiring complex individual processing capabilities. Future efforts are planned to explore different network geometries, perturbation analysis, and provide further theoretical and simulation-based proof of the system's operation within critical regimes.

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