Molecular Modeling Characteristics Based on Bio-inspired Ant Colony Optimization in Long-range Nanonetworks

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***Abstract*—This paper presents a bio-inspired molecular communication algorithm using ant colony optimization (ACO) to enable a target node to find the optimal path to a source node. The target node will attempt to find the next optimal node to the source using the molecules emitted and diffused by the source, which is analogous with the pheromones of an ant colony. The positions and velocities of the molecules determine the state in molecular dynamics. As the performance measures, the arrival time and number of contacts with molecules from the target to the source are evaluated two-dimensionally (2D) and three dimensionally (3D) with different time steps. On the basis of the simulation results in this study, the size of the time step is concluded to be a dominant factor in molecular communication.**

***Index Terms*—Molecular communication, Nanotechnology, Bio-inspired, Ant Colony Optimization (ACO)**

I. INTRODUCTION

In recent years, nanotechnology has become something of a buzzword and has started to be applied to many products and technologies. Nanotechnology is a tool that measures and manipulates phenomena and objects on the nanoscale. This technology is largely related to molecular communication [1].

Molecular communications combine communication technology and biochemistry. In molecular communications, a biological system is considered as a system of networking devices [2]. The idea of molecular communications is basically derived from the communications between the cells in a biological system because the cells communicate with each other using the molecules [3]. Molecular communications are based on chemical signals, unlike the electrical signals in data communications [4]. Molecular communications over a long distance (i.e., a distance larger than one molecule) can be analyzed using molecular dynamics. Research on molecular communication can be performed with experiments and computer simulations. Molecular Dynamics (MD) is a famous and accurate simulation that is currently used [5].

MD generates and predicts the movement of molecules to guide an assembly of large molecules. The movement of molecules is expressed by integrating the equations of Newtonian motions during the time step[6],[7]. The time step represents the time interval for the source to diffuse. The time step will control the distances among the diffuse molecules. Time steps are required to avoid collisions in the molecular dynamics by managing the movement of molecules.

These integrated results during a time step will determine the trajectories of the molecules. By holding and positioning these molecules, a molecular dynamics algorithm will control how the molecules react and create complex structures with atomic precision [8]. The structure of the molecules can be two-dimensional (2D) or three-dimensional (3D).

A typical example of a complex molecular structure is a protein. The global characteristics of a protein structure in a 3D cubic lattice were investigated in [9] through the use of ant colony optimization (ACO). ACO is a population-based stochastic search method for solving a wide range of combinatorial optimization problems.

In this paper, we propose a new molecular communication algorithm using the principle of ACO. For that, ACO is applied to one of integration algorithms of molecular dynamics. By applying ACO, we want to exploit the ability of ants to find food while minimizing the time by optimal path selection to molecular communications. To the best of our knowledge, using the characteristics of a single molecule in molecular dynamics by utilizing ACO has not been reported yet.

Previously, the movement of target is based on zig-zag pattern which consumes a larger time for the target to arrive at the source position and not all of the targets arrive at the source position [10], [11].

Based on nanotechnology, it is known to be impossible to control the behavior of a single molecule. However, we can control the number of molecules in one place, the degree of diffusion and position of the target, and the source position [12]. The target is a molecule that has to meet with the source molecule. For that, the source molecule diffuses molecules. The contributions of this paper are as follows:

Table 1
Differentials between traditional communcation and molecular communcation

Communication method	Traditional	Molecular
Communication carrier	Electromagnetic waves	Molecules
Signal type	Electronic and optical (Electromagnet)	Chemical
Propagation speed	3x108m=s (i.e., speed of light)	Extremely low
Medium conditions	Wired: Almost immune	Affect communication
Noise	Electromagnetic fields and signals	Particles and molecules in medium
Encoded information	Voice, text and video	Phenomena, chemical states or processes
Energy consumption	High	Low

- to investigate the characteristics of a molecule based on ACO by controlling the number of molecules and the positions of source and target
- to evaluate the performance of molecular communications using Molecular Dynamic simulation

In our simulation, it is assumed that the molecules diffuse unidirectionally in two dimensions in all time steps. As the measures of performance, the time required for the target molecule to arrive at the source position, i.e., travel time, and the number of contacts faced by the target molecule are investigated.

Figure 1 shows an illustrative example of the diffusion process in the molecular communication simulation for this study. First, a random number of molecules will be generated and diffused from the source. If the random molecules approach the target, the target will choose the closest molecule before moving to that position. The operation will stop when the target arrives at the source position. Both 2D and 3D fields are considered for the simulation.

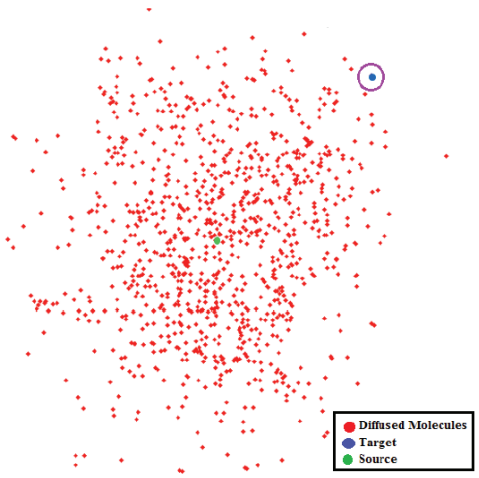


Figure 1: Illustrative example of molecular communication simulation

The rest of the paper is organized as follows. Section II explains the theory of nanoscale network. Section III explains the molecular dynamic simulation and theory of Verlet algorithm. Section IV explains the proposed algorithm that combines the molecular dynamics and ACO. Section V presents the simulation of the study. Finally, the conclusions are given in Section VI.

II. Theory of Nanoscale Network

A nanonetwork or nanoscale network is a set of interconnected devices of several hundred nanometers or several micrometers at most in size. In this network, the devices are only able to perform very simple tasks such as computing, data storage, sensing, and actuation. In order to expand the capabilities of a nanonetwork in terms of complexity and the range of operation, coordinating, sharing, and fusing information among the devices show good potential [13]. Nanonetworks are predicted to improve technology in biomedical fields, environment research, military technology, and industrial and consumer goods applications. There are many types of communication in the nanoscale network, but the main alternative is based on molecular communication. In molecular communication, individual molecules have the ability to code, transmit, decode and encode the signal.

The means of molecules in the transmission and reception information determine the transmission signal. The paradigms of molecular communication are different from those of traditional communication. Table 1 shows the differences between traditional communication and molecular communication [14].

Three main techniques to propagate molecules in molecular communication are as follows [15]:

1. Walkaway-based communication: molecules propagate along predefined pathways using carrier substances. One example is the molecular motor.
2. Flow-based communication: molecules propagated by diffusion in a medium, and the flow is guided and predictable. Hormonal communication through blood vessels in the human body is one example.
3. Diffusion-based communication: molecules propagated by spontaneous diffusion in a fluidic medium. Unlike that based on the flow, this type of communication can be affected by non-predictable turbulence present in the fluidic medium (air, water, etc.). Examples include diffusion of pheromone and calcium signaling among cells.

Research on molecular communication can be performed by experiments and computer simulations. MD is a famous and accurate simulation that is currently used in computer simulations. Table 2 shows the similarity between the MD simulation and real experiments.

Table 2
Illustrative example of molecular communication simulation

Step	Experiment	MD simulation
1	Prepare the sample	Setup and equilibrate a system model
2	Connect the sample to a measuring instrument and measure the properties of interest for a certain time	Perform MD simulations for a certain time and measure one or various observable that can be expressed as function of the position and momentum of the particle

III. Molecular Dynamic Simulation

Molecular dynamics simulations should be considered as good tools when involving molecular-level time scales [16]. A molecular dynamics simulation is based on Newton's second law or the equation of motion. Newton's equation of motion can be expressed as the relation between the derivative of the velocity, V to the change in position as a function of time.

From the knowledge of the force on each molecule, it is possible to determine the acceleration of each atom in the system. A time step is one of the protocols for a molecular dynamics simulation. It is used for the integration of an equation of motion. Integration of the equations of motion then yields trajectories that describe the positions, velocities, and accelerations of the molecules as they vary with time. Many different techniques are widely used to generate molecular dynamic trajectories. The basic idea of the molecular dynamic concept is as follows [17]:

1. The integration is broken down into fixed time intervals
2. The total force on each particle in the configuration is calculated at time t as a vector sum of its interaction with other particles
3. The acceleration of the particle is determined from the calculated force and then combined with the position and velocity at time t to calculate the position and velocity at time (t+dt).
4. Forces are assumed to be constant during the time step.
5. The force on the particle at the new position is calculated to determine the position and velocity at time (t+2dt) and so on.

Many numerical algorithms have been developed for integrating the equation of motion. The Verlet algorithm is commonly used in molecular dynamics calculations [18].

The Verlet algorithm is one of the most widely used methods for integrating the equations of motion in molecular dynamic simulations. In this algorithm, in order to find the positions of the next iteration, the positions $\mathbf{r}$, velocities $\mathbf{v}$, and accelerations $\mathbf{a}$ at time $\mathbf{t}$ and the positions from the previous step need to be calculated first. The Verlet algorithm uses positions and accelerations at time t and the positions from time (t-dt) to calculate new positions at time $(\mathbf{t} + \partial\mathbf{t})$ [19].

$$\mathbf{r}(t + \partial t) = \mathbf{r}(t) + \mathbf{v}(t)\partial t + \frac{1}{2}\mathbf{a}(t)\partial t^2$$
$$\mathbf{v}(t + \partial t) = \mathbf{v}(t) + \frac{1}{2}[\mathbf{a}(t) + \mathbf{a}(t + \partial t)]\partial t;$$

This algorithm is known to be straightforward and have modest storage requirements.

IV. Molecular Communication using ACO

A. Ant Colony Optimization

Individual ants are simple insects with limited memory and are capable of performing simple actions. However, an ant colony expresses complex collective behavior providing intelligent solutions to problems such as finding the shortest route from the nest to a food source [20].

This behavior of ants is applied to the molecular communications as follows. An ant in the colony and the nest are considered as the target and the source molecules. Pheromone diffused by an ant can be considered as the molecules diffused by the source. The ant successively finds the shorter routes by detecting the density of deposited pheromone. However, the target does not exploit the density of the diffused molecules by the source but successively tries to find the shorter routes by considering acceleration and force of the molecules near itself. As the ant finally finds the shortest path to the nest, we could expect that the target will travel to the source using the shortest path. For example, in Figure 2, node 1 is the target (ant) and node 2, 3 and 4 are the positions of molecules (pheromone) which are diffused from the source. Once the molecules gets near the target circle location, the target will calculate and search which the nearest molecule among them and move to that position by following $F = ma$; where F is force, m is mass and a is acceleration.

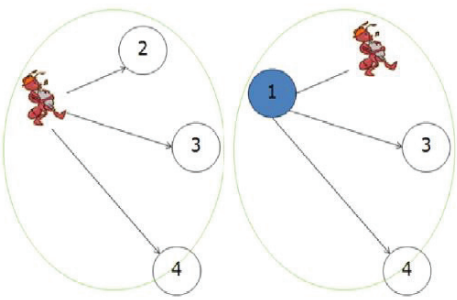


Figure 2: Proposed Algorithm Method

B. Molecular Communication based on ACO

An interesting question is how the target (which is an ant in ACO) finds the shortest route, i.e., the next step closer to the source based on the diffused molecules by the source. As ants successively find the shorter routes by detecting pheromones on the path, the target will attempt to find the nearest molecule considering the acceleration and force of the molecules near the target. In this study, it is assumed that the target attempts to move to the source node on the basis of the feasible shortest route.

The proposed algorithm can be applied by considering three basic parts: node initialization, a molecular dynamic process, and the ACO approach. The relationship among the three parts in the proposed method is shown in Figure 3. Node initialization is initializing the position of target and source, initial velocity and initial position of the released molecules from the source. Details are shown in Algorithm 1.

Molecular dynamic process will be started by updating the force of each diffused molecule. Then, the equations of

motions will be numerically solved over a short time, i.e., time step, for calculating the velocity and the position of diffused molecule using the Verlet algorithm. During ACO approach, the target will investigate the existence of molecules around it. Once it detects the existence of molecules near itself, it will calculate and define the nearest molecule position by considering the highest force between the target and the molecules. The target will move to that position and count the number of contacts it has faced. This process will be continued until the target arrives at the source. The detail is shown in the molecular communication based on ACO algorithm. The pseudocode for ACO approach is in the molecular dynamic.

In this paper, the speed of the target is assumed to be fast enough to travel within the target circle during the time step. In addition, the speed is not important in molecular communication simulation since the time will be mostly spent on calculating no bonded interactions and forces rather than integrating the equations of motion.

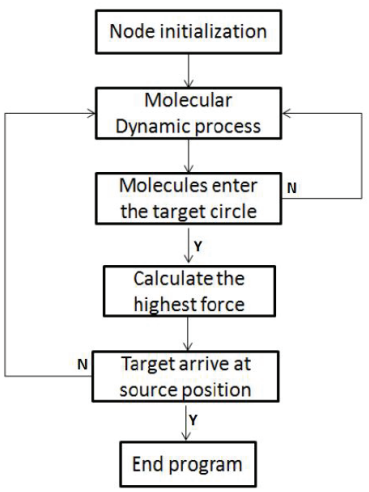


Figure 3: Algorithm of Proposed Method

Algorithm 1 Node initializing

1: Initialize position of each molecules diffuse, $r_i(t)$
2: Initialize velocity of each molecules diffuse, $v_i(t)$
3: Initialize target, p and source, n
4: Initialize angle of target position, k
5: Iteration set to zero
6: Contact set to zero, d_i
7: Set the number of molecules diffuse, x
8: Set value of time step, Δt
9: Set type of dimension, (2D or 3D)

V. Simulation

Algorithm 1 is simulated in MATLAB with a constrained environment that is described in Table 3. A number of molecules diffused in molecular dynamic are from 1000 to 10000 in all direction; 360 degrees. Since the purpose of this simulation is to investigate the time for target to arrive at the source of diffused molecule according to time step, we plotted the iteration of molecules dynamics for each step from 0.1, 0.01, 0.001 and each iteration have 0.5 second delay from the next iteration. The random amount of molecules will be generated in molecular dynamics systems. The source node and the target node are assumed in the distance of 20 cm with 45 degree. The target circle is assumed in 0.5 cm from the target node.

Table 3
Simulation Environment Parameters

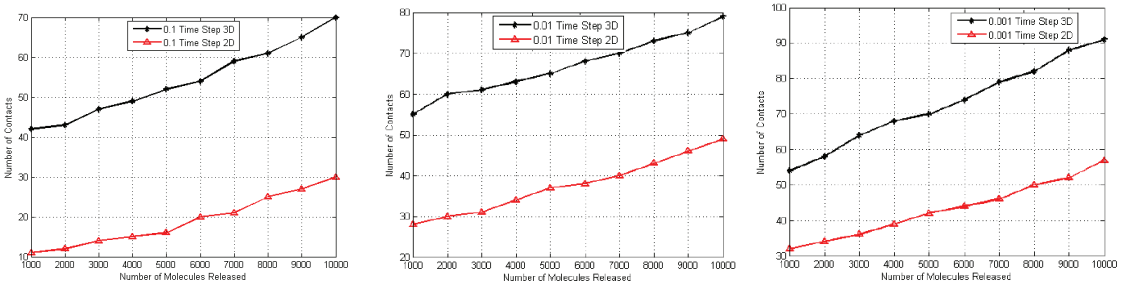
Parameters	Values
Number of molecules diffused per time step	From 1000 to 10000
Diffusion degree	360
Time step	0.1, 0.01, 0.001
Delay time of each iteration	0.5 seconds
Distance between target and source position	20 cm with 45 degree
Target circle size	0.5 cm radius from target

Algorithm 2 Molecular Communication based on ACO

1: Start counting the traveling time of the target
2: while (if the target do not arrive at the source)
3: Calculate and update force, $f_i(r_i)$ of each diffused molecule
4: Update the new position of molecules by solve the equation of motion numerically over Δt
5: $r_i(t) > r_i(t+\Delta t)$
6: $v_i(t) > v_i(t+\Delta t)$
7: if the molecules enter the target circle
8: Calculate the highest force among the molecules in the target circle
9: Update the new position of the target, p, to nearest molecule position based on $fi(r_i)$
10: Increment the number of contacts, $d_i = d_i+1$
11: if the position of target, p, equal to position of the source n
12: end if
13: end if
14: Calculate number of contacts face by the target before arrive at the source
15: Stop and calculate travel time for the target to arrive at the source
16: end while

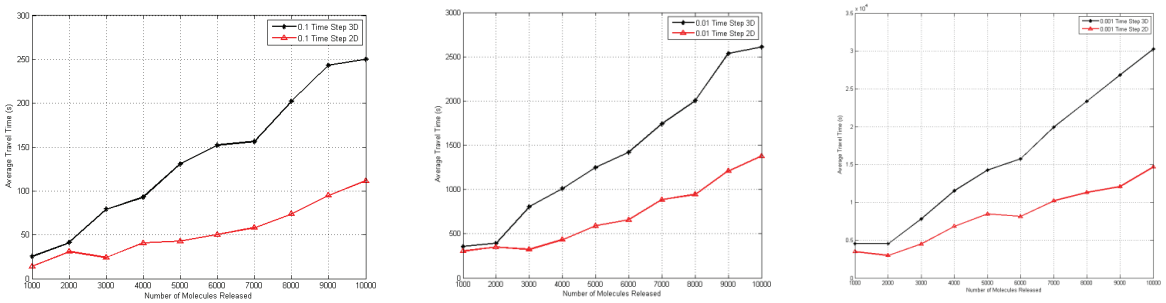
In this study, the simulations in different time step are compared using the proposed algorithm. The result are simulated in two types of structure; 3D and 2D simulation.
In molecular communication simulation, the position of molecules will change in specific location at the desired time with the random directions. Every molecule begins at the origin, i.e., the source node and travels at different direction and distance, which are related to their proximity to the time step.We continuously simulated the time step by a loop. Every iteration of the loop defined the time step.

As mentioned before, the time step will control the distances among the diffuse molecules by managing the movement of molecules. Figure 4 shows the smaller values of time step, the bigger number of contacts for the target to reach at the source, increasing numbers of molecules experienced higher number of contacts for both structure. Integrating a small value of time step resulted in molecules diffussion in close proximity to each other in the target circle, which subsequently causes a lot of contacts to be around the target. A 3D simulation has higher contacts compared with a 2D simulation. This is because there is a higher possibility of choosing the next position of the target in 3D simulation than the 2D. The 2D field is computed in cross-section XY plane; thus, it takes less computational effort, memory and time. In the 3D field, it computes in all directions and currents surrounding the arbitrary 3D area. It takes a lot of computational effort, memory and time.



(a) Time step 0.1 (b) Time step 0.01 (c) Time step 0.001

Figure 4: Average number of contacts between the target and diffused molecules in each time step



(a) Time step 0.1 (b) Time step 0.01 (c) Time step 0.001

Figure 5: Average arrival time of the target to the source over the number of diffused molecules

Figure 5 shows the increasing numbers of molecule that take a longer time for the target to arrive at the source in all the time steps either in 2D and 3D simulation. As the number of molecules rises, the area of the target circle becomes crowded and requires more complex calculation for the target to choose the next position. The more crowded the target circle, the more time is needed for the target to choose the nearest position.

The smaller is the time step, the higher is the average travel time for the target to arrive at the source. The average arrival time for 0.1 time step is ten times longer than 0.01. Furthermore, for 0.01 time step, the average arrival time is ten times longer than 0.001.

As the time step decreases, the distance of molecules diffused in the molecular communication becomes closer to each other. The average arrival time from the target to the source will increase since the target required more complicated calculation to choose the shortest route to be moved. As mentioned before, the 3D analysis is usually much more time consuming because it is computed in a cross section XYZ plane. Therefore, 3D simulation requires more average arrival time compared to 2D simulation.

As it can be seen, the average number of contacts faced by the target to arrive at the source position is proportional to the average travel time. As the number of molecules released increases, the number of contacts and average travel time also increases. This situation is the same in both 2D and 3D fields. Based on our simulations, all of the targets arrive successfully at the source position.

VI. Conclusion

This paper investigated the characteristic of bio-inspired molecular communication using ACO approach. The target successively finds the shorter routes by considering the acceleration and force of the molecules near the target. As the performance measures, the average travel time and the number of contacts faced by the target to the source are evaluated in molecular communication environment.

In this paper, the position and velocity of the molecules are determined in the state of molecular dynamics. To find the optimal route from the target to the source, ant colony optimization approach is used. To measure the performance, the arrival time and the number of contacts with molecules from the target to the source are evaluated in two-dimensional (2D) and three-dimensional (3D) with different time steps.

Based on the results from the simulations, we can draw the following conclusions. The average travel time is inversely proportional with the time step. The number of contacts is proportional to the time step; the results is similar in 3D and 2D simulation. The time step is concluded as a dominant factor for average arrival time for the target to arrive at the source of destination position and the number of contact faced. The three-dimensional simulations have higher time arrival

from target position to the source and higher number of contact compared to the two-dimensional simulation.

For future study, the comparison between this routing algorithm (ACO approach) and zig-zag pattern will be investigated.

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