Effect of Reflection Strategies on Diffusion

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1 Introduction

1.1 Particle Movement Model

We are going to try to understand the movement of particles in biological systems that takes role in the molecular communication, for example movement of neurotransmitter between the transmitter neuron and the receptor. Transmitters (particles diffusing in a synaptic cleft) are responsible for carrying information from the one neuron to the other. We can model the movement of particles with Brown Motion because these particles are suspended in liquid medium and the motion of particles are random and following a stochastic process.

Particle Movement Model:

$$\begin{aligned} x_t &= x_{t-\Delta t} + \Delta x, \quad \Delta x \sim \mathcal{N}(0, 2D\Delta t) \\ y_t &= y_{t-\Delta t} + \Delta y, \quad \Delta y \sim \mathcal{N}(0, 2D\Delta t) \\ z_t &= z_{t-\Delta t} + \Delta z, \quad \Delta z \sim \mathcal{N}(0, 2D\Delta t) \end{aligned} \tag{1}$$

Here, (x_t, y_t, z_t) represents the particle's position at time t, and Δx, Δy, and Δz are random displacements drawn from normal distributions with mean 0 and variance $2D\Delta t$ (mean square displacement). The parameter D is diffusion coefficient.

1.2 Simulation parameters

We will conduct simulations in two different environments. The first simulation will be in a 3D space with one point source (transmitter) and one receiver node with a radius r_{rx}. The transmitter node will emit neurotransmitters at t=0, and as time progresses, the neurotransmitters will diffuse with Brownian motion. If a transmitter reaches the receiver node, it will be absorbed by the receiver. Fortunately, we have an analytical solution for such a diffusion process, and we will compare the simulation results with it. For the second simulation, we will add reflecting obstacles in a 2D environment, with same one transmitter node point and one receiver node with a radius r_{rx} . We will use two different reflecting strategies: one involving roll-back and the other reflecting with respect to a line. The reflecting line's position relative to the transmitter and receiver will be adjusted. We will simulate both reflecting strategies and compare the results.

2 System Model

2.1 Topology

3D Simulation Topology:

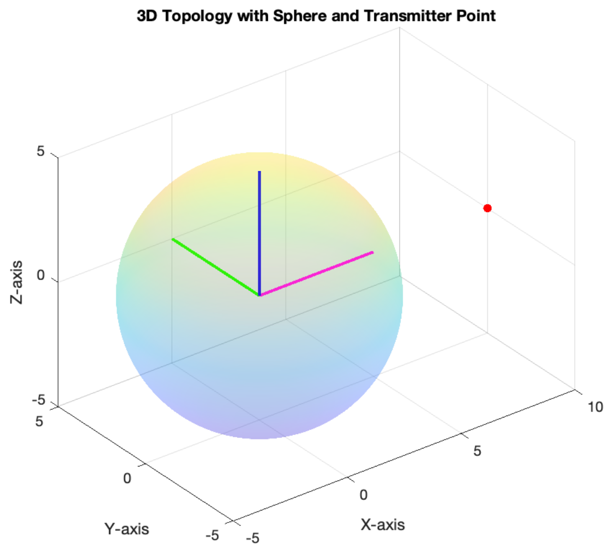


Figure 1: 3D Simulation Topology

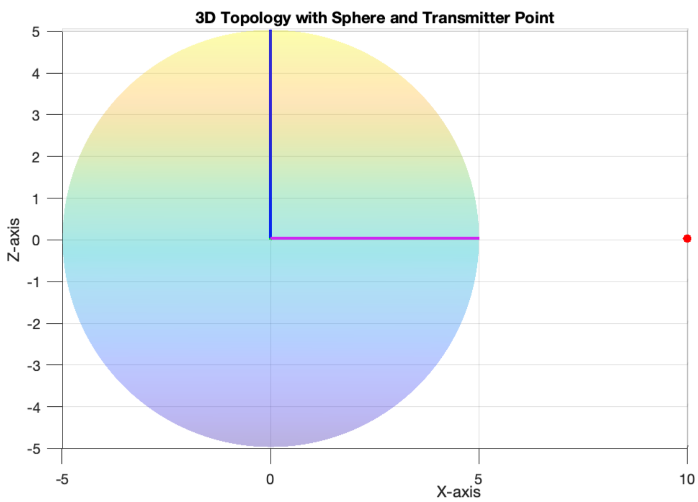


Figure 2: 3D Simulation Topology

2D Simulation Topology:

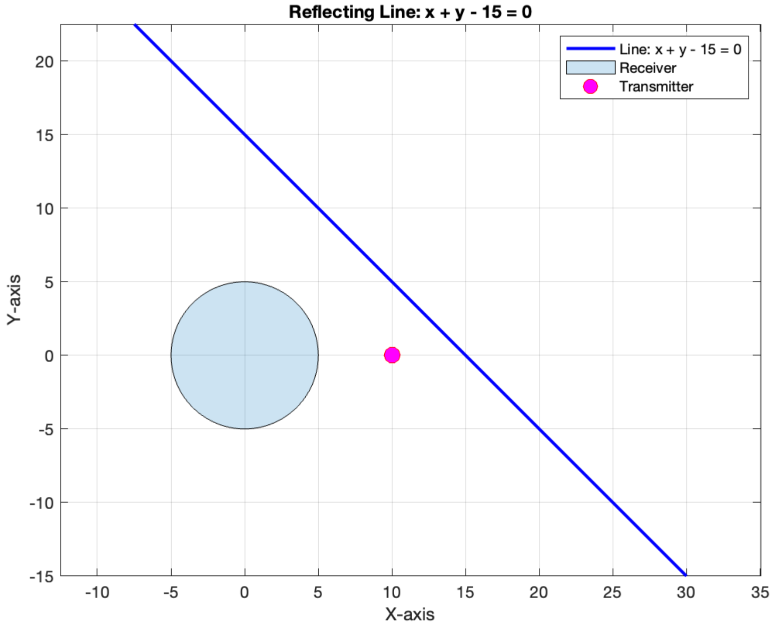


Figure 3: 2D Simulation Topology 1

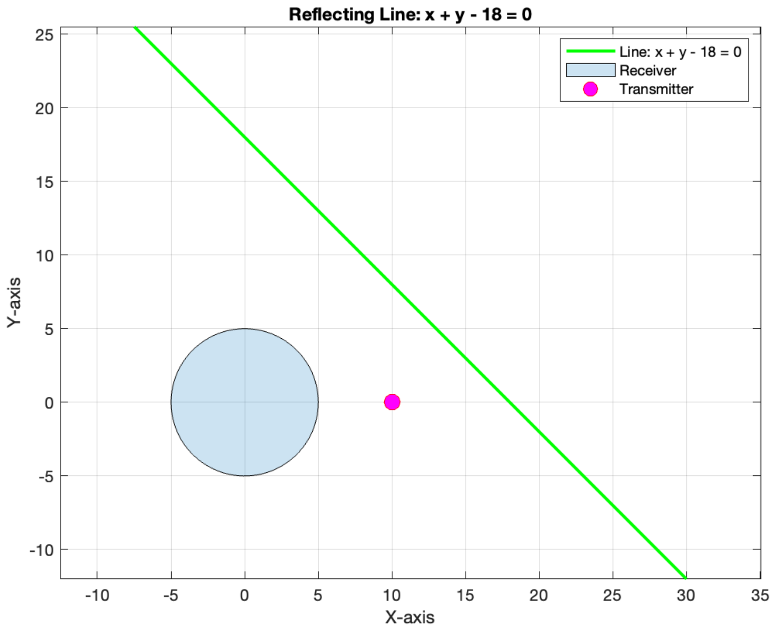


Figure 4: 2D Simulation Topology 2

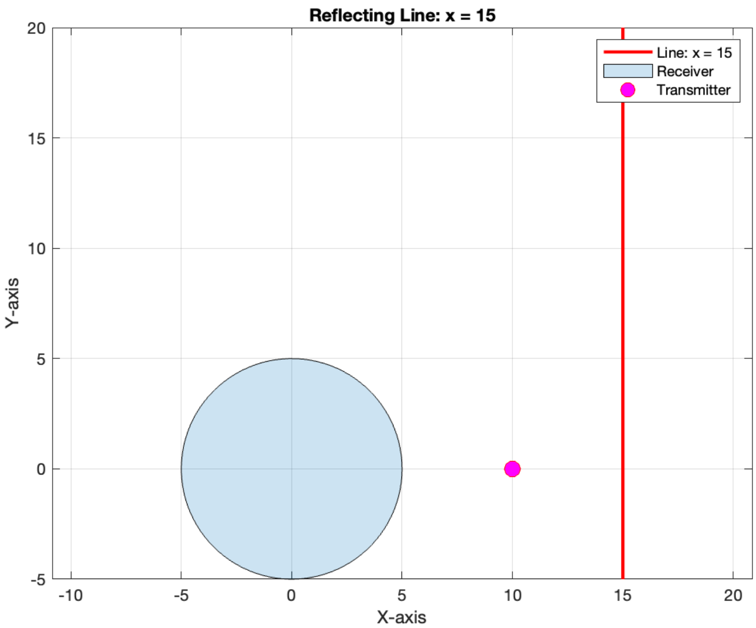


Figure 5: 2D Simulation Topology 3

2.2 Diffusion Simulations in 3D

In 3D simulations, we fixed the number of molecules, radius of the receiver, position of the transmitter and receiver, time step, and simulation time. The only variable we changed was the diffusion coefficient to observe the speed of the diffusion process. We expect faster convergence for higher D. Fortunately, we have an analytic solution for this setup in a 3D environment.

The cumulative distribution formula for the number of particles reaching the receiver ($nrx\_cumulative$) in a 3D environment is given by:

$$nrx\_cumulative(t) = \frac{r_{rx}}{r_{rx} + d} \cdot \operatorname{erfc}\left(\frac{d}{\sqrt{4Dt}}\right)$$

$$\begin{aligned} r_{rx} &: \text{Radius of the spherical receiver} \\ d &: \text{Distance between the emitter and the center of the receiver} \\ D &: \text{Diffusion coefficient} \\ t &: \text{Time of observation} \end{aligned}$$

2.3 Diffusion Simulations in 2D

In 2D simulations, we maintained fixed values for the number of molecules, radius of the receiver, position of the transmitter and receiver, time step, and simulation time. The only parameter adjusted was the alignment of the reflecting line, aimed at observing its impact on the number of received molecules. We will compare these simulations with identical parameters but without the presence of a reflecting object. In our initial Topology 1 , the reflective line is positioned to the right side of the transmitter, so that potential reflections are directed towards to the receiver node. The same logic is applied to the other two simulations. We only changed the closeness and slope of the line.

3 Numerical Results

In all of the simulations regardless of the dimension, the number of molecules emitted at time $t = 0$, is 50 000.

3.1 3D Simulations

We changed only the diffusion coefficient from $D = 75$ to $D = 200$, as expected particles received to the receiver node much earlier and faster, overall simulation converged faster for $D = 200$. Also the simulation results are very close to the analytic solution.

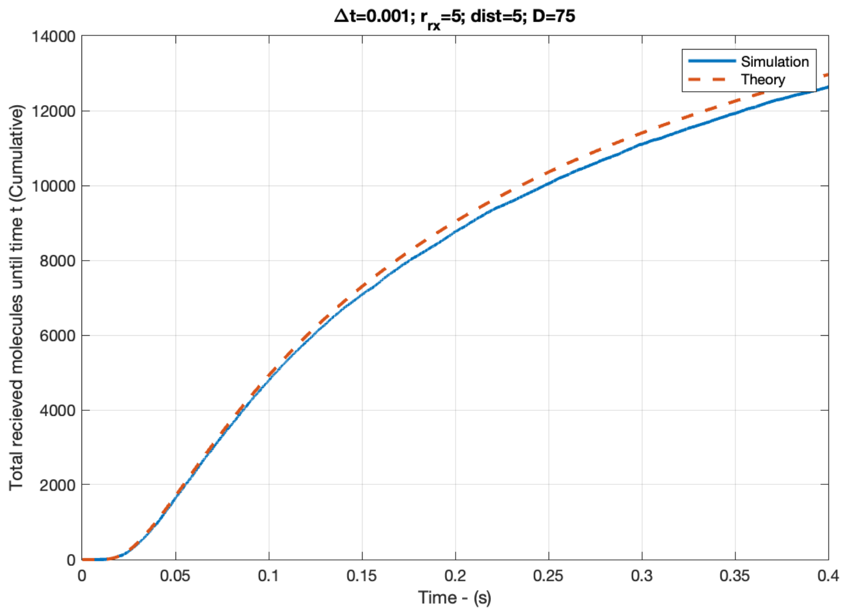


Figure 6: 3D Simulation with $D = 75$
Topology of the simulation

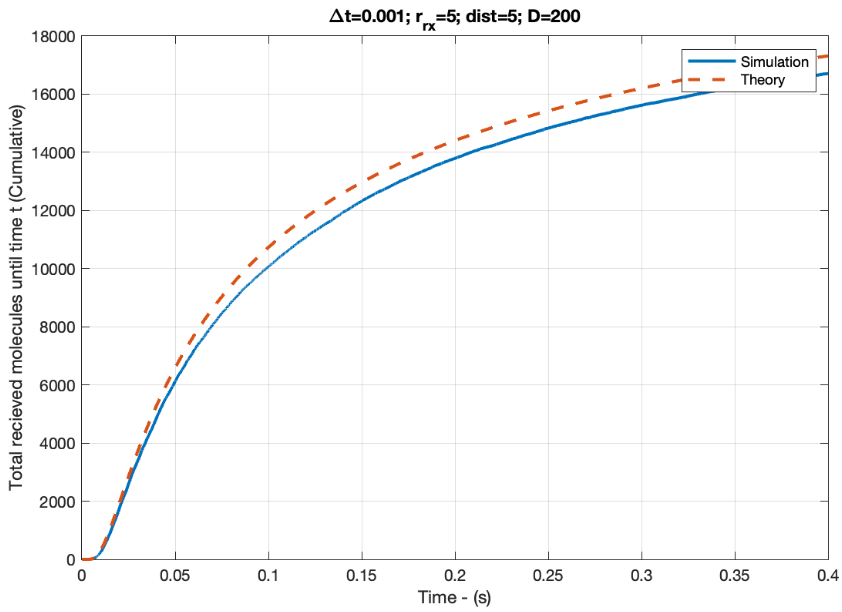
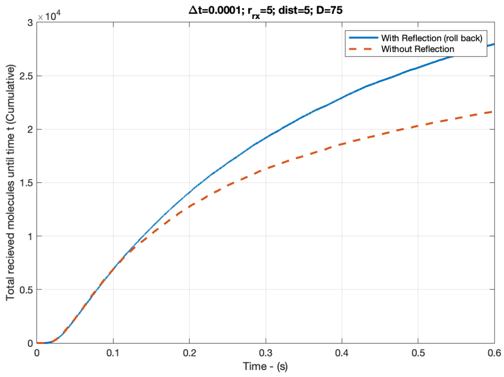
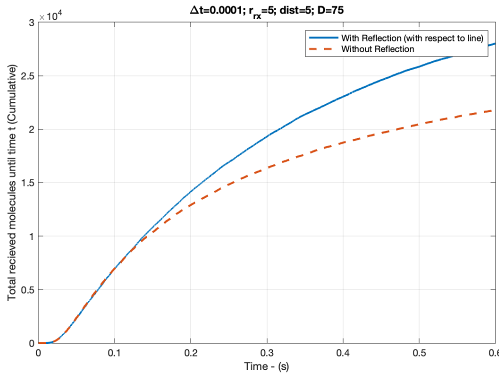


Figure 7: 3D Simulation with $D = 300$
Topology of the simulation

3.2 2D Simulations

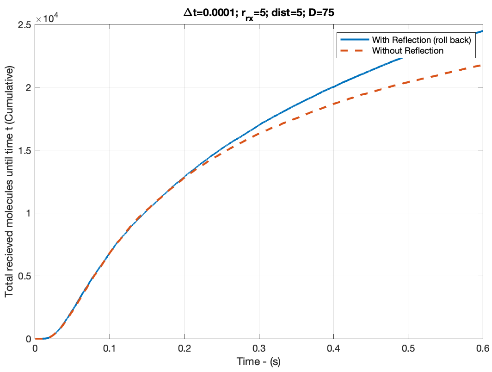


(a) roll-back

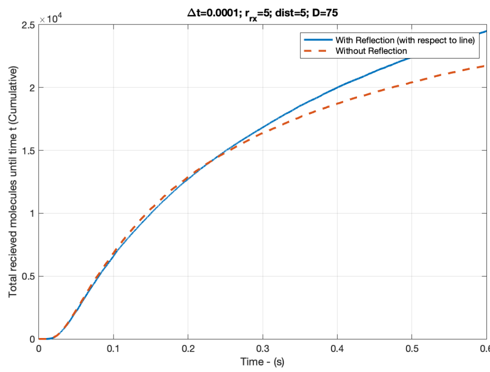


(b) reflection with respect to line

Figure 8: Topology of $x + y - 15 = 0$



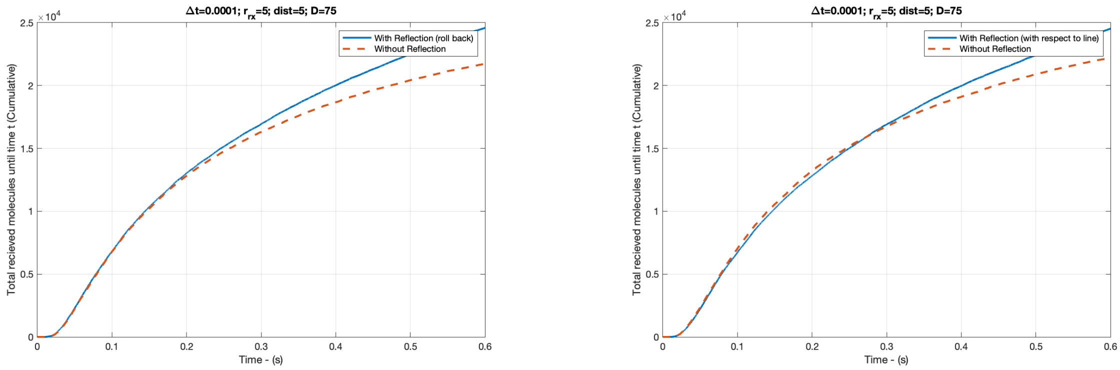
(a) roll-back



(b) reflection with respect to line

Figure 9: Topology of $x + y - 18 = 0$

In 2D simulations we can easily see that the reflection strategy does not change simulation results considerably. Also we can say that presence of reflecting object (line) increases the number received particles to the receiver significantly. The orientation of reflecting line is important, for the first set up the reflecting line $x + y - 15 = 0$ is closer to the transmitter and compared to second set up of the line $x + y - 18 = 0$, this increases the number of reflected molecules towards to the receiver, increasing the number of received molecules. Comparing line $x+y-18 = 0$ and $x = 15$ we don't observe important difference between results although the sloped line of the first set up. From visual perspective we except the set up 2 will end up more received particles but in reality final results are very close, this can be associated with distance from the transmitter to the sloped line is large enough that only small part of the particles receive and reflect in the direction receiver.



(a) roll-back (b) reflection with respect to line

Figure 10: Topology of $x = 15$

4 Conclusion

In 3D simulations, higher diffusion coefficients (D) led to faster convergence and simulations are really close to analytic solution. 2D simulations with reflecting obstacles showed negligible differences between strategies, but the presence of a reflecting object increased the number of particle received to the receiver node.

The orientation of reflecting lines in 2D simulations such as slope, distance to the transmitter and position with respect to receiver was critical. The effect on the final results depend on these factors.