# KMC Bacteria Hopping And Trapping Notes

by Carlos Alas and Trinh Lan Hoa

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## I. Problem Description

In a 3D domain, some flagellated bacteria will swim with a two state motion called a "run" and "tumble". The flagella "runs" in a straight direction for a few body lengths by bundling and rotating its flagella. After a few body lengths, the flagella unravels its bundle, which causes it to slow and tumble. It then goes off in a new random direction having been re-oriented by its tumble. In doing this, it is believed that bacteria sample the domain to construct a gradient of a food source or a specific chemical. In this motion, it is often presumed that the "run" time is much longer than its tumble time and so the diffusion can be estimated by considering its average run length and run time.

In a porous medium, it has been observed that flagellated bacteria employ a different two state motion called "hopping" and "trapping" [**?** ]. The bacteria will swim or "hop" in a straight direction until it gets stuck or "trapped" due to the confinement of neighboring pores. While trapped, the bacteria re-orients and goes off in an almost random direction; it has a slightly higher chance of going back the way it came from, but we will assume its re-orientation angle to be uniformly distributed. The bacteria spends a larger time trapped than in its hop state. Hence an estimation of their diffusivity through the porous medium can be obtained from the average hop length and trapped time –instead of the average hop time as in the homogenous space "run" and "tumble" motion.

The motion of flagellated bacteria through porous media was observed and measured in porous distributions with pores of characteristic sizes (a) 3.6 $\mu$m, (b) 2.5 $\mu$m, and (c) 1.9 $\mu$m [**?** ]. The experimenters ran tests to measure the effect of bacteria crowding and concluded this effect on their results to be minimal. They measured t velocity distributions of the bacteria during their experiments and set the threshold between the two states, hopping and trapping, to be half their measured value of the run velocity in a homogeneous domain; the threshold is 14 $\mu$m/s. They ran tests using several threshold velocities and found their choice of the threshold had little to no effect on their results. The experimenters all measured re-orientation angle distributions of the bacteria during both their hopping and trapping states and found that in the hopping state, the bacteria swim straight ahead without much deviation and in the trapped state, the motion is almost random, with a slight tendency of the bacteria to turn around and head back the way it came from. We will assume the re-orientation angle to be random during that trapped state, and to be straight ahead in the hopping state.

The group also measured distributions of the hopping lengths and reported their means, $\langle \ell \rangle$, as (a) 3.24 $\mu$m, (b) 2.79 $\mu$m, and (c) 2.14 $\mu$m and distributions of the trapped times, but do not report the means, $\langle \tau \rangle$, of the trapped times. The group also reported their measurements of the diffusivities of the bacteria through the different pore distributions to be (a) $(2 \pm 0.25)$ $\mu$m$^2$/s, (b) $(1 \pm 0.25)$ $\mu$m$^2$/s, and (c) $(0.5 \pm 0.25)$ $\mu$m$^2$/s. They compared their measurements to a simple model in which the bacteria are assumed to perform a random walk of step length $\langle \ell \rangle$ and step time $\langle \tau \rangle$ and an estimated diffusivity $D_{RW}$ given by

$$D_{RW} = \frac{\langle \ell \rangle^2}{3\langle \tau \rangle}. \tag{1}$$

To compare their predicted diffusivities to their measured diffusivities, they plotted them against each other and fit a line. Their line fit gave that the measured diffusivities, on average, were about 0.3 times that of the predicted diffusivites, or in other words, the measured diffusivities were about $\langle \ell \rangle^2/10\langle \tau \rangle$. From their predicted diffusivities, (a) 7 $\mu$m$^2$/s, (b) 3 $\mu$m$^2$/s, and (c) 2 $\mu$m$^2$/s, we can approximate their measurements of the mean trapped times, $\langle \tau \rangle$, by eqn. (1). We estimate the mean trapped times as (a) 0.5s, (b) 0.8649s, and (c) 0.7633s.

In order to simulate for the diffusivity, we will only require one bacteria in our simulations, which can be placed anywhere in the domain.

## II. Subvolume KMC method

Here we will present a KMC method that is essentially an alteration of the subvolume KMC method to allow for a distributed hop length $\ell$ to be sampled. Similar to the subvolume KMC method, we sample the amount of time spent in the lattice cell before hopping to another state, where the time spent in the lattice cell is called the trapped time $\tau$. We apply this method to study the diffusion of bacteria in a porous media [**?** ].

## III. Results

We simulated the diffusion of a single bacteria in these mediums for 10 minutes per iteration. Our results, averaged over the iterations, for the different pore size distributions are shown in figure 1. Our averaged diffusivity, over $10^5$ iterations, for the pore size distributions are (a) 2.3 $\mu$m$^2$/s, (b) 1.0 $\mu$m$^2$/s, and (c) 0.67 $\mu$m$^2$/s. We plotted the

measured diffusivities from the experiments [**?** ] against our simulated diffusivities in figure 2. The line fit $y = 0.88 * x$ demonstrates that on average the percent error is less than 14% which is quite good considering the hop times and re-orientation direction distributions are ignored; we assumed the hop times and re-orientation directions to be negligible and uniformly distributed, respectively.

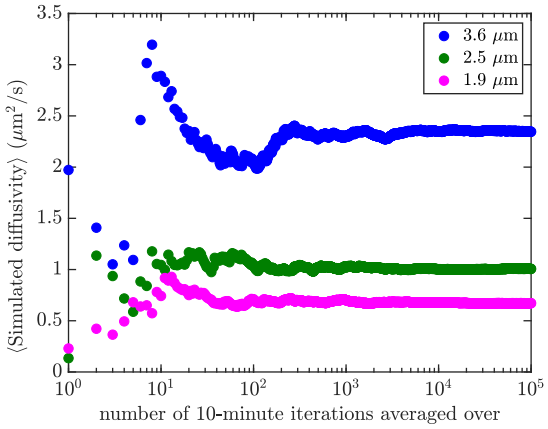


Figure 1.

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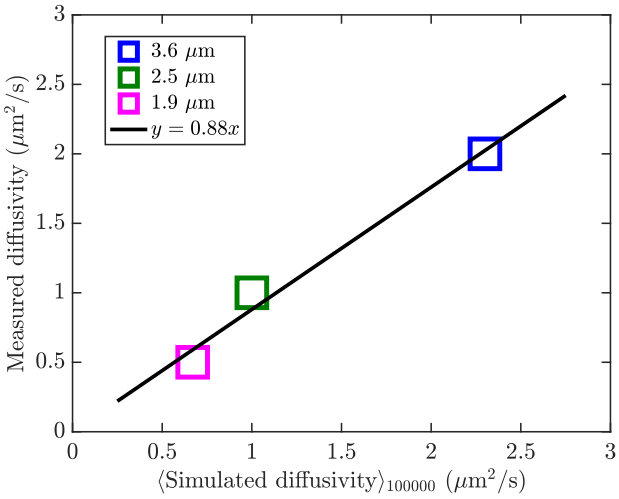


Figure 2.

## Bibliography

[1] Yiwei Li, Osman Kahraman, and Christoph A. Haselwandter. Distribution of randomly diffusing particles in inhomogeneous media. *Physical Review E*, 96(3), Sep 2017.

[2] Johan Elf, Andreas Doncic, and Mans Ehrenberg. Mesoscopic reaction-diffusion in intracellular signaling. In Sergey M. Bezrukov, Hans Frauenfelder, and Frank Moss, editors, *Fluctuations and Noise in Biological, Biophysical, and Biomedical Systems*. SPIE, May 2003.