A Computational Model of *Escherichia coli's* Chemotactic Motion in Chemical Concentration Gradients

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Abstract

Amongst the most critical and common bacteria for human and animal health are *Escherichia coli*, commonly referred to as *E.coli*. Behavioral information of this bacterium is of immense clinical and environmental importance because this bacterium is a causative agent for diseases like enteritis, urinary tract infections, septicemia, neonatal meningitis, and diarrheal diseases in humans and animals. Furthermore, *E.coli* shows chemotaxis, moving towards or away from chemical stimuli [1]. Therefore, it is an excellent model organism for the study of microbial navigation. Here, we showed a computational approach to simulate the chemotactic navigation of *E.coli* along chemical gradients using a biased random walk simulation. By changing between random tumbles and directed runs, the simulation mimics how bacteria as a group sense and migrate toward higher chemical concentration gradients. The model is coded in Python with a modular and object-oriented design, enabling changing parameters such as population size and time steps. Visualization of bacterial paths, spatial distributions, and concentration fields captures emergent behavior, which verifies our analysis of the impacts of different simulation parameters on collective motion. While the model simplifies real biological systems, it makes instructive contributions to microbial self-organization and may find practical applications in microbiology, synthetic biology, and environmental modeling.

Keywords: *E.coli* **(***Escherichia coli)*, chemotaxis, biased random walk, chemical gradients, microbial motion, Monte Carlo simulation, gradient sensing, Python, object-oriented modeling, trajectory analysis
Abbreviations: *E.coli*

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1. Introduction:

The scientific inquiry into how microorganisms perceive and react to their surroundings is central to biology and computational science. One of the ubiquitous microorganisms, *E.coli*, remains one of the most common causes of various common bacterial infections in humans and animals. For example, *E.coli*, a causative agent for enteritis, urinary tract infection, septicemia, and other clinical infections such as neonatal meningitis in humans, is also a significant cause of diarrhea in pets and farm animals [2]. Additionally, It is known for displaying chemotaxis, the ability to move toward or away from chemical stimuli.

Why *E.coli* chemotaxis simulation? Many aspects of *E.coli* behavior have been uncovered by experimental methods (e.g. microfluidics, capillary, and tethered-cell assays). However, these methods have limitations, such as the inability to maintain stable, well-characterized gradients over time and space, isolate single variables without confounding variables, track single-cell paths and population statistics at the same time, probe rare regimes (very shallow/steep gradients), and replicate identical conditions despite biological variability and noise. These studies are complemented by a computational model that allows mapping the relationship between microscopic rules and macroscopic patterns through controlled, repeatable in silico perturbations and counterfactuals. For example, systematically sweeping gradient shapes and steepness, run/tumble kinetics, and initial spatial distributions.

As cells integrate local concentration information over time, alternating random "tumbles" and directed "runs" produce a net drift up attractant gradients, which is the basis for chemotactic motion in *E.coli* [3,4]. This work simulates the run-tumble process in a two-dimensional concentration field and asks how essential parameters, such as population size, step sizes, and gradient width/steepness, shape collective outcomes like radial distributions, drift velocity, chemotactic index, and spatial aggregation.

Our Python implementation uses a modular, object-oriented design, allowing direct control of concentration profiles, time step, and population size. We visualize trajectories, spatial distributions, and concentration fields to interpret system behavior over time and to generate testable predictions that can guide targeted experiments.

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2. Methods:

Simulation Overview: We simulated the chemotactic movement of *E.coli* in a two-dimensional concentration field using a tumble–run biased random walk. Each bacterium was treated as a point particle moving during runs, with stochastic changes in direction during tumbles. The bias in movement was introduced through gradient sensing, allowing bacteria to adjust their tumble–run behavior toward favorable regions (high concentration regions) in the concentration field.

Concentration Field: The concentration field was represented as a radially symmetric Gaussian profile, the analytical solution to Fick's second law of diffusion (eq.1) for a point source:

$$\varphi(r,t) = \frac{1}{4\pi Dt} \exp\left(-\frac{r^2}{4Dt}\right)$$

(eq.1. Fick's second law of diffusion)

where φ is the concentration function, r is the radial distance from the source center, t is time, and D is the diffusion coefficient. For fixed t values, this yields a Gaussian distribution in space with a peak at the source center and an exponential decrease in concentration with distance [5].

Gradient Descent: Gradient descent is a general optimization technique used to find the minimum of a function by iteratively moving in the direction of the negative gradient. The gradient provides the slope of the function at a given point, and by taking steps opposite to this slope, the method steadily approaches a local or global minimum [6]. Gradient descent is usually used to find the smallest value, but in this simulation, we changed it so that it looks for the direction where the chemical concentration increases instead of decreases.

Biased Random Walk: The movement of the bacterium was modeled as two repeating phases: tumble and run. In the tumble phase, the bacterium chooses a new direction randomly, representing exploratory movement. In the run phase, the bacterium moves in the direction it chose during the previous tumble at a faster speed. The chosen direction is based on the outcome of the last tumble and the sensed concentration changes. A bias is added by sensing changes in concentration over time: if the concentration is higher than before, the bacterium is more likely to keep running; if it is lower, the cell is more likely to tumble and choose a new direction. This approach demonstrates how bacteria use both random motion and gradient sensing to move toward favorable conditions [7].

3. Implementation:

The package implements a comprehensive *E.coli* bacterial chemotaxis simulation using a multi-class architecture that models individual bacterial behavior and population-level dynamics. The 'ConcentrationProfile' class provides static methods for generating different radial concentration gradients (standard, steep, and shallow), while the 'EcoliBacterium' class models individual bacterial behavior using a run-and-tumble mechanism where bacteria alternate between random movement (tumbling) and directed movement (running) based on concentration gradients calculated from their movement history.

The main 'ChemotaxisSimulation' class orchestrates the entire simulation by managing populations of bacteria within a 2D grid, tracking their positions over time, and providing comprehensive visualization capabilities, including concentration profiles, bacterial trajectories, radial distributions, and time evolution plots. The package includes analysis functions that compare different population sizes (N = 10, 100, 1000 bacteria) across various gradient types, demonstrating how bacterial populations collectively migrate toward higher concentrations through individual chemotactic responses, with extensive matplotlib-based visualization tools for examining both individual trajectories and emergent population-level patterns via radial distribution histograms [8].

The core of the simulation relies on the tumble and run logic for exercising *E.coli* movement and direction. The "state" object of the bacteria is updated between two instances: "tumble" and "run", which dictate which movement function, tumble_step or run_step, is called. With a predefined tumble speed, the function tumble_step randomly selects a tumble angle for the *E.coli* to move. Similarly, the run_step function moves the bacteria at a predefined run speed; however, the angle is controlled by the run_direction object, as defined in the update_state function.

The update_state function utilizes the "state" object and a calculated gradient to determine whether the bacteria need to continue tumbling for another time step (four total), transition to the "run" state (as four tumble steps have been completed), or transition back to the "tumble" state (if no increasing concentration gradient is found). If the *E.coli* is in its run state and a concentration gradient increase has been found, the run direction is determined via the two most recent instances of the history_x and history_y objects, which track the *E.coli*'s most recent x and y positions.

The movement of the *E.coli* is performed in the step function, where the current concentration value and historical concentration values along the bacteria's tumble are called to calculate the gradient. The gradient is used in the update_state function to determine if a bacterium can transition to the "run" state. Finally, the bacteria are moved according to their current state via the tumble_step and run_step functions. This entire process (four tumble steps and one run step) is repeated until the *E.coli* no longer finds optimal moves during the tumble step that increase its concentration gradient, i.e., it has found the highest concentration location, representing the nutrient's source.

4. Evaluation:

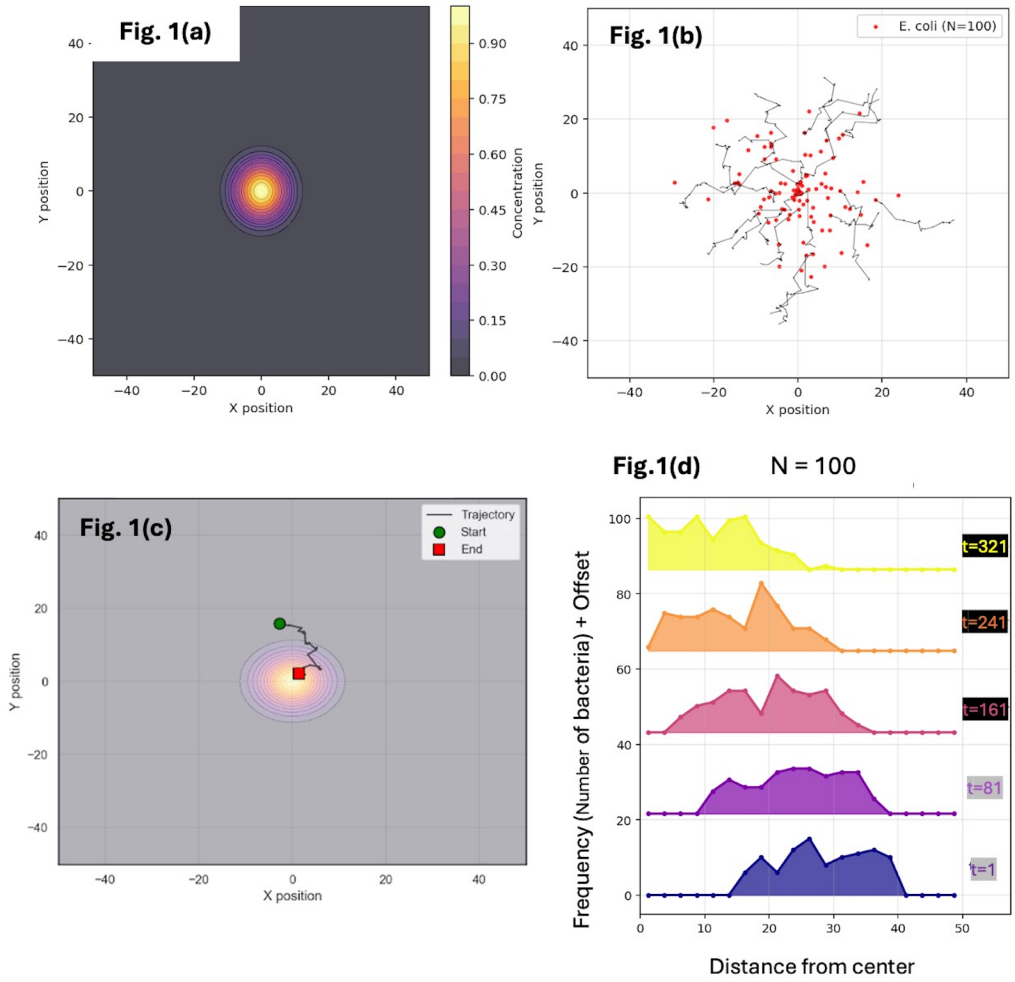

Fig 1. Example plots with a standard concentration gradient for N=100 of *E.coli*: (a) concentration field, (b) trajectories of all bacteria showing movement towards the maximum concentration (center), (c) trajectory of a single bacterium with concentration profile, and (d) distributions of *E.coli* at different time points (t=1, 81, 161, 241, 321).

Fig 1(a) shows the radial Gaussian concentration field, with the maximum at the center and an exponential decay outward. In this environment, a population of 100 bacteria (N = 100) moves from random starting positions toward a high-concentration center, as seen in Fig 1(b). The path of a single bacterium, shown in Fig 1(c), illustrates its tumble-run motion and gradual approach to the center. Fig 1(d) further depicts the temporal evolution of the movement toward the center. The resulting Gaussian distributions of *E.coli* broaden as time progresses, reflecting gradual spread of the population during migration. The combination of these plots demonstrates that the model successfully reproduces the biased random walk of chemotaxis, where random movements of individual bacteria result in an overall movement toward the concentration source.

5. Discussion:

The simulation reproduced key features of E. coli chemotaxis. The bacteria moved directionally toward the point of maximum concentration, gathered near this location, and dispersed outward over time, following the pattern of a biased random walk. These patterns align with behaviors reported in experimental studies of motile microbes, indicating that the model effectively captured both directed movement and the natural variability in bacterial trajectories.

Effect of Model Parameters: Changes in model parameters altered the strength and clarity of these patterns. Steeper gradients increased drift velocity and central clustering, while shallower gradients reduced drift and produced a broader, more dispersed population. Smaller populations tended to move in more random paths, whereas larger populations showed more consistent migration toward the center. Higher running speeds or larger step sizes improved exploration but risked overshooting narrow peaks unless run lengths were shorter or bias was stronger. Smaller step sizes allowed bacteria to detect curvature in the gradient more effectively and maintain stability near high-concentration zones.

Limitations: This model provides a simplified representation of chemotaxis, which inevitably omits several important biological and physical processes. At the biological level, it does not explicitly account for receptor methylation, CheY signaling, adaptive feedback mechanisms, or phenotypic variability among cells. Physically, the simulated environment is restricted to a static two-dimensional concentration field, without steric or hydrodynamic interactions, collision handling, nutrient depletion, swarming, or trail formation. Numerically, the parameters are not expressed in physical units, and the reliance on fixed time steps can introduce discretization artifacts. As a result, the outcomes are qualitative rather than quantitatively predictive [9].

Potential Improvements: Addressing these limitations would make the model more realistic and useful. For example, adding a minimal adaptation module or an empirically derived temporal kernel could give the bacteria logarithmic sensing and more realistic reaction times, producing responses closer to those seen in experiments. Changing the fixed concentration map to a reaction–diffusion setup could create effects like band formation, moving fronts, and nutrient shadowing. The model's accuracy could also be improved by matching parameters to real-world units and using continuous-time (e.g., Gillespie) or adaptive time-step simulations to reduce artifacts and better track changes over different time scales. These upgrades would make the simulation match lab results more closely and allow for clearer, quantitative comparisons with error estimates and sensitivity checks.

6. References

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