

# Modelling Population Growth

Andrew Martin and Eric Stubley

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## 1 Background, Purpose, and Hypothesis

This project came about as a fusion between cellular automata, such as Conway's Game of Life, and biological theory. This program combines the framework of a cellular automaton with complex mathematical application of biological theory.

The purpose of this project was to create a computer program in C++ capable of modelling the growth of a bacterial population by simulating the behaviour of individual cells and allowing the interactions between them and their environment to cause a natural emergence of the expected population behaviour. It was hoped that this model would be accurate enough to be applicable as both an academic and industrial tool.

For this computer program to be considered successful, it should be able to accurately model the exponential growth, stationary, and death phases of bacterial populations, while adhering to the law of conservation of mass-energy.

## 2 Program Design and Procedure

### 2.1 Framework

The simulation occurs within a 100 by 100 grid. Each node on this grid contains mass or energy values for a cell, nutrients, waste, and temperature. By taking small advances in time ("timesteps") and recalculating the values in the grid using the equations described below

at every timestep, the passage of time is simulated. Note that all quantities are in arbitrary units.

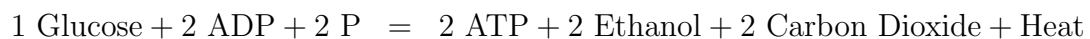
When a cell reaches a specified mass limit, it undergoes binary fission. If there is an adjacent node which does not contain a cell the dividing cell will split its mass in two. One half will stay in the original node, and the other half will form a new cell in the adjacent node. If there is no adjacent node the cell will continue growing until it reaches an upper mass limit.

Cells die when they reach either an upper or lower mass limit. When a cell dies, its mass is removed from the simulation and added to a counter which stores all dead cell mass.

## 2.2 Equations

We chose to model the growth of a cell with an equation representing the rate of change of the cell's mass, as simulating the entire inner workings of a cell would be too complex to easily simulate. This equation is based on the current mass of the cell and the local nutrient, waste, and temperature conditions. Each of these other substances also has an equation governing its rate of change. Two concepts were used in creating these equations: the process of anaerobic respiration, and the law of conservation of mass. The cellular equation was the first to be developed and the other three equations were formulated around it.

While there are several variations on the process of anaerobic respiration, a common one is given by the following formula<sup>1</sup>:



By determining the energy in each molecule using their bond enthalpies<sup>2</sup>, the energy lost

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<sup>1</sup>Andrew Allot, *Biology for the IB Diploma* (Oxford: Oxford University Press, 2007), 20, 73.

<sup>2</sup>Geoffrey Nauss, *Chemistry for the IB Diploma* (Oxford: Oxford University Press, 2007), 30.

to heat can be solved for. The efficiency of this form of anaerobic respiration can then be calculated. By taking each of the products as a percentage of the reactants (nutrients) we obtain: 23% ATP (cell mass), 70% ethanol and carbon dioxide (waste mass), 7% heat. These constants provide the basis of the equations.

The equations contain mechanisms for the uptake of nutrients, increased rate of reaction with increased temperature, denaturation, starvation, and degradation.

## 2.3 Solver

The numerical integration engine is an important aspect of this model. At the beginning of the simulation only the mass values are known. By numerically integrating the above equations, the actual masses a short time later can be found. This process is then repeated using the new masses until there are no more cells. This program uses the Runge-Kutta method<sup>3</sup> to solve the differential equations. This method approximates numerical solutions to differential equations by taking a weighted average of four different slopes in a single timestep.

## 2.4 Testing Methods

In order to prove the preliminary validity of this model, it needed to accurately model two concepts: the phases of a bacterial population and conservation of mass.

The growth of a bacterial population can be expressed in three phases: exponential growth, stationary, and death<sup>4</sup>. The latter two can be verified simply by visual inspection of a biomass vs. time graph, whereas the first requires further study. If the natural logarithm is taken of exponential data, a straight line should be produced. It is expected that the initial growth will be almost completely exponential, with the exponentiality dwindling over time due to the buildup of waste mass and loss of nutrients. In order to test the exponentiality

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<sup>3</sup>John H. Mathews and Kurtis D. Fink, *Numerical Methods Using Matlab* (Upper Saddle River, Prentice Hall, 1999), 458 - 461.

<sup>4</sup>Allot, *Biology for the IB Diploma*, 36.

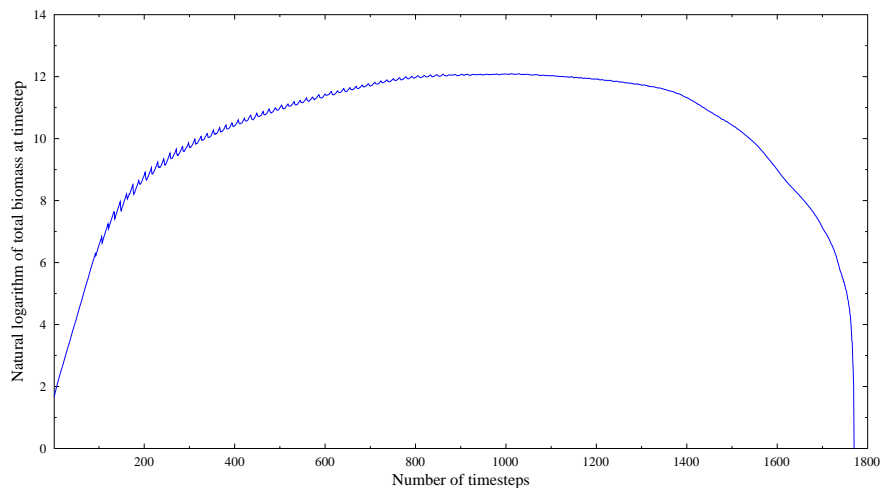
of the model, a series of linear regressions were performed on the natural logarithm of the data at intervals of 50 timesteps up to 500 timesteps.

Compared to exponential growth, conservation of mass is relatively easy to test. By simply adding up all the masses at each timestep, the conservation of mass can be verified. If the total mass remains constant throughout the simulation, mass is being conserved.

### 3 Observations and Conclusions

Figure 1 below shows an example of the natural logarithm of the total cellular mass in a test run of the model.

Figure 1: Logarithm of Total Biomass vs. Time

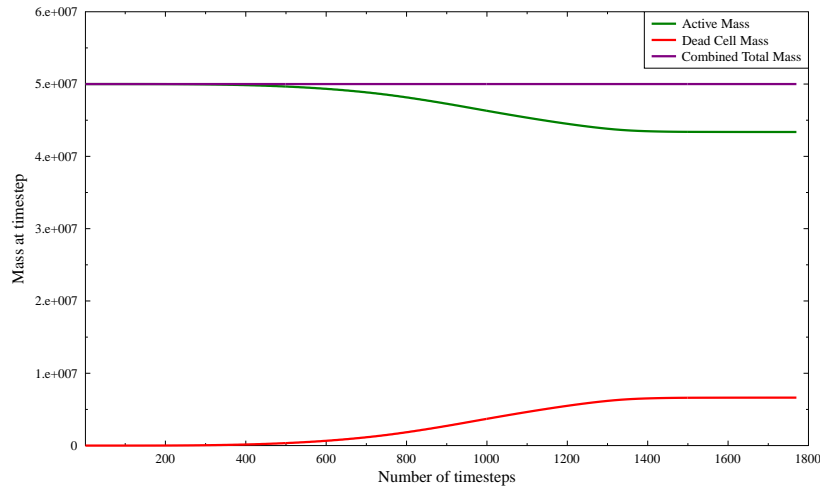


The stationary and death phases can be clearly seen on the graph, with the stationary phase starting at 800 timesteps and going to 1400 timesteps, and the death phase from 1400 timesteps until the end.

The results of the regression analyses on the growth phase of the population support the hypothesis of diminishing exponential growth. After 150 timesteps, the linear fit was 0.9852, meaning that the growth was still almost perfectly exponential. After 500 timesteps, the linear fit was 0.8414, meaning that the growth was tending losing exponentiality.

Figure 2 below displays the total active mass, the dead cell mass, and the combined total mass at each timestep in the simulation.

Figure 2: Active Mass, Dead Cell Mass, and Combined Total Mass vs. Time



Observation of this graph would suggest that conservation of mass was achieved, as the combined total mass seems to remain constant. A slight variation in the total combined mass was found, but this can be attributed to numerical errors inherent in the solver. As the mass is still conserved to eight or more decimal places, this variation can be ignored.

Thus both elements of the hypothesis were proved. The model exhibited a diminishing exponential growth phase, a stationary phase, and a death phase. The model was shown to conserve mass accurately to eight decimal places.

Further analyses are being conducted in preparation for the Canada-Wide Science Fair.

## 4 Acknowledgements

We would like to thank Mrs. Shaw and Mr. Fryer-Davis of Cameron Heights.

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