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Digital Simulation of Bioluminescent Bacteria Cells *Tweeting* via Quorum-Sensing Molecules

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In this paper, we propose a computational multiagent model of a bacterial light-producing communication system, termed quorum sensing (QS). Specifically, we propose a bottom-up agent-based approach combined with Ordinary Differential Equations, which abstract the intracellular dynamics, such as a proposed bioluminescence model. Results show that bacteria cells have a metabolism allowing them to grow, reproduce, interact, and cooperate at the population level to exhibit near-optimal light producing behaviors. The ultimate goal is to develop a self-regulated network in which the rules governing the formation of the network are linked to the internal dynamics of its units without any centralized control. Such a bacterial-inspired networks, can address issues such as mobility, and energy that are key factors for the development of new self-organized network such as mobile Ad-hoc networks.

Cellular Dynamics Model

To simulate cell-to-cell communication, we use a generic *LuxI/LuxR* QS. All *LuxI/R* systems are mediated by autoinducers, such as acylated homoserine lactone (*AHL*). Explicitly, the *AHL* and the receptor *LuxR* form a dimerized complex (*C*) that regulates the expression of both *LuxI* and *LuxR* genes. The QS model is based on the ODE-models proposed in (Melke et al., 2010). We model bioluminescence or light production as a function of the dimerized complex (*C*) as follows:

$$\frac{d[L]}{dt} = \frac{L_{max}[C]}{K_L + [C]}$$

where *L* is the light production rate, L_{max} is the maximum light production rate and K_L is the concentration of *C* at which *L* is at half-maximum. Bioluminescence is expressed as the accumulation of the green fluorescent protein *gfp*. The bacterial metabolism (ATP cycle) is implemented as follows:

$$\Delta ATP = (ATP_0 + E \cdot ATP_S + ATP_G + ATP_D + ATP_L + ATP_M)(\Delta t)$$

Where:

- ATP_0 is the basal energy.
- ATP_S represents the energy produced from substrates and is calculated as follows:

$$\frac{d[ATP_S]}{dt} = Y_{ATP/S} \cdot \frac{d[S]}{dt}$$

Where $Y_{ATP/S}$ is the energetic substrate yield *i.e.* the amount of *ATP* produced by per a unit of substrate (*S*).

- E is the substrate metabolism efficiency.
- ATP_G represents consumption of *ATP* due to the cell growth and is calculated as follows:

$$\frac{d[ATP_G]}{dt} = -\frac{1}{Y_{X/ATP}} \cdot \frac{d[X]}{dt}$$

Where $Y_{X/ATP}$ is the energetic growth yield coefficient.

- ATP_D is the division energy.
- ATP_L is the light energy. The consumption of energy due to light production is given by:

$$\frac{d[ATP_L]}{dt} = -\frac{1}{Y_{L/ATP}} \cdot \frac{d[L]}{dt}$$

Where $Y_{L/ATP}$ is the energetic light yield coefficient.

- ATP_M is the maintenance energy.

Results

The experiments were conducted using "gro" (Jang et al., 2012). The number of bioluminescent cells represents 73% of the population. This corresponds to the empirical rates found in real populations of bacteria (Anetzberger, Pirsch, & Jung, 2009). At the population level, figure 1.d shows a self organized behavior of the microbial population. Figure 2a shows the amount of autoinducer over time. In our simulations the accumulation of *AHL* exceeds the rate achieved in (Melke et al., 2010) (0.6 against 0.1). This shows that the cells in our model provide self-sustainable behaviors that allow them to exploit metabolism (figure 2b) to grow, survive and produce more *AHL* molecules, which in turn triggers communication.

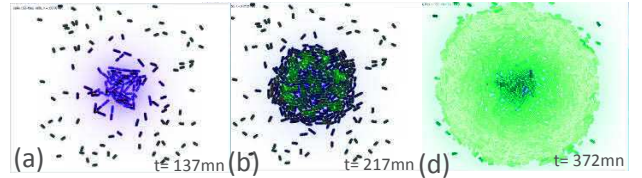


Figure 1: Evolution of bioluminescence. Substrate is shown in purple, *AHL* in blue, black cells are non-fluorescent. (a) cells grow and divide. In (b) the quorum is being reached, fluorescent cells begin to appear. (c): Bioluminescent cells organize themselves around the colony to be located at the edges of it.

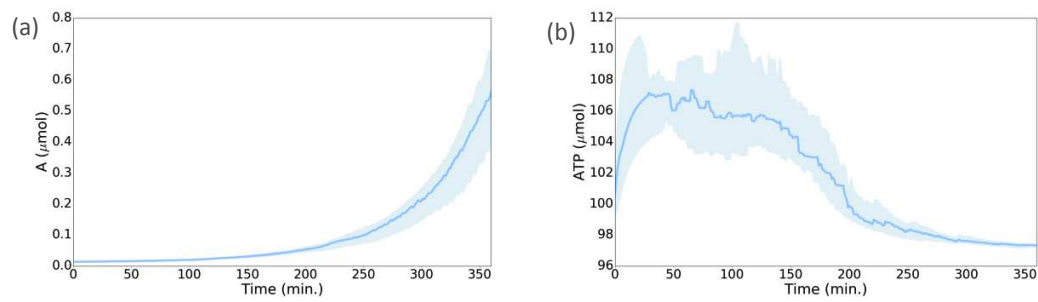


Figure 2: Evolution of the average amount of autoinducer (a) and ATP (b) inside cells over time : median and interquartile range of 20 independent runs of the simulation)

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