Bacterial Self-Assembly and Computation

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1 Introduduction

Researchers in the field of complex systems are often concerned with the study of collections of motile elements, such as fish, birds, insects and bacteria. These organisms may exhibit characteristic patterns of self-organized collective behaviour such as shoaling, flocking, swarming and aggregation. We are particularly interested in bacteria, as the ability to reliably predict and control the dynamical behaviour of microbial colonies has profound implications, both on the study of the biological system *per se* and also on the potential for their use in a diverse range of computational and engineering applications.

When millions of bacteria act collectively as a group (as is the case in any bacterial colony), a large variety of different patterns arise as a result of how the individual cells respond to the others in their neighbourhood and to the conditions in their environments (which will be different for different individual bacteria, even if they are relatively close to each other) [3, 6, 9, 10]. The physical appearance of these patterns lies (largely) due to cells clumping together in different ways at different positions. These patterns are the emergent result of local interactions and environmental conditions, and can be usefully viewed as being *programmed* by both the particular way the bacteria in question interact, and by the particular way these bacteria respond to environmental signals. Also, these patterns are widely regarded as functional; for example, in stress conditions (such as a toxic chemical in the environment), the pattern formed will be ideal for protecting a maximal number of individuals (e.g. by minimising the number of cells without immediate neighbours) while promoting the colony's "search" for a less harmful environment (by, e.g., extending "arms" of cells which explore the environment). This spontaneous development of functional patterns, purely as a result of environmental conditions and local interactions between individuals, is a form of computation which is extremely common and useful in nature, but which is currently very poorly understood and highly unexplored and unexploited in computer science.

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It may be possible to harness the sophisticated environment-driven pattern generation capabilities of bacteria for the purposes of providing concrete applications in which environmental input (to, for example, an aircraft's "smart-skin" or to nodes in a sensor network) leads to adaptive and functional emergent spatio-temporal organisation (such as, respectively, a surface pattern which stabilises against turbulence, or a connection pattern which optimises power). Such work would shed further light on the underlying biological mechanisms as well as investigating the potential for the "bottom up" engineering of micro-structures assembled from huge numbers of individual elements. These techniques would form a family of novel computational architectures with potential applications ranging from purely *in silico,* such as distributed optimisation, to direct applications in domains as varied as bio-nanotechnology, tissue engineering, bio-film and bio-filter engineering, bio-sensing and drug development.

2 Objectives

Previous work has focussed solely on the simulation of bacterial colonies, and coarse levels of similarity between actual and simulated pattern generation have already been achieved by previous researchers. Our goals are much more ambitious. We wish not only to be able to *predict* the final pattern, given the initial conditions, but to *control* the form of a final pattern by discovering the initial conditions that give rise to it. The level of control required for microtechnological applications can be gained only by a much better understanding of the effects of the factors contributing to pattern determination. These factors include environmental conditions (both physical and chemical), the rules and processes underlying bacterial interaction and the initial "program" manifest by the starting conditions. The fundamental questions that we seek to address are: **(1)** Is it possible to simulate the growth and movement of bacterial populations such that the complex patterns they generate *in vitro* can be *specified in advance* in computationally feasible times? **(2)** If achieved, how may the associated abstract computational architectures, as well as the directed self-assembly of bacteria *in vitro* be applied in various domains? **(3)** What level of complexity at the individual (bacterial) level is required to generate the observed complexity at the collective level? Additionally, how much of the observed complexity at the collective level is a reflection of environmental rather than individual complexity?

3 Impact

The first question is important if the great commercial potential for this field can be realised. An approach whereby repeated adjustments of growth parameters is driven by a series of laboratory trials would be very costly in time and is likely to be infeasible for this reason.

The second question is motivated by the search for practical applications of the technology generated in response to the first question. We would seek not only to study the biological system in question but to apply the computational system inferred from these studies to real-life problems. Potentially high-impact applications exist in a broad range of domains, and we list only a few of them here:

Optimisation. Models of bacterial movement (chemotaxis) have already been successfully applied to the training of artificial neural networks [2, 4], multimodal function optimisation [8], the design of aerofoils [8], the control of robots for environmental monitoring [5], and the modelling of pedestrian evacuation processes [7]. It is clear that this phenomenon has inspired a powerful optimisation strategy that is competitive with existing nature-inspired methods. However, what is lacking from the majority of these chemotactic models is a consideration of the communication strategies employed by bacteria in order to coordinate pattern formation. By including such mechanisms, we may further enrich the possibilities for *distributed* bacterial optimisation.

Pattern classification. The abstract computational model of bacterial self-assembly will give us a rich framework for the construction of non-linear maps between input values and final patterns. There are many possible applications for such a novel computational method. For example, there may exist categories of data that are difficult to distinguish using traditional techniques such as artificial neural networks. We will investigate the application of the model to see if different input categories give rise to very different types of final pattern (for example, one set of data may result in patterns characterised by patches, whilst another may give rise to patterns of circles). In particular, we could apply this in cases where traditional methods fail badly.

Micro-scale construction. The physical patterns of bacteria will find many applications in the biological and engineering domains. Self-assembly will clearly play a strong role in determining the future direction of (bio)nanotechnology [11]. This work will have implications for any application that requires spatially registered cellular engineering. These may include the development of novel biomaterials, the design of biosensors, and tissue engineering. We also anticipate its eventual application to the construction of structured microbial consortia [1], whose functioning in applications such as wastewater treatment and bioremediation is dependent on their precise structural ordering.

Questions 2 and 3 are closely related in that the abstraction of the computational architecture is closely informed by complexity issues. Answering question 3 will also help to address the fundamental issue of biological complexity, and may also give greater insight into the biological basis of bacterial self-organisation.

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