The Evolution of Active Droplets in Chemorobotic Platforms

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Abstract

There is great interest in oil-in-water droplets as simple systems that display astonishingly complex behaviours. Recently, we reported a chemorobotic platform capable of autonomously exploring and evolving the behaviours these droplets can exhibit. The platform enabled us to undertake a large number of reproducible experiments, allowing us to probe the non-linear relationship between droplet composition and behaviour. Herein we introduce this work, and also report on the recent developments we have made to this system. These include new platforms to simultaneously evolve the droplets' physical and chemical environments and the inclusion of self-replicating molecules in the droplets.

Introduction

The compartmentalisation of prebiotic chemicals is considered an essential step in abiogenesis – allowing a system to exist in a non-equilibrium state and preventing its dilution within the environment [1]. There is great interest in oil-in-water droplets both as protocell models and as simple systems that display astonishingly complex behaviours [2, 3], whilst they also inherently satisfy the need for a protocell to be compartmentalised. Interestingly, such systems are particularly suited to robotically assisted evolution because experiments can be performed on automated platforms while simple inputs lead to complex behaviours – making the search problem challenging. Recently, we reported the development and use of a chemorobotic platform capable of evolving these droplets to optimize given characteristics - such as movement or division [4]. A genetic algorithm was then used to optimize droplet behaviour by observing the effects of varying the composition of the oil droplets. This was the first example of robotically assisted evolution of a physicochemical system, expanding from the fields of engineering and robotics and inspired from the realm of biology. Herein, we briefly present results from robotically assisted experiments as well as more recent work undertaken in several new directions:

- How does the physical environment affect protocell behaviour?
- How does the chemical environment affect protocell behaviour?
- Can we expand the behaviours of the droplets – for example by morphological differentiation, replication or agency?

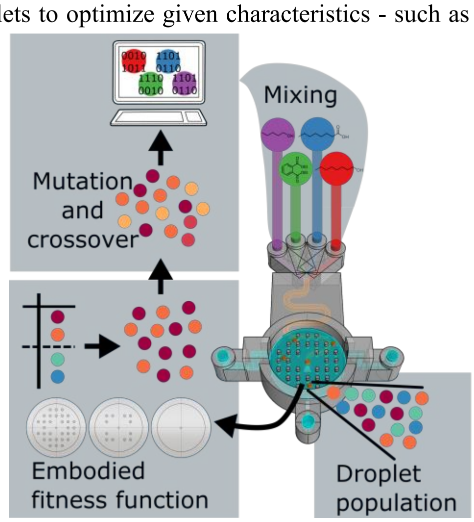

Figure 1– A 3D printed chemorobotic platform designed for the study of the effect of the physical environment on droplets.

Evolution of Oil Droplets in a Chemorobotic Platform

Our oil droplets were composed of four oils, which were mixed in various compositions (their genotype) and their behaviour (phenotype) was then observed. The platform was based upon an open-source 3D printer modified for liquid handling, droplet placement and video capture (Figure 1). Using computer vision each experiment was analysed and droplet movement, division and vibration were quantified, thus allowing evolution via mutation and crossover of the compositions. Not only were these behaviours optimized (Figure 2), but fitness landscapes – models of the composition-behaviour space – were built, whilst various type of droplets were also shown to be able to coexist. We believe this system – incorporating the hardware, software and physical components, allows the exploration of the minimal requirements for evolution and complex behaviours.

Co-Evolution of Oil Droplets with their Physical Environment

To probe the dynamics of the interaction between the droplets and their physical environment we developed a new platform (Figure 1). This simplified 3D printed platform is cheaper, more reliable and more easily customized. Obstacles can be printed inside the dish, thus customising the physical environment in which the droplets evolve, whilst these obstacles can be changed in between evolutionary generations. Indeed, the environment plays a defining role in evolution via natural selection – different environments lead

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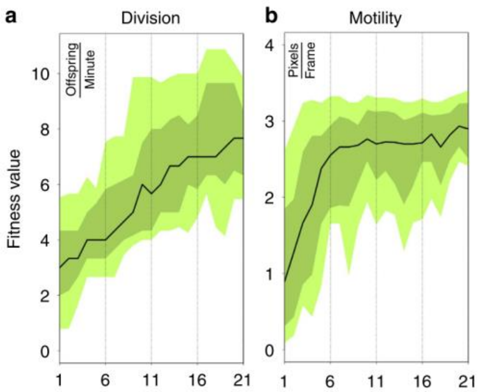

Figure 2– The evolution of droplet division (left) and movement (right) with genetic algorithm generation.

to different evolutionary niches and can lead to both extinction and speciation. This is also what we observed for our droplets – whilst a certain population may be highly evolved to a given environment, if this environment changes the individuals are less adapted to the new environment, and a drop in fitness is observed. Subsequently, the fitness rises again as the droplets adapt to their new environment – a process which can be repeated. Interestingly, genotypes resulting from evolution in a number of environments may not be suited to all those environments – in adapting to new situations, they are no longer as well suited to those they have previously observed.

Co-Evolution of Oil Droplets with their Chemical Environment

As well as the physical environment of the droplets - represented by physical pillars and caves - , the chemical environment may also be modified. Previously, all of our droplets have existed in the same chemical environment – a high pH tetradecyltrimethylammonium bromide (TTAB) containing aqueous phase. We have subsequently developed a chemorobotic platform capable of varying this environment to contain various ratios of up to six aqueous phase constituents. Using the platform we can screen for interesting droplet behaviours and utilise a genetic algorithm to optimise both the oil and aqueous phases simultaneously. Doing this, we have identified new droplet behaviours, such as swarming, where a large number of droplets move together in concert. We have also shown that the co-evolution of an entity with its environment allows the discovery of behavioural niches unreachable by independent evolution. Indeed, despite a significantly larger compositional space – some 9.2×10^{15} possible recipes, rapid optimization above that achieved for sequential oil then aqueous phase optimization was observed.

Expanding the Chemistry Set – Molecular Replicators and Self-Sustaining Droplets

Autocatalysis and molecular replication are thought to have been crucial for the emergence of the first evolvable life-like chemical systems [5]. In an attempt to further push our droplets to become more interesting and life-like, we are investigating new chemistries to apply to the droplets. For example, artificial self-replicating molecules may enable active droplets to grow and divide in cycles, evolving over time without requiring the input of a robotic assistant. Specifically, we have developed an amphiphilic template self-replicator, formed from a hydrophilic and a hydrophobic precursor, which are connected *via* a template self-replication process. As template self-replication leads to more surfactant production in a chloroform oil phase, the surface tension is reduced leading to division of these chloroform droplets. We believe that further developments combining molecular replication with evolvable droplets could truly lead them to survive, grow, reproduce and thrive.

Conclusion

In summary, we believe that oil-in-water droplets are uniquely suited as protocell models, due to their ability to exhibit widely varied behaviours based on simple inputs. They contain a phase boundary, considered a fundamental characteristic of droplets, whilst the incorporation of functionalities including metabolism and heredity are feasible. Over and above work utilising oil-in-water droplets, we believe that cheap, robust and customisable automated platforms, in conjunction with advanced computer science methods, represent a hugely underdeveloped opportunity for chemists to apply to a wide range of research areas including complex systems, chemical synthesis and materials chemistry. Of particular interest are recent developments on novelty seeking and curiosity driven algorithms that opens the way to the genuine autonomous exploration of what can be done with a new system rather than a more directed optimization of a specific property [6, 7]. Evolution *in materio*, using artificial intelligence in combination with a liquid handling robot for autonomous exploration of chemical spaces is rapidly proving its utility for tackling wider chemical problems.

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