Thesis summary:
Hydrodynamics of micro-swimmers in complex fluids and environments

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This thesis covers a myriad of interconnected topics concerning biological micro-organisms and synthetic micro-robots. Via intricate propulsion strategies these micro-swimmers can move through strongly viscosity-dominated liquids to achieve their goals, be it to invade new territories or to deliver drugs to infected regions. Therefore, the understanding of bacterial motility immediately impacts medicine and the food industry, and provides a direct stepping stone for microbial ecology, global health and biomedical solutions.

On a more fundamental level, suspensions of self-propelled particles can form 'active fluids'. Contrary to conventional fluids that dissipate energy through a cascade from large to smaller vortices, active fluids inject energy at the smallest length scales to construct macroscopic features. Like often in nature, many puzzling phenomena emerge, which could one day be used in new 'smart materials' capable of self-assembly, self-healing or abiotic self-reproduction.

With the intend to comprehend or even regulate these processes, we developed a hydrodynamic framework to compute the effects of swimmer-generated flows in complex environments. These currents can affect the surroundings, or the motion of the swimmer itself via reflections in surfaces. Moreover, they can act as mechanical signals that enable self-propelled particles to sense one another's presence and establish collective functionality.

Using this framework, we studied the accumulation of microbes on surfaces in relation to biofilm formation, and computed the strength required for external flows to detach and wash them away. Moreover, we evaluated the ability to swim upstream in complex biological fluids and uncovered that viscoelasticity could provide a natural sorting mechanism for sperm cells. Main results also included a model for the transport of particles by micro-robots, and how collisions with channel walls may be avoided. More recent work is aimed to estimate the attachment probability of viruses and physical limitations to motile cell-cell communication.

To verify results, we compare our theories to extensive simulations that also mimic biological fluctuations. This allows to determine previously unknown model parameters, and hence make suggestions that might improve micro-organism treatment and micro-robot design. This work is currently ongoing in the department of bioengineering at Stanford University. Meanwhile, I would like to express my warmest thanks to you all for sharing this curiosity and enthusiasm.

Ultrafast quantum effects and vibrational dynamics in organic and biological systems, a lay person's summary

Sarah Morgan, Cambridge

Over the last 100 years, the advent of quantum mechanics has revolutionised our understanding of how nature works. Our ability to understand and manipulate matter at the microscopic scale has given us cheap, powerful computers and enabled us to collect and store incredible quantities of information. Biology has already benefitted immensely from our ability to interrogate biological systems with ever greater resolution and it is tempting to see the role of physics as being to provide tools to biology. Yet the complex intricacies of biological organisms make our man-made systems look clunky. Nature has had billions of years to evolve highly efficient, robust systems, which operate far from equilibrium with astonishing stability. Could biology have something new to teach us about physics?

Recently, intriguing observations of quantum mechanical effects in biological systems have emerged which suggest that could indeed be the case. Examples include long-lived quantum signals in photosynthetic light harvesting complexes as well as proposals that quantum compasses might enable migratory birds to detect the Earth's magnetic field. These glimpses of the quantum world in biology are surprising due to the wet, warm and noisy environments that these systems operate in, which are normally expected to destroy quantum signals. Further work is needed to explain how these quantum signatures are maintained in living systems and whether they play a functional role.

One of the main experimental approaches to observing quantum effects is a non-linear laser experiment known as '2D electronic spectroscopy' (2DES), which was developed around 15 years ago. To better understand the observations, it is essential to be able to analyse and model these complex laser spectroscopy experiments. However, they contain many overlapping signals, which makes the results difficult to unravel. Hence the first part of my dissertation focuses on analysing 2DES results from an organic semiconductor known as pentacene. Studying organic materials is an ideal first step towards understanding biological light harvesting systems because they are simpler but have similar photophysics. They also exhibit interesting photovoltaic properties in their own right, for example pentacene can undergo an unusual chemical process called 'singlet fission' in which a single charge carrier can generate two charge carriers. This '2 for 1' process has attracted significant interest recently because it provides a way to side step the theoretical limit for the energy efficiency of solar cells of 34%. My work provides key insights into the mechanism behind singlet fission in pentacene and suggests that molecular vibrations play a crucial role in the fission process.

Could vibrations also increase the energy efficiency of biological light harvesting systems? Inspired by the importance of molecular vibrations in organic light-harvesting systems, in the second part of my dissertation I examined the role that nonlinear vibrations might play in a large light harvesting protein. To do this I used a computationally efficient network model. Remarkably, I found that these vibrations might be able to funnel energy to biologically relevant parts of the protein, opening up exciting possibilities for novel types of energy transfer and control.

Overall, examining organic and biological systems in tandem can help to build a better understanding of both. Organic materials provide an excellent testing ground to study quantum effects, whilst biological systems are well placed to inspire the next generation of efficient materials and devices, based on cheap, renewable components. Ultimately, living systems could open the doorway to a very different regime of physics. In the words of Stanislaw Ulam, 'Ask not what physics can do for biology, ask what biology can do for physics'.

An electronically coarse grained molecular model of water",

Flaviu Cipcigan Edinburgh

Research challenge. Atomistic materials modelling has become an integral part of research in condensed matter. Today, we can simulate entire viruses with atomic detail and use modelling to discover new medicine and materials.

Two fundamental challenges still limit the predictive power of atomistic materials modelling: the accuracy of the approximations and the timescales reached in simulations with atomic detail. My thesis addresses the former – improving the accuracy of atomistic materials modelling. This was achieved by constructing a model of the water molecule using electronic coarse graining, a fundamentally new class of materials modelling techniques based on a simplified description of the electrons.

Electronic coarse graining. The standard approach to constructing molecular models is to use fixed charges arranged in a rigid geometry and parameterised to experimental observables. Such models are efficient to simulate, but typically perform poorly away from their region of parameterisation due to the lack of *polarisation* (the redistribution of charge in a molecule due to the interactions with neighbouring molecules) and *many-body dispersion* (attractive forces caused by electron correlation between neighbouring molecules). Electronic coarse-graining is a fundamentally new technique that unites polarisation and many-body dispersion into a single element (namely a quantum harmonic oscillator), parameterised from the properties of isolated molecules. Such a parameterisation *generates all long–range forces to all orders*.

Electronically coarse-grained water. Water is a challenging substance to model, the literature containing many and diverse water models, with no transferable one. On the other hand, water is an important substance to model accurately. Proteins, for example, maintain their functional form only in the presence of water. Thus, constructing a model of water is an important challenge for a new atomistic modelling technique. In my thesis, I have constructed an electronically coarse grained model of water and demonstrated that this model is transferable to the following environments: ice II (a proton-ordered ice); the liquid–vapour interface (a prototypical hydrophobic interface); supercritical water; supercooled water; and ambient temperature water.

Adding to these predictions, the model revealed insights into the molecular structure of water. At the liquid- vapour interface, I discovered an asymmetry between hydrogen donor and hydrogen acceptor bonds. In supercritical water, I revealed a novel line separating liquid-like from gas-like regions, linked to molecular properties. Finally, in supercooled water, the model revealed qualitative differences between the behaviour of the first and second coordination shells of water, with the former having positive thermal expansion and the latter negative thermal expansion.

Perspective. My thesis has demonstrated the predictive power of electronic coarse graining. A water model parameterised from the properties of single molecules and a dimer generated a realistic condensed phase. This puts the foundation to further applications of electronic coarse graining to more complex molecules, enabling scientists to confidently predict the properties of materials from knowledge of their molecular structure.