Bridging the gaps at the physics–chemistry–biology interface

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It is commonly agreed that the most challenging problems in modern science and engineering involve the concurrent and nonlinear interaction of multiple phenomena, acting on a broad and disparate spectrum of scales in space and time. It is also understood that such phenomena lie at the interface between different disciplines, such as physics, chemistry, material science and biology. The multiscale and multi-level nature of these problems commands a paradigm shift in the way they need to be handled, both conceptually and in terms of the corresponding problem-solving computational tools.

The triple interface between biology, chemistry and physics provides a most fertile ground for these kinds of phenomena; the design of environmentally friendly catalytic devices or smart-drug delivery devices for nanomedicine purposes being just two examples in point where atomic-scale details organize coherently.

The above phenomena take place far from equilibrium, where the organizing power of nonlinearity is fully exposed and macroscopic universality is compromised by the necessary degrees of microscopic (molecular) individualism. Indeed, the ability to integrate universality and molecular individualism is perhaps the most challenging task of modern multiscale modelling.
Computer science and technology, key to enabling the quantitative modelling of such complex phenomena across scales, have experienced an extraordinary and relentless growth in both computational processing power and memory, along with dramatic cost reduction, all encouraging increased access to these approaches. At the same time, the recent decades have also witnessed substantial progress in the development of modelling methodologies at all scales, including, for example, \textit{ab initio} molecular dynamics and so-called QM/MM (quantum mechanics/molecular mechanics) techniques for atomic and nano-scales, lattice Boltzmann, Brownian and dissipative particle dynamics for mesoscales, and various grid-based methods for the several macroscales. The importance of all these efforts was recognized with the award of the 2013 Nobel Prize in Chemistry ‘for the development of multiscale models for complex chemical systems’ [1].

The papers contained in this theme issue of \textit{Philosophical Transactions of the Royal Society A} are the peer-reviewed products of a call for papers under the title of the theme issue. They and their authors were in large part brought together under the auspices of an exciting and enjoyable Solvay Workshop (which was held between 19 and 21 April 2016 at the Université Libre de Bruxelles, Belgium; figure 1). The meeting itself was similarly centred on the rising multiscale modelling paradigm, with particular focus on emergent phenomena flourishing at the physics–chemistry–biology interface. The meeting helped not only to put a focus on the present state of the art in the field, but, most importantly, also to foster and shape new cooperative research efforts so as to advance this exciting frontier of modern science.

The present theme issue starts with an opinion piece [2] discussing the ‘big data’ issue posed to conventional scientific methods of inquiry. Without conventional theoretical understanding of the structural characteristics of the system under investigation, we lack the principles by means of which to guide the optimal acquisition of data which we would expect to be forthcoming in any experimental design activity. The article provides a logical introduction to the multiplicity of research topics discussed in the following papers [3–17], which report findings spanning the full gamut of domains from physics and chemistry to biology. The first five research articles [3–7] address issues associated with the development and implementation of a range of methodologies...
for handling multiscale problems in molecular and condensed matter physics as well as fluid dynamics. These include innovative combinations of consolidated atomistic and mesoscale techniques, such as adaptive molecular dynamics, direct simulation Monte Carlo and lattice Boltzmann. In particular, the notion of Chimaera simulation is introduced to denote the intriguing ability of mesoscale methods to ‘morph’ from continuum to quasi-atomistic tools by tuning the amount of molecular details. The following two articles [8,9] consider multiscale situations arising in polymer and materials chemistry. The final eight articles [10–17] deal with the most complex and challenging aspects of multiscale modelling at the physics–chemistry–biology interface. The papers address problems which span many biologically relevant scales of organization, from the molecular and genomic levels through cellular to organ and organism levels.

According to Einstein’s famous statement ‘the most incomprehensible thing about our Universe is that it is comprehensible’ [18]. Today, we appreciate that a principal ingredient of real-world complexity is the hierarchical nature of multiple inter-connected layers of organization. Multiscale modelling is a scientifically motivated approach to apprehend such hierarchical organization, as opposed to avoiding the challenge by merely seeking correlations between observed processes. We hope that the present theme issue represents a valuable contribution along this fascinating road towards a better understanding of the marvellous complexity of the world around and within us.

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through the peer review process, to final publication at least one month ahead of the original schedule. As a result, the present issue has appeared less than six months after the Solvay Workshop took place. One of us (P.V.C.) wishes to thank Laura Parshotam for her able editorial assistance in connection with the publication of this theme issue.

Lastly, two of us (P.V.C. and S.S.) wish to dedicate this theme issue to our long-term colleague and friend, Jean Pierre Boon, on the occasion of his 80th birthday (figure 2). He has enjoyed a very distinguished and productive scientific career: we wish him well for many more years to come.

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References