Multiscale modelling: approaches and challenges

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Multiscale systems that are characterized by a great range of spatial–temporal scales arise widely in many scientific domains. These range from the study of protein conformational dynamics to multiphase processes in, for example, granular media or haemodynamics, and from nuclear reactor physics to astrophysics. Despite the diversity in subject areas and terminology, there are many common challenges in multiscale modelling, including validation and design of tools for programming and executing multiscale simulations. This Theme Issue seeks to establish common frameworks for theoretical modelling, computing and validation, and to help practical applications to benefit from the modelling results. This Theme Issue has been inspired by discussions held during two recent workshops in 2013: 'Multiscale modelling and simulation' at the Lorentz Center, Leiden (http://www.lorentzcenter.nl/lc/web/2013/569/info.php3?wsid=569&venue=Snellius), and 'Multiscale systems: linking quantum chemistry, molecular dynamics and microfluidic hydrodynamics' at the Royal Society Kavli Centre. The objective of both meetings was to identify common approaches for dealing with multiscale problems across different applications in fluid and soft matter systems. This was achieved by bringing together experts from several diverse communities.

As discussed in the contribution by Hoekstra et al. [1] (which opens this issue), one of the first questions that arise is what exactly constitutes the multiscale modelling that is inherent in multiscale systems and the issues that it involves. For example, it can be observed that multiscale problems do not typically have a closed solution (except for some idealized situations when a single-scale model at the finest level, e.g. a solution of the time-dependent Schrödinger equation in quantum mechanics, can be used as a first-principles direct solution method). To simulate a large enough system with multiple scales at the level of detail required, one has to combine models at various scale resolutions and invariably deal with different physics. Multiscale systems can be characterized by the fact that there is a form of approximation or coarse graining involved in the multiscale modelling, corresponding to an error below some threshold scale of interest. The specific terminology used for coarse graining and scale bridging in multiscale systems varies in different subject areas. For instance, terms such as projection, upscaling, model reduction and physical analogy could be used to describe the procedure of reducing the full complexity of the multiscale problem to an insightful, but tractable, representation. Coarse graining is implemented in order to reproduce interesting quantities at longer length and time scales. This, in turn, extends the modelling to a wider scale range at an affordable computational cost. On the other hand, it is not possible to coarse grain everything, as it incurs a loss of information at each step. Coarse graining also involves the exchange of information between the fine scale and the coarse scale. In some cases, this can be approximated as a one-way coupling between the scales, but, in others, a fully two-way coupling framework is required.

Despite the differences in the application methods, there is a good deal of similarity found in the application of scale separation and computational implementations in many multiscale problems. These can be analysed at the abstract level, as discussed in the contribution by Chopard et al. [2]. The exchange of information between multiple scales leads to error propagation within the multiscale model, thus affecting the stability and accuracy of the solution. Furthermore, it probes the question as to whether any mutual approaches for careful error analysis can be carried out at a theoretical level. Some examples of possible a priori estimates are discussed in the contribution by Abdulle & Bai [3] in applications to continuum fluid dynamics equations with multiscale coefficients based on homogenization theory.

Without thorough analysis or a priori guidance for computational modelling, it is necessary to make a comparison by empirical validation, or with a high-fidelity single-scale model, if that is computationally tractable. In numerous multiscale systems, a sequential approach is adopted when building a hierarchy of models. These begin with a high-fidelity model at a single scale well established with regard to the experiment or observation, which sequentially transfers information to a more coarse-grained level. For example, Booth et al. [4] discuss a 'boxed dynamics'

approach to accelerate atomistic simulations for capturing the thermodynamics and kinetics of complex molecular-dynamics systems. In the area of biological fluid flows, examples of multiscale models are discussed in the contribution by Li et al. [5] in application to multicomponent blood cell interactions in small capillary vessels. Validation is also discussed in the contribution by Wu et al. [6], who consider the interactions of platelets, blood flow and vessel walls that occur during blood clotting. In the area of coupling continuum flow and discrete particle dynamics, Srivastava et al. [7] provide an example of a multiscale model for two-phase granular systems and Markesteijn et al. [8] discuss a hybrid method for bridging continuum and molecular dynamics representations of liquids.

In addition to the physical and mathematical complexity at the conceptual level, another issue present in many domains is how to implement multiscale models in practice at the computational level. For example, there is the issue of coupling different codes written for single-scale single- physics simulation in a unified framework. It is necessary for the latter to be flexible enough to accommodate new codes written in an object-oriented environment in addition to legacy ones used in different communities for many years and based on more traditional data structures. These issues are discussed by van Elteren et al. [9] in the context of astrophysics and by Mahadevan et al. [10] in nuclear engineering applications. The scalability of such heterogeneous computational frameworks becomes important as the size of the multiscale system increases and requires the development of specialized custom-made software as discussed by Borgdorff et al. [11]. For efficient modelling of complex systems such as large biomolecular systems, including software optimization, it can be beneficial to implement custom-made hardware accelerators, such as those where the molecular interactions are implemented at the chip level, as discussed by Ohmura et al. [12].

To summarize, the contributions within this Theme Issue discuss the different aspects (conceptual, theoretical, algorithmic, applied) of various multiscale and multiphysics problems. Although this issue illustrates the diversity of the underlying scientific challenges, the solutions share common methodologies that can potentially be re-used and may possibly constitute the basis of a general theory of multiscale modelling and simulation.

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