Approaches and challenges of multiscale modelling in fluids and soft matter

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Multiscale systems that are characterised by a large range of spatial-temporal scales that naturally occur in many areas, from the study of protein conformational dynamics to multiphase processes in granular media or hemodynamics and from nuclear reactor physics to astrophysics. Despite the difference in subject areas and terminology, there are many common challenges in multiscale modelling, validation, and design of tools for programming and executing multiscale simulations. This special issue seeks to establish common frameworks for theoretical modelling, computing, validation, and helping practical applications to benefit from the modelling results. The issue has been inspired by discussions held during two recent workshops in 2013: 'Multiscale Modelling and Simulation' at the Lorentz Center Leiden[1] and 'Multiscale systems: linking quantum chemistry, molecular dynamics, and microfluidic hydrodynamics' at the Royal Society Kavli Centre. The idea

[1] http://www.lorentzcenter.nl/lc/web/2013/569/info.php3?wsid=569&venue=Snellius

behind both meetings was to identify common approaches for dealing with multiscale problems across different scientific domains by bringing together experts from different communities.

As discussed in the contribution by **Hoekstra et al**, which opens the issue, one of the first questions one might ask is what exactly constitutes multiscale modelling and what are the current open issues here. For example, it can be observed that multiscale problems do not typically have a closed solution. To simulate a large enough system with multiple scales at the level of detail required, one has to combine models at various scale resolution and invariably deal with different physics. Multiscale systems can be characterised by the fact that there is often some sort of approximation or coarse graining involved in the multiscale modelling, corresponding to an error below some threshold quantity of interest. The specific terminology used for coarse graining and scale bridging in multiscale systems varies in different subject areas, for instance, the terms: projection, up-scaling, interpolation, coarse-graining, filtering, averaging, homogenization, constitutive relations, boundary conditions, model reduction, and physical analogy could be used to describe the procedure of reducing the full complexity of the multiscale problem to some insightful but tractable representation. The idea of coarse graining is to reproduce interesting quantities at high scales to extend the modelling to a wider scale range at an affordable cost. On the other hand, it is not possible to coarse grain everything, as it incurs a loss of information at each step. The coarse graining also involves exchange of information between the fine scale and the coarse scale, which in some cases 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 details, there seems to be a lot in common at the scale separation and computing side in many multiscale problems, which can be analysed at the abstract level, as discussed in the contribution by **Chopard et al**. For example, the best practice for multiscale modelling may comprise the following steps: (i) consider the problem of interest and estimate what scale this problem is at, (ii) define which scales are less relevant and can be ignored, (ii) select scales below and above the threshold scale limits which need to be accounted for, (iii) select relevant models for the scales selected and the data which correspond to these scales; for example, a parameterisation can be done with respect to some characteristic scale, (iv) implement the modelling in a computational framework that has to integrate across the diversity of space-time steps of the multiscale/multiphysics models involved.

The exchange of information between multiple scales leads to error propagation through the multiscale model, which affects stability and accuracy of the solution. An open question here is if there are any common approaches for sharp error analysis at the theoretical level. Some examples of possible apriori estimates are discussed in the contribution by **Abdulle and Bai** applied to continuum fluid dynamics equations with multiscale coefficients based on the homogenization theory.

Without sharp analysis to provide apriori guidance for computational modelling, there is a need for validation where a multiscale model needs to be compared with nature and/or with a high fidelity single scale model. Hence, in many fields a sequential approach is adopted where a hierarchy of models is built, starting with a lower fidelity model at a single scale established with regard to the experiment or observation and then moving on to the next level. This is because the validation of the multiscale model actually makes some

assumptions and goes through several scales, which depend on the system size. This is quite different from the verification of an algorithm for a single scale problem. In particular, validation is very difficult to assess with separate scales and typically one needs to concentrate on the quantity of interest. For example, **Booth et al** 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 flows, examples of multiscale models are discussed in the contribution by **Li et al** in application to multi-component blood cell interaction in small capillary vessels and, at a higher level, in the contribution by **Wu et al** who consider the interaction of platelets, blood flow, and vessel walls which occurs during blood clotting. In the area of coupling continuum flow and discrete particle dynamics, **Luding et al** provide an example of a multiscale model for the two-phase granular systems and **Markesteijn et al** 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 areas is how to implement the multiscale models in practice at the computational code level. For example, there is an issue of coupling different codes written for single-scale and single-physics simulation in a unified framework. The latter needs to be flexible enough to be tailored both for the new codes written in an object oriented environment as well as for the ones used in different communities for a long time and based on old-fashioned data structures. These issues are discussed by **van Elteren et al** in application to astrophysics and **Mahadevan at al** in application to nuclear engineering. The scalability of such heterogeneous computational frameworks becomes important as the size of the multiscale system increases and may require the development of specialised custom made software as discussed by **Borgdorff et al.** For efficient modelling of complex systems

such as large biomolecular systems, in addition to the software optimisation, there is a need to use custom made hardware accelerators, such as those where the molecular potentials are implemented at the chip level, as discussed in the contribution by **Ohmura et al**.

Overall, the contributions to this special issue cover a range of aspects (conceptual, theoretical, algorithmic, applied) of various multiscale/multiphysics problems. They illustrate that despite the diversity of the underlying scientific challenges, the solutions share common approaches that can potentially be reused and, perhaps, even constitute the basis for a general theory of multiscale science.