Towards efficient tools for multiscale modelling of soft matter

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Recently, we have reviewed the variety of available methods for modelling soft matter ranging from the atomic to the meso-scale *[1]*. A principal observation was that the combination of different scales in the same calculation is still rare. One of the underlying reasons might be that we lack tools facilitating the combination of and exchange between calculation methods. This makes it difficult to use multiple physical models or multiple scales concomitantly. With this in mind, we are currently developing a generic software platform called ***FVNano*** *[2]* combining both a Virtual Reality-enabled visualisation interface and a generic coupling approach for calculation modules. In this perspective, ***FVNano*** aims at providing methods for moving between scales and for bridging different time and length scales (Fig. 1.). It is designed as an easy-to-use tool that allows to draw on existing and well-established simulation software in order to set up novel multi-scale approaches. Several scientific applications such as the Molecular Dynamics software *Gromacs*, our docking tool *Attract* and a molecular spring representation are already interfaced with our framework.

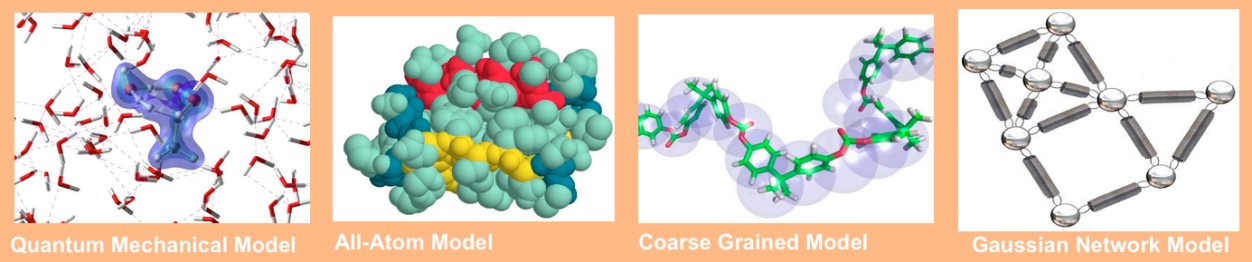

Fig. 1: Multiple scales that will be available in the FVNano application framework.

First, we will provide some guidelines on the design of new methodology for multiscale simulations. Our approach is based on *ad hoc* coupling of existing models rather than on developing an exhaustive theoretical framework specific to a given combination of multiple scales. Then we will discuss the basic concepts of the ***FVNano*** framework as an example of a possible implementation. We will present tangible scientific applications to membrane systems, including models of multiple lipid bilayers and membrane proteins. Another opportunity provided by multi-scale models of soft biological matter concerns the possibility of performing interactive simulations. As an example, we will discuss the use of coarse-grained *[3]* modeling methods within interactive simulations. This approach was tested on a large selection of complex biological systems. The immediate feedback from the interactive simulation, both visual and haptic, opens up new ways of dealing with simulations of soft matter systems.

1. Baaden & Lavery, There's plenty of room in the middle: multi-scale modelling of biological systems, in Recent Advances in Protein engineering (Research Signpost, India), edited by A.G. de Brevern (2007)
2. http://www.baaden.ibpc.fr/projects/fvnano/
3. Bond, Holyoake, Ivetac, Khalid & Sansom, J. Struct. Biol. (2006), 157, 593 ; Bond & Sansom, J. Am. Chem. Soc. (2006), 128, 2697 ; Bond & Sansom, Proc. Natl. Acad. Sci. U.S.A. (2007), 104, 2631