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Multi-Scale Approaches in Computational Materials Science

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INTRODUCTION

The term ”multi-scale” is presently very much en vogue, one almost gets the impression that this term very often is simply used to emphasize the ”importance” of a particular scheme or to impress an audience with a ”buzz word”. In the applied mathematics literature [1] it seems that essentially two types of multi-scale schemes are in discussion, namely ”one shot” schemes in which one approach is combined in a consecutive manner with another one of different mathematical origin, and procedures by intertwining two such approaches ”iteratively”, or, to use a term more common in physics and chemistry, ”selfconsistently”.

Clearly enough the easiest way to define multi-scale procedures in particular in the realm of physics and chemistry would be to state that a combination of say two different kinds of differential equations is required. Although this in principle would be a valid definition it is too narrow, since, e.g., any use of density functional theory (DFT) requires already the application of two differential equations of different kind, namely the Kohn-Sham equations (effective Schrödinger or Dirac equation) and the Poisson equation, in an ”iterative” manner. Surely enough nobody would call ab-initio type calculations in terms of the DFT a ”multi-scale” procedure. This simple counter-example indicates that it is perhaps quite appropriate to discuss the concept of ”multi-scale” only in the context of a particular field of research or discipline. In the present paper such a discussion is devoted to computational physics, in particular to computational materials science, since this is a well-established field of research in which many different types of computer simulations are performed.

FORMAL DISTINCTIONS

Suppose multi-scale schemes refer to a combination of different levels in physics such as, e.g., by combining quantum mechanical approaches with phenomenological ones, or, phrased differently, by combining microscopical with macroscopical schemes. A ”one shot” multi-scale procedure would then consist of a quantum mechanical calculation (e.g., within the framework of the DFT) followed by a phenomenological one, in which the results of the former are used; an ”iterative” procedure combines both in a kind of selfconsistent manner [2 – 7]. In the latter case of course great care has to be taken that fundamental concepts are not violated (microcosmos versus macrocosmos), i.e., that only quantities can be varied that are well-defined on both ”conceptual” levels.

Two typical situations will be discussed, namely augmenting a time-independent quantum mechanical scheme with (1) the concept of time (e.g., in terms of the phenomenological Landau-Lifshitz-Gilbert equation), and (2) with a method typical for statistical mechanics (e.g., Monte Carlo simulations based on ab-initio determined parameters), both schemes in fact can be operated in an iterative manner. Most frequently in computational materials science ”one-shot” multi-scale procedures are used, in which typically physical properties of materials are calculated in terms of the results of ab-initio approaches. In order to be classified as a multi-scale approach the evaluation of these properties has to be based on a scheme, which by definition is different from a typical DFT method such as, e.g., the Kubo equation for evaluating electric and (magneto-) optical transport, i.e., by requiring “physically separate” computer program packages that in the end provide macroscopic quantities. Very

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often also multiple combinations of ”one shot” multi-scale procedures are used as for example in evaluating magnetic domain wall properties [8 – 10], the switching times (pico-second regime) in current induced switching [11 – 13], or, rotation and ellipticity angles in the magneto-optical Kerr-effect [14 – 16].

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