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Multiscale simulations of complex systems: computation meets reality

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Abstract Multiscale simulations are evolving into a powerful tool for exploring the nature of complex physical phenomena. We discuss two representative examples of such phenomena, stress corrosion cracking and ultrafast DNA sequencing during translocation through nanopores, which are relevant to practical applications. Multiscale methods that are able to exploit the potential of massively parallel computer architectures, will offer unique insight into such complex phenomena. This insight can guide the design of novel devices and processes based on a fundamental understanding of the link between atomistic-scale processes and macroscopic behavior.

Keywords Multiscale simulations · Biomolecules · Corrosion

1 Introduction

Most physical phenomena of interest to humankind involve a large variety of temporal and spatial scales. This generic statement applies to systems as diverse as the brittle fracture of solids under external forces, which can lead to the failure of large structures such as bridges or ships starting at nanometer-scale cracks, to tidal currents in bays extending over many miles, whose behavior is dictated by the water viscosity determined from the molecular-scale interactions of water molecules.

Analytical models are typically formulated to capture the behavior of simple, homogeneous systems, or small deviations from such idealized situations, which are expressed as

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linear terms of a variable that describes the departure from uniformity. Such theories cannot cope with situations far from equilibrium, or involving very large deviations away from homogeneity, as is the case for many interesting phenomena in the spirit of the examples mentioned above. By necessity, a realistic description of such complex phenomena must rely on computational models, and more specifically on the use of multiscale approaches. This last requirement is dictated by the need to use the available computational resources in the most effective manner, allocating them judiciously to resolve the finer scales of the physical systems (which are usually the most computationally demanding) only where and when absolutely necessary. We feel that this notion is so central to computational approaches that it deserves the status of a "principle", and we will refer to it as the *Principle of Least Computation* (PLC). In other words, multiscale approaches aim at using the least possible computer power to describe satisfactorily the behavior of a complex physical system. The fact that these approaches often employ the latest and most sophisticated computer technology that is available, is a testament to the complexity of the problem at hand.

In the present article we wish to motivate the need for multiscale approaches by discussing the essential features of two specific examples of complex physical phenomena from very different domains. Through these examples, we hope to demonstrate how multiscale approaches can be formulated to satisfy the PLC, and what their prospects are for answering important scientific questions and addressing specific technological needs. We do not attempt to provide extensive references to the relevant literature, as this is beyond the scope of a perspective article and has already been done elsewhere [1]. We will only point to certain publications which have contributed key ideas on the way toward a comprehensive framework of multiscale modeling.

2 Two representative examples

Our first example has to do with Stress Corrosion Cracking (SCC): in this phenomenon, solids that are normally tough (ductile) become weak (brittle) and crack under the influence of external stresses due to the exposure to a hostile environment in which chemical impurities affect the structure at the microscopic, atomistic scale (corrosion). SCC is relevant to the stability or failure of systems in many practical applications [2]. The length scale at which this phenomenon is observed in everyday-life situations is roughly millimeters and above. At this scale cracks are detectable by naked eye, and if not arrested they can lead to the failure (occasionally catastrophic) of large structures such as ships, airplanes, bridges, etc. Evidently, the presence of chemical impurities changes the nature of bonds between the atoms, which is crucial in the region near the tip of the crack, where bonds are being stressed to the point of breaking. These atomic scale changes are ultimately responsible for the macroscopic scale change in the nature of the solid and can turn a normally ductile material into a brittle one leading to cracking. A breakdown of the different length and scale regimes relevant to this phenomenon is illustrated in Fig. 1.

A portion of a solid of linear dimension 1 mm contains of order 10^{20} atoms. Treating this number of atoms with chemical accuracy is beyond the range of any present or foreseeable computational model. Moreover, such a treatment would be not only extremely computationally demanding but terribly wasteful: most of the atoms are far away from the crack tip, they are not exposed to the effect of chemical impurities, and have little to contribute to the cracking phenomenon, until the crack tip reaches them. Thus, a sensible treatment would describe the vast majority of atoms in the solid by a simple continuum model, such as continuum elasticity theory, which is well suited for the regions far from the crack tip. Closer to the

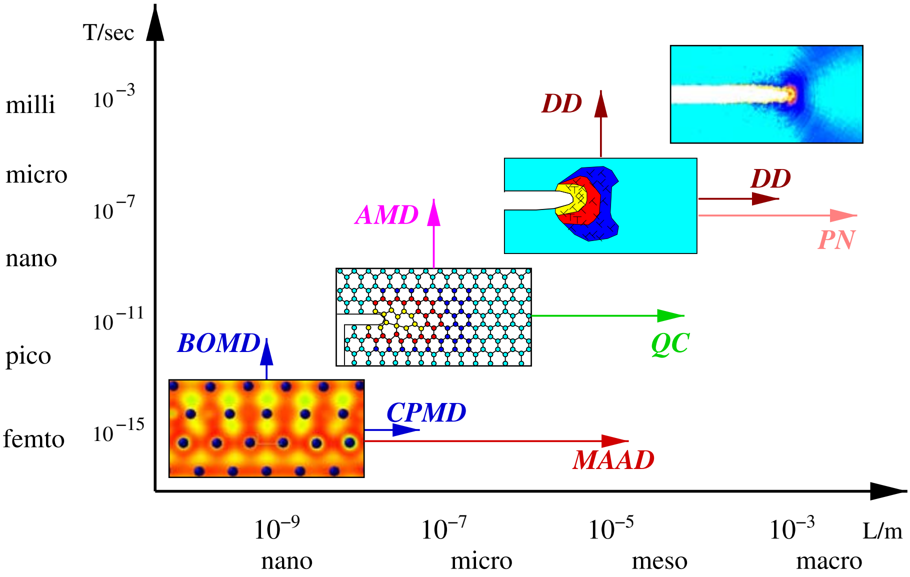

Fig. 1 Illustration of the length and time scales in Stress Corrosion Cracking, with the four different length scales, macro- (a continuum description of the crack in an otherwise elastic solid), meso- (a description of the plastic zone near the crack tip in terms of dislocations), micro- (a resolution of the dislocation structure at the atomistic level with classical interatomic interactions) and nano-scale (with the ions and corresponding valence electrons, treated quantum mechanically). The various acronyms refer to methodologies for extending the reach of conventional approaches, or coupling approaches across several scales (see text for details)

tip, several scales become increasingly important. First, the plastic zone, a scale on the order of μm, contains a large number of dislocation defects the presence of which determines the behavior of the system. The nature and interaction of these defects is adequately described by continuum theories at large scales [3,4]. However, atomistic scale simulations are required to derive effective interactions between these defects when they directly intersect each other, or in any other way come into contact at length scales equal to interatomic separation, when the continuum level of description breaks down. This introduces the need to couple atomic-scale structure and motion to dislocation dynamics [5], a coupling that has already been demonstrated and provided great insight to the origin of crystal plasticity [6]. Finally, in order to include the effects of chemical impurities on the crack tip, where the important processes that determine the brittle or ductile nature of the material take place, it is necessary to turn on a quantum mechanical description of the system, including ions and electrons.

These four levels of description, continuum at the macro-scale (mm), defect dynamics at the meso-scale (μm), atomistic scale dynamics at the micro-scale (100 nm) and quantum-mechanical calculations for the nano-scale (1–10 nm), are shown schematically in Fig. 1, together with the corresponding time scales which range from femto-seconds for the coupled motion of ions and electrons to milli-seconds and beyond for the macroscopic scale. This separation of spatial and temporal scales is only intended to show the conceptual division of the problem into regions that can be successfully handled by well developed computational methodologies. Such methodologies may include Density Functional Theory at the quantum-mechanical level, molecular dynamics with forces derived from effective interatomic potentials at the the scale of 100 nm, dislocation dynamics at the scale of several microns, and continuum elasticity (using, for instance, finite elements to represent a solid of arbitrary shape) in the macroscopic region. The goal of mutliscale simulations is to couple the various regimes, as appropriate for a particular problem, in order to achieve a satisfactory description of this complex phenomenon.

A number of computational schemes have already been developed to address this type of phenomenon. The work of Car and Parrinello [7] from over two decades ago, is a general method for extending the reach of quantum-mechanical calculations to systems larger than a few atoms, and can be viewed as a pioneering attempt to couple the purely quantum-mechanical regime to the classical atomistic. More recently, Parrinello and coworkers [8] have developed a method that extends the reach of this type of approach to significantly longer time-scales. The multiscale-atomistics-*ab initio*-dynamics (MAAD) [9] approach was an attempt to couple seamlessly within the same method three scales, the quantum-mechanical one, the classical atomistic, and the continuum, that enabled the first realistic simulation of brittle fracture in silicon. A direct link between the atomistic scale and the scale of defect (dislocation, domain boundaries, etc.) dynamics was accomplished by the quasi-continuum (QC) method [10], that enabled realistic simulations of large deformation of materials in situations like nano-indentation [11] and polarization switching in piezoelectrics [12]. The methods originally developed by Voter [13] for accelerating molecular dynamics (AMD) can extend the time-scales of classical atomistic approaches by a few orders of magnitude, addressing an important bottleneck in multiscale simulations. Finally, dislocation dynamics (DD) and continuum formulations like the Peierls-Nabarro (PN) theory, can make the connection to truly marcoscopic scales; however, these approaches depend crucially on input from finer scales to determine the values of important parameters, so they cannot by themselves have predictive power unless a connection is made to the finer scales.

We turn next to our second example. This has to do with ultrafast sequencing of DNA through electronic means, a concept that is being vigorously pursued by several experimental groups [14,15]. The idea is to form a small pore, roughly of the same diameter as the DNA double helix, and detect the DNA sequence of bases by measuring the tunneling current across two electrodes at the edges of the pore during the translocation of the biopolymer from one side of the pore to the other. Estimates of the rate at which this sequencing can be done are of order 10 kbp/s, which translates to sequencing the entire human genome in a time frame of a couple of days. While this goal has not been achieved yet, the successful demonstration of this concept has the potential to produce long-lasting changes in the way medicine is practiced.

This system is also a very complex one, involving several scales that are shown schematically in Fig. 2. At the coarsest scale, the biopolymer in solution needs to be directed toward the nanopore. The scale of the biopolymer in solution is of order μm, and the time scale involved in finding the pore is of order fractions of a second. At these scales, the system can be reasonably modeled as consisting of a continuous polymeric chain in a uniform solvent, possibly under the influence of an external non-uniform but continuous field that drives it toward the pore. In experiments, this can be achieved either by a concentration gradient on the two sides of the pore, or by an electric field acting on a polymer with uniform charge distribution. Understanding the translocation process itself involves modeling the polymer at scales set by the persistence length ($\sim$100 nm for DNA), while including the effect of the solvent. This is already a demanding proposition, because the number of molecules that constitute the solvent is macroscopic (10^{24}) and in fact it makes no sense to monitor their dynamics at an individual basis, since it is only the cumulative effect that is felt by the polymer.

We have recently succeeded in producing an efficient coupling between the solvent motion, described by the Lattice Boltzmann approach to model fluid dynamics [16], and the polymer motion, described by beads representing motion at the scale of the persistence length and

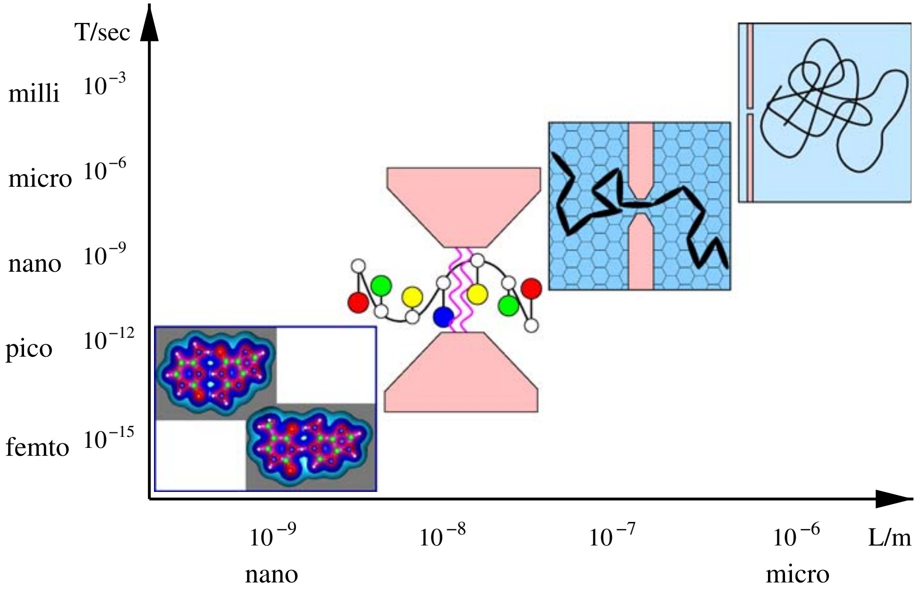

Fig. 2 Illustration of the length and time scales in ultrafast DNA sequencing by electronic signals during translocation through a nanopore. At the micro-scale, the biopolymer is a continuous line moving in a homogeneous solvent under external fields, at the next level (100 nm) the biopolymer is resolved at the persistence length and the fluid is modeled by a transport theory on a grid (the Lattice Boltzmann Equation), at the 10 nm scale the biopolymer structure is resolved at the level of individual bases (color coded) and electron current across the leads can be modeled by quantum transport equations, and at the nm scale the individual bases are modeled explicitly in terms of their atomic and electronic structure

following newtonian dynamics under the influence of local friction from the fluid [17]. This lattice-Boltzmann plus molecular-dynamics (LBMD) description was very successful in reproducing details of the observed translocation process in a realistic manner, as observed in experiments for both single-file and multi-file translocation [18]. Nevertheless, the approach is still far from capturing the full problem of electronic DNA sequencing. What is missing is the information at the 10 nm scale, with the biopolymer described as a sequence of individual DNA bases, the electronic properties of which will determine the electron current across the two leads on either side of the pore. The electron current can be calculated from quantum-transport theories, once the relevant electronic states are known. To this end, detailed calculations of the electronic properties of DNA bases need to be carried out, at the level of quantum chemistry, including all the details of the base-pair atomistic structure. Assembling the entire picture in a coherent model is a serious challenge to current computational capabilities and is likely to require profound conceptual and mathematical innovations in the way we handle the phase-space of complex systems [19,20].

3 Problems and prospects

The cases described above are representative of complex systems which by their nature demand multiscale approaches. There are many subtle issues on how multiscale approaches are formulated, both at the practical level, with each approach requiring great attention to computational details, as well as at the fundamental level, where questions of basic notions arise when degrees of freedom are eliminated in the process of coarsening [19], but these are well beyond the scope of the present article. Here, we wish to address only two general points. The first is the bottleneck of time-scale integration; the second is the bottleneck of efficient allocation of computational resources.

As the two examples mentioned earlier make clear, it is usually feasible to produce multiscale methods that successfully integrate several spatial scales, spanning many orders of magnitude in length. However, it is much more difficult to integrate temporal scales. Most often, the time-step of the simulation is dictated by the shortest time scale present. Even if ingenious approaches can be devised to accelerate the time evolution, they can produce a speedup of a couple orders of magnitude at best, which is rather restricted compared to the vast difference in time scales for different parts of the process (see Figs. 1, 2). At present, we are not aware of coupling schemes that can overcome this bottleneck in a satisfactory way, integrating over many orders of the time variable [21].

Second, we suggest that it may be necessary to rethink traditional algorithmic approaches in view of recent developments in computer architectures. Specifically, taking advantage of massively parallel architectures or streamlining in graphics-processing units, can produce very significant gains, at the cost of writing codes that are specifically suited for these architectures. We have found that in our LBMD scheme, speedups of order 10^4 in computation time could be achieved by using a multi-processor architecture, the IBM BluGene/L, because when properly formulated, the problem scales linearly with the number of available processors with excellent parallel efficiency. The mapping of the physical system to the computer architecture is not trivial and required specialist's skills. We feel that this aspect of the computational implementation should not be overlooked in trying to construct useful multiscale models.

As closing remarks, we express our conviction that multi-scale approaches are essential in faithfully capturing the nature of physical reality in a wide range of interesting phenomena. We are hopeful that carefully planned and executed computational efforts will indeed come very close to an accurate and useful representation of complex phenomena. This challenge has not been met yet, in other words, computation is still shy of full success in meeting physical reality. But the gap is closing fast.

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