Introduction

Nanorobotics is an emerging area of scientific and technological opportunity. It is a new and rapidly growing interdisciplinary field addressing the assembly, construction and utilization of molecular devices based on nanoscale principles and/or dimensions. The size-related challenge is the ability to measure, manipulate, and assemble matter with features on the scale of 1–100 nm. In order to achieve cost-effectiveness in nanotechnology it will be necessary to automate molecular manufacturing. The engineering of molecular products needs to be carried out by robotic devices, which have been termed nanorobots. A nanorobot is essentially a controllable machine at the nanometer or molecular scale that is composed of nano-scale components and algorithmically responds to input forces and information. Bio-nanorobotics, namely biomolecular robots, represents a specific class of nanorobots where proteins and DNA could act as motors, mechanical joints, transmission elements, or sensors. If all of these different components were assembled together they can form bio-nanorobots with multi-degree-of-freedom, able to apply forces and manipulate objects in the nanoscale world. These bio-components seem to be a very logical choice for designing nanorobots. In addition since some of the core applications of nanorobots are in the medical field, using bio-components for these applications seems to be a good choice as they both offer efficiency and variety of functionality. This idea is clearly inspired by nature's construction of complex organisms such as, bacteria and viruses which are capable of movement, sensing and organized control.

The design of nanorobotic systems requires the use of information from a vast variety of sciences ranging from quantum molecular dynamics to kinematic analysis. So far, there does not exist any particular guideline or a prescribed manner that details the methodology of designing a bio-nanorobot. As research development is at the interface of physical sciences and biology it requires multi-skilled teams. To achieve this it is essential for the future molecular roboticians to be able to design and prototype the bio-nanomechanics, to develop dynamic and kinematic models, to study their dynamic performances and to optimize their structure. Although many of the described technologies have been developed into more or less mature products for robots acting in the macro-world, the nano-size of the molecular robots poses ex-

treme challenges and requires a complete rethinking of the design and prototyping methodologies.

Based on the general research issues of design, modeling and prototyping, we have proposed the following research agenda for this thesis:

Chapter 1 presents a state-of-the-art in the emerging field of nano and bio-nanorobotics and its applications. First, it discusses some of the essential properties and dynamical laws which make this field more challenging and unique than its macro-scale counterpart. Second, we review the relation between molecular behavior and system/device response, by analyzing the current trend in modeling and simulation tools, which can analyze phenomena spanning the wide spectrum of length and time scales. This cannot be accomplished with one theory or simulation method. Finally, we describe some of the emerging applications of virtual reality coupled to molecular dynamics simulations recently completed or currently underway in the field of bio-nanotechnology with envisioned applications into molecular robotics.

In Chap. 2, we investigated computational nanotechnology methodologies, i.e., physics-, biology- and chemistry-based modeling and simulation, dedicated to the design and optimization of bio-nano structures. An attempt has been made to emphasize the paradigm of how computational nanotechnology can be used to not only understand and characterize the systems under experimental investigation, but also as to how predictions can be made for novel applications because there is a strong coupling between the structural, mechanical, and biological properties at multiple length-time-scale. Two prototyping methodologies, namely, *interactive multiscale design* using virtual reality techniques and *co-prototyping design* using experimental measurements and molecular modeling algorithms are proposed and discussed in detail.

Then, Chap. 3 presents the design hypothesis, architectures and computational analysis of novel bio-nanorobotic structures. Towards this end, we used an interactive prototyping platform using multiscale, multiphysics and virtual reality advanced techniques. Virtual Reality technology is applied here, which not only provides immersive visualization but also gives an added functionality of CAD-based design, simulation, navigation and interactive manipulation of molecular graphical objects. The present study demonstrates that the mechanical properties of protein-based nanodevices can be controlled by using rational design based on protein and/or DNA engineering principles. We proposed novel concepts of protein-based and DNA-based actuation nanomechanisms that have been computationally simulated and analyzed through multiscale modeling. These designs pave the way for future position and force control nano servomotors operating in water environments.

Finally, Chap. 4 introduces a new co-prototyping approach based on a dual paradigm, i.e., experimentation and molecular modeling. Usually, nanodevice optimization is only based on experimental investigation of nanodevice characteristics. As all design parameters are not accessible by experimental measurements, the designer is not able to characterize deeply the nanodevice operating principles leading to optimal performances. As alternative, we propose to use jointly modeling tools to support the designer in order to characterize novel phenomenons, evaluate

energy densities or new operational principles. Such principles have been applied to high-density electromechanical switches based on bi-directional linear bearing. Computational models provide new insights into the structural and energetic stability aspects of these unique nanomechanical elements.



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