Preface

The idea of building unimaginable small things at the atomic level is nothing new. Already in 1959, *R. Feynman*, the 1965 *Nobel* prize winner in physics, described during his famous dinner talk, "There's plenty of room at the bottom!" how it might be possible to print the whole 24 volumes of the *Encyclopedia Brittanica* on the head of a stick pin. He even speculated on how to store information at atomic levels or how to build molecular-sized machines:

"*I am not afraid to consider the final question as to whether, ultimately in the great future we can arrange atoms the way we want; the very atoms, all the way down! ⋯ The principles of physics, as far as I can see, do not speak against the possibility of maneuvering things atom by atom. It is not an attempt to violate any laws ⋯ but in practice, it has not been done because we are too big ⋯ The problems of chemistry and biology can be greatly helped if our ability to see what we are doing, and to do things on an atomic level, is ultimately developed — a development which I think cannot be avoided*". [Feynman, 1960]

Now, some decades later, new laboratory microscopes can not only visualize but manipulate individual atoms. With this recently developed ability to measure, manipulate and organize matter on the atomic scale, a revolution seems to take place in science and technology. And unfortunately, wherever structures smaller than one micrometer are considered the term *nanotechnology* comes into play. But nanotechnology comprises more than just another step toward miniaturization!

While nanotechnology may be simply defined as technology based on the manipulation of individual atoms and molecules to build structures to complex atomic specifications [Policy Research Project, 1989], one has to

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consider further that at the nanometer scale qualitatively new effects, properties and processes emerge which are dominated by quantum mechanics, material confinement in small structures, interfacial volume fraction, and other phenomena. In addition, many current theories of matter at the micrometer scale have critical lengths of nanometer dimensions and therefore, these theories are not adequate to describe the new phenomena at the nanometer scale.

Nevertheless, the concept of nanotechnology goes much further. It is an anticipated manufacturing technology giving thorough, inexpensive control of the structure of matter where other terms, such as molecular manufacturing, nano-engineering, etc. are also often applied. In other words, the central thesis of nanotechnology is that almost any chemically stable structure that can be specified can in fact be built. Researchers hope to design and program nano-machines that build large-scale objects atom by atom. With enough of these *assemblers* to do the work, along with *replicators* to build copies of themselves, we could manufacture objects of any size and in any quantity using common materials like dirt, sand, and water [Drexler, 1981; Drexler *et. al*, 1991; Regis, 1995; Merkle, 2001]. Computers 1000 times faster and cheaper than current models; biological nano-robots that fix cancerous cells; towers, bridges, and roads made of unbreakable diamond strands; or buildings that can repair themselves or change shape on command might be futuristic but likely implications of nanotechnology.

Today, while nanotechnology is still in its infancy and while only rudimentary nanostructures can be created with some control, this seems like science fiction. But respected scientists agree that it is possible, and more and more of the pieces needed to do it are falling into place. Nanotechnology has captured the imaginations of scientists, engineers and economists not only because of the explosion of discoveries at the nanometer scale, but also because of the potential societal implications. A White House letter (from the Office of Science and Technology Policy and Office of Management and Budget) sent in the fall of 2000 to all Federal agencies has placed nanotechnology at the top of the list of emerging fields of research and development in the United States. The *National Nanotechnology Initiative* was approved by Congress in November 2000, providing a total of $422 million spread over six departments and agencies [NNI; Roco, Sims, 2001]. And this certainly doesn't seem like science fiction!

Now, let us discuss nanotechnology from the educational point of view. What might be the most important scientific branch with respect to the development of nanotechnological applications?

To apply nanotechnology, researchers have to understand biology, chemistry, physics, engineering, computer science, and a lot of other special topics, such as protein engineering or surface physics. But the complexity of modern science forces scientists to specialize and the exchange of information between different disciplines is unfortunately not very common. So the breadth is one of the reasons why nanotechnology proves so difficult to develop.

But even today, one tendency is clearly visible: nanotechnology makes *design* the most important part of any development process. If nanotechnology comes true, the traditional production costs would drop to almost nothing, while the amount of design work would increase enormously due to its complexity. Further, the field of engineering design will become much more complex. Someone has to design these atomic-sized assemblers and replicators as well as nano-materials and others. And if we can build anything in any quantity, the practical question of "What can we build?" becomes a philosophical one: "What do we choose to build?". And this in turn is a design question. Answering it and planning for the widespread change each nano design could bring makes design planning incredibly important [Milanski, 2000].

As a conclusion, we may summarize: design will change radically under nanotechnology and for nano-engineers or nano-designers, respectively, a broad knowledge will become even more important in the future.

As long as we are still far away from the realization of complex nanotechnological applications, nano-engineering and nano-design almost exclusively take place on computers. Computational nano-engineering is an important field of research aimed at the development of nanometer scale modeling and simulation methods to enable and accelerate the design and construction of realistic nanometer scale devices and systems. Comparable to micro-fabrication which has led to the microelectronics revolution in the 20th century, nano-engineering and design will be a key to the nanotechnology revolution in the 21st century.

Therefore, the intention of this monograph is to give an introduction into the procedures, techniques, problems and difficulties arising with computational nano-engineering and design.

For the sake of simplicity, the focus is laid on the *Molecular Dynamics method* which is well suited to explain the topic with just a basic knowledge of physics. Of course, at some points we have to go further into detail, i.e. quantum mechanics or statistical mechanics knowledge is needed. But such subsections may be skipped without loosing the picture.