Literature Review

(Editor's Note: Eric Drexler's book on nanotechnology, which he defines as "technology based on the manipulation of individual atoms and molecules to build structures to complex, atomic specifications," has raised a number of issues of potential concern to the CAMD community. This month, ***CDA News*** *features a review of Drexler's book and of the course it inspired last spring at Stanford University , where Drexler is a Visiting Scholar. The course is reviewed by a participating graduate student. Readers should note that nanotechnology has some serious followers besides Drexler. The Massachusetts Institute of Technology's Artificial Intelligence Laboratory holds Nanotechnology Study Group meetings twice each month to discuss such relevant subjects as robotics, AI and molecular graphics; the group also publishes a newsletter, along with a bibliography of related topics.)*

Drexler's *Engines of Creation* Probes Consequences of Design at the Nano Level

In *Engines of Creation,* K. Eric Drexler urges us to ponder and plan for a world based on a new level of technology potentially more pervasive than any now known. We are accustomed to miniaturization; microcomputers and microelectronics are common currency. Drexler dubs the engineering of the next level of smallness "nanotechnology."

There is much to criticize and commend in this book. It is easy to pass of *Engines of Creation* as popular science, or worse, science fantasy; and the book may make chemists uncomfortable with the author's treatment of atomic and molecular systems as purely mechanical systems. *Engines of Creation* is also notably absent of chemically-based reasoning: there is no analysis of assemblers in terms of new enzymes that would transport and deposit, say, metal atoms on a growing part; yet we know many enzymes that play a carrier role. Nevertheless, the reader should consider suspending criticisms to give serious consideration to the real, practical questions the book raises about the possibility of a totally new ability to re-engineer the world.

The fundamental assertion of *Engines of Creation* is that miniaturization technology will soon progress from the mini- and micro- to the nano- level: in other words, engineers will be able to manipulate matter, molecule by molecule and atom by atom. This is not a ridiculous concept. For years chemists have been studying single atoms and molecules in molecular beam experiments, and as readers of ***CDA News*** know, chemical design tools are emerging to provide the theoretical basis for the evaluation of molecular interactions at a detailed, mechanistic level.

The underlying engineering apparatus of nanotechnology are nanomachines, or assemblers and nanocomputers; these are the actuators and control systems, respectively, of nanontechnology. The first three sections of the book describe them and discuss their applications and the potential benefits and dangers. The second part of the book deals with the potential benefits of the cleanest manufacturing technology imaginable, the ability to obtain resources not now practical and the ability to detect and correct physiological diseases and accidents at the molecular level. The last part of the book explores the dangers of armies of nanomachines running out of control, optimizing and replicating themselves while human beings become the victims of a mechanized Darwinian antiselection. Professor Hans Moravec of

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Seminal Book on Nanotechnology Inspires New Course at Stanford

This past spring, K. Eric Drexler, Visiting Scholar at Stanford University, taught CS404: Nanotechnology and Exploratory Engineering. According to Drexler, this was the first full-scale course taught on the subject of nanotechnology. During the quarter, we looked at several paper designs of systems built to atomic specification, explored the social ramifications of nanotechnology and examined some possible paths to nanotechnology.

The first complicated system we studied was a mechanical nanocomputer with logic elements that consisted of pyridazine- and thiopene-based knobs positioned on carbyne rods. The nanocomputer performed logic operations by moving these rods along tunnels in a solid block of material. Each logic operation would take on the order of several picoseconds, as opposed to fractions of a nanosecond for today's fastest production integrated circuit logic elements.

This mechanical nanocomputer illustrates several aspects of Drexler's design nethodology. The most important aspect is that Drexler designed the nanocomputer to atomic specifications: every atom had to be in the correct place for the device to function correctly. Because the systems that Drexler designs cannot be built and tested using current technology, Drexler uses mathematical models of the behavior of atoms and molecules, such as molecular mechanics, to argue that these systems will operate correctly. It is worth noting that the nanocomputer, like other objects Drexlers designs, is not made of protein molecules but of

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Carnegie-Mellon University explored this possibility when he was a guest lecturer at the MIT Nanotechnology Study Group in December, 1987 (this group meets twice each month to hear lectures on such subjects as robotics, artificial intelligence and molecular graphics).

While it is tempting to dismiss *Engines of Creation* as some lightweight, futuristic "technobabble" from a mechanical engineer who thinks chemistry is a Tinker-Toy set, the author clearly anticipated a quasi-Luddite reception and prepared plausible arguments to support his fundamental assumptions. Overall, *Engines of Creation* is perhaps best viewed as the proverbial "artist's conception" rather than as a detailed engineering drawing.

One of the most startling things about technological progress, as emphasized in the text and Foreword by Marvin Minsky, is how difficult it has been to predict and anticipate it. A world based on nanotechnology may seem foreign and implausible on the surface, but how many scientists of past generations accurately anticipated the global communications and microelectronics that we know today? *Engines of Creation* offers a reasoned "look-ahead," and suggests that we prepare ourselves better than we have in the past to use new technology more wisely.

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more constrained, rigid organic molecules.

Another major aspect of Drexler's approach is that he is more interested in demonstrating firm lower bounds on the achievable performance of devices built to atomic specifications than coming up with an optimal design for a specific task. Therefore, his devices are both built with large margins for error and designed for easy analysis. Even though Drexler believes that electrical nanocomputers may very well perform many times faster than mechanical nanocomputers, he designed a mechanical nanocomputer because molecular mechanics is a more tractable formalism than those used to model electrical charge at an atomic level.

Drexler used the same design methodology for other atomically precise parts such as bearings, gears and an electric motor. He also spent a fair amount of time on a robot assembler arm that could be used to position individual atoms as part of an atom-by-atom construction process. This arm would be the critical part of a general-purpose assembler that could build a wide range of systems and materials to atomic specifications.

Because Drexler makes extremely conservative design decisions, he can tolerate inaccuracies in the mathematical models he uses to reason about his systems. Under the assumption that these mathematical models provide a reasonable approximation to reality, it is clear that if built, Drexler's systems would work as designed.

The key problem here is that nobody knows how to build systems to atomic specifications. Drexler reduced this problem to the problem of constructing a general-purpose assembler consisting of assembler arms mounted on the base of a cylindrical housing with a nanocomputer for control. To build this assembler, Drexler envisions a sequence of progressively more complex assemblers, each of which builds its successor. In such a scenario, the first assembler might be made of protein molecules using conventional protein synthesis techniques. Drexler is quick to point out that building such as assember requires only enough knowledge to design proteins that will fold up into certain predetermined shapes, not a general solution to the protein folding problem.

Although this bootstrapping sequence seems intuitively plausible, it is so sketchy that it is hard to say whether or not it can be done any time in the foreseeable future.

The final large segment of the course dealt with the social implications of nanotechnology. Some of these are straightforward—for example, using nanotechnology, one could build nearly flawless materials with many times the strength to weight ratio of current materials. These extremely strong materials could revolutionize transportation and architecture.

Other contemplated effects seemed much less certain. Drexler claims that nanotechnology would lead to cell repair machines that could, for example, reverse aging effects. Given our current lack of knowledge about the precise workings of the human body and the enormous problems computer scientists face when trying to build machines that respond sensibly to real-world sensory input, I find these speculations farfetched. On the other hand, there is certainly no proof that such systems are impossible to build.

One lecture focused on dealing with the danger of nanotechnology. A typical scenario involved the use of small, smart machines to selectively kill large numbers of people. The only contemplated defense against such a terrifying weapon is a world-wide "living shield" designed to find and destroy any unauthorized objects in the environment. At this point we are dealing

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with pure speculation about what is actually scientifically possible.

Despite the uncertainty of mankind's ever actually acquiring nanotechnology and the difficulty of predicting the social ramifications of such an acquisition, contemplating these ramifications is a worthwhile activity. It is clear that mankind's acquisition of nanotechnology would bring about enormous social changes, and that many of these social changes may not be desirable. By considering the possible social repercussions of nanotechnology, we can prepare ourselves to deal with its emergence.

I enjoyed the class very much and found it intellectually stimulating. Unlike most science and engineering courses, which concentrate on known techniques and results, this course speculated on future technological developments. Also unlike most science and engineering courses, this course tried to examine the social repercussions of technological dedvelopments.

In a world in which technology is developing rapidly and having an increasingly large impact on our lives, there should be a place in every science and engineering curriculum for courses that address these two issues.

By Martin Rinard, Department of Computer Science, Stanford University, Stanford, CA 94304. ■

SCS

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Example 4: GAMESS - I/O performance on the SCS-40

wall clock time (seconds)

	DISK (1.8 MB/s.)	DISK 11 MB/s.)	XMSD (178 MB/s.)
BENCH1	457 s.	312 s.	217 s.
BENCH 2	252 S.	202 s.	124 s.
BENCH4	1950 s.	1331 s.	880 s.

Example 5: GAUSSIAN 86 Link 502 (solve SCF equations)

wall clock time (seconds)

	DISK (11 MB/s.)	XMSD (178 MB/s.)
TEST052	129 s.	91 s.

ample, can never be modelled by an O(N**4) method. In spite of these limitations, *ab initio* methods have now reached the point of being practical adjuncts to the laboratory chemist for the detailed study of properties of small molecules.

By Rick R. Castrapel, Scientific Computer Applications Analyst, Scientific Computer Systems Inc., 10180 Barnes Canyon Road, San Diego, CA 92121 (619-546-1212).

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New Products

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For integration into VAX environments, the FX/82 Computational Center includes VIP, Alliant's VAX integration package.

The new product is priced at $1.25 million and includes dual eight-ACE FX/80 systems, the ANSR/LCX and VIP software and Ethernet. Each FX/80 is configured with 64M bytes of memory, 1.1G bytes of disk and tridemsity tape drive and software licenses for the Concentrix operating system and FX/Fortran. Further details are available from Alliant Computer Systems Corporation, One Monarch Drive, Littleton, MA 01460 (617-486-4950). ■