Abstract

This paper describes the novel area of nano-planning—the study of automated planning in an eutactic environment. We begin by describing the evolution of present technology towards nanotechnology and the rationale for engineering nano-robots. The various established fields of research that will contribute to the creation of the first nano-robot are reviewed.

The discussion then focuses on the role of artificial intelligence (AI) in nanotechnology. We argue that AI techniques are the most appropriate means of control for nano-robots, and will facilitate a major improvement in the cost-effectiveness of molecular manufacturing. As molecular manufacturing is concerned with finding suitable assembly sequences for end-specified molecules, automated planning techniques will be essential.

Nano-planning is presented as a novel area of research comprising knowledge representation and domain modeling, traditional planning, scheduling and constraint satisfaction, machine learning and adaptive planning, nano-robotic fine motor control, computer aided economic analysis and advanced graphical simulation.

1 Introduction

1.1 The Evolution Towards Nanotechnology

Since the era of ENIAC, the first successful digital high-speed computer developed in the 1930s, the dominant feature of the evolution of computer science and computer engineering has been the continued reduction in the size of computer hardware [23]. The reduction in the size of pre-fabricated computer components, such as silicon chips and electronic circuits, has made it possible to build powerful computer systems in a physical space that had previously been considered impossible [46, 24, 21].

As our knowledge of quantum physics and quantum chemistry has increased [75, 78], it has become clear that the basic building blocks of all matter, namely individual atoms, may themselves be seen as pre-fabricated components [61]. Atoms may be assembled in an environment where individual atoms follow paths that seldom deviate from a nominal trajectory by more than an atomic
diameter while executing complex motions in an extended region from which freely-diffusing molecules are rigorously excluded. This is known as a *eutactic environment* [22].

The structures that will result from this type of manufacturing, termed *molecular manufacturing* [17], will be measured in nanometers [29, 84]. The new branch of computer science and engineering that deals with the assembly and disassembly of atoms in molecular manufacturing is called *Nanotechnology* [71].

### 1.2 The Potential of Nanotechnology

Nanotechnology represents a fundamental breakthrough in that both non-biological and biological problems may be perceived from an atomic engineering point of view. Numerous applications based upon the idea of the rearrangement of atomic species have been proposed:

1. Almost all physical illnesses that affect the human body, such as cancer, AIDS, or the common cold, cause pathology at the atomic level. As nanotechnology will allow for atomic assembly, disassembly and rearrangement, the task of treating disease can be viewed as simply a task of atomic engineering. For example, nanotechnological devices may be used to disassemble cancer cells or invading viral material, alter deoxyribonucleic acid (DNA) and ribonucleic acid (RNA) chains, or repair damaged tissue [24]. Moreover, nanotechnology will facilitate the ability to routinely diagnose disease at the atomic level, the level at which pathology is actually caused [23, 35].

2. Nanotechnology will enable the production of large quantities of bulk chemicals by making it possible to assemble these from either simple molecular structures or single atoms one at a time [22, 69]. Molecular manufacture of materials promises to be extremely energy efficient as energy will be able to be directed specifically at breaking and creating those bonds that result in the production of end-specified molecules.

As reactions are exogeric or endogeric in a eutactic system, as opposed to being endothermic and exothermic as occurs in a solution-phase environment [13], any non-utilized or mis-directed energy may still be held within the system in the form of mechanical energy which can then be used for further synthetic reactions [22].

3. The world faces enormous pollution problems due to the production of toxic chemicals as by-products of many heavy industrial applications [82, 3]. The application of nanotechnology will allow for many present pollutants to be either dismantled or altered on an atomic scale and rendered harmless and innocuous [71].

4. Space-Aeronautical Institutions such NASA [55, 30, 31] are conceptualizing the use of nano-robotic devices in the colonization of space [26] due to the ease with which a nanotechnological approach could be used to build housing and equipment for cosmic settlement [79]. In the face of the problem of world over-population nanotechnology will play an important role
in the first steps of mankind to colonize other planets and find new living space for human beings.

1.3 The Necessity for Nano-Robots

The above examples illustrate the extent to which nanotechnology may impact upon the world. However, if nanotechnology is to be accepted by the industrial community it must be able to accomplish its objectives in a manner that is cost-effective when compared to the present level of technology [22, 83]. This is vitally important since if the cost of utilizing nanotechnology does not prove to be as cheap or cheaper than the present modalities of manufacturing it is unlikely that nanotechnology will gain broad acceptance as a new and competitive alternative [66].

Useful structures such as chemical compounds may be built from thousands of individual atoms [33] and it is commonplace to manufacture quantities of bulk materials ranging from kilos to tonnes of active compounds. It is therefore impossible for large scale molecular manufacturing to be carried out by human operators using atomic movers such as scanning tunneling microscopes [11, 9]. Such a mode of manufacture would be prohibitive in terms of the investment of labour into such a slow and expensive process [71].

In order to achieve cost-effectiveness in nanotechnology it will be necessary to automate molecular manufacturing [23]. That is, the engineering of molecular products will need to be carried out by robots which are also nano-size in dimension. These robots have been termed nano-robots and are known as assemblers when referring to the ability to assemble molecules from atoms [59] and replicators when referring to the ability to produce exact copies of themselves [23, 56].

1.4 Contribution of Established Fields to Nano-Robotics

Building the first functional nano-robot is a challenge facing the world-wide scientific and industrial communities [53]. It is likely that the first assembler will emerge out of the evolution of established technologies including:

1. Quantum chemistry, surface physics, and engineering. The fields of quantum chemistry, surface physics involving scanning tunneling microscopy (STM) [9], and engineering are integral for understanding how molecules can be assembled [63] in an environment where the structures to be built will obey the laws of quantum mechanics [22]. Understanding these areas is critical in the calculation of the various mechanical strains and forces to which a nano-robot will be subjected.

2. Quantum computing or quantum dots. An important challenge for nanotechnologists involved in creating the first nano-robot will be the ability to design information storage architectures for on-board nano-computers without unduly increasing the size of the nano-robotic device. At present, one of the most promising solutions to this problem lies in the field of quantum computing [8] which uses the quantum mechanics principle of superposition in order to store information simultaneously as 1 and 0. This is termed a quantum bit or a qubit.
As $L$ qubits can store $2^L$ numbers at once, a memory register based upon this approach is able to perform operations simultaneously akin to there being $L$ parallel central processor units working together [19]. At present, two-spin experiments using chloroform (since the nucleus of common carbon with chloroform, carbon 12, has no spin and thus chloroform containing carbon with one extra neutron imparts an overall spin) have shown the practical application of this concept [27].

An alternative method of data storage may be the use of quantum dot cellular automata. A quantum dot is an artificial atom isolated on (or in) a semiconductor substrate. When a pair of electrons within a cell of four closely spaced dots is lost this creates a bit: the configuration of the electrons establishes either a 1 or 0. Situating many of these cells together creates a programmable cellular automata network [44]. Data input and output occurs at the periphery of the cell ensemble which acts like a connectionist network as the computing is performed by the quantum interactions within the array [43].

3. Reversible logic. Contemporary computers erase a bit of information every time they perform a logic operation. Such operations are called “irreversible”. Each time a bit of information is erased the computational system must dissipate approximately the kinetic energy of a single air molecule at room temperature [54].

As the design of nano-computers will require a greater number of logic elements in smaller and smaller volumes, together with being run at increasingly higher frequencies [81, 45], this will result in an increased dissipation of heat leading to potential overheating. In order to overcome this problem research is being carried out into “reversible” logic systems that do not erase information when performing a logic operation [62, 58, 57].

An area which is not as yet established in the field of nanotechnology is that of artificial intelligence [52, 20]. This is despite the fact that artificial intelligence will be essential to automate nanotechnology since it represents the most appropriate means of controlling nano-robotic devices [24, 72]. In addition, artificial intelligence will aid in the design, construction and testing of nano-robotic devices and will allow nanotechnologists to put into place the necessary moral safeguards and quality control standards such that nanotechnology will operate within all appropriate environmental and ethical guidelines [23, 24].

In the remainder of the paper we focus on a particular area of artificial intelligence—automated planning—which will be vital in controlling nano-robots and automating molecular manufacturing.

2 From Nanotechnology to Nano-Planning

Nanotechnology will involve the planning and scheduling of assembly sequences [25, 38] in a eutactic environment. Automated planning [2, 7, 6] therefore is essential for its development. As discussed below, automated planning in a eutactic environment will present problems unique to the process of molecular manufacturing. This novel area of research, which we term *Nano-Planning*, will comprise several components.
2.1 Knowledge Representation and Domain Modeling

The aim of knowledge representation in nanotechnology is to express knowledge about an atomic environment in computer-tractable form such that it can be used by a nano-robot to perform molecular manufacturing. It will be necessary to choose or develop the appropriate acquisition methods for characterizing planning knowledge [28, 77] in a eutactic system. Tasks will include representing the laws of quantum mechanics, representing the sizes of different atoms and the electron distributions about these atoms, representing the position in space of atomic species and the nano-robot itself, and representing the variety of molecular bonds that can form when atomic species are brought together.

Domain modeling will consist of using this knowledge to construct a computer model of the environment [73] which will enable the assembler to move, locate and manipulate atoms in order to build molecular structures from given specifications.

2.2 Traditional Planning

Traditional planning concentrates on how to generate a sequence of actions, considered at an abstract level as state transitions, that can be executed in a given situation in order to reach a goal state [72]. Important research topics will include efficiently searching the range of possible solutions to atomic engineering problems and dealing effectively with time and resource constraints.

As the issues of error rates and the flawless repeatability of eutactic systems are paramount in molecular manufacturing, there will also be a need to combine traditional planning with plan execution systems which will facilitate immediate re-planning as soon as a failure in execution is detected.

Task planning in nano-robotics will involve integrating goals, resources and time with several other domain specific agents [51] devoted to navigation and the manipulation of atomic species [63].

2.3 Scheduling and Constraint Satisfaction

Scheduling is concerned with ordering a set of actions that satisfy certain quality criteria. In nanotechnology this will focus on consuming as little time as possible since the time allocated to a synthetic process is an important determinant of the overall cost-effectiveness of the manufacturing system [42].

In relation to this, constraint satisfaction will be particularly important when manufacturing is carried out interactively [40] by a large group of assemblers termed a swarm [79]. It will be necessary to optimize the organization of swarms, each of which will be subject to energy and spatial constraints [37].

2.4 Machine Learning and Adaptive Planning

The theoretical study of nano-robotic devices raises several issues in regards to how assemblers will be able to optimize their plans in order to achieve their goal state in the most labour and time efficient manner.

Assemblers will have multiple ways to move in order to solve the same task. Problems involving many sub-optimal solutions or many local optima will mean searching a space of permutations for assembling molecules that will be of the
order of $10^{10}$ atoms or greater [22] while simultaneously navigating a three-dimensional space in order to locate and position atoms.

Assemblers will be required to work at speeds of up to one million molecules per second (akin to naturally occurring enzymes) [23]. It will be important that the planning algorithms which are implemented are fast at finding near optimal solutions.

It will also be important for nano-robotic devices to learn [64] from failures in nano-engineering, such as unwanted intra-molecular and inter-molecular interactions, when trying to adapt a previous plan to a new specification [50]. This will require supplying the planning system with appropriate retrieval strategies as well as making use of automated reasoning techniques that will allow a planner to prove the formal properties of plans and domain models. This will include the correctness and applicability of actions and plans and the consistency of domain models.

Automated planning has historically utilized traditional search algorithms such as hill-climbing, A*, IDA* and simulated annealing [72]. However, the fact that automated planning in a eutactic environment will need to be fast and make use of previous plans suggests that the use of adaptive planning or case-based planning algorithms [49, 36] will expedite the process of finding near optimal synthetic pathways. At present, little research has been carried out on the application of adaptive algorithms, such as genetic algorithms or particle swarm optimization (PSO) [41, 4] in automated planning [10, 48]. This will form a major component of research into nano-planning.

2.5 Nano-Robotic Fine Motor Control

Software will be needed to control the mechanical movement of nano-robots which will carry out a set of path actions leading to the completion of a goal task [47]. This will include implementing systems that will deal with perception and monitoring changes in the eutactic environment that will affect the performance of the robot [12, 16, 15]. The need for a nano-robot to have autonomy over these actions will be great since an increase in autonomy [68, 5] will lead to a decrease in the need for supervision by a nanotechnologist with a resulting decrease in labour costs.

Problems in providing fine motor control for assemblers will include noise in sensing action [39], positional (thermal) uncertainty [60] of reacting species, and errors in structural manufacturing due to unwanted inter-molecular or intra-molecular reactions.

2.6 Computer Aided Economic Analysis

Computer aided economic analysis has been utilized extensively in the manufacturing industry due to the complexities of analyzing manufacturing processes [18]. While the components of nano-planning described above deal with creating plans, it will be important to cost these plans [76, 34] for several reasons.

First, it will be important to ascertain the input costs of a proposed synthetic route [14, 32] before committing to the actual process of molecular manufacturing [76]. This is to ensure a nett positive monetary return on the product given the anticipated sales performance of the material [1].
In addition, it will be necessary to evaluate the cost-effectiveness of a nanotechnology-based approach compared with using present technology, principally solution-phase reactions [35]. This is essential in order to demonstrate any improvement in cost-effectiveness from using a nanotechnological approach and thereby show that nanotechnology is an economically acceptable alternative [67].

2.7 Advanced Graphical Simulation

A recent methodology called object-based evolutionary algorithms (OBEA) emphasizes the advantages of graphically displaying the results of experiments as animations [70]. Molecular manufacturing will require that the results of automated planning be viewed as graphical output since the ability to view molecular structures in three dimensions greatly assists in making informed judgements about chemical and biological properties, manufacturing feasibility [65], and checking for or anticipating errors in molecular structure [35].

The field of nano-planning will require the creation of advanced graphical simulations which can accurately reflect a nano-scale landscape [80]. In order to obtain realism in the simulation, however, it will be necessary to incorporate the constraints imposed by the laws of quantum mechanics [74].

3 Conclusion

Technology is evolving towards the ability to build structures of nano-scale size with atomic precision. This new field of research, a branch of computer science and engineering, is called nanotechnology. The potential benefits of nanotechnology for mankind are immense and include curing diseases, energy efficient and pollution free manufacturing, and the colonization of space.

In order to achieve the potential of nanotechnology and render it cost-effective it will be necessary to engineer nano-robots. Various established fields of research will contribute to the creation of the first nano-robotic device. In order to control nano-robots it will be necessary to devise the appropriate advanced artificial intelligence systems. As nanotechnology will predominantly involve finding suitable assembly sequences for end-specified molecular structures, automated planning is vital for its development.

Automated planning in a cutactic environment, or nano-planning, will present unique problems. Nano-planning will draw on aspects of knowledge representation and domain modeling, traditional planning, scheduling and constraint satisfaction, machine learning and adaptive planning, nano-robotic fine motor control, computer aided economic analysis and advanced graphical simulation.

References


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Nano-engineered materials in automotive products include high-power rechargeable battery systems; thermoelectric materials for temperature control; tires with lower rolling resistance; high-efficiency/low-cost sensors and electronics; thin-film smart solar panels; and fuel additives for cleaner exhaust and extended range. Nanostructured ceramic coatings exhibit much greater toughness than conventional wear-resistant coatings for machine parts. Nanotechnology-enabled lubricants and engine oils also significantly reduce wear and tear, which can significantly extend the lifetimes of moving parts. Will nanotechnology impact future global security? According to Jayshree Pandya, such technology is indeed about to change large-scale security dynamics, defense policies and possibly even the global balance of power. All states are eager to benefit from nanoscience, nano-engineering and nanotechnology initiatives - either directly or indirectly. While most states do not yet have dedicated nano-defense initiatives, rapid advances within the aforementioned fields are exciting many and becoming a cause of concern for the rest. Nano-planning is presented as a novel area of research comprising knowledge representation and domain modeling, traditional planning, scheduling and constraint satisfaction, machine learning and adaptive plan. Practical approaches for nano-planning systems have been presented [24] as a first step towards automating assembly tasks in nanorobotics, where was presented a 2D assembly tasks automation.