Nano Technology

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Abstract: We present a new approach using genetic algorithms, neural networks, and nano robotics concepts applied to the problem of control design for nanoassembly automation and its application in medicine. As a practical approach to validate the proposed design, we have elaborated and simulated a virtual Environment focused on control automation for nano robotics teams that exhibit collective behavior. This collective behavior is a suitable way to perform a large range of tasks and positional assembly manipulation in a complex three-dimensional workspace. We emphasize the application of such techniques as a feasible approach for the investigation of nano robotics system design in nano medicine. A theoretical and practical analysis of control modeling is one important aspect that will enable rapid development in the emerging field of nanotechnology.

Keywords: Assembly nanao manipulation, nano medicine, proposed Design, nanotechnology.

1. Introduction

First steps toward molecular manufacturing in the 1980s and 1990s in the sense of nano scale building blocks, we now face more complex challenges in achieving the next generation of nanotechnology advances, in the sense of building bio nano electronics and molecular machines.

This paper presents the simulation of mobile multirobot teams operating at atomic scales to perform biomolecular assembly manipulation for nanomedicine [20]. In such a virtual nanoworld, the teams must cooperate with each other in order to achieve a productive result in assembling biomolecules into larger biomolecules. The assembled biomolecules must be sequentially delivered into a set of predefined organ inlets, and the nanorobot teams must also keep the nutritional levels of the larger organism under control [8], [9]. The motivation for such study is the likelihood that in the emerging era of molecular engineering, the development of methodologies that help focus experimental investigations enabling the automation and the evaluation of new approaches for a better comprehension and visualization of virtual nanoworlds can have a great impact on effective design and on the future development of nanotechnology. One important challenge that has become evident as a vital problem in nanotechnology industrial applications is the automation of atomic-scale manipulation.

The starting point nanotechnology to achieve the main goal of building systems at the nanoscale is the development of control automation for molecular machine systems, which could enable the massively parallel manufacture of nanodevice building blocks. Governments all around the world are directing significant resources toward the fast development of nanotechnology. In Germany, the Federal Ministry of Education and Research has announced 50 million Euros to be invested in the years 2002–2006 in new research and development on nanotechnology. The U.S. National Science Foundation has launched a program in “Scientific Visualization” in part to harness supercomputers in picturing the nanoworld. A US$1 trillion market consisting of devices and systems with some kind of embedded nanotechnology is projected by 2015 [14]. More specifically, the firm Display Search predicts rapid market growth from US$84 million today to $1.6 billion in 2007. A first series of commercial nanoproducts has been announced as foreseeable by 2007. To reach the goal of building organic electronics, firms are forming collaborations and alliances that bring together new nanoproducts through the joint efforts of companies such as IBM, Motorola, Philips Electronics, Xerox/PARC, Hewlett-Packard, Dow Chemical, Bell Laboratories, and Intel Corp., among others [22]. For such goals, new methodologies and theories to explore the nanoworld are the key technology [13].

2. Assembly Nano Manipulation

Building patterns and manipulating atoms with the use of scanning probe microscopes (SPMs) as in atomic force microscopy (AFM) and scanning tunneling microscopy (STM) has been demonstrated with satisfactory success as a promising approach for the construction of nano electromechanical systems (NEMS) with three-dimensional (3-D) precision at 0.01-nm resolution. However, such manual manipulations require much time, and even for a repetitive task these manipulations tend to produce imprecise work when performed manually for a large number of molecules. Practical approaches for nano planning systems have been presented as a first step toward automating assembly tasks in nanorobotics, as, for example, in two-dimensional (2-D) positional assembly automation. The use of artificial intelligence as the appropriate means to enable some aspects of intelligent behavior in the control of nanorobots during molecular manufacturing automation has been discussed in the nanoco community. The use of concepts derived from collective robotics and behavior control was investigated for nanomedicine dealing with a common goal to destroy malignant tissues in the human body.

More recent work is progressing toward the development of 1536-1241/$20.00 © 2005 IEEE 134 IEEE TRANSACTIONS ON NANOBIOSCIENCE, VOL. 4, NO. 2, JUNE 2005 a nanorobotics autonomous system capable of performing 200 000 accurate measurements per second at atomic scale [39]. An Intel prototype 90-nm process facility has already produced a fully functional 52-Mb SRAM with transistor gate lengths of 50 nm and SRAM cell sizes of just 1 m, or roughly half the cell size of today’s most advanced...
SRAMs [22]. This downscaling will continue, according to the Semiconductor Industry Association’s roadmap. By 2016, high-performance ICs will contain more than 8.8 billion transistors in a 280 nm area—more than 25 times as many as on today’s chips built with 130-nm feature size[22].

Through the use of nanotechnology techniques [22], genetics advances, and biomolecular computing [1], we may also have biological nanorobots being applied in specific biomedical and environmental applications. For example, in microbiology engineering the construction of digital circuits in living cells has been demonstrated.

The Synthetic Biology Lab at the Massachusetts Institute of Technology, Cambridge (MIT), is creating a standardized set of biological building block components designed for logic operations inside a cell and are being accumulated in the MIT Registry of Standard Biological Parts. Bacteria have been used as physical system component [32], and radio remote control of biological processes has been demonstrated experimentally [27]. Following similar proposals on nanorobots being injected inside living cells and controlled for biomedical purposes [20], we can expect the first artificial biological nanorobots, a possibility extensively reviewed elsewhere [15]-[17], to become available in five years or less. More complex nanorobots will be manufactured using diamondoid or other similarly rigid materials awaiting primarily our ability to perform positional mechanoassembly, and work leading in this direction has progressed recently. Initial uses of nanorobots in health care are likely to emerge within the next ten years [20], with potentially broad biomedical applications [15], [20].

A useful starting point for achieving the main goal of building nanoscale devices is the development of generalized automation control for molecular machine systems which could enable a manufacturing schedule for positional nanoassembly manipulation.

In this paper, we consider a more specialized scheduling problem with a focus on nanomedicine: describing in a detailed fashion the nanorobot control design and the surrounding virtual workspace modeling that is required for the main kinematics aspects of a physically based nanoworld simulation.

Here the biomolecular assembly manipulation is automatically performed by smart agents, which are given the task of improving the nutritional state of an organism via the injection of appropriate assembled substances into pre-established delivery points in a complex 3-D environment.

3. Nano Medicine

In future decades the principal focus in medicine will shift from medical science to medical engineering, where the design of medically active microscopic machines will be the consequent result of techniques provided from human molecular structural knowledge gained in the 20th and early 21st centuries [20].

For the feasibility of such achievements in nanomedicine, two primary capabilities for fabrication must be fulfilled: fabrication and assembly of nanoscale parts. Through the use of different approaches such as biotechnology, supramolecular chemistry, scanning probes, both capabilities had been demonstrated to a limited degree as early as 1998 [20]. Despite quantum effects which impart a relative uncertainty to electron positions, the quantum probability function of electrons in atoms tends to drop off exponentially with distance outside the atom. Even in most liquids at their boiling points, each molecule is free to move only 0.07 nm from its average position [20].

Developments in the field of biomolecular computing [1] have demonstrated positively the feasibility of processing logic tasks by biocomputers [26], a promising first step toward building future nanoprocesors with increasing complexity. There has been progress in building biosensors and nanokinetic devices [2], which also may be required to enable nanorobotic operations and locomotion. Classical objections related to the feasibility of nanotechnology, such as quantum mechanics, thermal motions, friction, have been considered & resolved and discussions of techniques for manufacturing nanodevices are appearing in the literature with increasing frequency [29].

4. Proposed Design

Assemblers are molecular machine systems that could be described as systems capable of performing molecular manufacturing at the atomic scale [8]. The collective nanorobotic approach presented here is one possible method to perform a massively parallel positional nanoassembly manipulation. In our described workspace representing a simplification of the human body, the multinanorobot teams perform a pre-established set of tasks building nutrient molecules, crudely analogous to the work done by a ribosome which is a natural assembler.

Three well-known design approaches for nanomanipulation in liquid and air environments [13] include the telescoping robotic arm, the Stewart platform, and the five-strut crank model. For our experiment we chose a robotic arm with nanomanipulation in a liquid environment, the most suitable for an in vivo nanomedical application. It is also well known that computation is relatively cheap for macroscale robotic actuators, whereas arm motion is relatively cheap for nanoscale robotic actuators [13], [20].

Thus, the moment-by-moment computer control of arm trajectories is the appropriate paradigm for macroscale robots, but not for nanoscale robots. For nanoscale robots, the appropriate manipulator control paradigm is often trajectory trial and error, also known as sensor based motion control [31].

4.1 Virtual Environment and Nanorobot Design

Techniques to enable rapid design while incorporating complex aspects of physical principles used for production of final 3-D prototypes have been progressing rapidly. Virtual reality techniques are currently being explored...
successfully in the nano-science and nanotechnology research to provide researchers with an intuitive way to interact with materials and devices at the nanoscale. Guthold [24] tried to provide a virtual-environment interface to SPMs, giving a virtual tele-presence on the surface but downscaled by a factor of about a million to one.

The introduction of direct human–SPM interaction creates not only enhanced measurement capability (for instance, special transducers can provide a sense of touch to the nanomanipulator), but also presages a more fully automated technology that will enable nanofabrication and/or repair of nanostructures. A 3-D bionanomanipulation system integrated with a real-time virtual reality simulator has been proposed [21]. Nanoscale object manipulation systems have been applied with the use of computer graphics for teleoperation, where the requirements for such systems have been clearly established.

Virtual reality was considered a suitable approach for nanorobot design and for the use of macro- and micro robotics concepts given certain theoretical and practical aspects that focus on its domain of application.

The nanodevice design must be robust enough to operate in an aqueous environment with movement having six degrees of freedom (see Fig. 1). The virtual environment in our study is inhabited by nanorobots, biomolecules, obstacles, and organ inlets. Each nanorobot measures 650 nm in length and 160 nm in diameter. The biomolecule has a diameter of 10 nm and each obstacle has a diameter of 120 nm. The organ inlets are 400 nm in height and width with inlet orifices 720 nm in diameter. The trajectories and positions of each molecule which must be captured and assembled were generated randomly, and each one also has a probabilistic velocity and acceleration.

In the simulation, while some molecules have been captured (Fig. 2) other molecules are manipulated and assembled internally by the robot arm inside the proposed nanorobot. The nanorobot design is derived from biological models and is comprised of components such as molecular sorting rotors and a robot arm (telescoping manipulator) [13], [20]. The nanorobot exteriors considered in our design assumes a diamondoid material to which may be attached an artificial glycopilaxyl surface that minimizes fibrinogen (and other blood protein) adsorption and bioactivity, thus ensuring sufficient biocompatibility for the nanorobot to avoid immune system attack [18].

Different molecule types are distinguished by a series of chemotactic sensors whose binding sites have a different affinity for each kind of molecule [20].

Some concepts provided from underwater robotics were assumed for nanorobot locomotion. The nanorobot kinematic response can be predicted using state equations, positional constraints, inverse kinematics, and dynamics, while some individual directional component performance can be simulated using control system models of transient and steady-state response [6]. Plane surfaces (three fins total) and bidirectional propellers provide navigation, while two simultaneously counter rotating screw drives provide the propulsion [20]. The nanorobot lives in a world of viscosity, where friction, adhesion, and viscous forces are paramount and the gravitational force here is relatively negligible [13], [20]. In this world, a very low Reynolds number \( Re \) is assumed for the kinetic calculations, where the fluid mechanics in small structures can usually be described by the classical continuum equations [13]. The ratio of inertial to viscous forces is determined by as expressed in (1)

\[
Re = \frac{\rho v L}{\eta}
\]

where \( \rho \) is the absolute viscosity of the fluid, \( v \) is the velocity, \( L \) is the fluid density, and \( L \) is a characteristic dimension. \( Re \) indicates whether the flow will be laminar or turbulent around an object of a given shape at a given flow velocity. For nanoscale dimensions in fluids of ordinary viscosities and velocities, \( Re \) is low and the flow is laminar [20]. The inertial force on the object is of order and the viscous drag force is of order. In order to keep moving forward, a nanorobot of size \( m \) and velocity \( m/s \) must apply \( (\text{femtonewtons}) \) and a much larger of motive force [20]. For instance, if motive power to a swimming nanorobot with radius \( m \), and velocity \( cm/s \), is suddenly stopped, then the nanorobot will “coast” to a halt in a time given by (2)

\[
\tau_{\text{coast}} = \frac{\rho L \text{max}^2}{15\eta} = 0.1
\]
where $0.1$ is expressed in microseconds, and in a distance $\text{nm}$ [4].

By using the nanorobot’s local perception as much as possible and by sending the fewest possible messages to other nanorobots, unnecessary communication between the agents is reduced, thus minimizing energy consumption by the nanorobots.

Nanorobots satisfy their energy requirements via the chemical combination of oxygen and glucose [20], both of which are plentiful in the human body. The nanorobot includes external sensors to inform it of collisions and to identify when it has encountered an obstacle which will require a new trajectory planning. Aspects of the nanorobot's behavior in the human body include the interior of the body where the nanorobot is acting, and must be considered in the navigational sensing design.

In robotics fields, there are often many kinds of sensors, such as infrared, computer vision, chemical sensors, and so forth, which are normally used for robotics navigational purposes. Optical sensors have been widely applied in terrestrial mobile robotics, but these have an extremely limited range in a liquid environment. Types of sensors such as laser rangefinders [6] could be also used for underwater robotics but not for nanorobots sensing because, for instance, the laser energy might excite or chemically alter the surrounding biomolecules that the nanorobot is trying to capture. Although the infrared sensor seems preferable for macro scale terrestrial robots, for underwater robots the most common sensor approach involves the use of sonar systems. Similarly, the most addressable approach for nanorobots in nanomedicine is to use acoustic waves [20]. The blue cones shown in Fig. 2 represent regions that the robot’s sonar can “hear.” Scientific visualization techniques permit rapid and precise geometric analysis to simulate a sonar classification system [6].

We used physically based simulation [3] to consider kinematics and frictional aspects specifically required for rigid body motion with hydrodynamics at low $Re$ number for molecular assembly manipulation.

### 4.2 Evolutionary Decision

We intend to construct and demonstrate the applicability of multirobot teams in timely sequenced work for capture, assembly, transport, and delivery of biomolecular pieces to a predefined set of organ inlets.

The use of multirobot teams to work cooperatively to achieve a single global task applied to nanotechnology is a field of research that is relatively new [9]. Research on collective robotics suggests that we should consider emulating the methods of the social insects to build decentralized and distributed systems that are capable of accomplishing tasks through the interaction of agents with the same structures and preprogrammed actions and goals. Thus, a careful decomposition of the main problem task into subtasks with action based on local sensor-based perception could generate multirobot coherent behaviors [33].

The approach for the nanomedicine problem here could be described as two multirobot teams which must cooperate...
interactively to feed a set of organ inlets in the virtual environment under study. The importance of cooperative teamwork has led us to choose a high-level decision control model with adaptive evolutionary characteristics. Note that the proposed nanorobot model here includes no kind of nanorobot self-replicating behavior [12]. Instead, our model uses an evolutionary approach strictly for the combinatorial analyses, allowing the nanorobots to react cooperatively in an uncertain environment with a well-defined preprogrammed set of actions. The model used here, often cited in the literature as Genetic Algorithms (GA), relies on concepts derived from evolution and genetics [8]. Each solution here is described as a chromosome regarding the nanorobot decision on how, when, and which organ inlets to attend in the dynamic scenario. Each decision required to be taken by the nanorobot always follows the programmed set of actions rigidly pre-established in our design by the fitness/objective function.

Equation (4) represents our fitness function, where the nanorobots maximize the protein levels for the selected organ inlets. The variable induces the nanorobot to catch a number of molecules as closely as possible to the desired delivery mean, while brings the nutritional levels as close as possible to

$$\max f = \sum_{i=1}^{n} \sum_{j=1}^{m} u_{ij} - |x_{ij} - z_{ij}|$$

We have decomposed the total set of organ inlets, assigning for each pair of nanorobots a specified number of organ inlets to be attended by the nanorobots at each time step of the simulation.

Each pair is comprised of nanorobots from team A and B. The organ inlets selected to be fed at time have to be fed first by the agent A, then by B, and so forth. Both agents must take care to avoid applying an overdose or deficiency of the injected substances.

Table 1

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>$\tau$</td>
<td>robot time</td>
</tr>
<tr>
<td>$\omega$</td>
<td>organ inlets' desirable nutritional target level</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>surplus/deficit to the desired assembled mean</td>
</tr>
<tr>
<td>$\Delta$</td>
<td>keep the nutritional levels close to the target</td>
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<td>$\Omega_A$, $\Omega_B$</td>
<td>respective robot teams</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>size of time in the simulated scenario</td>
</tr>
<tr>
<td>$\beta$</td>
<td>total of organ inlets to be fed</td>
</tr>
<tr>
<td>$L$</td>
<td>robot load capacity</td>
</tr>
<tr>
<td>$Q_e$</td>
<td>substance amount injected in the organ inlet $e$</td>
</tr>
<tr>
<td>$C_e$</td>
<td>total assembled molecule by $r$ in $e$</td>
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<tr>
<td>$x_{ij}$</td>
<td>chemical state of the organ inlet $j$ at time $t$</td>
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<tr>
<td>$z_{ij}$</td>
<td>nutrients consumption by the organ inlet $j$</td>
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<tr>
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</tr>
<tr>
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<td>$\Delta$</td>
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<td>$\tau_{\max}$</td>
<td>maximum to be injected at organ $j$ in $t$</td>
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We used real time and parallel processing techniques, where both teams react adaptively to any stimulus produced by their partners' decisions, with the model visualization in real time. The study of smart multirobot behavior in a single global environment enables concepts related to the use of local perception for reactive agents [5], [33]. Multidisciplinary control design addresses the nanorobot's multimodular system architecture [10]. A feed forward neural networks model discussed below was used for the nanorobot motion control, wherein each nanorobot visits in a shorter time the organ inlets that were pre-attributed to that nanorobot in order to gather information for the next time step decision from the 3-D workspace.

4.3 Neural Motion

A connectionist model using artificial neural networks was chosen for the motion control and shortest-path problem solution, beginning with a dynamic combinatorial problem for each time step simulation. The classical problem of finding an optimal three-dimensional shortest path avoiding 3-D polygonal obstacles is typically NP-hard [3]. The use of a nondeterministic approach to solve the motion control seems to be the appropriate technique in such cases [23].

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We have decomposed the total set of organ inlets, assigning for each pair of nanorobots a specified number of organ inlets to be attended by the nanorobots at each time step of the simulation.
have implemented a feed forward or acyclic network due to its suitability for probabilistic calculations. The particular model implemented here is a stochastic feed forward neural network [28], which requires a lower computational effort in comparison with a back propagation algorithm [25] and a better performance in comparison with a greedy heuristic approach [59]. The features of the algorithm for the implemented neural network could be represented by (16)

$$p_a(X_j) \subseteq \{X_1, X_2, \ldots, X_{j-1}\}$$

(16)

where represents a vector, consisting of the two-valued random variables, defining a topology composed of stochastic neurons. With representing the range of hidden layers, which leads the network to be optimized at the time step, it represents each destiny to be achieved for throughout the simulation. The units in the network are organized into a 2-D matrix, with rows by columns, where and are the costs matrix of destinations for each evolutionary agent, which tries to complete its set of tasks successfully as fast as possible. Let the output of the unit in row and column be, where. This means that the referred destination is visited at the th stop, with otherwise. Therefore, a solution cost for each agent routing could be expressed by (17)

$$\min P^{*} = \sum_{m=1}^{n} \sum_{c=1}^{m} r_{m}\text{w}_{c}.$$  

(17)

Once having obtained both routes (route on and route off), which are composed respectively of the organ inlets to be supplied and the organ inlet whose nutritional level is to be verified, then the nanorobot performs the trajectory visiting the subset of organ inlets assigned to it, first executing the whole delivery route, and afterwards beginning the verification routine. One positive aspect of a feed forward neural network is that it requires low computational effort to achieve motion control in a workspace with six degrees of freedom [25]. We use binary cues to trigger the behavioral response as a common mechanism for action and for governing different phases of activity in tasks— as is done by social insects [11]. In this manner, activation of a motor behavior is not dependent on a specific perceptual cue, but rather on the decision that results from sensor processing. The advantage is that the design of the motor behavior does not change when different sensor types or alternate feature extraction techniques are used, since the information needed by the motor behavior is the same binary vector in both cases [33].

5. Simulation and Conclusion

Biomolecular machine system designs that are capable of accomplishing successfully a set of preprogrammed tasks in a 3-D workspace is a new challenge for control investigation. We describe the study of an automation model and the respective visualization tools to follow up the analyses for the control theory development based on experimental results. Nanorobots’ monitoring nutrient concentrations in a 3-D workspace is a possible application of nanorobots in medicine, among other biomedical problems [20]. One interesting nanorobot application is to assist inflammatory cells (or white cells) leaving blood vessels to repair injured tissues [7]. Also the nanorobot could be used to process specific chemical reactions in the human body as ancillary devices for injured organs. Nanorobots equipped with nanosensors could be developed to detect glucose demand in diabetes patients [30]. Nanorobots could also be applied in chemotherapy to combat cancer through superior chemical dosage administration and a similar approach could be taken to enable nanorobots to deliver anti-HIV drugs. Such drug-delivery nanorobots have been termed “pharmacytes” by Freitas [20].

The neural motion control was successfully used with real-time response for the circumstance where the nanorobots must capture molecules and visit a predefined set of delivery points, avoiding random obstacles and collision with other mobile nanorobots, and trying at the same time to minimize the time required.

These tasks were satisfactorily accomplished using the neural networks approach, wherein the nanorobots calculated their complete trajectories with a cost minimization of 37% in the required distance good improvement in comparison with a greedy solution for the motion control optimization. Realizing revolutionary applications of nanorobots to health or environmental problems raises new control challenges.

The design and the development of complex nanosystems with high performance should be addressed via simulation to help pave the way for future medical nanorobotic systems.

References


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