Nanosystem Design with Dynamic Collision Detection for Autonomous Nanorobot Motion Control using Neural Networks

Adriano Cavalcanti
Darmstadt University of Technology, Computer Science Department
Darmstadt, Germany

Robert A. Freitas Jr.
Zyvex Corporation
Richardson, USA

Abstract

The authors present a new approach within advanced graphics simulations for the problem of nano-assembly automation and its application in medicine using collective robotics. The problem under study concentrates its main focus on autonomous control for nanorobot teams coordination as a suitable way to perform a large range of tasks and assembly manipulation in a complex environment. The presented paper summarizes distinct aspects of some techniques required to achieve a successful nano-planning system design for a large number of cooperating autonomous agents and illustrates their three dimensional visualization in real time.

Keywords: *Virtual Reality, Physically Based Simulation, nanoCAD, Motion Control, Autonomous Nanorobotics, Nanomedicine.*

1. INTRODUCTION

The starting point of nanotechnology to achieve the main goal of building nanoscale systems is the development of autonomous molecular machine systems. The presented paper describes the design and simulation of autonomous multi-robot teams operating at atomic scales with distinct assembly tasks. Teams must cooperate with each other in order to achieve a productive result in assembling biomolecules into larger biomolecules. These biomolecules will be delivered to "organs" (into a set of predefined organ inlets), and such deliveries must also to be coordinated in time.

Building patterns and manipulating atoms with the use of Scanning Probe Microscopes (SPM) as in Atomic Force Microscopy and Scanning Tunneling Microscopy [14] is a promising approach for the construction of nanoelectromechanical systems (NEMS) with 3D precision at up to 0.01 nm resolution. However, these manual manipulations require much time and at present such repetitive tasks give imprecise results when performed manually on a large number of molecules. Approaches for nano-planning systems have been presented [14] as a first step towards automating 2D assembly tasks in nanorobotics, and the possible use of artificial intelligence as the appropriate means to enable some aspects of intelligent behaviour for the control of nanorobots in molecular manufacturing automation has been discussed in the nano community [05]. Theoretica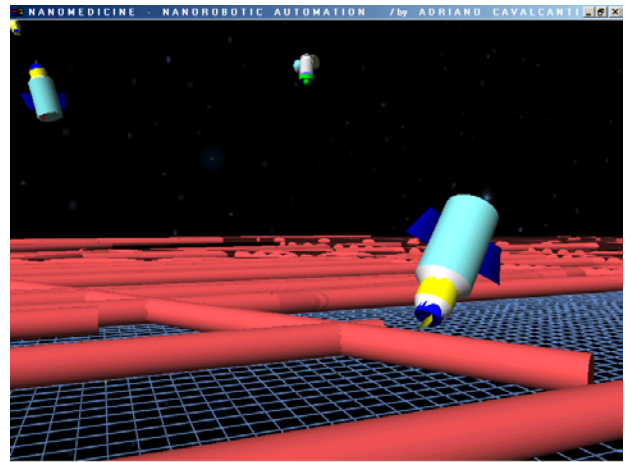l work in molecular manufacturing has emphasized the need for very small and very accurate manipulators which simultaneously have a wide range of motion to enable the task of assembling molecular components [06]. More recent work in the possible automation of nanoscale manipulation has produced a fully autonomous motion manipulator system capable of performing 200,000 accurate measurements per second at the atomic scale [15].

2. NANOMEDICINE

The principal focus in medicine is going to shift from medical science to medical engineering, where the design of medically-active microscopic machines will be the consequent result of the techniques provided from human molecular structure knowledge derived during the 20th (and the beginning of the 21st) century [07]. For the feasibility of such achievements in nanomedicine [07] two primary capabilities are required: fabrication of parts and assembly of parts. Through the use of different approaches such as biotechnology, supramolecular chemistry, and scanning probes, both capabilities had been demonstrated in limited fashion as early as 1998 [07]. Despite quantum effects which impose a relative uncertainty to electron positions, such objections are resolved by recognizing that the quantum probability function of electrons in atoms tends to drop off exponentially with distance outside the atom, giving atoms a moderately sharp "edge". Even in most liquids at their boiling points, each molecule is free to move only ~0.07 nm from its average position [07]. Recent developments in the field of biomolecular computing [01] have demonstrated positively the feasibility of processing logic tasks by bio-computers [09], which is a promising first step to enable future nanoprocessors with increasing complexity, and nanoscale information storage and data processing capacity, which could be considered as an indispensable component of a real autonomous nanosystem. Other advances in the sense of building biosensors [20] and nano-kinetic devices [19] have advanced recently too, which could be considered as well a prerequisite for making nano-automation feasible and enabling nanorobotics control and locomotion. Many classical objections to the feasibility of nanotechnology, such as quantum mechanics, thermal motions and friction, have already been considered and resolved [06]. The presented nanorobot will be required to perform a pre-established set of tasks in the human body similarly like a ribosome, which is a natural molecular machine system [07].
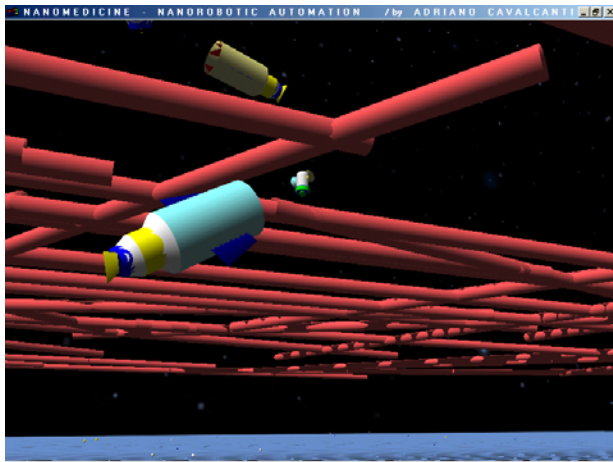
(1.a) Nanorobot finding path   **(1.b)** Nanorobot avoiding obstacles

Figure 1. Collision detection.

3. PROPOSED DESIGN

A multi-robot molecular machine system could be described as a system to perform molecular manufacturing at the atomic scale, whose constituent entities are capable of cooperating collectively. Three main design approaches in nano manipulation for the liquid and air environment are: robotic arm, Stewart platform and a five-strut crank model. For our experiments we chose nano-manipulation in a liquid environment, which is most relevant within the presented application in nanomedicine. It was demonstrated that computation is relatively cheap for macroscale robotic actuators while arm motion is relatively cheap for nanoscale robotic actuators. Thus the moment-by-moment computer control of arm trajectories is the appropriate paradigm for macroscale robots, but not for nanoscale robots [07]. For nanoscale robots, the appropriate manipulator control is often trajectory trial and error, also known as sensor based motion control [11].

3.1 Virtual Environment

Virtual Reality was used for the nanorobot design where the use of macro and microrobotic concepts is considered a practical approach once the theoretical and practical assumptions here have focused on its domain of appliance. The design should be robust enough to operate in a complex environment with movement in six-degrees-of-freedom. Nanoscale object manipulation systems have been applied with the use of computer graphics for teleoperation. The requirements for such systems have been clearly established [18]. A starting point for our hypotheses and experiments was to consider the robot design derived from biological models and comprised of some basic nanoscale components such as *molecular sorting rotors* and a *telescoping manipulator* (robot arm) [06]. The robot design adopted concepts provided from underwater robotics [21] - keeping in mind however the kinetics assumptions that the nanorobot lives in a world of viscosity, where friction, adhesion, and viscous forces are paramount and gravitational forces are of little or no importance [07]. The obstacles will be located in unknown positions (figure 1). The delivery positions that represent organ inlets requiring proteins to be injected are located in a well-known position for the nanorobot teams

- if these organ inlets are (or are not) scheduled for injection at time t, they will change their colours, indicating the opening or closing of the team *A* (blue nanorobots) and *B*'s (yellow nanorobots) delivery orifice, which will indicate for the agents if they could perform their delivery in the correct order (figure 2). The trajectories and positions of each molecule is generated randomly and each molecule also has a probabilistic motion acceleration. The nanorobot navigation uses plane surfaces (three fins total) and bi-directional propellers, which is comprised of two simultaneously counter-rotating screw drives for the propulsion [07]. The nanorobot has sensors which report collisions and identify when an encountered object is an obstacle to be avoided or a molecule to be caught. While some molecules are being captured (figure 3), other molecules will be assembled internally by the robot arm.

3.2 Physically Based Simulation

The study of non-penetrating rigid bodies in virtual reality for dynamic constrained simulation is a field of research in computer graphics that has an enormous impact for physically based simulation and a large range of works in this field have produced good achievements. Particularly in calculating motions of many objects that move under changing constraints and frequently make collisions, one of the key issues of dynamic simulation methods is calculation of collision impulse between rigid bodies. The correlation between contact force and relative normal acceleration could be expressed as a linear programming problem [02], what permits to calculate the collision impulse that works between rigid bodies colliding at multiple points. Furthermore the relation between collision impulse and relative normal velocity could be also expressed as a linear complementary problem. A simple and fast algorithm for calculating contact force with friction by formulating the relation between force and relative acceleration as a linear complementary problem was equally demonstrated [03], and this model was based on Dantzig's algorithm or solving linear complementary problem. Baraff's algorithm has achieved great performance for real-time and interactive simulation of two-dimensional mechanisms with contact force, friction force and collision impulse, although friction impulse at collision was not completely covered in such model.
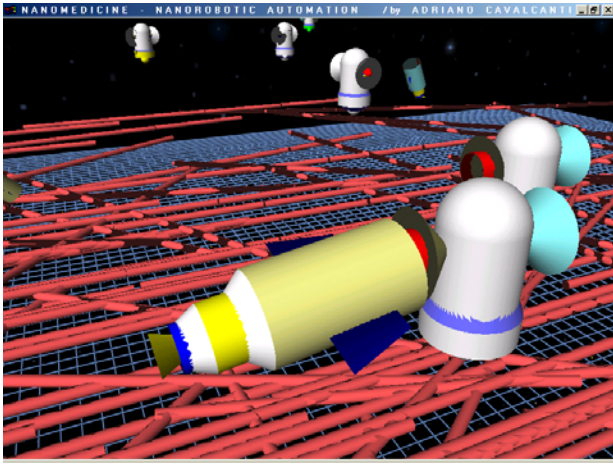
Figure 2. Nanorobot molecule delivery to the organ inlet - represented by the white cylinder.

Figure 3. Molecular identification by collisions contact.

Therefore was established a complementary algorithm covering as well the "impulse-based" aspects, which can trace in detail the change of friction force at a single colliding point by numerical integration of both contact force and friction force [16]. In the physical world, there are no perfectly planar faces or perfectly straight edges, and specifically at a nanoscopic level all contacts can be modelled as a composition of point contacts. Basically the problem of collision detection corresponds to determining whether there is any contact between two objects. We can express the exact conditions for dynamically contact forces as a vector C of contact force magnitude, which is correct if it satisfies some of the basic conditions discussed next. There is no object interpenetration through contact forces for rigid body, and any contact force can only push any related object. The contact force could not be used to pull any 3D object, it affects just the contact points and anything else otherwise. For dynamic collision detection the contact force express a continuous behaviour related to the function of time. Such assumptions are necessary for any correct contact force function that intends to produce a dynamically correct motion. It is possible to happen multiple correct contact force and when some similar circumstances arises the right solution is given using an equation of compatibility, what is precluded by the rigid body assumption, nevertheless any correct result provided by the contact force C result in the same correct motion [02]. The motion of a rigid body subject to external forces is described by the Newton-Euler motion equations as follows:

$$\dot{v} = \frac{1}{m}\sum_{i=1}^{k} f(C)_i \qquad (01)$$

$$\dot{w} = I^{-1}\left(\sum_{i=1}^{k} C_i \times f(C)_i - w \times Iw\right) \qquad (02)$$

where $\dot{v}$ is the dotted velocity vector, $\dot{w}$ is the dotted normal contact distance vector, $f(C)_i$ are the external forces (including contact forces), C_i are the vectors which point from the center of mass to the points where the force apply,
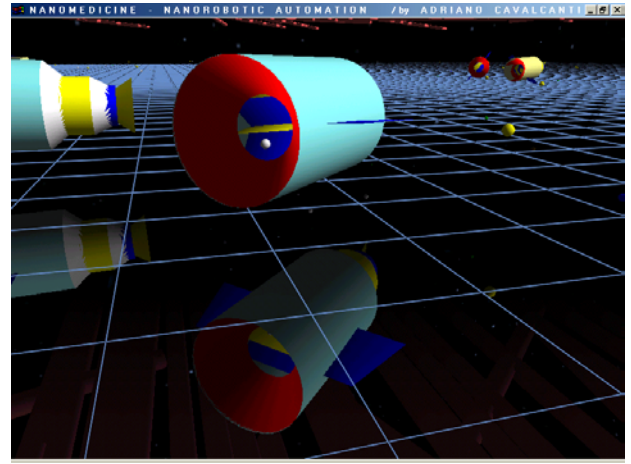
I denotes the inertia tensor, and m the object mass. We are interested to verify when the objects begin to their motion if there is any contact between the objects. For rigid body simulation there are two types of contacts [13] that we could identify as *tangential collision* and *boundary collision*.

Tangential Collisions: this corresponds to a tangential intersection between two surfaces at a geometric contact point. The contact point lies in the interior of each surface and the normal vectors at that point are collinear. Equation 03 expresses a tangential intersection.

$$E(s,t) = P(u,v) \qquad (03)$$

$$(E_s(s,t) \times E_t(s,t)) \bullet P_u(u,v) = 0 \qquad (04)$$

$$(E_s(s,t) \times E_t(s,t)) \bullet P_v(u,v) = 0 \qquad (05)$$

with E(s,t) and P(u,v) representing two parametric surfaces, we assume that the Bézier surface has an algebraic formulation in homogeneous coordinates as:

$$E(s,t) = (X(s,t), Y(s,t), Z(s,t), W(s,t)) \qquad (06)$$

$$P(u,v) = (\overline{X}(u,v), \overline{Y}(u,v), \overline{Z}(u,v), \overline{W}(u,v)) \qquad (07)$$

where E_s, E_t, P_u, P_v correspond to the partial derivatives and $\bullet$ corresponds to the dot product. Equation 03 corresponds to a contact between the two surfaces; equation 04 and 05 represent the fact that their normals are collinear. They are expressed as scalar triple product of the vector. This is an over constrained system and has a solution only when the two surfaces are touching each other tangentially. For such equations, after cross multiplication we get 3 polynomial equations of degree 2n each. The dot product results in the addition of degrees of the numerator polynomials. Similarly for two algebraic surfaces, the problem of tangential intersection can be formulated as:

$$e(x,y,z) = p(x,y,z) = 0 \qquad (08)$$

with

$$\begin{pmatrix} e_x(x,y,z) \\ e_y(x,y,z) \\ e_z(x,y,z) \end{pmatrix} = \theta \begin{pmatrix} p_x(x,y,z) \\ p_y(x,y,z) \\ p_z(x,y,z) \end{pmatrix} \cdot \qquad (09)$$

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Equation 08 and 09 correspond equally to an over constrained system.

Boundary Collisions: this intersection lies on the boundary curve of one of two surfaces. Thus given a Bézier surface, defined over the domain, $(s,t) \in [0,1] \times [0,1]$, we obtain the boundary curves by substituting s or t to be 0 or 1. The resulting problem reduces to solving the equation:

$$E(s,1) = P(u,v) . \tag{10}$$

Two objects collide if equations 03 or 10 for parametric surfaces and the 06 for algebraic surfaces have a common solution in their domain. Physically based simulation was used to consider kinetics and frictional aspects required specially for rigid body motion with hydrodynamics at low Reynolds number [07] and molecular assembly manipulation.

3.3 Cooperative Multi-Robot Teams

The approach for the nanomedicine problem here could be described as two multi-robots teams which must cooperate interactively to feed a set of organ inlets in the virtual environment under study. Research on multi-robot teams working cooperatively to achieve a single global task suggests that we should consider emulating the methods of the social insects [17], because nature is showing us how to build decentralized and distributed systems that are autonomous and capable of accomplishing tasks through the interaction of agents with the same structures and pre-programmed actions and goals. Kube [12] has pointed out that a careful decomposition of the main problem task into subtasks with action based on local sensor-based perception could generate multi-robot coherent behaviours without explicit communication. 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 t have to be fed first by the agent A and so forth. Both agents must take care to avoid applying an overdose or deficiency of the injected substances. The multi-robot team behaviour interaction rule is described at table 1, with Ω denoting if the robot r belongs to team A or B, where e, g and h represent the kind of molecule to be assembled by each multi-robot team, therefore:

Table 1. Multi-Robot teams interaction rule.

Step 1:	r_Ω walk randomly to capture β and δ;
Step 2:	if $\sum \beta = \sum \delta$ → assemble f(r_Ω)= β + δ;
Step 3:	if $\sum$ f(r_Ω) < min repeat step 1;
Step 4:	r_Ω achieve next delivery goal;
Step 5:	if delivery_permition = true → delivery: f(r_Ω) = f(r_Ω) -1;
Step 6:	if f(r_Ω)>0 repeat step 4;
Step 7:	repeat step 1;

$$\beta \begin{cases} \Omega = A & \Rightarrow & \beta = e, \\ \Omega = B & \Rightarrow & \beta = h, \end{cases} \tag{11}$$

$$\delta = g . \tag{12}$$

The *min* denotes the minimum defined to be captured by each nanorobot at time step t. The decision control model uses adaptive evolutionary characteristics [04], thus each autonomous decision is represented as a chromosome describing the agent decision on how, when and what organ inlets to attend at time t. Next is described the multi-objective model for the dynamic decision problem.

$$Max \quad f(r_\Omega) = \sum_{t=1}^{n} \sum_{i=1}^{m} w_i^t - \left| y^t \right| \tag{13}$$

$$\text{s.t.} \quad y^t = Q^t - d \; ; \tag{14}$$

$$Q^t = \sum x_i^t \le L ; \tag{15}$$

$$x_i^t = \mu_i^t x_i^{max} ; \tag{16}$$

$$\mu_i^t \le \Delta_i^{max} ; \tag{17}$$

$$w_i^{t+1} = w_i^t - \gamma z_i^t + x_i^t ; \tag{18}$$

$$w_i^{min} \le w_i^t \le w_i^{max} ; \tag{19}$$

$$\mu_i^t \in \{\{0,1\} \vee \{0.00,...,1.00\}\}; \tag{20}$$

where

r, t, i:	subscript denoting: robot, time, organ inlet.
max, min:	maximum and minimum relative capacity;
n:	size of time in the simulated scenery.
m:	total of organ inlets to be fed.
L:	robot load capacity.
y^t :	surplus/deficit to the desired assembled mean.
x_i^t :	substance amount injected in the organ inlet i.
Q^t :	total assembled molecule by r in t.
w_i^t :	chemical state of the organ inlet i at time t.
z_i^t :	substance consumption by organ inlet i.
d :	desired assembled substances rate.
γ :	parameter to look ahead nutritional levels.
μ_i^t :	boolean variable.
Ω:	determines if r belongs to team A or B.
Δ :	maximum to be injected in organ inlet i;

Equation 13 represents our fitness function, where the robots maximize the protein levels for the selected organ inlets; the variable y induces the robot to catch a number of molecules as closely as possible to the desired delivery mean. The proposed nanorobot model here includes no kind of nanorobot self-replicating behaviour. Instead, it uses an evolutionary approach strictly for the combinatorial analyses, allowing the nanorobots to react cooperatively in an uncertain environment with a well defined pre-programmed set of actions. In our architecture implementation, we use real time and parallel processing techniques which was required to provide a real time coherent multi-robot collective behaviour.
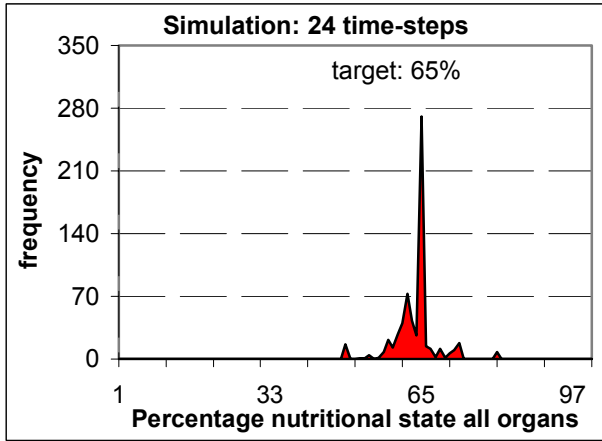
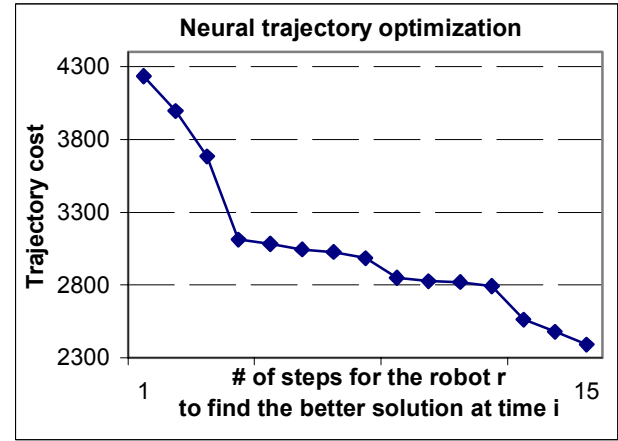**Figure 4.** Multi-robot cooperative reaction.

Figure 5. Motion control cost minimization.

3.4 Neural Motion

A connectionist model using artificial neural networks (ANN) was chosen for the motion control and shortest-path problem solution, where we are going to lead with a dynamic combinatorial problem for each time-step simulation. The classical problem of finding an optimal three-dimensional shortest path avoiding polygonal obstacles was demonstrated as typical NP-hard [10]. The use of a non-deterministic approach to solve the motion control seems to be the appropriate technique in such cases [08]. In our case we have implemented a feedforward or acyclic network due to its suitability for probabilistic calculations. The model particularly implemented here is known as a Neural Sigmoid Belief Network (NSBN) (table 2) [10], which requires a lower computational effort in comparison with a backpropagation approach. The properties of a NSBN could be described by equation 21:

$$pa(X_j) \subseteq \{X_1, X_2, ..., X_{j-1}\} \qquad (21)$$

Table 2. NSBN pseudo code.

```
timeSeconds=Φ;
time_begin = time(NULL);
do{//Generate NSBN Solutions
j=0;
for(move=0;move<nDestiny;move++)
{ neuronActive=randomLayer(nDestiny-move);
// Take the activated neurons.
search.sequence[j]=neuronSelect[neuronActive];
for(i=neuronActive;i<(nDestiny-move)-1;i++)
{ neuronSelect[i]=neuronSelect[i+1];
}
j++;
}
// Compare the actual cost and take this
// solution if it has the best cost.
reckonNeuralCost();
time_end = time(NULL);
}while(time_end - time_begin < timeSeconds);
```

where X represents a vector, consisting of the two-valued random variables $X1, X2, ..., Xn$, defining a topology composed of N stochastic neurons. With n representing the range of hidden layer, which leads the network to be optimised at the time-step t, it represents each destiny to be achieved for each agent through the simulation. The units in the network are organized into a two-dimensional n rows by m columns matrix A_{mn}, where n and m is the costs matrix of destinations to be performed by each evolutionary agent, which tries to complete its set of tasks successfully as fast as possible. Let the output of the unit in row i and column j be $v_{ij} = 1$, where $i \neq j$. This means that the referred destination is visited at the ith stop, with $v_{ij} = 0$ otherwise. Therefore, a solution cost for each agent routing could be expressed by equation 22.

$$Min \quad P_r^t = \sum_i \sum_j v_i w_{ij} \qquad (22)$$

4. SIMULATION AND CONCLUSIONS

The present work (1) considers the importance of nanosystems design in nanomedicine using multi-robot teams exhibiting cooperative autonomous behaviour, and (2) presents an advanced three-dimensional graphic environment using neural motion and physically based simulation applied to assembly tasks. A coherent team behaviour with a fast adaptive reaction was suitably achieved with the parameter organs' nutritional level starting at 65%. It could be demonstrated (figure 4) that the implemented model has generated satisfactory performances for maintaining the organs' nutritional levels, where just a few levels were a bit higher or lower and most values ranged around 65%, clearly indicating that there were no overdoses or deficiencies of the nutritional levels, as the most ideal state was considered to be a level ranging between 50% and 70%. We considered in the simulation a level of 90% as a near to an overdose and 10% as near to deficiency state. The nanorobot has required a motion control model based on either of two main aspects: optimization of the trajectory distance, and real time analyses for a required trajectory which enables the delivery of assembled biomolecules with avoidance of obstacles. The use of Artificial Neural Networks appears to be a suitable approach for the nanorobot motion analysis in a 6-degrees-of-freedom virtual

environment. Neural motion control achieves suitable results (figure 5) with a low processing requirement, providing shortest-path values ~ 44% better than a *greedy* solution for the route distance minimization problem. The coherent behaviour displayed for the transport task can also be attributed to the common goal shared by the individual medical nanorobots along with an identical set of interaction rules, similar to the effect observed by collective decision-making in honey-bees. These results indicate that the approach described in this work might also be a promising system design for assembly automation in nanotechnology.

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Adriano Cavalcanti is a fellow of the technical staff at Fraunhofer Institute for Computer Graphics, where he develops works on several research projects related to virtual reality, autonomous systems, and 3D physically based simulation. He holds a BS in Computer Science from Sao Paulo State University, and a MS in Electrical Engineering focusing on automation and control from Campinas State University, Brazil. He is currently a PhD student in the Computer Science Dept. at Darmstadt University of Technology. Fraunhoferstr. 05 Darmstadt 64283 Germany, E-mail: adasilva@igd.fhg.de .

Robert A. Freitas Jr. is a Research Scientist at Zyvex Corp. in Richardson, Texas, a Research Fellow at the Institute for Molecular Manufacturing in Palo Alto, California, and the author of Nanomedicine, Volume I (Landes Bioscience, 1999), the first technical book on the medical applications of molecular nanotechnology and medical nanorobotics. He holds degrees in physics, psychology, and law. Richardson TX 75081 USA, E-mail: rfreitas@zyvex.com .