Assembly Automation with Evolutionary Nanorobots and Sensor-Based Control applied to Nanomedicine

Adriano Cavalcanti, *Member, IEEE*

***Abstract*—The author presents a new approach within advanced graphics simulations for the problem of nano-assembly automation and its application for medicine. The problem under study concentrates its main focus on nanorobot control design for assembly manipulation and the use of evolutionary competitive agents as a suitable way to warranty the robustness on the proposed model. Thereby the presented paper summarizes as well distinct aspects of some techniques required to achieve a successful nano-planning system design and its simulation visualization in real time.**

***Index Terms*—Biomedical computing, control systems, genetic algorithms, mobile robots, nanotechnology, virtual reality.**

I. Introduction

The presented paper describe the design and simulation of a mobile nanorobot in atomic scales to perform biomolecular assembly manipulation for nanomedicine [12]. For the model robustness investigation we present a competitive scenery where the nanorobot must react adaptively in face of an adversary agent in a dynamic environment. The assembled biomolecules will be delivered into a set of predefined organ inlets, and such deliveries must also keep the nutritional levels of the organism under control. The motivation for such study is the fact that with the emerging era of molecular engineering, the development of methodologies that aims the experimental investigation enabling the automation, and evaluation of new approaches for a better comprehension of the nanoworlds, has a great impact for an effective design and development on nanotechnology.

The most important challenge and that has become evident as a vital problem for the nanotechnology fast development with its industrial application is the automation of atoms manipulation [4]. The starting point of nanotechnology to achieve the main goal of build systems at nanoscale is the development of control automation for molecular machine systems, which could enable a massively manufacture of nano-device building blocks. For such aim new methodologies and theory to explore the nano-world are the key technology [9]. Governments all around the world have addressed significant resources for a fast development of nanotechnology. In Germany only the Federal Ministry of Education and Research has announced 50 million Euros to be invested in the years 2002-2006 in research and development on nanotechnology [21]. More specifically the firm DisplaySearch predicts rapid market growth from US$ 84 million today to $ 1.6 Billion in 2007 [20]. A first series of commercially nanoproducts has been announced also as foreseeable for 2007, and to reach this goal of build organic electronics, firms are forming collaborations and alliances that bring together new nanoproducts through the joint effort from companies such as IBM, Motorola, Philips Electronics, PARC, Xerox, Hewlett Packard, Dow Chemical, Bell Laboratories, Intel Corp., just to quote a few ones [13], [20].

Building patterns and manipulating atoms with the use of Scanning Probe Microscope (SPM) such as Atomic Force Microscopy and Scanning Tunneling Microscopy has been used with satisfactory success as a promising approach for the construction of nanoelectromechanical systems (NEMS) with 3D precision on 0.01nm resolution [22], however such manual manipulations require much time and once that is a repetitive task, it tends to be an imprecise work when performed manually for a large number of molecules. Practical approaches for nano-planning systems has been presented as a first step towards automating assembly tasks in nanorobotics, where was presented a 2D positional assembly automation [17]. Arguments on the appliance of artificial intelligence as the appropriate means to enable some aspects of intelligent behavior to control of nanorobots for molecular manufacturing automation has been discussed in the nano community [25]. More recent work has converged to the advances onto development of a nanorobotics autonomous system capable of performing 200,000 accurate measurements per second at atomic scale [18]. An Intel's prototype 90nm process facility has already produced a fully functional 52Mb SRAM with transistor gate lengths of 50nm and SRAM cell sizes of just $1\mu m^2$, or roughly half the cell size of today's most advanced SRAMs [13]. This downscaling will continue, according to the Semicondutor Industry Association's roadmap, high-performance ICs will contain by 2016 more than 8.8 billion transistors in an area 280 mm^2 - more than 25 times as many as on today's chips built with 130-nm feature sizes [13].

II. Nanomedicine

The principal focus in the medicine is going to shift from medical science to medical engineering, where the design of

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A. Cavalcanti is with the Fraunhofer Institute for Computer Graphics, Fraunhoferstr. 5, Raum 109, 64283 Darmstadt, Germany (phone: +49-6151-155-409; fax: +49-6151-155-499; email: adrianocavalcanti@ieee.org).

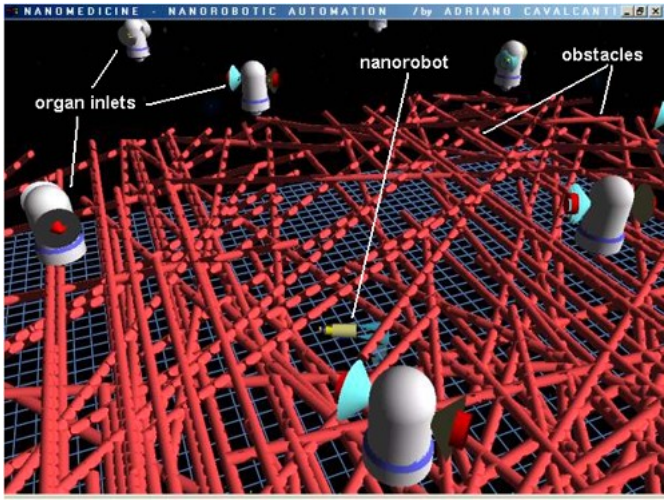

Fig. 1. Virtual environment, top camera view.

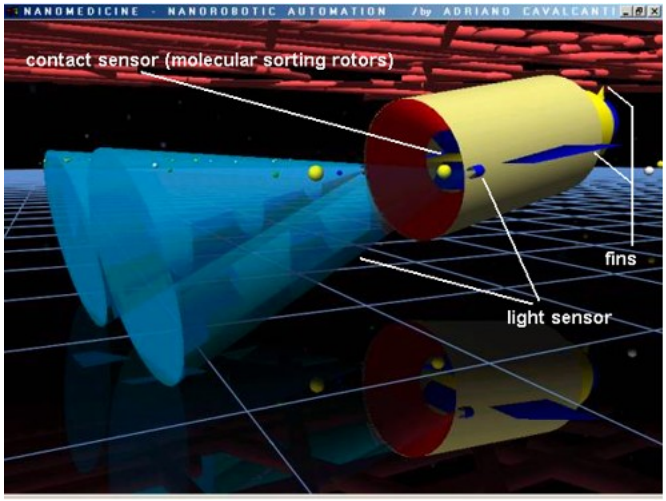

Fig. 2. Molecular identification.

medically-active microscopic machines will be the consequent result of the techniques provide from human molecular structure knowledge derived of 20th and beginning of 21st century [6]. For the feasibility of such achievements in nanomedicine two primary capabilities fabrication has to be fulfilled: fabrication of parts and assembly of parts. Through the use of different approaches such as biotechnology, supramolecular chemistry, and scanning probes, both capabilities were demonstrated in 1998 [12]. In despite of quantum effects which gets a relative uncertainty to electron positions, the quantum probability function of electrons in atoms tends to drop off exponentially with distance outside the atom, and even in most liquids at their boiling points, each molecule is free to move only ~0.07 nm from its average position [12]. Recent developments on the field of biomolecular computing [1] has demonstrated positively the feasibility of processing logic tasks by bio-computers [14], which is a promising first step to enable future nanoprocessors with increasingly complexity. Studies in the sense of building biosensors [24] and nano-kinetic devices [23], [2], which is required to enable nanorobotics operation and locomotion, has been advanced recently too. Classical objections related to the real feasibility of nanotechnology, such as quantum mechanics, thermal motions and friction, has been considered and resolved [12] and discussions about the manufacturing of nanodevises is growing up [10].

III. Proposed design

Molecular machine systems could be described as a system capable to perform molecular manufacturing in atomic scale [4]. The nanorobot presented here will be required to perform a pre-established set of tasks in the human body similarly like a ribosome [12], which is a natural molecular machine system.

Actually the three main design approaches in nano manipulation for liquid and air environment are: robotic arm, Stewart platform and a five-strut crank model [6]; for our experiments we chose a robotic arm with nano-manipulation in liquid environment, which is more suitable within the presented application for nanomedicine. It was demonstrated that computation is relatively cheap for macroscale robotic actuators while arm motion is relatively cheap for nanoscale robotic actuators [12]. 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 is often trajectory trial and error, also known as sensor based motion control [15], [5], [6].

A. Virtual Environment and Nanorobot Design

Virtual Reality was used for the nanorobot design where is considered as a suitable approach the use of macro and microrobotics concepts once the theoretical and practical assumptions here was done focusing on its domain of appliance, which intends to be robust enough to operate in an environment with movement in six-degrees-of-freedom (see figure 1). The nanorobot design (figure 2) is derived from biological models and comprised by some components such as *molecular sorting rotors* and a robot arm (*telescoping manipulator*) [9], meanwhile for the nanorobot locomotion was assumed some concepts provided from underwater robotics [26]. The trajectories and position of each molecule, which has to be captured and assembled, were generated randomly and each one has also a probabilistic motion acceleration. In the simulation while some molecules have been captured (figure 2), other molecules are manipulated and assembled internally by the robot arm into the proposed nanorobot.

The nanorobot uses a macrotransponder navigational system that has been addressed for the main aspects of the nanorobot positioning, which may keep high positional accuracy to each nanorobot's orientation [12]. Such a system might involve externally generated signal from beacons placed at fixed positions outside the skin [19]. Thus the delivery positions that represent organ inlets requiring proteins to be injected are located in a well-known location for the nanorobot; if these organ inlets are or not schedule for injection at time t, they change their delivery orifice's colors getting it open or closed

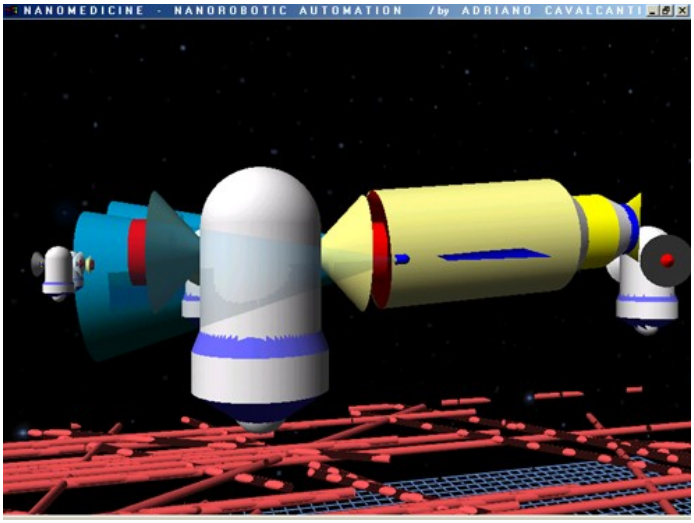

Fig. 3. Nanorobot molecule delivery.

(figure 3). Thus assembled molecules are delivered to specific locations by nanorobot's docking at 2 micron^2 (~1.4-micron square) embedded at appropriate spatial intervals across the organ inlets orifice, which is open for the delivery. The assembled molecule can be pumped by the molecular sorting rotors in ~10 seconds [11].

The nanorobot is comprised by sensors [24] that inform if a collision happens and identify when it is an obstacle, which in such cases will require a new trajectory planning. Plane surfaces (three fins total) and bi-directional propellers are used for the navigation, which is comprised by two simultaneously counter-rotating screw drives for the propulsion [6]. We are using binary cues to trigger the behavioral response as a common mechanism for action and for governing different phases of activity in tasks as done by social insects [8]. 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 information can be provided by either touch sensors or infra-red sensors. For example, a motor behavior created to make a robot rotate $\sin(\Phi)$, where Φ assumes a set of possible predefined values, changes the robot route avoiding a collision between the nanorobot and some undesirable obstacle. If infra-red sensor are used then about the point of contact, it could specify when both light sensors are in contact with some obstacle as illustrated in figure 4, and return a binary "11" value. 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 [16].

For the kinetics assumptions the nanorobot lives in a world of viscosity, where friction, adhesion, and viscous forces are paramount [12]. Observing environmental characteristics related to nano-worlds the gravitational force here is negligible [9]. The author used physically based simulation [4] to consider kinetics and frictional aspects required specially for rigid body motion with hydrodynamics at low Reynolds number [12] and molecular assembly manipulation. The

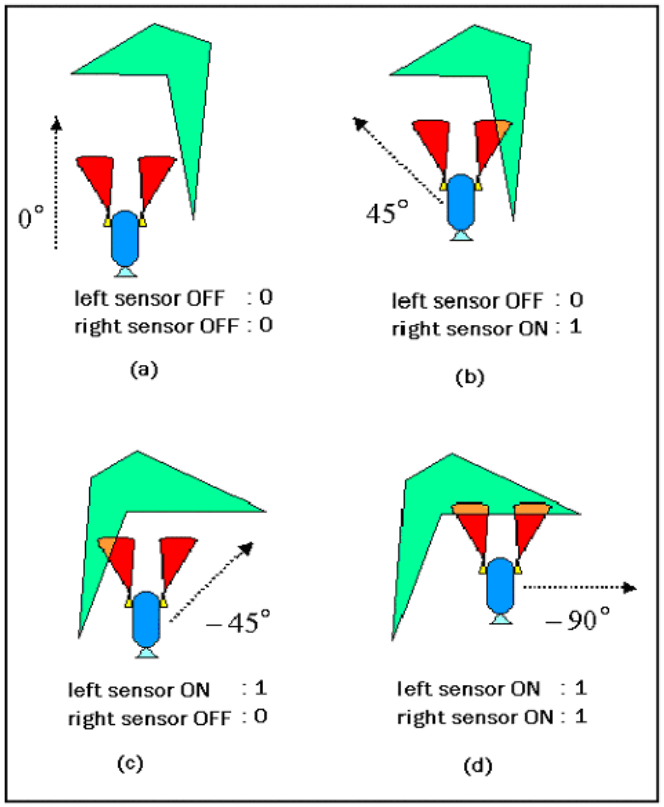

Fig. 4. Sensor-based navigational behavior.

obstacles are located in probabilistic positions (figures 5 and 6).

B.Evolutionary Decision

We intend to construct and validate a nano-planning system, where through the use of competitive evolutionary agents shall enable a better tuned validation for the control automation of our nanorobot under study, thus they compete against each other (figure 7) in the sense that meanwhile one agent try to improve the organism health in the represented living three-dimensional environment, the reagent try to debilitate the same organism through the injection of inappropriate assembled substances into the organ inlets. The evolutionary model, which is used here is cited in the literature as Genetic Algorithms (GA), relies on concepts derived from evolution and genetics [4].

Each solution here is described as a chromosome regarding the agent decision on how, when and what organ inlets to attend in the dynamic scenery, and each decision required to be taken by the nanorobot is always attaining the programmed set of action rigidly pre-established in our design by the fitness function. Equation 1 represents our fitness/objective function, where the agent maximizes the protein levels for the selected organ inlets, meanwhile the reagent minimizes the same parameter. The variable y induces the nanorobot to catch a number of molecules as closely as possible to the desired delivery mean, while z brings the nutritional levels as close as possible to w_i^*.

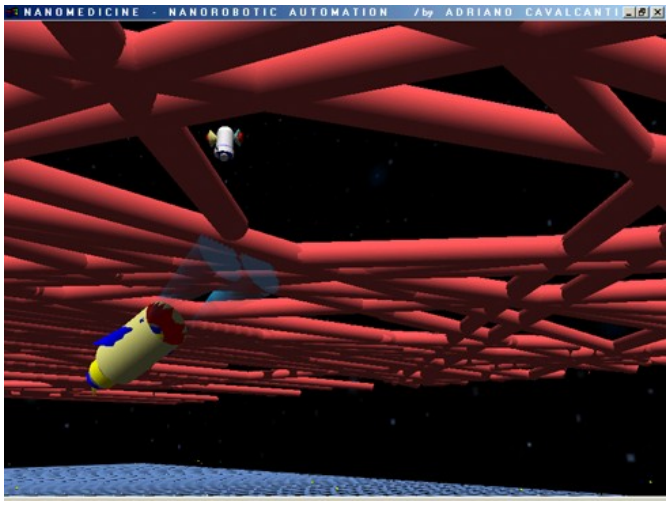

Fig. 5. Sensing obstacles.

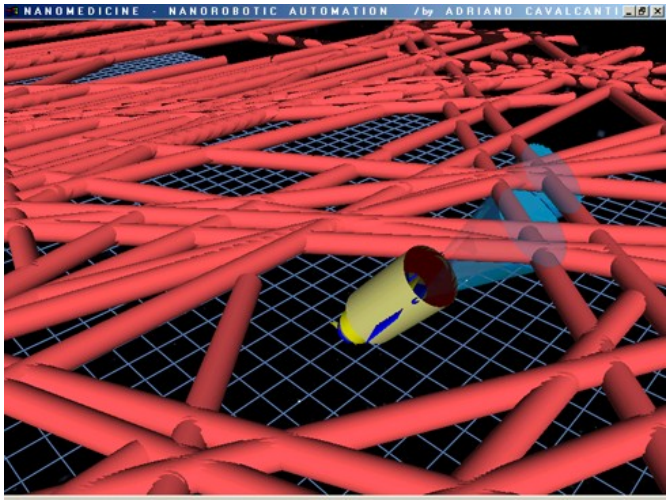

Fig. 6. Nanorobot obstacle avoidance.

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

s.t.
$$z_i^t = w_i^{t+1} - w_i^* \tag{2}$$
$$y^t = Q^t - d \tag{3}$$
$$Q^t = \sum x_i^t \le L \tag{4}$$
$$x_i^t = \mu_i^t x_i^{\max} \tag{5}$$
$$\mu_i^t \le \Delta_i^{\max} \tag{6}$$
$$w_i^{t+1} = w_i^t - \gamma\psi s_i^t + \psi x_i^t \tag{7}$$
$$w_i^{\min} \le w_i^t \le w_i^{\max} \tag{8}$$
$$\mu_i^t \in \{\{0,100\} \vee \{0,1\}\} \tag{9}$$
$$\Omega \in \{A, B\} \tag{10}$$
$$\psi \begin{cases} \Omega = A \Rightarrow & \psi = 1; \\ \Omega = B \Rightarrow & \psi = -1; \end{cases} \tag{11}$$

where

r, t, i:	subscript denoting: robot, time, organ inlet.
w_i^*:	organ inlets' desirable nutritional target level.
y^t:	surplus/deficit to the desired assembled mean.

Fig. 7. Competitive agent and reagent in action.

TABLE I
COMPETITIVE NANOROBOT INTERACTION RULE

Step 1: r_Ω walk randomly to capture β and δ;
Step 2: if $\sum \beta = \sum \delta \rightarrow$ assemble $f(r_\Omega) = \beta + \delta$;
Step 3: if $\sum f(r_\Omega) <$ min repeat step 1;
Step 4: r_Ω achieve next delivery goal regarding the delivery queue;
Step 5: if $\Omega = B$ go to step 7, otherwise next step;
Step 6: if delivery_NOT_overdose = true $\rightarrow$ next step; otherwise go to step 8;
Step 7: delivery: $f(r_\Omega) = f(r_\Omega) - 1$;
Step 8: if $f(r_\Omega) > 0$ repeat step 4;
Step 9: repeat step 1;

z:	keep the nutritional levels close to the target.
max, min:	upper and lower bound parameter.
A, B:	agent and reagent respectively.
n:	size of time in the simulated scenery.
m:	total of organ inlets to be fed.
L:	robot load capacity.
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*.
s_i^t:	adversary substance injected to organ inlet *i*.
d:	desired assembled substances rate.
γ:	parameter to look ahead nutritional levels.
μ_i^t:	boolean variable.
ψ:	determines the kind of behavior for *r*.
Ω:	determines if *r* is agent or reagent.
Δ:	maximum to be injected at organ *i* in *t*.

The competitive nanorobot interactive rule is described in the table 1, where e, g and h represent the kind of molecule to be assembled by *r*, therefore:

$$\beta \begin{cases} \Omega = A \Rightarrow & \beta = e, \\ \Omega = B \Rightarrow & \beta = h, \end{cases} \tag{12}$$

$$\delta = g. \tag{13}$$

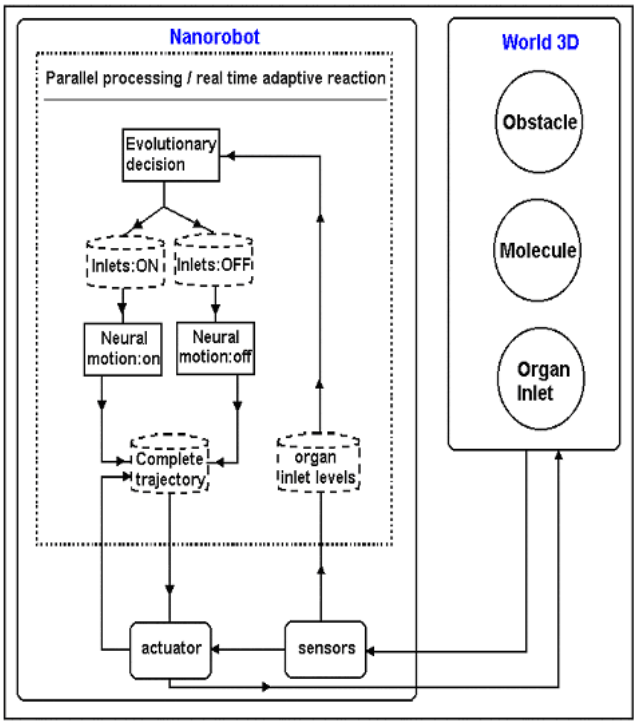

Fig. 8. Multi-modular system architecture.

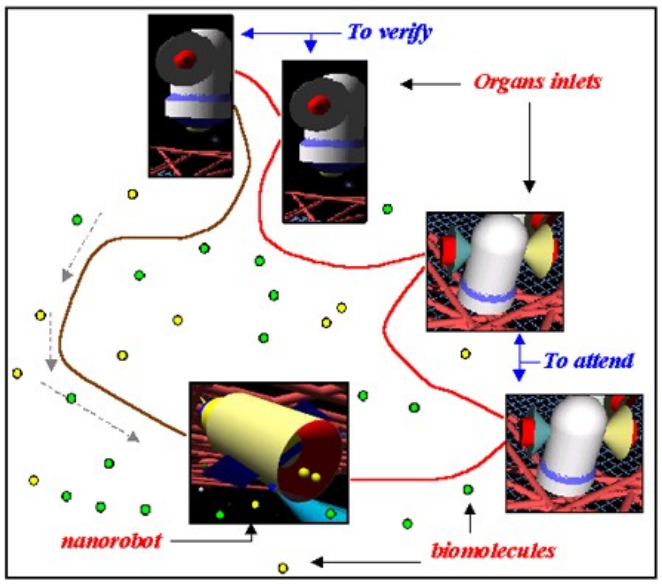

Fig. 9. Nanorobot gathers information and biomolecules.

Multidisciplinary control design (figure 8) has been taken to address the nanorobot's multi-modular system architecture [7]. A feedforward neural networks model was used for the nanorobot motion control [5], where the nanorobot visits each organ inlet to gather information for the next time-step decision in the 3D workspace (figure 9). We used real time and parallel processing techniques [27], where both agents react adaptively to any action performed by its adversary decision with the model visualization in real time [4]. The study of intelligent multi-robot behavior in a single global environment has enabled the most of concepts related to the use of local perception for reactive agents [3], [16], [6].

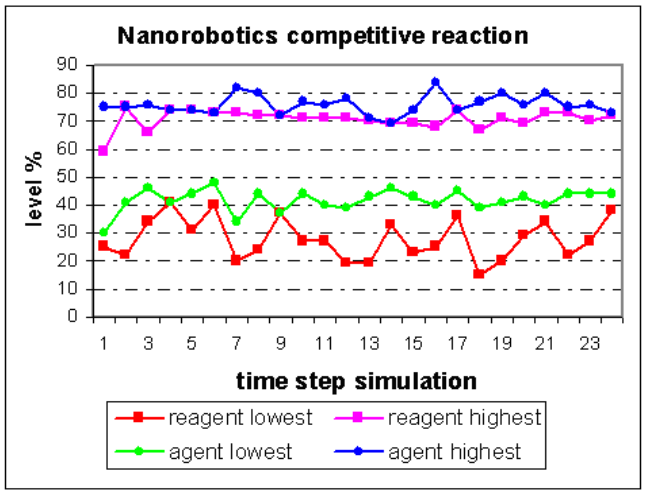

Fig. 10. Highest/lowest organ inlets' nutritional levels.

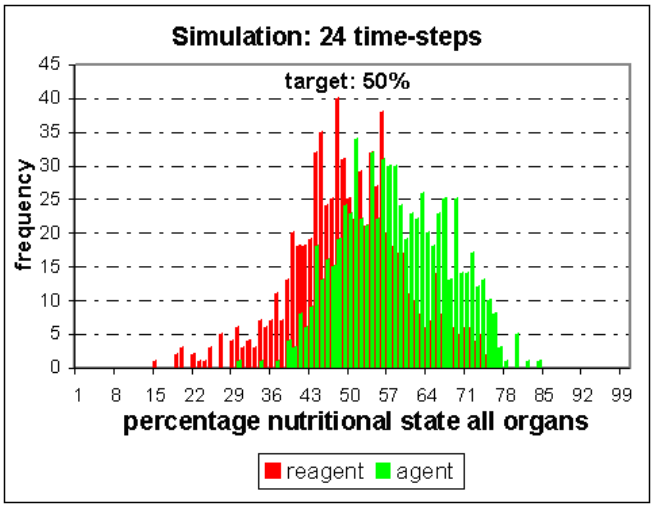

Fig. 11. Histogram with nutritional levels behaviors.

IV. Simulation and Conclusions

Many aspects of control theory and automation models for nanotechnology are still an open and challenging issue demanding further investigation. The use of Computer Graphics as an enabling technology to make feasible many of chemical, physical, and kinetic studies for theoretical and practical analyses of nano-worlds are expected to be playing an important role for the fast development of nanotechnology.

The presented work has intended to elaborate an advanced three-dimensional graphic environment applied to nanosystems design for nanorobotics assembly simulation in nanomedicine, as well as to postulate the use of competitive agents as a systematic way to verify the model robustness in attending real-time control constraints under a large range of uncertainty. We have adopted for the organ inlets' nutritional levels values rounding 50% of the relative organ inlet nutritional capacity as most ideal target. Levels lower than 20% or higher than 80% are characterized as a possible deficiency or overdose case. As we can observe (figures 10 and 11), few occurrences was registered with nutritional levels out from desired ranges, and in such cases the nanorobot agent acts immediately in the

sense to bring the nutritional level into the desirable levels. Thus the main aspects in the proposed study was successfully fulfilled, these results indicating 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 (M'02) received the BS CS from Sao Paulo State University, Brazil, in 1996, and a MS EE focusing on control automation from Campinas State University, Brazil, in 1999. Actually he is a PhD candidate at the Computer Science Department at Darmstadt University of Technology, Germany. He is a fellow of the technical staff at Fraunhofer Institute for Computer Graphics, where he has been developing works on several projects related to virtual reality, autonomous systems, and parallel processing. He is a member of the IEEE.