Space Bionanorobotic Systems: Design and Applications

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Abstract

This paper describes novel concepts of space bionanorobotic systems that are based on revolutionary bio-nano-mechanisms formed by protein and DNA based nano-components. Nano-robots are controllable machines at the nano ($10^{-9}$) meter or molecular scale that are composed of nano-scale components. With the modern scientific capabilities, it has become possible to attempt the creation of nanorobotic devices and interface them with the macro world. There are countless such machines that exist in nature and there is an opportunity to build more of them by mimicking nature. A roadmap towards the progression of this field is proposed and some design concept and philosophies are illustrated. Two macro-scale devices with important space application that will be using bio-nano-component assemblies are proposed. These are the Networked TerraXplorer (NTXp) and The All Terrain Astronaut Bio-Nano Gears (ATB).

1. Introduction

Peering into the future, we can envision a world where life does not take place before our eyes, yet at a level where the building blocks of life are interacting [1]. This world of nanotechnology will enable us to explore, venture, and inhabit places beyond our current realms of reality. But to reach this state of technology, we must begin with the basics. We must understand the biological components that draw a parallel to current macro-robotics. With this knowledge in hand we can continue forward and join these components into assemblies. Some of these assemblies will execute specific tasks, while others perform a number of different operations. Eventually these bio-nano-robots will interact with one another, collaborating to build, repair, and manipulate other objects in the nano-world. Once these nano-robots are shown to sustain and create life, transporting them to far away planets will yield results not currently possible.

1.1 The Roadmap

The roadmap for the development of bio nano systems for space applications is shown in Figure 1. The roadmap progresses through the following four steps that are described in this section.

![Figure 1: The Roadmap, illustrating the system capability targeted as the project progresses](image-url)
constructing newer and complex devices. These nanostructures are potential candidates for integrating and housing the bio-nano components within them. Proteins such as rhodopsin and bacteriorhodopsin are a few examples of such bio-nano components [2]. Our team’s initial work focused on bio-nano actuators, such as the viral protein linear motor concept [3]. These bionano sensors and actuators will form an integral part of the proposed bio-nano assemblies, where these will be integrated within a nano structure and will get activated, as programmed, for gathering the required information at the nano scale.

**Step 2: Assembled Bio Nano Robots**

The next step involves the assembly of functionally stable bio-nano components into complex assemblies. Some examples of such complex assemblies or bionano robots are shown in Figure 2. Figure 2A shows a bio-nano robot with its ‘feet’ made of helical peptides and its body of carbon nano tubes, while the power unit is a biomolecular motor. Figure 2B shows a conceptual representation of modular organization of a bio-nano-robot. The modular organization defines the hierarchy rules and spatial arrangements of various modules of the bio-nano-robots such as: the inner core (brain and energy source for the robot); the actuation unit; the sensory unit; and the signaling and information processing unit. By the beginning of this phase the “library of bio-nano components” will include various categories such as, actuation, energy source, sensory, signaling etc. Thereon, we will be able to design and develop such bionano systems that will have enhanced mobile characteristics, and will be able to transport themselves as well as other objects to desired locations at nano scale.

**Step 3: Distributive Intelligence & Control**

With the design of fully functionalized bio-nano-robots at hand, the issue of collaboration would be studied further. We envision that this phase will lay the foundation to the concept of distributive bio-nano robots (see Figure 3A). Designing bio-nano robots capable of carrying out such complex tasks and capable of computing and collaborating amongst the group will be the focus here. Therefore, the basic computational architectures needs to be developed and rules would need to be evolved for the bio-nano robots to make decisions at nano scale.

**Step 4: Automatic Fabrication and Information Processing Machines**

For carrying out complex missions (such as sensing, signaling and storing), there is a need to create colonies of these bio nano robotic systems. This step would see the emergence of automatic fabrication (Figure 4) of such bio-nano machines in vitro (or maybe in vivo). Development of information processing capabilities, which will involve learning (or error correction) and decision making abilities, would be a major objective of this phase. This would enable distributive bio-nano robots to have ability to self-repair based on its environment and stored information.

**Figure 2 (Step 2):** (A) the bio-nano components would be used to fabricate complex bio robotic systems. A vision of a nano-organism: carbon nano-tubes form the main body; peptide limbs can be used for locomotion and object manipulation and the biomolecular motor located at the head can propel the device in various environments. (B) Modular Organization concept for the Bio Nano robots. Spatial arrangements of the various Modules of the robots are shown. A single bio nano robot will have actuation, sensory and information processing capabilities.

**Figure 3 (Step 3):** (A) shows the basic bio nano robot forming a small swarm of five robots. The spatial arrangement of the individual bio nano robot will define the arrangement of the swarm. (B) A basic bio-nano computational cell. This would be based on one of the properties of the bio molecules, which is “reversibility”.

**Figure 4 (Step 4):** An automatic fabrication Floor layout. Different color represents different Functions in automatic fabrication mechanisms. The arrows indicate the flow of components on the Floor layout. Section 1 ➔ Basic Stimuli storage – Control Expression; Section 2 ➔ Bio molecular component manufacturing (actuator / sensor); Section 3 ➔ Linking of bio-nano components; Section 4 ➔ Fabrication of Bio-nano robots (assemblage of linked bio-nano components)
2. Design Philosophy and Architecture

2.1. Modular Organization

Modular organization defines the fundamental rule and hierarchy for constructing a bio-nano-robotic system. Such construction is performed through stable integration of the individual 'bio-modules' which constitutes the bio-nano-robot. For example, if the entity ABCD, defines a bio-nano-robot having some functional specificity then, A, B, C, and D are said to be the basic bio-modules defining it. The basic construction will be based on the techniques of molecular modeling with emphasis on principles such as Energy Minimization on the hyper surfaces of the bio-modules; Hybrid Quantum-Mechanical and Molecular Mechanical methods; Empirical Force field methods; and Maximum Entropy Production in least time. Further, Modular organization also enables the bio-nano-robots with capabilities such as, organizing into swarms, a feature which is extremely desirable for our proposed space applications. Figure 5 A shows the conceptual representation of Modular Organization. Figure 5 B shows a more realistic scenario in which all the modules are defined in some particular spatial arrangements based on their functionality and structure.

2.2. The Universal Template

The modular construction concept involves designing a universal template for bio-nano systems, which could be 'programmed and grown' into any possible Bio Nano coded system. This concept mimics the embryonic stem cells found in the human beings, that are a kind of primitive human cells which give rise to all other specialized tissues found in a human foetus, and ultimately to all the three trillion cells in an adult human body. Our Bio Nano Stem system will act in a similar way. This universal growth template will be constituted of some basic Bio Nano Codes, which will define the Bio-Nano-STEM system. This STEM system will be designed in a manner that could enable it to be programmed at run-time to any other required bio-module.

2.3. Information Processing and Programming

Capability of information processing is one of the most novel features of the proposed bio-nano system. Here we underline some design aspects on memory storage mechanisms and bio-nano intelligence (decision making and error corrections). The main hypotheses considered for designing such a mechanism are: i) reversibility of the bio-chemical reactions and molecules, and ii) Functions arises from conformations. The basic storage and retrieval mechanism is represented in Figure 6 below.

Figure 6: Showing the Bio Nano Code and the Fractal Modularity Principle. The dotted line represents the "reversibility" of the bio-chemical reaction.

A "Parent Cell" contains two stable structure of DNAs (DNA 1 and DNA 2) which bind within themselves four trigger ions or similar bio-molecule (Trigger A, Trigger B, Trigger C and Trigger D). These specific numbers of bio-components are used only for illustration purposes, exact number would vary upon the required bio-chemical reactions and the reactants involved in the reaction. Additional four different ions (Ion A, Ion B, Ion C & Ion D) are defined, which would react with the stable conformations of the two DNAs in the parent cell. The working principle is illustrated in the following equations (these equations are representative of the plausible bio-chemical reactions):
Where, the four basic ions are represented by: \( \text{IonA} \); \( \text{IonB} \); \( \text{IonC} \); \( \text{IonD} \) and the DNAs are represented by the following two symbols (for \( j = 1, 2 \)); \( \text{DNA}_{j}^{a};\text{DNA}_{j}^{b} \). The ‘a’ & ‘b’ sub-script represents one of the chains of the double helix of the DNA. The trigger ions are designed to bind with the child DNAs so as to change their conformations. When these trigger ions are released, altered conformations of the DNAs are left in the parent cell. These new conformations should also be stable at those ionic concentrations and field gradients. These released trigger ions flows into the adjacent “memory child” cells thereby changing the conformation their DNAs. Hence, this change in conformation of the DNAs of the child cell along with the parent cell DNAs constitutes the data storage (and retrieval) mechanism (as shown in Figure 7). Four memory child cells are defined in accordance with the possible number of trigger ions generated as a result of the biochemical reactions in the Parent Cell DNAs. This change in conformation will act as the memory storage mechanism for us. This change in the conformation of the DNAs has to be long-term and stable and at the same time reversible under the application of specific conditions (ions, temperature, pressure and pH value of the environment).

While storing the data, the ions (A, B, C & D) are passed through the ion channels connected with the parent cell. Retrieval of the data is the reversible process where the trigger ions are flowed through the ion channels of the memory child cells towards the parent cell (mechanism shown in Figure 7 B). Hence a reversible mechanism is established between the Parent Cell and the Memory child cells. Hence, this efficient information storage device could be used to program the behavior of the bio-nano system which will embed this in its “inner core” module.

**Figure 7 (A): Basic Information Processing Bio Nano Cell; (B) Trigger Release Mechanism - reversible reaction.**

### 2.4. Bio Nano ‘Intelligence’

Integrating bio-nano information storage and programming capability with the functionality of growth and evolution, lays the foundation of Bio-nano intelligence. What exactly is intelligence and how we can simulate intelligence is still an open area of research. Programming, learning and hence evolving could be one combination of events which can quantitatively describe intelligence. Therefore, we equate bio nano intelligence with the ability to “grow” coupled with basic information processing capabilities. Figure 8 depicts our basic concept. The bio-nano computational cells are embedded along the two axes. These axes have different functionalities. **Axis I** is the axis where the information is filtered and various components are sequentially isolated and stored in the bio-nano computational cell. The stimuli obtained by activation of the first block, triggers a reaction, which activates the subsequent blocks along the **Axis I**. The number of blocks would depend upon the bio chemical reaction employed. But there would be facility of increasing this axis at runtime. **Axis G** is the Growth Direction. Along this axis copy of the initial data is made. Once a row is finished along the
Axis I, the Axis G elements are activated. And again the sequencing along the Axis I would start. A single stimulus could trigger multiple outputs through this mechanism. Axis G would also enable parallel computations, thereby accelerating the response to a given input. This is typical of an intelligent living system, where the past stimuli are responded to faster when felt.

**Figure 8:** Mechanism for achieving bio-nano intelligence

Ions play a very crucial role in triggering and controlling the biochemical reaction in our scheme and hence, form the basic element in concept of “experience gathering”. This capability coupled with the above explained advanced information processing mechanism would constitute bio-nano intelligence in our proposed systems. **Ion types** could be related to the **variations in behavior** and **Ion Concentration** could be related to the **intensity** of the behavior of a bio-nano robotic system.

3. Space Applications

3.1. Networked TerraXplorers (NTXp)

Mapping and surveying a vast planetary terrain still remains a very difficult and expensive task. Some of the difficulties faced are limited area of landing for sophisticated planetary probes and rovers (estimated only 5% of the area is suited for landing). The planetary terrains and the atmospheric conditions pose a lot of difficulties for surface as well as air probes. Hence, only limited mobility could be achieved. Also, the investment required would be enormous for designing such rovers with capabilities of exploring the vast and difficult terrains.

Networked TerraXplorers is a concept (Figure 9) in which we exploit various advantages of the proposed bio-nano robotic systems. Advantages such as their extremely light weight; low cost of manufacturing; Mass scale production and bulk usage and their ability to self-assemble and self–replicate. NTXp is a network of channels containing the bio nano robots having the enhanced sensing and signaling capabilities. This essentially is a static device, which could be easily projected onto a surface which we intend to explore. The length of this device could be in miles, and yet it would be very light in weight. These could be easily packaged into small volumes appropriate for space missions. Also the power consumption for this device would be considerably less. The main consumption of power would be to maintain gradients for transporting the bio-nano components inside these channels and for signaling and communicating with the main receiver.

The bio-nano robots will move inside the channels of the network and would have ‘limited’ window of interaction, through special valves with the outside environment. They will interact with the outside terrain and chemically sense the presence of water or other targeted resources / minerals (Figure 10 A & B).

They would also act like a position sensor on the surface of the terrain enabling it with the capability to map the terrain geometrically. It would communicate with their main nodes and would pass the information about the terrain through them to the main receiver (which could be a low altitude orbiter). These networks could be spread throughout the terrain irrespective of the topological constraints. Their mass production would be cheap as compared to any technology available now which could be used to map a terrain.

**Figure 9:** A realistic scenario where the Networked TerraXplorers (NTXp) are employed. These meshes would be launched through the parachute and these would be spread open on the target surface. These NTXps could be launched in large quantities (hundreds) and hence the target terrain could be thoroughly mapped and sensed. A single NTXp could run into miles and when integrated with other NTXPs could cover a vast terrain.
to move its internal contents in a specific direction (depending upon the direction of the target). It could also be triggered such that it concentrates internally towards a particular location of interest so as to generate higher capabilities. Further, the locations from where these NTXps signal could be further explored based on the importance of the discovery. These networks would be designed to be integratable with similar networks. Once these networks are integrated the whole terrain could be mapped by a single “super network”.

NTXps could be designed in two variants: Macro level (as described above) and Micro level. The design of these variants would be based on their level of reach. Macro level variant could be miles long and integrated to a unitary central unit, whereas the micro variant would be only few millimeters (or smaller) in dimensions. The Micro variant (as shown in the Figure 11 below) called as Micro Networked TerraXplorers, is the extension of the NTXp concept. In this concept, the bio-nano robots would perform sensory function, but the signaling function would be performed by the “communication microchip” integrated with the bio-nano system. This microchip would signal the data gathered to the central receiver. This Micro NTXp would be very small in size (few mms or smaller) and could be sprayed from the air borne rover or orbiter to the desired location. These devices would form a sensory network amongst them and would act in collaborative and distributive way. The bio-nano robots would sense and then trigger the micro processor with the findings. These micro networks could be dynamic in nature as these could be easily flown by the high surface winds and currents and in effect would let us know more about the inside details of the structure of the storms and winds on the planet. Figure 11 describes the concept of this device.

3.2. The All Terrain Bio-nano Gears

To ensure enhanced health management capability for astronauts on future space missions, a multifunction system is needed to perform environment monitoring and serve as early warning and protection system against chemicals, radiations, temperature and pressure for the astronauts. This system will be like an adaptive shield protecting...
astronauts from possible health hazards. This device will form a complementary layer beneath the current or any other future space suits. The proposed ATB gear is one such concept that has the above-mentioned capabilities and functionalities. It will not only be lightweight but also flexible enough for allowing the astronauts to wear it all the time.

The ATB gear shown in Figure 12 is like an extra layer of shield on the human body, which will have the capability of sensing dangerous and harmful environments (such as radiations or chemicals) long before they could significantly harm the human. These will not only act like early warning and detection systems but will aid in healing through current process and medicines and curing the damages that may be caused to the astronaut. These “skins” are meant to be all terrain in the sense that these could be worn at any time and anywhere by the astronaut, either inside the space shuttle or on a planetary terrain. They could further be designed to cover specific areas of interest on the space suit, such as locations where the same may show fragility, and monitor these locations all the times. The bio gear will be made of various micro membranes and surface sheets as it is shown in Figure 13. Each one of these membranes and sheets will contain swarms of bio-nano robots capable of performing the required sensing and signaling tasks.

Figure 12: (A) The figure shows a representative structure of the ATB Gear. Shown is the arrangement of the bio-nano swarm inside one of the many channels which forms the ATB gear. (B) The swarms are shown to penetrate the inner layer of the channel for sensory and signaling purposes. The bio-nano swarms will have multiple layers having various layers of functionalities.

The Modular Architecture of the bio-nano robots and its design architecture as described before would give us an ability to manufacture and program them for complex tasks. At run-time we could decide the concentration and the Bio Nano code for the robots required at a particular location along the ATB gear surface. ATB gears could be programmed to form a self-healing layer for the astronaut’s space suit. Figure 14 shows various layers of the ATB gear interweaved with the inner layer of the “space suit” for astronauts. This interweaved concept is designed such that as soon as some breach is detected, the bionano robots inside these ATB gears will rush to the site and try and seal it, as it is shown in Figure 15, and block the effects to seep in through. This will give the astronaut valuable time to find a shelter or other alternative solution. This feature could be especially useful for the terrain mobile astronauts who don’t have immediate accessibility to the facilities of the main station. The ATB gears hence are made an integral part of the space suits, to protect and warn the astronaut against any possible health hazard from the outer environment and within.

Figure 13: The layered concept of the ATB gears. Shown are three layers for the ATB gears. The inner layer would be in contact with the human body and the outer layer would be responsible of sensing the outer environment. The middle layer would be responsible for communicating, signaling and drug delivery.

Furthermore, in case of a wound, these bio-nano robots will cover the skin of the astronaut so that the intensity of the wound is decreased. They could also be designed to deliver the wound healing drugs (stored inside the bio-nano robots) at the particular location of injury. The bio nano robots will have signaling capabilities that will trigger the flow of excess robots at such sites (stored in a stock on board the astronaut suit) and help accelerate the protection sequence. They can also help in sensing the temperature variations in the astronaut’s body and signal any un-natural event if it crosses any particular range.

Also, the harmful radiation protection layer on the outside of the layer will help the astronauts from getting affected by harmful radiations. If the radiations somehow penetrate through the outer layer then the bio robots will trigger an event and will alert the astronaut to seek a more protective place and simultaneously try to cover that breach through the movement of protective agents at that point. This interactive mechanism of ATB Gears to cover up or heal the gap in the ‘main pressure suit’ from where the radiation breach occurred will protect and give them a good
amount of time to seek a more protective place.

Figure 14: Interweaved Concept for the ATB gears

Figure 15: Mechanism of curing a wound by the ATB gear. Shown are the bio-nano robots flowing through various layers and binding amongst themselves and forming a cover over the wound. Also shown are the drug molecules which will be injected into the infected area and thereby will be enhancing the overall rate of recovery for the astronaut.

4. Computational Methods

Molecular modelling techniques [4, 5] in sync with extensive experimentations would form the basis for designing these bio-nano systems. As per the roadmap, various bio-nano components would have to be designed and then these functional elements would have to be bound into assemblies which could be controlled and programmed. The dynamics of these bio-nano component depends upon certain external parameters, such as, temperature, pressure, pH, light, other bio chemical molecules etc. At the same time we need to study the stability for the bio-nano system for the space conditions. The stability of the protein components in the complex environment where all the constraints will act at the same time depends in a very complex way to its primary sequence. Therefore we need to define and model the dynamics of the bio nano components based on these external variational parameters and stability conditions.

For studying the bio-nano system dynamics we would have to study Quantum-Classical and Quantum-Stochastic Molecular Dynamic Models (QCMD) [5] and hence form models for predicting its behavior. Time-dependent quantum mechanical models and theories would play a vital role in these studies related to dynamics of a protein, its interaction with the medium while in transition, its interaction with the other bio-components and modules. While a protein transits from initial conformational state to a subsequent state, while reaching the final state, each instant has to be clearly understood and defined. We propose to utilize bionano components as robotic elements, and hence we require the detailed dynamics of that system and its behavior. In QCMD models there exists a coupling of equation which considers two subsystems, quantum subsystem and classical subsystem. Schrödinger wave equation governs the quantum part and the classical molecular dynamics governs the classical subsystem [5]. The variations in the position and momentum of the classical particles in the system are evaluated using the \( \psi \), wave function of the quantum particles and using the potential energies of the classical and quantum regions.

Further, the dynamics of a bio-nano component or its complex assemblies should be such that they follow a reversible path given particular stimuli and energy for such transformations. This reversibility constraint further imposes stricter restrictions on us in terms of predicting the overall accurate dynamics of the system. To restore the reversibility all the interactions and the potentials have to be reversed, or there could be another path which would lead to the initial state. These studies are of paramount importance to us and would give us more insights into how the system could be designed and further optimized.

These dynamical models have to be coupled with iterative optimization kernels (consisting of expert systems, algorithms, and bio-nano conformation predictor). This would involve creating more optimized mutants of say a protein and sequentially subjecting it to the external parameters and stability conditions. Some of the classical molecular dynamic methods [4, 6, 7] include:

\( a) \) **Empirical force field methods:** (Molecular mechanics): In this method, motion of the electrons is ignored and energy of the system is calculated based on the position of the nucleus in a particular molecular configuration. There are several approximations which are used in this method the very basic is the Born-Oppenheimer. Modelling of bio nano components or the assemblies could be done by one of the energy functions:
\[ V(r^* ) = \sum_{n=0}^{2\pi} \left( \frac{k_n}{2} (l - l_{i, a})^2 + \sum_{\text{atms}} \frac{k_j}{2} (\theta - \theta_{i, a})^2 + \right. \\
\left. \sum_{\text{rest}} \frac{V_r}{2} (1 + \cos(n\omega - \gamma)) + \right. \\
\left. \sum_{\text{rest}} \sum_{\text{inter}} (4\epsilon_{ij} \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{6} + \frac{q_i q_j}{4\pi \varepsilon_r r_{ij}}) \right] \]

Where: \( V(r^* ) \) denotes the potential energy of \( N \) particles having position vector \( (r) \).

**b) Energy minimization methods:** The potential energy depends upon the co-ordinates of the molecular configuration considered. In this method, points on the hypersurface (potential energy surface) are calculated for which the function has the minimum value. Such geometries which correspond to the minimum energy are the stable states of the molecular configuration considered. By this method we can also analyze the change in configuration of the system from one minimum state to another. Methods such as the Newton-Raphson and Quasi-Newton are employed to calculate these minima. This method of finding minimum energy points in the molecule is used to prepare for other advanced calculations such as molecular dynamics or Monte-Carlo simulations. It is further used to predict various properties of the system under study.

**c) Molecular Dynamics Simulation methods:** To begin predicting the dynamic performance (i.e. energy and force calculation) of a bio component (e.g. a peptide) Molecular Dynamics (MD) is performed. This method utilizes Newton's Law of motion through the successive configuration of the system to determine its dynamics. Another variant of molecular dynamics employed in the industry is the Monte Carlo simulation, which utilizes stochastic approach to generate the required configuration of a system. Simulations are performed based on the calculation of the free energy that is released during the transition from one configuration state to the other. In MD, the feasibility of a particular conformation of a biomolecule is dictated by the energy constraints. Hence, a transition from one given state to another must be energetically favorable, unless there is an external impetus that helps the molecule overcome the energy barrier. When a macromolecule changes conformation, the interactions of its individual atoms with each other - as well as with the solvent - constitute a very complex force system. Molecular kinematic simulations [8] are also being used to study the geometric properties and conformational space of the bio molecules (peptides). The kinematic analysis is based on the development of direct and inverse kinematic models and their use towards the workspace analysis of the bio molecules. This computational study calculates all geometrically feasible conformations of the bio molecule i.e. all conformations that can be achieved without any atom interference. This analysis suggests the geometric paths that could be followed by a bio molecule during the transition from the initial to a final state, while molecular dynamics narrow downs the possibilities by identifying the only energetically feasible paths. The workspace analysis also characterizes the geometrically feasible workspace in terms of dexterity.

**d) Modular Pattern Recognition and Clustering Function:** The instantaneous value of the property \( A \) of a molecular system [4] can be written as \( A(p^r(t), r^r(t)) \), where \( p^r(t) \) and \( r^r(t) \) represent the \( n \) momenta and positions of a molecular system at time \( t \). This instantaneous value would vary with respect to the interactions between the particles. There are two parts to this function (termed as \( M \) function). One part (function \( A \)), evaluates and hence recognizes the equivalent modules (in term of properties) in the molecular system. The second part of the function \( D \), forms the cluster (like a bioisosteres, which are atom, molecules or functional groups with similar physical and chemical properties) of various modular patterns according to the characteristic behaviors as identified by function \( A \) and also tracks their variations with rest to time.

\[ M = \{ A(p^r(t), r^r(t), C^n[r]), D(A(p, r, C, t), f(x, y, \ldots), Bn(t)) \} \]

Where, \( C^n[r] \) is an \( n \) dimensional matrix element for the individual components of the molecular system, which would store the categorized values of the modular patterns. \( D \) is the second part of the function, and it takes on function \( A \) recursively. It also maps these clusters based on a fitness function and stores the time-variant value in sub-function \( B \). The \( M \)-function, is based on the hypothesis that in a complex molecular system, there are certain parts which have similar properties and behavior as the system goes from one state to the other. By identifying these property patterns we can considerably reduce the simulation and computational time frames and can have better predictability of the system.

Having established the design for the bio-nano components, computational studies would focus on determining the overall design and architecture of the bio-nano assemblies. One of the methods used in the industry is of Molecular Docking.

**e) Molecular docking & scoring functions:** Molecular docking [4, 9] method is very important for the design
of nanorobotic systems. This method is utilized to fit two molecules together in 3D space [9]. The method of molecular docking could be used to computationally design the bio-nano assemblies. Docking algorithm generates a large number of solutions. Therefore, we require scoring functions to refine the results so produced. Scoring functions in use today approximate the "binding free energy" of the molecules.

We are currently using NAMD (a molecular dynamics software) for running simulations on various bio-nano components. We are further developing the dynamical models and optimization kernels.

5. Conclusions

The recent explosion of research in nanotechnology, combined with important discoveries in molecular biology have created a new interest in bio nanorobotic systems. The preliminary goal in this field is to use various biological elements — whose function at the cellular level creates a motion, force or a signal — as nanorobotic components that perform the same function in response to the same biological stimuli but in an artificial setting. In this way proteins and DNA could act as motors, mechanical joints, transmission elements, or sensors. If all these different components were assembled together they can form nanorobots and nano devices with multiple degrees of freedom, with ability to apply forces and manipulate objects in the nanoscale world, transfer information from the nano to the macroscale world and even travel in a nanoscale environment.

The ability to determine the structure, behavior and properties of the nano components is the first step which requires focused research thrust. Only when the preliminary results on these nano components are achieved, steps towards actually building complex assemblies could be thought of. Still problems like protein (i.e. a basic bio nano component) folding and the precise mechanism behind the operation of the molecular motors like ATP Synthase have to be solved. The active control of nanorobots has to be further refined. Hybrid control mechanisms, where in, a molecular computer and external (navigational) control system work in sync to produce the precise results seem very promising. Further, concepts like swarm behavior in context of nanorobotics is still to be worked out.

Concepts for two macro-scale devices with important space application that will be using bio-nano-component assemblies have been presented in this paper. The Networked TerraXplorer (NTXp) will be a long and light-weight network of channels containing millions of bio-nano-robotic elements with ultra-enhanced sensing and signaling capabilities. NTXp could be used to map and explore in detail very large planetary surfaces. The All Terrain Astronaut Bio-Nano Gears (ATB) will serve as an extra layer of shield on the astronaut providing early detection and protection against dangerous and harmful environments or aiding in healing damages caused to the astronaut. The ATB gear will consist of micro membranes and surface sheets that contain swarms of bio-nano robots providing sensing and signaling capabilities.

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