TOPICAL REVIEW

Artificial Intelligence in Nanotechnology

G. M. Sacha and P. Varona

Grupo de Neurocomputación Biológica. Escuela Politécnica Superior,

Universidad Autónoma de Madrid, Cantoblanco, Madrid, Spain E-28049

Abstract

During the last decade there has been an increasing use of artificial intelligence tools in nanotechnology research. In this paper we review some of these efforts in the context of interpreting scanning probe microscopy, the study of biological nanosystems, the classification of material properties at the nanoscale, theoretical approaches and simulations in nanoscience, and generally in the design of nanodevices. Current trends and future perspectives in the development of nanocomputing hardware that can boost artificial intelligence based applications are also discussed. Convergence between artificial intelligence and nanotechnology can shape the path for many technological developments in the field of information sciences that will rely on new computer architectures and data representations, hybrid technologies that use biological entities and nanotechnological devices, bioengineering, neuroscience and a large variety of related disciplines.

1. Introduction

Modern scientific and technological development increasingly relies on nano, biological and information sciences. For more than a decade, the thought that the convergence of nanotechnology, artificial intelligence (AI) and biology will promote another technical and scientific revolution has been lingering. However, this expected integration of multidisciplinary research is still in progress. Nanotechnology combines the knowledge of physics, chemistry and engineering, while artificial intelligence has heavily relied on biological inspiration to develop some of its most effective paradigms such as neural networks or evolutionary algorithms. Bridging the link between current nanosciences and artificial intelligence can boost research in these disciplines and provide a new generation of information and communication technologies that will have a large impact in our society, probably providing the means so that technology and biology merge (see figure 1). In the meantime, different efforts have used tools from artificial intelligence in basic and applied nanoscience research, e.g. to interpret experimental techniques or to help in the design of nanomaterials and devices. There are also a few studies on how current and future artificial intelligence techniques will benefit from the increase in computational power than nanoscience will shortly provide. This paper addresses these issues in the context of a fast development in multiple disciplines that seem to be converging. Thus, we try to illustrate some answers to the questions: How can nanotechnology further benefit from computational intelligence developments, and how can nanotechnology be of use to implement novel AI paradigms, possibly expanding their uses and merging the gap to biotechnology.

There are several reasons why artificial intelligence paradigms are being used in nano research. Nanotechnology suffers the physical limitations of its working scale, where the physics is completely different from that of the macroscopic world. This means that the correct interpretation of the results obtained from any system or device at this scale is one of the issues that must be faced in nanotechnology [1]. To make the scenario even worse, it is frequent to find systems where many elements have a strong influence in the signal. In these cases, the development of analytical approximations is hard, and numerical simulations have become widely used to obtain accurate interpretations of experimental results. In this context is where AI tools such as machine learning paradigms can play a key role in producing scientific results and in the development of future nano applications.

Machine learning methods can represent and generalize complex or unknown functions or data, and they are very efficient in the parallel treatment of many interacting parameters [2,3]. Machine learning methods include approaches like artificial neural networks (ANNs), a set of interconnected nodes whose connection weights are determined through a supervised or unsupervised algorithm in order to learn these type of input-output functions. Other types of bio-inspired AI paradigms based on evolutionary or genetic algorithms also provide solutions to optimization and search problems. There is a wide variety of machine learning approaches that use single or combined methods including support vector machines (SVM), Bayesian

networks, decision trees, etc. which can be applied to complex classification, clustering, association, prediction, data mining and control problems in the context of nanotechnology research.

On the other hand, computer science in general, and AI in particular can benefit from the increased power that nanomaterials, nanodevices and nanocomputing will provide in the near future as effective architectures to implement machine learning methods. This bidirectional interaction between AI and nanotechnology is discussed in the next sections by using representative examples covering different uses and applications.

2. AI in Scanning Probe Microscopy

One of the most commonly used techniques to image the nanoworld is Scanning Probe Microscopy (SPM). This wide concept involves any technique that obtains images from the interaction between a probe and a sample. Depending on the nature of the interaction, many techniques have been developed. Although instruments such as the topografiner [4] had many of the main components of modern SPM, it is commonly accepted to consider the Scanning Tunneling Microscope in 1981 the first SPM technique to be developed [5]. In this case, the tunneling current between the probe and the sample is the interaction that allows the characterization of the sample topography with the microscope. By changing the interaction between the tip and the sample, several techniques were designed in the years following the discovery of this type of microscopes, or more precisely, nanoscopes. Some characteristic examples are the Scanning Capacitance Microscopy (SCM) [6], the Scanning Near-Field Optical Microscopy (SNOM) [7], and the Atomic Force Microscopy (AFM) [8]. In the case of the AFM, the first mode used to scan the surface of the sample was the Contact Mode. In 1986, the first SPM atomic resolution image appeared on the cover of a journal [9]. The magnetic force [10], the friction [11] or the electrostatic force [12] are other examples of interactions that have been commonly used to map surfaces at the nanoscale. SPM became also an effective tool for atomic-scale manipulation and several validating examples were shown in the literature [13,14] only a few years after the first SPM techniques were developed. Although many efforts have been made in the last years to improve the resolution [15,16] and the ability to manipulate atoms [17–20], the interpretation of the microscope signal is still a challenge nowadays [21]. The main problem is that most of the tip-sample interactions are not easy to understand and depend on many parameters. These are the kinds of problems where methods from artificial intelligence can be extremely helpful.

The last years have seen a great progress in multimodal SPM imaging in which multiple channels are acquired at the same time providing important complementary information about the image. Some examples are dual excitation frequency SPM [22], multiple harmonic imaging [23], 3D-modes [24], band excitation SPM [25] and the use of rapid digital lock-ins [26]. This huge amount of information rapidly increases the difficulty of interpreting specific properties of the material. To fight this issue, Nikiforov et al. [27] introduced a SPM approach, called functional recognition imaging (FR-SPM), which looks for

direct recognition of local behaviors from measured spectroscopic responses using neural networks trained on examples provided by an expert. This technique combines the use of ANNs with principal component analysis (PCA), which is used to simplify the input data to the neural network by whitening and decorrelating the data, reducing the number of independent variables. It is worth noting that the ANN would also work without this previous treatment since ANNs are able to extract relevant information from datasets that are redundant when they are well designed. However, by using PCA, the ANN is able to solve the task faster and with higher accuracy. The effectiveness of FR-SPM was demonstrated by the identification of *Micrococcus lysodeikticus* and *Pseudomonas fluorescens* bacteria deposited on a poly-L-lysine (PLL) coated mica substrate. The ANN used in this work was a multilayer perceptron trained by the standard back-propagation algorithm [28,29]. Specifically, it had six inputs, three outputs and three neurons in the hidden layer. The transfer functions used in each node were *sigmoid* in the hidden layer and *purelin* in the output layer. The output layer could give three different results that corresponded to the identification of the two different bacteria and the background.

In figure 2 we can see the topography image and the images where the recognition of the ANN is shown in a color scale for the three different elements involved in the identification process. In the first image, the dataset used for the training is shown inside a blue rectangle. It is worth noting that the dataset has to include a wide representation of the three elements that must be identified. The images demonstrate that the ANN correctly distinguishes the two bacteria and the background in most of the image.

The difficult interpretation of the electrostatic signal in SPM techniques such as Electrostatic Force Microscopy (EFM) [30] or Kelvin Probe Microscopy (KPM) [31] makes these kinds of microscopies especially suitable for the use of AI strategies oriented to perform image analysis. Moreover, the long-range nature of the electrostatic force involves many macroscopic parameters that must be taken into account. [32] The last factor that makes ANN a powerful tool in this framework is that frequently several important parameters are in fact unknown. To illustrate the effectiveness of ANN characterizing samples in EFM, a multilayer perceptron has been trained with numerical simulations to estimate the tip sample distance and dielectric constant of an EFM experiment where the tip is scanning over a carbon nanotube (CNT) placed on a semiinfinite dielectric sample.[33] The methodology has also been tested in a system where four parameters are not known: The tip shape (characterized by the tip apex radius, tip half-angle and length) and the sample dielectric constant. The ANN was able to accurately estimate the sample dielectric constant ε without knowing any geometrical parameter of the tip. Results are shown in figure 3a. In this example, we can see that the error increases as ε increases. This happens because the Force vs. Distance curves used for the training converge to the metallic case where ε increases and the difference between curves starts vanishing. When the input patterns during the training are similar, it is hard for the ANN to discriminate between them. Another factor that makes a strong influence in the signal is experimental noise. In figure 3b we show the error, due to

the experimental noise, measured from three F vs. D curves that were over a metallic sample at three different voltages. The curve associated with an applied voltage of 4V had the strongest noise level and corresponded to the curve where the ANN dielectric constant estimation was wrong.

This ANN already trained with numerical results was also used to estimate the effective dielectric constant of thin films. This numerical experiment confirmed the equivalency of a homogeneous dielectric sample and a system composed by two layers: A dielectric thin film over a semiinfinite dielectric sample. [34] The most notable result here is that only thin films with ultrahigh dielectric constants (at least ten times larger than typical values) can be detected when the thin film thickness is nanometric. Moreover, thin films with ultrahigh dielectric constants can be easily distinguished, which is something unexpected since they converge to the metallic case when the sample is macroscopic. In figure 4a we show the correspondence between the equivalent dielectric constant of the homogeneous sample and the one from the thin film. One can observe that values larger than 1000 correspond to effective values smaller than 50, which can be easily distinguished in standard EFM experiments. This fact is demonstrated in the inset of figure 4b, where we can see the difference between force curves with dielectric constants below 50. Figure 4b also illustrates how different the curves of thin films with dielectric constant 500 and 10000 are. These results predicted by the ANN were later confirmed in experiments made over graphene layers.[35]

Evolutionary optimization has been applied to automatize the process of imaging in SPM with a software that is able to tune the precise state of the probe and the associated control parameters [36]. In this way, high quality atomic resolution images are obtained with no human involvement further than the sample and tip preparation. This work was done using a prototypical tip-sample combination, which included a PtIr tip scanning over a highly oriented pyrolytic graphite (HOPG) sample. This sample is widely used as a test for the STM atomic resolution capabilities. The evolutionary algorithm employed in this system is based on a cellular genetic algorithm (cGA) [37], which belongs to a subclass of GAs where the individual only inherits characteristics from its closest neighbors during the breeding cycle. The cGA task is to evolve the imaging parameters in order to achieve the best match to a target image. The first generation is initialized with random parameter values. The parameters used in this example were the tunnel current setpoint, the sample bias, the integral gain and the proportional gain. At the end of the generation, when all the images have been taken, a fitness value is assigned to every image according to similarity to the target. Target images can be taken from previous cGA runs, theoretical representations or from the literature, among others. Figure 5 shows the evolution of the system as a function of the number of cGA generations. Inset shows the difference between the original image and the evolved one.

The image treatment in AFM has been also helped by using GA to select image filters with the proper type and order. [38]. These techniques significantly improve the quality of the images, helping in the location of nanoparticles.

3. Classification of material properties at the nanoscale

The characterization of structural properties of nanomaterials has also been solved by the use of ANNs [39]. For example, these algorithms have been employed to determine the morphology of CNT turfs by quantifying structural properties such as alignment and curvature.[40] First, the morphology was characterized by image processing of scanning electron microscopy (SEM) images and by applying stereological relations to quantify the sample structural properties. Then, the structural qualities were categorized using ANNs. Moreover, it was established that ANN models are an efficient quality evaluation tool to relate the physical appearance of CNT turfs to Raman features. As in most applications, one of the main challenges of using ANNs is the correct choice of the training set. In this case, two different strategies were used. First, a set of ideal rope images with defined values of curvature was used. Then, a training subset of CNTs images was manually analyzed to estimate the structural properties.

The characterization of different properties of thin films is a problem that has been widely solved by using neural networks. Because of the nonlinearities in the analysis of the signal in a film-substrate system, it is appropriate to use ANNs to process such complex systems. The determination of elastic [41] or electrostatic [33] properties by ANNs has been done by using theoretical simulations for the training set. Traditional numerical techniques in Nanotechnology such as the Finite Element Method (FEM) or the Generalized Image Charge Method (GICM) [42] are examples of different simulations that have demonstrated a large accuracy for the generation of complete training sets. To make the training task more realistic, Gauss noise can be directly added to the computer-generated training patterns.

The determination of material properties of functionally graded materials (FMG) assisted by ANNs has been also reported. [43,44] Using guided wave dispersion characteristics, an inverse method based on ANN has been employed to determine the material properties of FGM plates. The group velocities of several lowest modes at several lower frequencies are used as inputs to the ANN model, being the outputs the distribution function of the volume fraction of the FGM plate. The Legendre polynomials method is used to calculate the dispersion curves for the FGM plate. To improve the training process of the ANN model, the Levenberg-Marquardt algorithm has been used as a numerical optimization.

An ANN model has also been developed to accurately obtain physical characteristics of quantum-dot semiconductor optical amplifiers such as pulse amplification and four-wave mixing characteristics [45]. It has been demonstrated that this model requires smaller computation times compared with other numerical models, which is a great advantage for computer-aided applications.

Optical properties have been widely analyzed by AI techniques for two main reasons. [46] First, the fast growth of broadband communications, multimedia and Internet is closely related to the use of optical networks. Second, as the complexity of this kind of systems increases, AI becomes an extremely useful tool. Evolutionary strategies have been employed for the characterization of semiconductor quantum device properties such as transition energies, compositional parameters, applied electric field, or their geometry [47,48] focusing, for example, on the second harmonic generation for the production of multiple optical wavelengths.

Chemical reactions are another field where several works have studied the advantages of using AI methods as classification tools. It has been demonstrated that ANNs can evaluate chemical kinetic data parameters such as rate constants or concentrations of the reactants [49]. The advantage of using this technique is that new kinetic curves can be evaluated without solving again a system of differential equations. Using experimental results as learning data, ANNs have also been used to model the conversion rates of a heterogeneous oxidation reaction (oxidation of 2-octanol with nitric acid) [50]. It was found that this approach could successfully predict in most cases the behavior of a semi-batch reactor (i.e. its concentration and heat flow time profiles) within a singular series of experiments. A complete analysis of different neural network geometries has been done to study their usability in the estimation of the reaction rate of methanol dehydration in dimethyl ether synthesis [51]. The accuracy of the models was found to agree with experimental results over a wide range of experimental conditions. These results clearly establish that ANNs are powerful tools that can be used complementary or as an alternative to complex analytical equations.

Several previous works have used genetic algorithms to study the structural properties of small clusters or nanoparticles [52,53]. The use of GAs as an alternative tool to obtain equilibrium structures in self-organizing systems and clusters has been studied. [54–56] In contrast to the traditional methods, GAs have the advantage of searching among all lattice structures without having to fit any parameter at the beginning. These results provide a deeper understanding of the system's strategies to arrange particles in an energetically optimized fashion, leading to the competing self-assembly scenarios of cluster formation vs. lane formation. Combining GA with DFT calculations, the equilibrium state of small Pd clusters have been also obtained. [57] The role of the GA in these calculations is to provide a diverse set of initial unbiased cluster configurations. An important conclusion can be extracted from all these works: the use of GA and ANN is not restricted to only obtain the equilibrium state, but it also helps to gain insight of the physics underneath.

The use of AI techniques has begun to arise for the formulation of the properties and performances of concrete [58]. For example, ANN and GA have been used to predict the splitting tensile strength and water absorption values of concretes containing ZnO_2 or Cr_2O_3 nanoparticles.[59,60] The use of these techniques is justified by the large number of parameters that have a strong influence in the properties under study. Some of these parameters are the cement, nanoparticle and water

contents, the aggregate type, the amount of superplasticizer, the type of curing medium or the age of curing. The results obtained by both AI techniques are good. However, ANNs show a higher accuracy. This is compensated by fact that GA is an easier method to design and implement.

When the number of possible configurations shows a combinatorial explosion, the use of AI techniques becomes essential to overcome the problem of enormous computation times. [61] This problem appears for example when we combine the effects on the band structure of both nanostructuring and alloying to convert Si-based materials into strong light-absorber/emitters. Authors used a combination of a genetic algorithm and a semiempirical pseudopotential Hamiltonian for describing the electronic structures. They discovered some sequences which could offer both a direct bandgap and a strong oscillator strength. In this work we can find an example of new physics unveiled by the use of GA instead of a numerical solution. The results of this study provide simple design principles for the Si-based materials with strong optical activity.

4. Designing nanosystems

Recently, ANN has been used to draw the nonlinear relationship between input variables and output responses in the deposition process of transparent conductive oxide. This kind of thin films has been recently employed as electrodes in optoelectronic devices such as solar cells, organic light emitting diodes and flat panel displays. [62] Specifically, the processing effect on the electrical properties and the deposition rate of In_2O_3-ZnO thin films has been modeled.[63] Authors found out that the deposition rate of the thin films was affected by the RF power and the substrate temperature. Moreover, the carrier concentrations, mobility and resistivity of the thin films were controlled by O_2 ratio and the substrate temperature. It was found out that the effects of deposition processing parameters were nonlinear and highly complex. However, the output responses could be sufficiently estimated by ANN models.

Evolutionary optimization has also been used to find improved nanoantenna structures. These structures outperform the best radio wave-type reference antennas by a factor of 2. The analysis of the fittest antenna geometry reveals that it merges the features of the fundamental magnetic resonance of split-ring with the electric one of a linear dipole antenna.[64] To obtain the best configuration by a GA, authors decided to use as fitness parameter the normalized near-field intensity enhancement in the focus of an illuminating Gaussian beam. The GA used generations of 20 to 30 individual matrix antennas, where the five best structures were selected as parents for the next generation. In figure 6 we show the best matrix antenna structure obtained after running the GA for 100 generations with 20 individuals. It is also shown its maximal near-field intensity enhancement, which almost doubles the one from the reference antenna. This method is able to optimize nanoantenna

structures for various purposes, as well as to provide new design strategies by analyzing carefully the working principles of the resulting geometries.

The focusing quality of integrally gated CNT field emission devices have been optimized by numerical methods that include GA.[65] Using this design tool, a set of optimal structural and electrical parameters have been obtained. The devices designed with these parameters exhibited very good e-beam focusability. Authors suggested that this technique could be also used in various electro-optical systems, including micro- and nanofabrication processes (i.e. parallel electron-beam lithography), electron microscope imaging for material science, displays and lighting (i.e. field-emission pixels), and accelerator physics.

Genetic algorithms are very well established in radiofrequency antenna engineering because they can be easily implemented and because of their effective use of parallelism. In the last few years, GA has found also some applications in the field of nano-optics. For example, Ginzburg et al. presented a method for designing plasmonic particles with desired resonance spectra by exploiting the interaction of local geometry with surface charge distribution and applying evolutionary algorithm [66]. Forestiere et al. used GA to design metal nanoparticle arrays that produce broadband plasmonic field enhancement over the entire visible spectral range. [67] In another article from the same group, authors demonstrated how the designs of metallic nanoparticle arrays with large electric field enhancement can be performed using the optimization of a well-defined objective function. The results from this article leaded to general design criteria for best enhancement of electric fields, unveiling the fundamental interplay between the near-field plasmonic and radiative photonic coupling. It was also demonstrated how genetically optimized arrays can lead to a tenth order improvement of Raman enhancement over nanoparticle dimer antennas, and around one hundred improvement over optimal nanoparticle gratings. Authors noticed that a careful design of nanoparticle light concentrators could have a large impact in numerous nano-optics applications such as solar cells, optical manipulators, plasmon enhanced photodetectors, modulators or nonlinear optical devices.

Another example of computational tools that combine numerical methods, solutions of surface integral equations with a heuristic optimization based on evolutionary algorithms can be found in [68] The objective of this work is to set up the synthesis of metallic nanowires with optimized optical properties like the maximal scattering cross-section at a given wavelength. As in many other works, authors claim that their method is a versatile tool that may be used for the design of different configurations of interest in the field of plasmonics.

5. Artificial Intelligence in Nanoscale Simulations

One of the main problems that scientists must face when working at the nanoscale is related to the simulation of the system under study. The difference between macroscopic and nanoscopic images is that real optical images cannot be obtained at the nanoscale. Images at this scale must be interpreted and numerical simulations can be sometimes the best solution. At this time, there are many programs and applications that accurately simulate different systems where atomic effects are present. [69–73] When they are correctly employed, these techniques are extremely useful to get a precise idea of what is present in the image. However, in many cases they are still difficult to use and many parameters must be taken into account to obtain an accurate representation of the system. In this context, AI can be useful to improve the quality of the simulations and to make them easier to obtain and interpret.

The use of ANNs in numerical simulations, when working at the nanoscale, has been demonstrated useful in different ways. First, the software can be modulated manually to control the balance between numerical precision and physical meaning.[74] In these simulations, the numerical method underlying the calculations is a standard least-square minimization, where the error between the electrostatic potential at the tip surface is minimized. Sometimes, a minimization routine that changes the weights of the points at the tip has also been used. [75] The use of this minimization routine, which can be simulated by a single-layer perceptron, can serve to minimize problems where the surface charge density of a metallic sample is replaced by a set of charges inside the metallic objects (for example, an SPM tip). In traditional approximations, the value, position and number of charges are obtained after a standard least-squares minimization (LSM) routine for the electrostatic potential at the metallic surfaces. An alternative to the LSM is to use the single-layer perceptron formalism by considering the value of the charges q_i as the weights w_i and the potential at the metallic surfaces V_j as the expected output values y_j (see figure 7). The input patterns x_{ij} play the role of the Green functions G_i. Following this formalism, the electrostatic potential Vj can be expressed as

$$V_j = \sum_{i=1}^{N_C} q_i G_i = \sum_{i=1}^{N_C} w_i x_{ij} \qquad (1)$$

where N_C is the number of charged elements inside the tip. The right hand side term in (1) represents the electrostatic potential in the notation of a single output artificial neural network, where x_{ij} represents the inputs to the output neuron y_j and w_i are the connection weights from the inputs (i=1…N_c) to this neuron. The standard minimization routine always provides the best charge distribution to fit the potential at the points that were previously selected from the metallic surfaces. However, it does not take into account the physical properties of the system. It could happen that the best fit at the selected points also increases, at the same time, the error at other points that were not taken into account in the simulation. These kinds of effects are well-known in the ANN world under the concept “overtraining”. This concept refers to the case where an ANN learns too well the sets that were shown during the training reducing its capacity to generalize at the same time. Fortunately, this effect

can be controlled by monitoring the error during the training. For example, in figure 7 we show the equipotential distribution of an AFM tip over a semiinfinite dielectric sample where the tip surface has been obtained by using an ANN as the minimization algorithm. We can see how the potential distribution depends on the iterations. The last figure gives already a reasonable equipotential distribution. Although it may not be the most accurate calculation, we could decide to stop there the simulation and use those results, avoiding a possible overtraining effect, which could result in a potential distribution with no physical meaning.

A second application of ANNs in simulation software is to reduce the complexity associated to its configuration. In many numerical simulation methods [76–79], there is a great number of parameters that must be fitted to create the optimal configuration for an accurate simulation of the system. Most of these parameters are related to the physical geometry of the system, and must be known by the user. However, other kinds of parameters are only related to the algorithms used in the simulation and only users with an expertise in numerical methods are able to correctly manage them. This fact strongly reduces the usability of the software. To overcome this problem, ANNs have been proposed as a method to be included in the simulation packages with the objective of finding an adequate configuration automatically.[80] In figure 8 we show the graphical interface of the Generalized Image Charge Method (GICM), which is a freely available software package that simulates the electrostatic field around SPM tips. In this figure we can see that at least two different groups or parameters must be included before running the simulation. The first one, related to the SPM geometry, only deals with experimental features. The second one, however, is related to the configuration of the standard least-squares minimization used by the program to calculate the electrostatic magnitudes. This second type of parameters are only easy to set by users that are previously familiar with this kind of minimization algorithms and the specific effects that they may cause in the context of the problem addressed. Obviously, to acquire this knowledge would take an extra effort to the users that may make them consider different alternatives to this software. The solution proposed is to use an ANN to estimate the optimal configuration. This ANN is already trained with SPM configurations that have already been successfully simulated.

6. Nanocomputing and artificial intelligence

In the previous sections we have described several examples of how artificial intelligence and nanoscience can meet to solve problems in nanoscale microscopy, nanomaterial science and nanoscale simulation. Beyond these contexts, there is a large variety of potential applications arising from the combination of artificial intelligence and present and future nanocomputing, i.e. computation done with nanodevices [81–83]. From the early efforts in building nanocomputers [84,85], artificial intelligence paradigms were used in the different phases of modeling, designing and building prototypes of

nanocomputing devices [83,86]. Machine learning methods implemented by nanohardware instead of semiconductor-based hardware can also a basis for a new generation of cheaper and smaller technology that can implement high performance computing, including applications such as sensory information processing and control tasks. However the current development of nanocomputers is mainly at the level of manufacturing and analyzing individual components, e.g. nanowires as connectors or molecules as switches [86]. The largest expectations arise from nanotechnology enabled quantum computing and memory [87,88], which can significantly increase our capacity to solve very complex NP-complete optimization problems. These kinds of problems arise in many different contexts, but especially in those that require what is called computational intelligence in big data applications.

In this context, the concept of natural computing generally includes at least three different methods [89]: (1) Those that take inspiration from nature to the development of novel solving techniques, (2) those that are based on the use of computers to synthesize natural phenomena and (3) those that employ natural materials working at the nanoscale to compute. This last concept includes techniques such as DNA computing [90,91] or Quantum Computing [87,92,93] that are well-studied at the present.

There are other techniques and materials that have been used recently as new approaches for the simulation and modeling of natural computation [94]. For example, the behavior of synapses in neuromorphic electronic systems have been emulated using memristive nanodevices [95,96]. The main problem that must be solved with this proposal is the difficulty of implementing synapses in electronic circuits [97]. These materials are resistive and their resistance can be altered electrically. Although their state decays with time, they are stable for a long time and this characteristic makes them good candidates for use in synaptic circuits.

One of the topics that represents better the approximation between Nanotechnology, Biology and Computer Science is DNA computing. This is a discipline that aims at using individual molecules at the nanoscopic level for computational purposes. We could say that a DNA computer is a collection of selected DNA strands whose combinations will result in the solution to a problem. Nanocomputers are defined as machines that store information and make complex calculations at the nanoscale, which are commonly related to DNA since this kind of molecules have the required properties to success in both tasks. Thus, DNA computing is a promising development at the interface between computer science and molecular biology. It has emerged as a technology for information processing and a catalyst for knowledge transfer between information processing, nanotechnology and biology. As quoted by Ezziane Z [98], this area of research has the potential to change our understanding of the theory and practice of computing.

However, an interesting twist occurs when the number of variables in the calculation increases. The most common DNA computing strategies are based on enumerating all candidate solutions and using selection processes to eliminate incorrect

DNA. This means that the algorithm relates exponentially the size of the initial data pool with the number of variables. At some point, brute-force methods become unfeasible. This is a case where AI techniques in DNA computing become useful to get a final solution from a smaller initial data pool, avoiding using all candidate solutions. Another alternative is using evolutionary and genetic algorithms. The combination of the massive parallelism and high storage density in DNA computing with the search capability of genetic algorithms can break the limit of brute-force methods.

DNA computing has also received criticism from different authors who believe that the problems intrinsically associated to this technique would make it impractical. Some of these problems are the growing number of error-prone, time consuming operations and exponential growth of DNA volume according to problem size. A commonly extended solution to these problems has been the implementation in silico by computer architectures offering massive parallelism [99,100].

Overall, there is a wide variety of emerging nanotechnologies to implement nanocomputing devices, some of them are bio-inspired. These technologies, by adding novel physical basis of operation (photon, plasmon, molecular state, etc), reconfigurable architectures, memory and computational principles, will be able to use novel data representations to implement machine learning paradigms to solve complex problems in a wide variety of applications.

7. Nanotechnology for biology and medical applications

Many nanosystems have been proved to be useful for the interaction with living neurons. For example, some properties of CNT allow us to design nanotube detectors that might help implement the behavior of pulse-train neural networks because the detectors are threshold devices similar to spiking neurons.[101]

The detection of volatile organic compounds by carbon nanotube coated acoustic and optical sensors has also been successfully studied with the help of ANNs.[102] As in many other studies, a principal component analysis treatment was previously performed to improve the ANN classification efficiency. It was concluded that a significant improvement in the classification was achieved by combining various modules of acoustic and optical sensors, which is the scenario where ANNs demonstrate their full potential.

The use of microcantilevers as elements of sensor arrays to quantitatively detect components in vapor mixtures can be improved by ANNs for two main reasons.[103] First, every single detector reacts to the presence of the odor and the interaction of the components is not linear. Second, the use of ANNs to differentiate among the vapors to some extent mimics the highly efficient strategy of odor discrimination in the biological olfactory system.[104]

In the context of biotechnology development, carbon nanotubes possess high electrical conductivity, chemical stability and mechanical resistance, which make them promising materials to use in neuroscience research [105]. It has been demonstrated

that a CNT substrate can promote neural growth and facilitate signal transmission [106]. Many other studies have demonstrated the promising applications of combining CNT nanotechnology with neurons. For example, Xie et al have observed that the oxidation of CNT mats promotes cell adhesion and neurite extension [107]. It has been also demonstrated that a precise control of neurite outgrowth and branching can be achieved using CNT substrates [108]. The effect of chemical functionalization of multi-walled carbon nanotube arrays (MWTN-A) on neuron adhesion has been studied, as well as the establishment of neural networks.[109] It has been found that non-functionalized MWTN-A possess good neural adhesion properties, developing a neural network with the formation of clusters of neuronal bodies comprising local neurites and fascicles of neurites that connect neighboring clusters. The tendency of neurons to organize into clusters on the MWTN-A surfaces suggests that neurite-neurite interaction is preferred over neurite-surface interaction. In figure 9 we show a SEM image of neuron clusters on MWTN-A surfaces. In figure 10 a schematic illustration of a MWTN-A surface and SEM images taken from a side view is shown.

One of the main conclusions of this work is that neurons develop a preference for a given substrate, in agreement with previous works [110]. The affinity of neurons for different substrates found in these works can be used to control the location of neural development or to develop mixed chemical surfaces to study the neuron migration, with potential applications for the regeneration of neural tissues and future hybrid processing circuits composed of living neurons and artificial nanoelements.

The possible adverse effects in humans of the use and manipulation of nanoparticles is a critical issue for regulatory authorities. One of the main criticisms that has been recently heard is that nanosafety is far beyond the high technology level achieved in nanotechnology nowadays. Several models and studies have been proposed recently to address the influence of nanoparticles in biological systems. Some of these models are based in AI techniques, including support vector machines and nearest neighbors based regression [111]. In this field, where complex interactions that involve nanotechnology and biological systems, AI can be extremely helpful. [112]

On the other hand, ANNs have been proven to be a successful tool for nanoparticle preparation analysis and modeling in the context of pharmacology and nanomedicine, with high potential impact in cancer therapy [113,114]. The big data explosion in modem drug research requires effective analysis methods to deal with hidden causal relationships among a large set of properties and single or multiple responses. AI tools can meet some of the demands in the emerging field of drug discovery modeling [115–117]. Compared to traditional regression approaches, ANNs are able to model complex nonlinear relationships. For example, polymeric nanoparticles allow new ways for the administration and targeting of drugs. ANNs have been used to predict nanoparticle size and micropore surface area of polylactic acid nanoparticles [118] and to identify and model factors that affect the particle size [119]. ANN can also been combined with fuzzy logic systems for this kind of

problems [120]. The large variety of examples that include the use of A.I. tools in this field include the analysis of factors affecting the particle size and stability of nanoemulsions [121,122], the design of models that identify relationships between variables affecting drug nanoprecipitation [123], and the controlled release drug delivery systems [124].

8. Discussion

In this paper we have reviewed several problems arising in nanotechnology research that can be solved using methods from artificial intelligence. Table 1 summarizes some of the solutions provided by A.I. and the pending challenges in the nanotechnology problems discussed above. These solutions arise from the ability of artificial intelligence paradigms to generally deal with pattern association, recognition, classification, optimization and prediction tasks. In particular, we have discussed the application of artificial neural networks and genetic algorithms in many different contexts ranging from the interpretation of data in Scanning Probe Microscopy to the characterization and classification of material properties at the nanoscale. Many of these problems have one or both of the following characteristics: 1) The system under study is highly undetermined and 2) several interacting parameters have a strong influence in the results. We have also reviewed some recent efforts towards building nanocomputers and using them to implement modern artificial intelligence paradigms. These pioneering efforts call for a real convergence of nanotechnology and artificial intelligence in high performance computers enabled by nanocomputing devices including those based on biomaterials. Finally, we have also emphasized the large potential impact of using artificial intelligence tools when applying nanotechnology in the context of biomedical research and clinical applications.

Today's information technologies deal with big data, fast real time complex analysis and computations, security and encryption methods, high performance, multimodal and ubiquitous sensors, closed-loop interaction with complex systems or biological entities, etc. Bridging the gap between nanotechnology and artificial intelligence can lead to a more effective interaction between brains and machines and in fact provide the means for technology and biology to merge.

Nanotechnology research deals with building things bottom-up, while AI research typically provides a top-down approach to solve problems. The combination of these two disciplines will lead to solutions for many complex problems that require multiple description levels and interactions. One of such problems is to understand information processing in the nervous system [125], where complex computations are done from the molecular level all the way to the whole brain level at different but interacting time scales. As we have discussed above, Nanotechnology and artificial intelligence can help in this effort, which can return back novel bio-inspiration for these disciplines.

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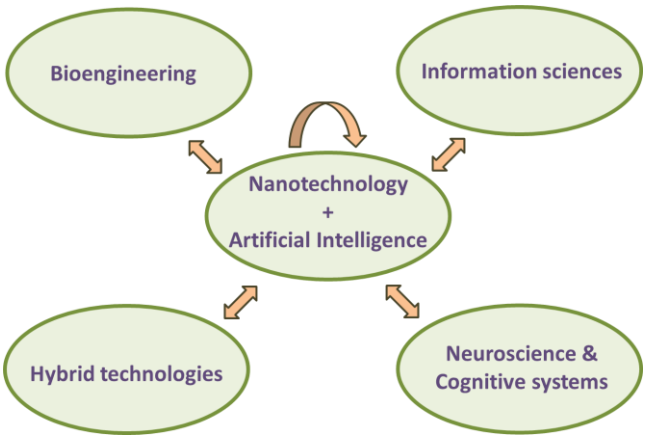

Figure 1. Convergence of nanotechnology and artificial intelligence has a large potential impact in many other scientific fields, e.g. bioengineering, novel information sciences based on new computer architectures and data representations, hybrid technologies that use biological entities and nanotechnological devices and research in neuroscience and cognitive systems, to name a few.

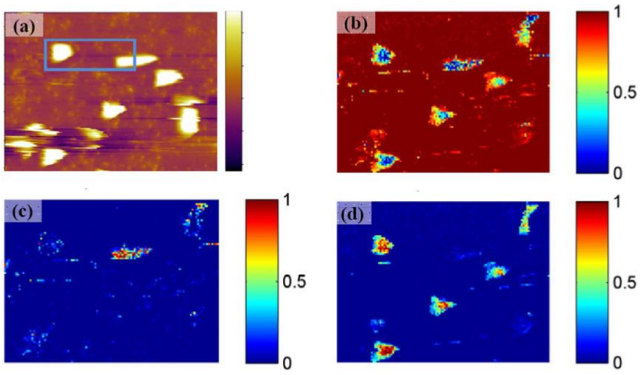

Figure 2. Identification of bacteria on a PLL coated mica substrate with ANN. (a) Topography image of the bacteria on PLL mica (the area within the blue rectangle was used for the training neural net). Output of the neural net in the form of recognition maps for the background (b), P. fluorescens (c) and M. lysodeikticus (d). Value 0 corresponds to the minimum likelihood of the point being the target when value 1 corresponds to the maximum one. Reprinted from Nanotechnology 20 (2009) 405708.

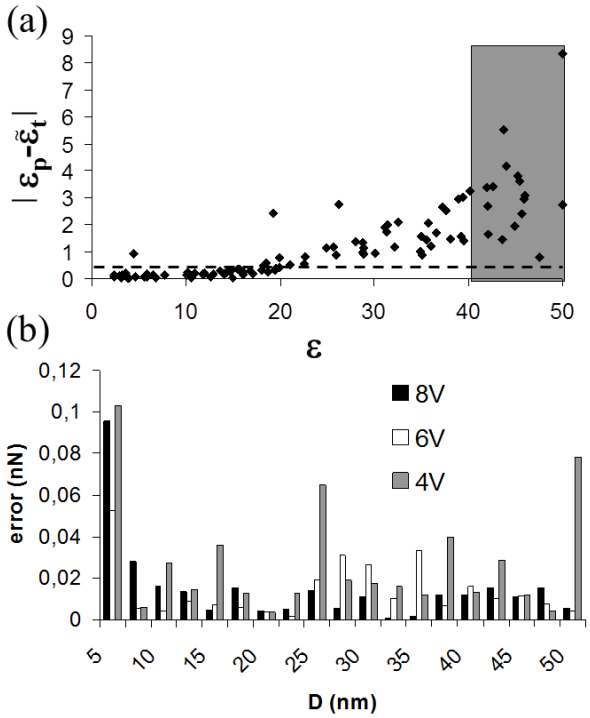

Figure 3. (a) Difference between the real and ANN predicted dielectric constant values from an Electrostatic Force Microscopy experiment. Dashed line corresponds to the error allowed in the training phase. (b) Normalized error of the experimental curves that were used in this work. Reprinted from Nanotechnology 20 (2009) 085702

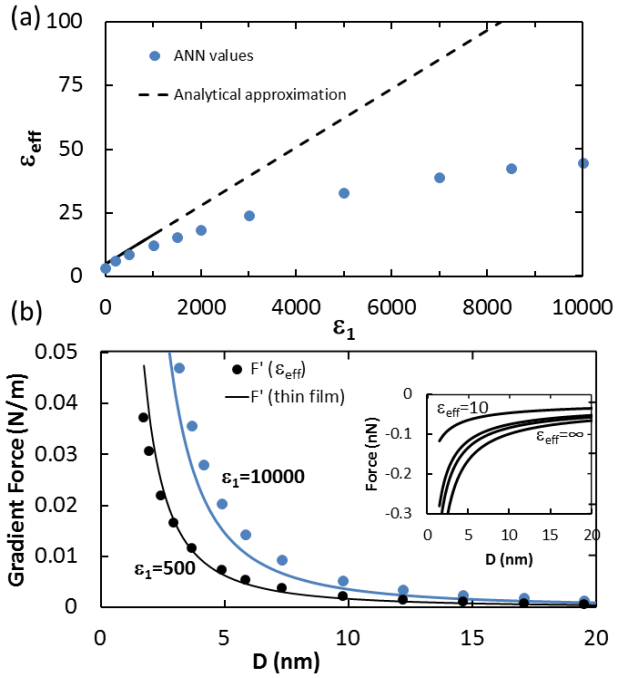

Figure 4. (a) Effective dielectric constant for ultrahigh thin film dielectric constants obtained by analytical approximations and ANNs. Values obtained with the ANN provide the most accurate results. (b) Gradient force for thin films with dielectric constants 500 and 10000. Inset shows the electrostatic force for semiinfinite dielectric constants with values 10, 30, 50 and ∞. Reprinted from Appl. Phys. Lett. 100, 023101 (2012).

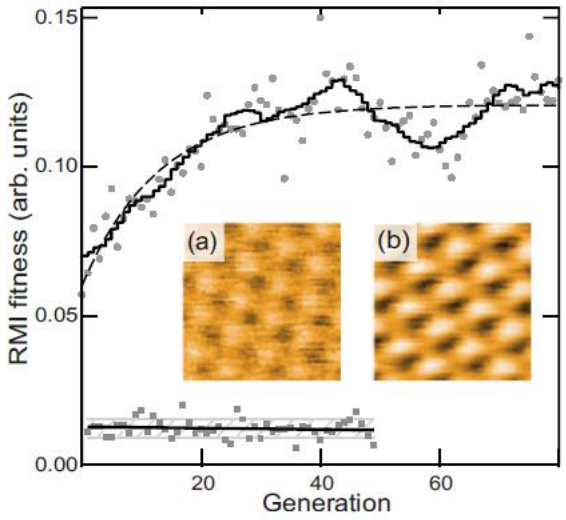

Figure 5. SPM imaging processing with evolutionary optimization. The average evolution of cGA image quality as a function of generation. The trend for increase in fitness is highlighted by a dashed line (an exponential fit to the data points). For comparison, the square markers show the lack of change in fitness for randomly selected imaging parameters deviation. Inset: 1x1 nm^2 (a) the starting image and (b) the evolved image. Reprinted from Appl. Phys. Lett. 98, 253104 (2011).

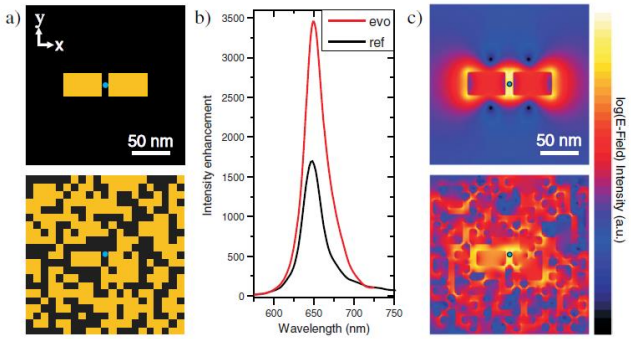

Figure 6. Comparison between a resonant linear dipole nanoantenna (reference) and a structure obtained with the GA described in the text. (a) shows the geometry of both structures. The blue spot denotes the position of the near-field optimization by the GA. The spectra in (b) are taken at this marked position during a broadband Gaussian excitation. (c) shows the logarithmic near-field intensities when the structures are illuminated by a monochromatic Gaussian focus. The scales are normalized and not comparable. Reprinted from Physical Review Letters 109 127701 (2012)

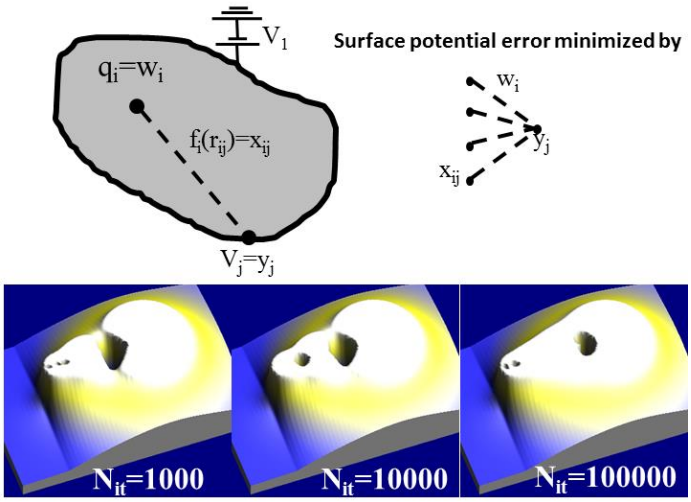

Figure 7. Schematic representation of the numerical method used to simulate the electrostatic potential around metallic objects and the Artificial Neural Network routine used to minimize the error at the surface. Equipotential distributions of an Atomic Force Microscopy tip over a dielectric sample are also shown as a function of the ANN iterations.

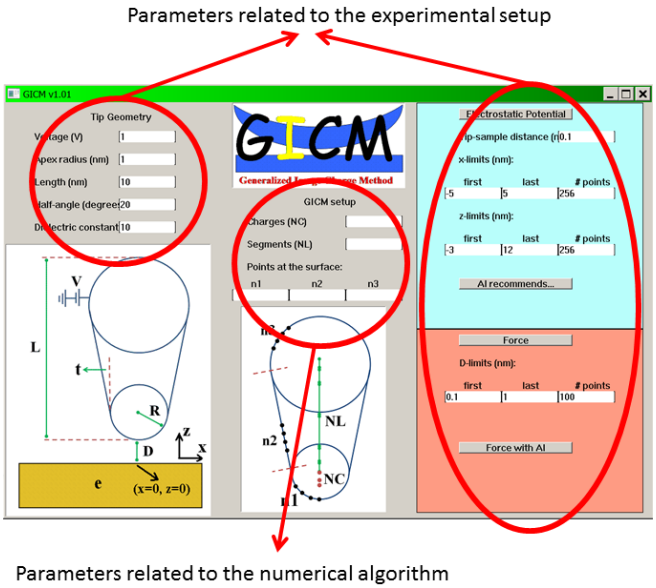

Figure 8. ANN application to reduce the complexity associated to simulation software confirgurations. In the figure, we explicitly show the parameters related to the SPM geometry (Atomic Force Microscope Parameters, Electrostatic Potential Calculation and Vertical Force Calculation) and the ones related to the GICM algorithms configuration (GICM Parameters) in the winGICM software. Reprinted from J. of Electromagn. Waves and Appl., 24, 1145–1155 (2010)

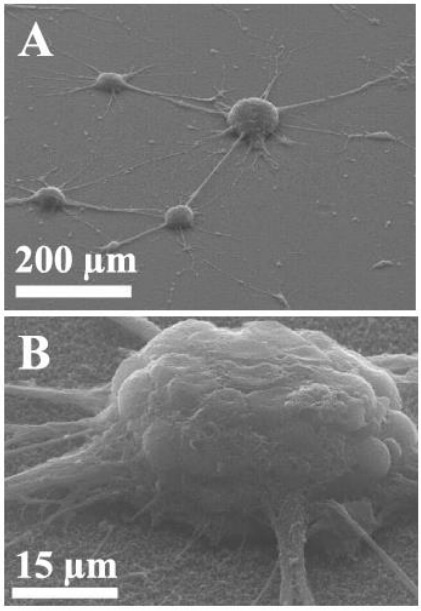

Figure 9. Use of nanomaterials in biotechnological applications (a) SEM image of neuron clusters growing on MWNT-A0 surface. (b) Zoom of a neuron cluster. Reprinted from Nanotechnology 22, 195101 (2011).

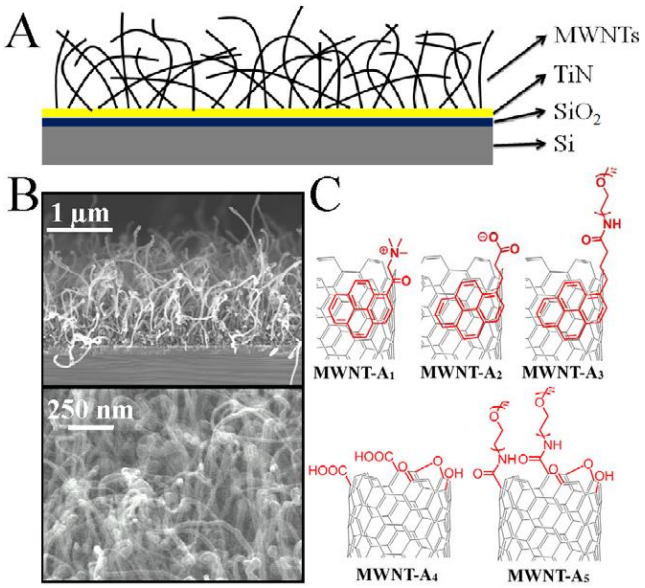

Figure 10. (a) Schematic illustration of a cross-section of a MWNT-A synthesized on Si substrate. (b) SEM images taken from a side view (upper panel) and top view (lower panel) of MWNT-A0. (c) Schematic illustration of the outermost graphene sheet of functionalized MWNT-A showing the different grafted molecules for each chemically modified MWNT-A (in red). Reprinted from Nanotechnology 22, 195101 (2011).

Nanoscience problem	Solution provided by A.I.	Pending challenges
Scanning Probe Microscopy	-Help in the interpretation of experimental results. -Multiple parameter account and estimation.	-Availability of experimental training sets. -Further developments to solve a wide variety of problems not addressable by human expertise.
Material properties at the nanoscale	-Characterization of material properties merging theory and experiments. -Inverse problem solutions. -Dealing with combinatorial explosion in configuration problems.	-Experimental constraints. -Increasing resolution and precision for specific technological applications.
Designing nanosystems	-Automatic characterization of complex input/output responses. -New design principles and system optimization.	-Suboptimal solutions if the parameter space is not fully explored.
Nanoscale Simulations	-Numerical system simulation and effective parameter estimation.	-Explore the vast variety of application fields. -Avoid the need of operators, making the software able to work autonomously when possible.
Nanocomputing	-Theoretical insights, data and algorithm design for nanocomputers.	-Moving from theory to real applications. -Reducing the computation time in new paradigms.
Nanotechnology for biology and medical applications	-Increasing biomedical research and applications, convergence between nanosystems and living cells and tissues.	-Truly hybrid systems, effective convergence among nano and living entities, including neural systems.

Table 1: Summary of solutions provided by A.I. and pending challenges in several nanotechnology problems