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STUDY OF NANO-SYSTEMS FOR COMPUTER SIMULATIONS

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***Abstract*— in the present paper the experimental study of Nanotechnology involves high cost for Lab set-up and the experimentation processes were also slow. Attempt has also been made to discuss the contributions towards the societal change in the present convergence of Nano-systems and information technologies. one cannot rely on experimental nanotechnology alone. As such, the Computer- simulations and modeling are one of the foundations of computational nanotechnology. The computer modeling and simulations were also referred as computational experimentations. The accuracy of such Computational nano-technology based experiment generally depends on the accuracy of the following things: Intermolecular interaction, Numerical models and Simulation schemes used. The essence of nanotechnology is therefore size and control because of the diversity of applications the plural term nanotechnology is preferred by some nevertheless they all share the common feature of control at the nanometer scale the latter focusing on the observation and study of phenomena at the nanometer scale. In this paper, a brief study of Computer-Simulation techniques as well as some Experimental result.**

***Index Terms* Nano-Systems, Computer-Simulations, global optimization method, Molecular Dynamics, hardware/software design Space.**

I. INTRODUCTION

As we enter in to the new century it is probably as good a time as any to look ahead and try to glimpse future trends in our society. With the abundance of powerful personal computer as well as plentiful supercomputer, time, available to researchers. Before that we should know about nanotechnology. In the Nanotechnology the manipulation of matter on an atomic and molecular scale. Generally, nanotechnology works with materials, devices, and other structures with at least one dimension sized from 1 to 100 nanometers**.** The design, characterization, production and application of materials, devices and systems by controlling shape and size of the nanoscale [1]. The computer simulation techniques are widely used for computational nano-technology[2]. The frequently used simulation approaches are Monte Carl, and Molecular Dynamics methodsis the manipulation of matter on a atomic and molecular scale. Generally, nanotechnology works with materials, devices, and other structures with at least one dimension sized from 1 to 100 nanometers. Nanotechnology is very diverse, ranging from extensions of conventional device physics to completely new approaches based upon molecular self assembly from developing new materials with dimensions on the Nanoscale to direct control of matter on the atomic scale. The computer- based simulation methods, developed for Nano-systems, generally consist of a computational procedure performed of few atoms or molecules confined in a small geometrical space. This geometrical space in which the simulation is performed is termed as cell. In the subsequent section, a brief classification of simulation methods based on Accuracy, Computational Time. This site features information about discrete event system modeling and simulation. It includes discussions on descriptive simulation modeling, programming commands, techniques for sensitivity estimation, optimization and goal-seeking by simulation ,and what-if analysis. Advancements in computing power, availability of PC-based modeling and simulation, and efficient computational methodology are allowing leading-edge of prescriptive simulation modeling such as optimization to pursue investigations in systems analysis, design, and control processes that were previously beyond reach of the modelers and decision makers. engineering mechanics provides excellent

theoretical descriptions for the rational design of materials and accurate lifetime prediction of mechanical structures. This approach deals with continuous quantities such as strain field that are functions of both space and time[7]. Constitutive relations such as Hooke's law for deformation and Coulomb's law for friction describe the relationships between these macroscopic fields. These constitutive equations contain material-specific parameters such as elastic module and friction coefficients, which are often size dependent. For example, the mechanical strength of materials is inversely proportional to the square root of the grain size, according to the Hall-Petch relationship. Such scaling laws are usually validated experimentally at length scales above a micron, but interest is growing in extending constitutive relations and scaling laws down to a few nanometers. This is because many experts believe that by reducing the structural scale (such as grain sizes) to the nanometer range, we can extend material properties such as strength and toughness beyond the current engineering-materials limit. In addition, widespread use of Nano electromechanical systems.

A. Classification of simulation methods based on accuracy and computational time

The computer based simulation method, being developed for nano-system, generally consist for computational procedure perform on a limited number of atoms, molecules, molecular building blocks or macromolecules confined to a limited, but small, geometrical space[12]. Generally the cell in which the simulation is performed could be replicated in all spatial dimensions, generating its own periodic images. computer based methods used for simulation of various properties of nano scale systems differ in their level of accuracy and time-complexity to perform such calculations. Based on it, the required time scale for these methods can be from tens of picoseconds to few microseconds or more (classical molecular dynamics simulation). There are also methods which require very long computational time such as cluster growth and may require super computers to achieve fast results. Based on these facts we may classify the methods into following groups (**i**) Methods with highest degree of accuracy (**ii**) Methods with second highest degree of accuracy (**iii**) Semi-empirical method and (**iv**) Stochastic method

The most important input to such computation is the antiparticle energy/force function for interaction between the entities composing the nano-system. Accuracy administered computer simulations can help in three different ways:

1-they can be used to compare and evaluate various molecular-based theoretical models.

2-they can help the evaluate and direct an experimental procedure for nano-system.

3- An ultimate use of computer simulations is its possible replacement of an experiment which otherwise may not be possible with the present state of the technology or may be too costly, but provided accurate intermolecular potentials are available to be use in their development.

B. Method with highest degree of accuracy

- Input: Atomic species, coordinate, system's symmetry, interaction parameter.
- Output: Total energy, excitation energy and spin densities, force on atoms
- Purpose: Investigation of both electronic and atomic ground state, optical and magnetic properties of weakly interacting and also strongly interacting correlated systems

C. Method with second highest degree of accuracy

- Input: atomic species and their coordinate and symmetry of the structure; eventually for the species considered.
- Output: Total energy, charge and spin densities, forces on atoms, electron energy eigen values, capability of doing Molecular Dynamics, vibration modes

and phonon spectrum.

- Purpose: Accurate calculations of ground state structure by local optimization; Calculation of mechanical, magnetic and optical properties of small clusters and perfect crystals of weakly interacting electron systems, estimation of reaction barrier and paths.

D. Semi-empirical methods

- Input: Atomic species, their coordinates; parameters of the inter-particle potential, temperature and parameters of the thermostat or other thermo-dynamic variables.
- Output: Output of Tight- Binding(TB): Total energy, charge and spin densities, force on atoms, particle trajectories, phonon calculation; mechanical magnetic and optical properties of clusters and crystals.
- Purpose: Search for ground state structure by GA, Simulated Annealing (SA) or local optimization if a good guess for the structure is known; simulation of growth or some reaction mechanisms; calculation of response functions.

Stochastic method: There are several methods that use stochastic representations of some or all of the physical processes responsible for ground shaking. In this paper I review the particular stochastic method that I and a number of others developed in the last several decades. The paper includes a few new figures and an improvement in the calculation of random vibration results that previously appeared only in an USGS open-file report, Other authors have published papers applying the stochastic method and extending the method in various ways.

Purpose: Investigation of long timescale non-equilibrium phenomena such as transport, growth, diffusion, annealing, reaction mechanisms and also calculation of equilibrium quantities and thermodynamic properties.

E. Molecular dynamics simulation methods

The two basic used simulation approaches are Monte Carlo (MC) and Molecular Dynamics (MD) methods. All the other various simulation methods come from these two basic methods. A brief over-view with areas of application of the both are discussed below. These concepts are essentially required to understand the methodology of classification of Computer-Based Simulation methods based on accuracy and time-complexity. MC method uses random numbers to perform calculations. There are many areas of application of MC Methods including Nano-material. Some important areas where we apply MC method are:- (i) Estimation of large-dimensional integrals (ii) Generating thermodynamic ensembles in order to compute thermal averages of physical equilibrium quantities of interest and simulation of non-equilibrium phenomena such as growth and (ii) Computation of distribution functions out of equilibrium known as Kinetic Monte Carlo [4]. MD deals with predicting the trajectories of atoms subject to their mutual interactions and eventually an external potential. Some important areas of application of MD are: - (i) Computation of transport properties such as response functions, viscosity, elastic module and thermal conductivity (ii) Thermodynamic properties such as total energy and heat capacity and (iii) Dynamical properties such as phonon spectra.

F. Global Optimization Methods

A much more challenging task than local optimization methods is to find the global minimum of a multi-valley energy landscape as shown in fig.1. global optimization problems involving a given cost function (minimization of energy or maximization of entropy) arise in many simulation problems dealing with Nano-systems. This subject has received a great deal of attention in recent year, mostly due to the rapid increase in computer power. The symbolic picture shown in fig.1. provides a rather simple tow- dimensional example of the global optimization paradigm.

A number of computational algorithms have been develop recently for global optimization of molecular simulations. Among those algorithms the simulated annealing and the genetic algorithms have found more applications in structural and dynamic simulation optimization of molecular clusters.

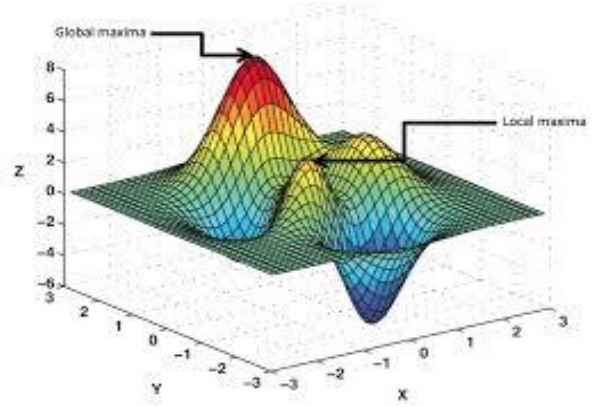

Fig.1. A two-dimensional example of global optimization of molecules energy $E_{(x,y)}$. the objective here is to locate the coordinates (x,y) for which the molecules energy has its absolute minimum.

This algorithm is basically search algorithm based on the machines of natural selection and nature genetics. It is the balance between efficiency and efficacy necessary for survival in many different environments. In order for GA to surpass their more traditional in the quest for robustness, GA must differ in some fundamental ways. GA are different from more normal optimization and search procedures in four ways:

- GA work with a coding of the parameter set, not the parameters themselves.
- GA search from a population of point not a single point.
- GA use pay off (objective function) not derivatives or other auxiliary knowledge.
- GA use probabilistic transition rules, not deterministic rules.

G. Optimization for Codesign to Molecular Dynamics

There are two applications address issues of the response of materials in extreme conditions and enabling the design of more effective and safe fission power plants, respectively. Hardware-Software codesign, perceived as a prerequisite exascale computing, needs to be put on a sound scientific basis such that design decisions for both hardware and software do not need to be made based on colloquial heuristic insights, but rather follow an established scientific procedure by sufficiently thorough search of realizable hardware and software options. Fig.1 illustrates our approach, where the left hardware design and the right software design boxes define a vast space of hardware and software solutions[5], whose combinations lead to performance prediction, the results of which in turn guide an optimization method towards new hw/sw solution to be tested. This resulting iterative process can be analyzed in formal and informal settings, thus opening doors to established optimization and analysis techniques, while at the same time incorporation sometimes superior but informal human ingenuity. The key research efforts in this approach are:

- Efficient enumeration method for the both hardware and software.
- Performance predication methods.
- Optimization methods to search the design spaces.

H. Simulation-based Optimization Techniques

Discrete event simulation is the primary analysis tool for designing complex Nano- systems. Simulation, however, must be linked with a optimization techniques to be effectively used for Nano-systems design. Simulations used as experiments:

1-Possible in case of coincidence between purposes of simulations and experiments

2-Discovering new explanatory hypotheses, confirming or refusing theories, choosing among competing hypotheses

3-Simulation with no experimental purposes in mind (simulation of a protein folding process for didactical Purposes)

I. Computer- Simulations and Results Obtained

In this paper work declares that a soft computing tool, GA is used to get the optimized system parameters of Ga As QW for a desired high frequency response characterized by a cutoff frequency (f3dB). QW is obtained for a high frequency under hot electron condition. In GA, a fitness function is the main criteria for reproduction. The fitness values are used to favor high fitness individuals over low fitness individuals to take part in the process of reproduction. in this work the application of GA, we get the f3dB for a semiconductor quantum structure for its different system parameters. Then we get cut off frequency it was low frequency value and one particular parameter of the system where the other parameters are optimized by the GA. By taking the other parameters in one form, we can be able to find the fitness values. These fitness values are converted to binary form and then proceed for further GA operation. After reproduction, simple crossover may proceed in the following steps. We note that the cut of frequency of mutation to get good results in GA studies.

II. Conclusions

The classification of simulation method presented in this paper important of the role of molecular dynamics and computer simulations in nanotechnology as well recognized for several reason:

1- Such simulation techniques will allow us to develop some fundamental understanding behavior of nano-systems for which there.
2- Since in a nano-system the number of particles involved is rather small and direct measurement of their collective behavior has not been well developed yet, computer simulations could help appreciable.
3- Computer simulation can produce data for testing and development of analytic predictive models on nano-systems.
4- demonstrates the various processes through which computer based simulations and optimizations are used in various field starting from classical to nano-levels.
5- The same will also help the reader to choose the best method suitable for a particular application of their interest. To give a better view we have given one example of computational technique that we have used for nano device simulation from one of our experimental work.

References

[1] B.D. Cullity, Elements of X-ray Diffraction (Addison-Wesley Publishing Company, Inc., 1956).
[2]. Narsingh Deo, System Simulation with Digital Computer, PHI Pvt. Ltd. (2001)
[3] Neel L 1961 C. R. Acad. Sci. Paris 252 4075, 253 9, 203, 1286
[4]. Lakhtakia A., A Handbook on Nanotechnology Nanometer Structures Theory, Modeling and Simulation, PHI Pvt. Ltd (2007).
[5]. Fox Keller, E. (2003) "Models, Simulation, and 'computer experiments', in Radder H. (ed.) The Philosophy of Scientific Experimentation, Pittsburgh University Press,198-21
[6]. Chandra S., Computer Application in Physics, Narosa Publishing House (2003).
[7]. Jorge J. More' et al, Optimization Software Guide, SIAM Publications (1993).
[8]. Das S. C., Neuro-Genetic Approach for Optimizing Parameters for the Polar Semiconductor, Proceedings of NATCOMNNAMTECH 2007.
[9] M. Sherif El-Eskandarany, Satoru Ishihara, Wei Zhang and A. Inoue, Met. Trans. 36 A (2005) pp. 141-147.
[10] S. Ogata et al., "Hybrid Finite-Element/Molecular-Dynamics/Electronic- Density-Functional Approach to Materials Simulations on Parallel Computers," to be published in Computer Physics Comm.
[11]R. Car and M. Parrinello, "Unified Approach for Molecular Dynamics and Density Functional Theory," Physical Rev. Letters, vol. 55, 1985, pp. 2471–2474.
[12]. Lakhtakia A., A Handbook on Nanotechnology Nanometer Structures Theory, Modeling and Simulation, PHI Pvt. Ltd (2007).
[13] Sheng-Hui Lin(2008)"Electrochromic properties of nano-structured nickel oxide thin film prepared by spray pyrolysis method". Volume 254, Issue 7, 30 January 2008, Pages 2017–2022

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