

MATERIALS AND PROCESS SIMULATION CENTER  
CALIFORNIA INSTITUTE OF TECHNOLOGY

PAN AMERICAN  
ADVANCED STUDIES  
INSTITUTE IN  
COMPUTATIONAL  
NANOTECHNOLOGY  
AND MOLECULAR  
ENGINEERING

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AN NSF FUNDED WORKSHOP

FINAL REPORT

FEBRUARY 2005

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## EXECUTIVE SUMMARY

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NSF sponsored a PASI Workshop at Caltech on Computational Nanotechnology and Molecular Engineering, both topics of great interest for advanced studies around the world. To capitalize on these advances, as well as to disseminate new theory and computer modeling ideas, the MSC organized this two week workshop for Latin American scientists, patterned after NATO workshops. In addition, the workshop provided close interactions between underrepresented minority graduate students at US institutions with postdoctoral level counterparts from various Latin American institutions. Such interactions fill a vacuum and help counterbalance the sociological factors that may hinder some of these students to pursue a life long career in science and engineering.

The workshop brought together scientists from institutions of higher education in Latin America, including Colombia, Mexico, and Guatemala with San Francisco State and a historically black university, Jackson State. The workshop included an advanced program of lectures and hands-on laboratory experiences. Although the PASI workshop dealt with such advanced topics as: Quantum Mechanics, Molecular Dynamics, mesoscale modeling, computational Nanotechnology and Molecular Engineering; it was also designed to generate spillovers into practical areas of research (industrial robotics, applications of massively parallel computing, computer science, environmental science) of current interest in Latin America. This was accomplished by focusing on fundamentals of computational chemistry common to advanced and current research topics. Successful developments in these areas of computational chemistry have broad implications for the national economies in the participating countries, as well as for the geopolitical interest of the USA. As a result, the workshop achieved a broader impact on the day-to-day industrial applications of computational chemistry such as in oil production in Mexico, on the environmental concerns surrounding the fate of tropical rain forests in Guatemala, and in the development of industrial robotics in Colombia.

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## ORGANIZING COMMITTEE

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The PI, Prof. William A. Goddard III, will be assisted by an Organizing Committee composed formally of three lecturers from the U.S. Dr. Mario Blanco and Dr. Mamadou Diallo senior staff members at Caltech and Dr. Sergio Aragon at SFSU. Colombia's regional organizer is Dr. Andres Jaramillo-Botero, Dean, School of Engineering, Pontificia Universidad Javeriana, Cali, Colombia. Mexico's regional organizer is Dr. Carlos Lira, Director, Molecular Engineering Division, Instituto Mexicano del Petroleo. Dr. Adrián Francisco Gil, PhD, Director, Department of Chemistry, Universidad Del Valle is the regional organizer for Guatemala. Additional lecturers and confirmed participants are included below. Academic and industrial sectors are represented in the PASI Regional Organizing Committee.

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PARTICIPANTS

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*Figure 1 PASI visiting teams from Mexico, Colombia, Guatemala, San Francisco State and Jackson State University pose for a group picture.*

San Francisco State University

- **Sergio Aragon (\*)**
- Andrew Ichimura
- Wanda Lew
- Shungo Miyabe
- Heather Harding

Jackson State University

- Tomekia Simon

California Institute of Technology

- **Mario Blanco (\*)**
- William A. Goddard III
- Mamadou Diallo
- Daniel Fisher
- Amos Anderson
- Santiago Solares

CalState Los Angeles

- Albert Cervantes

México

- **Dr. Carlos Lira-Galeana (\*)**
- Dr. Jose Manuel Martinez-Magadan
- Alejandro Ortega-Rodriguez,
- Dr. Alexandre Tkatchenko, Ph.D.
- Dr. Felipe Aparicio Platas, Ph.D.

Colombia

- **Dr. Andrés Jaramillo Botero (\*)**
- Antal Buss Molina
- Edgar Antonio Reyes
- Leonardo René Lareo
- Dr. Federico Sequeda

Guatemala

- **Dr. Adrian Francisco Gil (\*)**
- Cesar Antonio Estrada
- Roberto Estuardo Archila Diaz
- Paola Rivera Muñoz, UVG
- Ady Iveth Giordano, UVG

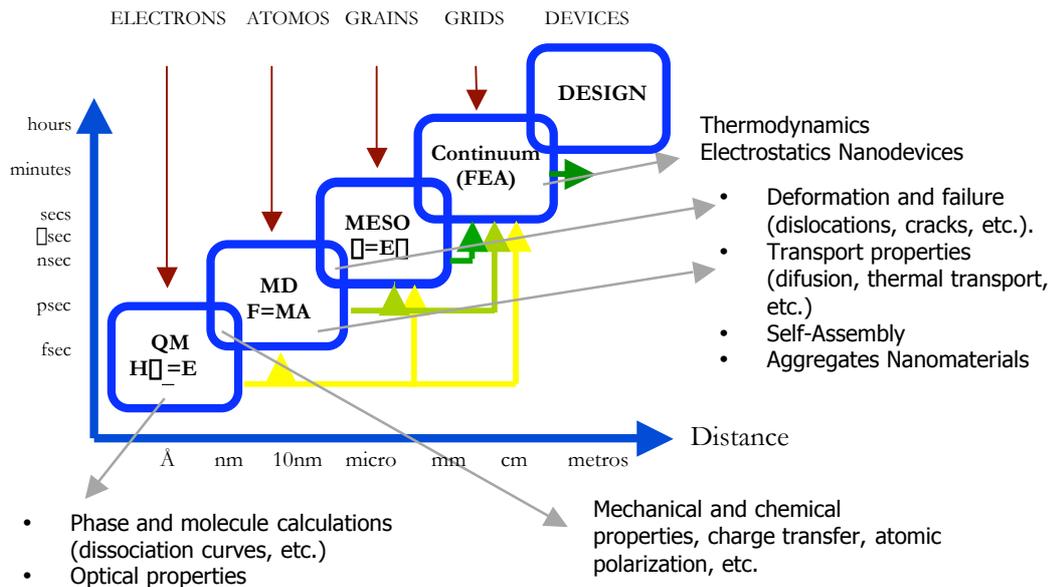
(\*) Regional Co-Organizer

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## INTRODUCTION

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The advent of affordable computer hardware, the ability to build one's own supercomputer (Beowulf) has made Computational Nanotechnology, i.e. computer modeling and simulation of molecular based components and devices for applications to nanotechnology, a topic of interest for postdoctoral and advanced graduate students around the world. Latin America is no exception. These Latin American research efforts will greatly benefit by direct interaction and exposure to advanced studies at a US institution. At the same time it is important to extend this opportunity to other institutions of higher education in the US (e.g., San Francisco State University, CalState) and to be inclusive of underrepresented minorities in research (Howard and Jackson State). The PASI workshop will help support such efforts, and the spillovers over other practical areas of research (industrial robotics, applications of massively parallel computing, computer science). It will encourage Latin American scientists through meetings with their US counterparts that may result in future collaborations. Additionally, the workshop seeks to impact day-to-day industrial applications of computational chemistry in oil producing countries, such as Mexico. Success in this area has broader implications to their national economy as well as to the geopolitical interest of the US. Cheaper and more stable sources of energy, through enhanced oil recovery for instance, are the main focus of computational efforts in Mexico. The use of commercial software dominates this area of research. A deeper understanding of the theory behind these computational tools can help enhanced the chances of success in oil field (upstream) and refinery (downstream) applications.



*Figure 2 Multi-Scale Hierarchical Approach to Computational Nanotechnology and Molecular Engineering*

The multi-scale modeling strategy (Figure 1) of the host institution, the Materials and Process Simulation Center (MSC) at Caltech, will provide the conceptual framework for the proposed workshop. The MSC has extensive experience and a distinguished track record in applying this strategy to outstanding problems in molecular engineering, bioengineering and nanotechnology 1-4. The MSC has pioneered the use of in-house developed computational chemistry codes, and commercialized versions of these, through numerous multi-year partnerships with the oil industry

(Exxon, Chevron, BP, Saudi Aramco) and through multi-year funded projects from DoE, DoD and NSF. The workshop will especially encourage papers and lectures on computational methods to be applied towards chemical synthesis of molecular components and/or fabrication and assembly of devices incorporating molecular components, papers and lectures reporting progress in molecular computer aided design and molecular structure elucidation in support of oil chemistries (asphaltenes, specialty chemicals, corrosion, scale, wax inhibitors, and computational evaluation of surfactants for enhanced oil recovery). Papers on massively parallel molecular dynamics formulations; suitable for the simulation of large molecular assemblies as well as multi-scale (Quantum to molecular dynamics, coupled particle/continuum) simulation methods will also be part of this workshop.

#### REGIONAL PARTICIPATION IN AMERICA

##### *Colombia (Dr. Andres Jaramillo-Botero)*

Colombia's effort around nanoscale science and engineering has been limited to a few individual efforts. In spite of this, interest and scientific contributions stemmed from these efforts have caught new advocates at the academic and industrial levels and are growing rapidly. Until now, work on the subject has concentrated mainly on theoretical aspects derived from quantum physics, quantum chemistry, molecular biology (bioinformatics, DNA engineering, protein structure and function), materials science (epitaxial growth, thin-films), dynamics (molecular design simple nanodevices) and computer science (large-scale, long-term molecular modeling and simulation, algorithmic complexity, and recently on quantum computation/information theory).

Experimental groups, from classical fields, are slowly turning their heads to related subjects or emerging, unfortunately with scarce resources and limited fundamental knowledge (first principles) to confront theory with experiment. Research at the nanoscale is naturally multi-disciplinary, furthermore, it requires the participation of worldwide effort in order to advance its development.

Attending participants will have an opportunity to contribute in the solution to still open problems and to learn about nanoscale systems from the perspectives of many different fields -- mathematics, science and engineering -- and to meet a diverse group of people providing a unique opportunity to form new collaborations or reaffirm existing ones. This cross-pollination between disciplines will prove a major asset when developing new ideas towards nanotechnology, in particular for developing countries given that the number of researchers in academia is low, as compared to technologically developed countries, and hence peers within a single field are limited. Furthermore, participants will have a chance to disseminate their acquired knowledge and augment interactions, in pertinent subjects, with other scientists around Colombia and Latin America. This will indeed promote teaching, training and learning of the fundamental subjects entailing the field on a wider scale within our country. Dr. Jaramillo will be lecturing on advanced topics in nanotechnology, new massively parallel molecular dynamics algorithms, as well as conduct a mini-workshop on how to build a custom Beowulf computer cluster.

##### *Mexico (Dr. Carlos Lira)*

Dr. Carlos Lira, Associate Professor at Universidad Autónoma de Mexico (UNAM) is the regional PASI co-organizer for Mexico. Dr. Lira is also the Director of Molecular Engineering Division of the Instituto Mexicano del Petroleo (IMP). A second contingent, under Dr. Lira's coordination also, is a group of scientist from Universidad Autonoma Metropolitana (UAM) – Iztapalapa, Mexico City.

This workshop would be useful to PhD candidates from UNAM (Universidad Nacional Autónoma de México) who are currently serving an internship at the IMP. These students work in close collaboration with the Molecular Engineering Division at IMP. In this Division most projects deal with the study of several phenomena associated with hydrocarbon phase behavior, physical properties of crude oils, phase separations and different physicochemical phenomena in crude oil fluids. In that sense, a number of molecular simulation techniques such as Monte Carlo (MC), Molecular Dynamics (MD), Brownian Dynamics (BD), and Molecular Mechanics (MM) are frequently used for representing such behavior in model systems. While many computer codes have been developed in-house, a significant number of programs utilized at IMP are of the commercial kind and thus prevent a full-knowledge of the theoretical/numerical approximations being used. In this regard, the training aspects of the PASI workshop would improve the background of our proposed students to better judge simulation results and even propose improvements over existing simulations. That, in turn, strengthens the profile and empowers the ability of our research group at the IMP and the PhD candidates from UNAM. Finally, having a molecular-simulation-trained individual in our group will broaden the possibilities of the UNAM group to solve problems related to heavy oil production and processing in the oil industry, a problem of critical importance to México.

The Division of Basic Sciences of the Universidad Autonoma Metropolitana-Iztapalapa has several research groups that are involved in Computational Chemistry. Prof. Nikola Batina adjunct Prof. Marcelo Galvan-Espinoza from UAM will attend the workshop. Dr. Batina is an experimentalist with emphasis on surface characterization by STM, SEM, and AFM. Dr. Galvan-Espinoza is a computational chemist and the UAM faculty coordinator and one of the PASI lecturers (biological simulations). In addition to Dr. Batina and Dr. Galvan-Espinoza 3 PhD students from UAM will be attending. Their research topics include Classical Molecular Dynamics, Quantum Chemistry, and Quantum Dynamics. All of them are linked to a Supercomputer Laboratory. In addition, there are experimental groups in materials sciences, in catalysis and in electrochemistry. Dr. Galvan-Espinoza remarks that “to build a bridge between these two types of academic bodies, it is important to improve the computational chemists skills in treating nano-scale systems. The acquisition of such capabilities will increase the possibility of interdisciplinary research, a major priority at UAM. Furthermore, interdisciplinary research requires not only intra-institutional but also inter-institutional cooperation. The workshop will enhance the skills of PhD students and faculty in Computational Nanotechnology and Molecular Engineering, allowing UAM to push for the opening of a special program in these fields. Also it could help to increase the cooperation of UAM groups with others in a Pan-American context.”

*Guatemala (Dr. Adrian Francisco Gil)*

The chemistry curriculum at Universidad del Valle de Guatemala actually does not include nanotechnology and related areas. However, the progress of nanotechnology in recent years and the wide range of possible applications in the future make it an important subject to cover in order to prepare our students for the world they may face soon. It becomes especially important because many of our chemistry students perform graduate studies abroad, a number of them in the USA and some in Europe, where they may be enrolled in nanotechnology-related research. Thus, the chemistry curriculum at UVG is designed to give the student a good fundamental academic background, but also to give the students a general vision of what the modern trends in science are. For this reason the curriculum includes several specialized courses, which the student may take in accordance to their interests.

“Our main interest in attending the workshop is to acquire the basic knowledge of the fundamentals of nano-technology in order to find new lines of research and collaboration with fellow researchers and institutions in the USA. It is very important to emphasize that we would be able to do some computational work in nanotechnology due the widespread availability of computers and online communications. In addition, the Chemistry curriculum in our University

would benefit from the concepts, techniques and seminal ideas obtained in this workshop”,  
remarks Dr. Adrian Gil.

**PROGRAM ACTIVITIES**

**WORKSHOP PROGRAM**

The entire program (including presentations) is available at

<http://www.wag.caltech.edu/PASI>

WEEK 1: Pan-American Advanced Studies Institute in Computational Nanotechnology and Molecular Engineering					
TIME	MONDAY 5	TUESDAY 6	WEDNESDAY 7	THURSDAY 8	FRIDAY 9
9:00-9:50 AM	Recent Advances in Computational Nanotechnology (CIT, W. A. Goddard III) <a href="#">Welcome Speech</a>	<a href="#">Introduction to Hartree-Fock Theory</a> (SFSU, A. Ichimura)	<a href="#">Gaussian basis sets &amp; performance</a> (SFSU, A. Ichimura)	<a href="#">Electronic Correlation: Post HF</a> (SFSU, A. Ichimura)	<a href="#">Density Functionals (DFT): Theory</a> (SFSU, S. Aragon) <a href="#">DFT in ppt</a>
9:50-10:40 AM	<a href="#">Introduction to Molecular Mechanics</a> (CIT, M. Blanco) <a href="#">Nanomotors</a>	First Principles Force Fields (CIT, William A. Goddard III)	<a href="#">Rigid Body Manipulator Design Criteria for Simplified Dynamics</a> (PUJ, A. Jaramillo-Botero)	<a href="#">Nanodevice Design Principles</a> (CIT, S. Solares)	Design of AFM based Nanoprobes (CIT, S. Solares)
10:40-11:00 AM	BREAK				
11:00-11:50 AM	<a href="#">Dendrimers in Environmental Engineering</a> (CIT, M. Diallo)	<a href="#">Massively Parallel Molecular Dynamics (O(log2))</a> (PUJ, A. Jaramillo-Botero)	Asphaltene Precipitation: Molecular Interactions, Aggregation, behavior and simulations (IMP, C. Lira)	Catalytic cracking of Hydrocarbons: paraffins and HZSM-5 and HUSY zeolites (IMP, F. Magadan)	Fundamentals of Molecular Dynamics (CIT, T. Cagin)
12-1:30	LUNCH				
1:30-4:30 PM COMP. LAB	<a href="#">Puzzle-like Algorithm to Predict Three-Dimensional Structures of Proteins</a> (PUJ, L. Lareo)  Visualization and Molecular Mech (Cerius2) (CIT, M. Blanco)	<a href="#">Electronic Structure</a> (Spartan) (SFSU, S. Aragon)	<a href="#">Electronic Structure</a> (G98) (SFSU, S. Aragon)	Electronic Structure (G98) (SFSU, S. Aragon)	<a href="#">DFT: Implementations &amp; Performance.</a>  Electronic Structure (G98) (SFSU, S. Aragon)
6:30-8:00 DINNER	Broad Café / Avery House / Chandler				

WEEK 2: Pan-American Advanced Studies Institute in Computational Nanotechnology and Molecular Engineering		
TIME	MONDAY 12	TUESDAY 13
9:00-9:50 AM	Dynamics at the Mesoscale: Boundary Element methods in Microhydrodynamics (SFSU, Aragon)	<a href="#">Nanocluster calculations for fuel cell c</a>
9:50-10:40 AM	Molecular Electronics I (CIT, Deng): tunneling Stoddart + design of rotary motor + pentacene mobilities.	Molecular Electronics II (CIT, Jang, S
10:40-11:00 AM		
11:00-11:50 AM	<a href="#">Applications of ReaxFF to nanotechnology</a> (CIT, van Duin)	<a href="#">Electronic Structure and Chemical Re</a>
12-1:30		
1:30-4:30 PM COMPUTER LAB	<a href="#">How to build a Beowulf Cluster Lecture I</a> (PUJ, A. Jaramillo-Botero)	<a href="#">How to build a Beowulf Cluster Lectu</a>
6:30-8:00 DINNER	Broad Café / Avery House / Chandler	

### TRAINING

The workshop provided training for a combination of commercial (Gaussian 98, Cerius2), national lab funded (LAMMPS, a CRADA DoE Sponsored project), and in-house developed software (SDK modules and LAMMPS extensions). The MSC provided access to all these programs during the course of the workshop. We made available to participants SDK modules free of charge (executables) for use at their home institutions. The workshop organizers provided assistance to the participants in requesting a license from Sandia National Labs for LAMMPS source code. Sandia provides LAMMPS freely for research purposes, but currently require a simple license agreement be signed before sending source code. The CRADA partner's only real concern with the intellectual property in LAMMPS is that it not be commercialized or further distributed by a user. U.S. participants (SFSU, Cal State LA and Howard University) obtained access to the code prior to the start of the workshop. Sandia currently provides a free license for all PASI participants, as long as foreign nationals comply with export-control regulations for LAMMPS.

[http://www.cs.sandia.gov/~sjplimp/docs/lammps/license\\_howto.txt](http://www.cs.sandia.gov/~sjplimp/docs/lammps/license_howto.txt)

The PASI workshop provided Caltech developed extensions to these softwares for the participants at no charge.

### CONFERENCE TALKS, PUBLICATIONS AND OTHER RESULTING ACTIVITIES

COLOMBIA (DR. ANDRÉS JARAMILLO-BOTERO)

#### *Technical Talks*

1. Invited talk, Pan American Advanced Studies Institute in Computational Nanotechnology and Molecular Engineering, Caltech, Pasadena, California, United States, January 2004.

Title: Massively Parallel Algorithms for Large Scale, Long-Term Molecular Constrained Dynamics Simulations

*Abstract:* The limitations of current size and time scales supported by Molecular Dynamics Simulations do not permit treatment of important problems, including: dynamics of self-assembled nano-scale devices and systems, state transformations in large biomolecules, structure and properties of complex biological systems (eg. globular proteins, DNA packing), among others. Significant improvements in computational efficiency are required to overcome these limitations, primarily due to the dominant computation of interatomic forces within the molecular system under simulation. The direct summation algorithm for calculating long-range interactions in  $O(n^2)$  can be reduced by the use of cutoff methods. On the other hand, this reduces precision from the truncation of long-range forces. Two approaches are common: 1) fast serial algorithms with time lower bound computational complexities (eg. Fast Multipole Method) and 2) fast strictly parallel algorithms (eg. Cell Multipole Method). This talk presents yet another approach consisting of strictly parallel algorithms for constrained rigid multibody dynamics that assure isoefficiency scaling for large molecular systems. It shows how the complexities involved in constrained dynamics turn the classical equations of motion for an atomistic model, from an ordinary differential equation, into a complex algebraic differential equation and how it requires an alternate computation based on a spatial decomposition strategy of the “intercluster” (constrained system) forces. In spite of these added complexities, for serially coupled multibodies, novel parallel solutions are presented for both steps involved in MD simulations leading to  $O(n)$  force computations and  $O(\log n)$  equations of motion in  $O(n)$  processors. Extensions are also presented to support hyperbranched and closed chain systems with time lower bound computational complexities. Results obtained from simulations on MIMD MPPs are presented for several large scale, long-range systems.

2. Invited talk, Pan American Advanced Studies Institute in Computational Nanotechnology and Molecular Engineering, Caltech, Pasadena, California, United States, January 2004. <http://www.wag.caltech.edu/PASI>

Title: Rigid-Body Nano-Manipulator Design Criteria for Simplified Constrained Dynamics.

*Abstract:* The ability to intentionally manipulate three-dimensional (3-D) irregular-shaped matter with atomic precision, abiding to physical laws, is considered as one of the ultimate goals of nanoscience and engineering. Nature has given us a vast assortment of biological molecular machines that demonstrate the viability of this goal, including, among others, the ribosome (which can translate mRNA instructions into proteins) and kinesin, an enzyme that acts as a molecular motor which pulls things toward the outer reaches of the cell. In nerve cells, it is kinesin that pulls vesicles or other cellular materials from the cell body to the nerve endings. These biological systems are primarily “application-specific molecular machines.” They are not universal assemblers that could, in principle, be used in a programmable fashion to perform alternate functions at the molecular level. Self-replicating programmable manufacturing systems able to arrange atoms for multiple “applications” would require a universal assembler with an appropriate end-effector and a corresponding controller. The scope of this talk explores design criteria for such a universal assembler. It reviews the requirements for creation of nanometer-scale spatial positioners, from a kinematic and dynamic standpoint, as one of the basic building blocks for an atomic-scale manipulator (to arrange differently functionalized molecular building blocks into a lattice or any other nanometer-scale object in a specified and complex pattern, it is necessary to introduce positional control). The development of theoretical criteria for the design of reduced constrained dynamic complexity of a nanoscale positioning device (that could in principle lead to the

construction of a molecular manipulator), based on the equations of motion (EOM) for spatial serially articulated rigid multibodies, is presented. By using a rigid-body semiclassical mechanics approach, it is shown how dynamic complexities, such as coupling and nonlinearities introduced by high-speed operation, complicate the control task and deteriorate performance. The first section of the presentation introduces the appropriate state space forms of the EOM for a serially coupled set of rigid bodies using internal coordinates. This allows a compact mathematical description of the problem at hand and exposes the intended solution by permitting concise physical insight. The EOM are expressed as a function of the articulated body inertia operator for the multibody, leading to a highly dependent form of the EOM on this operator. The internal matrix structure of the articulated body inertia is then revealed. Finally, the analysis that leads to a reduced set of EOM from the structural simplification of the articulated body inertia matrix is presented, as well as the general kinematics and mass distribution criteria for achieving these particular forms of the mass operator.

3. Invited talk, IEEE II International Congress for the Andean Region (Andescon 2004), <http://www.andescon2004.com>, Bogotá, Colombia, August 11-13, 2004.

Title: Molecular Nanotechnology: A Computational Perspective

*Abstract:* The growing interest around the development of practical applications in Nanotechnology has spurred an enormous effort from the research community worldwide. This talk covers the conceptual and scientific origins of bottom-up Nanotechnology, from the experiments that lead to the birth and development of quantum theory to the still useful classical formalisms applicable at the molecular scale. It introduces the subject from a computational perspective, from first principles, in an effort to demonstrate the available modeling and simulation techniques used to characterize, predict and design nanoscale devices and systems. The computational complexities involved in solving the exact wave equation for matter renders it useless (for today's technology) for practical applications, typically requiring the evaluation of molecular level mechanics or dynamics of large-scale systems, hence obliging approximations such as the separation of nuclear and electronic contributions via Born-Oppenheimer, or the determination of a multidimensional potential energy surface (PES) expressed from nuclear kinematics, or the elimination of electronic contributions by treating nuclei as classical particles moving on such a PES, depending on the simulation objectives. The talk covers a brief outline of Density Functional Theory (DFT) and introduces in a tutorial like manner the techniques involved in Molecular Mechanics and Molecular Dynamics as well as its application in nanodevice modeling and simulation. Several device models are exemplified, including nanogears, nanoactuators and more complex systems such as a carbon nanotube based 3D nanopositional device proposed by the author for molecular mechanosynthesis.

4. Invited talk, Colciencias (NSF counterpart in Colombia). Forum, "New Research and Development Policies for Colombia in the area of Electronics". Friday September 3rd 2004. Los Andes University, Bogotá, Colombia. 11:50-12:20pm.

Title: Research Perspective: Nanoelectronics and Molecular Electronics

*Abstract:* The downscaling of conventional silicon based CMOS circuits and devices continues. In spite of the physical limits that define the time lower bound switching capabilities (brick walls) of conventional semiconductors, silicon based CMOS still remains as the most cost-effective technology available for modern electronic

systems. It is estimated that no charged based system can outperform CMOS. Nonetheless, the grand challenges in its continued development include improvements in: process integration, power dissipation for high-speed switching applications, reduction of drain currents in oxinitride thin films for low power applications, front-end processes, manufacturing integration, immersion lithography, design, testing, assembly and packing, yield, and metrology, among others. The enormous investment in fabrication processes allows us to predict its continued use for the next 10-15 years provided no leap-frog technology comes into play. Such potential leap-frog technologies could be quantum structures, molecular electronics (based on self-assembled molecules) or bottom-up nanoelectronics. This talk presents a brief introduction to RTDs (Resonant Tunneling Diodes), Quantum Cell Automatas, Self Assembled organic Monolayers (SAM) for Molecular Electronics such as bistable rotaxanes - employing molecules as electronics components has been a mayor focus of nanotechnology research given the possibility to synthesize organic molecules, almost without limitations, with desired structure and functionality, and bottom-up nanoelectronics. A brief outline of enabling technologies for design and profiling of these devices is covered based on the available state of the art molecular simulations methods and tools that allow us to model quantum effects (eg. Electron Tunneling) and determine other electrical properties (eg. Conductance) of nanoscale circuits and devices.

5. Invited talk, Institute of Pure and Applied Mathematics, University of California at Los Angeles, Nanoscale Science and Engineering Program 2004 Reunion, June 2004, Lake Arrowhead.

Title: Design Criteria for a 3DOF Positional Nano-Manipulator based on a Simplified Constrained Dynamics Model

*Abstract:* The ability to intentionally manipulate three-dimensional (3-D) irregular-shaped matter with atomic precision, abiding to physical laws, is considered as one of the ultimate goals of nanoscience and engineering. Nature has given us a vast assortment of biological molecular machines that demonstrate the viability of this goal, including, among others, the ribosome (which can translate mRNA instructions into proteins) and kinesin, an enzyme that acts as a molecular motor which pulls things toward the outer reaches of the cell. In nerve cells, it is kinesin that pulls vesicles or other cellular materials from the cell body to the nerve endings. These biological systems are primarily “application-specific molecular machines.” They are not universal assemblers that could, in principle, be used in a programmable fashion to perform alternate functions at the molecular level. Self-replicating programmable manufacturing systems able to arrange atoms for multiple “applications” would require a universal assembler with an appropriate end-effector and a corresponding controller. The scope of this talk explores design criteria for such a universal assembler. It reviews the requirements for creation of nanometer-scale spatial positioners, from a kinematic and dynamic standpoint, as one of the basic building blocks for an atomic-scale manipulator (to arrange differently functionalized molecular building blocks into a lattice or any other nanometer-scale object in a specified and complex pattern, it is necessary to introduce positional control). The development of theoretical criteria for the design of reduced constrained dynamic complexity of a nanoscale positioning device (nanomanipulator), based on the equations of motion (EOM) for spatial serially articulated rigid multibodies, is presented. By using a rigid-body semiclassical mechanics approach, it is shown how dynamic complexities, such as coupling and nonlinearities introduced by high-speed

operation, complicate the control task and deteriorate performance. The presentation introduces the appropriate state space forms of the EOM for a serially coupled set of rigid bodies using internal coordinates. This allows a compact mathematical description of the problem at hand and exposes the intended solution by permitting concise physical insight. The EOM are expressed as a function of the articulated body inertia operator for the multibody, leading to a highly dependent form of the EOM on this operator. The internal matrix structure of the articulated body inertia is then revealed. Finally, the analysis that leads to a reduced set of EOM from the structural simplification of the articulated body inertia matrix is presented, as well as the general kinematics and mass distribution criteria for achieving these particular forms of the mass operator. From the resulting analysis, a set of compliant manipulator configurations that could, in principle, be built from carbon nanotubes, linked by direct-driven rotational molecular joints, is presented.

*Tutorials (4 hours) on Computational Nanotechnology*

6. IV IEEE National Robotics Competition, September 2004, Pontificia Universidad Javeriana, Cali, Colombia.
7. I National Congress on Biotechnology, October 11, 2004, Universidad de la Sabana, Bogotá, Colombia.

*Abstract:* Nanotechnology has become one of the fastest growing areas in science today. The promise of intentional and precise manipulation of matter at the atomic level using mechanosynthetic processes will bring about immense changes in almost every branch of life. This tutorial initiates engineering students into the fundamental principles of Nanotechnology, beginning with scaling of physical quantities down to the nanoscale, quantum theory and its approximations up to the use of classical physics to model and predict the behavior of rigid body macro molecules that could in principle serve as building blocks for complex nanosystems. A detailed explanation of Molecular Dynamics, for atomistic and rigid molecular multibodies, is included in order to simulate exploratory nanodevice designs. Among these, carbon based nanogears and other type of force actuators. The tutorial explores novel applications for nanotechnology in a varied number of areas, including: health, environmental engineering, military, and transportation, among others.

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## RESOURCES

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### LABORATORY

600+ sq.ft. computer lab at the Materials and Process Simulation Center (MSC) at Caltech.

- Clinical N/A
- Animal N/A
- Computers
  - 73 nodes, 146 processor 2.2 GHz Intel Xeon cluster, running Red Hat Linux, 2 GB nodes, 64 GB disk space.
  - One Silicon Graphics Origin 2000 supercomputer (16 CPU, R10000, 195 MHz, 7 GB RAM, 260 GB disk)
  - A Dell PC Cluster (20 node, 40 CPU, PIII, 866MHz, Beowulf/Linux, 20 GB RAM, 540 GB disk)
  - An IBM B80 Cluster (6 node, 24 CPU, Power3, 375MHz, 18GB RAM, 324 GB disk)
  - Two Dell PowerEdge 6300 Servers (4 CPU, PIII Xeon, 550 MHz, Linux OS, 1 GB RAM, 27 GB disk)
  - Two Dell 6100/200 PowerEdge Servers (4 CPU, PPro, 200 MHz, Linux OS, 512 MB RAM, 27 GB disk)
  - One Silicon Graphics Octane ESI graphics workstation (2 CPU, R12000, 300 MHz, 512 MB RAM, 27 GB disk)
  - One Silicon Graphics Octane SSI graphics workstation (2 CPU, R10000, 195 MHz, 128 MB RAM, 4 GB disk)
  - One Silicon Graphics Octane SI graphics workstation (1 CPU, R10000, 195 MHz, 256 MB RAM, 4 GB disk)
  - Six Dell Dimension 4100 Series workstations (1 CPU, PIII, 1GHz) (Linux OS, 256 MB RAM, 20 GB disk)
  - Three Dell Precision 410MT workstations (2 CPU, PIII, 600 MHz) (Linux OS, 256 MB RAM, 18 GB disk)
  - Three Dell Precision 410MT workstations (2 CPU, PIII, 450 MHz) (Linux OS, 256 MB RAM, 18 GB disk)
  - Four Silicon Graphics Indigo2 Solid Impact graphics workstations (R10000 CPU, 195 MHz, 192 MB RAM, 2 GB disk)
  - Fifteen Silicon Graphics O2 graphics workstations (R5000 CPU, 180 MHz, 192 MB RAM, 2 GB disk)
  - One Silicon Graphics Challenge DM server (2 CPU, R4400 CPU, 200 MHz, 192 MB RAM, 130 GB disk)
  - One Silicon Graphics Indigo2 Extreme graphics workstation (R4400 CPU, 250 MHz, 96 MB RAM, 2 GB disk)
  - Eight Silicon Graphics Indy graphics workstations (R4400 CPU, 175 MHz, 96 MB RAM, 1 GB disk)
  - One Seiko-Epson workstation (PIII, 800 MHz) (Linux OS, 512 MB RAM, 28 GB disk)
  - Two Seiko-Epson workstations (PIII, 600 MHz) (Linux OS, 128 MB RAM, 20 GB disk)
  - Two Dell Dimension XPS workstations (1 w/Linux OS, 1 w/NT 4.0) (PIII, 400MHz, 128 MB RAM, 13 GB disk)
  - One Dell Precision 410MT multi-user server (2 CPU, PIII, 500MHz) (NT 4.0 Terminal Server edition OS) (512 MB RAM, 9 GB disk)

- One Dell Dimension L workstation (1 CPU, PIII, 933MHz) (Win98 OS, 256MB RAM, 20 GB disk, 15" LCD)
- Several laptops (Sony and Dell) running Windows98/2K.
- There are also ~ 25 older SGI, HP, Sun, Apple, and IBM workstations available

#### **OTHER MAJOR EQUIPMENT**

- One Network Appliance F820 file server (1CPU, 733MHz, 1GB RAM, 504GB disk)
- In addition, we make use of supercomputers at Caltech (HP Exemplar), NPACI, NCSA, PNNL, LANL, LLNL, and SNL.

#### **WORKING AND LIVING FACILITIES**

6,500 square feet facility located at the Beckman Institute, office space for 40+ scientist, postdoctoral fellows, graduate students and Senior Personnel.

The Beckman Institute Auditorium with audiovisuals was reserved for the lecture series (mornings) and full duration of the workshop. Caltech's computer training room, with 15 additional (rental) personal computers was networked to the Caltech campus network and available for the use by the participants.

A block of 14 rooms was reserved at a local hotel, located in Old Pasadena, within walking distance of Caltech and urban amenities.

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**CALI, COLOMBIA WORKSHOP**

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**Date:**

February 14-18, 2005.

**Place:**

Pontificia Universidad Javeriana  
Calle 18 # 118-250  
Cali, Colombia

Pan American Advanced Studies Institute (PASI)  
NSF Funded Workshop in  
Computational Nanotechnology and Molecular Engineering

**Core Participants:**

**Organizers:**

- Andrés Jaramillo-Botero (co-organizer), Research Associate, Materials and Process Simulation Center, Caltech and Pontificia Universidad Javeriana Cali, Colombia.
- Mario Blanco (co-PI, co-organizer), Director, Molecular Process Simulation, Materials and Process Simulation Center, Caltech.

**Other Participants:**

- Daniel Fisher, Phd student, Materials and Process Simulation Center, Caltech
- Amos Anderson, Phd student, Materials and Process Simulation Center, Caltech
- Albert Cervantes, Phd student, Materials and Process Simulation Center, Caltech.
- Leonardo Lareo, Faculty of Science, Pontificia Universidad Javeriana, Bogotá, Colombia.
- Federico Sequeda, Center for Materials Research, Universidad del Valle, Cali, Colombia.
- Invited Speaker, Cenicaña, Cali, Colombia.
- Alba Lucía Ávila, Uniandes, Bogotá, Colombia.
- Camilo Rueda, Computer Science Department, Pontificia Universidad Javeriana, Cali, Colombia.
- Antal Buss, Computer Science Department, Pontificia Universidad Javeriana, Cali, Colombia.

**AGENDA**

**Saturday, Feb 12, 2005:**

**Arrival to Cali, (8:33pm) US participants will be transported to Faculty Housing.**

Stay at the Villa Javier House (PUJ-Cali)

**Sunday, Feb 13, 2005:**

**9:00-5pm** Short Tour of Cali and Visit to Calima Lake (lunch included)

**Monday, Feb 14, 2005:**

<b>Time</b>	<b>Activity</b>	<b>Responsible</b>	<b>Place</b>
<b>7:30-8:00</b>	Breakfast at CVJ	Ivette Ortiz	Casa Villa Javier
<b>8:00-8:15</b>	Meeting with PUJ Rector	Andrés Jaramillo-Botero	Rector Office
<b>8:15-10:00</b>	Picture of Group, Tour of PUJ Campus	Ivette Ortiz, Andrés Jaramillo-Botero	Oficina de Comunicaciones, Campus
<b>10:00-12:00</b>	Student Interaction Activities	Claudia Mora	TBA

12:00-2:00	Lunch	Ivette Ortiz	Casa Villa Javiera
2:00-5:00	Visit to labs and local project demonstrations		Andrés Jaramillo-Botero
	Labs		
5:00-7:00	Open		
7:00-9:00	Dinner	Andrés Jaramillo-Botero	Jaramillos

### Tuesday, Feb 14, 2005:

Time	Activity	Responsible	Place
7:30-8:00	Breakfast at CVJ	Ivette Ortiz	Casa Villa Javier
8:00-9:00	Workshop Registration	Local Coordinator	Auditorio Javeriano
9:00-9:15	Opening remarks	Andrés Jaramillo-Botero, Mario Blanco	Auditorio Javeriano
9:15-10:15	Talk: Opportunities for Molecular Simulations in Plant biology, drug design, or other (TBD)	Invited Speaker (cenicaña, ciat, pat)	TBA
10:15-10:45	Break		
10:45-11:45	Talk: First Principles Modeling and Simulation	TBD (Nelson Porras)	Auditorio Javeriano
11:45-12:45	Talk: Molecular Modeling in Biology and Material Science	Mario Blanco	Auditorio Javeriano (Caltech)
12:45-2:00	Lunch	Ivette Ortiz	Cafeteria Central (invitados especiales)
2:00-3:00	Talk: Computational Modeling and Simulation for Nanotechnology	Andrés Jaramillo-Botero (PUJ)	Auditorio Javeriano
3:00-4:00	Talk: Identification of sequences in biological processes	Leonardo Lareo	Auditorio Javeriano (PUJ)
4:00-7:00	Open		
7:00-9:00	Dinner	Andrés Jaramillo-Botero	Cali Viejo

### Wednesday, Feb 15, 2005:

Time	Activity	Responsible	Place
7:30-8:00	Breakfast at CVJ	Ivette Ortiz	Casa Villa Javier
8:00-9:00	Talk: Quantum Mechanical Solutions to Environmental Problems	Mario Blanco (Caltech)	Auditorio Javeriano
9:00-10:00	Talk: Modeling of Pollution Dynamics or Education for Nanotechnology Development	Clean Production Group (PUJ) / Alba Ávila (Uniandes)	Auditorio Javeriano
10:00-10:30	Break		
10:30-11:30	Talk: Constraint Programming for Biological System Simulations	Camilo Rueda (PUJ)	Auditorio Javeriano
11:30-12:30	Talk: Nanoparticle films for surface hardening	Federico Sequeda / Pedro Prieto (Univalle)	Auditorio Javeriano
12:30-2:00	Lunch	Ivette Ortiz	Cafeteria Central (invitados especiales)
2:00-3:00	Talk: Quantum Montecarlo Theory (A Primer)	Daniel Fisher (Caltech)	Auditorio Central
3:00-4:00	Talk: Teraflop computing with GPUs for Scientific Applications	Amos Anderson (Caltech)	Auditorio Javeriano
4:00-5:00	Talk: The Visual Human Project or CMDF Software Development	Albert Cervantes (Caltech?)	Auditorio Javeriano
5:00-7:00	Open		
7:00-9:00	Dinner	Andrés Jaramillo-Botero	TBD

### Thursday, February 16, 2005

Time	Activity	Responsible	Place
7:30-8:00	Breakfast at CVJ	Ivette Ortiz	Casa Villa Javier
8:00-9:00	Talk: Model for the NR1 subunits in glutamate receptors	Leonardo Lareo	Auditorio Javeriano (PUJ)

<b>9:00-10:00</b>	Talk: The Electronic Nose	Mario Blanco (Caltech)	Auditorio Javeriano
<b>10:00-10:30</b>	Break		
<b>10:30-11:30</b>	Talk: Towards Molecular Mechanosynthesis - design of nanometer scale 3D positioners	Andrés Jaramillo-Botero (PUJ)	Auditorio Javeriano
<b>11:30-12:30</b>	Talk: Software for Molecular Modeling and Simulation		Antal Buss (PUJ)
	Auditorio Javeriano		
<b>12:30-2:00</b>	Lunch and workshop closing (possible collaborative efforts)		Ivette Ortiz, Andrés Jaramillo-Botero, Mario Blanco
	Cafeteria Central		
<b>2:00-3:00</b>	Sightseeing	Local Coordinator	TBD
<b>3:00-4:00</b>	Sightseeing		TBD
<b>4:00-5:00</b>	Sightseeing		TBD
<b>5:00-7:00</b>	Sightseeing		TBD
<b>7:00-9:00</b>	Dinner and dance night (salsa)		TBD

### Friday, February 18, 2005:

Morning: Open (swimming pool, sports, etc.)

Afternoon: reunion de cierre (asado) en Casa Villa Javier

### Saturday, February 19, 2005:

Return US participants: 4:30am (pick-up time)

Information on Arrivals-Departures to-from Cali:

Driver assigned to the group during stay in Cali: Mr. Gerardo Ramón Lugo

a. Caltech members of the MSC (party of 5)

This party will stay at the “Casa Villa Javier” in the Pontificia Universidad Javeriana, Calle 18 # 118-250, Cali, Colombia.

b. PUJ-Bogotá (Biochemistry). TBA

c. Univalle (Materials Science). TBA

d. Others (Bogotá)

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**GUATEMALA CITY/HIGHLANDS, WORKSHOP**

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**Pan American Advanced Studies Institute (PASI)  
NSF FUNDED WORKSHOP IN  
COMPUTATIONAL NANOTECHNOLOGY AND MOLECULAR  
ENGINEERING  
Jan 15-23, 2005**

**Saturday, Jan 15:**

Morning: Visit to Universidad del Valle de Guatemala (UVG) campus.  
Tour of campus. Setup Computer  
laboratory/software. Afternoon: Visit "Guatemalan Museum of  
Archeology and Anthropology". Evening: visit "La Zona Viva",  
trendy area in Guatemala city.

**Sunday, Jan 16:**

Visit to Antigua Guatemala (old Colonial Capital City,  
Monument of the Americas) at the foot of "Agua" Volcano.

**Monday, Jan 17:**

Morning:

Introductory Overview of Quantum Mechanical Electronic Structure  
Calculations I : Andrew Ichimura  
Computer lab: Spartan, Illustration of Electronic Structure  
Calculations: Andrew

Afternoon

The Ethnobotany point of view of Medicinal Plants by Dr. E. Pöll.  
Presentation of ongoing projects on phytochemistry by UVG students.

**Tuesday, Jan 18:**

Morning

Presentation of Ady Giordano: Protein Crystallization Modeling, Fast Solvation Model  
Applications of Atomistic Modeling to Molecular Engineering  
Anthropological and Cultural Issues in the Practice Medicine, UVG Faculty Seminar

Afternoon

Computational Chemistry Solutions to Problems of Environmental  
Chemistry  
Student Seminars: These are 20 minute presentations by SFSU, Jackson State  
Presentations on their current research interests.

**Wednesday, Jan 19:**

Morning:

Isolation and Identification of Active Ingredients in Muerdago (Mistle Toe): Adrian Gil and Mario Blanco

Afternoon:

Free! Last chance for sightseeing in Guatemala city.

**Thursday, Jan 20:**

Morning:

Travel to UVG Altiplano (Universidad del Valle de Guatemala, Highlands Campus) for a mini-course in collection of medicinal plants.

Tour of Chichicastenango (market day).

Afternoon:

Arrive 1PM, to El Tablon, Solola, location of the campus

Tour of the campus, Introduction to the academic and research programs by the UVG staff (Dr. Poll)

**Friday, Jan 21:**

Morning:

Tour of Solola's Indian Open Market. Visit with local "naturalists" for a direct observation of herbal medicinal practices.

Afternoon: Tour to Panajachel and Santiago Atitlan

**Saturday, Jan 22:**

Morning:

Visit "Chalquijya" where the UVG promotes an agricultural project on medicinal plant cultivation and collection .

Afternoon: Wrap up of the PASI workshop. Evaluation and discussion session.

**Sunday, Jan 23:**

Travel back to Guatemala Airport

Departure: SFSU

Mario UA 0844 11:40 am

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Closer accommodations would be desirable, although some other priorities would have to be changed accordingly. Although the computer lab offered a comfortable environment (all new flat panel display computers) for the number of participants at all times, a handful of participants were asked not to use the computers during the lecture hours. Most restrain from this practice. In future opportunities a separate room for lectures will be reserved, or computers will be taken off line during lectures to avoid distractions. Printed lectures were contemplated but the cost was significant, considering the widespread use of Power Point presentations in color. Instead, the lectures were distributed in CD format, totaling over 194 Megabytes.

## TESTIMONIALS

### US PARTICIPANTS

“I enjoyed the ‘cramming’ of information into my head. Even the painful moments, when looked back on, were what made the workshop a ‘workshop’ ” (Heather Harding)

“Overall, I enjoyed the workshop, I learned new techniques that I can use in my present research. The implementation of this workshop was a great idea and I look forward to attending the next year” (Tomekia Simeon)

“I thought it was a good idea to allow students to apply the knowledge that they learned in the workshop” (Shungo Miyabe)

### LATIN AMERICAN PARTICIPANTS

“I express my complete gratefulness for the opportunity to assist to Caltech team efforts and to NSF financial support”, (Dr. Leonardo Lareo, Colombia)

“For the Guatemalan delegation this was a unique opportunity to start new work involving theoretical and computational chemistry. This will benefit research and teaching in our country”, (Dr. Cesar Estrada, Guatemala)

“A conference of possible interactions and stays at Caltech is needed.... Please let me know about the next event. I would like to start a collaboration” ( Dr. Jose-Manuel Martinez-Magadan, Mexico)

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**FINANCIAL AND BUDGET INFORMATION**

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(To be filed at completion of Workshop by Mr. Alvin Torres, Account Manager, Caltech,  
Feb 28th 2005)