DICA-016-2020
Santiago de Cali, 9 de julio de 2020

EL DECANO DE LA FACULTAD DE INGENIERÍA Y CIENCIAS
INFORMA QUE:

En el periodo 2020-1 (enero-junio) se dictaron los cursos que se relacionan a continuación, para los estudiantes del Doctorado de Ingeniería y Ciencias Aplicadas de la Pontificia Universidad Javeriana Cali, en el marco del Programa Ómicas:

Asignatura	Profesores
Análisis Probabilístico y Estadístico	Isabel García
Bioinformática	Mauricio Quimbaya y Fabián Tobar
Biología Celular y Molecular I	Mauricio Quimbaya
Biotecnología	Mauricio Quimbaya
Bases Matemáticas para no Ingenieros	Andrés Salazar
Química y Física de Materiales	Drochss Valencia
Matemáticas Discretas	Diana Bueno
Ciencia e Ingeniería de Nanoescala	Andrés Jaramillo
Verificación de Sistemas	Camilo Rocha y Camilo Rueda
Análisis de Redes para Grandes Volúmenes de Datos	Jorge Finke
Aprendizaje Automático	Diego Luis Linares
Bases Formales de la Computación	Frank Valencia

Cordialmente,

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Nano-scale Science and Engineering (400FIO002)

Professor Andrés Jaramillo Botero
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Class schedule: Tuesday and Wednesday, from 9-11am (3 hours of lecture and 1 hour discussion)
Consultation hours: Monday and Tuesday, from 10-noon (email, phone or in person)
Pre-requisites: prior knowledge of Physical Chemistry, introductory differential equations and numerical analysis

Motivation

The emerging ability to economically arrange atoms in most of the ways permitted by physical law will revolutionize life, as we know it. Controlling the expression of material properties in any of its phases (i.e. solid, liquid, gas or plasma) and at any scale depends on its atomic composition and arrangement in a 2D or 3D structure, both of which originate at the nano-meter scale.

In order to understand, characterize, manipulate or optimize such properties one must study and elucidate the interactions between the different material building blocks or constituents, fundamentally atoms, which live in the nano-meter scale. By today's standards, this requires the simultaneous contribution from theory, computation and experiments engaging a wide range of technical fields, from physics, chemistry and biology, to computer science and engineering. This course takes a computational approach, based on first principles quantum mechanics and classical approximations, to address these issues.

Computational nano-science now supplements and complements physical experiments, and in many cases constitutes an enabling tool to study problems that are otherwise extremely expensive, dangerous or even impossible to address through experiments alone. As our theoretical understanding of matter and material phenomena improves, materials and processes "by design" will become the norm, and this will entail solving large-scale numerical problems to predict atomic structure, composition, grain interfaces, etc., from engineering or at-scale property specifications and the use of fundamentally-derived models at the heart of computational optimization engines.

Nanotechnology is not only an exciting interdisciplinary research area, but also a technological and commercial reality that will continue to drive and shape the future and health of humanity, environment, transportation, energy, and space systems, education and almost everything else that we can think of.

Course description

The 16 week course will introduce the basic issues involved in nanotechnology and its broader applications, lay out the scientific end engineering foundations required to understand how the nano-scale atomic structure and composition of matter drives behavior, present the computational models and methods derived from first-principles quantum mechanics (QM), statistical mechanics, and classical mechanics and dynamics theory to characterize, design, and optimize materials, devices, systems and processes (biological, physical, chemical, etc.), and demonstrate their application for studying and solving critical challenges from a wide set of fields.

Goals and Objectives

The course is meant as a practical hands-on introduction to expose students to the tools of modern computational chemistry and computational materials science relevant to atomistic descriptions of the structures and properties of chemical, biological, and materials systems. It is aimed at experimentalists and theorists in chemistry, materials science, chemical engineering, applied physics, biochemistry, physics, geophysics, and from other engineering programs with an interest in characterizing and designing molecules, drugs, and materials.

After successful course completion, the attendant will:

- Achieve a conceptual, theoretical and applied understanding of how atomic structure and composition define material properties at all scales, and in particular at the nano-scale

- Acquire the fundamental knowledge about first-principles methods to study, characterize and optimize static and dynamic material properties, including but not limited to *ab initio* methods, density functional theory (DFT), adiabatic, non-adiabatic and coarse-grain force fields, molecular mechanics and molecular dynamics (MM/MD), and Monte Carlo (MC) methods.
- Learn about applications to materials design, energy storage and retrieval, tissue engineering, drug design, space exploration, and others addressed using the first-principles computational approach presented in the course.
- Understand the broader impact of nano-scale science, engineering, and nanotechnology.

Prerequisites

- Basic knowledge of C/C++, Python and Unix is required. Will also be used during the course lectures as well as in class assignments. Mathematica or Matlab are a plus.
- Background required in differential equations, statistical and classical mechanics, and linear algebra.
- The students must have successfully completed a course on Physical Chemistry.

Course contents and calendar

1. Introduction to computational nanoscale science and engineering (2 sessions)
- *Intentional manipulation of matter at the atomic scale*
- *Nature as a source of inspiration to nanotechnology (and vice versa)*
- *Current challenges in nanoscale science and engineering*
- *Theory and computation as enabling tools in advancing nanotechnology*
- *Time and length scales in atomic and sub-atomic motion*
- *Implications of a nano-scale world*

2. Computational Science: introduction to calculating material properties (1 sessions)

3. Theory and methods for first-principles based modeling and simulation (22 sessions)
- *Foundations of Quantum Mechanics – QM (ab initio methods)*
- *Adiabatic approximations to QM*
  - *Hartree-Fock approximation to many-body QM (Exchange)*
  - *Density Functional Theory: Kohn-Sham methods*
  - *LDA and GGA approximations to exchange-correlation energy*
  - *Electrons in periodic boundary conditions; reciprocal space and Brillouin-Zones.*
  - *Band-structure in solids*
  - *Basis sets – atomic and plane-wave*
  - *Pseudo potentials*
  - *SCF methods*
- *Approximations from statistical and classical mechanics, force fields, molecular mechanics and dynamics*
  - *Introduction to pair and valence potentials*
  - *Molecular mechanics: Energy minimization, geometry optimization, transition states*
  - *Molecular Dynamic: Ensembles*
  - *Conventional force fields (UFF[1], Dreiding[2], CHARMM[3-6], GAFF[7], etc.)*
- *Mixed QM-Classical Approximations: recovering chemical reactions and (some) electronic effects*
  - *Adiabatic reactive force fields (ReaxFF[8-10])*
  - *Non-adiabatic reactive force field (eFF-GHA[11-13])*
  - *Force field parameter optimization (GARFfield[14])*
- *Rigid body mechanics and coarse-grain molecular mechanics/dynamics methods*
  - *Coarse-grain force fields and constrained Molecular Dynamics (CoMoDyn[15])*
- *Monte Carlo (MC) Methods*
  - *Gran Canonical MC and kinetic MC*

4. Characterization of material properties using 1st principles computational methods (3 sessions)
- *Structure prediction – radial distribution function, XRD, neighbor analysis, etc.*
- *Thermodynamics properties – temperature, pressure, entropy, enthalpy, and free-energy*
- *Mechanical properties – stress-strain and elastic constants*
- *Transport properties (includes electrical, optical, thermal) - bandstructure*
- *Others (magnetic, rheological, tribological)*

5. Class research project (1 session)

- *Specification, requirements and deliverables*

6. Applications (1 sessions)

- *Health: Characterization and design of DNA nano-sequencers*
- *Tissue engineering: Molecular scaffolds for cartilage tissue*
- *Medicine: Nano drug delivery systems (DDS)*
- *Proteomics: G-protein coupled receptor structure prediction, conformational analysis and ligand interactions*
- *Materials characterization: Reaction kinetics during Portland cement hydration*
- *Space exploration: Hypervelocity impact ionization fragmentation in space missions (Cassini-Hyugens)*
- *Material synthesis in defense applications: Low-temperature atomic layer thin film deposition*
- *Energy storage and retrieval: Cementitious materials for CO2 sequestration*

Simulation packages and tools

We will be using different modeling and simulation tools to demonstrate and apply the theory and methods described during the lectures, among these:

- *ATK/VNL from http://www.quantumwise.com is a multi-paradigm framework capable of QM and MD. It is particularly well-suited for tunneling calculations using the Landauer formulation (good molecular builder and includes reaxFF).*
- *SeQuest general purpose electronic structure code for periodic systems, slabs or finite molecules (Sandia National Laboratory, SNL, http://dft.sandia.gov/Quest/)*
- *Quantum Espresso general purpose electronic structure code for periodic systems, slabs or finite molecules (http://www.quantum-espresso.org)*
- *Octopus time-dependent DFT code (http://www.tddft.org/programs/octopus/wiki/index.php/Main_Page)*
- *GAMESS general ab initio quantum chemistry package (http://www.msg.chem.iastate.edu/gamess/)*
- *LAMMPS (SNL, http://lammps.sandia.gov), including specific potentials:*
    - *Electronic (http://lammps.sandia.gov/doc/pair_eff.html)*
    - *Reactive (ReaxFF, http://lammps.sandia.gov/doc/pair_reax_c.html)*

A brief tutorial on the use of a sample QM, MD, MC package will given. The student will be responsible for learning other tools that he/she chooses to use for the same level of calculations as those listed here.

Other useful tools:

- VMD visual molecular dynamics (http://www.ks.uiuc.edu/Research/vmd/)
- Ovito molecular visualizer (http://www.ovito.org)
- Avogadro molecule builder (http://avogadro.cc/wiki/Main_Page)
- GARFfield (force field parameter optimizer, http://lammps.sandia.gov/offsite.html)
- Moltemplate text-based molecular builder for LAMMPS (http://www.moltemplate.org)

How to study for this course

Attend lectures, read the class notes ahead of time (if applicable), read the suggested scientific literature recommended during class sessions, practice simulation runs on local cluster, and solve all the assignments, including the class project individually (unless explicitly stated otherwise). Teamwork is encouraged, but you must hand in your own results for all assignments.

Evaluation

30% Assignments
20% Midterm
20% Journal reviews
20% Project

Journal reviews

Two (2) journal reviews will be due throughout the semester. Find a paper recently published in a scholarly journal and submit a review of the article to the course web page. The paper's topic should be based on the nanoscience concepts recently covered in class. The review should address the following: 1) purpose of the study; 2) methods/procedures used; 3) key findings and major points; 4) critical review. The length of the review should be no longer than the equivalent of a single spaced page (~600 words). The purpose of the article is to tie the nanoscience concepts covered in class to current or recent progress in nanotechnology and to expose you to additional nanotechnology material not covered in class. See the course schedule for due dates.

Assignments will be handed out each week during the first 8 weeks, and it will use generally available computer software implementing the basic methods on applications aimed at exposing the students to understanding how to use atomistic simulations to solve problems. Each calculation requires making decisions on the specific approaches and parameters relevant and how to analyze the results. The lowest homework score will be dropped from the final grade.

No late assignments will be accepted (because solutions will be posted on the day assignments are due.)

The midterm will require each student to submit a proposal for a project using the methods of this course to solve a research problem that can be completed in the final 8 weeks. The homework for the last 8 weeks is to turn in a one-page report on progress with the project.

Class project

The final project contains two parts: 1) a paper portion and 2) a PowerPoint presentation portion. In this project you are essentially designing a lecture that covers a nanotechnology and/or nanoscience topic from the list below. The purpose of the paper is to provide explanations and details of the presentation slides. But, the paper should tell a story and not simply catalogue the slides one by one.

Paper details

- 5-10 pages double spaced (not including figures, images, tables, etc.)
- Use at least 10 references, which may include journal articles, textbooks, news articles, web sites, etc. Be sure to include a bibliography. For web references you may simply use the web address.
- Publication dates for the main relevant topic should be recent (~ <5 years old).

Presentation details

- 10-15 slides
- Provide the appropriate citations for data/images/text that is not yours (including web addresses)

You can choose from the following list of broad sample topics (topics are very broad, so you may choose a more specific topic with in the given topic): Nanofluidics, Semiconductor nanostructures, Nanoparticles, nanocrystals, etc., Self-assembly of materials and devices, Physical processes in semiconductor nanostructures, Nanomagnetic materials and devices, Thermodynamics at the nanoscale, Electronics and electro-optic molecular materials and devices, Biomolecular Nanoscience, Biomimetic nanotechnology, Chemical Synthesis and modification of nanomaterials, Supramolecular Chemistry, Molecule-based devices, Nanowires, Therapeutic nanodevices, Friction and wear at the nano and atomic scale, Molecular films for lubrication, Nanotechnology for data storage applications, Molecular electronics, Photonic materials, structures, and devices.

The final will be a research report describing the calculations and conclusions, unless otherwise stated and agreed a priori.

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ACADEMIC INTEGRITY

Students are expected to exhibit the highest level of academic honesty. In particular, students are expected to read and follow all University policies and procedures (see the "Reglamento del Estudiante"); pursue their learning goals with honesty and integrity; demonstrate that they are progressing individually and in a timely fashion by meeting course deadlines and following outlined procedures; observe a code of mutual respect in dealing with Faculty, mentors, staff, and fellow students; behave in a manner consistent with the standards and codes of the profession they are studying for; and meet all other institutional obligations in a timely manner. Students not practicing good academic honesty may be subject to disciplinary action including suspension, dismissal, or holds on records (see section VI of the "Reglamento del Estudiante").

Academic Dishonesty

We expect all students to approach their education with academic integrity, i.e. the pursuit of scholarly knowledge free from fraud and deception. Academic dishonesty undermines this objective. Academic dishonesty can take many forms, including: cheating, gaining or providing unauthorized access to examinations, using unauthorized materials during exam administration, submitting credentials that are false or altered in any way, Plagiarizing (using someone else's work as your own; including copying and pasting from the Internet without using quotation marks and without acknowledging sources), forgery, fabricating information or citations, or falsifying documents, submitting the work of another person in whole or in part as your own, facilitating acts of dishonesty by others (including making tests, papers, and other course assignments available to other students), and tampering with the academic work of other students.

About Plagiarism

The Pontificia Universidad Javeriana takes a strong stance against plagiarism, and students found to be plagiarizing will be penalized according to section VI of the "Reglamento del Estudiante". If you copy sections or whole documents word-for-word—or if you paraphrase by changing a word here and there—without identifying the author, or without identifying it as a direct quote, then you are plagiarizing. This type of identification applies to Internet sources as well as to print-based sources. Copying and pasting from the Internet, without using quotation marks and without acknowledging sources, constitutes plagiarism. Always keep careful track of sources! [1]

Plagiarism defeats the purpose of education. If you plagiarize deliberately, you are not educating yourself, and you are wasting your time on courses meant to improve your skills. If you plagiarize, you are deceiving yourself.

Please acknowledge your understanding and acceptance by signing, dating and returning this page to the instructor, by the end of the first day of class.

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Student signature
Date: _____

[1] Adapted from http://www.tesu.edu/academics/catalog/Academic-Code-of-Conduct.cfm