# Long Form Course and Curriculum Proposal

## I. Heading and Proposal Number

A. University of North Carolina at Charlotte

New Graduate Course

Course Proposal from the Department of Physics and Optical Science

B. Proposal Number PHYS 8-1-08

C. Establishment of a new graduate course: Methods of molecular modeling and simulation in physics

## II. Content of Proposal

A. 1. **Summary.** The Department of Physics and Optical Science proposes to add the following course to the graduate curriculum, PHYS 6203.

II. A. 2. **Proposed Catalog Copy**

**PHYS 6203. Methods of molecular modeling and simulation in physics. (3)**
Prerequisite: Permission of the instructor. Numerical methods. Atomic models of soft-matter systems: liquids, polymers, and biomolecules. Molecular dynamics and Monte Carlo methods. Inter-particle potentials. Methods of efficient conformational sampling. Free energy calculations. Introduction to fundamental methods of molecular simulations designed to characterize and predict properties of microscopic systems in materials, phsics, and biology. Classical simulations and their connection to experimentally measurable properties. (*Spring, on demand*)

B. Justification

Our current understanding of the material world is complete: all objects are composed of atoms, all atoms are made up of nuclei and electrons. In theory, one should be able to predict all structural, mechanical, thermodynamic and other properties of objects surrounding us exactly. In practice, however, this task is faced with insurmountable challenges. Only for a few simple models in physics, such as ideal gases or crystal lattices, exact analytical solutions can be found. For the vast majority of all other objects in material science, physics, chemistry and biology, numerical methods are necessary. Over the past three decades, numerical and simulation techniques have evolved into a separate and fast-growing subfield of theoretical physics and chemistry. As the focus in modern natural sciences is shifting toward more complex objects that lie at the intersection of physics, chemistry and biology, the role of molecular simulations is set to

increase. For the increasingly interdisciplinary research landscape of tomorrow, it is essential that the researchers of today get familiar with as wide array of research tools and techniques as possible. With their ability to interrogate systems at the atomic level, computer simulations are one of such most valuable tools. The objective of the proposed course is to introduce fundamentals of computer simulations to the graduate curriculum. The main focus will be to familiarize graduate students with the most important simulation techniques that are available today to help aid their research.

C. Impact

1. Graduate students with an interest in materials, complex physicsal or biological systems will be served. This includes master's degree students in Applied Physics, including those in the medical physics concentration, and Ph.D. students in optics, engineering, biology, or a related field.
2. a. The course will be taught on-demand..
   b. Other courses will not be affected.
   c. Anticipated enrollment is 10-20 students per semester.
   d. Other course enrollment would not be affected in a large way. For example, the 30 credit hours required for a non-thesis master's degree requires the offering of 10 courses during a 2-year period. The Department of Physics and Optical Science currently offers about 16 courses on a regular basis.
   e. This course has not been offered before.
   f. Other areas of the catalog would not be affected.

D. Resources Required

1. a. There is no requirement for new faculty.

   b. Dr. Andriy Baumketner from the Department of Physics and Optical Science will initially teach the course.

2. Exisiting facilities can be used for access to a computer laboratory with 20 workstations.
3. There is an equipment requirement for 20 workstations which are in existance.
4. Existing computing resources can be used.
5. There is no requirement for additional audio-visual resources.

E. Consultation with the Library

1. Library Consultation is attached.
2. Other departments were not consulted.

F. Initiation and consideration of this proposal

1. The graduate studies committee of the Department of Physics and Optical Science approved this proposal and it was unanimously supported by the Department faculty.

G. Attachments

1. Library Consultation
2. Proposed course description and outline.

**Sample syllabus:**

**PHYS 6203. Methods of molecular modeling and simulation in physics. (3)**
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***Lecture textbooks:***

Required: A. Leach "Molecular modeling: Principles and applications"

Recommended: M. P. Allen and D. J. Tildesley "Computer simulations of liquids"
D. Frenkel and B. Smith "Understanding Molecular Simulation"

***The course:***

PHYS 6203 is intended to introduce the main ideas behind classical molecular simulations of physical systems in condensed state, such as liquids, polymers etc. The students will learn basic techniques of molecular dynamics and Monte Carlo simulations, will get practical skills required to setup simulations for a given physical system, analyze the results of these simulations and extract physically measurable quantities. Three simulation projects will be conducted as part of this course.

***Expectations of students:***

- Attendance and taking good lecture notes is expected. Supplementing the lecture notes with study notes based on the textbooks is a good way to improve your chances of being successful in this course. Recommended textbooks are intended for students who see their career in research or education.

- Three mid-term projects are scheduled. Students will be assigned specific simulation projects and will be asked to write a report following their completion. The projects will count toward the final grade.
- One oral presentation is scheduled. Students will be divided into 3 groups, each of which will be assigned a research article on topics covered in the class. Presentations will count toward the final grade.

- Grades are assigned using a 100-point grading scale: A = 90-100, B = 80-89, C=70-79, D<69. Your grade will be determined as follows:

| | |
|---|---|
| Simulation projects | 25%+25%+25%=75% |
| Final oral presentation | 25% |

***Academic integrity***

Students have the responsibility to know and observe the requirements of The UNCC Code of Student Academic Integrity (Catalog p. 275). This code forbids cheating, fabrication or falsification of information, multiple submissions of academic work, plagiarism, abuse of academic materials, and complicity in academic dishonesty. Any special requirements or permission regarding academic integrity in this course will be stated by the instructor, and are binding on the students. Academic evaluations in this course include a judgment that the student's work is free from academic dishonesty of any type; and grades in this course therefore should be and will be adversely affected for academic dishonesty. Students who violate the code can be expelled from UNCC. The normal penalty for first offense is zero credit on the work involving dishonesty and further substantial reduction of the course grade. In almost all cases the course grade is reduced to F. Students are expected to report cases of academic dishonesty to the course instructor.

- No cell phones or other electronics at all during exams.
- Students with cell phones, or other wireless communication devices during an exam will have the exam taken up and receive no credit for the exam.
- Students will be required to show their university ID upon turning in exams.

## *Tentative Lecture schedule:*

| *Lecture* | *Topics* |
|---|---|
| 1 | Computer simulation: motivation and applications |
| 2 | Model systems and interaction potentials |
| 3 | Constructing an intermolecular potential |
| 4 | Intro to Stat Mechanics: Sampling from ensembles |
| 5 | Common statistical ensembles. Transforming between ensembles. |
| 6 | Simple thermodynamic averages. Fluctuations. |
| 7 | Structural quantities. Time correlation functions. Transport coefficients |
| 8 | Molecular dynamics |
| 9 | Integration methods. Verlet algorithms |
| 10 | Rigid non-spherical bodies. Non-linear molecules. |
| 11 | Constraints. Linear molecules |
| 12 | Constant temperature and pressure methods |
| 13 | Hard-sphere systems. |
| 14 | Monte Carlo. Importance sampling |
| 15 | Metropolis method. Isothermal-isobaric ensemble. Gibbs ensemble. |
| 16 | Empirical force fields. |

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|---|---|
| 17 | Electrostatic interactions. Van der Waals interactions. |
| 18 | Hydrogen bonding. Many-body effects. |
| 19 | Force-field parametrization. Force fields for inorganic molecules. Force fields for solids. |
| 20 | Tools to analyze trajectories. Clustering. Principal component analysis. |
| 21 | Implicit solvent models |
| 22 | Methods of enhanced conformational sampling. Multicanonical ensemble. |
| 23 | Replica-exchange method. Multiple-histogram methods. |
| 24 | Free energy calculations. Perturbation method. Thermodynamic integration. |