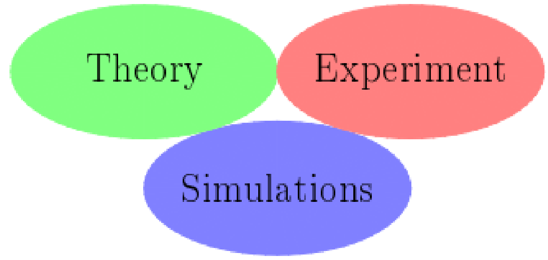
"Simple models of complex processes".

Introduction to Computational Physics by Oleg Kharshiladze (TSU)

7 Lectures (7*2=14 hours)



Course Rationale:

Computation is an integral part of modern science and the ability to exploit effectively the power offered by computers is therefore essential to a physicist. The proper application of a computer to modeling physical systems is far more than blind number crunching, and the successful physicist draws on a balanced mixture of analytically soluble examples, physical intuition, and numerical work to solve problems.

Computational research is an integral part of Theoretical and experimental physics. Course is geared for advanced bachelor students in physics, astrophysics, biophysics, materials science, geology, chemical engineering, electrical engineering, and related fields.

AIM OF SUBJECT

The course is aimed at refining computational skills by providing direct experience in using a computer to model physical systems and is facultative curse for Bachelor students.

CONTENT

Different numerical techniques will be applied to problems in classical and statistical physics. These problems will provide a vivid illustration of many basic and important concepts in theoretical physics. Special emphasis is directed to computer simulation methods, the Monte Carlo method and the molecular-dynamics technique, but also more traditional numerical methods will be included.

The different numerical techniques and the physical problems will be presented in a series of lectures. More specifically these will deal with: Solution of ordinary differential equations in classical mechanics, applied to non-linear dynamics and coupled anharmonic oscillators. The molecular-dynamics technique and various applications. Random-walk models, stochastic differential equations and Brownian dynamics, fast Fourier transform technique.

Deterministic Methods: Molecular Dynamics, Microcanonical Ensemble Molecular Dynamics, Isothermal-Isobaric Ensemble Molecular Dynamics. Stochastic Methods: Brownian Dynamics, Monte-Carlo Method.

The most important part is, however, the students' own activity in applying and solving some of the problems using computers. This part will be integrated with computer laboratory work, where instructors will be available for consultation.

LITERATURE

The course will be based on lecture notes. The following will be used as reference literature:

1. H. Gould & J. Tobochnik, *Computer Simulation Methods -- Applications to Physical Systems. Part 2*, Addison-Wesley, 1988.
2. D.W. Heerman: Computer Simulation Methods in Theoretical Physics (Springer, 1990) Steven E. Koonin and Dawn C. Meredith: Computational Physics (Addison Wesley, 1990)
3. Tao Pang, An Introduction to Computational Physics, University of Nevada, Las Vegas, 2006
4. K. Chen, Peter J. Giblin and A. Irving, Mathematical Explorations with MATLAB,2000
5. Germund Dalquist and Åke Björck, Numerical Methods in Scientific Computing, Society for Industrial and Applied Mathematics, 2008
6. Thomas J. Santner, Brian J. Williams, William I. Notz, The Design and Analysis of Computer Experiments, 2003
7. R. W. Hamming, Numerical Methods for Scientists and Engineers, Dover Pub., 1996
8. Benjamin A. Stickler, E. Schachinger, Basic Concepts in Computational Physics,2016

SUBJECT

Typical issues at lectures (lecture duration 2 hour):

1. Simple Monte Carlo simulation
2. Data analysis (Methods of: Nonlinear dynamics, theory of information, Statistical Mechanics)
3. Error analysis (averages, fluctuations, correlations, autocorrelations, confidence)
4. Simple molecular dynamics simulation
5. Kinetic simulations
6. Astrophysics simulations
7. Biophysics modeling

This course will be graded on prepared laboratories (in classical simulation and statistical analysis) and the following projects:

Monte Carlo Simulation (write your own simple code)
Molecular Dynamics Simulation (use a research code)
Reviews of published simulation work (written and oral presentation)

The examination will be based on an oral and written presentation of problems solved by the student.
The student will receive a written assessment by writing computer code and running a simulation.
The student will participate orally in the student conference "Simple models of complex processes". The student will be evaluated based on the conference presentation.