Syllabus for Special Topics in Physics - Condensed Matter Physics:
***Computational Methods in Condensed Matter Physics* – PHYS 790A**

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Semester:	Spring 2016 (Jan 18th – May 10th)
Lectures:	Tue & Thu, 14:15 – 15:30
Location:	Faraday West 227 / computer lab (FW 233)
Office hours:	Tue & Thu, 13:45 – 14:15, 15:30-16:00

(Planned) Contents

1. Introduction
    a. Floating-point numbers and numerical accuracy
    b. Overview of Numerical Mathematics
        i. Linear algebra
        ii. Numerical integration
        iii. Root finding
    c. Explicit and implicit PDE discretization
    d. Numerical stability
    e. (Pseudo) random number generators
    f. Data analysis
2. Monte Carlo methods
    a. Metropolis algorithm
3. Ordinary differential equations
    a. Single particle dynamics
4. Molecular dynamics
5. Partial differential equations
    a. Diffusion and heat equation
    b. Ginzburg Landau equations
6. Applied parallelization on Clusters and GPUs
    a. OpenMP
    b. MPI
    c. CUDA with practical examples
7. Exact diagonalization of quantum systems

Notes

1. Programming skills and some familiarity with the C programming language are expected. The knowledge of a data plotting software will be very useful.
2. This course is does not follow a single textbook. Changes sections 6&7 of the above lecture content are possible.

3. The main purpose of this lecture is to provide an overview of the most common methods in computational condensed matter physics (hard & soft) and introduce latest developments (see chapter 6). The main aim is to serve as a base for possible future computational research projects.
4. *Format of the lecture:* The first introductory chapter will be held as classroom lectures (about 3 weeks). The following chapters are taught as classroom + hands-on practice in the computer lab.
5. Homework is planned every other week involving writing & running codes plus data analysis. Lecture attendance is essential, in particular the hands-on practice lectures in order to get started with the homework.
6. One midterm exam, covering sections 1-3, is planned after completion of those sections.
7. Each student will work on a final project during the last month of the course and present a 10 min presentation during finals week. The presentation should cover the physics background, numerical realization, and results.
8. Lecture attendance is essential, see below.

Preferred prerequisites: linear algebra, classical mechanics, ED, QM, and statistical physics

Textbook suggestions

- **J. Franklin,** *Computational Methods for Physics***,** Cambridge University Press (July 15, 2013)
- **Nicholas J. Giordano, Hisao Nakanishi,** *Computational Physics,* Addison-Wesley; 2 edition (July 31, 2005)
- **Alfio Quarteroni, Riccardo Sacco and Fausto Saleri,** *Numerical Mathematics*, Springer; 2nd edition (October 19, 2006)
- **Curtis F. Gerald and Patrick O. Wheatley,** *Applied Numerical Analysis, Pearson*; 7 edition (August 10, 2003)
- **Germund Dahlquist and Åke Björck,** *Numerical Methods in Scientific Computing: Volume 1*, Society for Industrial and Applied Mathematics (September 4, 2008)
- **Jason Sanders and Edward Kandrot,** *CUDA by Example: An Introduction to General-Purpose GPU Programming*, Addison-Wesley Professional; 1 edition (July 29, 2010)

See course website for additional textbook references and online resources.

Grading

The final grade is determined according to

- 35%: homework percentage
- **20%: lecture attendance percentage**
- 20%: midterm exam percentage
- 25%: final project percentage

This results in a total score between 0 and 1, which is then multiplied by 12, rounded to the closed integer, divided by 3, and finally graded according to* http://www.niu.edu/regrec/grading/gradingfaqs.shtml

* values below 2 are round to the closed integer

Accessibility Statement

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