

## Slides PHY 480 and PHY 905 Lectures, introduction to the course

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## Overview of first two weeks

- First lecture: Presentation of the course, aims and content. Introduction to [github](#) with [tutorial](#).
- Second week (read sections 2.1-2.5 and 3.1-3.2 of lecture notes):
  - Introduction to C++ programming
  - Numerical precision and C++ programming (chapter 2 of lecture notes)
  - Numerical differentiation and loss of numerical precision (chapter 3 lecture notes)
  - Work on warm up exercise to demonstrate several programming elements

## Lectures and ComputerLab

- Lectures: 1-3pm Wednesdays (BPS4270) and 7-9pm Wednesdays (BPS1300).
- Lab: 2-4pm Thursdays and 1-3pm Fridays in BPS1240.
- Weekly reading assignments needed to solve projects.
- First part of a lab session may be used to discuss technicalities and issues related to additional software
- Detailed lecture notes, exercises, all programs presented, projects etc can be found at the homepage of the course.
- Weekly plans and all other information are at the [github](#) address of the course. Weekly emails about plans and progress will be sent to you all.
- Final oral exam to be determined

## Course Format

- Several computer exercises, 4 compulsory projects. Electronic reports only using [Git](#) for repository and all your material.
- Evaluation and grading: Each project counts 20% of the final mark. The final oral exam counts 20%. A tentative feedback form on projects can be found at the [github](#) address of the course
- The computer lab consists of 16 Linux PCs, but many prefer own laptops. C/C++ is the default programming language, but Fortran2008 and Python are also used.
- All source codes discussed during the lectures and for each chapter can be found at the [github](#) address of the course. We recommend either C/C++, Fortran2008 or Python as languages.

## Topics covered in this course

- Numerical precision and intro to C++ programming
- Numerical derivation and integration
- Random numbers and Monte Carlo integration
- Monte Carlo methods in statistical physics
- Quantum Monte Carlo methods
- Linear algebra and eigenvalue problems
- Ordinary differential equations
- Partial differential equations
- Parallelization of codes
- High-performance computing aspects

## Syllabus

### Linear algebra and eigenvalue problems, chapters 6 and 7

- Know Gaussian elimination and LU decomposition
- How to solve linear equations
- How to obtain the inverse and the determinant of a real symmetric matrix
- Cholesky and tridiagonal matrix decomposition

## Syllabus

### Linear algebra and eigenvalue problems, chapters 6 and 7

- Householder's tridiagonalization technique and finding eigenvalues based on this
- Jacobi's method for finding eigenvalues
- Singular value decomposition if time
- Cubic Spline interpolation

## Syllabus

### Monte Carlo methods (chapter 11)

- Brute force Monte Carlo integration
- Random numbers (simplest algo, ran0) and probability distribution functions, expectation values
- Improved Monte Carlo integration and importance sampling if time.

## Syllabus

### Monte Carlo methods in physics (chapters 12, 13, and 14)

- Random walks and Markov chains and relation with diffusion equation
- Metropolis algorithm, detailed balance and ergodicity
- Simple spin systems and phase transitions
- Variational Monte Carlo
- How to construct trial wave functions for quantum systems

## Syllabus

### Ordinary differential equations (chapter 8)

- Euler's method and improved Euler's method, truncation errors
- Runge Kutta methods, 2nd and 4th order, truncation errors
- How to implement a second-order differential equation, both linear and non-linear. How to make your equations dimensionless.

## Syllabus

### Partial differential equations, chapter 10

- Set up diffusion, Poisson and wave equations up to 2 spatial dimensions and time
- Set up the mathematical model and algorithms for these equations, with boundary and initial conditions. Their stability conditions.
- Explicit, implicit and Crank-Nicolson schemes, and how to solve them. Remember that they result in triangular matrices.
- How to compute the Laplacian in Poisson's equation.
- How to solve the wave equation in one and two dimensions.

## Additional learning outcomes

- has a thorough understanding of how computing is used to solve scientific problems
- knows some central algorithms used in science
- has knowledge of high-performance computing elements: memory usage, vectorization and parallel algorithms
- understands approximation errors and what can go wrong with algorithms
- has experience with programming in a compiled language (Fortran, C, C++)
- has experience with debugging software
- has experience with test frameworks and procedures
- can critically evaluate results and errors
- understands how to increase the efficiency of numerical algorithms and pertinent software
- understands tools to make science reproducible and has a sound ethical approach to scientific problems

## Overarching aims of this course

- Develop a critical approach to all steps in a project, which methods are most relevant, which natural laws and physical processes are important. Sort out initial conditions and boundary conditions etc.
- This means to teach you structured scientific computing, learn to structure a project.
- A critical understanding of central mathematical algorithms and methods from numerical analysis. In particular their limits and stability criteria.
- Always try to find good checks of your codes (like solutions on closed/analytical form)
- To enable you to develop a critical view on the mathematical model and the physics.

## Computing knowledge

### Our ideal about knowledge on computational science

Hopefully this is not what you will feel towards the end of the semester!



## And, there is nothing like a code which gives correct results!!

