

Computational Physics Lectures: Introduction to the course

Morten Hjorth-Jensen^{1,2}

Department of Physics, University of Oslo¹

Department of Physics and Astronomy and National Superconducting Cyclotron Laboratory, Michigan State University²

2017

© 1999-2017, Morten Hjorth-Jensen. Released under CC Attribution-NonCommercial 4.0 license

Overview of first week

- ▶ Tuesday (most likely):
 1. Presentation of the course, aims and content
 2. Introduction to C++ programming and numerical precision.
Exercises for first week.
 3. Numerical differentiation and loss of numerical precision
(chapter 3 lecture notes)
- ▶ Computer lab: Thursday (most likely)
 1. The first two weeks we focus on simple programming tasks, start to look at project 1 and to set up the software [Git](#) and a repository at [Github](#) as well as [Qt Creator](#) as one possible IDE. This week we discuss how to set up Git and obtain a Github account.

Reading suggestions and exercises

- ▶ 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 and/or start looking at project 1

Lectures and ComputerLab

- ▶ Lectures: Most likely Tuesdays from 3pm to 5pm (As of now not determined)
- ▶ Weekly reading assignments needed to solve projects.
- ▶ First hour of each lab session may be used to discuss technicalities, address questions etc linked with projects.
- ▶ Detailed lecture notes, exercises, all programs presented, projects etc can be found at the Github address of the course.
- ▶ Computerlab: Most likely Thursdays. We have reserved a time slot from 3pm to 7pm.
- ▶ Weekly plans and all other information are the github address of the course.
- ▶ Four projects, all have to be approved. The first project is pass/not passed only while the last three projects are graded and count 25% each of the final mark. The course ends with a final oral exam where you present a project of your choice. The final oral exam accounts for the remaining 25% of the

Course Format

- ▶ Use version control like [Git](#) for repository and all your material.
- ▶ C/C++ is the default programming language, but Fortran2008 and Python are also used. All source codes discussed during the lectures can be found at the webpage and [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
- ▶ Non-linear equations and roots of polynomials
- ▶ Ordinary differential equations
- ▶ Partial differential equations (may not be covered)
- ▶ Parallelization of codes
- ▶ High-performance computing aspects and optimization of codes

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
- ▶ Qubic Spline interpolation

Syllabus

Numerical integration, standard methods and Monte Carlo methods (chapters 4 and 11)

- ▶ Trapezoidal, rectangle and Simpson's rules
- ▶ Gaussian quadrature, emphasis on Legendre polynomials, but you need to know about other polynomials as well.
- ▶ Brute force Monte Carlo integration
- ▶ Random numbers (simplest algo, ran0) and probability distribution functions, expectation values
- ▶ Improved Monte Carlo integration and importance sampling.

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 (chapters 8 and 9)

- ▶ 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.
- ▶ Boundary value problems, shooting and matching method (chap 9).

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.

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 form)
- ▶ To enable you to develop a critical view on the mathematical model and the physics.

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

Computing knowledge

Our ideal about knowledge on computational science

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



©Zits Partnership

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



- ▶ J. J. Barton and L. R. Nackman, *Scientific and Engineering C++*, Addison Wesley, 3rd edition 2000.
- ▶ B. Stoustrup, *The C++ programming language*, Pearson, 1997.
- ▶ An excellent text is [Discovering Modern C++](#)
- ▶ D. Yang, *C++ and Object-oriented Numeric Computing for Scientists and Engineers*, Springer 2000.

Extremely useful tools, strongly recommended

and discussed at the lab sessions

- ▶ [Git](#) and a repository at [Github](#), this week and next weeks.
- ▶ ipython notebook
- ▶ [Qt Creator](#) as one possible IDE for editing and mastering computational projects (for C++ codes, see webpage of course), discussed during the whole semester. You can however use other IDEs as well such as [VisualC++](#).
- ▶ Armadillo as a useful numerical library for C++, highly recommended, discussed in connection with LinAlgebra lectures
- ▶ Unit tests, discussed throughout the whole semester
- ▶ Piazza for discussions and teaching material