

Lectures “Computational Methods”

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AIM

The aim of the course is that you learn to apply numerical techniques to solve problems that cannot be solved analytically. You should gain understanding of various techniques (e.g. Fourier transforms, integration, solving linear equations, etc), of errors and uncertainties related to the methods you use, and how to verify the results of your coding. You should also be able to find optimal algorithms and compare the performance of different algorithms.

BOOK

The lectures follow the book

“Numerical Recipes” by W.H. Press et al, Cambridge UP.

The first edition of this book is available on-line, see www.nr.com/index.html. There are C, C++ and FORTRAN versions of the code available, each can be used, although I will use the C++ code from edition 3 in the discussion of the exercises.

The routines from the second edition and from the third edition of the book are available from my home page:

<http://www.nikhef.nl/~henkjan/NUMREC/Cincludes.zip> and

<http://www.nikhef.nl/~henkjan/NUMREC/includes.zip>

The lecture notes, exercises and examples will be on my homepage too:

<http://www.nikhef.nl/~henkjan> click on Computational Methods

FIGURES

Probably you know how to make simple drawings and figures. A simple drawing may be made with xfig (/usr/local/bin/xfig

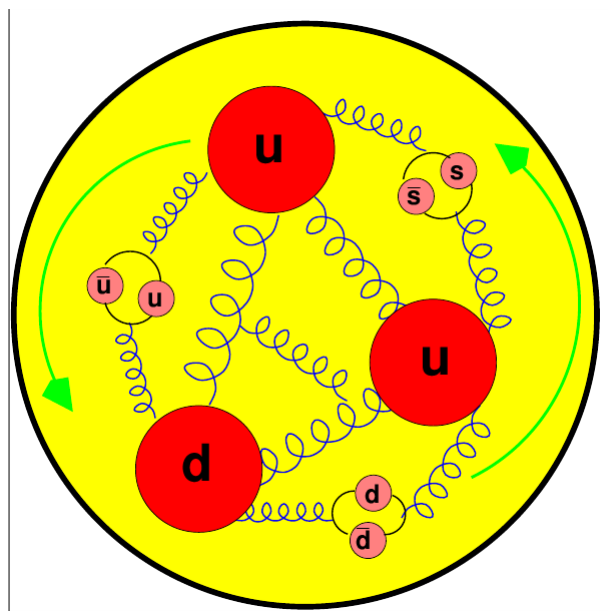


Fig. 1. Schematic display of quarks and gluons contributing to the spin of the proton in deep-inelastic scattering.

and e.g. with /usr/local/bin/xmgrace.

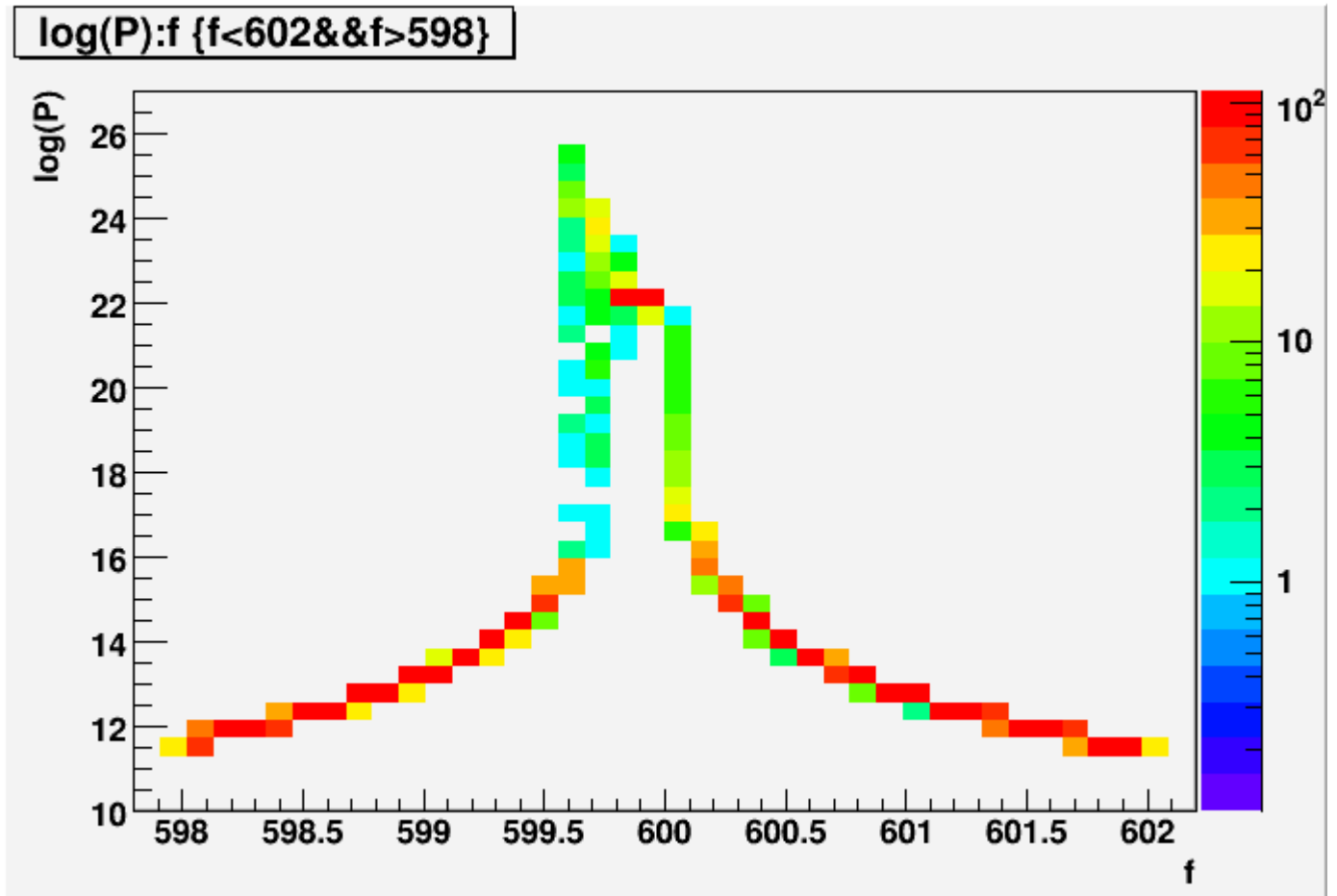


Fig. 2. Logarithm of the power as a function of the frequency. Plot produced with root.

Personally, I use root (<http://root.cern.ch>). It may be that you prefer mathematica or matlab to make figures like the above.

LIBRARIES

Apart from the methods, described in the book, there are several libraries available, such as NAG. These are described at the VU website (theory department). One handy library to have is the FFTW3 library from MIT, the fastest Fourier-transform in the west. That is used worldwide. Also, for particle physicists, there is the FORM package from Jos Vermaseren (<http://www.nikhef.nl/~t68/>). This package is extremely efficient and is used by theoretical physicists all over the world, e.g. to calculate Feynman diagrams with internal loops.

COURSE CONTENTS

Introduction, numerical techniques
Interpolation and extrapolation, chapter 3
Integration of functions, chapter 4
Evaluation of functions, chapter 5
Roots, Minima and maxima, chapters 9 and 10
Fourier methods, chapters 12 and 13
Systems of linear equations, chapter 2
Eigensystems, chapter 11
The Schroedinger equation
Integration of differential equations, chapter 17
Boundary value problems, chapter 18
Monte Carlo techniques chapter 7

In the later lectures, some of the techniques will be applied in a physics/engineering context. Monte Carlo techniques will only be introduced if time allows.

EXAM

During the course I assign several exercises. These will be discussed during the lecture immediately after the deadline for completion. The final grade will be based on the successful completion of these exercises. The first exercises are small and will have less weight in the final grade than later exercises. Exercises must be turned in in time, since they will be discussed during the course in the lecture following the deadline for completion.