COMPUTATIONAL PHYSICS LABORATORY NOTES

1. INTRODUCTION

The methodology of computational physics is intermediate between theoretical and experimental physics. Computer simulations are performed on the basis of theoretical models of the real world, formulated in terms of a set of mathematical relations. These are cast into a numerical form, an algorithm, which is run on the computer. The analysis and development of the results is closely akin to experiment, in that relationships between independent (input) quantities and dependent (output) quantities are identified in terms of numerical relations. In essence the simulation is the representation of an individual experiment, and may be used to give a prediction of the results of that experiment, if the model is accurate. Such simulation may be considerably easier to perform than the equivalent experiment. In consequence simulation has become established as an important technique extending the range of physics.
The techniques of computational physics embrace model design, numerical analysis, computer programming and experimentation. Included in these are the essential 'debugging' and validation skills, which check and verify the accuracy and correctness of the simulation model, without which no confidence in the predictions would be possible. In addition some understanding of the machine limitations on programme performance, and the application of graphic presentation is necessary if the full potential of the approach is to be realised. The laboratory is designed to help you to develop these skills by practical applications.

2. LABORATORY ORGANISATION

2.1 General
Laboratory sessions are held from 10.15 to 17.15 each Thursday. Lunch is from 13.00-14.00. You are expected to remain in the laboratory until 17.00 and to complete as much as possible of the practical, including writing up, in the laboratory. You will work individually.

2.2 Demonstrators
Supervision in the laboratory is by one academic and one graduate student demonstrator. Their job is to assist you with all aspects of your laboratory work. In addition the student demonstrator will mark your work during the day, and staff and student demonstrators will discuss simulation techniques in general.
Staff will be present in the laboratory for part of the time and available in his/her office for the remaining hours; the demonstrator will be present in the laboratory at all times.

2.3 Equipment
The laboratory is based around dual core workstations. These are provided on an individual basis: at present a total of twenty machines. The machines run a full virtual LINUX environment (Ubuntu), allowing you to use compilers and analysis tools on your own machine. Your files must be linked from the university unix server after which all files are stored on your filestore. Fortran 90 and C++ are the working languages using appropriate compilers with LINUX.

2.4 Availability
The laboratory will be open from 9.00 to 17.15 each day. Physics students may use the laboratory unsupervised during this period.

2.5 Attendance
Please note, that *attendance at laboratory classes is compulsory.* An attendance record will be kept.

2.6 Laboratory Programme
The laboratory programme consists of a series of experiments mostly designed to take two or three weeks. The experiments have been developed to co-ordinate with the lecture courses, and all students carry out the same programme.

Term 1: Weeks 1-9 will be devoted to an experiment on random number generation and numerical integration followed by a series of more complex physics experiments. Week 10 is to be used for writing up the first formal report

Term 2: Weeks 1-9 all sessions devoted to physics experiments. Week 10 is to be used for writing up the second formal report

3. LABORATORY PROCEDURES

3.1 Assignment of experiments
Experiments will be assigned to you as scheduled. You will receive the experiment in the form of a script. If parts of the necessary subroutines are to be provided, they will be stored on the file server and should be copied on to the local virtual machine.

3.2 Disk back-up
You cannot guarantee that your data or programme left on the hard disk of a machine will remain uncorrupted, nor that you will necessarily use the same machine each session. It is therefore essential that you make a copy of all your files on to a USB stick at the end of every session. *You are responsible for the safe keeping of your work.*

3.3 Laboratory notebooks
You are required to keep a laboratory notebook in which you enter the full details of your experiments. The notebook will be the main means of assessing your work. A guide on how to keep the notebook is given in section 4 of these notes.

3.4 Marking Procedures
Your experiment will be marked in the laboratory by the student demonstrator sometime in the week after you have completed it. Marking is based on your laboratory notebook. Furthermore, you should expect to be asked questions about the programme, your experiment and the results.

In assessing an experiment the points to be considered are the following:

- Identification of the objective of the experiment
- The planning of your work
- The difficulties and problems in executing your plan
- The amount of useful data collection you complete

- The discussion and interpretation of your data
- The accuracy, completeness and legibility of your notes
- Evidence of understanding of the background of the model and programme
- Your conclusions at the finish

During the year two project experiments will be written up for formal report. These will be marked separately. Your completed report should be handed in to the Departmental Office by 11.00 am on Tuesday of Week 1. *Reports submitted within a week after the deadline will have their marks reduced by 25%. Those submitted more than a week late will not be marked and will be given zero credit.*

3.5 Final Assessment

At the end of the academic year the marks you have obtained for both experiments and formal reports will be combined to produce your laboratory mark for the session. The pass mark will be 50%. Students who fail to pass will be reported to the Board of Studies for further action, *in extreme cases this could mean that you will not be allowed to do a project in your final year***.**

4. KEEPING OF LABORATORY NOTEBOOKS AND WRITING FORMAL REPORTS

4.1 Notebooks

The maintenance of a laboratory book remains an essential skill for a practicing scientist and the ability to write a concise account of what has been achieved is often necessary. Your lab book should be kept in an accepted style so that if necessary another scientist could continue your work

Maintenance of a Laboratory Book

A laboratory book should always be a hardback book, clearly labelled on the outside and inside of the front cover with your name and contact details i.e. e-mail address, mobile phone number etc. At the front of the book there should be a clearly labelled contents page showing the date on which an activity was undertaken, its title and the page number within the book where it can be found. You can keep other notes on lab briefings, etc, at the back of the book. In general a single hardback book will be sufficient for your entire laboratory course during the second year. Allowing for this there is still sufficient room in the book so that you can maintain rough notes, calculations or sketches on the left-hand side page and keep your neat tables of results and other comments on the right-hand side of the page. Under no circumstances should you be writing on bits of paper or scrap, and the demonstrators are instructed to tell you not to do this. Laboratory books should be neat and well organised and should be a contemporaneous record of what you have done. A laboratory notebook does not necessarily contain the same elements as are in a formal report. The laboratory script also forms part of your laboratory record and hence there is no information in the script that you need copy out into your book. Before starting any experiment read the script and plan the code either as a flowchart or as pseudocode

Introduction

This should summarise the main aims of the experiment, ideally as bullet points. Remember that the lab script can be taken as included in the report, you are not expected to copy the script verbatim. Key equations relating to the model should be included in the introduction.

Method

The next section in your account will obviously be your notes on your coding method and plan of calculations. The best way to develop the programme is via the use of a flowchart or pseudocode. This is central to the method section. You should also describe any code which you wrote to do analysis on the data.

Results

The results and analysis section varies in length depending on the experiment. However you should give some thought to the organisation of this section and in particular use sub headings so that another researcher could read your book, without you being present, and understand exactly what you had done, how you had done it and why you had done it.

Discussion

It is then necessary to have some discussion of the results you have obtained, what they mean, how they could have been improved, how any errors in the calculations could be reduced further and any other difficulties.

Assessment of Notebooks

Your laboratory notebook will be assessed on completion of the experiment by the academics and demonstrators. Your lab book should be handed in at the end of the final lab session of a given experiment. Be sure to have all calculations complete by lunchtime on the final day of the lab to allow for analysis of the data and completion of the notebook. The notebook will be marked and returned to you at the beginning of the next experiment. Brief verbal feedback will be provided to you as to where you have lost marks or need to improve.

Assessment will be by impression of the overall quality of your record keeping and your work on a scale of 1 to 20. There are 5 marks for the quality and neatness of the book, 7 for the quality of the data and 8 for the other work.

Lab Book Marking Scheme

Quality of Notebook	5 Marks
Introduction	2 Marks
Method	5 Marks
Quality of Results	6 Marks
Discussion	2 Marks
Total	20 Marks

4.2 Formal Reports

When writing your report you must not imagine that you are writing up a laboratory experiment for a member of staff, who almost by definition knows the answers! A good rule is to write as if your reader is scientifically literate but not familiar with the subject you are describing, except in the most general terms.

(i) General

Unlike your laboratory notebook a formal report must be written using stricter conventions. The report should read continuously. The reader should not be continually referred to other sections of the report. It must be written on loose sheets but these must be firmly attached together before submission. Reports can be submitted handwritten or typed.

Sections of the report, equations, figures (including graphs) and tables must be given numbers so that where cross-referencing is necessary, it can be achieved easily. Programme listings should not be included in the main text (they break up the flow of the report). They may be added as an appendix if useful. If it helps, a flowchart can be included in the main text. Graphs, tables, and flowcharts should be close to the section where they are discussed. They must also be referred to in the text otherwise the reader will not know they exist. As well as being numbered all graphs, figures, tables and flowcharts must have a brief descriptive title. The columns of tables must have a suitable notation and both axes of the graph must be labelled and the units given.
On occasions it will be necessary to use data you have not measured, or make reference to formulae that you have not derived etc when you do this some indication of the source of the data or formulae must be given. There are many conventions for "Referencing" information one of the simplest and the one you are recommended to use is to give each reference a number in square brackets in the text, giving the author’s name if appropriate. An example defining the reference style is given in appendix I.

(ii) Structure of the report

The following gives an outline of the general structure you are expected to follow in writing your report.

Title

The title should be a short concise summary of the experiment, and should be limited to ten to fifteen words. Underneath the title should be the author’s name.

Abstract

The abstract is one paragraph extending the title to include all the important details of the work. The past tense is used when referring to the contents of the report. It should be self-contained and intelligible in isolation from the rest of the report. It should only be sixty to eighty words long, but nevertheless it must indicate what was done and give an indication of the conclusions reached and their validity. This should probably be the last section you write.

Check points

- Define what the experiment was about and be intelligible without the rest of the report
- Include the main result(s)
- Compare results with accepted values from the literature where appropriate
- do not use references in the abstract

The Title and Abstract form the first page of your report. A typical layout would be:

Title

Date

Author

Abstract

Introduction
The introduction outlines the contents in order, puts the work being reported in context with other related work, and discusses the phenomenon in general terms.
This is usually one of the most difficult sections to write. It should not just be a copy of the laboratory script.

Check points

- Introduce the topic (Note how the authors in the article of appendix I describe the context of their work)
- Explain why it is important
- Provide some background for those who may not be expert in the field.
- Give examples of where the basic physics that you are studying is used.
- Place your experiment into an historical context if appropriate.
- Include your thinking behind the plan of your experiment
- Outline the methods used to identify the critical parameters that you needed to measure.

Theory
The theory section should be an *outline* of the *essential* background theory for your project. It is an extension of the introduction, *do not* give long standard derivations of well known equations, but make suitable references to standard textbooks.

Check points

- Give an outline of the origin of key equations and background theory
- Identify the final equation(s) that give the main result(s) which form the basis of the computational model

Method
The method etc, should give a detailed description of the method, the programme, the work done and how it was carried out. Be careful not to divert attention from the principle of your method by unnecessary discussion of detail. It is essential that this section and especially the description of the programme should read as continuous prose and not be just a list of procedures. Once again *do not* copy out sections of the laboratory script for this.

Check points

- Include a fairly complete, concise description of the computational model and how it was constructed. Flow diagrams help to outline the logic of the code.
- Give sufficient detail that one of your colleagues could repeat the experiment without reference to the script.
- Your colleagues should understand not only how you did certain things but why you did them.

Results
The results section gives a digest of the data, with graphs and tables, and the final conclusion. Once again care must be taken to ensure that this section reads continuously and is not just a collection of graphs and tables.

In a formal report it is not necessary to give the detailed arithmetical calculations.

Check points:

- It is almost always better to graph your results rather than to tabulate them
- Your graphical results should be labelled with a figure number and caption. The axes should be defined and the units associated with the axes given. Refer to all diagrams or graphical results by a figure number in the text of your report at least once.
- Tables these should have a table number and also be referred to at least once in the text
- The units should be stated.

Discussion and Conclusions

The discussion analyses the result, gives its probable worth and implication and compares it with other related results. In this section also give a summary of the uncertainties and if possible give a reasoned conclusion about the result and how it could be improved.

Check points:

- Discuss the technique and your procedure in the context of the results obtained
- Discuss the importance and implications of the result you have obtained

In the work you will be reporting it may not be worth separating the discussion and conclusions into different sections but as you progress in your career you will probably find this to be necessary.

References

This section should give a list of references to the material referred to in the report. The form these should take is given in appendix I.

Appendices

In these give any long theoretical derivations if you feel they are essential.

(iii) Marking of reports

Below is a list of the points that will be considered when marking formal reports. It may help to guide you to an acceptable standard. Note the high importance attached to the communication of ideas.

Structure and Presentation:

Has the student selected relevant material?
Does the general layout suit the material?
Does the report develop logically and continuously?
Is the English correct and the style good?

Abstract:

Is it intelligible without the rest of the report?
Does it summarise what was done and discovered?

Introduction:

Is the physics relevance established?
Is the phenomenon discussed in general terms?
Is the objective made clear?

Diagrams and Tables:
Are they necessary?
Are they to an acceptable standard?
Are they all labelled and referred to in the text?

Results and Conclusions:
Is the analysis correct and complete?
Are relevant conclusions extracted?
Is there an adequate discussion?

Appendix 1: Reference style

An example of text taken from the following article is given below to illustrate the reference style to be used:

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS D: APPLIED PHYSICS

J. Phys. D: Appl. Phys. 38 (2005) 3016–3027 doi:10.1088/0022-3727/38/17/S02

Numerical validation of a self-absorption model for plasma radiation

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1. Introduction

The profiles of spectral lines emitted by plasma light sources contain valuable information about the elementary processes that take place within the discharge. A special category of profiles is obtained for optically thick lines. In that case a part of the radiation is trapped inside the plasma by self-absorption. As a consequence, the observed line profile is altered appreciably. The final profile of the spectral line as observed outside the plasma depends chiefly on the distribution of the absorbing and emitting atoms along the line of sight. More specifically, it is largely determined by the population density-ratio of the emitters to absorbers, which is closely related to the source function. In most cases this quantity does not remain constant over the length of the plasma layer and decreases close to the plasma edge. As a consequence, intense emission lines, which are sufficiently affected by self-absorption, undergo self-reversal.

Most of the theoretical radiation models proposed for inhomogeneous plasma layers, which are symmetric along the line of sight, differ from each other mainly with respect to the method that is used to represent the source function [1–5]. A description of relevant theories and the existing simplified models [1–3] for inhomogeneous optically thick plasmas, which are applied in spectroscopic practice [6–9], was given in [10].

The main assumption of the Cowan–Dieke model [1] is that of the existence of a simplified functional form for the radial distribution of the population density-ratio between the levels of the spectral line, which is the density-ratio of the emitters to the absorbers. This form of a simple power law allows description of the source function of the considered line by one single parameter—the exponent of the power; the so-called inhomogeneity parameter. The resulting radiation model for optically thick spectral lines is independent of the assumption of the local thermodynamic equilibrium (LTE) and of the form of the spatial distribution of the temperature as well.

In contrast, the existence of LTE along with a parabolic radial temperature profile is the main assumption of Bartels

The references are then listed at the end of the text as follows:

References

[1] Cowan R and Dieke G 1948 *Rev. Mod. Phys.* **20** 418
[2] Bartels H Z 1950 *Z. Phys.* **127** 243
[3] Bartels H Z 1950 *Z. Phys.* **128** 546
[4] Preobrazhenskii N G 1964 *Opt. Spectrosc.* **17** 4
[5] Preobrazhenskii N G 1967 *Opt. Spectrosc.* **22** 95
[6] Karabourniotis D 1983 *J. Phys. D: Appl. Phys.* **16** 1267
[7] Karabourniotis D and Karras C 1985 *J. Appl. Phys.* **57** 4861
[8] Fishman I S, Ilin G G and Salakhov M Kh 1987 *J. Phys. D: Appl. Phys.* **20** 728
[9] Fishman I S, Ilin G G and Salakhov M Kh 1995 *Spectrochim. Acta* B **50** 947
[10] Karabourniotis D 1986 *Radiative Processes in Discharge Plasmas* (*NATO ASI Series B: Phys.* vol 149) (New York: Plenum) p 171