Computational Lab – Report Guidelines

The Advanced Labs aim to prepare you for independent research: teach you how to plan the study, formulate valid questions and hypotheses and select appropriate methods to verify those, collect and process the data, critically assess the consistency, validity and accuracy of the methods and of the results, and draw justified conclusions.

Effective communication is a critical part of scientific research. The Lab Report should be organised as a standalone research report, e.g. a journal article, presenting the entire cycle from the original practical problem to the conclusion on what has been achieved. In most respects, it will be similar to an Experimental Lab Report. It should contain the following sections:

Abstract

This is a concise summary of your report, and so should be written last. The first sentence should introduce the general topic. The second sentence should highlight the specific problem you want to solve. The next sentence should state your general approach and the answer to the question you just posed. It should start with "Here, I show that...". The next 1-2 sentences should give a high level overview of your most important methods and your main results. The final sentence should give some implications of your work, e.g., do your results influence your understanding or prompt further research?

Introduction

In this section, you should provide the relevant background information and clearly identify the problem you want to address. Start by placing your work in a broad context (e.g., the stability of mechanical systems), and then narrow the scope to discussing the specific problem you hope to solve (e.g., the motion of a damped, driven pendulum).

Clearly state the main problem that you are addressing (e.g., "Is the fourth-order Runge Kutte algorithm sufficiently accurate to model the advance of the perihelion of Mercury?"). This is a crucial piece of information – the 'narrative' or 'story' told by the rest of your Report should be shaped by how you answer this question.

Finish this section by providing a 1-2 sentence overview of your approach to the problem (e.g., "I will address this problem by ...") This will improve the 'flow' of the Report, making it easier to read.

Theory / Computational Methods

Depending on the Lab, this section can include a description of the relevant theory (e.g. Coulomb's Law) and/or a description of the computational method or algorithm (e.g., the Euler algorithm). Use subsections to make it easier to read.

Do not reproduce large pieces of code or your Jupyter notebooks in this section. If you want to make a specific point about your implementation, you may include short code snippets or pseudo-code.

Aim to give sufficient information that another student can reproduce your work without having to refer to the Lab Script. The method should be described and justified (i.e. explain why it is suitable for solving this particular problem), validated (i.e. demonstrated to produce correct

results in some simple test cases or to reproduce the exact analytical solution), and assessed for accuracy and consistency. The equations should be named and their origin indicated/cited.

The limitations of the method and the choice of parameters (such as time steps, initial values, number of trials) should be discussed.

Results

In this section present your key findings. Use subsections to make it easier to follow. Identify which graphs, tables and data will help you tell the 'story'. In some cases, the Lab Script will prompt you to include certain graphs. In other cases, you will have to decide what to include yourself. Write descriptive text explaining each graph you show.

Ensure each graph is readable, i.e., ensure all lines are visible and presented over a suitable range. If you scale graphs to place them in a Word or LaTeX document, ensure all text remains legible at the smaller size. (Rule of thumb: The font size of the axes labels should be the same size as the rest of the text.) Give mean values and uncertainties properly rounded with no junk digits remaining, etc. In case of stochastic modelling, make sure you have sufficient statistics.

If you use certain parameters or initial conditions to obtain a particular graph, make sure you include that information in the graph or in its caption.

Discussion

Note that it is not always necessary to have a separate Discussion section. In many cases, the discussion can be merged effectively with the Results section. Decide yourself which structure would allow you to tell the story more effectively.

The purpose of the Discussion is to present a high-level analysis of all results, describe what you see, and to state whether the observations are reasonable (matching the expectations, e.g. the trajectory is periodic and not divergent), whether they agree with the relevant laws (e.g. the total energy is conserved). At this point you also have a chance to a look at the results critically and spot any errors. Do the calculated quantities match what is expected? Is the effect of increasing or decreasing certain parameters what you would expect?

Conclusion

Briefly restate your main findings. State the significance of those results. Did you succeed in answering the specific question you posed in the Introduction? Place your results in a broader context – do any interesting questions arise from your work or does it prompt further research?

Appendix

Append all of your code at the end of your report.

If you have any questions about your Computational Lab, please contact me at nuala.caffrey@ucd.ie