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Computational Physics

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Preface

So, ultimately, in order to understand nature it may be necessary to have a deeper understanding of mathematical relationships. But the real reason is that the subject is enjoyable, and although we humans cut nature up in different ways, and we have different courses in different departments, such compartmentalization is really artificial, and we should take our intellectual pleasures where we find them. *Richard Feynman, The Laws of Thermodynamics.*

Why a preface you may ask? Isn't that just a mere exposition of a *raison d'être* of an author's choice of material, preferences, biases, teaching philosophy etc.? To a large extent I can answer in the affirmative to that. A preface ought to be personal. Indeed, what you will see in the various chapters of these notes represents how I perceive computational physics should be taught.

This set of lecture notes serves the scope of presenting to you and train you in an algorithmic approach to problems in the sciences, represented here by the unity of three disciplines, physics, mathematics and informatics. This trinity outlines the emerging field of computational physics.

Our insight in a physical system, combined with numerical mathematics gives us the rules for setting up an algorithm, viz. a set of rules for solving a particular problem. Our understanding of the physical system under study is obviously gauged by the natural laws at play, the initial conditions, boundary conditions and other external constraints which influence the given system. Having spelled out the physics, for example in the form of a set of coupled partial differential equations, we need efficient numerical methods in order to set up the final algorithm. This algorithm is in turn coded into a computer program and executed on available computing facilities. To develop such an algorithmic approach, you will be exposed to several physics cases, spanning from the classical pendulum to quantum mechanical systems. We will also present some of the most popular algorithms from numerical mathematics used to solve a plethora of problems in the sciences. Finally we will codify these algorithms using some of the most widely used programming languages, presently C, C++ and Fortran and its most recent standard Fortran 2003¹. However, a high-level and fully object-oriented language like Python is now emerging as a good alternative although C++ and Fortran still outperform Python when it comes to computational speed. In this text we offer an approach where one can write all programs in C/C++ or Fortran. We will also show you how to develop large programs in Python interfacing C++ and/or Fortran functions for those parts of the program which are CPU intensive. Such an approach allows you to structure the flow of data in a high-level language like Python while tasks of a mere repetitive and CPU intensive nature are left to low-level languages like C++ or Fortran. Python allows you also to smoothly interface your program with other software, such as plotting programs or operating system instructions.

¹ Throughout this text we refer to Fortran 2003 as Fortran, implying the latest standard. Fortran 2008 will only add minor changes to Fortran 2003.

A typical Python program you may end up writing contains everything from compiling and running your codes to preparing the body of a file for writing up your report.

Computer simulations are nowadays an integral part of contemporary basic and applied research in the sciences. Computation is becoming as important as theory and experiment. In physics, computational physics, theoretical physics and experimental physics are all equally important in our daily research and studies of physical systems. Physics is the unity of theory, experiment and computation². Moreover, the ability "to compute" forms part of the essential repertoire of research scientists. Several new fields within computational science have emerged and strengthened their positions in the last years, such as computational materials science, bioinformatics, computational mathematics and mechanics, computational chemistry and physics and so forth, just to mention a few. These fields underscore the importance of simulations as a means to gain novel insights into physical systems, especially for those cases where no analytical solutions can be found or an experiment is too complicated or expensive to carry out. To be able to simulate large quantal systems with many degrees of freedom such as strongly interacting electrons in a quantum dot will be of great importance for future directions in novel fields like nano-technology. This ability often combines knowledge from many different subjects, in our case essentially from the physical sciences, numerical mathematics, computing languages, topics from high-performance computing and some knowledge of computers.

In 1999, when I started this course at the department of physics in Oslo, computational physics and computational science in general were still perceived by the majority of physicists and scientists as topics dealing with just mere tools and number crunching, and not as subjects of their own. The computational background of most students enlisting for the course on computational physics could span from dedicated hackers and computer freaks to people who basically had never used a PC. The majority of undergraduate and graduate students had a very rudimentary knowledge of computational techniques and methods. Questions like 'do you know of better methods for numerical integration than the trapezoidal rule' were not uncommon. I do happen to know of colleagues who applied for time at a supercomputing centre because they needed to invert matrices of the size of $10^4 \times 10^4$ since they were using the trapezoidal rule to compute integrals. With Gaussian quadrature this dimensionality was easily reduced to matrix problems of the size of $10^2 \times 10^2$, with much better precision.

Less than ten years later most students have now been exposed to a fairly uniform introduction to computers, basic programming skills and use of numerical exercises. Practically every undergraduate student in physics has now made a Matlab or Maple simulation of for example the pendulum, with or without chaotic motion. Nowadays most of you are familiar, through various undergraduate courses in physics and mathematics, with interpreted languages such as Maple, Matlab and/or Mathematica. In addition, the interest in scripting languages such as Python or Perl has increased considerably in recent years. The modern programmer would typically combine several tools, computing environments and programming languages. A typical example is the following. Suppose you are working on a project which demands extensive visualizations of the results. To obtain these results, that is to solve a physics problems like obtaining the density profile of a Bose-Einstein condensate, you need however a program which is fairly fast when computational speed matters. In this case you would most likely write a

² We mentioned previously the trinity of physics, mathematics and informatics. Viewing physics as the trinity of theory, experiment and simulations is yet another example. It is obviously tempting to go beyond the sciences. History shows that trinities, trinites and for example triple deities permeate the Indo-European cultures (and probably all human cultures), from the ancient Celts and Hindus to modern days. The ancient Celts revered many such trinities, their world was divided into earth, sea and air, nature was divided in animal, vegetable and mineral and the cardinal colours were red, yellow and blue, just to mention a few. As a curious digression, it was a Gaulish Celt, Hilary, philosopher and bishop of Poitiers (AD 315-367) in his work *De Trinitate* who formulated the Holy Trinity concept of Christianity, perhaps in order to accommodate millenia of human divination practice.

high-performance computing program using Monte Carlo methods in languages which are tailored for that. These are represented by programming languages like Fortran and C++. However, to visualize the results you would find interpreted languages like Matlab or scripting languages like Python extremely suitable for your tasks. You will therefore end up writing for example a script in Matlab which calls a Fortran or C++ program where the number crunching is done and then visualize the results of say a wave equation solver via Matlab's large library of visualization tools. Alternatively, you could organize everything into a Python or Perl script which does everything for you, calls the Fortran and/or C++ programs and performs the visualization in Matlab or Python. Used correctly, these tools, spanning from scripting languages to high-performance computing languages and visualization programs, speed up your capability to solve complicated problems. Being multilingual is thus an advantage which not only applies to our globalized modern society but to computing environments as well. This text shows you how to use C++ and Fortran as programming languages.

There is however more to the picture than meets the eye. Although interpreted languages like Matlab, Mathematica and Maple allow you nowadays to solve very complicated problems, and high-level languages like Python can be used to solve computational problems, computational speed and the capability to write an efficient code are topics which still do matter. To this end, the majority of scientists still use languages like C++ and Fortran to solve scientific problems. When you embark on a master or PhD thesis, you will most likely meet these high-performance computing languages. This course emphasizes thus the use of programming languages like Fortran, Python and C++ instead of interpreted ones like Matlab or Maple. You should however note that there are still large differences in computer time between for example numerical Python and a corresponding C++ program for many numerical applications in the physical sciences, with a code in C++ or Fortran being the fastest.

Computational speed is not the only reason for this choice of programming languages. Another important reason is that we feel that at a certain stage one needs to have some insights into the algorithm used, its stability conditions, possible pitfalls like loss of precision, ranges of applicability, the possibility to improve the algorithm and tailor it to special purposes etc etc. One of our major aims here is to present to you what we would dub 'the algorithmic approach', a set of rules for doing mathematics or a precise description of how to solve a problem. To devise an algorithm and thereafter write a code for solving physics problems is a marvelous way of gaining insight into complicated physical systems. The algorithm you end up writing reflects in essentially all cases your own understanding of the physics and the mathematics (the way you express yourself) of the problem. We do therefore devote quite some space to the algorithms behind various functions presented in the text. Especially, insight into how errors propagate and how to avoid them is a topic we would like you to pay special attention to. Only then can you avoid problems like underflow, overflow and loss of precision. Such a control is not always achievable with interpreted languages and canned functions where the underlying algorithm and/or code is not easily accessible. Although we will at various stages recommend the use of library routines for say linear algebra³, our belief is that one should understand what the given function does, at least to have a mere idea. With such a starting point, we strongly believe that it can be easier to develop more complicated programs on your own using Fortran, C++ or Python.

We have several other aims as well, namely:

- We would like to give you an opportunity to gain a deeper understanding of the physics you have learned in other courses. In most courses one is normally confronted with simple systems which provide exact solutions and mimic to a certain extent the realistic cases. Many are however the comments like 'why can't we do something else than the particle in

³ Such library functions are often tailored to a given machine's architecture and should accordingly run faster than user provided ones.

a box potential?'. In several of the projects we hope to present some more 'realistic' cases to solve by various numerical methods. This also means that we wish to give examples of how physics can be applied in a much broader context than it is discussed in the traditional physics undergraduate curriculum.

- To encourage you to "discover" physics in a way similar to how researchers learn in the context of research.
- Hopefully also to introduce numerical methods and new areas of physics that can be studied with the methods discussed.
- To teach structured programming in the context of doing science.
- The projects we propose are meant to mimic to a certain extent the situation encountered during a thesis or project work. You will typically have at your disposal 2-3 weeks to solve numerically a given project. In so doing you may need to do a literature study as well. Finally, we would like you to write a report for every project.

Our overall goal is to encourage you to learn about science through experience and by asking questions. Our objective is always understanding and the purpose of computing is further insight, not mere numbers! Simulations can often be considered as experiments. Rerunning a simulation need not be as costly as rerunning an experiment.

Needless to say, these lecture notes are upgraded continuously, from typos to new input. And we do always benefit from your comments, suggestions and ideas for making these notes better. It's through the scientific discourse and critics we advance. Moreover, I have benefitted immensely from many discussions with fellow colleagues and students. In particular I must mention my colleague Torgeir Engeland, whose input through the last years has considerably improved these lecture notes.

Finally, I would like to add a petit note on referencing. These notes have evolved over many years and the idea is that they should end up in the format of a web-based learning environment for doing computational science. It will be fully free and hopefully represent a much more efficient way of conveying teaching material than traditional textbooks. I have not yet settled on a specific format, so any input is welcome. At present however, it is very easy for me to upgrade and improve the material on say a yearly basis, from simple typos to adding new material. When accessing the web page of the course, you will have noticed that you can obtain all source files for the programs discussed in the text. Many people have thus written to me about how they should properly reference this material and whether they can freely use it. My answer is rather simple. You are encouraged to use these codes, modify them, include them in publications, thesis work, your lectures etc. As long as your use is part of the dialectics of science you can use this material freely. However, since many weekends have elapsed in writing several of these programs, testing them, sweating over bugs, swearing in front of a `f*@?%g` code which didn't compile properly ten minutes before monday morning's eight o'clock lecture etc etc, I would dearly appreciate in case you find these codes of any use, to reference them properly. That can be done in a simple way, refer to M. Hjorth-Jensen, *Computational Physics*, University of Oslo (2011). The weblink to the course should also be included. Hope it is not too much to ask for. Enjoy!