

Introduction to Classical Mechanics with Computational Competences and skills

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Introduction

Classical mechanics is a topic which has been taught intensively over several centuries. It is, with its many variants and ways of presenting the educational material, normally the first **real** physics course many of us meet and it lays the foundation for further physics studies. Many of the equations and ways of reasoning about the underlying laws of motion and pertinent forces, shape our approaches and understanding of the scientific method and discourse, as well as the way we develop our insights and deeper understanding of physical systems.

There is a wealth of well-tested (from both a physics point of view and a pedagogical standpoint) exercises and problems which can be solved analytically. However, many of these problems represent idealized and less realistic situations. The large majority of these problems are solved by paper and pencil and are traditionally aimed at what we normally refer to as continuous models. As a consequence, it implies that we can seldomly venture beyond an idealized case in order to develop our understandings and insights about the underlying forces and laws of motion.

On the other, numerical algorithms call for approximate discrete models and much of the development of methods for continuous models are nowadays being replaced by methods for discrete models in science and industry, simply because **much larger classes of problems can be addressed** with discrete models, often also by simpler and more generic methodologies.

As we will see below, when properly scaling the equations at hand, discrete models open up for more advanced abstractions and the possibility to study real life systems, with the added bonus that we can explore and deepen our basic understanding of various physical systems

Analytical solutions are as important as before. In addition, such solutions provide us with invaluable benchmarks and tests for our discrete models. Such benchmarks, as we will see below, allow us also to discuss possible sources of errors and their behaviors. And finally, since most of our models are based on various algorithms from numerical mathematics, we have a unique opportunity to gain a deeper understanding of the mathematical approaches we are using.

With computing and data science as important elements in essentially all aspects of a modern society, we can then define Computing as solving scientific problems using all possible tools, including symbolic computing, computers and numerical algorithms, and analytical paper and pencil solutions. Computing is about developing an understanding of the scientific method by enhancing algorithmic thinking when solving problems.

The way we will teach this course reflects this definition of computing. The course contains both classical paper and pencil exercises as well as computational projects and exercises. The hope is that this will allow you to explore the physics of systems governed by the degrees of freedom of classical mechanics at a deeper level, and that these insights about the scientific method will help you to develop a better understanding of how the underlying forces and equations of motion and how they impact a given system. Furthermore, by introducing various numerical methods via computational projects and exercises, we aim at developing your competences and skills about these topics.

These competence will enable you to

- understand how algorithms are used to solve mathematical problems,
- derive, verify, and implement algorithms,
- understand what can go wrong with algorithms,
- use these algorithms to construct reproducible scientific outcomes and to engage in science in ethical ways, and
- think algorithmically for the purposes of gaining deeper insights about scientific problems.

All these elements are central for maturing and gaining a better understanding of the modern scientific process *per se*.

The power of the scientific method lies in identifying a given problem as a special case of an abstract class of problems, identifying general solution methods for this class of problems, and applying a general method to the specific problem (applying means, in the case of computing, calculations by pen and paper, symbolic computing, or numerical computing by ready-made and/or self-written software). This generic view on problems and methods is particularly important for understanding how to apply available, generic software to solve a particular problem.

However, verification of algorithms and understanding their limitations requires much of the classical knowledge about continuous models.

A well-known examples to illustrate many of the above concepts

Integration by the Trapezoidal Rule is given by following algorithm for an interval $x \in [a, b]$

$$\int_a^b (f(x))dx = \frac{1}{2} [f(a) + 2f(a+h) + \cdots + 2f(b-h) + f(b)] + O(h^3).$$

Python offers an extremely versatile programming environment, allowing for the inclusion of analytical studies in a numerical program. Here we show an example code with the **trapezoidal rule** using **SymPy** to evaluate an integral and compute the absolute error with respect to the numerically evaluated one of the integral $\int_0^1 dx x^2 = 1/3$. The following code for the trapezoidal rule allows you to plot the relative error by comparing with the exact result. By increasing to 10^8 points one arrives at a region where numerical errors start to accumulate.

This example shows the potential of combining numerical algorithms with symbolic calculations, allowing us to

- Validate and verify their algorithms.
- Including concepts like unit testing, one has the possibility to test and test several or all parts of the code.
- Validation and verification are then included *naturally* and one can develop a better attitude to what is meant with an ethically sound scientific approach.
- The above example allows the student to also test the mathematical error of the algorithm for the trapezoidal rule by changing the number of integration points. The students get **trained from day one to think error analysis**.
- With a Jupyter notebook you can keep exploring similar examples and turn them in as your own notebooks.

In this process we can easily bake in

1. How to structure a code in terms of functions
2. How to make a module
3. How to read input data flexibly from the command line
4. How to create graphical/web user interfaces
5. How to write unit tests (test functions or doctests)
6. How to refactor code in terms of classes (instead of functions only)
7. How to conduct and automate large-scale numerical experiments

8. How to write scientific reports in various formats (L^AT_EX, HTML)

The conventions and techniques outlined here will save you a lot of time when you incrementally extend software over time from simpler to more complicated problems. In particular, you will benefit from many good habits:

1. New code is added in a modular fashion to a library (modules)
2. Programs are run through convenient user interfaces
3. It takes one quick command to let all your code undergo heavy testing
4. Tedious manual work with running programs is automated,
5. Your scientific investigations are reproducible, scientific reports with top quality typesetting are produced both for paper and electronic devices.