Chapter 1

Introduction to Advanced Computational Laboratory

This is no ordinary laboratory manual. Indeed, it is not meant for an ordinary lab course. The experiments to be conducted will be in a "virtual" lab that exists only inside the student's computer and brain. These experiments are all based on computer programs ("codes") which either simulate nature or analyze complex physical phenomena. What's really unusual is that these codes are the real thing; they were written over decades by graduate students as part of their M.S. and Ph.D. degree research or by professors and research scientists as part of their scholarly investigations[1].

In a broad sense, the aim of the laboratory is to incorporate some authentic research experience into the undergraduate curriculum without all the pain and time required for a "wet" lab. We believe that is is an exciting approach that stimulates the intellectual growth of students by having them get close to the techniques, mindset, and research that generates new knowledge. Specifically, we have designed this lab to be accessible to undergradutes who have already had a junior- or senior-level course in Computational Physics, such as one based on the book *Computational Physics* [CP]. Although we make frequent reference to that book, in this lab we go beyond the small and simple codes in *Computational Physics* and work with real research codes that are bigger, more complex and not necessarily "user friendly" (welcome to the real world!).

In addition to the description that we have added to make the science and codes accessible to undergraduates, in most cases we also include a reprint of an original research article that used the code under study. We suspect that this may be the only true research paper encountered and read in an undergraduate curriculum. Although it may be a challenge for an undergraduate to understand an entire research paper (it surely is for professors!), we try to have the students reproduce a figure or two from the paper so that they

[1] Well, in some cases we may have cut out some confusing parts, while in other cases we may have removed parts which a researcher did not want their competition to get their hands on!

can know and feel the excitement of dealing with the "real thing". We suspect that many students may also carry away some memory of the style and contents of these papers (we did).

Whatever a "research experience" might be, it is probably not just one thing. Accordingly, in this lab we have a number of teaching goals. They include:

- To have each student, or maybe pair of students, works independently on a selected group of experiments as they might in a research setting. While this may start with some exploration just to figure out what the experiment is about, it should finish with inquiry-based ("what happens if?") independent investigation.
- To have the students interact with the science, math and the codes in a challenging yet also engaging and rewarding manner.
- To experience the excitement of actually getting a big and complex program to work for hours on end, and thereby to develop a deeper understanding of the need for high performance computing and for scaling computational problems to larger computer systems.
- To learn some of the techniques needed for solving complex problems.
- To gain some awareness that the codes used to solve realistic problems are often neither elegant nor written in a pleasing style or language; yet that it is still better to work with them than to write your own.
- To come to appreciate that codes are pieces of scientific literature, to be understood as a whole and in terms of their individual parts.
- To understand that a sustained and reliable level of high performance computing requires care, attention to details and tuning.
- To develop a critical view of the solution to complex problems in which there is a healthy questioning of the validity of the assumptions and of the numerical algorithms (in other word, to see the codes break).
- To understand why compromises are made between speed and precision.
- To learn to use visualization wherever possible to hasten and deepen understanding
- To be able to make the connection between the theory and results given in an actual research paper (reprints to be included) by using the code that generated those results.