COMPUTATIONAL PHYSICS

by
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Preface

The teaching of physics has traditionally placed a heavy emphasis on those systems in Nature for which there are analytic descriptions. But many natural phenomena either do not lend themselves to analytic treatment, or possess a functional description that has thus far evaded our discovery. Examples of systems that currently require a numerical approach range from the calculation of elementary-particle masses to the mechanical behavior of complex biological systems.

In this course, we explore several of these complex systems from a computational viewpoint, including
•linear polymers
•non-ideal gases
•spin systems.
Our task is both to solve these systems numerically, and to analyse our numerical results.

A variety of techniques is used in numerical approaches to physical systems, but only a subset of these is included in this course:
•numerical differentiation and integration
•molecular dynamics
•Monte Carlo simulation
•optimization methods
•neural networks.
While sufficient time will be devoted to each of these techniques to allow students to work comfortably with them, we emphasize that this is not a course in numerical analysis or algorithm development. However, such courses should be of interest to students considering a career in scientific computing.

The generation and analysis of numerical data involves statistical concepts. We devote one section of the course to data analysis, but refer the interested student to the appropriate literature or statistics courses for further study. Similarly, there are many algorithms, such as fast Fourier transforms, for which very efficient routines are available in standard numerical libraries. We introduce such libraries, but they are not a major component of this course.

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