**参考书目**

1. 计算物理(影印版)，作者：Purdue university, Nicholas J. Giordano and Hisao Nakanishi (清华大学，段文晖) (2007年)

由于计算方法的深入发展和过去几十年中高速计算机的出现和普及，随着物理学基础理论的进一步突破，物理学家们逐步可以应用一些更严格和更全面的复杂模型，来定量研究实际和复杂体系的物理性质。基于物理学基本原理的数值计算和模拟已经成为将理论物理与实验物理紧密联系在一起的一座重要桥梁：它不仅能够弥补简单的解析理论模型难以完全描述复杂物理现象的不足，而且可以克服实验物理中遇到的许多困难，例如直接模拟实验上不能实现或技术条件要求很高、实验代价昂贵的物理系统等。计算机模拟技术已经渗透到物理学的各个领域，包括凝聚态物理、核物理、粒子物理、天体物理等，导致了计算物理这一新学科的突破性发展和成熟。从20世纪40年代开始，计算物理学家们已经发展了大量新数值方法(Monte Carlo方法、分子动力学方法、快速Fourier变换等)，由此发展了很多未曾预料到的新现象，并给理论与实验物理学提出了许多新问题。总之，计算物理已成为物理学家揭示多层次复杂体系的物理规律的重要手段，同时也广泛应用于处理实验结果和提出物理解释。对一个成功的物理学家来说，掌握必要的计算物理学知识和手段已变得越来越重要。越来越多的大学已针对将要从事物理学及相关学科研究的研究生和本科生开设了计算物理课程。

过去十年中国际上已涌现出一些很好的计算物理专著和教材。由Purdue大学物理系的Nicholas Giordano教授和Hisao Nakanishi教授在其多年计算物理教学和科研工作基础上合作撰写的Computational Physics(Second Edition)一书就是其中的突出代表。该书紧扣一些非常基本但难以解析求解的物理问题逐步展开，围绕各个物理学专题介绍了物理学研究中各种基本数值方法。这样可以使读者通过学习，对物理学中应用的主要计算技术有一个全面的了解，从而具有利用计算机进行数值计算解决复杂体系物理问题的能力。该书的另一个特点是包含了很多的物理学专题，这使得该书作为教材使用时教师在教学内容及深度的选择方面有较大的灵活性。

1. An Introduction to Computational Physics (Second Edition), 作者：Tao Pang

The beauty of Nature is in its detail. If we are to understand different layers of scientific phenomena, tedious computations are inevitable. In the last half-century, computational approaches to many problems in science and technology have clearly evolved into a new branch of science, computational science. With the increasing computing power of modern computers and the availability of new numerical techniques, scientists in different disciplines have started to unfold the mysteries of the so-called grand challenges, which are identified as scientific problems that will remain significant for years to come and may require teraflop computing power. These problems include, but are not limited to, global environmental modeling, virus vaccine design, and new electronic materials simulation.

Computational physics, in my view, is the foundation of computational science. It deals with basic computational problems in physics, which are closely related to the equations and computational problems in other scientific and engineering fields. For example, numerical schemes for Newton’s equation can be implemented in the study of the dynamics of the large molecules in chemistry and biology; algorithms for solving the Schrodinger equation are necessary in the study of electronic structures in materials science; the techniques used to solve the diffusion equation can be applied to air pollution control problems; and numerical simulations of hydrodynamic equations are needed in weather prediction and oceanic dynamics.

1. Computational Physics (Second Edition) 作者： J. M. Thijssen, Delft University of Technology

Computational physics is concerned with performing computer calculations and simulations for solving physical problems. Although computer memory and processor performance have increased dramatically over the last two decades, most physical problems are too complicated to be solved without approximations to the physics, quite apart from the approximations inherent in any numerical method. Therefore, most calculations done in computational physics involve some degree of approximation. In this book, emphasis is on the derivation of algorithms and the implementation of these: it is a book which tells you how methods work, why they work, and what the approximations are. It does not contain extensive discussions on results obtained for large classes of different physics systems.

Solving a physical problem often amounts to solving an ordinary or partial differential equation. This is the case in classical mechanics, electrodynamics, quantum mechanics, fluid dynamics and so on. In statistical physics we must calculate sums or integrals over large numbers of degrees of freedom. Whatever type of problem we attack, it is very rare that analytical solutions are possible. In most cases we therefore resort to numerical calculations to obtain useful results. Computer performance has increased dramatically over the last few decades and we can solve complicated equations and evaluate large integrals in a reasonable amount of time.

Often we can apply numerical routines (found in software libraries for example) directly to the physical equations and obtain a solution. We shall see, however, that although computers have become very powerful, they are still unable to provide a solution to most problems without approximation to the physical equations. In this book, we shall focus on these approximations: that is, we shall concentrate on the development of computational methods (and also on their implementation into computer programs).

* 1. Classical mechanics and statistical mechanics
  2. Stochastic simulations
  3. Electrodynamics and hydrodynamics
  4. Quantum mechanics
  5. Relations between quantum mechanics and classical statistical physics
  6. Quantum molecular dynamics
  7. Quantum field theory

1. Computational Physics 作者：Steven E. Koonin and Dawn C. Meredith, 加州理工学院

Computation is an integral part of modern science and the ability to exploit effectively the power offered by computers is therefore essential to a working physicist. The proper application of a computer to modeling physical systems is far more than blind “number crunching”, and the successful computational physicist draws on a balanced mix of analytically soluble examples, physical intuition, and numerical work to solve problems that are otherwise intractable.

Unfortunately, the ability “to compute” is seldom cultivated by the standard university-level physics curriculum, as it requires an integration of three disciplines (physics, numerical analysis, and computer programming) covered in disjoint courses.

1. 计算物理学， 作者，顾昌鑫，复旦大学

计算物理学是物理学中实验物理学与理论物理学两大分支外的第三大分支。它是以现代计算机为工具，应用适当的数学方法，对物理问题进行数值计算及分析、对物理过程进行数值模拟的一门新的物理学分支学科，是物理学、数学与计算机科学三者相结合的交叉、综合学科。

计算物理学自20世纪中期诞生以来，它在研究复杂物理体系与近代科学技术的重大发明中所显示的无法替代的作用及强大的功能，日益被人们所认识和重视。经过半个多世纪的不平凡发展历程，随着现代科学技术的高速发展与复杂体系研究的不断深入，计算物理学及由此拓展而成的科学计算，已发展成为除了理论与实验之外的第三种研究手段，它在当代科学技术和工程应用领域研究中的重要性已经日益明显地体现出来。

计算物理学作为物理学的一个独立分支，不仅与传统的实验物理学及理论物理学一起成为现代物理学的鼎立三足，而且深入现代的实验物理与理论物理之中，发挥着从未有过的独特作用。理论物理没有计算物理学的支撑，研究以难以深入；而实验物理不用计算物理的方法对实验数据进行处理，也很难甚至无法从复杂的测量结果中得到有用的物理信息，计算物理学已成为现代物理学的基石。因此当代物理工作者，无论是进行理论物理研究，还是从事实验应用研究，都必须掌握计算物理的概念和方法，具备计算物理应用能力。同样，计算物理学工作者不仅需要具有坚实的理论物理基础、熟谙实验物理方法，更重要的是需要掌握计算方法和应用现代计算机，解决科学前沿领域和重大工程技术中传统的理论解析方法及目前实验技术无能为力的问题。