

# **Reformation and Practice of the Teaching of Computational Physics**

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*Abstract:* This paper focuses on the teaching reform and practice of computational physics around the training goal and ability development direction of physics professionals. The content of computational physics should be adjusted to meet the requirements of physics professional training. Strengthen the connection between computational physics and other professional courses. Add examples that are easy to understand and operate, and strengthen the practice of computational physics. The teaching materials of computational physics adapted to the course plan are compiled, the vivid and effective multimedia courseware is made and the online course is constructed.

Keywords: Computational Physics; Teaching Reform and Practice; Physics Major

With the further development of computational methods and the emergence and popularization of high-speed computers, computational physics has become an important means to reveal the physical laws of multi-level complex systems. At the same time, it is also widely used to deal with experimental results and propose physical explanations. It is more and more important to master the necessary knowledge and means of computational physics. At the same time, it also requires computational physics to keep pace with the times, curriculum, teaching content and teaching methods to carry out the necessary changes, in order to more adapt to the needs of scientific and social development.

The purpose of teaching reform and practice of computational physics is:

(1)Based on the cultivation of students' ability and quality education, infiltrate and promote the education of scientific computing ability, and cultivate qualified talents to adapt to social development.

(2)Enrich the classroom teaching content, improve the practicality and interest of the course.

(3)Strengthen computer practice, enhance students' application ability.

(4)Integrate teaching materials, optimize teaching content, and gradually establish a systematic and mature course of Computational Physics with characteristics.

## 1. Integrating teaching materials and optimizing teaching contents

The application of computer in physics can be roughly divided into four categories: computer numerical analysis, computer symbol processing, computer real-time control and computer simulation. Most of the existing textbooks of computational physics are based on these contents, but most of them are faced with the situation of less class hours and more contents, so it is difficult to make students have a deep understanding of the above contents in the limited class hours. In addition, the traditional teaching mode of computational physics only pays attention to the explanation of numerical calculation methods and

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principles, emphasizes the high abstraction and strict logic in theory, and ignores the interest, universality and high technicality of application, and involves complex mathematical deduction, which is easy to make students tired of learning and not easy to receive good teaching effect. And we think that in the teaching of computational physics, we should pay more attention to the establishment of physical model, the design of physical quantity algorithm, the simulation of physical process and the analysis of simulation results. Introduction to computational physics mainly talks about what is computational physics, the development and significance of scientific computing, high-performance computer, multi-scale simulation method system, review of computer simulation events, and the content setting and assessment methods of this course. The basis of computational physics mainly includes three parts: The first is the basic calculation method. The second is the material structure, including material dimension, crystal structure, chemical bond and phase transition, and the third is the interaction and potential function between substances. Monte Carlo method, molecular dynamics method and first principles are widely used in computational physics. Moreover, the complete implementation of these algorithms can fully enable students to learn physical model building, physical quantity algorithm design, physical process simulation and simulation result analysis.

### 2. Case teaching, enrich teaching means

In the above-mentioned teaching of computational physics, examples are supplemented. Specific examples can be divided into class analysis examples and computer training examples. Examples of class analysis can stimulate students' interest in learning and enhance their purpose of learning computational physics. The calculation and simulation of crystal structure phase transition induced by changing pressure and carbon nanotubes filled with transition metals are illustrated respectively. These examples focus on discussing the results and simply analyzing the implementation process. In the teaching of Monte Carlo method, the random number algorithm design examples, high-dimensional integration examples, electron double slit diffraction simulation examples and transition metal filled carbon nanotubes examples are arranged; In the molecular dynamics method, the melting simulation examples of AR clusters are mainly inserted; In the first principles introduction, the band structure and state density of intrinsic semiconductor silicon are simulated as examples. These examples are integrated with the teaching of methods and principles, focusing on the analysis of the implementation process of calculation, and the organization form of the content is gradually expanded with the deepening of the teaching methods and principles. This kind of teaching process of combining typical examples and methods has not only the application process of the learned knowledge, but also the reconstruction process of knowledge, which has practical significance for the cultivation of applied and innovative talents. Computer examples are selected from the examples in class, but more emphasis is placed on students' hands-on operation of the implementation process and corresponding conclusions.

#### 3. Modular programming training to enhance students' application ability

The teaching of computational physics is inseparable from the students' personal operation on the computer. In the course of computer programming language learning, students pay more attention to how to use programming language, such as mastering the grammar format, data format and key functions of the language. In the numerical algorithm course, most of the problem solving training is around the equation, such as heat conduction equation, wave equation and so on. These learning processes are only a small part of physical process simulation. In order to let the students accept the simulation of the physical process completely, combined with the practical examples, the modular programming training is implemented in the computer process. According to the practical examples, it is divided into the following modules: the program language with random function uniformity and independence test training, linear congruence programming to achieve random function training, cast point method to calculate the PI training, high-dimensional integral training, Lennard Jones potential programming training, physical model building training, distribution function programming training, metal atom filling stiffness training Monte Carlo simulation training of carbon nanotubes and molecular dynamics simulation melting training of AR clusters. The combination of early computer training modules is just a complete programming process of example simulation. Finally, the whole programming process of the example is divided into global variable declaration module, main program call module, initial model module, main method implementation module (Monte Carlo method or molecular dynamics method programming and physical quantity programming to be counted), energy calculation module and random function definition module in strict accordance with the modular subroutine programming format. It mainly emphasizes programming according to physical thought and calculation purpose. After fully debugging the program, simply run the results on your own machine and upload the complex results to the server. Such modular programming training can effectively enhance students' application ability.

# 4. Compiling teaching materials, making multimedia courseware and strengthening the construction of online courses

Starting from the trend of today's science and technology development, the curriculum reform should adapt to the international society, the information society, the quality education and the lifelong education system. Teaching materials are the main media of curriculum implementation. To do well in curriculum reform, we must pay attention to the reform of teaching materials, including the reform of the content and structure of teaching materials and the management system of teaching materials. In order to meet the needs of cross century talents training, the teaching materials of computational physics should be examined from the perspective of development. It is necessary to realize the modernization of curriculum content while ensuring the foundation, so as to make the education of computational physics "keep pace with the times". Expand vision, guide students' desire to explore, enhance students' sense of innovation.

Therefore, according to the needs of reform, we first compile the teaching materials of computational physics, and develop them into teaching materials after trial and improvement. The compilation of the handout will be closely linked to the goal of the curriculum reform. While ensuring the core theoretical knowledge and basic algorithm, it will increase the calculation examples to enhance the operability and practicability of the course. The theory part is concise, the example part is easy to implement, and can be closely linked with other courses of physics. Add the part of frontier project development, for the students who have spare time to think and research.

Computational physics is a very practical course. We will make rich and vivid multimedia courseware according to the content of the course, and increase interaction in the classroom as much as possible. We have completed the construction and application of online course of computational physics. At present, the number of visits to this course has exceeded 30000. With online courses, students can use the spare time to learn and complete online homework, and even complete the example operation online, which can not only improve the learning efficiency, but also enhance the attraction of the course. Teachers also have more time for example design and guidance, as well as interaction with students.

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