



Fudan Series in Graduate Textbooks



Fundamental of Advanced Computer Programming

高级计算机程序基础

周麟祥 编著

Linxiang Zhou

复旦大学出版社



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PREFACE

Scientific research of humankind has already been touching the field of sophisticated systems, which include those from the lowest hierarchy of atoms and molecules to the highest hierarchy of biological phenomena. For studying the sophisticated systems, besides using the traditional experimental measure and theoretic method, the large scale computational calculation and simulation have indispensably become the third approach. The basic task of computational physics, which has been the third branch of physics in addition to experimental physics and theoretic physics, is more and more relied on the large scale computer calculation and simulation.

As a student carrying out the large scale calculation and simulation, in general, he must be familiar with not only C language but also other computer languages, especially those advanced computer languages. Therefore, they would overcome the trouble due to the lack of basic computer knowledge of professional field in the future.

At present there are many kinds of advanced computer languages, and each language can be written as a professional book. However for non-computer science students who are going to take up the large scale computer simulation, the curriculum schedule does not allow them to learn all these advanced languages by taking different courses one by one. Could we teach them the basic knowledge of these languages in a single concise course? This is just our motivation to attempt editing this textbook. According to my teaching experience, the manuscript of this book has been lectured six times for both undergraduates and graduate students in the Department of Physics, Fudan University and the expected effect has been reached.

This book consists of three knowledge blocks: Unix operating system, computer languages (C/C++/Java/Matlab), and database language SQL. These three parts are treated by the following considerations:

(1) We take Unix as a unique work platform for operating these three knowledge blocks. All students can learn the whole course on a computer server opening for 24 hours every day.

(2) Various computer languages in this book are integrated as a whole to teach. For example, in C++ language we teach only the Class and its two characters, but omit the knowledge in common with C language. In Java, we do not describe the Class again, but only discuss

those characteristics different from C++ language. This is why we can compress several languages into a single course.

(3) The whole course is structured based on a guiding idea: "Any computer language consists of five elements: variable, operator, function, control, and input/output. The difference between different languages appears only on their different formats."

Relying on this idea, students can understand several languages easily. For example, teaching Matlab needs only two times with total six class hours. Also, we put Python and TCL languages in the attached compact disk (CD-ROM) as the appendix of this book. These two languages are often used in many big computer programs as the languages of input files. We believe that students could understand them easily.

(4) We take a unified handling for three knowledge blocks by combining Shell Script program with computer languages. That is a commonly used method and is also a powerful method in large scale computer programs, and a powerful method to edit programs. For example, in the case of C language, the students are asked to edit not only C program, but also the corresponding Shell Script file. Moreover, they are asked to edit M file of Matlab into Shell Script file.

Therefore, although this book includes fruitful contents, it is not a simple preliminary introduction relying on ignoring advanced materials. On the contrary, the core knowledge of each block in this book is intact.

(5) This book includes a lot of source codes attached on the CD-ROM. These source codes are the indiscrptible parts of the book. Students can really understand the contents of the book only if they learn these source codes in detail.

This book can be used for a one semester course with three class hours per week and three more hours for laboratory work on a public Linux server.

The whole book was carefully read by Professor Xun Wang and he made considerable corrections and many valuable opinions.

The author is grateful to the Physics Department, Surface Physics Laboratory of Fudan University, and the Fudan University Press for their kind support in publishing this book. Enthusiastic help and encouragement by Professors Xun Wang, Ling Ye, Ruibao Tao, and Yu Wang are sincerely appreciated.

Linxiang Zhou
June, 2005
Fudan University

前 言

人类已经进入复杂性系统的研究,包括从最低层次的原子分子到最高层次的生物学对象。对复杂性系统的研究,除了传统的实验手段和理论方法外,大规模计算和模拟已经是不可缺少的第三种方法。同样,在物理学的研究中,计算物理已经作为实验物理与理论物理之外的第三个分支而得到广泛的应用和发展。计算物理学研究也不可避免地越来越依靠与使用大规模计算和模拟。

从事大规模计算和模拟,一般需要掌握多种计算机语言。国内学生比较熟悉的 FORTRAN 语言在国外已经很少使用。虽然熟悉 C 语言的越来越多,但是,对于从事大规模计算和模拟的研究工作来说,仅仅 C 语言是远远不够的。我们需要熟悉更为高级的计算机语言,使学生在今后的专业领域内不再有计算机基础不足的麻烦。

现今发展的各种高级语言种类很多,每一种语言都可以有一本专门的书籍来叙述。对于使用这些语言来进行大规模计算机模拟的非主修计算机专业的学生来说,要一门一门地来读完这些语言的课程,在时间上是不允许的。是否可以用一门课程来传授最基本的知识,为他们应用这些语言打下基础,本书正是在这方面的一个尝试。根据本人的教学实践,本书的原稿作为一门课程的教材,在复旦大学物理系本科生和研究生中作了六次讲授,达到了预期的目标。

本书的内容由三个知识块组成:Unix 操作系统,计算机语言(C/C++/Java/Matlab)和数据库语言 SQL。具体安排上,有如下几点处理:

(1) 整个课程的三个知识块都在统一的一个 Unix 平台上操作。所有学生可在 24 小时开放的一个服务器上

学习。

(2) 各门计算机语言作为一个统一的整体讲授。如在 C++ 中只需讲授 Class (类) 及其两个特征, 不需再讲跟 C 语言相通的知识。在 Java 语言中, 则又不再讲述 Class, 只需讲述跟 C++ 差异之处。这就是为什么可以把多个语言压缩到同一课程的原因。

(3) 整个课程贯穿一个主要指导思想, 即任何计算机语言和程序都是由五个基本要素, 即由变量、算符、函数、控制、输入/输出组成的。不同语言只是书写格式不同而已。

由于这一指导思想, 学生可以很快掌握多个语言。一门 Matlab 只需讲授两次, 每次三课时即可基本掌握。因此又在光盘内附录了 Python 语言和 TCL 语言。这两种语言是目前很多大型科学计算程序中作为输入文件的语言。相信学生用这一指导思想也可以很快掌握它们。

(4) 本书还对三个知识块作了统一处理, 即把 Shell Script 的操作系统编程和计算机语言结合起来。这种方式, 也是当今大规模计算程序中普遍使用的方法, 是最强大的编程方法。以 C 语言为例, 不仅要求学生编出 C 的程序, 还要编出相应的 Shell Script 文件, 还要求把大型软件, 如 Matlab, 作为后台编进去。

因此, 虽然本书含有多个内容, 但绝不是靠牺牲内容的简单介绍。相反, 每个知识块, 在基础知识上都是完整的。

(5) 本书附有大量的源码, 放在所附光盘中。由于本书的例题有限, 大量、完整的练习则放在光盘内, 这也是本书不可分割的部分。只有通过这些源码, 才能真正掌握所讲授的知识。

本书内容可以作为一学期的课程, 每周讲授三课时, 学生上机练习三课时。

王迅院士仔细通读了全文, 并给予许多修订和宝贵意见。

在编写过程中,编者得到了复旦大学物理系和复旦大学应用表面物理国家重点实验室和复旦大学出版社的众多支持和帮助,也得到了王迅院士、陶瑞宝院士、叶令教授和王煜教授很多具体指导和热情帮助,在此表示深切的谢意。

编者

2005年6月

复旦园

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PART I UNIX OPERATING SYSTEM

To carry out the computer calculation, firstly, one must select an operating system as a platform, which is a piece of software. Unix is a common operating system, which is adopt by all the large scale computer calculation and simulation. Unix is like a 'tool kit'. It contains many small programs and tools, that can be used together to solve complex problems.

Unix possesses several unique features, which are different from other operating systems, namely it may have multi-user, multi-tasking, and is very stable. A Unix operating system is very rarely crashed. Especially, Unix has Shell Script file, which is a strong tool for writing program. We call it as second development of program. Also, Unix has X Windows providing a graphical interface.

If you run Internet web from PC machine instead of X-window in workstation, you should use **NetTerm** program, **Xwin32** program, **Xserver** program, or Windows/start/run. And if you have trouble to install Linux system, you can download a program winlinux2003 from [http:// www. winlinux. net/download](http://www.winlinux.net/download) to install on your Windows system.

EDITING AND MANAGING FILE

1.1 LOGIN AND LOGOUT

1.1.1 Login and Logout

1. Tool: **NetTerm** or **Xwin32**.
2. Login: use telnet program to type the command: % **telnet IP** and answer: login and password.
3. Logout: **logout** for telnet program (for other programs, often use: quit, exit and bye).

Please note that ① We use C-shell only. Its prompt is % .
 ② There are some Berkley commands called the remote operations, but they are only used on the Unix web.

Ex1 : % rlogin IP (remote login)

Ex2 : % rcp -r mylinux: /home/aaa /home/myfile (remote copy)

Ex3 : % rsh (remote shell command)

Ex4 : % rsh name_remote_machine unix_command

Ex5 : % rsh abc ls /home/aaa

1.1.2 File and Command

(1) Command format

In general, a complex Unix command consists of three parts:

% command -option filename or path.

Ex: % ls -l aaa

Where aaa is a file and % is prompt in C shell. We call 'ls', '-l' and 'aaa' as the parameters of the command line.

(2) File and directory

Directory: A directory is a collection of files or other subdirectories.

File: There are two kinds of files: **text file** and **binary file**. You can directly read a text file, but not a binary file. All executable file (i. e. program), sound file, image file, and encode file are binary files. To identify the property of a file, we should add an **extension** for a file.

Path: The structure in the Unix system is like a tree, so the position of one file or directory forms a path. If we call file name, it means filename or path/filename. We use **slash** '/' to represent path, for example, /usr/bin/ls.

Especially, the single mark '/' is root directory; '~/' is your home directory; the dot '.' is local directory and the double dot '..' is last directory.

Some file sorts are listed in the following:

Text file: *.txt *.html *.asc *.msg *.wpd

Video file: *.avi *.mov *.mpg

Graphics file: *.bmp *.eps (on PC) *.ras (image format)
*.ps *.pbm *.psm *.pnm *.ppm (data
format)
*.tiff *.gif *.jpg (on scanner or PhotoShop)
*.pdf

Sound file: *.au *.snd *.ra *.ram *.wav *.mid *.mp3

Program file: *.exe *.bat *.com

Compress file: *.Z *.gz *.tar.Z *.tar.gz *.iso

1.1.3 Set Up

When you enter into your account on the server, maybe, you should set up such commands:

```
% stty erase ' type backspace key'
```

(let the backspace key available)

```
% set term = vt100
```

(vt100 is PC machine's terminal)

```
% setenv DISPLAY = userIP : 0
```

(for workstation)

The command DISPLAY is only available for workstation or X-window. This command makes you be able to watch images from the server. And where '0' means the standard input, '1' is standard output, and '2' is standard error output.

1.2 EDITOR VI

1.2.1 Login and Logout

Login: % vi aaa (aaa is a file name you want to write).

Logout: ZZ (quit and save) or :q! (only quit, not save) in the escape status.

1.2.2 Two Statutes

The vi editor has two statutes:

i (insert) : type [i] key , then you can write any letter.

esc (escape): type [esc] key, then you can type any command.

1.2.3 Command

Cursor movement operators:

h j k l: move cursor to left, down, up and right, respectively.

nG: go to n-th line (only type G, the cursor will go to the end of a file).

H: move cursor to home.

o: move cursor to beginning of next line and enter insert status.

or \$: move cursor to the end of line.

Scroll:

^f: move forward one screen.

^b: move backward one screen.

Enter into the next line: press "Return" key (or call "Enter" key).

Move backward the parts of line behind cursor: press "bar".

Connect sentence: **J** (connect to behind cursor)

Deleting:

x: delete a single character on which the cursor is located.

dd: delete the line on which the cursor is located.

n dd: delete n lines on which the cursor is located.