A Book of

COMPUTATIONAL PHYSICS

T. Y. B.Sc. • PHYSICS (PH-335) • SEMESTER III

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NIRALI PRAKASHAN
ADVANCEMENT IN KNOWLEDGE

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COMPUTATIONAL PHYSICS

T.Y.B.Sc. Physics : PH - 335 : Semester-III

As Per New Revised Syllabus

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Preface ...

The present book entitled **"Computational Physics"** is written as per new revised syllabus prescribed for the IIIrd Semester of T.Y.B.Sc. (Physics) with effect from June 2015. This book is targeted mainly to the undergraduate students of Pune University, but will be found useful for the graduate students and Teachers of other universities also. The book is divided into six chapters. Each chapter begins with basic concepts containing theory, set of formulae and explanatory notes followed by a number of solved problems. Summary of contents in topic, short, long questions and unsolved problems are also given at the end of each topic.

The problems are judiciously selected and are given topic and section-wise. The approach is straight forward and step-by step solutions are elaborately provided. More importantly the relevant formulas used for solving the problems can be located in the beginning of each chapter. There are number of diagrams for illustration.

Chapter 1 in the book is devoted to the Concepts of Programming Chapter 2 is basically concerned with C Programming. Chapter 3 is concerned with Arrays and Pointers in C. Chapter 4 is basically related to User-Defined Functions. Chapter 5 is related to Graphics in C. Chapter 6 is concerned with Computational Physics.

All precautions have been taken to avoid mistakes and misprint in the book. However, it is possible that some mistakes and misprints might have passed unnoticed. Such mistakes and misprint, is brought to our notice will be thankfully acknowledged.

We are thankful to Shri Jignesh Furia and staff of Nirali publication for publishing the book in attractive look. We have a pleasure to thank Mr. Santosh Bare for the bulk of typing and Mr. Kiran Velankar for proof reading. I am indebted to Chaitali Takle for line drawings, to Ravi Walodare for designing cover page and all staff in the distribution of books network.

We are also thankful to all the Marketing Staff especially Mr. Nilesh Deshmukh and others for co-ordinating the matter well in time.

Suggestions to improve the quality of the book will be gladly accepted.

AUTHORS

Syllabus ...

1. Concepts of Programming (6 L)

Definition and Properties of algorithms.

Algorithm development.

Flow charts - Symbols and simple flowcharts.

Flow charts and Algorithms for Kinematic equations, Free fall, Equation of state, Factorial of a number.

Types of programming languages : Lower, middle and higher level languages.

2. C Programming (14 L)

Structure of C program, Character set, Keywords, Constants and variables, Variable names, Data types and their declarations, Symbolic constants.

Input/output functions: scanf ( ), printf ( ), getchar ( ), putchar ( ), getch ( ), gets ( ), puts ( ).

Operators and Expressions: Arithmetic operators, Relational operators, Logical operators, Assignment operators, Conditional operator.

Formatted input/output.

Control statements: If, if else, while, do while, for loop, nested control structures (nested if, nested loops), break, continue, switch-case statement, goto statement.

Use of Library functions: e.g. mathematical, trigonometric, graphics.

3. Arrays and Pointers in C (4 L)

Arrays: 1-D, 2-D and String

Examples: Arranging numbers in descending and ascending order, Sum of matrices, Multiplication of matrices.

Concept of Pointers.

4. User-Defined Functions in C (8 L)

User-Defined functions: Definitions and declaration of function, function prototype, passing arguments (Call by value, Call by reference).

Storage classes: Auto, External, Static, Register variables.

5. Graphics in C (4 L)

Some simple graphic commands : Line, Circle, Arc, Ellipse, Bar.

6. Computational Physics (12 L)

1. Errors in Computation: Inherent errors in storing numbers due to finite bit representation to use in Computer, Truncation error, Round-off errors (Explain with the help of examples).
2. Iterative methods: Discussion of algorithm and flowcharts and writing C programs for finding single root of equation using Bisection method, Newton-Raphson method.
3. Discussion of algorithm and flowcharts and writing C program for Trapezoidal rule and Simpson's $\frac{1^{rd}}{3}$ rule (Derivation of formula is not expected).

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Contents ...

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Chapter **1**...

Concepts of Programming

Contents ...

Introduction

- A computer is a useful tool for solving a great variety of problems. The word '*Computer*' is originated from the word "*compute*" (*means to calculate*). Normally computer was considered as a calculating device that can perform arithmetic operations with enormous speed. But more than 80 % of work done today is of non-mathematical or non-numeric in nature. Hence more accurately a computer may be defined as a *device that operates on information or data*. Data can be - biodata of various applicants, marks obtained by students, telephone calls or electric power/units consumed, passenger's reservations, scientific research programs, records of offices, payrolls, bank transactions, etc.
- Speed, accuracy, diligence, versatility and power of remembering (storage) are the main characteristics of computers. A computer system is made of hardware and software. *Hardware* means the physical device that make up the computer system. Hardware includes input devices (like keyboard, mouse, joystick, bar code reader, optical and magnetic ink character reader, etc.), output devices (like visual display unit, printer) and central processing unit and memory devices (floppy, hard disk, pen drive, CD, DVD etc).
- Computer *software* is a collection of programs and applications that manage and work with the hardware. To make a computer do anything (i.e. solve a problem), we have to write a computer program. In a computer program you tell a computer, step by step, exactly what you want it to do. Software is classified into system hardware (like operating system) and application software (like word processor graphic software, etc.). These softwares are the computer programs written in different languages.

- Before writing computer program, one must be clear about the processing steps to be performed by a computer. Thus, to write effective program one must first plan logic of the program. The computer then executes the program, following each step mechanically, to accomplish the end goal. Hence, before we learn how to write program in 'C' (next chapter), we will first learn how to plan the logic of computer program in this chapter.

1.1 Algorithms (April 17, Oct. 17)

Definition of Algorithm : *Algorithm is a finite sequence of instructions, which can be carried out to solve a particular problem in order to obtain the desired result.*

In computer systems, an algorithm is basically an instance of logic written in software by programmers to be effective for the intended "target" computer(s) to produce output from given input.

1.1.1 Characteristics of Algorithm

Algorithm is a sequence of logical steps required to perform a specific task. A good algorithm greatly reduces programming efforts. A good algorithm has following characteristics :

1. **Definiteness :** The instructions in the algorithm must be precise, clear, unambiguous.
2. Algorithm must be **organized** properly i.e. the instructions must be arranged in a meaningful way to solve the problem.
3. **Finiteness :** Algorithm must terminate after a finite number of steps. (Instructions should not repeat infinitely.)
4. **Input :** Algorithm must have zero or more inputs.
5. **Output :** Algorithm must have one or more outputs. After performing the instructions (i.e. after the algorithm terminates), the desired results should be obtained.
6. **Effectiveness :** It means guaranteed to give a correct answer. Every instruction should be performed in finite time.
7. Algorithm should be **independent** of the programming language.

1.1.2 Advantages of Algorithm

1. Algorithm is a general purpose tool, which is language and hardware independent.
2. It is easy to understand program logic using algorithm. If basic layout is known it is easy to write program in any language using algorithm.
3. Algorithm is written in English, hence it can be understood by everyone.
4. Identification of error is easier.

1.1.3 Limitations of Algorithm

1. It is a time consuming process.
2. It is difficult to show branching and repetitive task in algorithm.
3. For big task, algorithm can be lengthy and complicated.

1.2 Algorithmic Development

- Computers have provided a man the capability to handle many varied problems. The computer does not possess any common sense and cannot make any unplanned decision. The problem to be solved whether simple or complex, has to be broken into well defined steps. It should be kept in mind that the computers do not solve the problems, rather, they are used to implement the solutions to the problems.
- Computer cannot be used for problem solving until a proper method of solution has been evolved and detailed procedure has been prepared by the user. It is assumed that the user or programmer has a certain amount of background knowledge, knows certain facts about the problems and possesses deductive and reasoning skills. Thus problem solving involves following steps :
  1. studying the problems in detail,
  2. redefining and restarting the problem,
  3. identifying the output requirements, input data, conditions and limitations,
  4. generating and comparing alternative method of solution,
  5. selecting the method which is considered to be as the best method,
  6. preparing a logical and concise list of procedure or steps necessary for determining the solution,
  7. computing the results,
  8. examining the results for correctness.

The computer's help may be necessary in seventh steps. All the remaining steps are to be performed by user. Let us discuss following example.

Example :

Suppose you are income-tax consultant. You have to help one of your client to prepare his income-tax return.

Step 1 : Find more details about your client's profession, nature of income, category of income-tax, etc.

Step 2 : The problem is to calculate the income tax for the year 2009-2010 under individual category.

Step 3 : Output required is Tax for 2009-2010. Data available is monthly income, deduction from LIC, PF and other payment and tax rate, etc.

Step 4 : Find out the various approaches of calculating income tax.

Step 5 : Select the approach which benefits your client.

Step 6 : Prepare steps for calculating total salary, deduction, exemptions, taxable salary and procedure for tax calculations.

Step 7 : Write the program to compute the result using computer and get the results.

Step 1 to 5 relate to problem analysis. Step 6 provides logical and concise list of procedure required for solving the problem. This introduces the algorithmic approach for problem solving.

The logical and concise list of procedure for solving problem is an algorithm.

Example 1.1 : *Write algorithm to obtain Fibonnaci series.*

Solution : The first and second terms in this series are 0 and 1, subsequent terms are found by adding the preceding two terms in the sequence. A part of the sequence is :

0, 1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89, ...

Step 1 : Read N.

Step 2 : Assign first term $F_1 = 0$ and second term $F_2 = 1$.

Step 3 : Print F_1 and F_2.

Step 4 : Let counter = 3.

Step 5 : Calculate third term $F_3 = F_1 + F_2$.

Step 6 : Print F_3.

Step 7 : Add 1 to counter.

Step 8 : If counter > N, go to step 10.

Step 9 : $F_1 = F_2$, $F_2 = F_3$ go to step 5.

Step 10 : Stop.

Example 1.2 : *Write algorithm for finding square root of N numbers for finding square root of a set of N numbers.*

Solution :

Step 1 : Start.

Step 2 : Read the number of values for which square roots are to be evaluated.

Step 3 : Take a value.

Step 4 : Check whether the value is positive or negative. If positive, go to step 5, otherwise go to step 7.

Step 5 : Calculate square root.

Step 6 : Record the value and its square root.

Step 7 : Repeat steps 3 to 5 until all values are completed.

Step 8 : Stop.

Example 1.3 : *Algorithm to swap and print the values of two variables A and B.*

Solution :

Step 1 : Start.

Step 2 : Read A and B.

Step 3 : Let temp. = A.

Step 4 : A = B.

Step 5 : B = temp.

Step 6 : Print the values A and B.

Step 7 : Stop.

Example 1.4 : *Using equation of state PV = RT, find pressures for different volume.*

Solution :

Step 1 : Start.

Step 2 : Read R, dV, T and initial volume V_{in} and final volume V_f.

Step 3 : $V = V_{in}$.

Step 4 : Calculate P = RT/V.

Step 5 : Increase V by dV ($V \leftarrow V + dV$).

Step 10 : If $V \leq V_f$, go to step 4.

Step 11 : Print P.

Step 12 : Stop.

Example 1.5 : *Write an algorithm to solve the kinematic* $S = S_0 + ut + \frac{1}{2}gt^2$. **(April 16)**

Solution :

Step 1 : Start.

Step 2 : Initial position S_0, initial velocity u, final time t_0.

Step 3 : t = 0.

Step 4 : Calculate $S = S_0 + ut + \frac{1}{2}gt^2$.

Step 5 : $t \leftarrow t + dt$.

Step 6 : If $t <= t_0$ go to step 4.

Step 7 : Sum = sum + Term.

Step 8 : Print t and S.

Step 9 : Stop.

Example 1.6 : *Write algorithm to find sum of the following series :*

$$1 + \frac{1}{2!} + \frac{1}{3!} + \frac{1}{4!} + \frac{1}{5!} + \ldots\ldots$$

Solution :

Step 1 : Start.

Step 2 : Read number of terms as N.

Step 3 : Let sum = 0, ctr (counter) = 1.

Step 4 : Let j = 1 and fact = 1.

Step 5 : Calculate fact = fact * j.

Step 6 : Increase value of j by 1.

Step 7 : If $j \leq N$, then go to step 5.

Step 8 : Calculate sum = sum + $\frac{1}{\text{fact}}$

Step 9 : Increase value of counter by one.

Step 10 : If counter ≤ N, then go to step 4.

Step 11 : Print sum.

Step 12 : Stop.

1.3 Flow Charts **(April 16, 13, 11; Oct. 17, 16, 12)**

- A flow chart is a *pictorial representation of an algorithm that uses boxes of different shapes to denote different types of instructions*. It is the diagrammatic representation of the step-by-step solution to a given problem. The instructions are written within these boxes using clear and concise statements. These boxes are joined by lines having arrow mark to indicate flow of operation.
- Normally, an algorithm is first represented in the form of flow chart and then flow chart is expressed in some programming language. Such a two-step approach is essential in program writing because while drawing flow chart one is not concerned with the details of programming language. Hence user can fully concentrate on logic. Since flow chart shows flow of operations in a picture form, any error in the logic can be detected more easily than a program. Once flow chart is ready, a programmer can forget about logic and can concentrate on coding the operations in each box.
- A flow chart, therefore, is a picture of logic to be included in the computer program.

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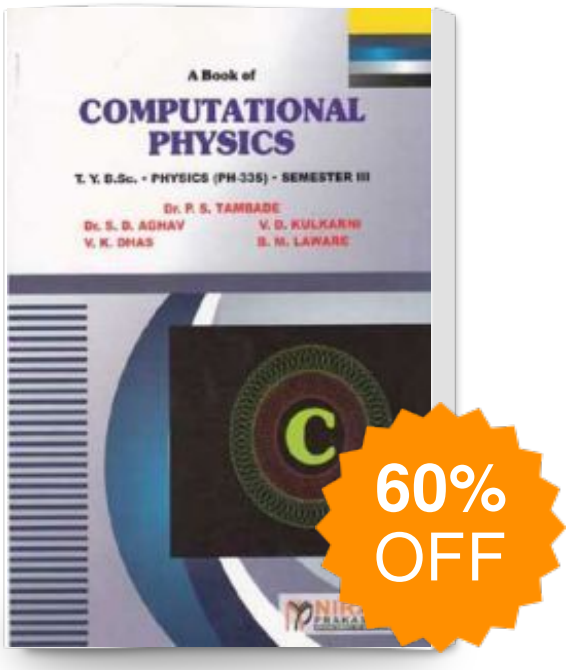

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