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E. Balaguruswamy, Numerical Methods, Tata McGraw Hill (2017). 4. V. Rajaraman, Computer oriented numerical methods, PHI Learning Pvt. Ltd., 4 th Ed. (2018). Course Title: Density Functional Theory Paper Code: CCC.529 Total Lecture: 45 Objective and Learning Outcomes: This is a specialization course for students of Computational Chemistry.

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This comprehensive text provides a thorough understanding of mathematical concepts and their applications with special emphasis on computational algorithms. The book gives a detailed discussion on all the relevant topics of both numerical and statistical methods, which are nowadays very important at computing level. It also includes the basic issues related to theory of estimation and testing of hypothesis, various sampling tests, and analysis of variance with plenty of illustrations. The topics covered in this book are supported by a large number of worked-out examples, C programs and algorithms to facilitate clear understanding of various theories discussed on numerical and statistical methods. The text is intended for the undergraduate students of computer engineering and postgraduate students of computer applications.

This work addresses the increasingly important role of numerical methods in science and engineering. It combines

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traditional and well-developed topics with other material such as interval arithmetic, elementary functions, operator series, convergence acceleration, and continued fractions.

The rapid development of high speed digital computers and the increasing desire for numerical answers to applied problems have led to increased demands in the courses dealing with the methods and techniques of numerical analysis. Numerical methods have always been useful but their role in the present-day scientific research has become prominent. For example, they enable one to find the roots of transcendental equations and in solving nonlinear differential equations. Indeed, they give the solution when ordinary analytical methods fail. This well-organized and comprehensive text aims at enhancing and strengthening numerical methods concepts among students using C++ programming, a fast emerging preferred programming language among software developers. The book provides an synthesis of both theory and practice. It focuses on the core areas of numerical analysis including algebraic equations, interpolation, boundary value problem, and matrix eigenvalue problems. The mathematical concepts are supported by a number of solved examples. Extensive self-review exercises and answers are provided at the end of each chapter to help students review and reinforce the key concepts. **KEY FEATURES** : C++ programs are provided for all numerical methods discussed. More than 400 unsolved problems and 200 solved problems are included to help students test their grasp of the subject. The book is intended for undergraduate and postgraduate students of Mathematics, Engineering and Statistics. Besides, students pursuing BCA and MCA and having Numerical Methods with C++ Programming as a subject in their course will benefit from this book.

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This concise introduction to Numerical Methods blends the traditional algebraic approach with the computer-based approach, with special emphasis on evolving algorithms which have been directly transformed into programs in C++. Each numerical method used for solving nonlinear algebraic equations, simultaneous linear equations, differentiation, integration, ordinary differential equations, curve-fitting, etc. is accompanied by an algorithm and the corresponding computer program. All computer programs have been test run on Linux 'Ubuntu C++' as well as Window-based 'Dev C++', Visual C++ and 'Turbo C++' compiler systems. Since different types of C++ compilers are in use today, instructions have been given with each computer program to run it on any kind of compiler. To this effect, an introductory chapter on C++ compilers has been added for ready reference by the students and teachers. Another major feature of the book is the coverage of the practicals prescribed for laboratory work in Numerical Analysis. Each chapter has a large number of laboratory tested programming examples and exercises including questions from previous years' examinations. This textbook is intended for the undergraduate science students pursuing courses in BSc (Hons.) Physics, BSc (Hons.) Electronics and BSc (Hons.) Mathematics. It is also suitable for courses on Numerical Analysis prescribed for the engineering students of all disciplines.

Provides a comprehensive coverage of the subject, Emphasis is laid to ensure the conceptual understanding of numerical methods, Formulae for different numerical methods have been derived in the simplest manner, algorithms for these methods are developed using pseudo language, Large number of programming exercises to test your for reference, large number of multiple choice questions and review exercises to test your programming skills acquired, Majority of

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the algorithms are implemented in C,C++ and FORTRAN languages.

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