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Real-Space Finite-Difference PAW Method for Large-Scale Applications on Massively Parallel Computers The Boxstep Method for large scale optimization An Iterative Tikhonov Method for Large Scale Computations Numerical Methods for Large Eigenvalue Problems Large Strain Finite Element Method Development of the Discontinuous Galerkin Method for High-resolution, Large Scale CFD and Acoustics in Industrial Geometries A Method for the Calculation of Large Numbers of Dipole and Quadrupole Transition Probabilities Large-Eddy Simulation Based on the Lattice Boltzmann Method for Built Environment Problems A Method for Ascertaining the Effect of Large Targets Present in Terrain Return Signals A New Method for Determining the Physical Parameters of Large Soil and Rock Samples in Situ Automated Method for the Large Deflection and Instability Analysis of Three-dimensional Truss and Frame Assemblies Iterative Methods and Preconditioning for Large and Sparse Linear Systems with Applications Stochastic Decomposition Interior and Exterior Newton Methods for Large-scale Quadratic Programming Iterative Solution of Large Linear Systems A Best Choice Numerical Method for Large Scale Computations in Nacelle Acoustics Computational Methods for Large Molecules and Localized States in Solids On Laplace's Method of Large Powers for Complex Functions Calculations on nonlinear optical properties for large systems A Parallel Solution Method for Large Sparse Linear Systems of Equations on Multicomputers A Parallel Bundle Method for Large-scale Semidefinite Programs Discourse on the Method Meshless Methods in Solid Mechanics Discourse on the Method Iterative Methods for Sparse Linear Systems An Optimal Solution Method for Large-scale Multiple Traveling Salesman Problems A Scaled Gradient Projection Method for Large Scale Optimization A Parallel Quasi-Newton Method for Partially Separable Large Scale Minimization A cyclic low rank Smith method for large sparse Lyapunov equations with applications in model reduction and optimal control Numerical Method for the Solution of Large Systems of Differential Equations of the Boundary-layer Type A Vector Method for Large Scale Configuration Interaction Problems Sequential Subspace Optimization Method for Large-scale Unconstrained Problems The Fragment Molecular Orbital Method Word Segmentation Method in Large Scale Protein and Genomic Research A Two-level Iterative Method for Large Sparse

Generalized Eigenvalue Calculations A Design Method for Large Diameter Reinforced Concrete Siphons Second Derivative Method for Nonlinearly Constrained Optimization Gradient-based Aerodynamic Shape Optimization Using ADI Method for Large-scale Problems Small Grain Varieties for Indiana Parallel Octree-based Multiresolution Mesh Method for Large-scale Earthquake Ground Motion Simulation

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A method for ascertaining the effect of large targets present in terrain return signals is presented along with a technique whereby this effect may be removed with a reasonable degree of confidence in order to study the behavior of scattering ground alone. A numerical method for the solution of large systems of nonlinear differential equations of the boundary-layer type is described. The method is a modification of the technique for satisfying asymptotic boundary conditions. The present method employs inverse interpolation instead of the Newton method to adjust the initial conditions of the related initial-value problem. This eliminates the so-called perturbation equations. The elimination of the perturbation equations not only reduces the user's preliminary work in the application of the method, but also reduces the number of time-consuming initial-value problems to be numerically solved at each iteration. For further ease of application, the solution of the overdetermined system for the unknown initial conditions is obtained automatically by applying Golub's linear least-squares algorithm. The relative ease of application of the proposed numerical method increases directly as the order of the differential-equation system increases. Hence, the method is especially attractive for the solution of large-order systems. After the method is described, it is applied to a fifth-order problem from boundary-layer theory. Good sense is, of all things among men, the most equally distributed; for every one thinks himself so abundantly provided with it, that those even who are the most difficult to satisfy in everything else, do not usually desire a larger measure of this quality than they already possess. And in this it is not likely that all are mistaken the conviction is rather to be held as testifying that the power of judging aright and of distinguishing truth from error, which is properly what is called good sense or reason, is by nature equal in all men; and that the diversity of our opinions, consequently, does not arise from some being endowed with a larger share of reason than others, but solely from this, that we conduct our thoughts along different ways, and do not fix our attention on the same objects. For to be possessed of a vigorous mind is not enough; the prime requisite is rightly to apply it. The greatest minds, as they are capable of the highest excellences, are open likewise to the greatest aberrations; and those who travel very slowly may yet make far greater progress, provided they keep always to the straight road, than those who, while they run, forsake it. This book covers the fundamentals of continuum mechanics, the integral formulation methods of continuum problems, the basic concepts of finite element methods, and the methodologies, formulations, procedures, and applications of various meshless methods. It also provides general and detailed procedures of meshless analysis on elastostatics, elastodynamics, non-local continuum mechanics and plasticity with a large number of numerical examples. Some basic and important mathematical methods are included in the Appendixes. For readers who want to gain knowledge through hands-on experience, the meshless programs for elastostatics and elastodynamics are provided on an included disc. In this paper we present an iterative method for the minimization of the Tikhonov regularization functional in the absence of information about noise. Each algorithm iteration updates both the estimate of the regularization parameter and the Tikhonov solution. In order to reduce the number of iterations, an inexact version of the algorithm is also proposed. In this case the inner Conjugate Gradient (CG) iterations are truncated before convergence. In the numerical experiments the methods are tested on inverse ill posed problems arising both in signal and image processing. The main objective of this work is the practical development of the discontinuous Galerkin method, arguably the most mature high-order discretisation, for the scale resolving simulations of turbomachinery flows. Abstract: "We propose a new parametrized gradient projection algorithm for solving constrained large scale optimization problems and, in particular, discrete optimal control problems with linear constraints. We demonstrate that an appropriate choice of parameters controls the behavior of the proposed algorithm between that of the well-known Frank-Wolfe and Rosen methods. We investigate the identification of those algorithm parameters that result in fast convergence to the solution by allowing many constraints to be added or dropped from the active set at each iteration. We show that an acceleration step based on the Fletcher-Reeves method can be easily added, and numerical results are provided for discrete optimal control problems with a large number (up to 10000) of control variables." An introductory approach to the subject of large strains andlarge displacements in finite elements. Large Strain Finite Element Method: A Practical Course,takes an introductory approach to the subject of large strains andlarge displacements in finite elements and starts from the basicconcepts of finite strain deformability, including finite rotationsand finite displacements. The necessary elements of vector analysisand tensorial calculus on the lines of modern understanding of theconcept of tensor will also be introduced. This book explains how tensors and vectors can be describedusing matrices and also introduces different stress and straintensors. Building on these, step by step finite element techniquesfor both hyper and hypo-elastic approach will be considered. Material models including isotropic, unisotropic, plastic andviscoplastic materials will be independently discussed tofacilitate clarity and ease of learning. Elements of transientdynamics will also be covered and key explicit and iterativesolvers including the direct numerical integration, relaxationtechniques and conjugate gradient method will also be explored. This book contains a large number of easy to followillustrations, examples and source code details that facilitateboth reading and understanding. Takes an introductory approach to the subject of large strainsand large displacements in finite elements. No prior knowledge ofthe subject is required. Discusses computational methods and algorithms to tackle largestrains and teaches the basic knowledge required to be able tocritically gauge the results of computational models. Contains a large number of easy to follow illustrations,examples and source code details. Accompanied by a website hosting code examples. For design purposes one needs to relate the structure of proposed materials to their NLO (nonlinear optical) and other properties, which is a situation where theoretical approaches can be very helpful in providing suggestions for candidate systems that subsequently can be synthesized and studied experimentally. This brief describes the quantum-mechanical treatment of the response to one or more external oscillating electric fields for molecular and macroscopic, crystalline systems. To calculate NLO properties of large systems, a linear scaling generalized elongation method for the efficient and accurate calculation is introduced. The reader should be aware that this treatment is particularly feasible for complicated three-dimensional and/or delocalized systems that are intractable when applied to conventional or other linear scaling methods. A computer program is presented which selects allowed transitions and calculates dipole and quadrupole transition probabilities for transitions with LS coupling and no equivalent electrons, based on an extension of the Coulomb approximation formalism to quadrupole and higher multipole transitions. Absorption oscillator strengths or f-values calculated by (1) the self-consistent-field method, (2) the scaled Thomas-Fermi method, (3) the Coulomb approximation method, (4) the variational method, and (5) the effective charge method for singlet and triplet transitions in neutral helium are presented and compared. The Coulomb approximation f-values calculated with the present computer program are found to be in good agreement with the results obtained by the more sophisticated methods. During the past few years, there has been dramatic progress in theoretical and computational studies of large molecules and local ized states in solids. Various semi-empirical and first-principles methods well known in quantum chemistry have been applied with considerable success to ever larger and more complex molecules, including some of biological importance, as well as to selected solid state problems involving localized electronic states. In creasingly, solid state physicists are adopting a molecular point of view in attempting to understand the nature of electronic states associated with (a) isolated structural and chemical defects in solids; (b) surfaces and interfaces; and (c) bulk disordered solids, most notably amorphous semiconductors. Moreover, many concepts and methods already widely used in solid state physics are being adapted to molecular problems. These adaptations include pseudopotentials, statistical exchange approxi mations, muffin-tin model potentials, and multiple scattering and cellular methods. In addition, many new approaches are being de vised to deal with progressively more complex molecular and local ized electronic state problems. A new method is introduced for determining the electrical and mechanical parameters of large samples of materials in situ. A set of linear electrodes in boreholes forms a square pattern; positive and negative electrical potentials on alternate electrodes create symmetry planes which define several 'cells'; a given fraction of electric current leaves an electrode and reaches a corresponding electrode. It is thus possible to obtain an impedance characteristic for each cell. The situation is basically two-dimensional, so a Schwarz-Christoffel transformation may be used followed with electrical calculations to obtain the conductivity and the permittivity of the cell material. The mechanical parameters of the cells are obtained in a similar manner. A mechanical disturbance is generated in the central borehole and the travel time to the other boreholes is measured along with the attenuation. The mechanical parameters are computed and correlated with the electrical parameters. (Author Modified Abstract). This book describes, in a basic way, the most useful and effective iterative solvers and appropriate preconditioning techniques for some of the most important classes of large and sparse linear systems. The solution of large and sparse linear systems is the most time-consuming part for most of the scientific computing simulations. Indeed, mathematical models become more and more accurate by including a greater volume of data, but this requires the solution of larger and harder algebraic systems. In recent years, research has focused on the efficient solution of large sparse and/or structured systems generated by the discretization of numerical models by using iterative solvers. Answering the need to facilitate quantum-chemical calculations of systems with thousands of atoms, Kazuo Kitaura and his coworkers developed the Fragment Molecular Orbital (FMO) method in 1999. Today, the FMO method can be applied to the study of whole proteins and protein-ligand interactions, and is extremely effective in calculating the propertie This book details the lattice Boltzmann method (LBM) applied to the built environment problems. It provides the fundamental theoretical knowledge and specific implementation methods of LBM from the engineering perspective of the built environment. It covers comprehensive issues of built environment with three detailed cases, solving practical problems. It can be used as a reference book for teachers, students, and engineering technicians to study LBM and conduct architecture and urban wind environments simulations, in the fields of architecture, building technology science, urban planning, HVAC, built environment engineering, and civil engineering. This self-contained treatment offers a systematic development of the theory of iterative methods. Its focal point resides in an analysis of the convergence properties of the successive overrelaxation (SOR) method, as applied to a linear system with a consistently ordered matrix. The text explores the convergence properties of the SOR method and related techniques in terms of the spectral radii of the associated matrices as well as in terms of certain matrix norms. Contents include a review of matrix theory and general properties of iterative methods; SOR method and stationary modified SOR method for consistently ordered matrices; nonstationary methods; generalizations of SOR theory and variants of method; second-degree methods, alternating direction-implicit methods, and a comparison of methods. 1971 edition. This revised edition discusses numerical methods for computing eigenvalues and eigenvectors of large sparse matrices. It provides an in-depth view of the numerical methods that are applicable for solving matrix eigenvalue problems that arise in various engineering and scientific applications. Each chapter was updated by shortening or deleting outdated topics, adding topics of more recent interest, and adapting the Notes and References section. Significant changes have been made to Chapters 6 through 8, which describe algorithms and their implementations and now include topics such as the implicit restart techniques, the Jacobi-Davidson method, and automatic multilevel substructuring. The computer program presented in this report was developed to predict large deflection behavior of three-dimensional truss and frame assemblies. The solutions are obtained by the direct minimization of the total potential energy with respect to the displacement variables rather than by solving nonlinear matrix equations. Sample problems are presented to demonstrate the analysis capability developed. Instructions for the preparation of the input data and the Fortran IV source program listing are included. Good sense is, of all things among men, the most equally distributed; for every one thinks himself so abundantly provided with it, that those even who are the most difficult to satisfy in everything else, do not usually desire a larger measure of this quality than they already possess. And in this it is not likely that all are mistaken the conviction is rather to be held as testifying that the power of judging aright and of distinguishing truth from error, which is properly what is called good sense or reason, is by nature equal in all men; and that the diversity of our opinions, consequently, does not arise from some being endowed with a larger share of reason than others, but solely from this, that we conduct our thoughts along different ways, and do not fix our attention on the same objects. For to be possessed of a vigorous mind is not enough; the prime requisite is rightly to apply it. The greatest minds, as they are capable of the highest excellences, are open likewise to the greatest aberrations; and those who travel very slowly may yet make far greater progress, provided they keep always to the straight road, than those who, while they run, forsake it. Motivation Stochastic Linear Programming with recourse represents one of the more widely applicable models for incorporating uncertainty within in which the SLP optimization models. There are several arenas model is appropriate, and such models have found applications in air line yield management, capacity planning, electric power generation planning, financial planning, logistics, telecommunications network planning, and many more. In some of these applications, modelers represent uncertainty in terms of only a few seenarios and formulate a large scale linear program which is then solved using LP software. However, there are many applications, such as the telecommunications planning problem discussed in this book, where a handful of seenarios do not capture variability well enough to provide a reasonable model of the actual decision-making problem. Problems of this type easily exceed the capabilities of LP software by several orders of magnitude. Their solution requires the use of algorithmic methods that exploit the structure of the SLP model in a manner that will accommodate large scale applications. Mathematics of Computing -- General.

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