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Nota di contenuto

An overview of the techniques in use for solving the coupled equations

of scattering theory -- Weyl's theory for second order differential equations and its application to some problems in quantum chemistry -- The discretization of continuous infinite sets of coupled ordinary linear differential equations: Application to the collision-induced dissociation of a diatomic molecule by an atom -- Extraction of continuum properties from L2 basis set matrix representations of the schrödinger equation: the sturm sequence polynomials and gauss quadrature -- Approximate solution of schrödinger's equation for atoms -- Numerical integration of linear inhomogeneous ordinary differential equations appearing in the nonadiabatic theory of small molecules -- Computation of solenoidal (divergence-free) vector fields -- Efficient solution of a nonlinear heat conduction problem by use of fast elliptic reduction and multigrid methods -- Are the numerical methods and software satisfactory for chemical kinetics? --Optimization of nonlinear kinetic equation computation -- Automatic detection and treatment of oscillatory and/or stiff ordinary differential equations -- Characterization of non-linearly stable implicit Runge-Kutta methods -- Compact deferred correction formulas -- Solving odes in quasi steady state -- A singular perturbations approach to

reduced-order modeling and decoupling for large scale linear systems -- Global codes for BVODEs and their comparison -- Global error estimation in ordinary initial value problems -- Lower bounds for the accuracy of linear multistep methods -- Asymptotic error expansions and discrete newton methods for elliptic boundary value problems --The use of sparse matrix techniques in ode — Codes -- On conjugate gradient methods for large sparse systems of linear equations -- A preconditioned tchebycheff iterative solution method for certain large sparse linear systems with a non-symmetric matrix -- On modified incomplete factorization methods -- Solving large sparse linear systems arising in queuing problems -- Large eigenvalue problems in quantum chemistry -- Variational pseudo-gradient method for determination of m first eigenstates of a large real symmetric matrix --Simultaneous rayleigh-quotient iteration methods for large sparse generalized eigenvalue problems -- Large sparse unsymmetric eigenvalue problems.