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# Abstracts of Papers to Appear in Future Issues

NUMERICAL INTEGRATION OF FUNCTIONS WITH A SHARP PEAK AT OR NEAR ONE BOUNDARY USING MÖBIUS TRANSFORMATIONS. Herbert H. H. Homeier and E. Otto Steinborn, *Universität Regensburg, Regensburg, WEST GERMANY (FRG).*

A class of coordinate transformations depending on a single parameter is studied as quadrature tool. Working rules for the choice of the parameter are proposed. Numerical tests for the method are presented. They show that these coordinate transformations, when combined with Gauss–Legendre quadrature rules, are well suited for the numerical integration of functions possessing a sharp peak *at or near* one boundary of the interval of integration. A method how to combine the transformations with automatic quadrature routines is also proposed; it seems to be useful for the numerical evaluation of integrals with the same kind of integrand behavior.

A VIEW-FACTOR METHOD FOR SOLVING TIME-DEPENDENT RADIATION TRANSPORT PROBLEMS INVOLVING FIXED SURFACES WITH INTERVENING, PARTICIPATING MEDIA. Douglas J. Drake, *KMS Fusion, Inc., Ann Arbor, Michigan, USA.*

A description is given of a view factor technique for solving time-dependent, non-linear radiative transfer problems. It is believed unique among view factor methods in having the ability to solve problems involving gases or plasmas with emissive and absorptive characteristics which vary in space and time. The radiative characteristics of the enclosing surfaces can also have an arbitrary space and time dependence, and these characteristics can be updated based on an appropriate physical model of the interaction of the background radiation field with the medium. Various sample problems are solved, including a time-dependent solution for concentric spheres filled with a participating medium of arbitrary opacity for a step function source.

A FINITE ELEMENT METHOD FOR CAPILLARY SURFACES WITH VOLUME CONSTRAINTS. Ulrich Hornung and Hans D. Mittelmann, *Arizona State University, Tempe, Arizona, USA.*

Capillary surfaces with prescribed volume are determined numerically. The obstacles that confine the given amount of liquid may be planes in space arbitrarily chosen. Parameters of the problem are the Bond number, the contact angle, and the volume. Results for several examples are presented, such as a drop in a corner and on an edge.

VECTORIZATION OF TREE TRAVERSALS. Lars Hernquist, *Princeton University, Princeton, New Jersey, USA.*

A simple method for vectorizing tree searches, which operates by processing all relevant nodes at the same depth in the tree simultaneously, is described. This procedure appears to be general, assuming that gather–scatter operations are vectorizable, but is most efficient if the traversals proceed monotonically from the root to the leaves, or *vice versa.* Particular application is made to the hierarchical tree approach for computing the self-consistent interaction of $N$ bodies. It is demonstrated that full vectorization of the requisite tree searches is feasible, resulting in a factor $\sim$4–5 improvement in cpu efficiency in the traversals on a CRAY X-MP. The overall gain in the case of the Barnes–Hut tree code algorithm is a factor $\sim$2–3, implying a net speedup of $\approx$400–500 on a CRAY X-MP over a VAX 11/780 or a SUN 3/50.



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VECTORIZATION OF A TREECODE. Junichiro Makino, *University of Tokyo, Tokyo, JAPAN.*

Vectorized algorithms for the force calculation and tree construction in the Barnes–Hut tree algorithm are described. The basic idea for the vectorization of the force calculation is to vectorize the tree traversal across particles, so that all particles in the system traverse the tree simultaneously. The tree construction algorithm also makes use of the fact that particles can be treated in parallel. Thus these algorithms take advantage of the internal parallelism in the $N$-body system and the tree algorithm most effectively. As a natural result, these algorithms can be used on a wide range of vector/parallel architectures, including current supercomputers and highly parallel architectures such as the Connection Machine. The vectorized code runs about five times faster than the non-vector code on a Cyber 205 for an $N$-body system with $N = 8192$.

A MODIFIED TREE CODE: DON'T LAUGH; IT RUNS. Joshua E. Barnes, *Princeton University, Princeton, New Jersey, USA.*

I describe a modification of the Barnes–Hut tree algorithm together with a series of numerical tests of this method. The basic idea is to improve the performance of the code on heavily vector-oriented machines such as the Cyber 205 by exploiting the fact that nearby particles tend to have very similar interaction lists. By building an interaction list good everywhere within a cell containing a modest number of particles and reusing this interaction list for each particle in the cell in turn, the balance of computation can be shifted from recursive descent to force summation. Instead of vectorizing tree descent, this scheme simply avoids it in favor of force summation, which is quite easy to vectorize. A welcome side effect of this modification is that the force calculation, which now treats a larger fraction of the local interactions exactly, is significantly more accurate than the unmodified method.

VARIATIONAL CALCULATION OF ELECTROMAGNETIC INSTABILITIES IN TOKAMAKS. X. Garbet, L. Laurent, F. Mourgues, J. P. Roubin, and A. Samain, *Association Euratom-CEA, Saint-Paul-Lez-Durance, FRANCE.*

A variational method is presented in order to determine and to study linear microinstabilities in tokamaks. Exploiting the existence of a system of action and angular variables for trapped and circulating particles, a functional, extremum in the turbulent electromagnetic field, is analytically established and implemented in the code TORRID. The coupling of poloidal harmonics due to toroidal effects is investigated within the frame of a WKB formalism whose zeroth order is equivalent to the ballooning analysis. The essential features of the code TORRID are described. Curvature effects on ionic mode profiles and stability thresholds are presented as an example of application.

A CONVERGENCE-IMPROVING ITERATIVE METHOD FOR COMPUTING PERIODIC ORBITS NEAR BIFURCATION POINTS. Michael N. Vrahatis and Tassos Bountis, *University of Patras, GREECE.*

The accurate computation of periodic orbits and the precise knowledge of their bifurcation properties are very important for studying the behavior of many dynamical systems of physical interest. In this paper, we present an iterative method for computing periodic orbits, which has the advantage of improving the convergence of previous Newton-like schemes, especially near bifurcation points. This method is illustrated here on a conservative, nonlinear Mathieu equation, for which a sequence of period-doubling bifurcations is followed, long enough to obtain accurate estimates of the two *universal scaling* constants $\alpha$, $\beta$, as well as the *universal rate* $\delta$, by which the bifurcation values of a parameter $q = q_k$, $k = 1, 2, 3, \ldots$, tend to their limiting value, $q_\infty < \infty$, as $k$ increases.

A PARTICLE METHOD FOR COLLISIONAL KINETIC EQUATIONS. I. BASIC THEORY AND ONE-DIMENSIONAL RESULTS. G. Russo, *Courant Institute of Mathematical Sciences, New York University, New York, New York, USA.*

A new method is introduced for describing the collisional term in the framework of a particle scheme. The equations of motion of the particles contain an additional term which takes into account the collisions. Numerical techniques are shown to compute this extra term and to solve the equations. Exact results concerning stability and consistency of the schemes for the diffusion equation are derived. Some numerical results for the one-dimensional case are reported.

DYNAMICS OF SHEAR FLOW OF A NON-NEWTONIAN FLUID. David S. Malkus, John A. Nohel, and Bradley J. Plohr, *University of Wisconsin, Madison, Wisconsin, USA.*

Viscoelastic materials with fading memory, e.g., polymers, suspensions, and emulsions, exhibit behavior that is intermediate between the nonlinear hyperbolic response of purely elastic materials and the strongly diffusive, parabolic response of viscous fluids. Many popular numerical methods used in the computation of steady viscoelastic flows fail in important flow regimes, and thus do not capture significant non-Newtonian phenomena. A key to satisfactory explanation of these phenomena is the study of the full dynamics of the flow. This paper studies the dynamics of shear flow, presenting a description of non-Newtonian phenomena caused by a non-monotone relation between the steady shear stress and shear strain rate. Analytical results for such phenomena are surveyed, and three distinct numerical methods are developed to accurately compute the dynamics. The computations reproduce experimental measurements of non-Newtonian "spurt" in shearing flow through a slit die. They also predict related phenomena (such as hysteresis and shape memory); experiments are suggested to verify these predictions.

SYMBOLIC COMPUTATION AND AUTOMATIC FORTRAN CODE GENERATION FOR EIGENVALUE DETERMINATION BY PHASE INTEGRAL METHOD. Jussi Luppi and Petri Pajunen, *University of Helsinki, Helsinki, FINLAND.*

An automatic FORTRAN code generation and determination of energy eigenvalues for periodic potentials with wells and barriers are presented. These problems serve as test cases in developing tools and techniques for generation of numerically efficient FORTRAN software and for more general, efficient, and flexible ways of programming. Several problems in different areas of science are described, and the advantages of the approach as well as limitations of the tools presently available are discussed.

COMPUTATION OF ZERO $\beta$ THREE-DIMENSIONAL EQUILIBRIA WITH MAGNETIC ISLANDS. A. H. Reiman, *Princeton University, Princeton, New Jersey, USA*; H. S. Greenside, *Duke University, Durham, North Carolina, USA.*

A Picard iteration scheme has been implemented for the computation of toroidal, fully three-dimensional, zero $\beta$ equilibria with islands and stochastic regions. Representation of the variables in appropriate coordinate systems has been found to be a key to making the scheme work well. In particular, different coordinate systems are used for solving magnetic differential equations and Ampere's law. The current profile is adjusted when islands and stochastic regions appear. An underrelaxation of the current profile modifications is generally needed for stable iteration of the algorithm. Some examples of equilibrium calculations are presented.

PERTURBATIVE SOLUTIONS OF QUANTUM MECHANICAL PROBLEMS BY SYMBOLIC COMPUTATION. T. C. Scott, R. A. Moore, G. J. Fee, M. B. Monagan, and E. R. Vrscay, *University of Waterloo, Waterloo, Ontario, CANADA.*

Symbolic computation provides excellent tools for solving quantum mechanical problems by perturbation theory. The techniques presented herein avoid the use of an infinite basis set and some of the complications of degenerate perturbation theory. The algorithms are expressed in the Maple symbolic computation system and are solved for both the eigenfunctions and eigenenergies as power series in the order parameter. Further, each coefficient of the perturbation series is obtained in closed form. In particular, this paper examines the application of these techniques to R. A. Moore's method for solving the radial Dirac equation. One is confident that the techniques presented will also be useful in other applications.

NUMERICAL COMPUTATION OF THE INCOMPLETE LIPSCHITZ–HANKEL INTEGRAL $Je_0(a, z)$. Stevel L. Dvorak and Edward F. Kuester, *University of Colorado, Boulder, Colorado, USA.*

Two factorial Neumann series expansions are derived for the incomplete Lipschitz–Hankel integral $Je_0(a, z)$. These expansions are used together with the Neumann series expansion, given by Agrest, in an algorithm which efficiently computes $Je_0(a, z)$ to a user defined number of significant digits. Other expansions for $Je_0(a, z)$, which are found in the literature, are also discussed, but these expansions are found to offer no significant computational advantages when compared with the expansions used in the algorithm.

IMPROVED RADIAL DIFFERENCING FOR THREE-DIMENSIONAL MAGNETOHYDRODYNAMIC EQUILIBRIUM CALCULATIONS. S. P. Hirshman, *Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA*; U. Schwenn and J. Nuhrenberg, *Max-Planck Institut für Plasmaphysik, Garching bei München, WEST GERMANY (FRG).*

Several numerical schemes are described for accurately discretizing the radial dependence of the magnetohydrodynamic (MHD) energy of a toroidal plasma configuration. Compared with previous schemes, the new methods have significantly improved mesh convergence properties for the energy, magnetic axis, and other equilibrium parameters. This has favorable implications for both stability analysis, where small numerical errors in the energy may significantly affect the computation of marginal points and transport applications, for which equilibrium computations on coarse meshes are desirable.

## NOTES TO APPEAR

ON THE VALIDITY OF VORTEX-TANGLE SIMULATIONS OF HOMOGENEOUS SUPERFLUID TURBULENCE. K. W. Schwarz, *IBM Research, T. J. Watson Research Center, Yorktown Heights, New York, USA.*

VORTEX-TANGLE SIMULATIONS. Thomas F. Buttke, *Princeton University, Princeton, New Jersey, USA.*