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Abstracts of Papers to Appear in Future Issues

THE ARC TAN/TAN AND KEPLER–BURGER MAPPINGS FOR PERIODIC SOLUTIONS WITH A SHOCK, FRONT, OR INTERNAL BOUNDARY LAYER. John P. Boyd. *Department of Atmospheric, Oceanic, Space Science and Laboratory for Scientific Computation, 2200 Bonisteel Boulevard, Ann Arbor, Michigan 48109, USA.*

Many periodic solutions have internal regions of rapid change—internal boundary layers. Shock waves and geophysical fronts are one class of examples. A second class is composed of functions which decay rapidly away from a central peak or peaks. Spherical harmonics, Mathieu eigenfunctions, prolate spheroidal wave functions, and geophysical Hough functions may all be locally approximated by Hermite functions (in the appropriate parameter range) and decay exponentially fast outside a narrow subinterval. Similarly, the large amplitude cnoidal waves of the Korteweg–DeVries equation are narrow, isolated peaks which are well approximated by the $\text{sech}^2(y)$ form of the solitary wave. In this article, we show that a change-of-coordinate is a powerful tool for resolving such internal boundary layers. In the first part, we develop a general theory of mappings for the spherical harmonic/cnoidal wave class of examples, which decay rapidly away towards the edges of the spatial period. The particular map $y = \text{arc tan}(L \tan(x))$ is a particularly effective choice. Four numerical examples show that this map and the Fourier pseudospectral method are a good team. In the second part, we generalize the earlier theory to describe mappings which asymptote to a constant but non-zero resolution at the ends of the periodicity interval. We explain why the "Kepler–Burger" mapping is particularly suitable for shock and fronts.

NUMERICAL COMPUTATION OF 2D SOMMERFELD INTEGRALS—DECOMPOSITION OF THE ANGULAR INTEGRAL. Steven L. Dvorak. *Electromagnetics Laboratory, Department of Electrical and Computer Engineering, University of Arizona, Tucson, Arizona 85721, USA*; Edward F. Kuester. *Electromagnetics Laboratory, Department of Electrical and Computer Engineering, Campus Box 425, University of Colorado, Boulder, Colorado 80309, USA.*

Spectral domain techniques are frequently used in conjunction with Galerkin's method to obtain the current distribution on planar structures. When this technique is employed, a large percentage of the computation time is spent filling the impedance matrix. Therefore, it is important to develop accurate and efficient numerical techniques for the computation of the impedance elements, which can be written as two-dimensional (2D) Sommerfeld integrals. Once the current distribution has been found, then the near-zone electric field distribution can be obtained by computing another set of 2D Sommerfeld integrals. The computational efficiency of the 2D Sommerfeld integrals can be improved in two ways. The first method, which is discussed in this paper, involves finding a new way to compute the inner angular integral in the polar representation of these integrals. It turns out that the angular integral can be decomposed into a finite number of incomplete Lipschitz–Hankel integrals, which in turn can be calculated using series expansions. Therefore, the angular integral can be computed by summing a series instead of applying a standard numerical integration algorithm. This new technique is found to be more accurate and efficient when piecewise-sinusoidal basis functions are used to analyze a printed strip dipole antenna in a layered medium. The incomplete Lipschitz–Hankel integral representation for the angular integral is then used in another paper to develop a novel asymptotic extraction technique for the outer semi-infinite integral.

NUMERICAL COMPUTATION OF 2D SOMMERFELD INTEGRALS—A NOVEL ASYMPTOTIC EXTRACTION TECHNIQUE. Steven L. Dvorak. *Electromagnetics Laboratory, Department of Electrical and Computer Engineering, University of Arizona, Tucson, Arizona 85721, USA*; Edward F. Kuester. *Electromagnetics Laboratory, Department of Electrical and Computer Engineering, Campus Box 425, University of Colorado, Boulder, Colorado 80309, USA.*

The accurate and efficient computation of the elements in the impedance matrix is a crucial step in the application of Galerkin's method to the analysis of planar structures. As was demonstrated in a previous paper, it is possible to decompose the angular integral, in the polar representation for the 2D Sommerfeld integrals, in terms of incomplete Lipschitz–Hankel integrals (ILHIs) when piecewise sinusoidal basis functions are employed. Since Bessel series expansions can be used to compute these ILHIs, a numerical integration of the inner angular integral is not required. This technique provides an efficient method for the computation of the inner angular integral; however, the outer semi-infinite integral still converges very slowly when a real axis integration is applied. Therefore, it is very difficult to compute the impedance elements accurately and efficiently. In this paper, it is shown that this problem can be overcome by using the ILHI representation for the angular integral to develop a novel asymptotic extraction technique for the outer semi-infinite integral. The usefulness of this asymptotic extraction technique is demonstrated by applying it to the analysis of a printed strip dipole antenna in a layered medium.

LOCATING THREE-DIMENSIONAL ROOTS BY A BISECTION METHOD. John M. Greene. *General Atomics, San Diego, California 92186-9784, USA.*

The evaluation of roots of equations is a problem of perennial interest. Bisection methods have advantages since the volume in which the root is known to be located can be steadily decreased. This method depends on the existence of a criterion for determining whether a root exists within a given volume. Here topological degree theory is exploited to provide this criterion. Only three-dimensional volumes are considered here. The result is of some use in locating roots and in illustrating the theory. The classification of roots as X-points or O-points and the generalization to three dimensions are also discussed.

CRYSTAL GROWTH AND DENDRITIC SOLIDIFICATION. James A. Sethian. *Department of Mathematics, University of California, Berkeley, California 94720, USA*; John Strain. *Courant Institute of Mathematical Sciences, New York University, 251 Mercer Street, New York, New York 10012, USA.*

We present a numerical method which computes the motion of complex solid/liquid boundaries in crystal growth. The model we solve includes physical effects such as crystalline anisotropy, surface tension, molecular

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kinetics, and undercooling. The method is based on two ideas. First, the equations of motion are recast as a single history-dependent boundary integral equation on the solid/liquid boundary. A fast algorithm is used to solve the integral equation efficiently. Second, the boundary is moved by solving a "Hamilton–Jacobi"-type equation (on a *fixed* domain) formulated by Osher and Sethian for a function in which the boundary is a particular level set. This equation is solved by finite difference schemes borrowed from the technology of hyperbolic conservation laws. The two ideas are combined by constructing a smooth extension of the normal velocity off the moving boundary, in a way suggested by the physics of the problem. Our numerical experiments show the evolution of complex crystalline shapes, development of large spikes and corners, dendrite formation and side-branching, and pieces of solid merging and breaking off freely.

AN EVALUATION OF THE SNIFFER GLOBAL OPTIMIZATION ALGORITHM USING STANDARD TEST FUNCTIONS. Roger A. R. Butler and Edward E. Slaminka. *Mathematics Department, Auburn University, Auburn, Alabama 36849-5310, USA.*

The performance of Sniffer—a new global optimization algorithm—is compared with that of Simulated Annealing. Using the number of function evaluations as a measure of efficiency, the new algorithm is shown to be significantly better at finding the global minimum of seven standard test functions. Several of the test functions used have many local minima and very steep walls surrounding the global minimum. Such functions are intended to thwart global minimization algorithms.

ORTHOGONAL MAPPING IN TWO DIMENSIONS. Ramani Duraiswami and Andrea Prosperetti. *Department of Mechanical Engineering, 127 Latrobe Hall, The Johns Hopkins University, Baltimore, Maryland 21218, USA.*

A method for the generation of orthogonal boundary-fitted curvilinear coordinates for arbitrary simply- and doubly-connected domains is developed on the basis of the theory of quasi-conformal mappings of quadrilaterals and of previous work by Ryskin and Leal. The method has useful applications in orthogonal grid generation in two-dimensional and axi-symmetric domains and in the extension of rapid elliptic solvers and spectral methods to complex geometries. A new technique for the calculation of the conformal module of quadrilaterals is also presented.

NUMERICAL INTEGRATION FOR POLYATOMIC SYSTEMS. G. te Velde and E. J. Baerends. *Afdeling Theoretische Chemie, Scheikundig Laboratorium der Vrije Universiteit, De Boelelaan 1083, 1081 HV Amsterdam, The Netherlands.*

A numerical integration package is presented for three-dimensional integrals occurring in electronic structure calculations, applicable to all polyatomic systems with periodicity in 0 (molecules), 1 (chains), 2 (slabs), or 3 dimensions (crystals). The scheme is cellular in nature, based on Gaussian product formulas and it makes use of the geometrical symmetry. Convergence of accuracy with the number of points is rapid and use of the program has been made easy.

A NUMERICAL METHOD FOR SOLVING SYSTEMS OF LINEAR ORDINARY DIFFERENTIAL EQUATIONS WITH RAPIDLY OSCILLATING SOLUTIONS. Ira B. Bernstein. *Department of Applied Physics, Yale University, Yale Station, New Haven, Connecticut 06520-2159, USA, and Center for Solar and Space Research, Yale University, P.O. Box 6666, New Haven, Connecticut 06511-6666, USA*; Leigh Brookshaw. *Department of Applied Physics, Yale University, Yale Station, New Haven, Connecticut 06520-2159, USA*; Peter A. Fox. *Center for Solar and Space Research, Yale University, P.O. Box 6666, New Haven, Connecticut 06511-6666, USA.*

A numerical method is presented which allows the accurate and efficient solution of systems of linear equations of the form $dz_i(x)/dx = \sum_{j=1}^{N} A_{ij}(x)\, z_j(x)$, $i = 1, 2, ..., N$, when the solutions vary rapidly compared with the $A_{ij}(x)$. The method consists of numerically developing a set of basis solutions characterized by new dependent variables which are slowly varying. These solutions can be accurately computed with an overhead that is substantially independent of the smallness of the scale length characterizing the solutions. Examples are given.

THE ASYMPTOTIC DIFFUSION LIMIT OF A LINEAR DISCONTINUOUS DISCRETIZATION OF A TWO-DIMENSIONAL LINEAR TRANSPORT EQUATION. Christoph Börgers. *Department of Mathematics, University of Michigan, Ann Arbor, Michigan 48109, USA*; Edward W. Larsen. *Department of Nuclear Engineering, University of Michigan, Ann Arbor, Michigan 48109, USA*; Marvin L. Adams. *Lawrence Livermore National Laboratory, University of California, Livermore, California 94550, USA.*

Consider a linear transport problem, and let the mean free path and the absorption cross section be of size ε. It is well known that one obtains a diffusion problem as ε tends to zero. We discretize the transport problem on a fixed mesh, independent of ε, consider again the limit $\varepsilon \to 0$, and ask whether one obtains an accurate discretization of the continuous diffusion problem. The answer is known to be affirmative for the linear discontinuous Galerkin finite element discretization in one space dimension. In this paper, we ask whether the same result holds in two space dimensions. We consider a linear discontinuous discretization based on rectangular meshes. Our main result is that the asymptotic limit of this discrete problem is *not* a discretization of the asymptotic limit of the continuous problem and thus that the discretization will be inaccurate in the asymptotic regime under consideration. We also propose a modified scheme which has the correct asymptotic behavior for spatially periodic problems, although not always for problems with boundaries. We present numerical results confirming our formal asymptotic analysis.

HYDRODYNAMIC MODELING OF PARTICLE AND ANGULAR MOMENTUM TRANSPORT IN ROTATING TOKAMAK PLASMAS WITH IMPURITIES. R. Zanino. *Energetics Department, Polytechnic Institute of Turin, Italy.*

We have developed a 1 + 1 D time dependent code for the description of ion-impurity transport in a rotating tokamak plasma, using a pseudo-spectral discretization in the poloidal angle θ and a staggered finite difference mesh in the minor radius r. The plasma is assumed to have a constant uniform temperature T, to be in the high collisionality (Pfirsch–Schlüter) regime, and to contain electrons "e," fuel ions "i," and a single impurity species "Z" of charge eZ, where e is the proton charge. We are particularly interested in the case when: (1) flow velocities in the toroidal (symmetry) direction ϕ are in the range typical of neutral beam injection experiments, i.e., $v_{thZ} < V_{\phi i,Z} \lesssim v_{thi}$, ($v_{thj} \equiv \sqrt{2T/m_j}$ is the thermal speed, m_j is the mass); (2) the relative concentration of impurities in the plasma, $\bar{n}_Z/\bar{n}_i$, is significant and comparable to that observed in present tokamaks, i.e., $\sqrt{m_e/m_i} \ll \bar{n}_Z Z^2/\bar{n}_i \approx 1$ in order of magnitude. The model fluid equations are obtained via a moment approach, and an expansion in powers of the small ordering parameter $\delta_{pi} \equiv (m_i v_{thi}/e\mathbf{B}_\theta)((1/\bar{n}_i)\,|\partial \bar{n}_i/\partial r|) \ll 1$ ($\mathbf{B}$ is the magnetic field) is then employed. The equations at each order in δ_{pi} up to the second are solved, and the characteristic features of the results presented: to lowest order, outboard impurity peaking on each magnetic surface appears due to centrifugal forces; to first order, radial gradients driven ion-impurity friction gives rise to up–down asymmetries in