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Abstracts of Papers to Appear in Future Issues

LOCALIZATION SCHEMES IN 2D BOUNDARY-FITTED GRIDS. Thomas Westermann. *Kernforschungszentrum Karlsruhe GmbH, Abteilung für Numerische Physik, HDI-3, P.O. Box 3640, 7500 Karlsruhe, Germany.*

A discussion of localization schemes in two-dimensional structured grids consisting of convex four-point meshes is presented. These algorithms are applicable to particle-in-cell codes based on two-dimensional boundary-fitted coordinates in order to localize particles inside the grid. They are fully vectorizable and two of them are directly applicable also to triangular meshes. Since all of them are exact, they avoid an overhead for a special treatment of particles near the boundary as is necessary for the approximate localization proposed by Seldner and Westermann (*J. Comput. Phys.* **79** (1988)). Hence, they are suitable for complicated geometries with outer and inner curved boundaries. Depending on the vector computer used, a speedup of 3.5 to 8 is achieved for the fastest algorithm.

A COMPARISON OF PARTICLE-IN-CELL AND FOKKER–PLANCK METHODS AS APPLIED TO THE MODELING OF AUXILIARY-HEATED MIRROR PLASMAS. Richard J. Procassini. *Electronics Research Laboratory, University of California, Berkeley, California 94720, USA*; Bruce I. Cohen. *Magnetic Fusion Energy Program, Lawrence Livermore National Laboratory, Livermore, California 94550, USA.*

The transport and confinement of charged particles in an auxiliary-heated mirror plasma is modeled via two diverse computational tools: an implicit particle-in-cell (PIC) code and a bounce-averaged Fokker–Planck (F-P) code. The results from the PIC simulation are benchmarked against those obtained via use of F-P techniques, which has been the preferred means of analyzing plasma confinement and transport in mirror devices. The computer time required by each code to solve a specific test problem is presented, along with an itemization of the cost of the major processes involved in each method of solution. A qualitative discussion of the advantages and disadvantages of each code is also included.

NUMERICAL MODELING OF MACRO AND MICRO BEHAVIORS OF MATERIALS IN PROCESSING: A REVIEW. A. A. Tseng and J. Zou. *Department of Mechanical Engineering and Mechanics, Drexel University, Philadelphia, Pennsylvania 19104, USA*; H. P. Wang. *General Electric R & D, Schenectady, New York 12301, USA*; S. R. H. Hoole. *Harvey Mudd College, Claremont, California 91711, USA.*

Numerical techniques used for modeling the macroscopic and microscopic behavior of materials in processing are reviewed. The macromodels are based on the concept of a material continuum for which the densities of mass, momentum, and energy exist in the mathematical sense of the continuum and the microstructure of matter can be ignored. The micromodels, on the other hand, are based on the concepts of micromechanics and statistics applied to the study of the microstructure of the material. In this paper, formulation of the partial differential equations that govern the macroscopic behavior of materials resulting from the material continuum assumption is first presented. The relevant numerical techniques for solving these equations and for handling the associated boundary conditions are then discussed. As a demonstration, a continuous drawing process is modeled to illustrate the procedure involved and the information revealed. In microscopic modeling, the numerical and statistical techniques used to simulate the microstructure formation of materials are reviewed. Examples applied to solidification and recrystallization as well as defect formation are then presented. Finally, following an examination of the approaches that incorporate the microscopic models into the macroscopic models, recommendations on the future development are given.

A NUMERICAL SOLUTION METHOD FOR BOUNDARY VALUE PROBLEMS CONTAINING AN UNDETERMINED PARAMETER. P. A. Ramachandran. *Department of Chemical Engineering, Chemical Reaction Engineering Laboratory, Box 1198, Washington University, St. Louis, Missouri 63130, USA.*

A number of physical problems can be described by a complex differential equation with an undetermined coefficient appearing as an explicit term. The problem is usually encountered in diffusion-reaction systems and in these cases the unknown parameter is the gradient at the diffusing interface. The problem is stiff and difficult to solve. This paper describes a new method for the solution of such problems. The procedure is based on the boundary integral element concepts where both the dependent variable and its gradient become the primary variables. This permits a direct iterative solution to this problem. Numerical studies presented here show that the proposed solution method is very accurate and rapidly convergent. Two case studies involving gas absorption with chemical reaction are also presented.

ABSORBING BOUNDARY CONDITIONS FOR ACOUSTIC AND ELASTIC WAVES IN STRATIFIED MEDIA. Robert L. Higdon. *Department of Mathematics, Oregon State University, Corvallis, Oregon 97331, USA.*

Absorbing boundary conditions are needed for computing numerical models of wave motions in unbounded spatial domains. Prior progress on this problem for acoustic and elastic waves has generally been concerned with waves propagating through uniform media. The present paper is concerned with waves in stratified media, which are of interest, for example, in geophysical problems. Suppose that the medium consists of homogeneous layers separated by parallel horizontal interfaces, and suppose that absorbing boundary conditions are needed along a vertical computational boundary. The boundary conditions that are described in this paper are based on a quantity known as the "ray parameter." According to Snell's law, this parameter remains the same when a plane wave propagates through a stratified medium and undergoes reflection, refraction, and, in the case of elastic waves, conversion. One can therefore use the same absorbing boundary conditions in all layers. For acoustic waves, the absorption properties are the same in all layers. For elastic waves, the absorption properties vary somewhat from one layer to another; however, one still obtains good absorption in all layers, even in the presence of strong contrasts between layers. The boundary conditions are also effective in

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absorbing Rayleigh waves, which propagate along free surfaces of elastic media. The boundary formulas developed here can be applied without modification to problems in both two and three dimensions.

A Comparative Study of Advanced Shock-Capturing Schemes Applied to Burgers' Equation. H. Q. Yang and A. J. Przekwas. *CFD Research Corporation, 3325-D Triana Boulevard, Huntsville, Alabama 35805, USA.*

In recent years, a number of new shock-capturing finite difference schemes, often called high resolution schemes, have been proposed. We have considered several variations of the TVD and FCT schemes and geometrical approaches such as MUSCL, ENO, and PPM. Included is an organized overview and classification of the schemes. Only essential features are described, and numerical implementation is discussed. Much of the mathematical theory is omitted, but a key source reference list is provided. In this paper we present a comparative study of these schemes applied to the Burgers' equation. The objective is to assess their performance for problems involving formation and propagation of shocks, shock collisions, and expansion of discontinuities.

Absorbing Boundary Conditions, Difference Operators, and Stability. R. A. Renaut. *Arizona State University, Tempe, Arizona 85287-1804, USA.*

In this paper we present a review of some of the methods currently used for solving the absorbing boundary problem for the two-dimensional scalar wave equation. We show the relationship between the methods of Lindman and Clayton and Engquist. Through this relationship we can derive discretizations of any rational approximation to the one-way wave equation. We prove that, for all the cases considered here, which can be solved in a manner similar to Lindman's approach, the bounds imposed on the Courant number for stability at the boundary are no more severe than the bound $1/\sqrt{2}$ required for stability of the interior scheme. These bounds are, however, necessary but not sufficient. We also compare the methods reviewed numerically. It is demonstrated that Lindman's scheme is no better than a sixth-order approximation of Halpern and Trefethen. For low-order approximations, Higdon's one-dimensional equations are satisfactory, but as the order increases the two-dimensional form of the equations, as derived by Halpern and Trefethen, is preferable.

A Combined Spectral-Finite Element Method for Solving Two-Dimensional Unsteady Navier–Stokes Equations. Ben-yu Guo and Wei-ming Cao. *Shanghai University of Science and Technology, Shanghai, China.*

In this paper, a combined Fourier spectral-finite element method is proposed for solving two-dimensional, semi-periodic, unsteady Navier–Stokes equations. The convergence is proved and the numerical results are presented.

A Finite Difference Procedure for a Class of Free Boundary Problems. Bengt Fornberg. *Corporate Research, Exxon Research and Engineering Company, Annandale, New Jersey 08801, USA*; and Rita Meyer-Spasche. *Max-Planck-Institute for Plasma Physics, IPP-EURATOM Association, D-W-8046 Garching, Germany.*

Finite difference schemes loose accuracy when free boundaries cross over rectangular grids. For a class of second-order equations, the leading error term at such a boundary can be eliminated by a simple correction strategy. This procedure works in any number of space dimensions and offers an alternative to (more costly and complicated) adaptive grid techniques.

Orthogonal Grid Generation in a 2D Domain via the Boundary Integral Technique. I. S. Kang. *Chemical Engineering Department, POSTECH, P.O. Box 125, Pohang, 790 Korea*; L. G. Leal. *Department of Chemical and Nuclear Engineering, University of California, Santa Barbara, Santa Barbara, California 93106, USA.*

A new numerical scheme is proposed for the generation of an orthogonal coordinate grid in an arbitrary simply connected two-dimensional domain. The scheme is robust and noniterative and is based on the conjunction of the familiar boundary integral technique with the covariant Laplace equation method for mapping. In the proposed scheme, two types of problems are considered: (1) Boundary correspondence is specified on two adjacent sides of the boundary, or (2) The distortion factor is specified in the product form $f(\xi, \eta) = \Pi(\xi)\, \Theta(\eta)$.

Global and Local Remeshing Algorithms for Compressible Flows. C. J. Hwang and S. J. Wu. *Institute of Aeronautics and Astronautics, National Cheng Kung University, Tainan, Taiwan, Republic of China.*

A new adaptive remeshing approach for unstructured meshes, which includes the error indicator, global, and local mesh regeneration techniques, has been developed in this paper. In this approach, nodes are first distributed according to the remeshing parameters, and those nodes are connected into a complete mesh. The concepts of side-based and vertex-based fronts are introduced to achieve the triangulation. According to the CPU time and the versatility, the vertex-based triangulation technique is proved to be more efficient. By using vertex-based triangulation approach, a local remeshing method, which regenerates only some regions of the flow domain, is presented. To demonstrate the reliability and availability of the proposed procedure, several compressible flow problems are investigated. The regular/stretched triangles and the mixed type of triangular and quadrilateral stretched elements are used. In this work, the Euler equations are solved by the multistep Runge–Kutta Galerkin finite element methods. From the numerical results, the approaches, which employ the directionally stretched elements, are effective and suitable for treating the flow problems with one-dimensional features. The development of the local remeshing algorithm for unsteady flows is worthwhile and important.

Spectral Methods in Time for a Class of Parabolic Partial Differential Equations. Glenn Ierley, Brian Spencer, and Rodney Worthing. *Department of Mathematical Sciences, Michigan Technological University, Houghton, Michigan 49931, USA.*

In this paper, we introduce a fully spectral solution for the partial differential equation $u_t + uu_x + vu_{xx} + \mu u_{xxx} + \lambda u_{xxxx} = 0$. For periodic boundary conditions in space, the use of a Fourier expansion in x admits of a particularly efficient algorithm with respect to expansion of the time dependence in a Chebyshev series. Boundary conditions other than periodic may still be treated with reasonable, though lesser, efficiency. For all cases, very high accuracy is attainable at moderate computational cost relative to the expense of variable order finite difference methods in time.

Time Domain Numerical Calculations of Unsteady Vortical Flows about a Flat Plate Airfoil. S. I. Hariharan and Yu Ping. *Department of Mathematical Sciences, University of Akron, Akron, Ohio 44325 USA*; J. R. Scott. *NASA Lewis Research Center, Cleveland, Ohio 44135, USA.*

A time domain numerical scheme is developed to solve for the unsteady flow about a flat plate airfoil due to imposed upstream, small amplitude, transverse velocity perturbations. The governing equation for the resulting unsteady potential is a homogeneous, constant coefficient, convective wave