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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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