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Abstracts of Papers to Appear in Future Issues

CALCULATING COMPLEX INTERACTIONS IN MOLECULAR DYNAMICS SIMULATIONS EMPLOYING LAGRANGIAN PARTICLE TRACKING SCHEMES. J. H. Dunn and S. G. Lambrakos. *Naval Research Laboratory, Washington, DC 20375-5000, U.S.A.*

In this report, we describe some general features of Lagrangian particle tracking and the method of table look-up that are important for calculating many different types of interactions of arbitrary complexity in large molecular dynamics simulations. Based on our experience using these approaches and state-of-the-art of computer technology, we state formally those properties of Lagrangian tracking and table look-up that are important to the design of optimal programming structures. We examine the relationship between Lagrangian indexing and list indexing of data and how this influences the complexity of programming structures for effecting vector operations. Included in this report are criteria for the efficient use of Lagrangian particle tracking schemes in molecular dynamics simulations.

FLUX-CORRECTED TRANSPORT IN A MOVING GRID. Kambiz Salari. *Ecodynamics Research Associates, Inc., P.O. Box 8172, Albuquerque, New Mexico 87198, U.S.A.*; Stanly Steinberg. *Department of Mathematics and Statistics, University of New Mexico, Albuquerque, New Mexico 87131, U.S.A.*

A flux-corrected transport algorithm in moving grids is developed and applied to transport problems involving solution adapted grids. The success of the algorithm is demonstrated numerically, as are certain limitations.

A SYNOPSIS OF MONTE CARLO PERTURBATION ALGORITHMS. Herbert Rief. *Commission of the European Communities, Ispra Establishment, I-21020 Ispra (Va), Italy.*

Fundamental aspects of correlated sampling and differential operator procedures applied to integrals and systems of linear equations modelling Markov processes are investigated. Algorithms providing sensitivities (gradients, Jacobians) and perturbation estimates obtained by a single simulation experiment are described in detail and explained by examples. Mathematical proofs are provided which show that under most conditions a finite relative variance can be obtained for arbitrarily small parameter variations.

A DIVERGENCE-FREE SPECTRAL EXPANSIONS METHOD FOR THREE-DIMENSIONAL FLOWS IN SPHERICAL-GAP GEOMETRIES. Guy Dumas and Anthony Leonard. *Graduate Aeronautical Laboratories, California Institute of Technology, Pasadena, California 91125, U.S.A.*

A spectral method for the solution of the incompressible Navier–Stokes equations in spherical-gap geometries is presented. The method uses divergence-free vector expansions which inherently satisfy the boundary conditions. Basis and test functions are constructed from Chebyshev polynomials and vector spherical harmonics (VSH) yielding a Petrov–Galerkin weighted-residual method that produces spectral convergence. No rotational nor equatorial symmetry of the flow field is simplicity imposed. The approach makes extensive use of the convenient properties of the VSH which are presented in a computationally suitable form whenever possible. The alias-free implementation of the method rests upon a standard, explicit–implicit time-integration technique. A VSH-Chebyshev vector transform with two "fast directions" is also developed and briefly presented. Several test cases are used to validate the resulting initial-boundary-value code. Axisymmetric, basic spherical Couette flow computations are compared with available numerical results while a three-dimensional spiral Taylor–Görtler vortex flow simulation is tested against experimental measurements. Very good agreement is found in all cases.

ACCURATE ONE-DIMENSIONAL COMPUTATION OF FRONTAL PHENOMENA BY PLIM. Markku Rajamäki and Mika Saarinen. *Nuclear Engineering Laboratory, Technical Research Centre of Finland, P.O. Box 208, 02151 Espoo, Finland.*

We introduce a new method for solving systems of one-dimensional hyperbolic partial differential equations and present the first applications of this method. The piecewise linear interpolation method PLIM is shown to have the capability to preserve the shape of a propagating distribution and great applicability. Various difficult flow problems, such as the strong convection problem, the convection–diffusion problem, and the reaction–diffusion problem, have been solved. In addition, the approximate hyperbolic equations technique to handle the diffusion terms is introduced.

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