

Abstracts of Papers to Appear

FAST EVALUATION OF TRANSIENT WAVE FIELDS USING DIAGONAL TRANSLATION OPERATORS. A. Arif Ergin,* Balasubramaniam Shanker,† and Eric Michielssen‡. *Center for Computational Electromagnetics, Department of Electrical and Computer Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801.* E-mail: *aergin@decwa.ece.uiuc.edu, †shanker@socrates.ece.uiuc.edu, and ‡michiels@decwa.ece.uiuc.edu.

This paper presents novel plane wave time domain (PWTd) algorithms which accelerate the computational analysis of transient surface scattering phenomena. The proposed PWTd algorithms permit the fast evaluation of transient fields satisfying the wave equation. The cost associated with the computation of fields at N_s observers produced by a surface bound source density represented in terms of N_s spatial samples for N_t time steps scales as $O(N_t N_s^2)$ if classical time domain integral-equation-based methods are used. It is shown that this cost can be reduced to $O(N_t N_s^{4/3} \log N_s)$ and $O(N_t N_s \log N_s)$ using two-level and multilevel PWTd schemes, respectively. These algorithms are the time domain counterparts of frequency domain fast multipole methods and make feasible the practical broadband analysis of scattering from large and complex bodies.

VLASOV SIMULATIONS USING VELOCITY-SCALED HERMITE REPRESENTATIONS. Joseph W. Schumer* and James Paul Holloway†. *Code 6770, *Naval Research Laboratory, Washington, DC 20375*; †2943 *Cooley Building, Nuclear Engineering and Radiological Sciences, 2355 Bonisteel Boulevard, University of Michigan, Ann Arbor, Michigan 48109-2104.* E-mail: schumer@calvin.nrl.navy.mil and hagar@engin.umich.edu.

The efficiency, accuracy, and stability of two different pseudo-spectral methods using scaled Hermite basis and weight functions, applied to the nonlinear Vlasov–Poisson equations in one dimension (1d-1v), are explored and compared. A variable velocity scale U is introduced into the Hermite basis and is shown to yield orders of magnitude reduction in errors, as compared to linear kinetic theory, with no increase in workload. A set of Fourier–Hermite coefficients, representing a periodic Gaussian distribution function, are advanced through time with an $O(\Delta t^2)$ -accurate splitting method. Within this splitting scheme, the advection and acceleration terms of the Vlasov equation are solved separately using an $O(\Delta t^4)$ -accurate Runge–Kutta method. The asymmetrically weighted (AW) Hermite basis, which has been used previously by many authors, conserves particles and momentum exactly and total energy to $O(\Delta t^3)$; however, the AW Hermite method does *not* conserve the square integral of the distribution and is, in fact, numerically unstable. The symmetrically weighted (SW) Hermite algorithm, applied here to the Vlasov system for the first time, can either conserve particles and energy (for N_u even) or momentum (for N_u odd) as $\Delta t \rightarrow 0$, where N_u is the largest Hermite mode number. The SW Hermite method conserves the square integral of the distribution and, therefore, remains numerically stable. In addition, careful velocity scaling improves the conservation properties of the SW Hermite method. Damping and growth rates, oscillation frequencies, E-field saturation levels, and phase-space evolution are seen to be qualitatively correct during simulations. Relative errors with respect to linear Landau damping and linear bump-on-tail instability are shown to be less than 1% using only 64 velocity-scaled Hermite functions. Comparisons to particle-in-cell (PIC) simulations show that as the number of particles increases to more than 10^6 , the PIC solutions converge to scaled SW Hermite solutions that were found in only 1/10 of the run-time. The SW Hermite method with velocity scaling is well-suited to kinetic simulations of warm plasmas.

MONTE CARLO CONFIGURATION INTERACTION. J. C. Greer. *National Microelectronics Research Centre, University College, Lee Maltings, Prospect Row, Cork, Ireland.* E-mail: Jim.Greer@computer.org.

A procedure for solving quantum many-body problems is presented and is shown to have properties which make it well suited for parallel computer architectures. The underlying method is an application of the linear variational principle using many-body expansion functions and is known as the configuration interaction or superposition of configurations method. By repeatedly generating expansion vectors using a Monte Carlo technique for configuration generation, a sequential improvement in the variational energy can be achieved. By performing independent samples of the expansion space concurrently on different processors, the results may be combined after a variational calculation to form an improved expansion vector. This sequence of steps is repeated until a desired level of convergence in the wavefunctions or energies is achieved. Analysis of the method is given within a parallel environment: efficiency, scaling, and a two-tiered approach to parallelism with the algorithm are discussed.

DATA ASSIMILATION IN A WAVE EQUATION: A VARIATIONAL REPRESENTER APPROACH FOR THE GRENOBLE TIDAL MODEL. F. H. Lyard. *Proudman Oceanographic Laboratory, Bidston Observatory, Birkenhead, Merseyside L43 7RA, United Kingdom.*

We propose in this paper a synthesis of both the hydrodynamic and assimilation aspects of the quasi-linearized tidal model developed by the Grenoble tidal group. Starting from the hydrodynamic model, which is represented by a linearized wave equation, we emphasize the different steps taken to lead to the final finite-element discrete system of the coupled hydrodynamic and assimilation problem. As the hydrodynamic formulation has been already detailed in many previous publications, we insist especially on the formulation of the assimilation part. The assimilation is based on a general inverse method using an L_2 norm-type cost function, weighted by the use of inverse error covariance operators. The full implications of choosing this kind of cost function are discussed. The least-square problem thus defined is developed by using the representer approach. The representers are a finite set of functions defined on the modeling domain. The solution is sought as a perturbation of the solution to the prior model and it is shown that this perturbation belongs to the vector subspace of finite dimension generated by the representers (i.e., it is a linear combination of the representers). The assimilation problem then involves first solving two systems, called backward and forward systems, to determine the representers. An alternative formulation of the boundary conditions associated with the forward system is developed, as the original one is somewhat unsuited to the finite-element discretization. The three resulting systems are solved under a variational formulation identical to the one of the hydrodynamic problem. Discretization of the assimilation problem, which is entirely described in the general continuous case, is performed as a last step, consistent with that of the hydrodynamic problem. Finally, the coefficients of the linear combination giving the model perturbation are obtained by solving a $K \times K$ system. As an illustration, we propose a realistic application performed on the M_2 tidal elevation problem in the South Atlantic by assimilating tidal gauge data in a solution of the Grenoble model.

AN ADAPTIVE, CARTESIAN, FRONT-TRACKING METHOD FOR THE MOTION, DEFORMATION AND ADHESION OF CIRCULATING CELLS. G. Agresar,* J. J. Linderman,† G. Tryggvason,‡ and K. G. Powell§. **Departments of Microbiology and Immunology and Biomedical Engineering;* †*Department of Chemical Engineering;* ‡*Department of Mechanical Engineering and Applied Mechanics;* and §*Department of Aerospace Engineering, The University of Michigan, Ann Arbor, Michigan 48109.* E-mail: *agresar@engin.umich.edu, †linderma@engin.umich.edu, ‡gretar@engin.umich.edu, and §powell@engin.umich.edu.

Cells in circulatory systems adhere through a competition between molecular interactions and colloidal repulsion, while the cells arbitrarily deform in the presence of external fluid forces. The complex coupling of the forces involved, the disparate length scales at which they, act and uncertainties in the mechanics of cell deformation have complicated the study of cell adhesion. To address these difficulties, a multi-fluid, front-tracking method with staggered, adaptively refined meshes has been developed. As a tool to study cell mechanics, the program allows the incorporation and testing of different mechanical models of the cell without significant changes in the setup. As a tool to study cell adhesion, the method models the coupling of the relevant forces resolving the disparate length scales involved. The method was validated by simulating various test cases, and the results were found to agree well with analytical and other numerical solutions. The capabilities of the method are demonstrated with the simulation of a common cell-mechanics experiment (a micropipet assay) and a common physiological situation for cell adhesion (the adhesion of two cells under shear flow).