

Abstracts of Papers to Appear

LARGE-WAVE SIMULATION (LWS) OF FREE-SURFACE FLOWS DEVELOPING WEAK SPILLING BREAKING WAVES.

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A methodology, called large-wave simulation (LWS), for the numerical simulation of free-surface flows past the appearance of spilling breakers is presented. LWS is designed to resolve only the large, energy-carrying scales of the flow and model the effect of the subgrid, small-wavelength scales of the flow spectrum. This part of the spectrum includes the characteristic frothy whitecaps associated with spilling breakers. Modeling in LWS is based on the consistent application of spatial filtering on both the velocity field and the free-surface elevation. The subgrid scale (SGS) effect is modeled by two sets of stresses: (i) the eddy SGS stresses, which are identical to those arising in large-eddy-simulation (LES) of flows without a free surface, and (ii) the wave SGS stresses, which incorporate the free-surface effect. Both SGS stresses are modeled by eddy-viscosity models with constant coefficients. The methodology is applied on two free-surface flows: (i) the interaction of a plane gravity wave with a surface wake layer, and (ii) the nonlinear evolution of a surface shear layer instability. *A priori* and *a posteriori* tests show good agreement between the proposed model and actual SGS stresses, while LWS of both flows successfully continue past the breaking point as opposed to corresponding direct numerical simulations. For the first flow, LWS predicts the post-breaking appearance of a recirculating flow region in the wake of the breaker in qualitative agreement with experimental observations.

INHERENTLY ENERGY CONSERVING TIME FINITE ELEMENTS FOR CLASSICAL MECHANICS. P. Betsch and P.

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In this paper, we develop a finite element method for the temporal discretization of the equations of motion. The continuous Galerkin method is based upon a weighted-residual statement of Hamilton's canonical equations. We show that the proposed finite element formulation is energy conserving in a natural sense. A family of implicit one-step algorithms is generated by specifying the polynomial approximation in conjunction with the quadrature formula used for the evaluation of time integrals. The numerical implementation of linear, quadratic, and cubic time finite elements is treated in detail for the model problem of a circular pendulum. In addition to that, concerning dynamical systems with several degrees of freedom, we address the design of nonstandard quadrature rules which retain the energy conservation property. Our numerical investigations assess the effect of numerical quadrature in time on the accuracy and energy conservation property of the time-stepping schemes.

A DISCRETIZATION SCHEME FOR AN EXTENDED DRIFT-DIFFUSION MODEL INCLUDING TRAP-ASSISTED PHENOMENA. F. Bosisio, S. Micheletti, and R. Sacco. Dipartimento di Matematica, "F. Brioschi," Politecnico di

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An extended drift-diffusion model to account for the kinetics of electrons trapped in defect states within a semiconductor material is considered. A discretization scheme based on Newton-Krylov iterations and mixed finite volumes is then proposed and applied to the model, even in the presence of Schottky contacts (i.e., Robin-type boundary conditions). Numerical results concerning the simulation of an electro-optical device under several working conditions are finally presented.

GENERALIZED DISCRETE SPHERICAL HARMONIC TRANSFORMS. Paul N. Swarztrauber and William F. Spitz.
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Two generalizations of the spherical harmonic transforms are provided. First, they are generalized to an arbitrary distribution of latitudinal points θ_i . This unifies transforms for Gaussian and equally spaced distributions and provides transforms for other distributions commonly used to model geophysical phenomena. The discrete associated Legendre functions $\bar{P}_n^m(\theta_i)$ are shown to be orthogonal, to within roundoff error, with respect to a weighted inner product, thus providing the forward transform to spectral space. Second, the representation of the transforms is also generalized to rotations of the discrete basis set $\bar{P}_n^m(\theta_i)$. A discrete function basis is defined that provides an alternative to $\bar{P}_n^m(\theta_i)$. On a grid with N latitudes, the new basis requires $O(N^2)$ memory compared to the usual $O(N^3)$. The resulting transforms differ in spectral space but provide identical results for certain applications. For example, a forward transform followed immediately by a backward transform projects the original discrete function in a manner identical to the existing transforms. Namely, they both project the original function onto the same smooth least-squares approximation without the high frequencies induced by the closeness of the points in the neighborhood of the poles. Finally, a faster projection is developed based on the new transforms.

LEVEL SET BASED DEFORMATION METHODS FOR ADAPTIVE GRIDS. Guojun Liao,* Feng Liu,† Gary C. de la Pena,* Danping Perg,‡ and Stanley Osher.§ **Department of Mathematics, University of Texas, Arlington, Texas 76019-0408*; †*Department of Mechanical and Aerospace Engineering, University of California—Irvine, Irvine, California 92027*; ‡*Barra, Inc., Berkeley, California 94704*; and §*Department of Mathematics, University of California—Los Angeles, Los Angeles, California 90095-1555*. E-mail: liao@uta.edu, fliu@uci.eng.edu, delapena@math.uta.edu, danpingpeng@barra.com, sjo@math.ucla.edu.

A new method for generating adaptive moving grids is formulated based on physical quantities. Level set functions are used to construct the adaptive grids, which are solutions of the standard level set evolution equation with the Cartesian coordinates as initial values. The intersection points of the level sets of the evolving functions form a new grid at each time. The velocity vector in the evolution equation is chosen according to a monitor function and is equal to the node velocity. A uniform grid is then deformed to a moving grid with desired cell volume distribution at each time. The method achieves precise control over the Jacobian determinant of the grid mapping as the traditional deformation method does. The new method is consistent with the level set approach to dynamic moving interface problems.