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Abstracts of Papers to Appear in Future Issues

DISCRETE TRANSPARENT BOUNDARY CONDITIONS FOR SCHRÖDINGER-TYPE EQUATIONS. Frank Schmidt* and David Yevick.† **Konrad-Zuse-Zentrum für Informationstechnik Berlin, D-14195 Berlin-Dahlem, Germany; †Queen's University, Department of Electrical Engineering, Kingston, Ontario, Canada K7L 3N6.*

We present a general technique for constructing nonlocal transparent boundary conditions for one-dimensional Schrödinger-type equations. Our method supplies boundary conditions for the θ-family of implicit one-step discretizations of Schrödinger's equation in time. The use of Mikusiński's operator approach in time avoids direct and inverse transforms between time and frequency domains and thus implements the boundary conditions in a direct manner.

SOLITON ANALYSIS IN COMPLEX MOLECULAR SYSTEMS: A ZIG-ZAG CHAIN. P. L. Christiansen,* A. V. Savin,† and A. V. Zolotaryuk.‡ **Institute of Mathematical Modelling, Technical University of Denmark, DK-2800 Lyngby, Denmark; †Institute for Problems of Physics and Technology, 119034 Moscow, Russia; ‡Bogolyubov Institute for Theoretical Physics, 252143 Kyiv, Ukraine.*

A simple numerical method for seeking *solitary wave* solutions of a permanent profile in molecular systems of big complexity is presented. The method is essentially based on the minimization of a finite-dimensional function which is chosen under an appropriate discretization of time derivatives in equations of motion. In the present paper, it is applied to a zig-zag chain backbone of coupled particles, each of which has *two* degrees of freedom (longitudinal and transverse). Both topological and nontopological soliton solutions are treated for this chain when it is (i) subjected to a two-dimensional periodic substrate potential or (ii) considered as an isolated object, respectively. In the first case, which may be considered as a zig-zag generalization of the Frenkel–Kontorova chain model, two types of kink solutions with different topological charges, describing vacancies of one or two atoms (I- or II-kinks) and defects with excess one or two atoms in the chain (I- or II-antikinks), have been found. The second case (isolated chain) is a generalization of the well-known Fermi–Pasta–Ulam chain model, which takes into account transverse degrees of freedom of the chain molecules. Two types of stable nontopological soliton solutions which describe either (i) a supersonic solitary wave of longitudinal stretching accompanied by transverse slendering or (ii) supersonic pulses of longitudinal compression propagating together with localized transverse thickening (bulge) have been obtained.

BGK-BASED SCHEME FOR MULTICOMPONENT FLOW CALCULATIONS. Kun Xu. *Mathematics Department, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong.*

This paper concerns the extension of the gas-kinetic BGK-type scheme to multicomponent flow calculations. In this new scheme, each component satisfies its individual gas-kinetic BGK equation and the equilibrium states for each component are coupled in space and time to have common temperature and velocity. The particle diffusion in gas mixtures is included naturally in the gas-kinetic model. The current scheme could handle strong shocks and be oscillation-free through the material interface. The scheme guarantees the exact mass conservation for each component and the exact conservation of total momentum and energy in the whole particle system. As a special application, the current scheme is applied to gas vacuum interaction case, where the mass densities for other components are set to zero in the whole domain. The extension of the current approach to three dimensions is straightforward. With the definition of $\varphi = \rho^{(1)} - \rho^{(2)}$ in the two-component gas flow, similar to the level set method we can follow explicitly the time evolution of the material interface ($\varphi = 0$). The numerical results confirm the accuracy and robustness of the BGK-type scheme.

INTEGRAL EQUATION METHOD FOR THE CONTINUOUS SPECTRUM RADIAL SCHRÖDINGER EQUATION. R. A. Gonzales,* J. Eisert,† I. Koltracht,* M. Neumann,* and G. Rawitscher.† **Department of Mathematics, †Department of Physics, University of Connecticut, Storrs, Connecticut 06269-3046.*

A new approach to the numerical solution of boundary value problems for differential equations, which originated in recent papers by Greengard and Rokhlin, is improved and adapted to the numerical solution of the radial Schrödinger equation. The approach is based on the conversion of the differential equation into an integral equation, together with the application of a spectral type Clenshaw–Curtis quadrature method. Through numerical examples, the integral equation method is shown to be superior to finite difference methods.

PDF MODEL CALCULATIONS OF COMPRESSIBLE TURBULENT FLOWS USING SMOOTHED PARTICLE HYDRODYNAMICS. Walter C. Welton and Stephen B. Pope. *Department of Mechanical & Aerospace Engineering, Cornell University, 139 Upson Hall, Ithaca, New York 14850.*

A particle method which applies the probability density function (PDF) method to compressible turbulent flows is presented. Solution of the PDF equation is achieved using a Lagrangian/Monte Carlo approach. A unique feature of the method is its ability to calculate the mean pressure gradient directly from the particles using a grid-free approach. This is accomplished by applying techniques borrowed from the field of smoothed particle hydrodynamics. Furthermore, these techniques have been implemented using a recently discovered algorithm which greatly reduces the computational work in 1D. The particle method also incorporates a variance-

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reduction technique which can significantly reduce statistical error in first and second moments of selected mean flow quantities. When combined with a second-order accurate predictor/corrector scheme, the resulting particle method provides a feasible way to obtain accurate PDF solutions to compressible turbulent flow problems. Results have been obtained for a variety of quasi-1D flows to demonstrate the method's robustness. These include solutions to both statistically stationary and nonstationary problems and to use both periodic and characteristic-based inflow/outflow boundary conditions. Convergence of the method with respect to four different kinds of numerical errors has also been studied. Detailed results are presented which confirm the expected convergence behavior of each error.