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Abstracts of Papers to Appear

Dissipative or Conservative Finite-Difference Schemes for Complex-Valued Nonlinear Partial Differential Equations. Takayasu Matsuo* and Daisuke Furihata.† *Department of Computational Science & Engineering, Graduate School of Engineering, Nagoya University, Nagoya, 464-8603, Japan; and †Research Institute for Mathematical Sciences, Kyoto University, Kyoto, 606-8502, Japan.

We propose a new procedure for designing finite-difference schemes that inherit energy conservation or dissipation property from complex-valued nonlinear partial differential equations (PDEs), such as the nonlinear Schrödinger equation, the Ginzburg–Landau equation, and the Newell–Whitehead equation. The procedure is a complex version of the procedure that Furihata has recently presented for real-valued nonlinear PDEs. Furthermore, we show that the proposed procedure can be modified for designing "linearly implicit" finite-difference schemes that inherit energy conservation or dissipation property.

An Efficient Numerical Method for Studying Interfacial Motion in Two-Dimensional Creeping Flows. M. C. A. Kropinski. Department of Mathematics and Statistics, Simon Fraser University, Burnaby, British Columbia, Canada V5A 1S6.

We present new methods for computing the motion of two-dimensional closed interfaces in a slow viscous flow. The interfacial velocity is found through the solution to an integral equation whose analytic formulation is based on complex-variable theory for the biharmonic equation. The numerical methods for solving the integral equations are spectrally accurate and employ a fast multipole-based iterative solution procedure, which requires only $O(N)$ operations where N is the number of nodes in the discretization of the interface. The interface is described spectrally, and we use evolution equations that preserve equal spacing in arclength of the marker points. A small-scale decomposition is performed to extract the dominant term in the evolution of the interface, and we show that this dominant term leads to a CFL-type stability constraint. When in an equal arclength frame, this term is linear and we show that implicit time-integration schemes that are explicit in Fourier space can be formulated. We verify this analysis through several numerical examples.

Exact Monte Carlo Perturbation Analysis by Forward-Adjoint Coupling in Radiation Transport Calculations. Taro Ueki* and J. Eduard Hoogenboom.† *3-44-1-13 Chiharadai, Ichihara, Chiba 290-0158 Japan; †Interfaculty Reactor Institute, Delft University of Technology, Mekelweg 15, 2629 JB Delft, The Netherlands.

An exact perturbation analysis method in Monte Carlo radiation transport calculations is investigated utilizing the coupling of forward and adjoint simulations. The vehicle chosen for this investigation is correlated-coupling for time-independent neutron or photon transport problems, which has been applied to material perturbation isolated from both the source and detector. By initiating forward and adjoint simulation histories (trajectories) in opposite directions at a position sampled from the interface between the perturbed and unperturbed materials, the correlated-coupling can exclusively construct the physical particle histories traversing the perturbed material. In other words, only those histories that have influence on the variation of the detector response are simulated. There exists no approximation in the sense that all the higher order perturbed terms in the response variation are kept. Moreover, the statistical error is estimated in the same way as in the confidence interval estimation in a standard forward or adjoint calculation. The theoretical basis lies in response decomposition with an enclosure containing both the source and detector. Numerical results are shown for multi-energy group problems.

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A Dual-Reciprocity Boundary Element Method for Evaluating Bulk Convective Transport of Surfactant in Free-Surface Flows. Samir N. Ghadiali,* David Halpern,† and Donald P. Gaver III.* *Department of Biomedical Engineering, Tulane University, New Orleans, Louisiana 70118; and †Department of Mathematics, University of Alabama, Tuscaloosa, Alabama 35487.

We present a dual-reciprocity boundary element method (DRBEM) to investigate bulk surfactant transport dynamics in a free-surface flow system under steady-state conditions. This free-surface flow system consists of semi-infinite bubble progression in a rigid axisymmetric capillary tube. Once adsorbed to the air–liquid interface with a surface concentration Γ, surfactant alters the interfacial surface tension γ. As the interfacial stress balance, which governs the fluid mechanics, is a function of γ, a strong coupling exists between surfactant transport dynamics and the fluid mechanics (physicochemical hydrodynamics). To model this problem over a range of bulk concentrations, C, the bulk convective/diffusive transport of surfactant to the interface must be calculated. In this paper, DRBEM is used to simulate the bulk convection–diffusion relationship while the boundary element method (BEM) is used to solve Stokes flow, and a finite-difference method is used to solve the surface transport equation under steady-state conditions. A nonlinear Langmuir adsorption model is used to determine the surfactant equation of state $\gamma = f(\Gamma)$. The validity of the DRBEM is first demonstrated by comparing computational and analytical solutions for a test problem. Next, the computational algorithm is used to calculate the bulk concentration field surrounding the bubble as a function of the far-downstream quantity of surfactant, C_o, and its influence on interfacial dynamics. These profiles clearly demonstrate the importance of accurately calculating the bulk concentration field under moderate C_o conditions. In addition, the variation of mechanical properties of this system as a function of C_o indicates that the interfacial pressure jump can be significantly larger when the bulk transport of surfactant to the interface is limited.

High Accuracy Iterative Solution of Convection Diffusion Equation with Boundary Layers on Nonuniform Grids. Lixin Ge and Jun Zhang. Department of Computer Science, University of Kentucky, 773 Anderson Hall, Lexington, Kentucky 40506-0046.

A fourth-order compact finite difference scheme and a multigrid method are employed to solve the two-dimensional convection diffusion equations with boundary layers. The computational domain is first discretized on a nonuniform (stretched) grid to resolve the boundary layers. A grid transformation technique is used to map the nonuniform grid to a uniform one. The fourth-order compact scheme is applied to the transformed uniform grid. A multigrid method is used to solve the resulting linear system. Numerical experiments are used to show that a graded mesh and a grid transformation are necessary to compute high accuracy solutions for the convection diffusion problems with boundary layers and dicretized by the fourth-order compact scheme.