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Abstracts of Papers to Appear in Future Issues

NUMERICAL CONSIDERATIONS IN THE COMPUTATION OF THE ELECTROSTATIC FREE ENERGY OF INTERACTION WITHIN THE POISSON–BOLTZMANN Theory Alexandru M. Micu,*,† Babak Bagheri,‡ Andrew V. Ilin,† L. Ridgway Scott,‡,† and B. Montgomery Pettitt,*,† **Department of Chemistry, †Texas Center for Advanced Molecular Computation, ‡Department of Mathematics, University of Houston, Houston, Texas 77204*

We evaluate two different ways of calculating the contribution of the electrostatic stress to the free energy integral based on Sharp and Hönig's method within the finite difference nonlinear Poisson–Boltzmann equation method with the University of Houston Brownian Dynamics program. We show that only one of these approaches gives consistent results in the limit of zero ionic concentration for interactions of the order of magnitude of the hydrogen bond. The results are compared with results from both the linear Poisson–Boltzmann equation and the Debye–Hückel theory, for ion concentrations within the limits of validity of these approximate methods. We demonstrate this by application to DNA molecules.

LATTICE BOLTZMANN METHOD ON CURVILINEAR COORDINATES SYSTEM: FLOW AROUND A CIRCULAR CYLINDER, Xiaoyi He,*,† and Gary Doolen,† **Center for Nonlinear Studies, MS-B258, †Complex Systems, Group T-13, MS-B213, Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545*

Using an interpolation-based strategy, the lattice Boltzmann method is extended to apply to general curvilinear coordinate systems. As an example, a cylindrical coordinate system is used to simulate two-dimensional flow around a circular cylinder. Numerical simulations are carried out for impulsive initial conditions with Reynolds numbers up to 10^{14}. The agreement of our results with previous computational and experimental results is satisfactory. Compared with previous lattice Boltzmann simulations of the same problem, our new approach greatly enhances the computational efficiency.

SIMULATION OF FLUIDIZED BEDS WITH LATTICE GAS CELLULAR AUTOMATA, B. G. M. van Wachem,* A. F. Bakker,† J. C. Schouten,* M. W. Heemels,† and S. W. de Leeuw,† **Chemical Reactor Engineering Section, Department of Chemical Process Technology, †Physics Informatics Section, Computational Physics, Faculty of Applied Physics, Delft University of Technology, The Netherlands*

This paper introduces an approach for the simulation of the hydrodynamic behaviour of gas–solid fluidized beds via the use of lattice gas cellular automata. This approach is based on a two-speed model, developed by U. Frisch, B. Hasslacher, and Y. Pomeau. Simulation runs for different configurations of the automaton produce results that can be compared to actual data. The simulations show when and how bubbling will occur. Values for the bubble diameters as a function of bed height, as well as bed porosities in two horizontal planes have been obtained from the simulations. From these results correlation diagrams and the Kolmogorov entropy are calculated. Generally, the results of the simulations are qualitatively in good agreement with experimental observations, showing that this new approach could provide a useful tool in predicting the fluid dynamic behaviour of fluidized beds.

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