Journal of Computational Physics **154,** 528–529 (1999)
Article ID jcph.1999.6352, available online at http://www.idealibrary.com on IDEAL®

Abstracts of Papers to Appear

AN ACCURATE CURVED BOUNDARY TREATMENT IN THE LATTICE BOLTZMANN METHOD. Renwei Mei,* Li-Shi Luo,† and Wei Shyy.* *_Department of Aerospace Engineering, Mechanics, and Engineering Science, University of Florida, Gainesville, Florida 32611-6250; and †ICASE, NASA Langley Research Center, Hampton, Virginia 23681-2199._ E-mail: rwm@aero.ufl.edu, wss@tiger.aero.ufl.edu, luo@icase.edu.

The lattice Boltzmann equation (LBE) is an alternative kinetic method capable of solving hydrodynamics for various systems. Major advantages of the method are owing to the fact that the solution for the particle distribution functions is explicit, easy to implement, and natural to parallelize. Because the method often uses uniform regular Cartesian lattices in space, curved boundaries are often approximated by a series of stairs that leads to reduction in computational accuracy. In this work, a second-order accurate treatment of boundary condition in the LBE method is developed for a curved boundary. The proposed treatment of the curved boundaries is an improvement of a scheme due to Filippova and Hänel [*J. Comp. Phys.* **143**, 426 (1998)]. The proposed treatment for curved boundaries is tested against several flow problems: 2-D channel flows with constant and oscillating pressure gradients for which analytic solutions are known, flow due to an impulsively started wall, lid-driven square cavity flow, and uniform flow over a column of circular cylinders. The second-order accuracy is observed with solid boundary arbitrarily placed between lattice nodes. The proposed boundary condition has well-behaved stability characteristics when the relaxation time is close to $1/2$, the zero limit of viscosity. The improvement can make a substantial contribution toward simulating practical fluid flow problems using the lattice Boltzmann method.

SIMULATIONS OF PARTICLE DYNAMICS IN MAGNETORHEOLOGICAL FLUIDS. H. V. Ly,* F. Reitich,† M. R. Jolly,‡ H. T. Banks,* and K. Ito.* *_Center for Research in Scientific Computation, North Carolina State University, Raleigh, North Carolina 27695-8205; †School of Mathematics, University of Minnesota, Minneapolis, Minnesota 55455; and ‡Material Division, Lord Corporation, 110 Lord Drive, Cary, North Carolina 27511._

We present particle dynamics simulations for the response of magnetorheological (MR) fluids upon application of a magnetic field. The particles' motion is considered to be governed by magnetic, hydrodynamic, and repulsive interactions. Fluid–particle interactions are accounted for via Stokes' drag while interparticle repulsions are modeled through approximate hard-sphere rejections. In accordance with their greater significance, on the other hand, (linear) magnetic interactions are fully simulated. The time evolution is considered to be magnetically quasi-static, and magnetostatic forces are derived from the solution of (steady) Maxwell's equations, recomputed at each instant in time. For this we use a potential theoretic formulation where the boundary integral equations are solved with a fast multipole approach. We show that the resulting numerical codes can be effectively used to study a number of experimental observables such as effective magnetic permeabilities and response timescales which are of crucial importance in the design of MR fluids.

A NEW DISCRETE VELOCITY METHOD FOR NAVIER–STOKES EQUATIONS. Michael Junk* and S. V. Raghurama Rao.† *_Fachbereich Mathematik, Universität Kaiserslautern, D-67663 Kaiserslautern, Germany; and †Institut für Techno- und Wirtschaftsmathematik, Erwin-Schrödinger-Straße, Kaiserslautern, D-67663 Kaiserslautern, Germany._ E-mail: junk@mathematik.uni-kl.de, raghu@itwm.uni-kl.de.

The relation between the lattice Boltzmann method, which has recently become popular, and the kinetic schemes, which are routinely used in computational fluid dynamics, is explored. A new discrete velocity method for the numerical solution of Navier–Stokes equations for incompressible fluid flow is presented by combining both the

0021-9991/99 $30.00

approaches. The new scheme can be interpreted as a pseudo-compressibility method, and for a particular choice of parameters, this interpretation carries over to the lattice Boltzmann method.

POSITIVITY OF FLUX VECTOR SPLITTING SCHEMES. Jérémie Gressier, Philippe Villedieu, and Jean-Marc Moschetta. *École Nationale Supérieure de l'Aéronautique et de l'Espace, ONERA BP 4025, 31055 Toulouse Cedex 4, France.* E-mail: gressier@onecert.fr, villedieu@onecert.fr, moscheta@supaero.fr.

Over the past ten years, robustness of schemes has raised an increasing interest among the CFD community. One mathematical aspect of scheme robustness is the positivity preserving property. At high Mach numbers, solving the conservative Euler equations can lead to negative densities or internal energy. Some schemes such as the flux-vector splitting (FVS) schemes are known to avoid this drawback. In this study, a general method is detailed to analyze the positivity of FVS schemes. As an application, three classical FVS schemes (Van Leer's, Hänel's variant, and Steger and Warming's) are proved to be positively conservative under a CFL-like condition. Finally, it is proved that for any FVS scheme, there is an intrinsic incompatibility between the desirable property of positivity and the exact resolution of contact discontinuities.

EFFICIENT AND RAPID EVALUATION OF THREE-CENTER TWO-ELECTRON COULOMB AND HYBRID INTEGRALS USING NONLINEAR TRANSFORMATIONS. H. Safouhi and P. E. Hoggan. *Ensemble Scientifique des Cézeaux, SEESIB, UMR 6504, 63177 Aubière Cedex, France.* E-mail: safouhi@chisg1.univ-bpclermont.fr.

Among the two-electron integrals occuring in the molecular context, the three-center Coulomb and hybrid integrals are numerous and difficult to evaluate to high accuracy. The analytical and numerical difficulties arise mainly from the presence of the spherical Bessel function and hypergeometric series in these integrals. The present work pursues the acceleration of convergence for three-center two-electron Coulomb and hybrid integrals. We have proven that the hypergeometric function can be expressed as a finite expansion, and that the integrand involving this series and a product of Bessel functions satisfies a linear differential equation with coefficients having a power series expansion in the reciprocal of the variable suitable for application of the nonlinear D and $\bar{D}$ transformations. These transformations depend strongly on the order of the differential equation that the integrand of interest satisfies. This work concentrates on reduction of this order to two, exploiting properties of spherical and reduced Bessel functions, leading to greatly simplified calculations to evaluate the integrals precisely by reducing the order of linear systems to be solved. It also avoids the long and difficult implementations of successive derivatives of the integrands. The numerical results section illustrates clearly the reduction of the calculation time we obtained for a high predetermined accuracy.