8th. World Congress on Computational Mechanics (WCCM8)
5th European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2008)
June 30 –July 5, 2008
Venice, Italy

A quadrature based moment approach for multi-component fluid mixtures using Boltzmann equations

*** Prakash Vedula**[1]

[1] School of Aerospace and Mechanical Engineering
University of Oklahoma, Norman OK 73019, USA
E-mail: pvedula@ou.edu

Key Words: *Multiphysics Problems, Applications, Computing Methods.*

ABSTRACT

The transport of mass and momentum among multiple species in a fluid mixture is important in a variety of applications in chemical process industries, gas turbine engines and micro-electro-mechanical fluid systems. Analysis of fluid mixtures using continuum approaches, based on Navier-Stokes equations, can be quite challenging due to the the lack of appropriate constitutive models for momentum transfer between the components of a mixture. An alternative approach based on kinetic theory can be used to provide a statistical description of macroscopic system properties using knowledge of microscopic dynamics involving particle or molecular motions. Macroscopic system properties of fluid mixtures can be obtained from the single particle distribution functions $f_i \equiv f_i(\mathbf{x}, \mathbf{v}_i, t)$, which correspond to the probability of locating a molecule of i^{th} species in six dimensional phase space $(\mathbf{x}, \mathbf{v}_i)$ at time t. The evolution of these distribution functions is given by the following Boltzmann equations [1],

$$\partial_t f_i + \mathbf{v}_i \cdot \partial_{\mathbf{x}} f_i + \mathbf{F}_i \cdot \partial_{\mathbf{v}_i} f_i = \sum_j \frac{1}{m_j} \int_{\mathbb{R}^3} \int_{\mathbb{R}^2} \left(f_i(\mathbf{v}'_i) f_j(\mathbf{v}'_{j*}) - f_i(\mathbf{v}_i) f_j(\mathbf{v}_{j*}) \right) \, B_{ij} \, d\sigma \, d\mathbf{v}_{j*} \quad (1)$$

where $\mathbf{F}_i$ denotes the external force per unit mass acting on a molecule of i^{th} species (with mass m_i) and the right hand side represents the collision operator, to account for the contribution due to collisions. The collision term involves pre-collision velocities ($\mathbf{v}_i$, $\mathbf{v}_{j*}$), post-collision velocities ($\mathbf{v}'_i$, $\mathbf{v}'_{j*}$) and the differential collision cross-section (related to B_{ij}). The set of equations in Eq. (1) constitutes a coupled system of nonlinear integro-differential equations, for which numerical solutions are difficult to obtain.

Our objective through this work is to propose an efficient numerical approach for the solution of this set of equations (Eq. (1)), capable of describing highly non-equilibrium behavior. The latter applicability to non-equilibrium flows attempts to partially overcome the limitations of several approaches in the literature (like Grad's moment approach [2]) that are restrictive due their assumption of a known form of the equilibrium (Maxwellian) distribution. We propose the use of a quadrature-based method, known as the direct quadrature method of moments (DQMOM) [3], for solving Boltzmann equations. It was previously shown that DQMOM leads to an efficient Eulerian implementation for multi-phase flow predictions involving polydispersity, aggregation and breakage [3]. Using DQMOM the velocity

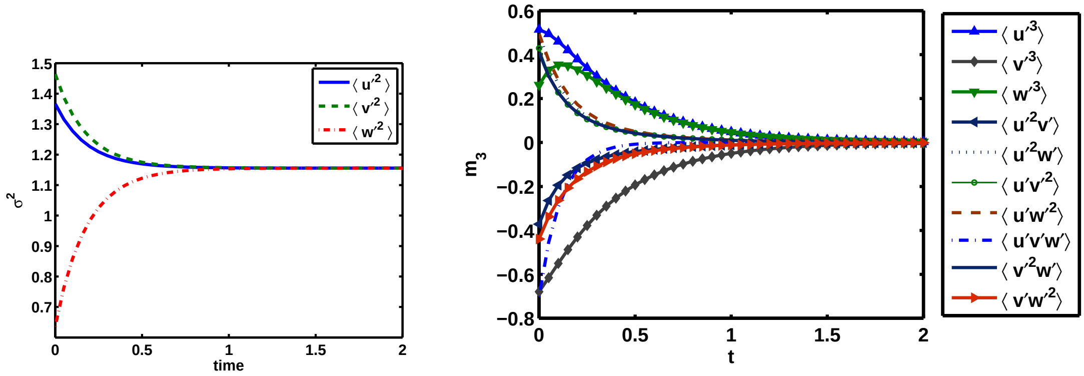

Figure 1: Evolution of velocity variances ((a), left) and third order moments ((b), right) with time

distribution function for each species i is approximated as a collection of discrete Dirac delta functions, with associated weights and abscissas in phase space, as

$$f_i(\mathbf{x}, \mathbf{v}_i, t) = \sum_{k=1}^{N} p_{i_k}(\mathbf{x}, t)\, \delta\left(\mathbf{v}_i - \mathbf{v}_{i_k}(\mathbf{x}, t)\right) \tag{2}$$

The unknown weights p_k and abscissas $\mathbf{v}_{i_k}$ are obtained as solutions of their evolution equations, which are in turn derived from the Boltzmann equation using constraints on generalized moments of velocity. These constraints are derived based on the complex collision integral present in Boltzmann equations (Eq. (1)), without resorting to the use of simplifying kinetic model approximations. The contributions to the evolution of generalized moments due to collisions involve eight-fold integrals. We show that these multi-dimensional integrals can be evaluated using Eq. (2) via algorithmic enumeration of terms resulting from products of multinomials, along with analytical evaluation of elementary integrals.

We evaluated the performance of our novel numerical method for solution of Boltzmann equation, applicable for the degenerate case of a spatially homogeneous, single-species fluid mixture, with elastic collisions. The results based on our new approach (see figure 1a) show that the variances of velocity components, which denote constituents of the total kinetic energy, approach a constant value at equilibrium through the process of redistribution of energy (while the total energy remains constant due to elastic collisions) among its constituents, as expected from the equilibrium Maxwellian distribution. The cross covariances and third order moments (in figure 1b) are also found to decay to zero, the equilibrium value, as expected from a Maxwellian distribution. These results on performance evaluation of our numerical approach are highly encouraging.

It may be noted that in our multi-component fluid mixture, collisions among molecules of the same species result in no net exchange of momentum or energy, while collisions among molecules of different species leads to exchange of momentum and energy. At the conference, we will present further detailed results on the behavior of multi-component fluid mixtures using our quadrature based approach.

REFERENCES

[1] C. F. Curtiss and J. O. Hirschfelder. “Transport properties of multicomponent gas mixtures”. *J. Chemical Phys.*, Vol. **17**, 550–555, 1949.

[2] H. Grad. “On kinetic theory of rarefied gases”. *Commun. Pure Appl. Math.*, Vol. **2**, 331–407, 1949.

[3] D. L. Marchisio and R. O. Fox. “Solution of population balance equations using the direct quadrature method of moments”. *J. Aerosol Sci.*, Vol. **36**, 43–73, 2005.