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

A mixed finite-element/spectral approach to solving the Boltzmann equation

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Key Words: *molecular-continuum flows, Boltzmann equation, FEM, discontinuous Galerkin, MD.*

ABSTRACT

Fluids are composed of molecules that behave in accordance with Hamiltonian Dynamics. For small systems, i.e. small number of molecules, all relevant properties of a fluid flow can be obtained from Molecular Dynamics (MD) simulations [1]. As the system size increases, the number of molecules however increases to a level that makes MD simulations infeasible. Fortunately, large number of molecules exhibit an ensemble behaviour which makes it possible to treat them as a continuum. All relevant properties of the fluid flow can therefore be determined by solving a system of partial differential equations such as the Euler or Navier-Stokes equations.

For problems that reside in the transitional regime, i.e., a system that includes regions characterized by molecular behaviour and regions where the continuum description is appropriate, some try to seek an adaptive model which couples the MD simulations with the partial differential equations. For problems in which the interest is restricted to average quantities of the fluid flow, such as temperature or pressure or heat-fluxes across a boundary, MD simulations do not make sense, as average quantities of a fluid are essentially independent of the properties of individual molecules. MD therefore provides severely redundant information. Such problems can be adequately described in terms of a probability distribution that specifies the probability density of a generic molecule in state space. This is precisely what the Boltzmann equation does.

The Boltzmann equation describes the evolution of a one-particle distribution function and is given by [2]:

$$\frac{\partial f}{\partial t} + u \cdot \frac{\partial f}{\partial x} = \frac{1}{\epsilon} \int (f' f'_* - f f_*) \mathcal{B}(u, u_*, \theta) \, d\omega du_*. \tag{1}$$

The main difficulty of this equation resides in the fact that it is posed in a high dimensional solution space: For a problem with d spatial dimensions, its solution is a scalar function $\mathbb{R}_+ \times \mathbb{R}^{2d} \rightarrow \mathbb{R}_+$.

Efficient solution techniques for the Boltzmann equation have formed an active area of research. There are simulation methods such as the one from Bird [5] or Nanbu. Another method solves (1) by reducing the number of possible velocities [6], known as the Discrete Velocity Method (DVM). Recently, a spectral Fourier method was introduced that, for some specific types of potentials, reduced the integral expression to one dimension [3, 4].

In this contribution, we will present a solution approach based on mixed finite-element/spectral formulation. The general idea is to use an approximation basis that contains the so-called Maxwellian solutions of the Boltzmann equation. These solutions have the form,

$$f = e^{a(x,t)+\mathbf{b}(x,t)\cdot\mathbf{u}+c(x,t)|\mathbf{u}|^2}. \tag{2}$$

In particular, instead of solving for $f(x,u,t)$, we now have to determine the $d+2$ coefficients $a(x,t)$, $b(x,t)$ and $c(x,t)$, which are however independent of u. This reduces the problem dimension with 3, but increases the degrees of freedom per node. With the form (2), only equilibrium behaviour can be represented, analogous to for instance the Euler equations. However, for areas where we expect significant non-equilibrium behaviour, the approximation can be *enriched* by introducing higher order terms (the full second-order tensor instead of $|\mathbf{u}|^2$, third-order terms, etc.). This approach increases the number of coefficients in regions with significant non-equilibrium behaviour.

To solve the Boltzmann equation for Maxwellian solutions, we use the *Discontinuous Galerkin* method (dG). The dG method has outstanding properties for solving hyperbolic equations such as (1). Moreover, in the dG method the enrichments can be introduced without essential complications. To get acquainted with the procedure, we first consider the prototypical projection problem:

Find α, β, $\gamma \in \mathcal{V}^3$ such that,

$$\begin{aligned}&\int_\Omega \int_V (a(x,t)+\mathbf{b}(x,t)\cdot\mathbf{u}+c(x,t)|\mathbf{u}|^2)\, e^{\alpha(x,t)+\beta(x,t)\cdot\mathbf{u}+\gamma(x,t)|\mathbf{u}|^2}\, dV d\Omega = \\ &= \int_\Omega \int_V (a(x,t)+\mathbf{b}(x,t)\cdot\mathbf{u}+c(x,t)|\mathbf{u}|^2)\, g(x,u,t)\, dV d\Omega \quad \forall\, a,b,c \in \mathcal{V}^3,\end{aligned} \tag{3}$$

where $\mathcal{V}$ represents a finite-element space and $g(x,u,t)$ is a prescribed function.

Furthermore, we consider a one-dimensional Boltzmann problem. In the one-dimensional case, the Boltzmann equation reduces to a Knudsen problem in which the collision term becomes zero [2] and the solution is completely determined by the boundary conditions. The FEM results are compared with the results of an equivalent molecular dynamics simulation.

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