LATTICE BOLTZMANN REPRESENTATION FOR GAS MIXTURES: PRELIMINARY STUDIES FOR THE GAS BLANKET DIVERTOR

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1. Introduction

There is considerable interest in developing schemes that can cope with the wide range of collisionalities encountered in the scrape-off-layer (SOL). Within the SOL, there are time varying spatial domains in which the neutral collisionality ranges from highly collisional (fluid) to the kinetic (Monte Carlo) regime. While attempts are being made to couple plasma-fluid codes to Monte Carlo codes, this coupling is necessarily numerically stiff due to the disparate length and time scales involved in these schemes.

Here we look at a thermal lattice Boltzmann (TLBE) solver for the fluid regime [1,2] which is (a) computationally more efficient than conventional Navier-Stokes sovlers, (b) ideal for parallel processors and (c) should provide for a much simpler coupling strategy to the weakly collisional Monte Carlo regime since both schemes are solved on the kinetic length and time scales. In particular, in the highly collisional regime, the exact form of the collision operator is not critical. Hence one can employ a simplified collisional operator that is much more amenable to efficient numerics but without sacrificing any of the essential physics. TLBE can be viewed as a maximally discretized molecular dynamics utilizing the minimal number of (discrete) molecular speeds needed to recover the correct fluid equations. The TLBE algorithm proceeds through two steps: (a) free-streaming to different lattice sites according to the (fixed) lattice velocity vectors, and (b) collisional relaxation at each lattice site. All operations are local and thus ideally suited for multiple PE's like the T3E. Moreover, since the free-streaming is nothing but linear advection there is no numerical diffusion or dissipation introduced when one employs the simple shift operator. This trivially avoids the major difficulty for Navier-Stokes solvers which have to resolve the nonlinear convection operators in the fluid equations - something that takes over 30% of the entire CPU.

TLBE methods can also be extended to solve the physics solved by the UEDGE code coupled to the Navier-Stokes neutrals [3]. One would consider a 2-species TLBE for the plasma and the neutrals. As a first step, we report on some results for a 2-species TLBE with modified BGK collision operators [4,5].

2. TLBE for binary gas mixtures

For a binary gas mixture, the governing equations of TLBE [1,2], which in local microscopic units of length and time, take the generic form in discrete phase space

$$N_{pi,s}(\mathbf{x} + \mathbf{e}_{pi}, t + 1) - N_{pi,s}(\mathbf{x}, t) = \Delta_{pi,s} \qquad (1)$$

where $N_{pi,s}$ is the s-species distribution function, and $\Delta_{pi,s}$ is the s-species collision operator. Here we shall consider 2D systems on a hexagonal lattice. The index p labels the number of sublattice required (here p = 1 and 2) and i labels the number of lattice links within each sublattice (for a hexagonal lattice, i = 0... 5). $\mathbf{e}_{pi}$ is the lattice vector for the moving particles in the system [for the hexagonal lattice $\mathbf{e}_{pi} = p. (\cos i\pi/6, \sin i\pi/6)$]. The particle speed on each sublattice is $|\mathbf{e}_{pi}| = p$. To recover the correct macroscopic behavior one must also include rest particles (with speed p = 0). The collisional operator $\Delta_{pi,s}$ is taken to be generalization of the standard BGK operator [3,4]

$$\Delta_{pi,s} = -\frac{N_{pi,s} - N^{eq}_{pi,s}}{\tau_{ss}} - \frac{N_{pi,s} - N^{eq}_{pi,ss'}}{\tau_{ss'}} \qquad (2)$$

where the collisional time τ_{ss} governs the relaxation rate of the same species (s → s) to its appropriately chosen equilibrium distribution function $N^{eq}_{pi,s}$ while $\tau_{ss'}$ governs the corresponding cross species (s → s') relaxation rate to $N^{eq}_{pi,ss'}$. The corresponding species moments of number density n_s, fluid velocity $\mathbf{v}_s$ and temperature θ_s are defined as usual (m_s is the mass of s-species)

$$n_s = \sum_{pi} N_{pi,s} = \sum_{pi} N^{eq}_{pi,s} \quad ; \quad n_s \mathbf{v}_s = \sum_{pi} N_{pi,s}\, \mathbf{e}_{pi} = \sum_{pi} N^{eq}_{pi,s}\, \mathbf{e}_{pi}$$

$$n_s\,\theta_s = \frac{m_s}{2} \sum_{pi} N_{pi,s}\,(\mathbf{e}_{pi} - \mathbf{v}_s)^2 = \frac{m_s}{2} \sum_{pi} N^{eq}_{pi,s}\,(\mathbf{e}_{pi} - \mathbf{v}_s)^2 \qquad (3)$$

The equilibrium functions are assumed to have a truncated power series in the fluid velocity $\mathbf{v}_s$:

$$N^{eq}_{pi,s} = A_{p,s} + B_{p,s}\,(\mathbf{e}_{pi} \cdot \mathbf{v}_s) + C_{p,s}\,(\mathbf{e}_{pi} \cdot \mathbf{v}_s)^2 + D_{p,s}\,\mathbf{v}_s^2 + E_{p,s}\,(\mathbf{e}_{pi} \cdot \mathbf{v}_s)^3 + F_{p,s}(\mathbf{e}_{pi} \cdot \mathbf{v}_s)\,\mathbf{v}_s^2 \qquad (4)$$

while the cross species N^{eq} has similar form. The coefficients $A_{p,s}(\theta_s)$ ... are determined from the constraints (3) and imposed local collisional invariants with relaxation times [5]

$$\tau_{ss'} = \left(\frac{m_s}{m_{s'}}\right)^{1/2} \frac{1}{n_{s'}\,\sigma_{ss'}} \frac{1}{(\theta_s/m_s + \theta_{s'}/m_{s'})^{1/2}} + \frac{1}{2} \qquad (5)$$

with $\sigma_{ss'} = \sigma_{s's}$. The temperature and number density dependence of the relaxation times are appropriate for a two-species plasma.

Performing a standard Chapman-Enskog expansion on (1), one finds the following transport equations for the mass, momentum and energy for each species [5]

$$\frac{\partial n_s}{\partial t} + \frac{\partial}{\partial x_\alpha}(n_\alpha\, v_{s,\alpha}) = 0 \qquad (6)$$

$$n_s\, m_s \left(\frac{\partial}{\partial t} + v_{s,\alpha}\frac{\partial}{\partial x_\alpha}\right) v_{s,\alpha} = -\frac{\partial\,(n_s\,\theta_s)}{\partial x_\alpha} - \frac{n_s\, m_s}{\tau_{ss'}}(v_{s,\alpha} - v_{s',\alpha}) - \frac{\partial\,\Pi_{s,\alpha\beta}}{\partial x_\beta} \qquad (7)$$

$$\frac{\partial}{\partial t}\left(\frac{n_s\, m_s\, \mathbf{v}_s^2}{2} + n_s\, \theta_s \right) + \frac{\partial}{\partial x_\alpha}\left(\frac{n_s\, m_s\, \mathbf{v}_s^2\, v_{s,\alpha}}{2} + \frac{5}{3}\, n_s\, \theta_s\, v_{s,\alpha} + v_{s,\beta}\, \Pi_{s,\alpha\beta} \right)$$

$$= - \frac{1}{\tau_{ss'}}\left[\frac{1}{2}\, n_s\, m_s\, (\mathbf{v}_s^2 - \mathbf{v}_{s'}^2) + n_s\, (\theta_s - \tilde{\theta}) \right] - \frac{\partial q_{s,\alpha}}{\partial x_\alpha} \tag{8}$$

The s-species pressure tensor

$$\Pi_{s,\alpha\beta} = -\mu_s \left[\frac{\partial v_{s,\alpha}}{\partial x_\beta} + \frac{\partial\, v_{s,\beta}}{\partial x_\alpha} - \frac{2}{3}\, \delta_{\alpha\beta}\, \frac{\partial v_{s,\gamma}}{\partial x_\gamma} \right] +$$

$$+ \frac{\tau_{ss}}{\tau_{ss'}} \left[(v_{s,\alpha} - v_{s',\alpha})\, (v_{s,\beta} - v_{s',\beta}) - \frac{1}{3}\, \delta_{\alpha\beta}\, (\mathbf{v}_s - \mathbf{v}_{s'})^2 \right] \tag{9}$$

includes the effects of the cross-species as does the heat flux

$$q_{s,\alpha} = -\kappa_s \frac{\partial \theta_s}{\partial x_\alpha} + \frac{5}{3}\, \frac{\tau_{ss}}{\tau_{ss'}}\, n_s\, (\theta_s - \tilde{\theta}\,)\, (v_{s,\alpha} - v_{s',\alpha}) -$$

$$- \frac{1}{2}\, \frac{\tau_{ss}}{\tau_{ss'}}\, n_s\, m_s\, (v_{s,\alpha} - v_{s',\alpha})\, (\mathbf{v}_s - \mathbf{v}_{s'})^2 \tag{10}$$

The viscosity μ_s and thermal conductivity κ_s coefficients are given by

$$\mu_s = \frac{2}{3}\left(\tau_{ss} - \frac{1}{2} \right) n_s\, \theta_s \quad , \quad \kappa_s = \frac{5}{3}\left(\tau_{ss} - \frac{1}{2} \right) n_s\, \theta_s \tag{11}$$

and

$$\tilde{\theta} = \frac{m_s\, \theta_{s'} + m_{s'}\, \theta_s}{m_s + m_{s'}} \tag{12}$$

The cross-correlation relaxation rate $\tau_{ss'}$ drives the species velocities and temperatures into equilibration.

3. Double shear turbulence

We now present some results on double shear turbulence in 2D neutral fluids of mass ratio $m_2/m_1 = 4$. The ratio of the relaxation parameters which couple to the two fluids have $\sigma_{ss'} / \sigma_{ss} = 10^{-6}$. In fluid '1' there is a double shear layer in the x-direction, while in fluid '2' the double shear layer is in the y-direction. Positivity vorticity is drawn with solid lines while negative vorticity is represented by dashed lines, as can be shown in the Figure. After 1K (TLBE) time steps, fluid '1' exhibits some vortex globs forming (lower of the two curves) while fluid '2' has mild oscillation in the vortex layers. At t = 1.5 K, there are major distortion in the vortex layers in fluid '1', while vortex globs are beginning to form in the vortex layers in fluid '2'. Note that there is some spatial correlation between the major vortex structures in the two species. Eventually equilibration occurs - as can be seen in the figure at t = 12.25 K where the system has relaxed to the same two large counter-rotating vortices, independent of species.

References

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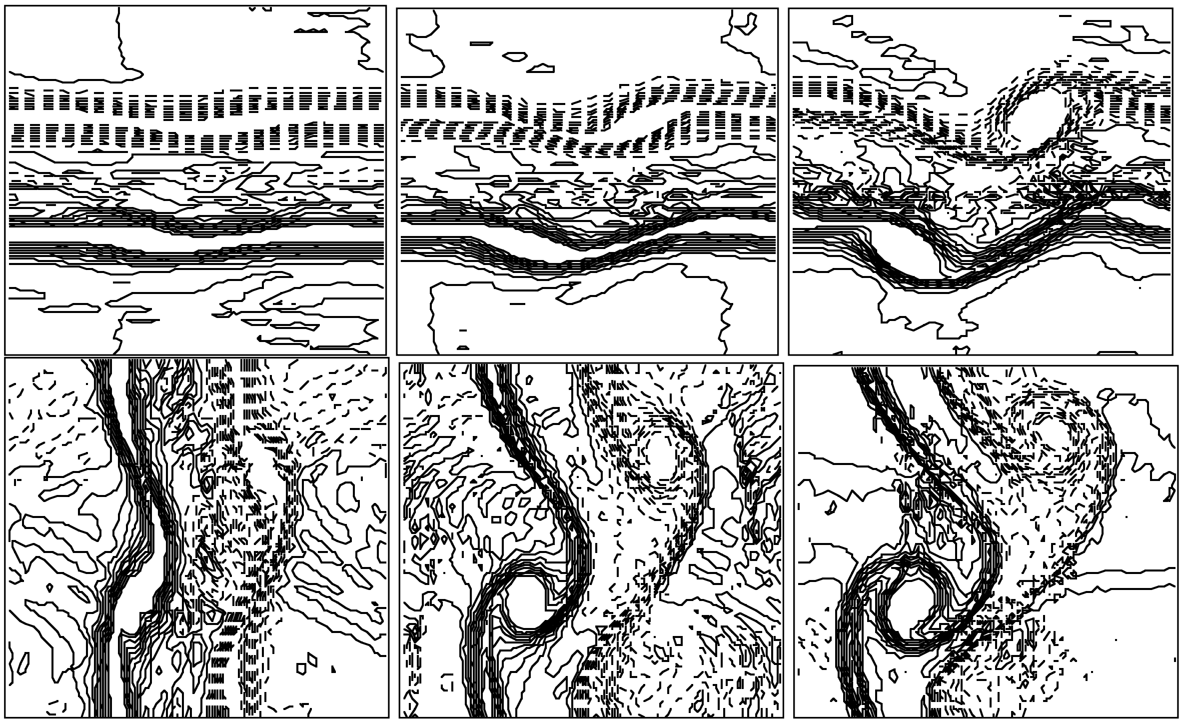
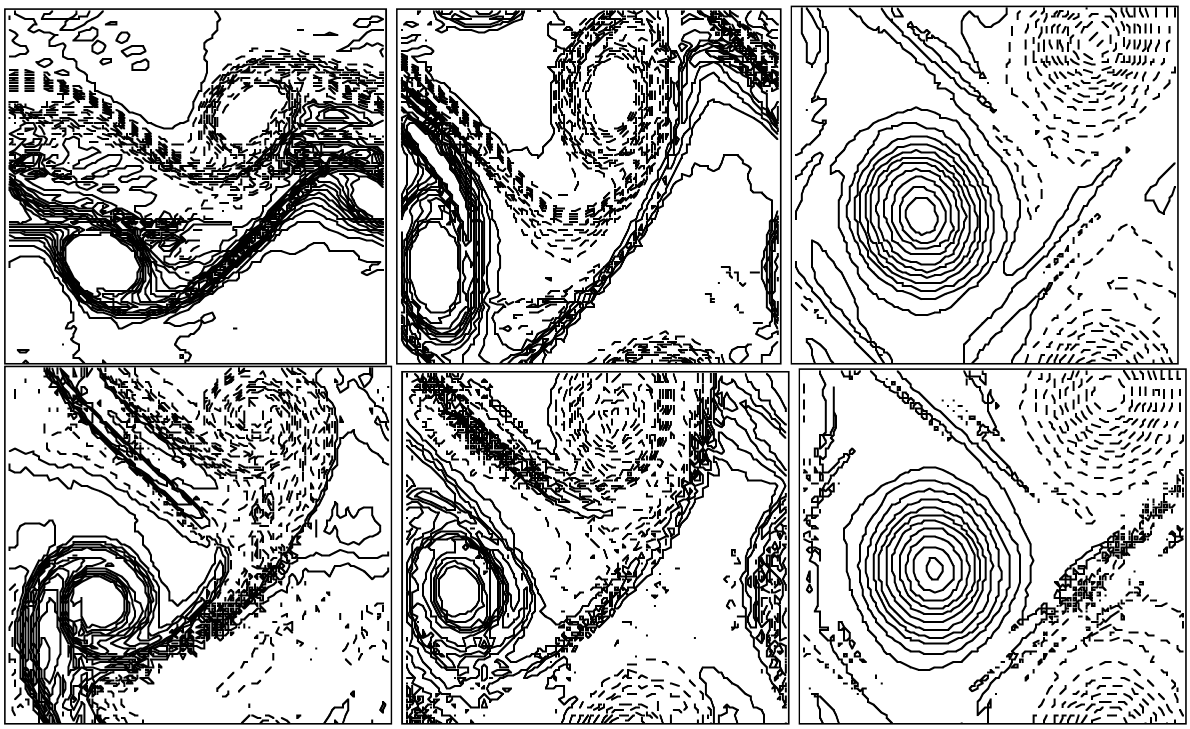


t = 1.0 K   t = 1.5 K   t = 2.0 K

t = 2.5 K   t = 3.75 K   t = 12.25 K



Time Evolution of the Vorticity Contours for Species 1 and 2
Initially Species 1 has double vortex layer in the x-direction, while that for Species 2 is in the y-direction
Solid Lines : positive vorticity contours, Dashed Lines : negative vorticity contours