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Coupling of the Boltzmann and Euler Equations with Automatic Domain Decomposition

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A criterion for automatic domain decomposition has been introduced for the coupling of the Boltzmann and Euler equations. This criterion is obtained by using the Grad's 13-moments expansion method. The Boltzmann and Euler equations have been solved by the particle method. This criterion has been further tested for the spatial homogeneous relaxation case and the coupling of the Boltzmann and Euler equations in two dimensional physical space. Some numerical results obtained from the particle code of the full Boltzmann equation are compared with those of coupling of the Boltzmann and Euler equations.

1. INTRODUCTION

In the kinetic theory of gases the Boltzmann equation gives the accurate description of a rarefied gas flow. To predict a hypersonic flow past a body flying at high altitude one considers usually the Boltzmann equation. Due to the complexity of this equation one has to solve it by some numerical methods. The most widely used numerical methods for the Boltzmann equation are particle methods, like the Direct Simulation Monte Carlo Method (DSMC) [2], the Finite Pointset Method (FPM) [1, 17], and some weighted particle methods [18, 19]. In the case of particle methods the mean free path of a particle (the average distance traveled by a molecule between collisions) is an important parameter. For example, in the reentry phase of the space shuttle into the atmosphere the gas becomes denser and denser so that the mean free path becomes smaller and smaller, which leads to a high computation time of a particle code for the Boltzmann equation. In fact, in the discretization of the Boltzmann equation a mesh size and a time step are proportional to the mean free path due to stability and accuracy of the numerical solution.

From the classical theory, as the mean free path tends to zero, the solution of the Boltzmann equation tends to a local Maxwellian distribution, in which the parameters are the approximate solutions of the compressible Euler equations. But in this regime, there are some regions, where the particle distribution function is far from a local Maxwellian

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distribution so that the limiting equations are not valid everywhere. In such a situation, one has to solve the Boltzmann equation only where it is necessary and the limiting equations wherever possible. This gives rise to two problems. The first one is to determine the domains of validity for these equations and the second is to solve these equations in the corresponding domains of validity. This means that the first problem corresponds to the domain decomposition of the Boltzmann and fluid dynamic equations and the second to solving matching (or coupling) problems. Moreover, one has to choose the suitable numerical methods for matching these two equations. Therefore the challenging task is to develop a hybrid code, which switches automatically from the fluid dynamic code to the Boltzmann code and vice versa.

In the past ten years many works have been reported with reference to both problems. In the coupling of the Boltzmann and Euler equations or that of Boltzmann and Navier–Stokes equations most of the authors have decomposed the computational domain a priori [15, 3, 4, 12, 20]. They assumed a Boltzmann domain in the vicinity of the body and that of Euler or Navier–Stokes away from the body. During the simulation of these equations the corresponding domains of validity do not remain fixed as shown in Fig. 4. Therefore, one needs criteria for domain decomposition. Tiwari *et al.* [22] have proposed the Sobolev norm as a criterion for the same. This criterion gives a correct domain decomposition, but its computational cost is very high compared to the criterion proposed in this paper [21].

The main objective of this paper is to develop a criterion for domain decomposition which has a low computational cost in comparison to the Sobolev norm and gives the required results. We have used the criterion which is obtained from Grad's 13-Moments expansion and can be monitored during the simulation. This criterion gives the suitable domain decomposition of the Boltzmann and fluid dynamic equations. We restrict ourselves to the coupling of the Boltzmann and Euler equations.

We organize the paper as follows. In Section 2, we give a short description of the Boltzmann and Euler equations and their numerical methods. In Section 3 we derive a criterion for a local thermal equilibrium. Finally, the coupling algorithm and some of the numerical results are given in Section 4.

2. THE EQUATIONS TO BE COUPLED AND NUMERICAL METHODS

2.1. *The Boltzmann and Euler Equations*

The Boltzmann equation is the time evolution of a distribution function $f(t, x, v)$ for particles of velocity $v \in \mathbb{R}^3$, at point $x \in \Omega \subset \mathbb{R}^d$ $(d = 1, 2, 3)$, at a time $t \in \mathbb{R}_+$ and is given by

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = \frac{1}{\epsilon} J(f, f), \tag{1}$$

with

$$J(f, f) = \int_{\mathbb{R}^3} \int_{S^2_+} k(|v - w|, \eta)[f(t, x, v') f(t, x, w') - f(t, x, v) f(t, x, w)] \, d\omega(\eta) \, dw,$$

where

$$v' = T_{v,w}(\eta) = v - \eta \langle \eta, v - w \rangle, \qquad w' = T_{w,v}(\eta), \tag{2}$$

$\eta \in S_+^2 = \{\eta \in \mathbb{R}^3/|\eta| = 1, \langle v - w, \eta\rangle \geq 0\}$, $k(|v - w|, \eta)$ is the collision scattering kernel, which describes the actual interaction potential. We have considered the hard sphere model which is given by

$$k(|v - w|, \eta) = \langle v - w, \eta\rangle \geq 0.$$

The constant ϵ is proportional to the mean free path λ. For more detail about the Boltzmann equation, we refer to [7]. If ϵ approaches zero, one can prove [6] that the Boltzmann distribution function f tends to a local Maxwellian

$$f_M := f_M[\rho, u, T](t, x) = \frac{\rho}{(2\pi RT)^{3/2}} e^{-\frac{|v-u|^2}{2RT}}, \tag{3}$$

where R denotes the gas constant and the parameters $\rho(t, x)$, $u(t, x)$, $T(t, x)$ approximate the compressible Euler equations:

$$\frac{\partial \rho}{\partial t} + \sum_{j=1}^{d} \frac{\partial}{\partial x_j}(\rho u_j) = 0 \tag{4}$$

$$\frac{\partial}{\partial t}(\rho u_i) + \sum_{j=1}^{d} \frac{\partial}{\partial x_j}(\rho u_i u_j) + \frac{\partial(\rho RT)}{\partial x_i} = 0 \qquad (1 \leq i \leq d) \tag{5}$$

$$\frac{\partial}{\partial t}\left(\rho\left(\frac{1}{2}|u|^2 + \frac{3}{2}RT\right)\right) + \sum_{j=1}^{d} \frac{\partial}{\partial x_j}\left[\rho u\left(\frac{1}{2}|u|^2 + \frac{5}{2}RT\right)\right] = 0. \tag{6}$$

In the coupling of these equations when we solve both of them by the particle methods, we can use the same initial and boundary conditions. The initial condition is given by

$$f(0, x, v) = f_0(x, v). \tag{7}$$

2.2. *The Boltzmann Solver*

We solve the Boltzmann equation by a particle method proposed by Babovsky [1] and described in [17]. The particle scheme for this equation is based on the time splitting of the equation. The first step consists of solving the free transport equation in $0 \leq t < \Delta t$

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = 0 \tag{8}$$

and the second consists of solving the equation

$$\frac{\partial f}{\partial t} = \frac{1}{\epsilon} J(f, f). \tag{9}$$

The particle simulation of (8) is based on the approximation of the initial density $f_0(x, v)$ by a discrete measure (a sum of Dirac masses)

$$f_0(x, v) \approx \sum_{i=1}^{N} \alpha_i \delta(x - x_i(0))\delta(v - v_i(0)), \tag{10}$$

where N is the number of particles with weights α_i. We have normalized the total mass of particles to 1 and considered the equal weight of all particles so that $\alpha_i = 1/N$ for all i. The positions $x_i(\Delta t)$ of particles change (during the free flow only) as per the following relation

$$x_i(\Delta t) = x_i(0) + \Delta t \cdot v_i(0), \tag{11}$$

where velocities change during the collision step. In the free flow step one has to consider boundary conditions.

For the simulation of (9) we introduce a spatial mollifier since the collision integral $J(f, f)$ is a local operator in space and time. We divide the computational domain into many regular cells C where the density $f(t, x, v)$ is substituted by $f_C(t, v)$ for $x \in C$ and

$$f_C(t, v) = \frac{1}{\mathrm{Vol}(C)} \int_C f(t, y, v)\, dy. \tag{12}$$

Now, it is sufficient to describe the particle simulation of the following spatially homogeneous Boltzmann equation

$$\frac{\partial f}{\partial t} = \frac{1}{\epsilon} J(f, f). \tag{13}$$

For the sake of simplicity, we rewrite f instead of f_C. To derive the particle scheme for (13) we used the explicit Euler discretization and obtained

$$f(\Delta t, v) = f(0, v) + \Delta t \frac{1}{\epsilon} J(f, f)(0, v). \tag{14}$$

To obtain a particle approximation one has to consider the weak formulation of (14) by multiplying by a test function Φ and integrate it with respect to v

$$\int_{\mathbb{R}^3} \Phi(v) f(\Delta t, v)\, dv = \int_{\mathbb{R}^3} \Phi(v) f(0, v)\, dv + \Delta t \int_{\mathbb{R}^3} \Phi(v) J(f, f)(0, v)\, dv. \tag{15}$$

Now, assuming that $\|f\| = 1$ and using the decomposition $J(f, f) = J^+(f) - f L(f)$, we have

$$\begin{aligned} \int_{\mathbb{R}^3} \Phi(v) f(\Delta t, v)\, dv = & \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \Phi(v) f(0, v) f(0, w)\, dw\, dv \\ & + \Delta t \int_{\mathbb{R}^3} \Phi(v) J^+(f)(0, v)\, dv \\ & - \Delta t \int_{\mathbb{R}^3} \Phi(v) L(f)(0, v)\, dv, \end{aligned} \tag{16}$$

where

$$J^+(f) = \frac{1}{\epsilon} \int_{\mathbb{R}^3} \int_{S^2_+} k(|v - w|, \eta) f(0, v') f(0, w')\, d\omega(\eta)\, dw$$

$$L(f) = \frac{1}{\epsilon} \int_{\mathbb{R}^3} \int_{S^2_+} k(|v - w|, \eta) f(0, w)\, dw(\eta)\, dw.$$

In the integral over the gain term J^+ we can use the collision transformations (2) to change the variable (v, w) into (v', w') and obtain

$$\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \Phi(v)k(|v-w|,\eta)\, f(0,v')\, f(0,w')\, dw\, dv = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \Phi(v')k(|v-w|,\eta)\, f(0,v)\, f(0,w)\, dw\, dv. \tag{17}$$

From (16) and (17) we obtain

$$\begin{aligned}\int_{\mathbb{R}^3} \Phi(v)\, f(\Delta t, v)\, dv &= \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{S^2_+} \Phi(v)(1-\Delta t\, k(|v-w|,\eta))\, f(0,v)\, f(0,w)\, d\omega(\eta)\, dw\, dv \\ &\quad + \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{S^2_+} \Phi(v')\Delta t\, k(|v-w|,\eta)\, f(0,v)\, f(0,w)\, d\omega(\eta)\, dw\, dv. \end{aligned}\tag{18}$$

In order to guarantee the positivity of the function $f(\Delta t, v)$ we need the restriction on time step which must satisfy

$$1 - \frac{\Delta t}{\epsilon} k(|v-w|,\eta) \geq 0. \tag{19}$$

Assuming the condition (19), we introduce an artificial variable s on the interval $[0, 1]$ and a appropriate mapping Ψ to transform (18) into

$$\begin{aligned}\int_{\mathbb{R}^3} \Phi(v)\, f(\Delta t, v)\, dv &= \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{S^2_+}\int_{[0,1]} (\Phi\circ\Psi)(v,w,\eta,s)\, f(0,v)\, f(0,w)\, ds\, d\omega(\eta)\, dw\, dv, \end{aligned}\tag{20}$$

where

$$\Psi(v,w,\eta,s) = \begin{cases} v', & \text{if } \Delta t k(|v-w|,\eta) \leq s \\ v, & \text{else.} \end{cases} \tag{21}$$

This leads to the following time discretized equation for the corresponding measures

$$\mu_{\Delta t} = (\mu_0 \times \mu_0 \times \omega \times \nu)\circ\Psi^{-1}, \tag{22}$$

where ω denotes the surface measure on S^2_+ and ν the uniform measure on $[0, 1]$.

For a particle simulation we considered first a particle set μ_0, which yielded an approximation of $f(0, v)$, i.e.,

$$f(0,v) \approx \delta_{\mu_0} = \frac{1}{N}\sum_{i=1}^{N} \delta(v - v_i(0)), \tag{23}$$

where all particles have equal weight $1/N$. Next, one approximates the product measure $\mu_{\Delta t}$ with the help of μ_0. For details of this procedure we refer to [1, 17].

2.3. *The Euler Solver*

We solve the Euler equations also by the particle method based on the kinetic scheme. Earlier workers [8, 9, 11], have reported this scheme in detail. It is the direct consequence of the solution scheme for the Boltzmann equation. The main idea of the kinetic scheme is that one considers the problem on a kinetic level or in a position-velocity space and defines the macroscopic quantities as moments of the density $f(t, x, v)$ by

$$\rho(t, x) = \int_{\mathbb{R}^3} f(t, x, v)\, dv, \tag{24}$$

$$\rho u(t, x) = \int_{\mathbb{R}^3} v f(t, x, v)\, dv, \tag{25}$$

$$T(t, x) = \frac{1}{3\rho R} \int_{\mathbb{R}^3} |v - u|^2 f(t, x, v)\, dv, \tag{26}$$

finding a simple evolution for the density f such that this evolution approximates the compressible Euler equations for $\rho, u,$ and T. This evolution also consists of two steps as in the case of the Boltzmann equation. The first free flow step is exactly the same as in the case of the Boltzmann equation. In the second step we consider the relaxation.

$$J(f, f) = 0, \tag{27}$$

where the solution of the Boltzmann equation is relaxed to a thermodynamic equilibrium (a local Maxwellian) whose parameters solve the compressible Euler equations. In this step we compute the macroscopic quantities ρ, u, T as moments of the solution of the free transport equation and then generate the particles according to a local equilibrium distribution function such that the conservations of mass, momentum, and energy hold. As an equilibrium distribution function one considers usually a Maxwellian. The computational time for a generation of particles according to a Maxwellian is larger than the collision process. In this case, an equilibrium distribution function proposed by Kaniel is more convenient. The numerical results obtained from both functions are very close. The function, for a monoatomic gas, proposed by Kaniel, is given by [11]

$$f_K = \begin{cases} \frac{3}{4\pi} \frac{\rho}{(5RT)^{3/2}}, & |v - u| \le \sqrt{5RT} \\ 0, & |v - u| > \sqrt{5RT}. \end{cases} \tag{28}$$

3. THE CRITERIA FOR A LOCAL THERMAL EQUILIBRIUM

Since the Euler equations can be approximated from the Boltzmann equation if particles are distributed according to a local Maxwellian or near enough to it, we need a test to determine whether a particle distribution is close enough to a local Maxwellian, that is, in a local thermal equilibrium, or not.

For a criterion of equilibrium, we assume that the distribution function $f(t, x, v)$ deviates from a local Maxwellian. Suppose

$$f = f_M(1 + \phi). \tag{29}$$

Local thermal equilibrium can be assumed if $\|\phi\| \ll 1$, with some appropriate norm. This suggests defining a Hilbert space, where the scalar product is [7]

$$\langle \phi, \psi \rangle = \int_{\mathbb{R}^3} \frac{f_M}{\rho} \phi \overline{\psi}\, dv \tag{30}$$

and the corresponding norm is given by

$$\|\phi\| = \left(\int_{\mathbb{R}^3} \frac{f_M}{\rho} |\phi|^2\, dv \right)^{1/2}. \tag{31}$$

While deriving fluid dynamic equations from the Boltzmann equation, the moments can be defined by [7]

$$\rho = \int_{\mathbb{R}^3} f\, dv, \qquad \rho u = \int_{\mathbb{R}^3} v f\, dv, \qquad \rho E = \int_{\mathbb{R}^3} \frac{|v|^2}{2} f\, dv \tag{32}$$

$$q = \frac{1}{2} \int_{R^3} (v - u)|v - u|^2 f\, dv, \qquad \tau = \int_{\mathbb{R}^3} (v - u)(v - u)^t\, f\, dv - p\delta_{ij}, \tag{33}$$

where E is the specific energy, q is the heat flux vector, τ the stress tensor, p the static pressure, and δ_{ij} is the Kronecker symbol. $(v-u)^t$ denotes the transpose of the vector $v-u$. We assume that the first five moments ρ, u, E of f are those of f_M. Then

$$\int_{\mathbb{R}^3} \phi f_M\, dv = 0 \tag{34}$$

$$\int_{\mathbb{R}^3} v \phi f_M\, dv = 0 \tag{35}$$

$$\int_{\mathbb{R}^3} |v|^2 \phi f_M\, dv = 0. \tag{36}$$

We also have

$$\frac{1}{2} \int_{\mathbb{R}^3} (v - u)|v - u|^2 \phi f_M\, dv = q \tag{37}$$

$$\int_{\mathbb{R}^3} (v - u)(v - u)^t \phi f_M\, dv = \tau. \tag{38}$$

The non-vanishing of the stress tensor τ and the heat flux vector q are due to deviation from a Maxwellian distribution. Thus, ϕf_M describes the deviation from a Maxwellian distribution.

With the help of the above 13 equations (34)–(38) we intend to express ϕ in a polynomial,

$$\phi = a + \langle b, v - u \rangle + (v - u)^t C (v - u) + \langle d, v - u \rangle |v - u|^2, \tag{39}$$

where a is a scalar, b, d are vectors in $\mathbb{R}^3$, and C is a (3×3) symmetric matrix.

This is the Grad's 13 moments expansion method [10]. Now, substituting ϕ in (34)–(38) one can compute all the coefficients of the polynomial (39) and gets [21]

$$\phi = \frac{\langle q, v-u\rangle}{\rho(RT)^2}\left[\frac{|v-u|^2}{5RT}-1\right] + \frac{1}{2\rho(RT)^2}\big[\tau_{11}(v_1-u_1)^2+\tau_{22}(v_2-u_2)^2 - (\tau_{11}+\tau_{22})(v_3-u_3)^2\big] + \frac{1}{\rho(RT)^2}[\tau_{12}(v_1-u_1)(v_2-u_2) + \tau_{23}(v_2-u_2)(v_3-u_3)+\tau_{13}(v_1-u_1)(v_3-u_3)]. \tag{40}$$

We are interested in estimating the quantity $\|\phi\|$ with the help of the norm defined in (31). In order to calculate the integral on the right hand side of (31), we write (40) in the form

$$\phi = \frac{1}{\rho(RT)^2}\left[|q|\,|v-u|\cos\theta\left(\frac{|v-u|^2}{5RT}-1\right)\right] + \frac{1}{2\rho(RT)^2}\big[\tau_{11}(v_1-u_1)^2 + \tau_{22}(v_2-u_2)^2-(\tau_{11}+\tau_{22})(v_3-u_3)^2\big] + \frac{1}{\rho(RT)^2}[\tau_{12}(v_1-u_1)(v_2-u_2) + \tau_{23}(v_2-u_2)(v_3-u_3)+\tau_{13}(v_1-u_1)(v_3-u_3)]. \tag{41}$$

Squaring (41) on both sides and substituting into the right hand side of (31), the integrals containing the odd powers of v_i-u_i, $i=1,2,3$, vanish and we get

$$\begin{aligned}\|\phi\|^2 = \frac{1}{\rho^2(RT)^4}\frac{1}{(2\pi RT)^{3/2}}\int_{\mathbb{R}^3}\Bigg[&|q|^2|v-u|^2\cos^2\theta\left(\frac{|v-u|^2}{5RT}-1\right)^2 \\ &+\frac{\tau_{11}^2}{4}(v_1-u_1)^4+\frac{\tau_{22}^2}{4}(v_2-u_2)^4+\frac{(\tau_{11}+\tau_{22})^2}{4}+\tau_{12}^2(v_1-u_1)^2(v_2-u_2)^2 \\ &+\tau_{23}^2(v_2-u_2)^2(v_3-u_3)^2+\tau_{13}^2(v_1-u_1)^2(v_3-u_3)^2 \\ &+|q|\tau_{11}|v-u|\cos\theta\left(\frac{|v-u|^2}{5RT}-1\right)(v_1-u_1)^2 \\ &+|q|\tau_{22}|v-u|\cos\theta\left(\frac{|v-u|^2}{5RT}-1\right)(v_2-u_2)^2 \\ &-|q|(\tau_{11}+\tau_{22})|v-u|\cos\theta\left(\frac{|v-u|^2}{5RT}-1\right)(v_3-u_3)^2 \\ &+\frac{\tau_{11}\tau_{22}}{2}(v_1-u_1)^2(v_2-u_2)^2-\frac{\tau_{11}(\tau_{11}+\tau_{22})}{2}(v_1-u_1)^2(v_3-u_3)^2 \\ &-\frac{\tau_{22}(\tau_{11}+\tau_{22})}{2}(v_2-u_2)^2(v_3-u_3)^2\Bigg]e^{-\frac{|v-u|^2}{2RT}}\,dv.\end{aligned} \tag{42}$$

Now, we compute each integral separately by transforming $v-u$ in spherical coordinates and integrating. We get

$$\int_{\mathbb{R}^3}(v_i-u_i)^2(v_j-u_j)^2 e^{-\frac{|v-u|^2}{2RT}}\,dv = 2\pi(RT)^3\sqrt{2\pi RT}, \qquad i,j=1,2,3\,(i\neq j)$$

$$\int_{\mathbb{R}^3}(v_i-u_i)^4 e^{-\frac{|v-u|^2}{2RT}}\,dv = 6\pi(RT)^3\sqrt{2\pi RT}, \qquad i=1,2,3.$$

Next, we consider the first integral of (42), in which we first transform $v-u$ in spherical coordinates in such a way that the polar angle is equal to the angle in a spherical coordinate system between $v-u$ and q, that is, θ. Then, we have

$$\int_{\mathbb{R}^3}|v-u|^2\cos^2\theta\left(\frac{|v-u|^2}{5RT}-1\right)^2 e^{-\frac{|v-u|^2}{2RT}}\,dv = \frac{4\pi}{5}(RT)^2\sqrt{2\pi RT}$$

$$\int_{\mathbb{R}^3}|v-u|\cos\theta\left(\frac{|v-u|^2}{5RT}-1\right)(v_i-u_i)^2 e^{-\frac{|v-u|^2}{2RT}}\,dv = 0, \qquad i=1,2,3.$$

Now, substituting all the values of the integrals in (42) and simplifying, we get

$$\begin{aligned}\|\phi\|^2 &= \frac{1}{(\rho RT)^2}\left[\frac{2}{5}\frac{|q|^2}{RT}+\tau_{11}^2+\tau_{22}^2+\tau_{11}\tau_{22}+\tau_{12}^2+\tau_{23}^2+\tau_{13}^2\right]\\ &= \frac{1}{(\rho RT)^2}\left[\frac{2}{5}\frac{|q|^2}{RT}+\frac{1}{2}\left(\tau_{11}^2+\tau_{22}^2+(\tau_{11}+\tau_{22})^2\right)+\tau_{12}^2+\tau_{23}^2+\tau_{13}^2\right]\\ &= \frac{1}{(\rho RT)^2}\left[\frac{2}{5}\frac{|q|^2}{RT}+\frac{1}{2}\|\tau\|_E^2\right],\end{aligned}$$

where we use the relation $\sum_{i=1}^3\tau_{ii}=0$.

Therefore, we have

$$\|\phi\| = \frac{1}{\rho RT}\left[\frac{2}{5}\frac{|q|^2}{RT}+\frac{1}{2}\|\tau\|_E^2\right]^{1/2}, \tag{43}$$

where $\|\tau\|_E$ is the Euclidean norm of the stress tensor matrix τ.

The quantity $\|\phi\|$ gives a criterion for a local thermal equilibrium, which identifies Boltzmann and Euler cells during the simulation of the Boltzmann or Euler code. If the quantity $\|\phi\|$ is very small compared to unity, we assume that a particle system is very close to a local Maxwellian. This criterion consists of the heat flux vector q and the shear stress tensor τ, which have to be vanished in order to yield the closure relations for the Euler equations [7]. These quantities vanish if the particle distribution is Maxwellian. Therefore, the higher the norm of ϕ obtained in (43), the more a particle system deviates from a Maxwellian distribution.

If we do not take into account the shear stress tensor, we have

$$\|\phi\| = \sqrt{\frac{2}{5}}\frac{|q|}{\rho(RT)^{3/2}}. \tag{44}$$

We take $R = 1$ for the sake of simplicity. In the case of Navier–Stokes equations we use the Fourier law

$$q = -k\nabla T,$$

where k is the heat conduction coefficient. We substitute this value in (44) and get

$$\|\phi\| \leq \frac{k|\nabla T|}{\rho T^{3/2}}.$$

In the kinetic theory for a hard sphere, k is proportional to $\sqrt{T}$ and also the mean free path λ is inversely proportional to the density ρ. Therefore, we can write

$$\|\phi\| \leq C\frac{\lambda|\nabla T|}{T}, \tag{45}$$

where C is a constant. This is exactly the same criterion of a local thermal equilibrium, which is used in Refs. [5, 13, 16].

Similarly, if we neglect the effect of the heat flux vector in the criterion given by (43), we obtain $\|\phi\|$ equal to the quantity used in Ref. [14] as a criterion for a local thermal equilibrium.

The use of both the heat flux and the shear stress tensor gives a correct domain decomposition. As we solve the Boltzmann and Euler equations by particle methods, it is very easy to compute the heat flux vector and the stress tensor, that is, the criterion represented by (43). If the quantity $\|\phi\|$ is less than a small number, then, we assume that the cell is a Euler cell, otherwise, a Boltzmann one. The small number depends on the number of particles per cell at the initial time and other input parameters, like the Mach number. This quantity gives the correct domain decomposition for the Boltzmann and Euler equations and is displayed in Fig. 4.

4. NUMERICAL RESULTS

4.1. *A Spatial Homogeneous Relaxation Case*

First, we check the above criterion by considering a spatial homogeneous relaxation problem. Generally, a gas tends to approach a Maxwellian distribution due to intermolecular collisions as expressed by Boltzmann's H-theorem. This implies that if we start the simulation of the spatial homogeneous Boltzmann equation with a non-Maxwellian distribution as an initial condition, the quantity $\|\phi\|$ is usually large at the initial time $t = 0$ and decreases to a small number as time increases. As the distribution function relaxes to an equilibrium, the quantity $\|\phi\|$ becomes smaller and smaller as shown in Fig. 1.

We consider the spatial homogeneous Boltzmann equation

$$\frac{\partial f}{\partial t} = J(f, f) \tag{46}$$

with the initial condition

$$f(0, v) = \frac{\rho}{2(2\pi R\hat{T})^{3/2}}\left(e^{-\frac{|v-\hat{u}|^2}{2R\hat{T}}} + e^{-\frac{|v+\hat{u}|^2}{2R\hat{T}}}\right). \tag{47}$$

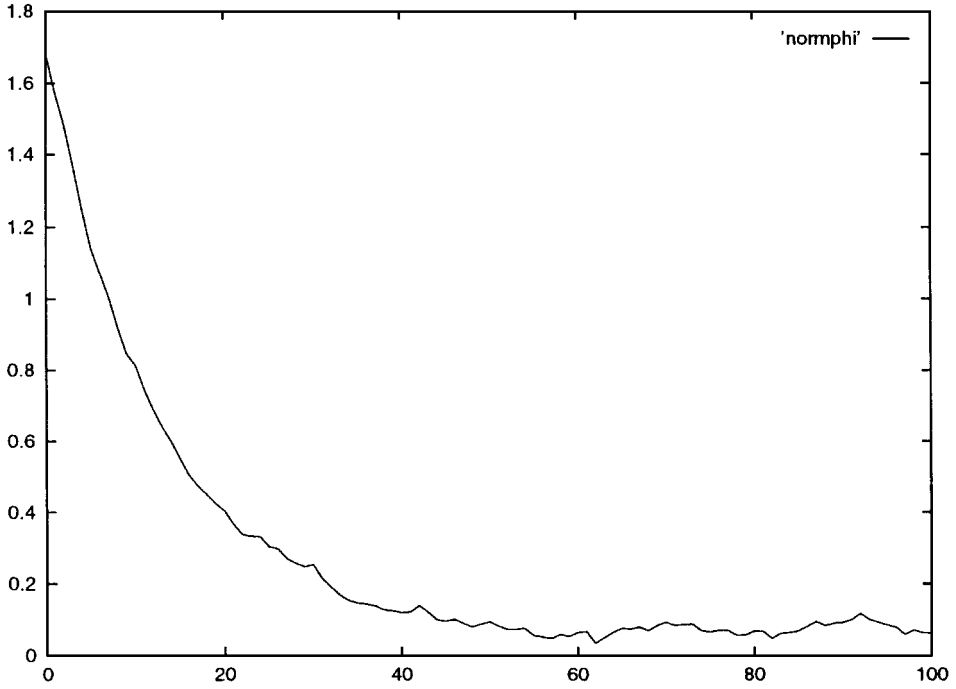

FIG. 1. $\|\phi\|$ for 1000 particles.

As time t tends to infinity, the solution of the problems (46)–(47) tends to an equilibrium distribution with the density, mean velocity, and the temperature obtained from the initial value $f(0, v)$. Therefore, the quantity $\|\phi\|$ must decrease to a small constant as time tends to infinity.

We solve the problems (46)–(47) by the particle method, developed at the University of Kaiserslautern, Germany. The simulation is performed with 1000 particles. At each time step we compute the quantity $\|\phi\|$ and then collisions. In Fig. 1 we observe that the quantity $\|\phi\|$ decreases asymptotically to a very small constant as time advances.

4.2. *The Coupling of the Boltzmann and Euler Equations in the 2D Case*

Our main objective is to apply the above criterion as a switching criterion from the Euler code to the Boltzmann code and vice versa. We considered a two dimensional flow of a perfect monoatomic gas flowing at hypersonic speed around an ellipse with major and minor axes $1.0m$ and $0.5m$, respectively. The computational domain Ω is a rectangle with size $6m \times 4m$ as shown in Fig. 2.

As an initial condition we use the following Maxwellian distribution

$$f(0, x, v) = \frac{\rho_\infty}{(2\pi RT_\infty)^{3/2}} e^{-\frac{|v-u_\infty|^2}{2RT_\infty}} \tag{48}$$

and the following boundary conditions:

(i) diffuse reflection with complete thermal accommodation at the boundary Γ_3,

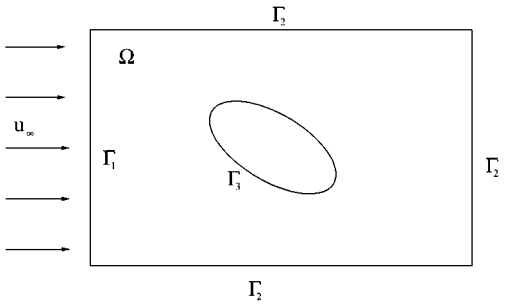

FIG. 2. Computational domain.

(ii) on Γ_1 an ingoing function of the form

$$f(t, x, v) = \frac{\rho_\infty}{(2\pi RT_\infty)^{3/2}} e^{-\frac{|v-u_\infty|^2}{2RT_\infty}}, \tag{49}$$

(iii) non-reflecting boundary conditions at the other three boundaries Γ_2.

We divided the computational domain Ω into many rectangular cells of the size of the global mean free path, that is, $dx = \lambda$. We have chosen the time step $\Delta t = dx/|u_\infty|$, and computed until the steady state is reached.

The Coupling Algorithm. From Section 2 we see that the only difference between solving the Boltzmann and Euler equations is the treatment of collisions and projection procedures after free flow at the end of time step Δt. The advantage of using the particle code for the Euler equations is that one can easily adjust the Euler solver in the particle code for the Boltzmann equation. We have the following coupling algorithm:

(i) Approximate the initial distribution function by Dirac masses.
(ii) For time step 1 to L:
- Generate particles having a Maxwellian distribution in the velocity space and a uniform distribution in the physical one at the boundary cells.
- Advance the particles in a free flow

$$x_i(t + \Delta t) = x_i(t) + \Delta t \cdot v_i(t).$$

- If the particle collides with the surface boundary, then, we reflect it according to a boundary condition and continue the free flow with a new velocity until Δt is over.
- Erase the particles that leave the domain.

(iii) Check whether the cells are either Euler or Boltzmann cells using the criterion described in the next section.
(iv)(a) Consider intermolecular collisions in Boltzmann cells.
(iv)(b) Project the distribution function into a local thermal equilibrium in Euler cells.
(v) Go to step (ii).

The input parameters are the following: at infinity the characteristics of the flow are $u_\infty = (ux_\infty, 0, 0)$ with $ux_\infty = 4126\,\text{m/s}$, $T_\infty = 200\,\text{K}$, gas constant $R = 208\,\text{Jkg/K}$ which approximately corresponds to a Mach number 15. Furthermore, the temperature of the

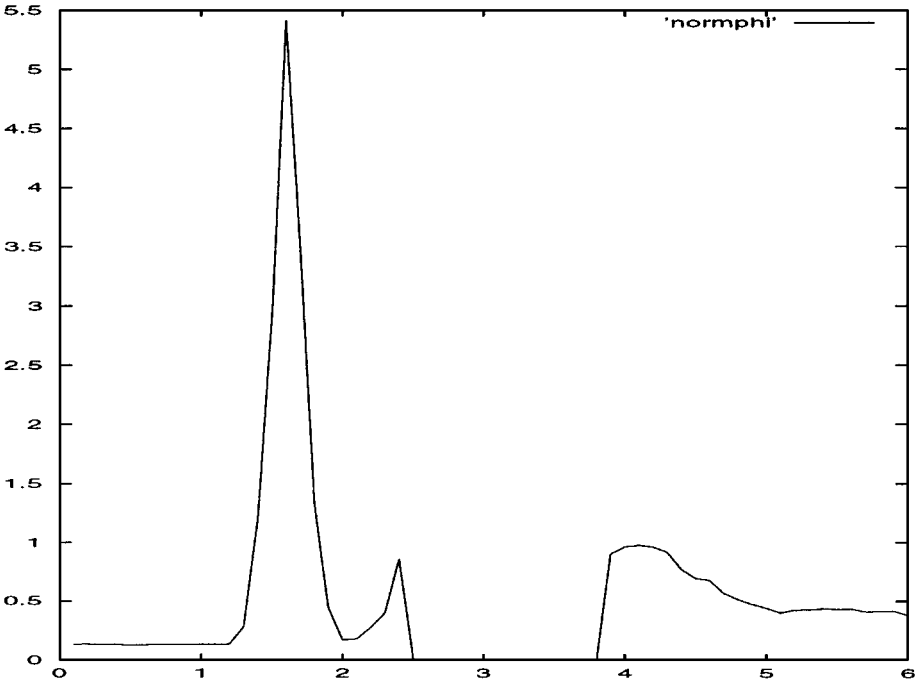

FIG. 3. $\|\phi\|$ on 20th row at at steady state.

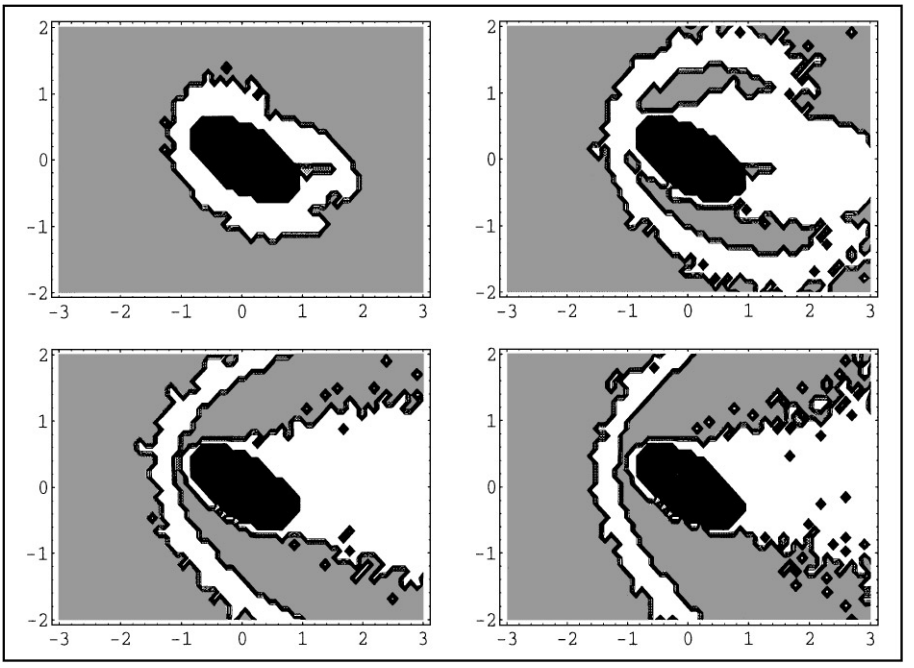

FIG. 4. The domain decomposition of Boltzmann and Euler equations. In the upper half the domain decomposition is shown at time steps 10 (left) and 25 (right) and in the lower half for time steps 50 (left) and 100 (right). White and gray domains represent the Boltzmann and Euler ones.

body $T_W = 1000\,\mathrm{K}$, angle of attack $= 30^\circ$, the number of particles per cell at the beginning $N = 50$, the mean free path $\lambda = 0.1m$ and the total time steps $L = 400$.

As in the space homogeneous case we plot the value of the term $\|\phi\|$ from (43). In Fig. 3 we have plotted, in a steady state, the value of this quantity on the middle row. We observed that this value is small in front of the bow shock and is large in the shock region, on the solid boundary and in the wake. Between the bow shock and the solid boundary this quantity is also low. On the ellipse we put $\|\phi\|$ equal to 0.

As a criterion of a local thermal equilibrium we assume that if $\|\phi\|$ is less than 0.4 in each cell, the cell is a Euler cell, otherwise, a Boltzmann one. Then, we do collisions in the Boltzmann cells and regenerate the particles according to a local thermal equilibrium in Euler cells. As a local thermal equilibrium function we have considered the function f_K. We perform the above processes in every cell and at every time step.

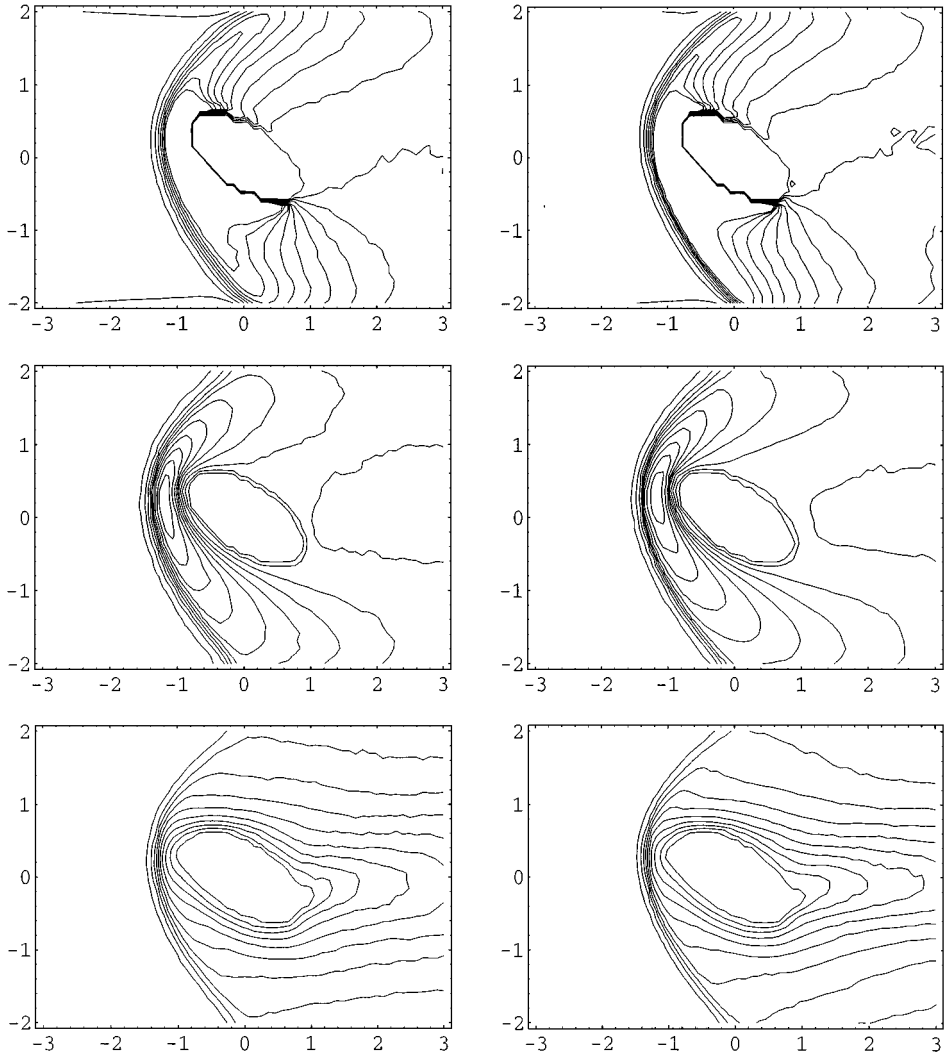

FIG. 5. Contour plots of densities (row 1), temperatures (row 2), and Mach numbers (row 3) obtained from both the codes. Pictures on the left are from the pure Boltzmann code and those on the right are from the coupling code.

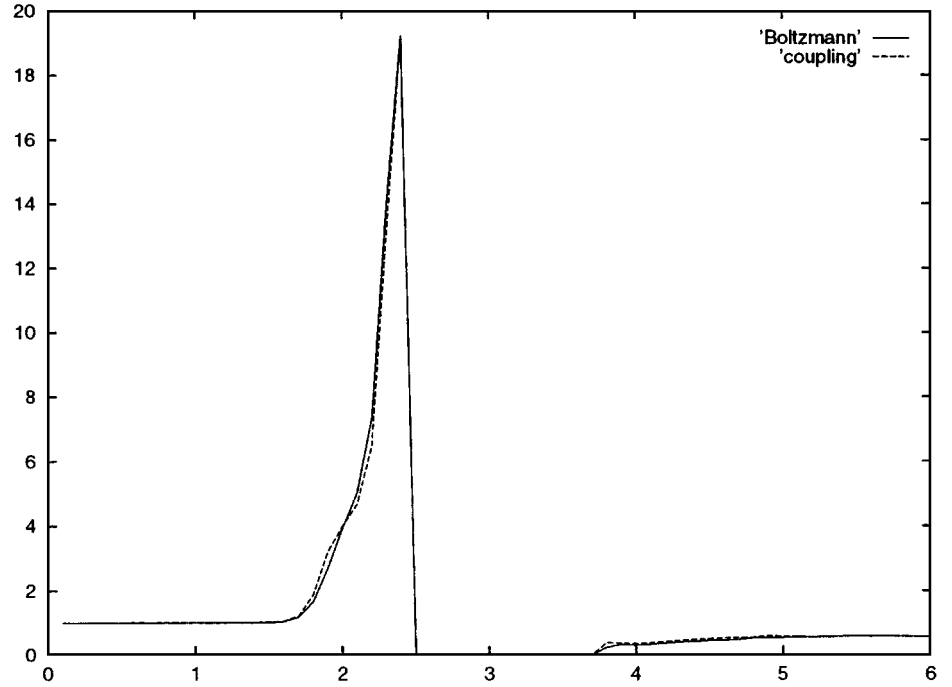

FIG. 6. Densities on the middle row obtained from both codes.

The tuning parameter of $\|\phi\|$ is not a global one. It depends upon users and the input parameters. In a particle simulation for the Boltzmann equation a number of particles per cell depends on the capacity of the computer memory. Usually one considers 30 particles per cell. In this case the criterion of $\|\phi\|$ also gives similar results, but with a different tuning parameter. For the same estimate with a small number of particles one might get a larger Boltzmann domain than that given in Fig. 4.

In the beginning we find all the cells are Euler cells. As the time increases, the Boltzmann and Euler domains separate automatically. We have plotted such domain decompositions in time steps 10, 25, 50, and 100. The white part indicates the Boltzmann domain and the gray part that of Euler as shown in Fig. 4.

Our reference solution is the solution of the pure Boltzmann code. We compare the results of the coupling code with those of the pure Boltzmann code. In Fig. 5 we have plotted the density, temperature, and the Mach number for the coupling and pure Boltzmann code. We have noted that the results are similar. Further, in Fig. 6 we have plotted the density along the middle row (20th row) of the computational domain. The values of the density obtained from both codes are almost the same. In Fig. 7 we have plotted again the densities from both codes along the 7th row of the computational domain. We see that the error is not very large.

Finally, in Fig. 8 we have plotted the temperature ratio T/T_∞ along the middle of the computational domain by both codes. All of these figures show that the results obtained from the coupling code are very close to those of the Boltzmann one. In this simulation the computational cost for the coupling code is 20% lower than that of the pure Boltzmann code.

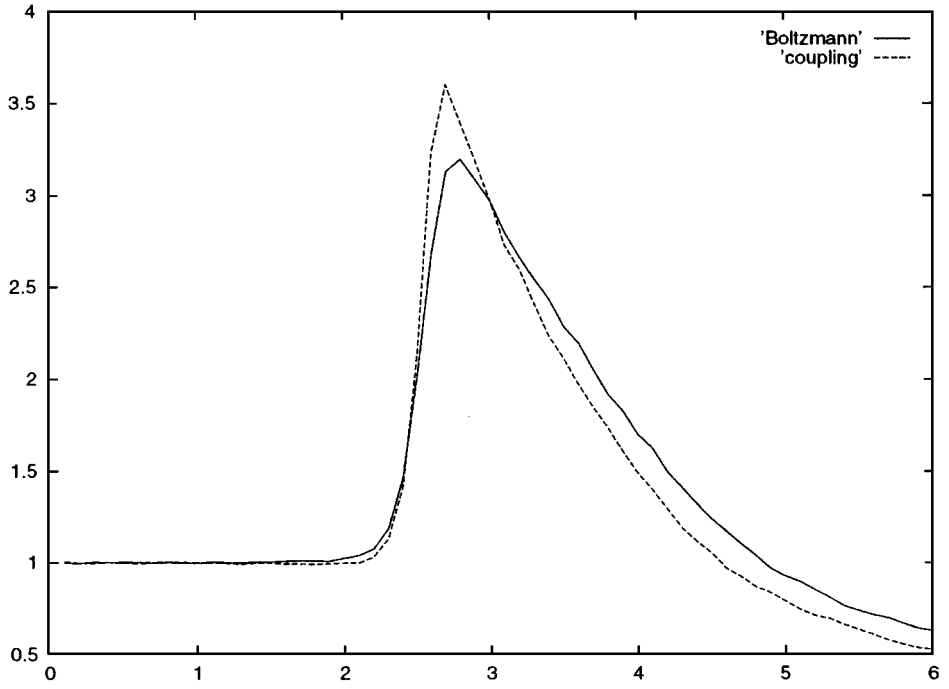

FIG. 7. Densities on the 7th row (from below) obtained from both codes.

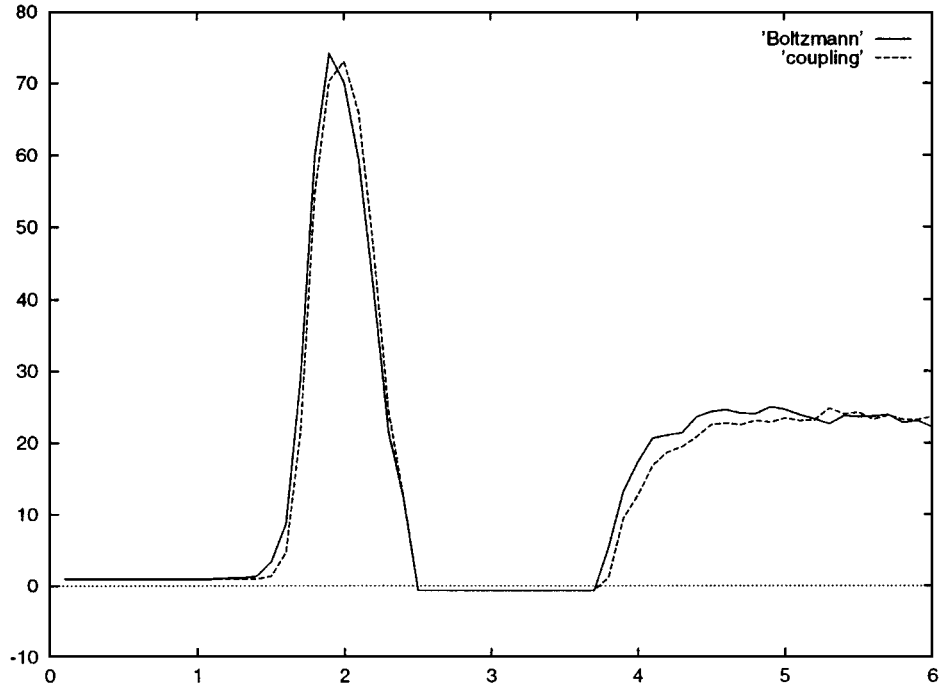

FIG. 8. Temperature ratios obtained from both codes.

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