

A new decoupled rotational energy exchange scheme for DSMC calculations

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Abstract. We present a new scheme for modeling rotational energy exchange with the direct simulation Monte Carlo (DSMC) method. This new scheme is fundamentally different to conventional Borgnakke-Larsen (BL) procedures, in which energy exchange is performed at the time of collision. In the new scheme, all collisions are performed elastically. Rotational energy exchange is performed after the collision routine, in an independent step. The rotational energy of all particles in each cell is adjusted by a factor, to satisfy the desired macroscopic relaxation behaviour. To conserve the total energy in a cell, the thermal velocities of all particles in the cell are adjusted. DSMC calculations of shock structure show that the new scheme gives results in reasonable agreement with those provided by conventional BL procedures. The new scheme has a potential advantage over BL procedures: It is easy to use with *any* DSMC collision model.

Keywords: Direct simulation Monte Carlo, rotational energy exchange

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INTRODUCTION

The direct simulation Monte Carlo (DSMC) method [1] captures general non-equilibrium gas behaviour and is the most useful computational tool for modeling rarefied gas flows of engineering interest. To obtain the non-equilibrium distribution of molecular velocities, the DSMC collision routine must perform collisions such that the distribution of relative speeds g for colliding particles is correct. This is achieved by using the no-time counter (NTC) method [2], which selects collision partners within each DSMC cell.

The non-equilibrium distribution of rotational energy captured by the DSMC method depends on the details of the rotational energy exchange scheme. Usually, a version of the phenomenological Borgnakke-Larsen (BL) scheme [3] is used in DSMC calculations to perform rotational energy exchange. BL exchange procedures cannot be expected to accurately model the complex exchange processes that occur in real intermolecular collisions, so they are unlikely to capture the real distribution of rotational energies. In a typical DSMC engineering calculation, the distribution of rotational energies is rarely important; rather the mean rotational energy (or rotational kinetic temperature T_{rot}) is the required information. There is therefore some justification in a new scheme that simplifies the complex problem of rotational-translational energy exchange by concentrating only on this mean value of rotational energy, and does not attempt to capture the non-equilibrium distribution of rotational energy.

This paper describes a new rotational energy exchange scheme for DSMC calculations that applies a decoupled approach to rotational energy exchange in which all intermolecular collisions are performed elastically and energy exchange is performed independently, after the DSMC collision routine. The distribution of rotational energies is ignored. Rotational energy exchange is performed for each computational cell according to a macroscopic adiabatic relaxation equation. We test the decoupled scheme with DSMC shock calculations and demonstrate that it can capture detailed shock structure, including T_{rot} , with reasonable accuracy relative to standard BL procedures. The new scheme can be readily applied to any DSMC collision model. This flexibility represents a potential advantage over conventional BL procedures.

Macroscopically, rotational relaxation is described in terms of T_{rot} or a mean rotational energy $\bar{\epsilon}_{\text{rot}}$ per molecule. Jeans [4, p. 120] gives

$$\frac{d\bar{\epsilon}_{\text{rot}}}{dt} = \frac{2\bar{\epsilon}_{\text{tr}}/3 - \bar{\epsilon}_{\text{rot}}(t)}{\tau_{\text{rot}}} \quad (1)$$

to describe the instantaneous rotational relaxation of diatomic molecules. Here $\bar{\epsilon}_{tr}$ is the mean translational energy per molecule and τ_{rot} is some characteristic time. Under isothermal conditions, $\bar{\epsilon}_{tr}$ is constant and Eq. 1 has the solution

$$\frac{\bar{\epsilon}_{rot}(t) - 2\bar{\epsilon}_{tr}/3}{\bar{\epsilon}_{rot}(0) - 2\bar{\epsilon}_{tr}/3} = \exp \left[- \int_0^t \frac{dt}{\tau_{rot}(t)} \right].$$

This may be written in the pure exponential form

$$\Delta \hat{\epsilon}_{rot} = \exp(-\hat{t})$$

where

$$\Delta \hat{\epsilon}_{rot} = \frac{\bar{\epsilon}_{rot}(t) - 2\bar{\epsilon}_{tr}/3}{\bar{\epsilon}_{rot}(0) - 2\bar{\epsilon}_{tr}/3} = \frac{\bar{\epsilon}_{rot}(t) - \bar{\epsilon}_{rot}(\infty)}{\bar{\epsilon}_{rot}(0) - \bar{\epsilon}_{rot}(\infty)}$$

is a normalized mean rotational energy and

$$\hat{t} = \int_0^t \frac{dt}{\tau_{rot}(t)}$$

is a non-dimensional time. This may be regarded as the total number of relaxing collisions between time 0 and time t [5]. $\bar{\epsilon}_{rot}(\infty)$ is the mean rotational energy at equilibrium for isothermal conditions, which equals $2\bar{\epsilon}_{tr}/3$. Under adiabatic conditions, $\bar{\epsilon}_{tr}$ varies with time and Eq. 1 has the solution

$$\frac{\bar{\epsilon}_{rot}(t) - 2\bar{\epsilon}/5}{\bar{\epsilon}_{rot}(0) - 2\bar{\epsilon}/5} = \Delta \hat{\epsilon}_{rot} = \exp \left(-\frac{5}{3} \hat{t} \right) \quad (2)$$

where $\bar{\epsilon} = \bar{\epsilon}_{tr}(t) + \bar{\epsilon}_{rot}(t)$ is constant and $2\bar{\epsilon}/5 = \bar{\epsilon}_{rot}(\infty)$ is the mean rotational energy at equilibrium. This expression for adiabatic relaxation has a characteristic relaxation time which is smaller than that for the isothermal case by a factor of 3/5. A dimensionless rotational collision number may be defined by $Z_{rot} = \tau_{rot}/\tau_c$, where τ_c is the mean time between intermolecular collisions. In effect, Z_{rot} characterizes the number of collisions required for rotational energy to equilibrate after a perturbation to the equilibrium state.

BORGNAPKE-LARSEN ENERGY EXCHANGE PROCEDURES

Most DSMC codes employ versions of BL procedures to model rotational energy exchange. It has been shown [5, 6] that these procedures can recover the macroscopic adiabatic relaxation behaviour described by Eq. 2. BL rotational energy exchange proceeds in two steps: Particle selection followed by energy exchange between translation and rotation.

The selection procedure identifies those particles that are to participate in the energy exchange process. Selection occurs within the DSMC collision routine, when the collision occurs. It is a probabilistic process that is performed according to some exchange probability ϕ_{rot} that may be applied to each individual particle (particle-based) or to each collision pair (pair-based). The exchange probability is effectively controlled by the required macroscopic relaxation rate and is usually described in terms of Z_{rot} . It is possible to capture relaxation rates that depend on the macroscopic temperature by including collision energy dependencies in ϕ_{rot} .

The second step of BL procedures performs the exchange of energy between rotation and translation. Post-exchange energies are sampled from appropriate equilibrium energy distributions. This is also a probabilistic process and is performed subject to the constraints of energy conservation and detailed balancing.

Here, we used the particle-based selection scheme of Gimelshein *et al.* [7] to select particles for BL energy exchange. In this scheme, each collision partner is assigned an exchange probability. For particles A and B, these are denoted $(\phi_{rot})_A$ and $(\phi_{rot})_B$ respectively. Multiple exchange events are prohibited, meaning that particle A or particle B can exchange rotational energy in a given collision, but not both. A random fraction R_f that is uniformly distributed between 0 and 1 is generated, and then particle selection is performed according to:

If	$0 \leq R_f < (\phi_{rot})_A$	Particle A exchanges rotational energy with translational mode
If	$(\phi_{rot})_A \leq R_f < (\phi_{rot})_A + (\phi_{rot})_B$	Particle B exchanges rotational energy with translational mode
If	$(\phi_{rot})_A + (\phi_{rot})_B \leq R_f \leq 1$	Elastic collision with no rotational energy exchange

This selection scheme allows different relaxation rates for different species to be captured, and is simpler and more versatile than pair-based selection schemes. Recently, Lilley [8] showed that the selection probability for this particle-based selection scheme must be

$$\phi_{\text{rot}} = \frac{1}{Z_{\text{rot}}} \left(1 + \frac{\zeta_{\text{rot}}}{\zeta_g} \right) \quad (3)$$

to provide the macroscopic relaxation behaviour of Eq. 2 with constant Z_{rot} . Here, ζ_{rot} is the number of rotational degrees of freedom (DOF) in the relaxing molecules and ζ_g is the effective number of DOF in the relative translational energy of colliding molecules. This ϕ_{rot} expression compares to

$$\phi_{\text{rot}} = \frac{1}{Z_{\text{rot}}} \left[1 + \frac{(\phi_{\text{rot}})_A + (\phi_{\text{rot}})_B}{\zeta_g} \right]$$

given by Lumpkin *et al.* [6] for pair-based selection. For the particle-based selection scheme of Gimelshein *et al.* in which multiple exchange events are prohibited, $(\phi_{\text{rot}})_A = 0$ or $(\phi_{\text{rot}})_B = 0$, so Eq. 3 is equivalent to the expression given by Lumpkin *et al.* Eq. 3 has been checked by performing a zero-dimensional DSMC simulation of a rotationally relaxing gas [8]. The results are shown in Fig. 1, and demonstrate that Eq. 3 is correct. For the DSMC calculation, \hat{t} for time step s was calculated from

$$\hat{t}(s) = \frac{2}{Z_{\text{rot}}N} \sum_{j=1}^s N_{\text{colls}}(j)$$

where N is the number of simulator particles and $N_{\text{colls}}(j)$ is the number of collisions performed during time step j [8].

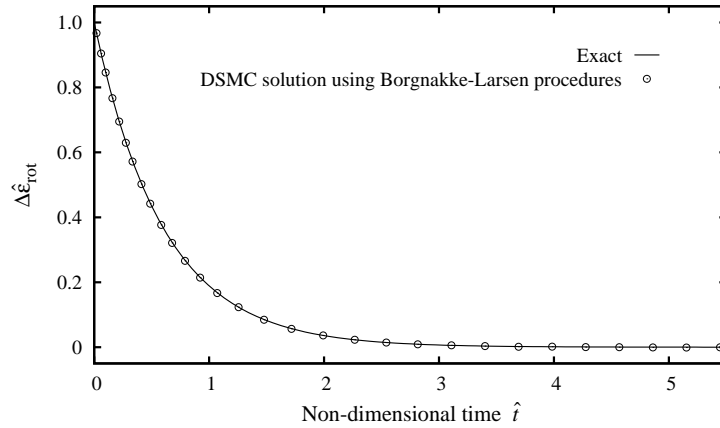


FIGURE 1. Exact adiabatic rotational relaxation history from Eq. 2 compared to DSMC solution using BL procedures with the particle-based selection scheme of Gimelshein *et al.* [7] and ϕ_{rot} calculated from Eq. 3. Constant $Z_{\text{rot}} = 5$ was used. Lilley [8] gives full details of the DSMC simulation.

THE NEW DECOUPLED ROTATIONAL ENERGY EXCHANGE SCHEME

The decoupled exchange scheme is fundamentally different to conventional collision-based BL procedures. We decouple the rotational energy exchange process from the intermolecular collisions and perform rotational energy exchange as an independent step, after the DSMC collision routine. We based the decoupled scheme on the adiabatic relaxation behaviour described by Eq. 2. The mean rotational energy $\bar{\epsilon}_{\text{rot}}$ at the end of a DSMC time step of duration Δt is given by

$$\bar{\epsilon}'_{\text{rot}} = \bar{\epsilon}_{\text{rot}}(t + \Delta t) = F \bar{\epsilon}_{\text{rot}}(t) + (1 - F) 2\bar{\epsilon}/5, \quad (4)$$

where $\bar{\epsilon}_{\text{rot}}(t)$ is the mean rotational energy at the start of the step and

$$F = \exp \left(-\frac{5}{3} \frac{1}{Z_{\text{rot}}} \frac{\Delta t}{\tau_c} \right). \quad (5)$$

This assumes that the mean collision time τ_c is constant, which is sufficiently accurate when the DSMC time step Δt is small relative to τ_c . This is satisfied by the standard DSMC time step criterion in which $\Delta t \lesssim \tau_c/3$. The local collision frequency in a DSMC calculation can be estimated with

$$\tau_c = \frac{N}{N_{\text{colls}}} \frac{\Delta t}{2}, \quad (6)$$

where N is the number of particles in the cell and N_{colls} is the number of collisions performed in the cell by the DSMC collision routine during time step Δt . Substituting Eq. 6 into Eq. 5 gives

$$F = \exp\left(-\frac{10}{3} \frac{1}{Z_{\text{rot}}} \frac{N_{\text{colls}}}{N}\right).$$

The decoupled exchange scheme forces the mean rotational energy of all particles in each cell to be the new mean rotational energy $\bar{\epsilon}'_{\text{rot}}$ as dictated by Eq. 4. To implement this, we define an adjustment factor $f = \bar{\epsilon}'_{\text{rot}}/\bar{\epsilon}_{\text{rot}}(t)$, and assign new rotational energies to each individual particle according to

$$\epsilon'_{\text{rot}} = f \epsilon_{\text{rot}}.$$

The net change in total rotational energy in a cell is $\Delta E_{\text{rot}} = (f - 1)E_{\text{rot}}$, where E_{rot} is the total rotational energy in the cell at the start of the time step. This amount of energy is removed from the translational thermal energies of all particles in the cell. To achieve this, we use the factor

$$\Psi = (1 - \Delta E_{\text{rot}}/E_{\text{tr}})^{1/2},$$

where E_{tr} is the total translational thermal energy in the cell at the start of the time step. We then adjust the velocity \mathbf{v} of each particle in the cell according to

$$\mathbf{v}' = \Psi \mathbf{v} + \bar{\mathbf{v}}(1 - \Psi),$$

which requires the mean velocity $\bar{\mathbf{v}}$ in each cell.

DETAILS AND RESULTS OF DSMC SHOCK CALCULATIONS

To test the decoupled exchange scheme, we applied it to simulate shocks in nitrogen with the DSMC method at Mach numbers of 1.2, 1.7, 3 and 10. Bird [1] gives DSMC shock modeling procedures. We compared the resulting profiles of density, translational kinetic temperature T_{tr} and rotational kinetic temperature T_{rot} to those obtained with conventional BL exchange procedures. Vibrational excitation was ignored. The variable hard sphere (VHS) collision model [9] which has the collision cross-section $\sigma(g) = \sigma_r(g_r/g)^{2v}$ was used. We used $\sigma_r = 4.991 \times 10^{-19} \text{ m}^2$, $g_r = 1089 \text{ m/s}$ and $v = 0.26$ for diatomic nitrogen [10]. The simulation domain contained 1000 cells, each with six subcells. Each simulation had about 495×10^3 simulator particles in total. The simulation time step Δt was set to $(\tau_{\text{VHS}})_2/4$ where $(\tau_{\text{VHS}})_2$ was the mean collision time for VHS molecules at the downstream conditions. Bird [1] gives the formula for τ_{VHS} . The number of DSMC time steps between flowfield samples was $\lfloor \Delta x / (\Delta t u_2) \rfloor + 1$, where Δx was the cell size and u_2 was the downstream flow speed. The flowfield was sampled 2000 times. For VHS molecules, the effective number of translational DOF for colliding molecules ζ_g is simply $4 - 2v$ [6]. Using Eq. 3 with $\zeta_{\text{rot}} = 2$ and constant $Z_{\text{rot}} = 5$, we obtained $\phi_{\text{rot}} = 0.315$. The shock profiles are shown in Figs. 2 to 5. Table 1 includes some further details of the DSMC simulations.

TABLE 1. Details of DSMC simulations using the decoupled rotational exchange scheme. Here $(\lambda_2)_{\text{VHS}}$ is the downstream mean free path for VHS molecules [1].

Mach number	Mean particles per cell		$\Delta x / (\lambda_2)_{\text{VHS}}$	CPU time relative to BL solution
	Upstream	Downstream		
1.2	423	567	0.104	1.18
1.7	310	680	0.159	1.38
3	204	786	0.119	2.13
10	147	843	0.104	2.59

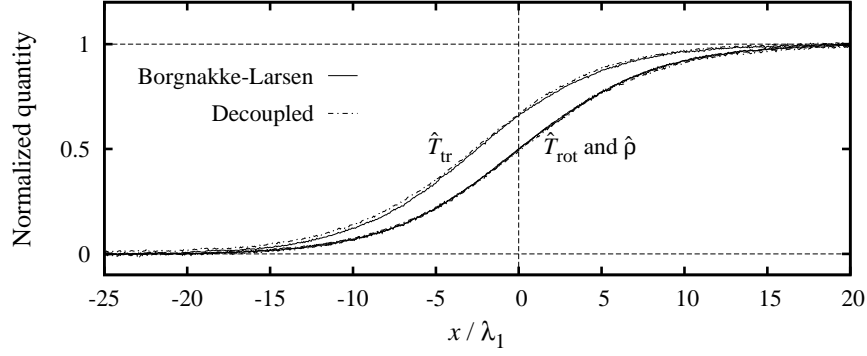


FIGURE 2. Normalized profiles of density ρ , translational kinetic temperature T_{tr} and rotational kinetic temperature T_{rot} within a Mach 1.2 shock in nitrogen. Flow is from left to right. The normalized density $\hat{\rho}$ is given by $\hat{\rho} = (\rho - \rho_1)/(\rho_2 - \rho_1)$ where ρ_1 and ρ_2 are the respective densities in the upstream and downstream flows. Similar normalization was applied to obtain \hat{T}_{tr} and \hat{T}_{rot} . Here $\lambda_1 = 2\mu_1/(\rho_1 \bar{c})$ is the nominal mean free path in the upstream gas, where μ_1 is the upstream viscosity and \bar{c} is the upstream mean thermal speed. $x/\lambda_1 = 0$ was set at $\hat{\rho} = 0.5$.

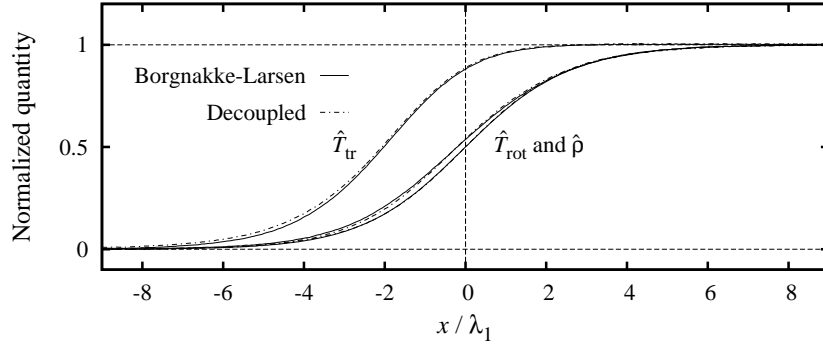


FIGURE 3. Normalized profiles of ρ , T_{tr} and T_{rot} within a Mach 1.7 shock in nitrogen. For other details see caption of Fig. 2.

DISCUSSION AND CONCLUSIONS

The profiles in Figs. 2 to 5 show that the decoupled scheme gives shock solutions that are generally in close agreement with those obtained using conventional BL exchange procedures. Agreement is best for lower Mach numbers.

A major perceived advantage of the decoupled exchange scheme is that it is simple to apply for *any* DSMC collision model. In contrast, conventional BL procedures have been developed primarily for the VHS model. Variants have been developed for the Sutherland hard sphere model [11] by Boyd [12] and for the generalized hard sphere model [13] by Hassan & Hash [13] and Hash *et al.* [14]. From Boyd and Hash *et al.*, it is evident that particle selection procedures are quite complicated for these models, due to the difficulty associated with determining ζ_g for colliding molecules. General BL procedures do not exist for realistic intermolecular potentials such as the Lennard-Jones and Morse potentials. The decoupled scheme could be readily applied to such models.

A disadvantage of the decoupled scheme in its present form is its poor computational efficiency compared to BL procedures, as shown by the relative CPU times in Table 1. However, there may be scope for improvements to the decoupled exchange algorithm that could improve its efficiency relative to BL procedures.

Our results show that the new decoupled exchange scheme gives shock structure in reasonable agreement with that given by conventional collision-based BL exchange procedures. This shows that the detailed distribution of rotational energies is not important for obtaining the density and kinetic temperatures, which are the macroscopic flowfield properties of engineering interest. Given its accuracy relative to conventional BL exchange procedures, and the fact that it is easy to implement for any DSMC collision model, it is clear that the decoupled exchange scheme is worthy of further investigation. A possibility is the extension of the decoupled approach to model vibrational energy exchange.

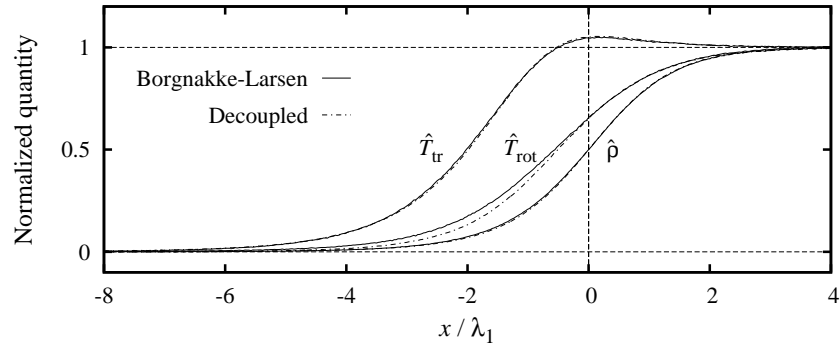


FIGURE 4. Normalized profiles of ρ , T_{tr} and T_{rot} within a Mach 3 shock in nitrogen. For other details see caption of Fig. 2.

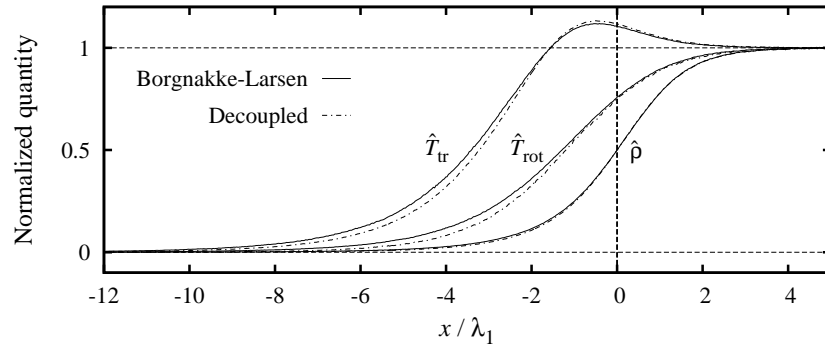


FIGURE 5. Normalized profiles of ρ , T_{tr} and T_{rot} within a Mach 10 shock in nitrogen. For other details see caption of Fig. 2.

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