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Methods for implementing the stream boundary condition in DSMC computations

Charles R. Lilley[*,†,‡] and Michael N. Macrossan[§,¶]

Centre for Hypersonics, School of Engineering, The University of Queensland, Brisbane, Queensland 4072, Australia

SUMMARY

In the direct simulation Monte-Carlo (DSMC) method for simulating rarefied gas flows, the velocities of simulator particles that cross a simulation boundary and enter the simulation space are typically generated using the acceptance–rejection procedure that samples the velocities from a truncated theoretical velocity distribution that excludes low and high velocities. This paper analyses an alternative technique, where the velocities of entering particles are obtained by extending the simulation procedures to a region adjacent to the simulation space, and considering the movement of particles generated within that region during the simulation time step. The alternative method may be considered as a form of acceptance–rejection procedure, and permits the generation of all possible velocities, although the population of high velocities is depleted with respect to the theoretical distribution. Nevertheless, this is an improvement over the standard acceptance–rejection method. Previous implementations of the alternative method gave a number flux lower than the theoretical number required. Two methods for obtaining the correct number flux are presented. For upstream boundaries in high-speed flows, the alternative method is more computationally efficient than the acceptance–rejection method. However, for downstream boundaries, the alternative method is extremely inefficient. The alternative method, with the correct theoretical number flux, should therefore be used in DSMC computations in favour of the acceptance–rejection method for upstream boundaries in high-speed flows. Copyright © 2003 John Wiley & Sons, Ltd.

KEY WORDS: direct simulation Monte-Carlo; boundary condition; acceptance–rejection

1. INTRODUCTION

The direct simulation Monte-Carlo (DSMC) method is a computational fluid dynamics (CFD) scheme that recognizes the discrete molecular character of gases and models the macroscopic gas behaviour by simulating the motions of and collisions between representative simulator particles within a spatial array of computational cells. Most rarefied gas flows of engineering

[*]Correspondence to: C. R. Lilley, Centre for Hypersonics, School of Engineering, The University of Queensland, Brisbane, Queensland 4072, Australia.
[†]E-mail: c.lilley@uq.edu.au
[‡]PhD Research Student, Student Member AIAA.
[§]E-mail: m.macrossan@uq.edu.au
[¶]Senior Lecturer, Member AIAA.

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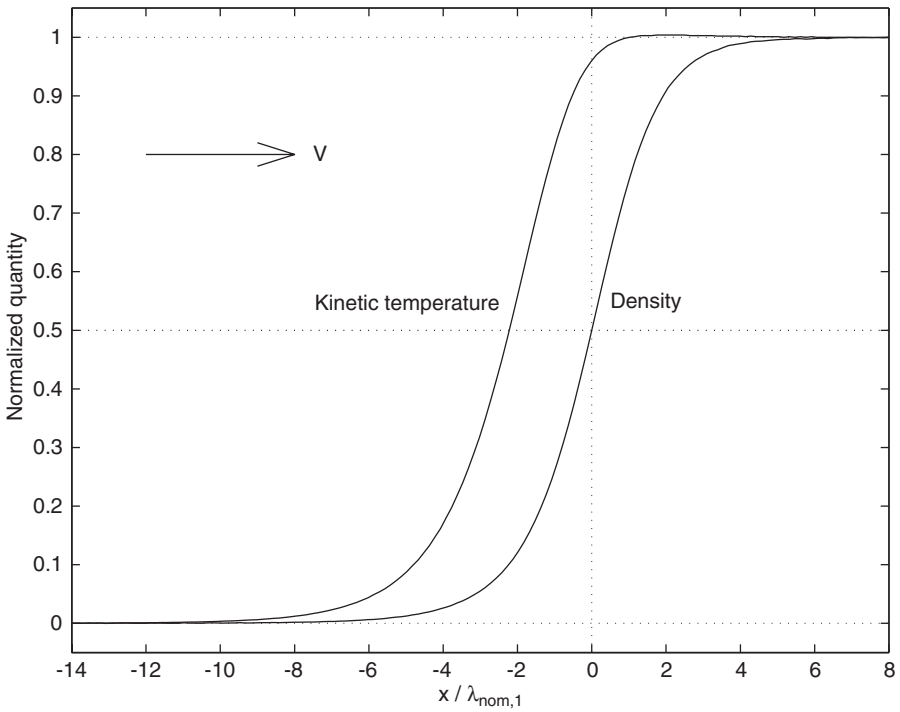

Figure 1. Kinetic temperature and density profiles within a Mach 5 normal shock for a gas with viscosity $\mu \propto T^{0.72}$, as calculated using the DSMC1S code of Bird [2]. The flow direction is indicated by V. The temperature and density are normalized according to the general expression $\hat{q} = (q - q_1)/(q_2 - q_1)$, where q is the quantity of interest, $\hat{q}$ is the normalized quantity and the subscripts 1 and 2 refer to upstream and downstream conditions, respectively. Upstream and downstream sample sizes were approximately 5×10^6 and 1.7×10^7, respectively. The x co-ordinate is normalized with respect to the upstream nominal mean free path $\lambda_{\text{nom},1} = 2\mu_1/(\rho_1 \bar{c}_1)$.

interest are simulated using the DSMC method. The DSMC method was introduced by Bird [1], and has been described in detail by Bird [2]. An essential DSMC approximation is that convection and collision processes are decoupled, and are performed independently and sequentially after time increments less than the mean molecular collision time. Essentially, the DSMC procedure is comprised of four basic steps, as summarized below ([3]):

1. Perform convection step and enforce boundary conditions.
2. Index simulator particles and cross-reference to cells and subcells.
3. Select collision partners within subcells and perform intermolecular collisions and chemical reactions. In the DSMC method, these processes are performed probabilisitically.
4. Sample the flowfield.

As an example of the use of the DSMC method, the internal structure of a normal shock has been calculated, and presented in Figure 1. In such a simulation, a method for obtaining the

velocities of simulator particles crossing the upstream and downstream simulation boundaries and entering the simulation space is required.

Consider the flow across a typical stream boundary in a DSMC computation. The unit vector normal to the boundary $\hat{\mathbf{n}}$ is directed into the simulation space. If the flow velocity vector is $\mathbf{V}$, the component of $\mathbf{V}$ normal to the boundary V is given by $V = \mathbf{V} \cdot \hat{\mathbf{n}}$. For an upstream boundary, $V > 0$, while $V < 0$ for a downstream boundary. Molecular and thermal velocity components normal to the boundary are denoted by v and $c = v - V$, respectively. The requirement is to obtain the normal velocity components v of those particles crossing the boundary and entering the simulation space, according to the velocity distribution characteristic of the external flow. After v is obtained for a particle, the velocity components parallel to the boundary, denoted $v_{p,q}$, must be obtained. These are obtained in a process separate to that used to obtain v, by sampling from the velocity distribution characteristic of the external flow. The sampling process for obtaining $v_{p,q}$ is independent of the method for obtaining v.

Only equilibrium conditions in the external flow are considered in this paper, which are represented by the Maxwell–Boltzmann velocity distribution $f_0 \propto \exp(-\beta^2 c^2)$, where $\beta = (2RT)^{-1/2}$ is the reciprocal of the most probable thermal speed, R is the specific gas constant and T is the temperature. For this case, the theoretical distribution of entering velocities is given in Section 2. The analysis could readily be extended to other distributions, such as the Chapman–Enskog distribution.

In the DSMC technique, the acceptance–rejection procedure is usually employed to select normal velocity components from the distribution function characteristic of those particles crossing the boundary [2]. The acceptance–rejection method for obtaining samples from a prescribed probability density distribution function $f(v)$ is a two-step process. Firstly, a possible random value of v, denoted v^*, is generated, which is uniformly distributed within the range of interest. Secondly, the value v^* is accepted if $f(v^*)/f_{\max} > R_f$, where $f_{\max}$ is the maximum of the distribution f and R_f is a uniformly distributed random fraction in the range $0 \leqslant R_f \leqslant 1$. In this paper, this acceptance–rejection method is referred to as the standard method, and will be discussed in detail in Section 3.

Hybrid CFD methods that employ the DSMC technique for rarefied regions of the flow and continuum solvers elsewhere typically use buffer cells adjacent to the periphery of the DSMC domain. An example of such a hybrid method is described by Garcia *et al.* [4]. The buffer cells are filled with particles during the DSMC convection phase, and those particles that cross the boundary into the DSMC domain are retained. Macrossan [5] used this method for generating the velocities of particles entering a DSMC normal shock simulation. This method extends the DSMC simulation procedures to the region adjacent to the simulation boundary, and may be considered as a form of acceptance–rejection procedure. In this paper, this method will be referred to as the alternative method, and is discussed in detail in Section 4.

2. THE THEORETICAL VELOCITY DISTRIBUTION

The probability of a gas particle crossing a boundary is proportional to the velocity normal to the boundary v. Therefore, for an equilibrium gas, the theoretical velocity distribution for particles crossing the boundary and entering the simulation space, denoted f_t, is

given by

$$f_t(v) = K_t^{-1} v \exp(-\beta^2 c^2) \tag{1}$$

where K_t^{-1} is the normalization constant. The flow conditions V, T and number density n outside the boundary adjacent to the simulation space are known. The normalization constant K_t^{-1} in Equation (1) is calculated using the normalization condition

$$\int_0^\infty f_t \, dv = 1$$

and is given by

$$2\beta^2 K_t = S\sqrt{\pi}(1 + \operatorname{erf} S) + \exp(-S^2)$$

where $S = \beta V$ is the non-dimensional speed ratio. The maximum value $f_{t,\max}$ of f_t is

$$f_{t,\max} = \phi \exp(-\chi)(2\beta K_t)^{-1} \tag{2}$$

where

$$\phi = S + (S^2 + 2)^{1/2} \quad \text{and} \quad 2\chi = 1 + S[S - (S^2 + 2)^{1/2}]$$

The theoretical number flux of particles crossing the simulation boundary, denoted $\dot{N}$, is given by

$$\dot{N} = n\beta K_t / \sqrt{\pi}$$

3. THE STANDARD ACCEPTANCE–REJECTION METHOD

The standard method for generating the velocities of particles entering a DSMC computation space makes use of the acceptance–rejection technique, as described in Section 1, to select velocities from the theoretical velocity distribution of Equation (1) [2]. In applying the acceptance–rejection procedure to this distribution, it is necessary to limit the range of v^*, because when $f_t(v^*)/f_{t,\max}$ is small, there is a low probability of acceptance, which results in poor computational efficiency. Using $v_{\min} \leqslant v \leqslant v_{\max}$, the distribution of entering normal velocities for the standard method, denoted f_s, is given by

$$f_s(v) = \begin{cases} K_s^{-1} v \exp(-\beta^2 c^2) & \text{if } v_{\min} \leqslant v \leqslant v_{\max} \\ 0 & \text{otherwise} \end{cases}$$

The normalization constant K_s^{-1} for f_s is given by

$$2\beta^2 K_s = S\sqrt{\pi}(\operatorname{erf} x_{\max} - \operatorname{erf} x_{\min}) + \exp(-x_{\min}^2) - \exp(-x_{\max}^2)$$

where $x_{\min}$ and $x_{\max}$ are non-dimensional thermal speeds defined by $x_{\min} = \beta(v_{\min} - V)$ and $x_{\max} = \beta(v_{\max} - V)$, respectively. For computational efficiency, $v_{\min}$ and $v_{\max}$ may be selected such that

$$v_{\min} = \max(V - 3\beta^{-1}, 0) \quad \text{and} \quad v_{\max} = \max(V + 3\beta^{-1}, \beta^{-1}) \tag{3}$$

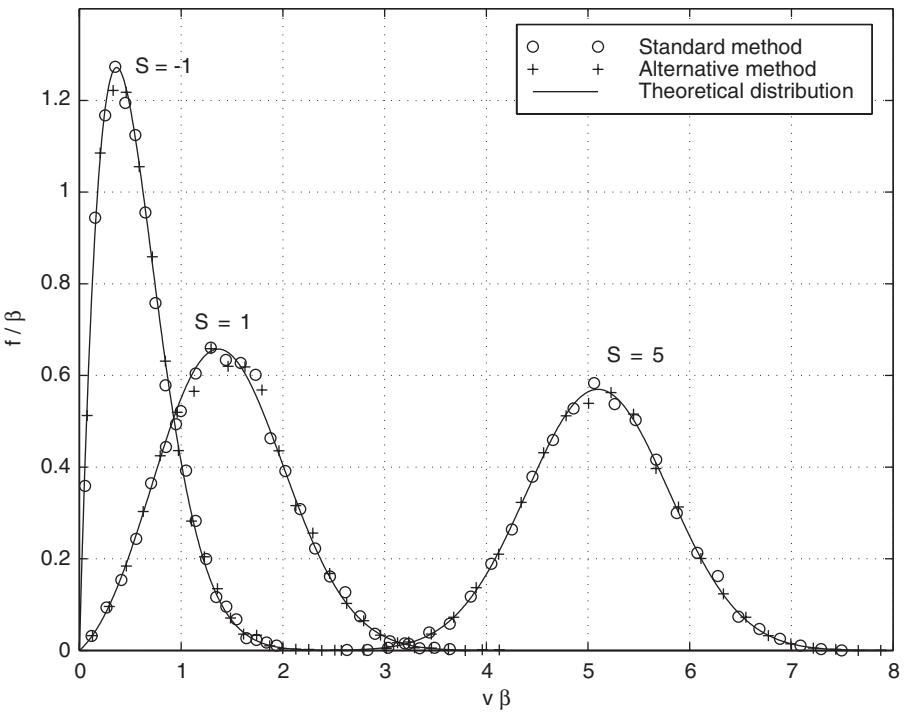

Figure 2. Comparison between the theoretical distribution and the distributions generated using the standard acceptance–rejection and the alternative methods for various values of S. For the standard acceptance–rejection method, $v_{\min}$ and $v_{\max}$ are given by Equation (3). For the alternative method, v' is given by Equation (7). The sample size in each case was 10^5 velocities.

This corrects an anomalous effect in the DSMC coding provided by Bird [2], where $v_{\min} = 0$ at $S = -3$, so that no velocities can be accepted for that singular case. It also avoids the unnecessary generation of values of $v^* \leqslant 0$, which can never be accepted.

A velocity v^* is generated, uniformly distributed in the range $v_{\min} \leqslant v^* \leqslant v_{\max}$, and is accepted if $f_s(v^*)/f_{s,\max} > R_f$, where $f_{s,\max} = \phi \exp(-\chi)(2\beta K_s)^{-1}$, as in Equation (2). The acceptance criterion for the standard method may therefore be expressed as

$$2\beta v^* \exp(\chi - \beta^2 c^{*2})/\phi > R_f \tag{4}$$

where $c^* = v^* - V$. The distribution of accepted normal velocities is shown in Figure 2, for $S = -1$, 1 and 5.

The acceptance–rejection procedure is applied to obtain the velocities of particles entering the simulation space. The location of entering particles is determined by the generation of further values of R_f. One value of R_f gives the fraction of the DSMC time step Δt that the particle travels within the cell, so that the distance normal to the boundary at the end of the time step is specified by $v\Delta t R_f$. For an N_d-dimensional simulation, a further $N_d - 1$ values of R_f are required to determine the location at which the particle crosses the simulation boundary.

The standard method is conventionally applied until the theoretically required number of velocities is obtained, which is based on the theoretical number flux [2]. If N_g possible values of v^* are generated and subjected to the acceptance criterion of Equation (4), the mean number accepted N_a is given by

$$N_a = \frac{N_g}{(v_{max} - v_{min}) f_{s,max}} = \frac{\beta N_g}{(x_{max} - x_{min}) f_{s,max}}$$

where $f_{s,max} = \phi \exp(-\chi)(2\beta K_s)^{-1}$. A variant of the standard method may therefore be implemented where a fixed number of velocities N_g are generated, and then subjected to the acceptance criterion of Equation (4) such that a varying number of velocities are accepted at each time step, with the mean number accepted N_a equal to the number calculated from the theoretical number flux.

4. THE ALTERNATIVE METHOD

In the alternative method of Garcia *et al.* [4] and Macrossan [5], the DSMC simulation procedures are extended to an external region adjacent to the DSMC simulation domain. Particles with velocities v^* are created in this region at each time step. The particles are uniformly distributed in the direction $-\hat{\mathbf{n}}$ to a distance $v'\Delta t$ from the boundary, where v' is a constant with the dimensions of velocity that is used to specify the extent of the region. The number of particles created depends on the number density n of the external flow, and the velocities v^* are generated according to the distribution of velocities characteristic of the external flow conditions. The particles are then moved at velocity v^* for time Δt, and those that cross the simulation boundary and enter the simulation space are retained. Particles are created at distances $v'\Delta t R_f$ from the boundary, and move a distance $v^*\Delta t$. Therefore, those particles with $v^* > v' R_f$ are accepted, so the acceptance criterion for the alternative method may be written

$$v^*/v' > R_f \tag{5}$$

The final position of each accepted particle relative to the boundary is simply the position to which the particle moves after Δt. As for the standard method, the location at which each accepted particle crosses is determined by generating $N_d - 1$ values of R_f for an N_d-dimensional simulation.

As noted in Section 1, the alternative method may be cast in the form of an acceptance–rejection procedure to replace the acceptance–rejection procedure of the standard method. In that case, no buffer cells are required, and potential values of v^* are generated according to the distribution function characteristic of the external flow, which is in this case the equilibrium distribution f_0, and then are either accepted or rejected according to the criterion of Equation (5). The velocity distribution function of accepted particle velocities for the alternative method, denoted f_a, is given by

$$f_a(v) = \begin{cases} K_a^{-1} v \exp(-\beta^2 c^2) & \text{if } 0 \leqslant v \leqslant v' \\ K_a^{-1} v' \exp(-\beta^2 c^2) & \text{if } v > v' \end{cases} \tag{6}$$

The normalization constant K_a^{-1} for f_a is given by

$$2\beta^2 K_a = S\sqrt{\pi}(1 + \text{erf}\, S) + x'\sqrt{\pi}(1 - \text{erf}\, x') + \exp(-S^2) - \exp(-x'^2)$$

where x' is a non-dimensional thermal speed defined by $x' = \beta(v' - V)$. This method gives a varying number of accepted velocities at each time step. Equation (6) shows that for $v > v'$, a fraction v'/v of the theoretical number required will be accepted. Therefore, the mean number of velocities accepted using this method is slightly lower than the theoretical number required, due to the depleted population of $v > v'$ relative to the theoretical distribution. The ratio of the number accepted to the theoretical number required is K_a/K_t.

In the standard method, no velocities $v^* > v_{max}$ are generated, due to the use of v_{max} for computational efficiency. Therefore the alternative method, despite the depleted population of $v > v'$, gives a more accurate distribution function, relative to the theoretical distribution of Equation (1), than the standard method, because some high velocities can still be accepted. Further, the alternative method gives the correct number of low velocities, whereas in the standard method the generation of velocities $v^* < v_{min}$ is again prevented for computational efficiency.

Distribution functions of entering velocities obtained using the alternative method are shown in Figure 2 for $S = -1$, 1 and 5, using

$$v' = V + 3\beta^{-1} \quad \text{which gives} \quad x' = 3 \tag{7}$$

It is apparent that the velocities provided by the alternative method conform closely to the theoretical distribution.

As noted above, the alternative method gives a variable number of velocities accepted at each time step, with the mean number accepted slightly less than the theoretical number required. The deficiency in accepted velocities is due to the depleted population of high-speed particles, which depends on the constant v', as implied by the dimensions of the buffer cells. The theoretically correct number of acceptances may be obtained simply by repeated generation of velocities v^*, followed by application of the selection criterion of Equation (5), until the required number of new particles is obtained. If buffer cells are used, the number density of simulator particles generated outside the simulation boundary should be increased to a higher value n' given by

$$n' = nK_t/K_a$$

which will result in a variable number of particles crossing the simulation boundary at each time step, with the mean number crossing equal to the theoretical number required. For the alternative method, the fraction of particles accepted N_a/N_g is given by

$$\frac{N_a}{N_g} = \frac{\beta K_a}{\sqrt{\pi} v'} = \frac{\beta^2 K_a}{\sqrt{\pi}(S + x')}$$

It is important to recognize that obtaining the correct number flux for the alternative method does not involve correcting the depleted population of high-speed particles. Correcting the number flux simply means that the theoretically correct number of particles enter the simulation space at each time step. The distribution of entering velocities, after the correction is applied, will still be depleted in high velocities relative to the theoretical distribution. Again,

it is important to recognize that this is still an improvement over the standard method, because all velocities can be represented, whereas in the standard method, the velocities v are restricted to the range $v_{\min} \leqslant v \leqslant v_{\max}$.

The alternative method is implicit in hybrid CFD schemes, such as that described by Garcia *et al.* [4]. However, the method of Macrossan [5] permits specification of the distance from the boundary to which particles are generated through the parameter v'. In hybrid schemes, the distance is dictated by the dimensions of the buffer cells for the DSMC simulation domain. As indicated in Equation (6), higher values of v' give distributions in better agreement with the theoretical distribution of Equation (1).

5. COMPARISON OF COMPUTATIONAL EFFICIENCY

The computational efficiency of the standard and alternative methods, both with a fixed number of velocities accepted at each time step, was examined using C codes. The inverse of the CPU time required per velocity accepted, which is indicative of computational efficiency, is shown in Figure 3 for $-5 \leqslant S \leqslant 10$. The results have been normalized with respect to the standard method at $S = 0$. The alternative method is more efficient that the standard method for

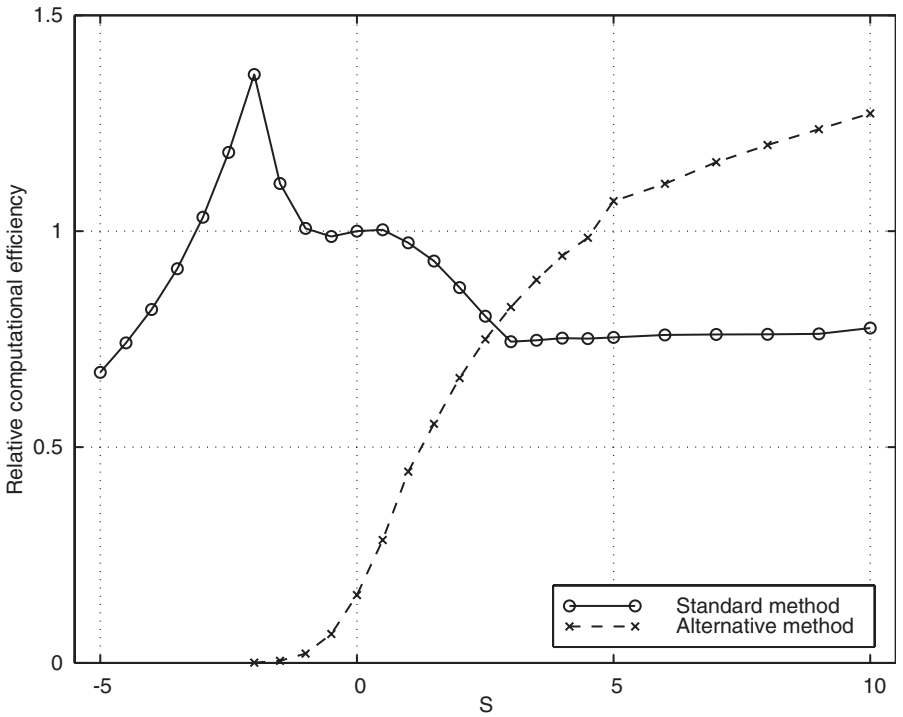

Figure 3. Comparison of computational efficiency, relative to the standard acceptance–rejection method at $S = 0$, determined using C codes compiled with maximum optimization. Downstream boundaries are represented by $S < 0$. For the standard acceptance–rejection method, $v_{\min}$ and $v_{\max}$ are given by Equation (3). For the alternative method, v' is given by Equation (7).

$S \gtrsim 2.5$, and is extremely inefficient for downstream boundaries where $S < 0$. The computational efficiency of the standard method is approximately constant for $S > 3$. Increasing the value of v' would decrease the computational efficiency of the alternative method.

6. CONCLUSIONS

The alternative implementation of the stream boundary condition for DSMC computations, as used in hybrid CFD schemes such as that of Garcia *et al.* [4] and as used by Macrossan [5], gives a more accurate distribution of entering velocities than the standard acceptance–rejection procedure of Bird [2]. Further, for $S \gtrsim 2.5$, the alternative method is more computationally efficient than the standard method. For downstream boundaries, where $S < 0$, the alternative method is extremely inefficient. The original implementations of the alternative method by Garcia *et al.* and Macrossan resulted in a number flux that was slightly lower than the theoretical number flux, due to a depleted population of high velocities. Two methods for obtaining the theoretically correct number flux using the alternative method have been presented.

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