Methods for implementing the stream boundary condition in DSMC computations

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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 method that samples the velocities from the theoretical velocity distribution. 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 technique. The number flux obtained using the alternative method is slightly lower than the theoretical number flux, due to a depleted population of high velocities. Methods of obtaining the correct number flux are presented. The alternative method allows acceptance of all possible velocities, and represents an improvement over the acceptance-rejection method where some velocities are excluded to improve computational efficiency. 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 favour of the acceptance-rejection method only for upstream boundaries in DSMC computations.

1   Introduction

The direct simulation Monte Carlo (DSMC) method is a computational fluid dynamics (CFD) scheme that recognises 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 cells. Most rarefied gas flows of engineering 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 summarised below (Oran *et al.* [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.

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 Fig. 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 domain 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 generate velocity components v of those particles crossing the boundary, according to the velocity distribution characteristic of the external flow. Velocity components parallel to the boundary are generated independently. Only equilibrium conditions in the external flow are considered in this paper, which are represented by the Maxwell-Boltzmann velocity distribution $f_0 \propto \exp\left(-\beta^2 c^2\right)$. The analysis could readily be extended to other distributions, such as the Chapman-Enskog distribution.

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

$$f_1(v) = K_1^{-1} v \exp\left(-\beta^2 c^2\right),\qquad(1)$$

where $\beta = (2RT)^{-\frac{1}{2}}$ is the reciprocal of the most probable thermal speed, R is the specific gas constant, T is the temperature and K_1^{-1} is the normalisation constant. The flow conditions V, T and number density n outside the boundary adjacent to the simulation space are known. The normalisation constant K_1^{-1} in Eq. 1 is calculated using the normalisation condition

$$\int_0^\infty f_1 dv = 1,$$

and is given by

$$2\beta^2 K_1 = S\sqrt{\pi}\left(1 + \operatorname{erf} S\right) + \exp\left(-S^2\right),$$

where $S = \beta V$ is the non-dimensional speed ratio. The maximum value $f_{\max}$ of a function of the form of Eq. 1 is

$$f_{\max} = \phi \exp\left(-\chi\right) \cdot \left(2\beta K_i\right)^{-1}, \tag{2}$$

where K_i^{-1} is the appropriate normalisation constant,

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

In the DSMC technique, the acceptance-rejection method is usually employed to select normal velocity components from the distribution function of Eq. 1 [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 and R_f is a uniformly distributed random fraction in the range $0 \leq R_f \leq 1$. In this paper, this acceptance-rejection method is referred to as the standard method, and will be discussed in detail in §2.

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 region. 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 method. This method will be referred to as the alternative method in this paper, and is discussed in detail in §3.

The alternative method, as implemented by Garcia *et al.* and Macrossan, results in a variable number of velocities being accepted at each time step, with the average number accepted being slightly less than the number required, based on the theoretical number flux. The deficiency in accepted velocities is due to a depleted population of high speed particles, which is dependent on the dimensions of the buffer cells. Methods for correcting this deficiency are discussed in this paper. The computational efficiency of the standard and alternative methods is also compared in this paper.

2   The standard method

The standard method for generating the velocities of particles entering a DSMC computation space makes use of the acceptance-rejection technique to select velocities from the theoretical velocity distribution of Eq. 1 [2]. In applying the acceptance-rejection procedure to this distribution, it is necessary to limit the range of v^*, because when $f(v^*)/f_{\max}$ is small, there is a low probability of acceptance, and therefore poor computational efficiency. Using $v_{\min} \leq v \leq v_{\max}$, the distribution of entering speeds is given by

$$
f_2(v) = \begin{cases} K_2^{-1}\, v \exp\left(-\beta^2 c^2\right), & \text{if} \quad v_{\min} \leq v \leq v_{\max}; \\[2mm] 0, & \text{otherwise.} \end{cases} \tag{3}
$$

The normalisation constant K_2^{-1} for Eq. 3 is given by

$$
2\beta^2 K_2 = S\sqrt{\pi}\left(\operatorname{erf} x_{\max} - \operatorname{erf} x_{\min}\right) + \exp\left(-x_{\min}^2\right) - \exp\left(-x_{\max}^2\right),
$$

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, $v_{\max}$ and $v_{\min}$ may be selected such that

$$v_{\max} = \max\left(V + 3\beta^{-1}, \beta^{-1}\right) \quad \text{and} \quad v_{\min} = \max\left(V - 3\beta^{-1}, 0\right). \tag{4}$$

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. The present method also avoids the unnecessary generation of values of $v^* \leq 0$, which can never be accepted.

A velocity v^* is generated, uniformly distributed in the range $v_{\min} \leq v^* \leq v_{\max}$, and is accepted if $f_2(v^*)/f_{2,\max} > R_f$, where $f_{2,\max}$ is given by Eq. 2 with $K_i = K_2$. The acceptance criterion may therefore be expressed as

$$2\beta v^* \exp\left(\chi - \beta^2 c^{*2}\right)/\phi > R_f, \tag{5}$$

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

The procedure described above 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. The first 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.

As noted in §1, the standard method is conventionally applied until the theoretically required number of velocities is obtained [2]. The required number is determined from the theoretical number flux $\dot{N}$, given by

$$\dot{N} = \frac{n\beta K_1}{\sqrt{\pi}} \tag{6}$$

If N_g possible values of v^* are generated and subjected to the acceptance criterion of Eq. 5, the

average number accepted N_a is given by

$$N_a = \frac{N_g}{(v_{\max} - v_{\min}) f_{2,\max}} = \frac{\beta N_g}{(x_{\max} - x_{\min}) f_{2,\max}}.$$

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 Eq. 5 such that a varying number of velocities are accepted at each time step, with the average number accepted N_a being equal to the number calculated from the theoretical number flux.

3 The alternative method

In the alternative method, particles with velocities v^* are created outside the simulation space 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 is based on the number density n of the flow. The velocities v^* are generated according to the distribution function 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

$$v^*/v' > R_f. \tag{7}$$

As noted in §1, the alternative method may be considered as form of acceptance-rejection method. Potential values of v^* are generated according to the distribution function characteristic of the external flow, which is in this case an equilibrium distribution, and then are either accepted or rejected according to the criterion of Eq. 7. The position of each accepted particle relative to the boundary is simply the position to which the particle moves after Δt. The location at which each accepted particle crosses the boundary is determined from its trajectory.

The velocity distribution function of accepted particle velocities is given by

$$
f_3(v) = \begin{cases} K_3^{-1} \, v \exp\left(-\beta^2 c^2\right), & \text{if} \quad v \le v'; \\[2mm] K_3^{-1} \, v' \exp\left(-\beta^2 c^2\right), & \text{if} \quad v > v'. \end{cases} \tag{8}
$$

The normalisation constant K_3^{-1} is given by

$$
2\beta^2 K_3 = S\sqrt{\pi}\left(1 + \operatorname{erf} S\right) + x'\sqrt{\pi}\left(1 - \operatorname{erf} x'\right) + \exp\left(-S^2\right) - \exp\left(-x'^2\right),
$$

where x' is a non-dimensional thermal speed defined by $x' = \beta\left(v' - V\right)$. This method gives a varying number of accepted velocities at each time step. As noted in §1, the average 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. As demonstrated in Eq. 8, for $v > v'$, a fraction v/v' of the theoretical number will be accepted. The theoretically correct number of acceptances may be obtained simply by repeated application of the selection criterion of Eq. 7 until the required number of velocities is obtained.

In the standard method, no velocities $v^* > v_{\max}$ are generated, due to the selection 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 Eq. 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.

As noted in §1, 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. As indicated in Eq. 8, higher values of v' give distributions in better agreement with the theoretical distribution of Eq. 1.

Distribution functions of entering velocities obtained using the alternative method are shown

in Fig. 2 for $S = -1$, 1 and 5, using

$$v' = V + 3\beta^{-1}, \quad \text{which gives} \quad x' = 3. \tag{9}$$

It is apparent that the velocities provided by the alternative method conform closely to the theoretical distribution. The distribution for $S = -5$ was not generated, for reasons of computational efficiency which will be discussed in §4.

The number of velocities accepted N_a from N_g generated velocities is given by

$$N_a = \frac{\beta K_3 N_g}{\sqrt{\pi} v'} = \frac{\beta^2 K_3 N_g}{\sqrt{\pi}(S + x')}.$$

This expression may be utilised to provide a variant of the alternative method that gives a varying number of velocities accepted at each time step, with the average number accepted being equal to the number required based on the correct theoretical number flux.

4   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 a FORTRAN code. The inverse of the CPU time required per velocity accepted is shown in Fig. 3 for $-5 \leq S \leq 10$. The CPU time has been normalised with respect to the standard method at $S = 0$. The alternative method is more efficient that the standard method for $S \gtrsim 2.5$, and is extremely inefficient when $S \lesssim -1$. The computational efficiency of the standard method is approximately constant for $S > 3$.

5   Conclusions

The alternative implementation of the stream boundary condition for DSMC computations, as utilised in hybrid schemes such as that of Garcia *et al.* [4] and as used by Macrossan [5], gives a number flux that is slightly lower than the theoretical number flux, due to a depleted population

of high velocities. The alternative method may be used to obtain the theoretically correct number of accepted velocities by repeated application of the selection criterion until the required number of velocities is accepted, as calculated from the theoretical number flux. Alternatively, the fraction of velocities accepted using the alternative method can be used to generate a fixed number of velocities that will, after application of the selection criterion, give a varying number of accepted velocities such that the average number accepted is equal to the theoretical number required. The alternative method allows the generation of all possible velocities entering the simulation space, and therefore represents an improvement over the standard acceptance-rejection method where some velocites are excluded for computational efficiency.

A variant of the standard acceptance-rejection method has been introduced that allows the acceptance of a variable number of particle velocities at each time step, with the average number accepted equal to the theoretical number required.

For $S \lesssim 1$, which corresponds to a supersonic downstream boundary, the alternative method is extremely inefficient. However, for boundaries where $S \gtrsim 2.5$, the alternative method is more efficient than the standard acceptance-rejection method. It is therefore apparent that the alternative method, with the correct theoretical number flux, should be adopted for upstream boundaries in DSMC computations.

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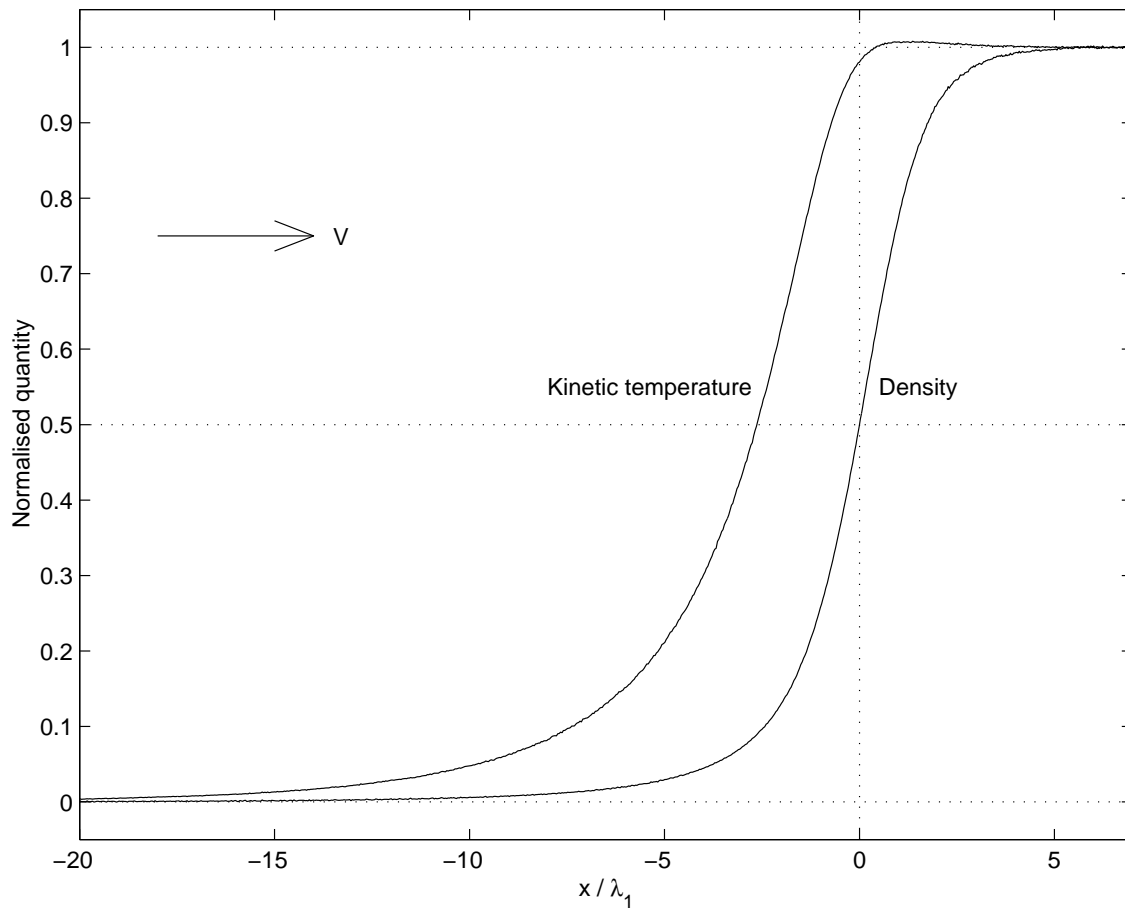
Figure 1: Example of kinetic temperature and density profiles within a normal shock as determined using the DSMC method. The flow direction is denoted by V. The temperature and density are normalised according to the general expression $\hat{q} = (q - q_1)/(q_2 - q_1)$, where q is the quantity of interest, $\hat{q}$ is the normalised quantity and the subscripts 1 and 2 refer to upstream and downstream conditions respectively. The x coordinate is normalised with respect to the upstream mean free path λ_1.
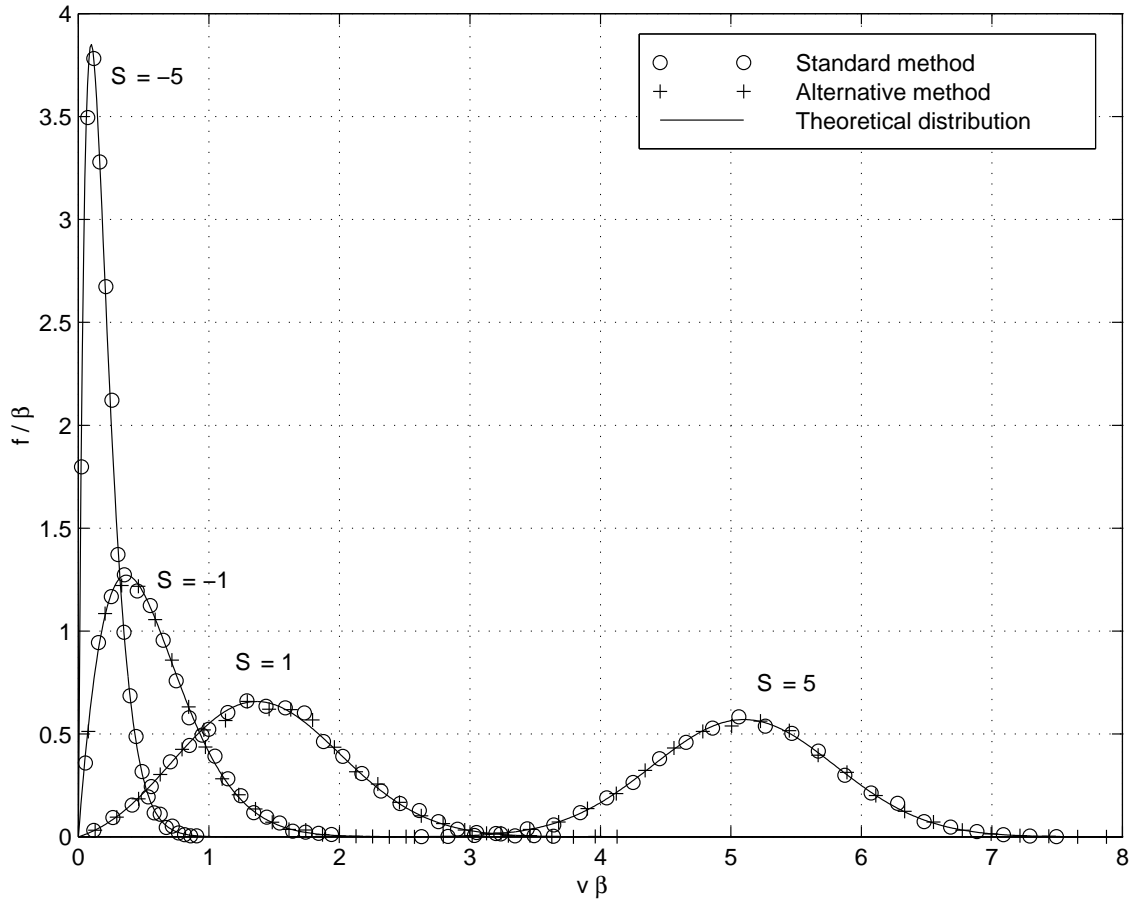
Figure 2: Comparison between the theoretical distribution and the distributions generated using the standard acceptance-rejection and the alternative methods for various values of S. For the standard acceptance-rejection method, $v_{\min}$ and $v_{\max}$ are given by Eq. 4. For the alternative method, v' is given by Eq. 9. The sample size in each case was 10^5 velocities.
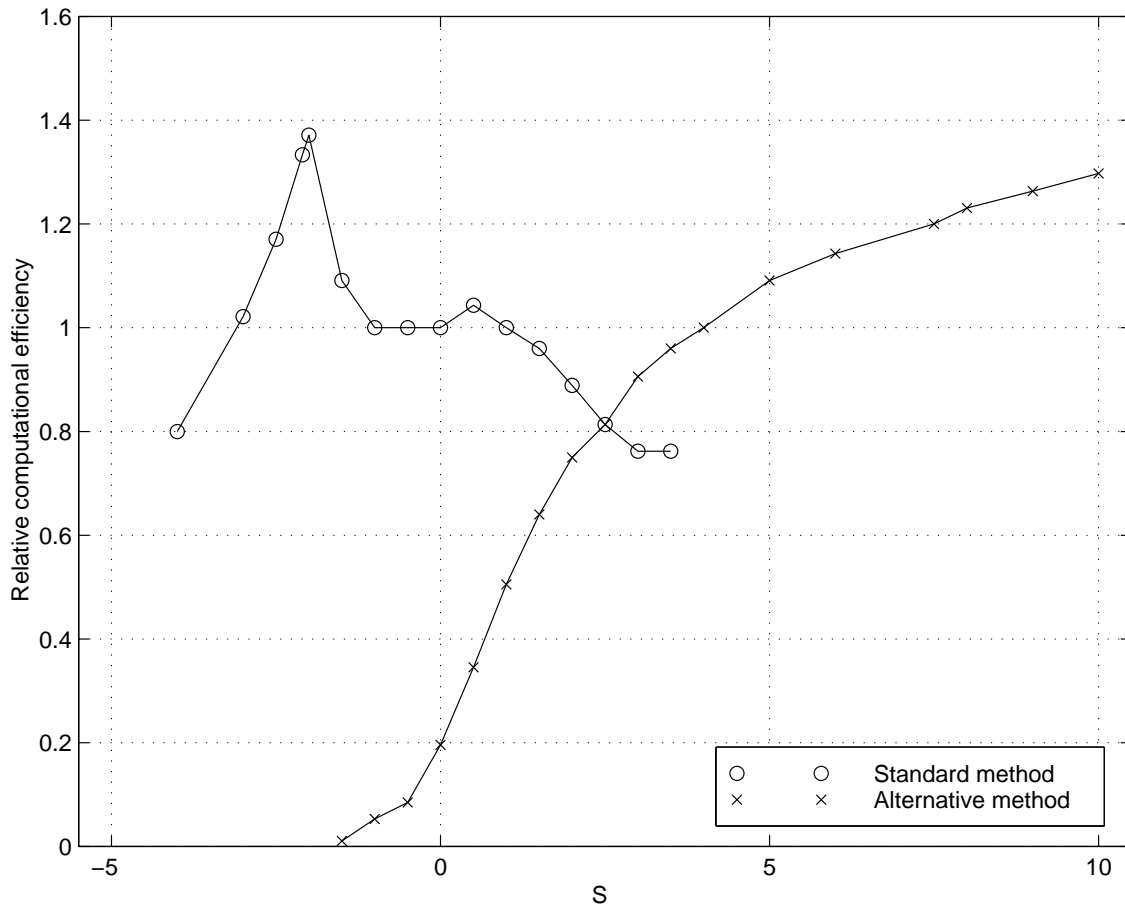
Figure 3: Comparison of computational efficiency, relative to the standard acceptance-rejection method at $S = 0$, determined using FORTRAN code. Downstream boundaries are represented by $S < 0$. For the standard acceptance-rejection method, $v_{\min}$ and $v_{\max}$ are given by Eq. 4. For the alternative method, v' is given by Eq. 9.