# Detecting equilibrium cells in DSMC to improve the computational efficiency

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**Abstract.** DSMC in the large collision rate limit [1, 2, 3] has previously been used as an approximate Euler solver. Macrossan [4] suggested that therefore a particle-only approach could be taken to flows which contain a mixture of rarefied and continuum or near-continuum conditions; in those parts of the flow that would more conventionally be solved by a continuum Navier-Stokes or Euler solver, DSMC could be invoked in its 'Euler solver mode'. The regions where the Euler solver can be invoked were determined (as is usual in such hybrid codes) by evaluating the breakdown parameter which compares the local collision time $\tau$ to the flow transit time through a local characteristic flow length. The flow length is derived from the gradient of some flow property. Here we investigate a different, but related, approach to this problem. In regions where the Euler equations apply, the velocity distribution function has the Maxwell form. If the velocity distribution in a cell is examined after the particles have been moved, but before the collisions are calculated, it could be established that the cell is already in, or very close to, its equilibrium state. Such 'equilibrium cells' may be found anywhere in the flow where the flow gradients are small; it is only when the movement of the particles brings to one 'recipient cell' particles which started in different 'donor cells' with different flow conditions that a non-equilibrium velocity distribution is established in the recipient cell. Here two different measures derived from the velocity distribution were used to identify the equilibrium cells: the ratio of shear stress to pressure and a measure of the departure of all temperature components from the overall kinetic temperature. These were evaluated from the time-averaged flow state found from flow samples taken before the collision calculations were performed. In the equilibrium cells there would appear to be no need to calculate any collisions; the effect of the collisions would merely be to bring about a new statistical representation of the same equilibrium distribution. To maintain stability it was found that new velocities must be established in these equilibrium cells. Two different methods were used to set new velocities in equilibrium cells. These were (1) Pullin's EPSM method [1] by which new particle velocities are *selected* from an equilibrium distribution and (2) a form of 'collision limiting' in which a reduced number of collisions are calculated in equilibrium cells. These methods were tested for a Mach 5, blunt body flow with freestream Knudsen numbers of 0.1 and 0.064. Savings of CPU times of 10% (over standard DSMC) were achieved. We believe the general method could lead to greater savings in the CPU times for flows at lower Knudsen numbers, where the collision calculations could become more time consuming.

**Keywords:** DSMC, near-continuum, equilibrium, collision-limiting, EPSM, breakdown criteria
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## INTRODUCTION

In a typical DSMC computation there are many cells throughout the computational domain where the flow is in thermodynamic equilibrium. These regions of equilibrium are found where the mean time between collisions is negligible compared to the time required for the flow to traverse the local characteristic gradient length of the flow, that is where the 'breakdown parameter' $u\tau\nabla Q/Q$ is small. Here $Q$ is a flow property, $Q/\nabla Q$ is the 'gradient length', $u$ is the flow speed in the direction of the gradient and $\tau$ is the collision time. Regardless of the collision rate or overall density of the flow, any region which has zero or sufficiently low flow gradients will be in local thermodynamic equilibrium, and special procedures can be applied to these regions.

Macrossan [4] suggested that Pullin's Equilibrium Particle Simulation Method [1] could be combined with DSMC to yield an Euler solution in equilibrium cells. In EPSM, new particle velocities for a cell are selected so that they conform to an equilibrium distribution, while preserving total momentum and energy in the cell. Another method of establishing equilibrium velocities is to calculate a sufficient number of collisions amongst the particles, but not necessarily the theoretically large number that may be required according to the local cell density and temperature. This 'collision-limiting' has been proposed to make DSMC an 'Euler solver' [2, 3]. Here we calculate only half the theoretically correct number of collisions for equilibrium cells, with an upper limit of $N_{colls} = N_p/2$, where $N_p$ is the number of particles in the cell. Both EPSM and 'collision limited DSMC' were originally applied in all cells throughout the flow at every time step, and the velocity distribution in each cell after the convection calculation could

**TABLE 1.** Flow about thin plate normal to flow. Surface temperatures: front (windward) $T_f$; back (leeward) $T_b$. Gas is monatomic (molecule mass = $6.63\times10^{-26}$kg, $\gamma=5/3$). VHS scattering, with $\mu=\mu_\infty(T/T_\infty)^\omega$. $H=0.15$m is the semi-height of the plate. Computational region was $L_x\times L_y$ = 0.10m×0.08m.

| Case | $V_\infty$ m/s | $T_\infty$ K | $T_f$ K | $T_b$ K | $\rho_\infty$ kg/m$^3$ | $\mu_\infty$ Pa.s | $\omega$ | $\lambda_\infty$ * m | $\lambda_\infty/H$ | $\Delta t/\tau_s$ † | $\Delta x/\lambda_s$ ** |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1317.3 | 200 | 1867 | 200 | $6.63\times10^{-6}$ | $1.645\times10^{-5}$ | 0.81 | $1.52\times10^{-2}$ | 0.101 | 0.45–0.56 | 2.9 |
| 2 | 1613.4 | 300 | 2800 | 500 | $1.42\times10^{-4}$ | $1.983\times10^{-4}$ | 0.83 | $7.00\times10^{-4}$ | 0.046 | 0.64 | 1 |

* *Nominal* mean free path $\lambda_\infty\equiv 2\mu_\infty/(\rho_\infty\bar{c}_\infty)$, $\bar{c}_\infty=(8RT_\infty/\pi)^{1/2}$.
† $\tau_s=\lambda_s/c_s=(\pi/4)(\mu_s/p_s)$ is the nominal collision time for conditions immediately behind the normal bow shock.
** $\lambda_s$ is the nominal mean free path immediately behind the bow shock.

be highly non-equilibrium. Here we apply both these methods to enforce or maintain equilibrium in near-equilibrium cells only; in the remaining cells the normal DSMC procedures are applied.

To detect where the special collision procedures may be applied we propose a method which does not rely on the explicit evaluation of flow gradients. At periodic intervals we sample the flow state between the movement and collision steps of the calculation. Thus we can examine the (time-averaged) pre-collision distribution of velocities in each cell, *i.e.* the distribution of velocities established by the movement of molecules between cells. If the pre-collision state in a cell is sufficiently close to equilibrium, according to measures of non-equilibrium discussed later, we tag the cell as an 'equilibrium cell' in which special procedures can be applied. Although the flow gradients are not explicitly calculated, it is only when there are significant gradients of flow properties (*i.e.* gradients of the distribution function) that a non-equilibrium pre-collision velocity distribution is established by the movement of the particles.

The greatest potential saving in CPU time from the use of these methods arises when the there are large regions of high density (high collision rate) flow which are in thermal equilibrium. The time step $\Delta t$ must be less than the mean collision interval in non-equilibrium cells only, and can be significantly larger the small collision time in those high density, equilibrium cells. The larger time step does not in itself lead to a significant reduction of CPU time, because if the collision rate is preserved (*i.e.* the standard collision procedures are applied) just as many collisions have to be calculated. CPU time can only be saved by reducing the total number of collisions, which occurs here because new velocities in equilibrium cells can be established by a reduced number of collisions, or by the EPSM procedure. Here we are not primarily concerned with the computational efficiency, but with showing what measure of equilibrium must be used to identify equilibrium cells.

Rebrov and Skovorodko [5] have shown that pre-collision samples can be combined with post-collision samples to give a better representation of the true flow state than post-collision samples alone. Here we keep the pre- and post-collision samples separate, so that pre-collision equilibrium can be detected, but use the combined samples to give the best estimate of the flow state. The pre- and post-collision samples were not taken at the same time step but alternated in time, separated by half the nominated sampling time interval.

## Test cases

The 2D code supplied by Bird [8] was adapted to test the new methods. The Mach 5 flow of a monatomic gas about a flat plate normal to the freestream velocity was calculated. The VHS collision model with viscosity exponent $\omega$ was used. Four-subcells in each cell were used in the collision routines. Both EPSM and a form of collision limiting were added to the code, and a different measure of non-equilibrium was used in each case. The flow conditions and collision model parameter $\omega$ were slightly different in each case, as shown in Table 1. The freestream Knudsen number in the test flow is 0.10 or 0.046, and hence these are not what are considered near-continuum flows. We have chosen these rarefied conditions to illustrate that the method of dividing the flow into 'equilibrium' and 'non-equilibrium cells' is a general procedure, not one that depends on a certain collision rate.

# FIRST MEASURE OF NON-EQUILIBRIUM

The flowfield pressure and the shear stress throughout the flow are shown in Fig. 1 for test Case 1. The pressure contours show the bow shock, the high pressure region near the windward surface stagnation point and the expansion

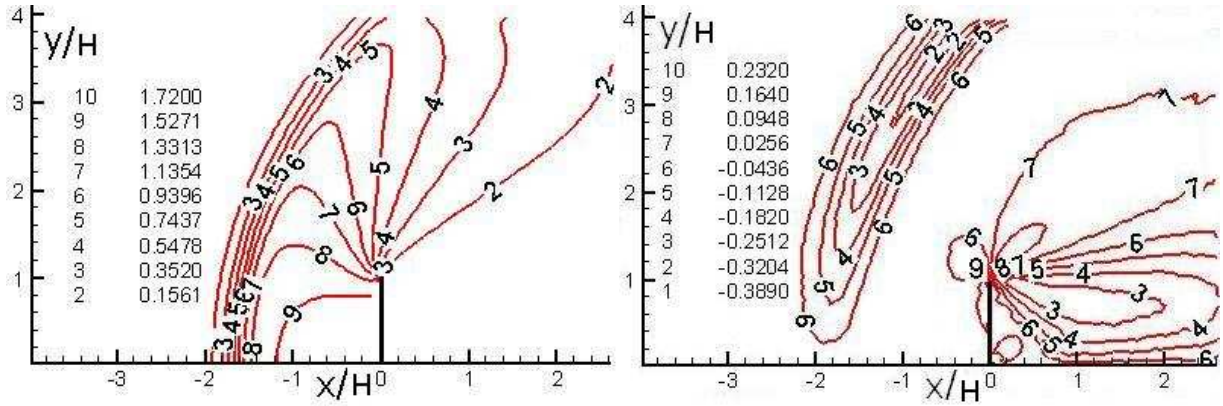


**FIGURE 1.** Flow case 1. Left: Pressure coefficient $2p/\left(\rho_\infty V_\infty^2\right)$. Right: normalized shear stress $\zeta = \left\langle c_x c_y/RT \right\rangle$.

of the flow around the end of the wall (at $y/H = 1$). The gas viscosity is related to the mean free time and pressure as $\mu \approx p\tau$. Hence the shear stress relative to the pressure can be expressed as $\mu\nabla u/p \sim \tau\nabla u \sim u\left(\lambda/\bar{c}\right)\left(\nabla u/u\right) \sim SKn$ where $S = u/\left(2RT\right)^{1/2}$ is the local speed ratio and $Kn = \lambda/\left(u/\nabla u\right)$ is the local Knudsen number based on the flow length derived from the velocity gradient. Thus this ratio is a form of the breakdown parameter [6, 7] and where it is large the correct DSMC collision procedures should be applied. The shear stress contours in Fig. 1 indicate a large degree of non-equilibrium in the bow-shock, as expected, and also show that the leeward flow ($x/H > 1$ and $y/H < 1$) is significantly non-equilibrium.

For our first measure of departure from equilibrium conditions in any cell we take the ratio of shear stress to pressure

$$\zeta = \left|\left\langle c_x c_y/RT \right\rangle\right|, \tag{1}$$

as calculated from the time-averaged *pre-collision* flow samples. Here $c_j = v_j - \left\langle v_j \right\rangle = v_j - u_j$, is a thermal velocity component, $v_j$ is the molecular velocity, the angle brackets denote the average taken over the distribution function, $u_j = \left\langle v_j \right\rangle$ is the local flow velocity (mean molecular velocity), $R$ is the ordinary gas constant and $T$ is the kinetic temperature. This ratio can be calculated in each cell from samples accumulated during the course of the calculation. These samples are regularly cleared during the development of the flow, but accumulated after steady state is reached.

At periodic time intervals, a new estimate of the flow state was calculated and written to disk storage, and it was at this stage that the value of $\zeta$ for each cell was determined from the pre-collision flow samples. All cells for which $\zeta \leq \zeta_c$ were then marked as equilibrium cells, based on a specified 'cut-off' value of $\zeta_c$. This designation as equilibrium or non-equilibrium remained in force for each cell until the next update of the flow state, when the cell status was re-calculated. The time step was based on the 'collision fraction', *i.e.* the average number of collisions per particle in one time step, given by $2\sum N_{coll}/\sum N_p$, where $\sum N_{coll}$ was the total number of collisions in the cell since the last update and $\sum N_p$ was the total number of particles in the cell over all the time steps since the last update. The time-step was set so that the largest collision fraction in *any non-equilibrium cell* was less than 0.8. In practice this meant that the collision fraction was less than 0.5 in virtually all the non-equilibrium cells. Thus the time step was about 25% greater than that used in the standard DSMC calculations.

Calculations were performed for different values of $\zeta_c$, including (in effect) $\zeta_c \to \infty$. For those cells which were designated as equilibrium cells, no collisions were calculated. Instead, as described by Macrossan [4], new particle velocities were selected from the local equilibrium distribution, while preserving the total momentum and energy in the cell. For $\zeta_c \to \infty$ equilibrium is enforced in every cell, and the method reduces to Pullin's Equilibrium Particle Simulation Method [1]. Fig. 2 shows the pressure and shear stress coefficients on the windward (front) surface, for various values of $\zeta_c$. These are virtually independent of $\zeta_c$, and hence the front surface properties can tell us little about what value of $\zeta_c$ is appropriate. On the other hand, Fig. 3 shows that the pressure and shear on the rear surface are sensitive to the value of $\zeta_c$. The large difference between the DSMC results and the results for $\zeta_c \to \infty$ indicate that rarefaction effects are significant in this flow. The scatter in the results is considerable, but it appears that a value of $\zeta_c = 0.01$ is sufficiently small (the results for $\zeta_c = 0.004$ do not appear to be significantly closer to the DSMC results). The new method required 90% of the CPU time required for the DSMC calculations.

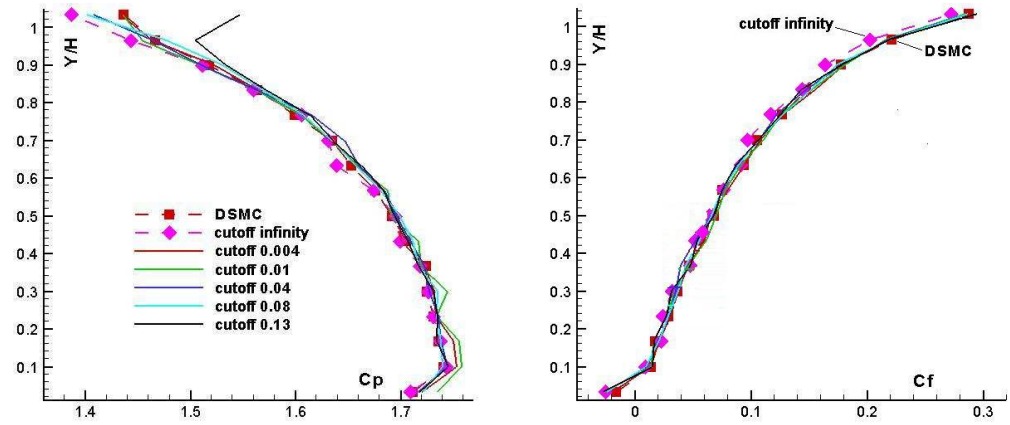


**FIGURE 2.** Pressure (left) and shear stress (right) distribution over the windward face, for standard DSMC and various cut-off values of the breakdown parameter *zeta* (Eq. 1). If $\zeta < \zeta_c$ (cutoff value), equilibrium is enforced in the cell. If $\zeta_c \to \infty$ equilibrium is enforced in all cells and the method is equivalent to Pullin's Equilibrium Particle Simulation Method [1].

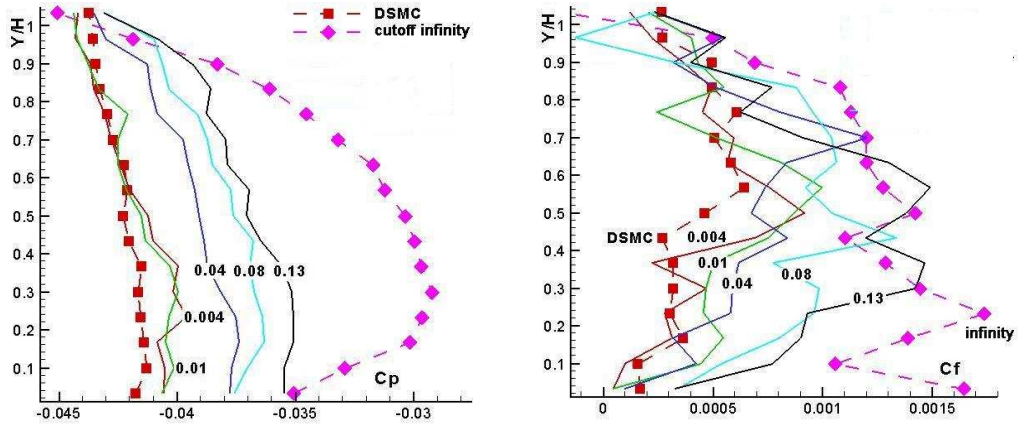


**FIGURE 3.** Pressure (left) and shear stress (right) distribution over the leeward face. The data is more scattered but it can be seen that the results for this more rarefied flow are more sensitive to $\zeta_c$.

## SECOND MEASURE OF NON-EQUILIBRIUM

We have tested another measure of non-equilibrium, the deviation of the temperature components from the mean kinetic temperature in the cell, which will be zero for the Maxwell (equilibrium) velocity distribution. Thus we define a 'breakdown parameter'

$$B = \frac{\sqrt{(T_x - T)^2 + (T_y - T)^2 + (T_z - T)^2}}{T} \tag{2}$$

where $T_x$, $T_y$ and $T_z$ are the three components of kinetic temperature and $T = (T_x + T_y + T_z)/3$ is the overall kinetic temperature in the cell. For molecules having more than three thermal degrees of freedom, other temperatures can be included in the evaluation of $B$. This parameter was calculated from the pre-collision velocity samples, at periodic time intervals. A cell was designated as an equilibrium cell if $B < B_c$, where $B_c$ was a specified cut-off value.

It is tempting to think that no collisions at all might be needed in cells which are already in equilibrium. However, we found that instabilities developed unless at least some of the particles in the equilibrium cells were given new velocities at every time step. As an alternative to using EPSM in equilibrium cells we have tested a method which requires minimal modification of an existing DSMC collision routine. In designated equilibrium cells, we calculated *half* the correct number of collisions. This was achieved with the addition of a few lines to the standard collision procedure which halved the number of potential collision pairs tested against the accepetance/rejection criteria. The

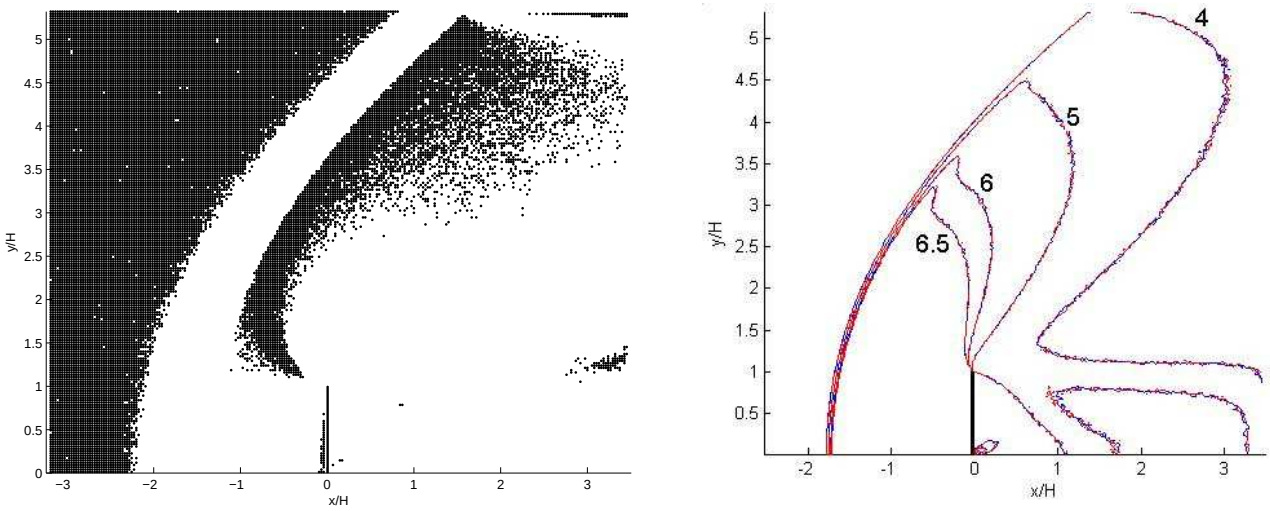


**FIGURE 4.** Left: 'Equilibrium' cells, $B \leq 0.015$ (Eq. 2), in which collision rate was halved and Maxwell collision probability was applied (40% of total); Right: Overlaid contours of $T_x/T_\infty$ as calculated for standard and collision-reduced DSMC. Flow case 2. Accumulated flow samples from $19 < tV_\infty/L_x < 101$. Cell sample sizes 71,000 to 550,000 particles (approximately).

halved collision rate, in effect, doubles the viscosity and thermal conductivity of the simulation gas in these cells, but this is of no consequence if the cell is already in its equilibrium state before the collisions are calculated. Looking at it another way, the greater viscosity and thermal conductivity are insignificant in regions of the flow where the gradients of velocity and temperature are negligible. It is in precisely those regions of negligible gradient that the non-equilibrium measures should approach zero.

In this second test case, the time step was constant as shown in Table 1. With a cut-off value of $B_c = 0.015$, 40% of the cells were found to be in equilibrium and these equilibrium cells are shown in Fig. 4. Virtually all of the freestream ahead of the bow shock was in equilibrium (as expected) and there is also an equilibrium region behind the bow shock. The appearance of single 'non-equilibrium' cells surrounded by equilibrium cells suggests that it might be advantageous to consider a cell to be in equilibrium if most of its neighboring cells are in equilibrium. A few cells near the stagnation point and along the front surface of the wall were also detected as equilibrium cells. The flow calculated using the collision-reducing procedures in these equilibrium cells agrees closely with that calculated by DSMC. This can be seen in the second part of Fig. 4, where some contours of the kinetic temperature component $T_x$ for both standard and collision-reduced DSMC are overlaid. These temperature contours are virtually indistinguishable for the two methods. In addition, Fig. 5 shows that the pressure and shear stress on the rear wall for the new method agree closely with the standard DSMC results. These results show that the value of $B_c = 0.015$ was safe in this case. The collision-reduced calculation required 90% of the CPU required for standard DSMC.

## DISCUSSION AND CONCLUSIONS

The velocity distribution at the end of the movement stage in DSMC (the 'pre-collision velocity distribution') will be non-equilibrium whenever there are significant gradients of flow properties. Hence this velocity distribution is an indirect measure of the flow gradients and can be used to determine the 'breakdown parameter'. Two measures of non-equilibrium have been tested here: (1) the ratio of shear stress to pressure and (2) a measure of the departure of the separate temperature components from the overall kinetic temperature.

We have shown that simplified or alternative collision procedures can be applied in DSMC cells which are found to be sufficiently close to their equilibrium state before collisions are calculated. Because the cell is already close to, or at, its equilibrium state the details of how new velocities are established are not important. What matters is that the new velocities conform to the local equilibrium state and that the mass, momentum and energy in each cell are conserved. For instance, we might apply equal probability to all collision pairs in equilibrium cells, which could be convenient.

Significant saving in CPU time can only be expected when there are large regions of high collision rate combined with low flow gradients, *i.e.* many designated equilibrium cells which have a high collision rate. In that case, the global

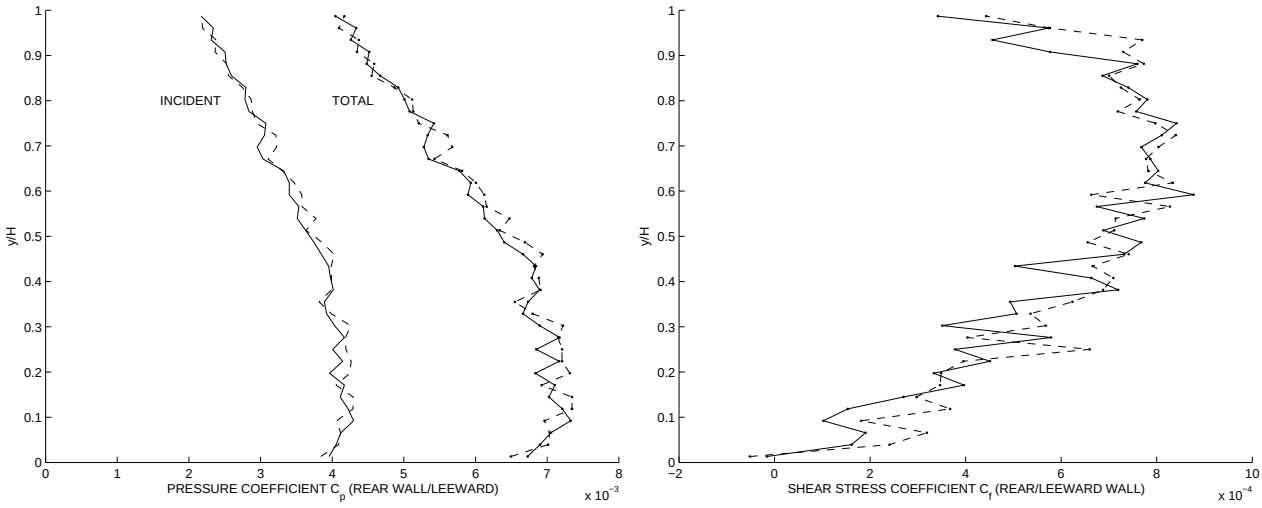


**FIGURE 5.** Pressure and shear stress coefficients on front surface, with (broken line) and without collision limiting (solid lines). Conditions correspond to those for Fig. 4. Pressure contributions from incident molecules only, as well as total (incident + reflected) are shown. Surface cell samples sizes ranged from 1400 to 2200 particles.

time step can be set larger than the theoretical collision time in those cells and the theoretical number of collisions required in those cells need not be calculated. Although the improvements in efficiency reported here were modest we believe the general method is capable of improvement and shows promise for the calculation of near-continuum flows with DSMC.

It might be asked why we cannot base our measures of non-equilibrium on samples of the post-collision state. In that case, if the EPSM procedure is used in a cell which is detected as an equilibrium cell, the cell would remain as an equilibrium cell for the remainder of the calculation, regardless of the development of flow gradients in its vicinity. This may not happen when collision-reduction (rather than EPSM) is used but, in any case, the post-collision state will always be expected to be closer to equilibrium than the pre-collision state. Thus the non-equilibrium pre-collision state is a better sign that the correct DSMC collision procedures must now be applied, regardless of whether the cell was previously in equilibrium. On the other hand, if one uses a continuum (Navier Stokes) solver for those cells deemed to be in equilibrium, one needs to detect where the flow calculated by the continuum solver is significantly non-equilibrium. Our first measure of non-equilibrium, the ratio of shear stress to pressure, can be used by continuum solvers. The shear stress and pressure are routinely calculated by the Navier Stokes solver for every cell as part of the flux calculations; no separate evaluation of flow gradients is required to calculate the breakdown parameter.

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